



**Existence of dynamic phase transitions in a one-dimensional  
lattice model with piecewise quadratic interaction potential**

*Hartmut Schwetlick and Johannes Zimmer*

**Bath Institute For Complex Systems**

Preprint 9/09 (2009)



# Existence of dynamic phase transitions in a one-dimensional lattice model with piecewise quadratic interaction potential

Hartmut Schwetlick and Johannes Zimmer

## Abstract

The existence of travelling waves in an atomistic model for martensitic phase transitions is the focus of study. The elastic energy is assumed to be piecewise quadratic, with two wells representing two stable phases. We develop a framework such that the existence of subsonic heteroclinic waves in a bi-infinite chain of atoms can be proved rigorously. The key is to represent the solution as a sum of a (here explicitly given) profile and a corrector in  $L^2(\mathbb{R})$ . It is demonstrated that the kinetic relation can be easily inferred from this framework.

## 1 Introduction

Phase transitions in solids have been a focus of research activities in mathematics and physics alike. A very simple discrete model of elasticity allowing for phase transitions is as follows. Given a one-dimensional chain of atoms  $\{q_j\}_{j \in \mathbb{Z}}$  on the real line, let the deformation of each atom be given by  $u_j: \mathbb{R} \rightarrow \mathbb{R}$ . If neighbouring atoms are linked by springs, then the evolution governed by Newton's law takes the form

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

for every  $j \in \mathbb{Z}$ . A main challenge of phase transitions is that they are commonly characterised by a nonconvex energy  $V$ .

In this article, we prove the existence of subsonic travelling waves for the system (1) in the special case of a piecewise quadratic interaction potential  $V$  with two wells of equal depth. We say that a travelling wave solution represents a phase transition if its strain lives in both wells of the energy. Here, the wells meet at 0, so a solution with positive and negative strains exhibits a phase transition. We say that a phase-transforming solution is *heteroclinic* if the strain belongs asymptotically to the two different variants or phases of the material, that is, the two wells of the potential energy.

Modelling the elastic or plastic behaviour of materials with chain models with bistable or multistable springs is common in engineering and physics; see, for example, the seminal work [4] by Frenkel and Kontorova on dislocation dynamics (where an additional periodic on-site potential is introduced), or the analysis of a static snap-spring model by Müller and Villaggio [5]. The specific problem under consideration in the present work has been studied in a number of papers, notably by Balk, A. Cherkaev, E. Cherkaev, and Slepyan [7, 2, 3], and Truskinovsky and Vainchtein [10, 11]. In particular, the setting of [7, 10] is very similar to the one considered here. Yet, the methods employed in the present article are entirely different, and we believe that the tools we develop are of wider interest for lattice dynamical systems.

One of the difficulties of proving the existence of travelling waves in the lattice model (1) is as follows. We express the solution in the strain variable  $\varepsilon$ . It is easy to see that the Fourier transform  $F[\varepsilon]$  of the solution, if it exists, has non-integrable real poles stemming from zeros of the dispersion relation. The natural approach of finding the solution by applying the inverse Fourier transform  $F^{-1}$  to  $F[\varepsilon]$  is thus not rigorous. This is acknowledged in the physics literature. There, instead of integrating along the real axis  $\Gamma_0 := \mathbb{R}$ , the Fourier transform and its inverse are computed along suitable paths  $\Gamma_s$  such that the paths converge in the limit  $s \rightarrow 0$  to  $\Gamma_0$ ; the solution is then found

in the limit  $s \rightarrow 0$  of the Fourier-like transform along  $\Gamma_s$ . The mathematical justification of this method is not immediate, as the result depends on the choice of the paths. However precisely this thought amounts to the physical beauty of the argument: a selection principle is applied to choose physically reasonable solutions. This is called the *causality principle for a steady-state solution*, see [8].

One aim of this paper is to show that a rigorous framework can be established using Fourier methods. The idea is very simple. Indeed, it is already implicitly stated in the physics literature [7]. Namely, the aforementioned difficulties stem from the singularities that occur in the Fourier transform  $F[\varepsilon]$ , and here these singularities can be traced back to 0 and  $\kappa_0 > 0$  being zeros of the dispersion relation; the positive zero, in turn, defines the oscillation frequency in the asymptotic tails of the solution. Therefore, we represent the solution as a sum of a *profile* and *corrector*; the former captures the non-decaying oscillatory tails, and the latter will be shown to be in  $L^2(\mathbb{R})$ . We will demonstrate that this splitting allows a rigorous application of Fourier methods to the equation for the corrector.

We emphasise that this is more than a mere mathematical subtlety. One advantage of the rigorous framework is that there is no need, and in fact no space, for a selection principle; the selection is made by the dispersion relation. The new mathematical framework thus has a very elementary physical interpretation.

A second advantage of the method presented here is that a central argument can be made rigorous, apparently for the first time. This is the *key difficulty*, which can be described as follows. Effectively, one wants to solve a non-homogeneous linear equation, where the inhomogeneity depends on the solution. This is formulated in a precise manner in (7), where the inhomogeneity depends on the solution  $\varepsilon$ . *Only* if the solution satisfies the sign condition (8), then the inhomogeneity becomes a function of the spatial variable  $x$  alone, as shown in (9). With any approach that we are aware of a solution to the latter non-homogeneous equation is found, that is, with inhomogeneity  $f = f(x)$ . It is, however, evident that this solution is *not* a solution of the former (original) system if the sign condition (8) is violated. Yet, we could not find a rigorous proof of the sign condition in the literature. Since the deformation of integration paths leads to a representation of the solution as an infinite sum of residues, even a numerical verification of the sign condition will be difficult. Our proof in the setting introduced in this article is presented in Subsection 3.4 and Section 4.

We hope that the method of combining a profile with a corrector, as described here, may be of interest for related problems as well. This study seems to present the first rigorous results for heteroclinic waves for a double-well potential. In addition, though the verification of the sign condition is cumbersome, the decomposition of the solution as sum of a profile and corrector is in principle simple and may be useful in numerical investigations as well as a stability analysis.

One attractive feature of the approach presented here is that relevant information can be easily read off from the profile. This is demonstrated in Section 5. There, we determine the *kinetic relation* of the evolving interface, which relates the velocity of a phase boundary to a configurational force. Kinetic relations are relevant for the continuum limit of (1), which is elliptic-hyperbolic and thus genuinely ill posed. Namely, kinetic relations serve as a selection criterion [1, 9]. As shown in Section 5, it is easy to deduce from the symmetry of the profile that the kinetic relation here is zero. (The kinetic relation should not be confused with the pressure difference. In the situation under consideration, the region of atoms with high average pressure pushes the interface into the region of atoms with low average pressure; the asymptotic difference of the averaged pressure is explicitly calculated in Section 5 and shown to be strictly positive.)

Mathematically, an attractive feature of lattice systems is that a lot less is known about them in comparison to PDEs, and some methods are not easily applicable. For example, the use of the Wiener-Hopf technique for lattice equations is more subtle than for continuous problems. This is since the interface between the two linear half-spaces to be glued together is no longer a hypersurface, but a set of full measure, due to the atomistic spacing. This already indicates that the consistency check of a solution candidate is a much more involved process.

## 2 Description of the problem

We consider a one-dimensional chain of atoms  $\{q_j\}_{j \in \mathbb{Z}}$  on the real line. For each atom, the deformation is given by  $u_j: \mathbb{R} \rightarrow \mathbb{R}$ . The argument of the elastic potential is the discrete strain, which is given by the difference of the deformations  $u_{j+1}(t) - u_j(t)$ . In particular, only nearest neighbour interaction (NN) is considered. The elastic potential  $V: \mathbb{R} \rightarrow \mathbb{R}$  will be nonconvex to model phase transitions. As in several previous studies [2, 3, 10, 11], we consider the simplest possible elastic potential  $V$ , namely a piecewise quadratic function. Specifically, we define

$$V(\varepsilon) := \frac{1}{2} \begin{cases} (\varepsilon + 1)^2 & \text{for } \varepsilon < 0, \\ (\varepsilon - 1)^2 & \text{for } \varepsilon \geq 0. \end{cases} \quad (2)$$

This choice of the interaction potential sets the sound speed to  $\sqrt{V''} = 1$ . It is obvious that the corresponding stress-strain relation is piecewise linear and exhibits a jump discontinuity at  $\varepsilon = 0$ . Let  $H$  be the symmetrised Heaviside function,

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

then

$$\sigma(\varepsilon) := \varepsilon + 1 - 2H(\varepsilon) = \varepsilon + H(-\varepsilon) - H(\varepsilon) \quad (3)$$

equals  $V'(\varepsilon)$  wherever  $V$  is differentiable, that is, for every  $\varepsilon \neq 0$ .

We make two more assumptions, the first being that the equations of motion are governed by Newton's law,

$$\ddot{u}_j(t) = V'(u_{j+1}(t) - u_j(t)) - V'(u_j(t) - u_{j-1}(t)) \quad (4)$$

for every  $k \in \mathbb{Z}$ . In particular, it is assumed that dissipative effects can be neglected. In fact, Equation (4) is a Hamiltonian system with Hamiltonian

$$\mathcal{H} := \sum_{j \in \mathbb{Z}} \int_0^1 \left[ \frac{1}{2} \dot{u}_j(t)^2 + V(u_{j+1}(t) - u_j(t)) \right] dt.$$

The second assumption is that the movement of a phase boundary can be described as a travelling wave with strains in both wells of the potential  $V$ . A travelling wave is a solution of the form

$$u_j(t) = u(j - ct) \text{ for } j \in \mathbb{Z}. \quad (5)$$

With the travelling wave ansatz (5), Equation (4) reduces to

$$c^2 u''(x) = V'(u(x+1) - u(x)) - V'(u(x) - u(x-1)).$$

It is convenient to reformulate the travelling-wave equation for the discrete strain  $\varepsilon(x) := u(x) - u(x-1)$ . Then, after defining the discrete Laplacian as

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

the travelling wave equation for the discrete strain can be formulated as

$$c^2 \varepsilon''(x) = \Delta_1 V'(\varepsilon(x)).$$

For the special potential  $V$  defined in (2), this becomes

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

For the sake of clarity, we order into linear and nonlinear part and rewrite (6) as

$$c^2 \varepsilon'' - \Delta_1 \varepsilon = -2\Delta_1 H(\varepsilon). \quad (7)$$

The aim of this article is to study the existence of heteroclinic travelling wave solutions for this nonlinear advance-delay equation.

### 3 Waves on the real line

The purpose of this section is to prove the existence of solutions  $\varepsilon$  to (7) which are defined on the real line and have the property that

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

Since a solution with this property has asymptotic strains in the different wells of the potential, we call it *heteroclinic*.

If (8) holds, and only in this case, it follows directly that

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

that is, the nonlinear right-hand side turns into a linear function depending on the spatial variable alone.

Note that the right-hand side  $-2f$  of equation (7) is then, as a consequence of the sign condition (8), compactly supported on  $[-1, 1]$ , and hence its Fourier transform exists. Recall that for  $g: \mathbb{R} \rightarrow \mathbb{R}$ , the Fourier transform (if defined) is  $F[g] := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} g(x) \exp(-i\kappa x) dx$ ; the Fourier sine transform (if defined) is given by

$$F_s[g](\kappa) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \sin(\kappa x) g(x) dx = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \sin(\kappa x) g(x) dx. \quad (10)$$

The relation

$$F[g] = -iF_s[g]$$

holds for odd functions  $g: \mathbb{R} \rightarrow \mathbb{R}$ .

The dispersion relation for the linear part  $c^2\varepsilon'' - \Delta_1\varepsilon$  of Equation (6) will play a central rôle in the analysis to come; it can be defined by the calculation

$$F [c^2\varepsilon'' - \Delta_1\varepsilon] = D(\kappa) F[\varepsilon], \quad (11)$$

where

$$D(\kappa) := -c^2\kappa^2 + 4 \sin^2\left(\frac{\kappa}{2}\right) \quad (12)$$

is the *dispersion relation*. Let us define the function

$$d(\kappa) := \frac{\sin\left(\frac{\kappa}{2}\right)}{\frac{\kappa}{2}} \quad (13)$$

and rewrite  $D(\kappa) = (d^2(\kappa) - c^2)\kappa^2$ . It follows that  $\kappa_0$  is a zero of  $D$  if and only if  $d^2(\kappa_0) = c^2$ , where  $c^2 < 1$  for subsonic speeds, see Fig. 1 for a graph of  $d^2(\kappa)$ .

To simplify technicalities in the proof below, we restrict ourselves to consider positive values of  $\kappa_0$  such that  $\kappa_0^2 < \frac{1}{2}$ . The first implication is that such a zero of the dispersion relation  $D$  is the *unique* positive real zero once we define

$$c := d(\kappa_0) = \frac{\sin\left(\frac{\kappa_0}{2}\right)}{\frac{\kappa_0}{2}}. \quad (14)$$

The choice of the sign of  $c$  is immaterial for the proof and we choose without loss of generality the positive one. The second implication of the choice  $\kappa_0^2 < \frac{1}{2}$  is that quantitative estimates in the proof will be sufficiently small, uniformly for arbitrarily small choices of  $\kappa_0$ .

For further reference, we rewrite Equation (11) in terms of the Fourier sine transform,

$$F_s [c^2\varepsilon'' - \Delta_1\varepsilon] = D(\kappa) F_s[\varepsilon]. \quad (15)$$

The existence result of this article can be formulated as follows.

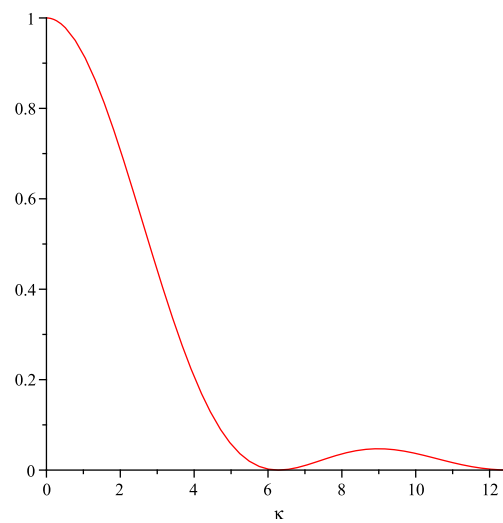


Figure 1: The graph of  $d^2(\kappa)$  for  $0 < \kappa < 4\pi$ .

**Theorem 3.1** *Suppose  $\kappa_0^2 < \frac{1}{2}$ . Then there exists a heteroclinic solution to Equation (7) with speed  $c$  given by (14). The solution has the odd symmetry and satisfies the sign condition (8).*

The outline of the proof is as follows. The first step is to show that Equation (7) has a solution if the right-hand side is of the form given in (9). In a second step, we need to verify the sign condition (8) to show that the solution also solves the original problem (7).

For an impression of the shape of the solution, we refer to Fig. 2 (see also Section 6 for numerical solutions of the initial value problem for different interaction potentials).

### 3.1 A rigorous setting for Fourier analysis

We pause for a moment to describe the difficulties of solving (7) on the real axis with the special nonlinearity  $f$  given by (9). By (11) and (12), the solution  $\varepsilon$  is formally given by the inverse Fourier transform of

$$\frac{F[-2f]}{D(\kappa)} \quad (16)$$

(and analogously for the Fourier sine transform). The attempt to solve (7) with Fourier methods thus faces the obvious difficulty that the inverse Fourier transform of (16), which would yield  $\varepsilon$ , is not well-defined. Namely, we had to integrate over the singularities of (16), that is, every real zero of the dispersion relation  $D$ , including  $\kappa = 0$ . These zeros necessarily exist; the singularity at 0 corresponds to non-zero asymptotic values of  $\varepsilon$ , whereas singularities at other real zeros reflect asymptotic oscillations of the solution with a frequency given by the corresponding dispersion frequency.

This problem is acknowledged in the physics literature, where the so-called *causality principle for a steady-state solution* [8] has been introduced as a formal solution method. Specifically, the singularities of (16) are avoided by choosing suitable paths around the singularities. Then, the limit of the Fourier-like transform along these paths is considered; the inverse Fourier-like transform can then be applied and the limit of vanishing deformations of the paths is considered. The solution is then expressed as a sum over residues. A particular difficulty of this approach is that this representation of the solution as a formal sum makes it at least difficult to verify the sign condition (8). However, the solution is a solution to (7) with  $f$  given by (9). If the sign condition is not satisfied, then  $f(x) \neq \Delta_1 H(\varepsilon(x))$ , so the solution is not a solution to the original system we set out to solve. See also the discussion in Section 1.

We thus propose an alternative approach. Namely, we write the solution  $\varepsilon$  of (7) (with the sign condition (8)) as a linear combination of a *profile* and a *corrector*, that is,

$$\varepsilon := \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}. \quad (17)$$

The profile function collects all parts of the solution  $\varepsilon$  corresponding to the singularities of (16), so that the corrector is a function in  $L^2(\mathbb{R})$  and satisfies an equation which can be solved by Fourier methods in  $L^2(\mathbb{R})$ .

We show that this method does not require us to compute the Fourier (sine) transform of the profile. Indeed, in the calculations below, only those quantities derived from the profile enter Fourier arguments which are in  $L^2(\mathbb{R})$ .

There are several possible choices for the profile function. Different profile functions obviously have different corrector functions, and the crucial sign condition (8) has to be estimated from the Fourier image of the corrector. The explicit choice of the profile function made below has the advantage that these estimates can be obtained relatively easily, while the estimates needed from the profile function itself can be read off directly. As motivation for the profile, let us consider the linearised problem of (7),

$$c^2 \varepsilon'' - \Delta_1 \varepsilon = 0. \quad (18)$$

Linear waves, e.g.,  $\cos(\kappa_0 x)$  for  $\kappa > 0$ , travel with speed  $c = d(\kappa_0)$ . Note that, by definition, such speeds are subsonic ( $c < 1$ ). The specific profile we use contains such linear waves, located in either well of the potential  $V$ , thus satisfying the sign condition (8). In particular, the profile

is heteroclinic. Thus, if we can show that the solution is close to the profile, we are able to infer that the phase transition from left to right well is travelling with subsonic speed  $c$  given in (14).

Now, we turn our attention to the profile  $\varepsilon_{\text{pr}}$ , which we define as follows. Let  $\alpha$  and  $\beta$  be constants, with

$$\alpha := c^2 \frac{\kappa_0^2}{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}} \quad (19)$$

and  $\beta > 0$  chosen such that

$$\gamma^2 := \left(1 + \frac{\kappa_0^2}{\beta^2}\right)^{-1} := c^2 \alpha \frac{1 - c^2}{\kappa_0^2} = c^4 \frac{1 - c^2}{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}. \quad (20)$$

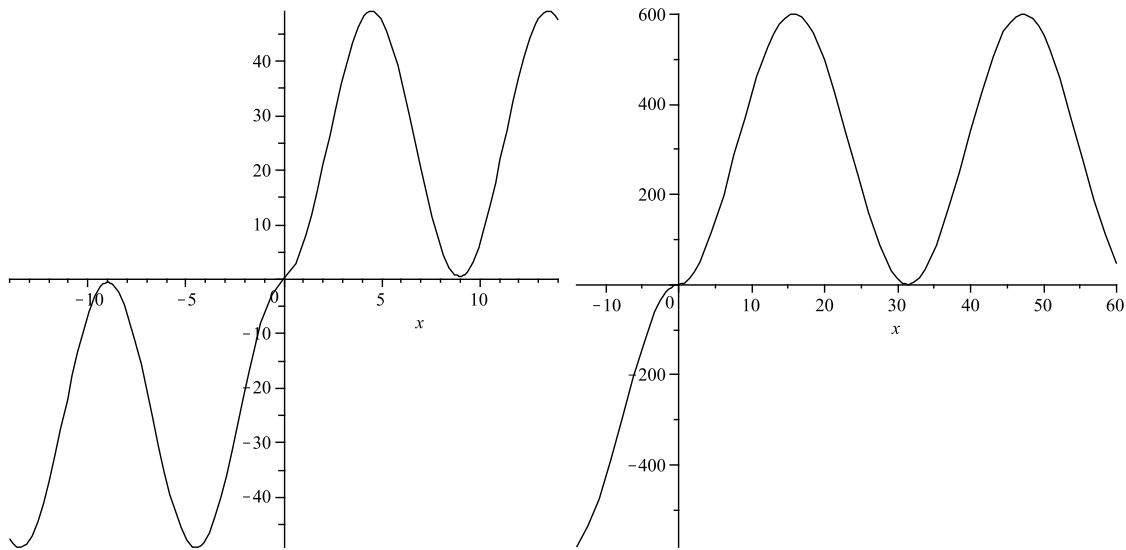


Figure 2: The profile function  $\varepsilon_{\text{pr}}$  for  $\kappa_0 = 0.7$  (left panel) and  $\kappa_0 = 0.2$  (right panel).

Then, we define the profile function as

$$\varepsilon_{\text{pr}}(x) := \varepsilon_{\text{pr}}^{\text{osc}}(x) + \frac{-2}{c^2} \Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}](x) + \varepsilon_{2\text{nd}}(x), \quad (21)$$

with

$$\varepsilon_{\text{pr}}^{\text{osc}}(x) := \text{sign}(x) \cdot \alpha \left( \frac{2 \sin^2(\frac{\kappa_0}{2} x)}{\kappa_0^2} + \frac{1 - \exp(-\beta|x|)}{\beta^2} \right) \in C^2(\mathbb{R}), \quad (22)$$

$$\varepsilon_{\text{pr}}^{\text{jump}}(x) := \text{sign}(x) \cdot \frac{1}{4} |x|^2, \quad (23)$$

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

$$\varepsilon_{2\text{nd}}(x) := \text{sign}(x) \cdot \frac{7}{60} \frac{129}{128} \frac{|x| \exp\left(-\frac{\sqrt{30}}{2} |x|\right)}{c^2} \left( \sqrt{30} + 15|x| - \frac{115}{86} \sqrt{30} |x|^2 \right). \quad (24)$$

We remark that  $\frac{1}{2}(1 - \cos(\kappa_0 x)) = \sin^2(\frac{\kappa_0}{2} x)$ , which shows the connection to linear waves discussed above. All other terms use exponentials since their expressions in Fourier space are simple.

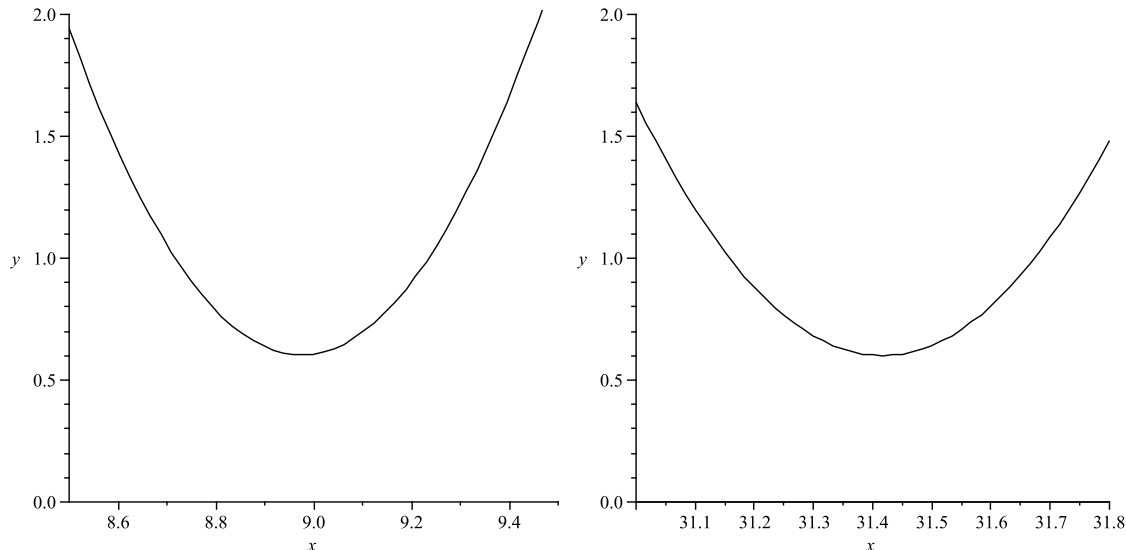


Figure 3: A zoom to the first positive minimum of the profile function  $\varepsilon_{\text{pr}}$ , again for  $\kappa_0 = 0.7$  (left panel) and  $\kappa_0 = 0.2$  (right panel).

See Figure 2 for plots of the profile for  $\kappa_0 = 0.7$  and  $\kappa_0 = 0.2$ . Figure 3 shows a zoom to illustrate the main challenge of Subsection 3.4: the solution  $\varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$  will satisfy the sign condition (8) only if the corrector  $\varepsilon_{\text{cor}}$  is in amplitude small enough so that the sign for  $\varepsilon$  agrees with the sign for the profile  $\varepsilon_{\text{pr}}$ .

Observe that  $\varepsilon_{\text{pr}}^{\text{jump}} \in C^{1,1}(\mathbb{R}) \cap C^2(\mathbb{R} \setminus \{0\})$  has a unit jump in the second derivative at 0, that is,  $\llbracket \partial^2 \varepsilon_{\text{pr}}^{\text{jump}}(0) \rrbracket = 1$ .

As for the profile  $\varepsilon_{\text{pr}}$ , the first part of  $\varepsilon_{\text{pr}}^{\text{osc}}(x)$  represents the oscillatory tails, while the additional exponential term ensures that  $\varepsilon_{\text{pr}}^{\text{osc}}(x)$  is  $C^2(\mathbb{R})$  for all choices of the parameters  $\kappa_0$  and  $\beta$ . The properties of the function  $\varepsilon_{\text{pr}}^{\text{jump}}(x)$  imply that the jumps in the second derivative of  $\frac{-2}{c^2} \Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}](x)$  compensate the jumps in the right-hand side of (7), see (9).

We call  $\varepsilon_{2\text{nd}}$  a second order correction since the oscillatory tails and the discontinuities in the second derivative of the solution  $\varepsilon$  are already taken care of by the first two terms  $\varepsilon_{\text{pr}}^{\text{osc}}$  and  $\varepsilon_{\text{pr}}^{\text{jump}}$  in (21). This correction is by no means unique. However, the specific choice of  $\varepsilon_{2\text{nd}}$  makes it possible to obtain a quantitatively small estimate for  $F_s[\varepsilon_{\text{cor}}](\kappa)$  for all values of  $\kappa \in \mathbb{R}$ . The second order correction  $\varepsilon_{2\text{nd}}$  is plotted in Figure 4.

We now outline the construction of the solution. We will show that the profile function  $\varepsilon_{\text{pr}}$  satisfies an equation

$$(c^2 \partial^2 - \Delta_1) \varepsilon_{\text{pr}}(x) = -2f(x) + \Phi(x), \quad (25)$$

where  $\Phi$  is a continuous localised function. In particular, we will prove that  $\Phi \in L^2(\mathbb{R})$ .

If, for the moment, we take this for granted, Equation (25) shows that  $\varepsilon_{\text{pr}}$  is a solution to (7) up to an error  $\Phi$ . The definition of the corrector is thus obvious; it is defined as a solution  $\varepsilon_{\text{cor}} \in L^2(\mathbb{R})$  of

$$(c^2 \partial^2 - \Delta_1) \varepsilon_{\text{cor}}(x) = \Phi(x). \quad (26)$$

Hence, by Equations (25) and (26) we deduce that  $\varepsilon = \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$  solves

$$(c^2 \partial^2 - \Delta_1) \varepsilon(x) = -2f(x). \quad (27)$$

This would be exactly the identity of Equation (7) we set out to solve. However, there is a subtle issue; the explicit form of  $f$  in (9) was derived under the assumption that the sign condition (8) is valid; we thus need to prove that the solution  $\varepsilon$  has the sign distribution prescribed by (8).

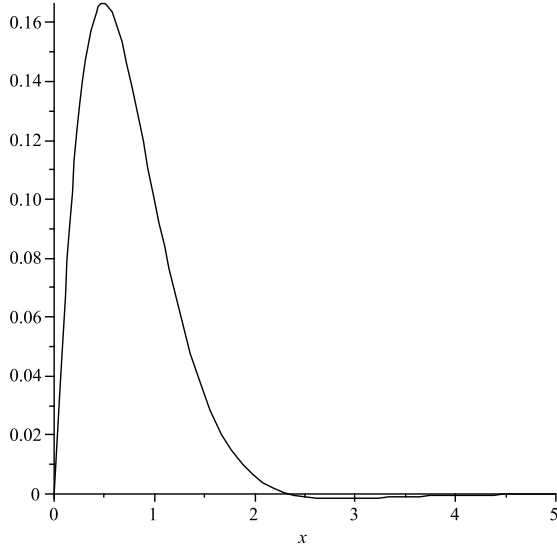


Figure 4: A plot of the second order correction  $\varepsilon_{2\text{nd}}$  of Equation (24).

In summary, two key assumptions made in this derivation need to be verified, as formulated in the claim below.

**Claim 3.2** *We claim that the following two statements are true.*

- (i) *Equation (26) can be solved in  $L^2(\mathbb{R})$ .*
- (ii) *The sign condition (8) holds for  $\varepsilon = \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$  uniformly in  $\kappa_0^2 \leq \frac{1}{2}$ .*

Theorem 3.1 follows immediately once Claim 3.2 is verified. However, to achieve uniformity in (ii), it turns out to be necessary to derive a sequence of technical estimates.

**Remark 3.3** *We remark that as long as  $D$  has a unique positive root  $\kappa_0$ , the profile has to include tails which oscillate exactly with frequency  $\kappa_0$ . The bounds, as a function of  $\kappa_0$ , are likely to diverge as  $\kappa_0$  approaches the first double root  $\kappa_1$  of  $D$ . For larger values of  $\kappa_0$ , that is, for smaller values of  $c$ , the decomposition can be generalised to include a superposition of oscillations with frequencies given by all positive roots of  $D$  as long as all these roots have single multiplicity. Note that for fixed  $c \in (0, 1)$ , there are at most finitely many roots of multiplicity two, and none of multiplicity three or higher. The technical difficulties to derive the necessary estimates will be significantly higher, and they cease to be uniform in  $0 < \kappa_0 < \kappa_1$ .*

*The fact that  $D$  always has for subsonic speeds, that is,  $c \in (0, 1)$ , a positive zero is in contrast to the Frenkel-Kontorova model (Klein-Gordon chain), where a positive zero can, but does not need not to exist. In the former case, the decomposition technique introduced here carries over (in preparation).*

In the following we present some auxiliary results, and verify the two claims (i) respectively (ii) of Claim 3.2 in Subsection 3.3 respectively Subsection 3.4.

### 3.2 Auxiliary statements

For the arguments to follow, it will be useful to be familiar with the behaviour of the constants  $\alpha$  and  $\beta$  as we vary the frequency  $\kappa_0$ . The expansions given below imply for (19) that  $\alpha = 12 - \frac{1}{5}\kappa_0^2 + O(\kappa_0^4)$ , and  $\gamma^2 = 1 - \frac{2}{15}\kappa_0^2 + O(\kappa_0^4)$ , by (20). This in turn determines an order of magnitude which will be relevant in Subsection 3.4,

$$\frac{1}{\beta^2} = \frac{2}{15} + O(\kappa_0^2). \tag{28}$$

For  $\kappa_0^2 \leq \frac{1}{2}$ , we obtain the more precise estimate

$$\left| \frac{1}{\beta^2} - \left( \frac{2}{15} + \frac{247}{25200} \kappa_0^2 \right) \right| \leq \varepsilon_2 \kappa_0^4, \quad \text{with } \varepsilon_2 := \frac{1}{1000}. \quad (29)$$

We approximate  $\eta(\kappa) := 4 \sin^2\left(\frac{\kappa}{2}\right)$  by a truncated Taylor series in powers of  $\kappa$ . Since  $|\eta^{(8)}(\kappa)| \leq 2$ , it holds that

$$\left| \eta(\kappa) - \kappa^2 \left[ 1 - \frac{1}{12} \kappa^2 \left( 1 - \frac{1}{30} \kappa^2 \right) \right] \right| \leq \varepsilon_0 \kappa^8, \quad \text{with } \varepsilon_0 := \frac{1}{20160}. \quad (30)$$

Thus, recalling  $c^2 = \frac{\eta(\kappa_0)}{\kappa_0^2}$ , we find

$$\left| c^2 - \left[ 1 - \frac{1}{12} \kappa_0^2 \left( 1 - \frac{1}{30} \kappa_0^2 \right) \right] \right| \leq \varepsilon_0 \kappa_0^6. \quad (31)$$

A division by  $\frac{1}{12} \kappa_0^2$  gives

$$\left| \frac{1 - c^2}{\frac{1}{12} \kappa_0^2} - \left( 1 - \frac{1}{30} \kappa_0^2 \right) \right| \leq 12 \varepsilon_0 \kappa_0^4. \quad (32)$$

Similarly, we obtain

$$\left| \frac{\sin(\kappa_0)}{\kappa_0} - \left( 1 - \frac{1}{6} \kappa_0^2 \left( 1 - \frac{1}{20} \kappa_0^2 \left( 1 - \frac{1}{42} \kappa_0^2 \right) \right) \right) \right| \leq \varepsilon_1 \kappa_0^8, \quad \text{with } \varepsilon_1 := \frac{1}{362880}. \quad (33)$$

The last two estimates imply by direct calculation that

$$\left| \frac{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}{\frac{1}{12} \kappa_0^2} - \left( 1 - \frac{1}{15} \kappa_0^2 + \frac{1}{420} \kappa_0^4 \right) \right| \leq \kappa_0^4 (12 \varepsilon_0 + 12 \kappa_0^2 \varepsilon_1). \quad (34)$$

### 3.3 Solvability in $L^2$

Here, we turn to the verification of point (i) of Claim 3.2. We need to show that, with the profile  $\varepsilon_{\text{pr}}$  given in (21) and for the choice of the constants  $\alpha$  in (19) and  $\beta$  in (20), the corrector  $\Phi$  on the right-hand side of equation (26) has *no* contribution on the Fourier mode associated with  $\kappa = 0$  and  $\kappa = \kappa_0$ . Recall that the choice of  $c$  is such that there is exactly one real positive root  $\kappa_0$  of the dispersion relation  $D$  given in (12).

We base our arguments on the following essential calculation of the Fourier sine transformation of  $L\varepsilon_{\text{pr}}$ ; here,  $L := (c^2 \partial^2 - \Delta_1)$  is the operator of Equation (25).

$$F_s[L\varepsilon_{\text{pr}}] = \sqrt{\frac{2}{\pi}} D(\kappa) \left( \frac{\alpha}{\kappa (\kappa_0^2 - \kappa^2)} \frac{\beta^2 + \kappa_0^2}{\beta^2 + \kappa^2} - \frac{4 \sin^2\left(\frac{\kappa}{2}\right)}{\kappa} \frac{1}{c^2 \kappa^2} + \frac{\phi}{c^2} \right), \quad (35)$$

where

$$\phi = \frac{7}{60} \kappa \frac{1 + \frac{44}{100} k^2}{\left( 1 + \frac{2}{15} \kappa^2 \right)^4}. \quad (36)$$

Further, the right-hand side  $-2f$  of equation (27), with  $f$  given by (9), transforms as

$$F_s[-2f](\kappa) = \sqrt{\frac{2}{\pi}} \frac{4 \sin^2\left(\frac{\kappa}{2}\right)}{\kappa}. \quad (37)$$

**Proposition 3.4** *The function  $\Phi$  on the right-hand side of Equation (25) and, hence, Equation (26) is in  $L^2(\mathbb{R})$ , provided the profile function  $\varepsilon_{\text{pr}}$  in (21) is chosen such that  $\alpha$  and  $\beta$  satisfy the relations (19) and (20), respectively. The unique  $L^2$  solution  $\varepsilon_{\text{cor}}$  of (26) has a bounded Fourier (sine) transform.*

*Proof:* First, we establish that  $\Phi \in L^2(\mathbb{R})$ . Equations (25), (35) and (37) imply

$$\begin{aligned} F_s[\Phi](\kappa) &= F_s[L\varepsilon_{\text{pr}}] - F_s[-2f] \\ &= \sqrt{\frac{2}{\pi}} \left[ D(\kappa) \left\{ \frac{\alpha}{\kappa(\kappa_0^2 - \kappa^2)} \frac{\beta^2 + \kappa_0^2}{\beta^2 + \kappa^2} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{c^2 \kappa^2} + \frac{\phi}{c^2} \right\} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \right]. \end{aligned} \quad (38)$$

It follows that the Fourier (sine) transform of  $\Phi$  has, at most, singularities at  $\kappa = 0$  and  $\kappa = \kappa_0$ . For  $\kappa = \kappa_0$ , only the first term in (38) has a singularity, but a removable one since  $D(\kappa_0) = 0$ . Similarly, for  $\kappa = 0$ , since  $D(0) = 0$ , the first two terms in (38) are singular, but again with a removable singularity; the same applies for the last term. Thus,  $F_s[\Phi]$  has, for the given profile independently of the choice of  $\alpha$  and  $\beta$ , no singularity. It is then easy to see that  $F_s[\Phi] \in L^2(\mathbb{R})$  and thus  $\Phi \in L^2(\mathbb{R})$  by Parseval's identity.

It remains to be shown that the Fourier (sine) transform of  $\varepsilon_{\text{cor}}$  is bounded. The argument resembles the previous one; we show that the singularities are removable. Unlike in the previous argument, this is only true for the specific choices of  $\alpha$  and  $\beta$  in (19) and (20). Equation (26), written in Fourier space, shows that

$$\begin{aligned} F_s[\varepsilon_{\text{cor}}](\kappa) &= \frac{F_s[\Phi](\kappa)}{D(\kappa)} = \sqrt{\frac{2}{\pi}} \left[ \frac{\alpha}{\kappa(\kappa_0^2 - \kappa^2)} \frac{\beta^2 + \kappa_0^2}{\beta^2 + \kappa^2} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{c^2 \kappa^2} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{D(\kappa)} + \frac{\phi}{c^2} \right] \\ &= \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{\kappa(\kappa_0^2 - \kappa^2)} \left[ \alpha \frac{\beta^2 + \kappa_0^2}{\beta^2 + \kappa^2} - \frac{(4 \sin^2(\frac{\kappa}{2}))^2 \kappa^2 (\kappa_0^2 - \kappa^2)}{c^2 (k^2)^2 D(\kappa)} \right] + \frac{\phi}{c^2} \right\} \\ &= \sqrt{\frac{2}{\pi}} \left\{ \frac{1}{\kappa(\kappa_0^2 - \kappa^2)} \left[ \frac{\alpha}{x^2 + \gamma^2 (1 - x^2)} - \frac{\kappa_0^2}{c^2} \left( \frac{\sin(\frac{\kappa}{2})}{\frac{\kappa}{2}} \right)^4 \frac{\kappa^2 (1 - x^2)}{D(\kappa)} \right] + \frac{\phi}{c^2} \right\}. \end{aligned} \quad (40)$$

Taking the limit  $\kappa \rightarrow \kappa_0$ , for the quotient on the right-hand side we find with L'Hospital's rule that it equates to

$$\sqrt{\frac{2}{\pi}} \frac{1}{\kappa_0} \left( \alpha - c^2 \frac{\kappa_0^2}{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}} \right) = 0, \quad (41)$$

which vanishes by the choice of  $\alpha$  in (19). Thus,  $F_s[\varepsilon_{\text{cor}}]$  is bounded for  $\kappa = \kappa_0$  by (40). Similarly, a twofold application of L'Hospital's rule yields that the limit of the quotient in (40) as  $\kappa \rightarrow 0$  is

$$\sqrt{\frac{2}{\pi}} \frac{1}{\kappa_0} \left( \alpha \left( 1 + \frac{\kappa_0^2}{\beta^2} \right) - \frac{1}{c^2} \frac{\kappa_0^2}{1 - c^2} \right) = 0,$$

now vanishing by the definition (20) of  $\beta$ . Thus,  $F_s[\varepsilon_{\text{cor}}]$  is bounded for  $\kappa = 0$ . Since  $\kappa = 0$  and  $\kappa = \kappa_0$  are the only potential singularities, we have shown that the choices of the profile  $\varepsilon_{\text{pr}}$  and for  $\alpha$  and  $\beta$  ensure that the Fourier sine transform  $F_s[\varepsilon_{\text{cor}}]$  is bounded for all  $\kappa \in \mathbb{R}$ .  $\square$

**Remark 3.5** *As demonstrated, the choice for  $\alpha$  and  $\beta$  ensures that the Fourier sine transform  $F_s[\varepsilon_{\text{cor}}]$  is bounded for all  $\kappa \in \mathbb{R}$ , in particular when  $\kappa$  passes through 0 and  $\pm\kappa_0$ . It is possible to strengthen this result and to show that  $\frac{F_s[\varepsilon_{\text{cor}}](\kappa)}{\kappa}$  stays bounded as  $\kappa$  goes to 0. Furthermore, we show in Lemma 3.9 that  $F_s[\varepsilon_{\text{cor}}]\kappa^5$  stays bounded for  $\kappa > 4$ , provided  $\kappa_0^2 < \frac{1}{2}$ . Thus, the Fourier transform  $F_s[\varepsilon_{\text{cor}}]$  of the corrector  $\varepsilon_{\text{cor}}$  is in  $L^2(\mathbb{R})$ , and so is the corrector itself. Furthermore, the corrector is a classical (in fact,  $C^4(\mathbb{R})$ ) solution of Equation (26).*

We prove the remarks regarding the corrector  $\varepsilon_{\text{cor}}$  itself. It follows from Proposition 3.4 and Lemma 3.9 that  $F_s[\varepsilon_{\text{cor}}]$  belongs to  $L^2(\mathbb{R})$ . Thus,

$$\varepsilon_{\text{cor}}(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty \sin(\kappa x) F_s[\varepsilon_{\text{cor}}](\kappa) \, d\kappa$$

belongs to  $L^2(\mathbb{R})$  as well. The fact that  $\varepsilon_{\text{cor}}$  is a solution of Equation (26) follows from the solvability of linear equations in  $L^2(\mathbb{R})$ ; the smoothness of the solution is a consequence of the decay of the Fourier (sine) transform at infinity.

A direct consequence of the preceding considerations is that the full profile  $\varepsilon = \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$  has a well-defined local average at  $x = \pm\infty$ . Thus, point (i) of the list in Claim 3.2 above is verified.

### 3.4 Verification of the sign condition for $\varepsilon$

Now we turn to the task of verifying point (ii) of Claim 3.2, that is, estimating the sign of  $\varepsilon$ . The estimates are lengthy, since the sign of  $\varepsilon$  has to be inferred from the amplitude of  $F_s[\varepsilon_{\text{cor}}]$  for all  $\kappa \in \mathbb{R}$ . The overarching assumption is that  $\kappa_0$  is sufficiently small. Specifically, as stated in Theorem 3.1, we assume throughout that

$$\kappa_0^2 < \frac{1}{2}. \quad (42)$$

Under this condition, we are going to prove a quantitatively small weighted estimate for  $F_s[\varepsilon_{\text{cor}}](\kappa)$  for all values of  $\kappa \in \mathbb{R}$ . Hence, we are able to employ the straightforward integral estimate

$$|\varepsilon_{\text{cor}}(x)| = \left| \sqrt{\frac{2}{\pi}} \int_0^\infty F_s[\varepsilon_{\text{cor}}](\kappa) \sin(\kappa x) \, d\kappa \right| \leq \sqrt{\frac{2}{\pi}} \int_0^\infty |F_s[\varepsilon_{\text{cor}}](\kappa)| \, d\kappa$$

to bound the supremum of  $\varepsilon_{\text{cor}}$  in real space. This is the key issue to prove that the sign condition (8) holds for the solution

$$\varepsilon(x) = \varepsilon_{\text{pr}}(x) - \varepsilon_{\text{cor}}(x),$$

as can be seen from Figure 3: the profile  $\varepsilon_{\text{pr}}$  satisfies the sign condition (8), see Figure 2. Thus, the solution  $\varepsilon$  has the same sign and is thus a solution of (7), if the corrector  $\varepsilon_{\text{cor}}$  is so small that it fits in the gap between the real axis and the profile. This gap is shown in Figure 3. To make the estimate more digestible, we break it into four parts, depending on the value of  $\kappa$  and the scaled frequency  $x := \frac{\kappa}{\kappa_0}$ . (We work in Fourier space throughout this section and Section 4; thus,  $x$  always denotes the rescaled variable and not the coordinate in real space, unless used to denote the arguments of the functions  $\varepsilon_{\text{cor}}$  and  $\varepsilon'_{\text{cor}}$  in Theorem 3.11 and its proof, as well as the statement of Corollary 3.10.) The four regimes are:  $0 < \kappa < 2$  and  $|x^2 - 1| > \frac{1}{2}$ , investigated in Lemma 3.6;  $0 < \kappa < 2$  and  $|x^2 - 1| \leq \frac{1}{2}$ , see Lemma 3.7;  $2 \leq \kappa \leq 4$ , studied in Lemma 3.8 and finally  $4 < \kappa$ , topic of Lemma 3.9. We approach the estimates in Lemma 3.6 and 3.7 by carefully expanding terms around the respective zeros of the dispersion relation. It turns out that for large values of  $\kappa$  (Lemma 3.9), we need to invoke a different asymptotic argument. To achieve the necessary quantitative smallness of the corrector, we have to join the different ranges of  $\kappa$  considered so far by an intermediate regime, as done in Lemma 3.8, which exploits uniform continuity on bounded intervals.

To emphasise the flow of the argument, we first state the results for these four regimes, and postpone the proofs to Section 4.

**Lemma 3.6** *Assume  $\kappa \in I_1 := (0, 2) \setminus \left[ \sqrt{\frac{1}{2}}, \sqrt{\frac{3}{2}} \right] \kappa_0$ , that is,  $\kappa < 2$  and  $|x^2 - 1| > \frac{1}{2}$ . Then there holds*

$$\sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| \leq \frac{2}{c^2} \left( 0.181\kappa + \frac{0.24\kappa}{1+x^2} \right).$$

In the second step, we investigate  $F_s[\varepsilon_{\text{cor}}]$  near  $\kappa_0$ .

**Lemma 3.7** *Assume  $\kappa \in I_2 := \left[ \sqrt{\frac{1}{2}}, \sqrt{\frac{3}{2}} \right] \kappa_0$ , that is,  $\kappa < 2$  and  $|x^2 - 1| \leq \frac{1}{2}$ . Then there holds*

$$\sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| \leq \frac{2}{c^2} \left( 0.219\kappa + \frac{1}{c^2} \cdot \frac{0.13}{x^4(1+x)^2} \cdot \kappa \right).$$

**Lemma 3.8** Assume  $\kappa \in I_3 := [2, 4]$ . Then

$$\sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| \leq \frac{2}{c^2} \left( 14 \left( \frac{0.18}{\kappa^5} + \frac{0.54}{\kappa^7} \right) + 0.032 \right).$$

**Lemma 3.9** Assume  $\kappa \in I_4 := (4, \infty)$ . Then

$$\sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| \leq \frac{2}{c^2} \frac{1}{\kappa^3} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \cdot 22.$$

Now it is relatively easy to gather together the results.

**Corollary 3.10** Let  $\kappa_0^2 \leq \frac{1}{2}$ . Then for all  $x \in \mathbb{R}$  it holds true that

$$|\varepsilon_{\text{cor}}(x)| < \frac{0.48}{c^2} =: E_{\text{cor}} \quad (43)$$

and

$$|\varepsilon'_{\text{cor}}(x)| < \frac{1.1}{c^2} =: E'_{\text{cor}}. \quad (44)$$

*Proof:* (i) Since

$$|\varepsilon_{\text{cor}}| \leq \sqrt{\frac{2}{\pi}} \int_0^\infty |F_s[\varepsilon_{\text{cor}}]| \, d\kappa \leq \sqrt{\frac{2}{\pi}} \int_{I_1 \cup I_2 \cup I_3 \cup I_4} |F_s[\varepsilon_{\text{cor}}]| \, d\kappa,$$

it is possible to proceed by integrating the estimates of the four preceding steps of Lemma 3.6 to Lemma 3.9. Note that

$$\int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{3}{2}}} \frac{dx}{x^3(1+x)^2} \leq 0.19.$$

Hence, since  $\kappa = \kappa_0 x$ ,

$$\frac{1}{c^2} \int_{I_2} \frac{1}{x^4(1+x)^2} \cdot \kappa \, d\kappa = \frac{\kappa_0^2}{c^2} \int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{3}{2}}} \frac{dx}{x^3(1+x)^2} \leq \frac{\kappa_0^2}{c^2} \cdot 0.19 < 0.2\kappa_0^2.$$

Further, for the range of  $\kappa_0$  under consideration, it holds that

$$\int_0^2 \frac{\kappa}{1+x^2} \, d\kappa = \kappa_0^2 \int_0^{\frac{2}{\kappa_0}} \frac{x}{1+x^2} \, dx = \frac{\kappa_0^2}{2} \ln \left( 1 + \frac{4}{\kappa_0^2} \right) < 0.55.$$

Now, observe that for all  $\kappa \in I_2$ , i.e.,  $|1 - x^2| \leq \frac{1}{2}$ , we know that

$$0.219 \leq 0.181 + \frac{0.24}{1+x^2}.$$

Hence, we infer from Lemma 3.6 and Lemma 3.7 that

$$\begin{aligned} & \sqrt{\frac{2}{\pi}} \int_{I_1 \cup I_2} |F_s[\varepsilon_{\text{cor}}]| \, d\kappa \\ & \leq \frac{2}{c^2} \left( 0.181 \int_0^2 \kappa \, d\kappa + \int_0^2 \frac{0.24\kappa}{1+x^2} \, d\kappa + 0.13 \cdot \frac{1}{c^2} \int_{I_2} \frac{\kappa \, d\kappa}{x^4(1+x)^2} \right) \\ & \leq \frac{2}{c^2} (0.181 \cdot 2 + 0.24 \cdot 0.55 + 0.13 \cdot 0.2\kappa_0^2) < \frac{2}{c^2} \cdot 0.508. \end{aligned}$$

An integration of the estimate in Lemma 3.8 yields

$$\sqrt{\frac{2}{\pi}} \int_{I_3} |F_s[\varepsilon_{\text{cor}}]| \, d\kappa < \frac{2}{c^2} \cdot 0.121.$$

Finally, the integrated version of Lemma 3.9 reads

$$\sqrt{\frac{2}{\pi}} \int_{I_4} |F_s[\varepsilon_{\text{cor}}]| \, d\kappa \leq \frac{2}{c^2} \int_{I_4} \frac{1}{\kappa^3} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \cdot 22 \, d\kappa = \frac{2}{c^2} \left( \frac{\ln(2)}{3} - \frac{\ln(47)}{15} + \frac{1}{32} \right) \cdot 22 < \frac{2}{c^2} \cdot 0.124.$$

Thus, the sum of these four integral estimates gives the desired bound

$$|\varepsilon_{\text{cor}}| < \frac{2}{c^2} (0.508 + 0.121 + 0.124) \leq \frac{0.48}{c^2}.$$

(ii) The argument is similar to the preceding one, but now we consider

$$\begin{aligned} |\varepsilon'_{\text{cor}}(x)| &= \left| \sqrt{\frac{2}{\pi}} \int_0^\infty F_s[\varepsilon_{\text{cor}}](\kappa) \kappa \cos(\kappa x) \, d\kappa \right| \\ &\leq \sqrt{\frac{2}{\pi}} \int_{I_1 \cup I_2 \cup I_3 \cup I_4} |F_s[\varepsilon_{\text{cor}}](\kappa)| \kappa \, d\kappa. \end{aligned}$$

Thus, the second estimate can be inferred from a multiplication of the integrands in Lemma 3.6 to Lemma 3.9 by  $\kappa$  followed by an integration.

This time,

$$\int_{\sqrt{\frac{1}{2}}}^{\sqrt{\frac{3}{2}}} \frac{x \, dx}{x^3(1+x)^2} \leq 0.17$$

implies

$$\frac{1}{c^2} \int_{I_2} \frac{1}{x^4(1+x)^2} \cdot \kappa^2 \, d\kappa \leq \frac{\kappa_0^3}{c^2} \cdot 0.17 < 0.18\kappa_0^3,$$

and a similar calculation shows that

$$\int_0^2 \frac{\kappa^2}{1+x^2} \, d\kappa = \kappa_0^3 \int_0^{\frac{2}{\kappa_0}} \frac{x^2}{1+x^2} \, dx < 0.57.$$

Thus, analogously to the calculation for  $I_1 \cup I_2$  in the first step of the proof,

$$\begin{aligned} &\sqrt{\frac{2}{\pi}} \int_{I_1 \cup I_2} |F_s[\varepsilon_{\text{cor}}]| \kappa \, d\kappa \\ &\leq \frac{2}{c^2} \left( 0.181 \int_0^2 \kappa^2 \, d\kappa + \int_0^2 \frac{0.24\kappa^2}{1+x^2} \, d\kappa + 0.13 \cdot \frac{1}{c^2} \int_{I_2} \frac{1}{x^4(1+x)^2} \cdot \kappa^2 \, d\kappa \right) \\ &\leq \frac{2}{c^2} \left( 0.181 \cdot \frac{8}{3} + 0.24 \cdot 0.57 + 0.13 \cdot 0.18\kappa_0^3 \right) < \frac{2}{c^2} \cdot 0.63. \end{aligned}$$

It is thus immediate to conclude from Lemmata 3.8–3.9

$$\begin{aligned} |\varepsilon'_{\text{cor}}(x)| &\leq \frac{2}{c^2} \left[ 0.63 + \int_{I_3} \left( 14 \left( \frac{0.18}{\kappa^5} + \frac{0.54}{\kappa^7} \right) + 0.032 \right) \kappa \, d\kappa + \int_{I_4} \frac{1}{\kappa^3} \frac{1}{1 + \frac{2}{15}\kappa^2} \cdot 22\kappa \, d\kappa \right] \\ &\leq \frac{2}{c^2} [0.63 + 0.33 + 0.68] < \frac{1.1}{c^2}. \end{aligned}$$

□

It is now not hard to prove the main statement of this subsection. The following theorem shows that point (ii) of Claim 3.2 is true; its proof relies on the following estimate, which follows directly from the expansion formulae in Subsection 3.2.

$$\frac{1}{\mathring{\beta}^2} := \frac{2}{15} \leq \frac{1}{\beta^2} \leq \frac{1}{\mathring{\beta}^2} \left(1 + \frac{1}{20}\right). \quad (45)$$

Here and in the following, we use the general notation  $\mathring{X} := \lim_{\kappa_0 \rightarrow 0} X$  for a quantity  $X$  that depends on  $\kappa_0$ .

**Theorem 3.11** *Let  $\kappa_0^2 \leq \frac{1}{2}$ . Then the solution  $\varepsilon$  satisfies the sign condition (8), that is*

$$\varepsilon(x) \geq 0 \text{ as } x \geq 0.$$

*Proof:* Let us recall the definition (21) of the profile function

$$\varepsilon_{\text{pr}}(x) := \varepsilon_{\text{pr}}^{\text{osc}}(x) + \frac{-2}{c^2} \Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}](x) + \varepsilon_{2\text{nd}}(x),$$

where, as in (22),

$$\varepsilon_{\text{pr}}^{\text{osc}}(x) = \text{sign}(x) \cdot \alpha \left( \frac{2 \sin^2(\frac{\kappa_0}{2} x)}{\kappa_0^2} + \frac{1 - \exp(-\beta|x|)}{\beta^2} \right).$$

Thus, we obtain

$$c^2 \varepsilon_{\text{pr}}(x) \geq t_4 (1 - \exp(-\beta|x|)) - 2\Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}](x) + c^2 \varepsilon_{2\text{nd}}(x), \quad (46)$$

where, with (20),

$$t_4 = t_4(\kappa_0) := \frac{\alpha c^2}{\beta^2} = \frac{\frac{\kappa_0^2}{1-c^2}}{\kappa_0^2 + \beta^2}.$$

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

$$1.57 \leq t_4 \leq \mathring{t}_4 := \lim_{\kappa_0 \rightarrow 0} t_4 = 1.6. \quad (47)$$

Furthermore, the monotonicity of  $\beta$  in  $\kappa_0$  yields via (45)

$$\begin{aligned} \left| \exp(-\beta x) - \exp(-\mathring{\beta} x) \right| &= \left| e^{-\frac{\beta+\mathring{\beta}}{2} x} \sinh\left((\beta - \mathring{\beta})x\right) \right| \\ &\leq \exp\left(-\mathring{\beta} \sqrt{\frac{20}{21}} x\right) \sinh\left(\mathring{\beta} \left(\sqrt{\frac{20}{21}} - 1\right) x\right) < 0.01. \end{aligned} \quad (48)$$

Let us define

$$W(x) := \mathring{t}_4 \left(1 - \exp(-\mathring{\beta} x)\right) - 2\Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}] + c^2 \varepsilon_{2\text{nd}}, \quad (49)$$

which is a function that only depends on  $x$  and not on  $\kappa_0$ . We collect two properties of  $W(x)$ ,

$$W(x) > 0.58 \quad \text{for } x > 0.385, \quad (50)$$

$$W(x) > 1.5 \cdot x \quad \text{for } 0 < x \leq 0.385. \quad (51)$$

Essential for the forthcoming arguments is that both lower bounds will turn out to be larger than the bounds in Corollary 3.10, that is,  $E_{\text{cor}}$  and  $E'_{\text{cor}}$ , respectively.

We break the argument showing the positivity of  $\varepsilon$  for  $x > 0$  in two parts,  $0 < x \leq 0.385$  and  $x > 0.385$ .

(i)  $x > 0.385$ . Since  $\varepsilon = \varepsilon_{\text{pr}} - \varepsilon_{\text{cor}}$ , we estimate with (46) and

$$W_1 := t_4 \exp(-\beta x) - \mathring{t}_4 \exp(-\mathring{\beta} x)$$

that

$$\begin{aligned}
c^2 \varepsilon_{\text{pr}} &\geq t_4 (1 - \exp(-\beta x)) - 2\Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}] + c^2 \varepsilon_{2\text{nd}} \\
&= \left( t_4 - 2\Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}] + c^2 \varepsilon_{2\text{nd}} - \dot{t}_4 \exp(-\dot{\beta} x) \right) - W_1 \\
&= t_4 - \dot{t}_4 + W - W_1.
\end{aligned}$$

It follows from (47) that

$$|t_4 - \dot{t}_4| \leq 0.03. \quad (52)$$

Hence, we estimate with (52), (48) and (47) in the second step that

$$\begin{aligned}
|W_1| &\leq |t_4 - \dot{t}_4| \frac{\exp(-\beta x) + \exp(-\dot{\beta} x)}{2} + \left| \exp(-\beta x) - \exp(-\dot{\beta} x) \right| \frac{t_4 + \dot{t}_4}{2} \\
&< 0.03 \cdot 1 + 0.01 \dot{t}_4 \leq 0.046 =: E_1.
\end{aligned} \quad (53)$$

Thus, (50) ensures for all  $x > 0.385$  that

$$W(x) > 0.58 > 0.03 + c^2 E_{\text{cor}} + E_1 = 0.556, \quad (54)$$

where  $E_{\text{cor}}$  is defined in (43). Hence, (43), (54), and (53) imply

$$c^2 \varepsilon \geq c^2 \varepsilon_{\text{pr}} - c^2 |\varepsilon_{\text{cor}}| > W(x) - (|t_4 - \dot{t}_4| + c^2 E_{\text{cor}} + |E_1|) > 0, \quad (55)$$

which proves the sign condition for all  $x > 0.385$ .

(ii)  $0 < x \leq 0.385$ : For this range of  $x$ , we base our argument on estimating the derivative of  $\varepsilon$ . We investigate all terms in

$$\varepsilon' = \varepsilon'_{\text{pr}} - \varepsilon'_{\text{cor}}.$$

Since  $\kappa_0^2 \leq \frac{1}{2}$ , we observe

$$\begin{aligned}
c^2 \varepsilon'_{\text{pr}} &\geq \frac{\sin(\kappa_0 x)}{\kappa_0^2} + \beta t_4 \exp(-\beta x) + (-2\Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}] + c^2 \varepsilon_{2\text{nd}})' \\
&\geq \dot{\beta} \dot{t}_4 \exp(-\dot{\beta} x) + (-2\Delta_1 [\varepsilon_{\text{pr}}^{\text{jump}}] + c^2 \varepsilon_{2\text{nd}})' - W_2 \\
&= W' - W_2,
\end{aligned} \quad (56)$$

where  $W$  is defined in (49), and

$$W_2 := \dot{\beta} \dot{t}_4 \exp(-\dot{\beta} x) - \beta t_4 \exp(-\beta x).$$

Next, we want to show that  $W_2$  is small. Since (45) and (47) imply

$$\dot{\beta} \dot{t}_4 \geq \beta t_4 \geq \dot{\beta} \sqrt{\frac{20}{21}} \cdot 1.57 > 0.95 \cdot \dot{t}_4 \dot{\beta},$$

we deduce  $|\dot{\beta} \dot{t}_4 - \beta t_4| < 0.05 \dot{t}_4 \dot{\beta}$ , and can estimate

$$\begin{aligned}
|W_2| &\leq \left| \exp(-\beta x) - \exp(-\dot{\beta} x) \right| \frac{\dot{\beta} \dot{t}_4 + \beta t_4}{2} + |\dot{\beta} \dot{t}_4 - \beta t_4| \left( \frac{\exp(-\beta x) + \exp(-\dot{\beta} x)}{2} \right) \\
&\leq 0.01 \cdot \dot{t}_4 \dot{\beta} + |\dot{\beta} \dot{t}_4 - \beta t_4| \cdot 1 < 0.06 \dot{t}_4 \dot{\beta} < 0.3 =: E_2.
\end{aligned} \quad (57)$$

Thus, we deduce from (44), (56), and (57)

$$c^2 \varepsilon \geq \int_0^x (c^2 \varepsilon'_{\text{pr}} - c^2 |\varepsilon'_{\text{cor}}|) d\xi \geq W(x) - (E_2 + c^2 E'_{\text{cor}}) x = W(x) - 1.4 \cdot x,$$

which is strictly positive for all  $0 < x \leq 0.385$  by (51).

The claimed statement for  $x < 0$  follows by symmetry.  $\square$

## 4 Proof of the integral estimates for the corrector

In this section, the proofs of Lemma 3.6–Lemma 3.9 are given. The estimates are delicate, but can be skipped by a reader who is mainly interested in the logic of the argument.

Before we start with these calculations, we collect a few estimates on terms depending on  $\kappa_0$  alone, which follow directly from the expansion formulae in Subsection 3.2.

$$1 \leq \frac{1}{c^2} \leq 1.05, \quad (58)$$

$$\frac{(1-c^2)}{\frac{1}{12}\kappa_0^2} \leq \lim_{\kappa_0 \rightarrow 0} \frac{(1-c^2)}{\frac{1}{12}\kappa_0^2} = 1, \quad (59)$$

$$\frac{\frac{1}{12}c^2\kappa_0^2}{1-c^2} \leq \lim_{\kappa_0 \rightarrow 0} \frac{\frac{1}{12}c^2\kappa_0^2}{1-c^2} = 1. \quad (60)$$

### 4.1 Proof of Lemma 3.6

We now give the proof of Lemma 3.6. Recall from (30) and (31) in Subsection 3.2 that  $\eta(\kappa) := 4\sin^2\left(\frac{\kappa}{2}\right)$  and  $c^2 = \frac{\eta(\kappa_0)}{\kappa_0^2}$  satisfy

$$\begin{aligned} \left| \eta(\kappa) - \kappa^2 \left[ 1 - \frac{1}{12}\kappa^2 \left( 1 - \frac{1}{30}\kappa^2 \right) \right] \right| &\leq \varepsilon_0 \kappa^8, \\ \left| c^2 - \left[ 1 - \frac{1}{12}\kappa_0^2 \left( 1 - \frac{1}{30}\kappa_0^2 \right) \right] \right| &\leq \varepsilon_0 \kappa_0^6. \end{aligned}$$

A division of the second inequality by  $\frac{1}{12}\kappa_0^2 \left( 1 - \frac{1}{30}\kappa_0^2 \right)$  yields for  $\kappa_0^2 < \frac{1}{2}$

$$\left| 1 - \frac{1-c^2}{\frac{1}{12}\kappa_0^2 \left( 1 - \frac{1}{30}\kappa_0^2 \right)} \right| \leq 12 \frac{\varepsilon_0 \kappa_0^4}{\left( 1 - \frac{1}{30}\kappa_0^2 \right)} \leq 12.5 \varepsilon_0 \kappa_0^4. \quad (61)$$

To simplify the expressions in this proof, it is convenient to introduce

$$t_0 := \frac{1-c^2}{\frac{1}{12}\kappa_0^2 \left( 1 - \frac{1}{30}\kappa_0^2 \right)} \quad (62)$$

to rewrite Equation (61) in more compact form,

$$|1 - t_0| \leq 12.5 \varepsilon_0 \kappa_0^4. \quad (63)$$

As the dispersion relation  $D$  introduced in (12) satisfies  $D(\kappa) = \eta(\kappa) - c^2\kappa^2$ , an analogous procedure shows that

$$\left| \frac{D(\kappa)}{(1-c^2)\kappa^2} - \left[ 1 - \frac{\frac{1}{12}\kappa^2}{1-c^2} \left( 1 - \frac{1}{30}\kappa^2 \right) \right] \right| \leq \frac{\varepsilon_0 \kappa^6}{1-c^2}. \quad (64)$$

We now express  $\kappa = x\kappa_0$  in the rescaled variable  $x$  to find  $t_0$  in this estimate,

$$\left| \frac{D(\kappa)}{(1-c^2)\kappa^2} - \left[ 1 - \frac{1}{t_0} x^2 \frac{1 - \frac{1}{30}\kappa^2}{1 - \frac{1}{30}\kappa_0^2} \right] \right| \leq \frac{\varepsilon_0 \kappa^6}{1-c^2}. \quad (65)$$

We multiply by  $1 - \frac{1}{30}\kappa_0^2$  and expand  $\frac{1}{t_0} = \frac{1}{t_0} - 1 + 1$ . This yields

$$\begin{aligned} \left| \frac{D(\kappa) \left( 1 - \frac{1}{30}\kappa_0^2 \right)}{(1-c^2)\kappa^2} - \left[ 1 - \frac{1}{30}\kappa_0^2 - x^2 \left( 1 - \frac{1}{30}\kappa^2 \right) \right] \right| \\ \leq \frac{\varepsilon_0 \kappa^6}{1-c^2} \left( 1 - \frac{1}{30}\kappa_0^2 \right) + \left| \frac{1}{t_0} - 1 \right| x^2 \left( 1 - \frac{1}{30}\kappa^2 \right). \end{aligned} \quad (66)$$

We divide by  $1 - \frac{1}{30}\kappa_0^2 - x^2(1 - \frac{1}{30}\kappa^2) = (1 - x^2)\left(1 - \frac{\kappa_0^2}{30}(1 + x^2)\right)$  and arrive at

$$|\delta_1 - 1| \leq \frac{\frac{\varepsilon_0 \kappa^6}{1-c^2} \left(1 - \frac{1}{30}\kappa_0^2\right) + |t_0^{-1} - 1| x^2 \left(1 - \frac{1}{30}\kappa^2\right)}{(1 - x^2) \left(1 - \frac{\kappa_0^2}{30}(1 + x^2)\right)},$$

where we have introduced

$$\delta_1 := \frac{D(\kappa)}{(1 - c^2) \kappa^2 (1 - x^2)} \frac{1 - \frac{1}{30}\kappa_0^2}{1 - \frac{\kappa_0^2}{30}(1 + x^2)} = \frac{D(\kappa)}{(1 - c^2) \kappa^2 (1 - x^2)} \frac{1}{1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}}. \quad (67)$$

We continue the estimate as follows: the second estimate uses the trivial bound 1 for the terms in parentheses in the nominator and the scaled variable  $\kappa = x\kappa_0$  as well as (63). The third inequality invokes (58), (60) and, for the denominator,  $\kappa_0^2 \leq 1$  and the assumption  $\kappa^2 \leq 2$  stated in Lemma 3.6. Altogether,

$$\begin{aligned} |\delta_1 - 1| &\leq \frac{\frac{\varepsilon_0 \kappa^6}{1-c^2} \left(1 - \frac{1}{30}\kappa_0^2\right) + |t_0^{-1} - 1| x^2 \left(1 - \frac{1}{30}\kappa^2\right)}{(1 - x^2) \left(1 - \frac{\kappa_0^2}{30}(1 + x^2)\right)} \\ &\leq \varepsilon_0 \kappa_0^4 x^2 \frac{\frac{1}{c^2} \frac{c^2 \kappa_0^2}{1-c^2} x^4 + \frac{12.5}{1-12.5\varepsilon_0 \kappa_0^4}}{|1 - x^2| \left(1 - \frac{\kappa_0^2}{30} - \frac{\kappa^2}{30}\right)} \\ &\leq \varepsilon_0 \kappa_0^4 \frac{x^2}{|1 - x^2|} \frac{12.6}{1 - \frac{1}{30} + \frac{2}{30}} (1 + x^4) \\ &\leq 15\varepsilon_0 \kappa_0^2 \kappa^2 \frac{(1 + x^4)}{|1 - x^2|}. \end{aligned} \quad (68)$$

Now we have all ingredients to estimate  $\frac{F_s[\varepsilon_{\text{cor}}](\kappa)}{\kappa}$  with  $F_s[\varepsilon_{\text{cor}}]$  from (39). The second equality below uses the dispersion relation (12) to rewrite the term  $4\sin^2\left(\frac{\kappa}{2}\right)$  and the scaled variable  $x = \frac{\kappa}{\kappa_0}$ , while the third line employs (20) for the first term.

$$\begin{aligned} \frac{F_s[\varepsilon_{\text{cor}}](\kappa)}{\kappa} &= \sqrt{\frac{2}{\pi}} \frac{1}{\kappa} \left[ \frac{\alpha}{\kappa(\kappa_0^2 - \kappa^2)} \frac{\beta^2 + \kappa_0^2}{\beta^2 + \kappa^2} - \frac{4\sin^2\left(\frac{\kappa}{2}\right)}{\kappa} \frac{1}{c^2 \kappa^2} - \frac{4\sin^2\left(\frac{\kappa}{2}\right)}{\kappa} \frac{1}{D(\kappa)} + \frac{\phi}{c^2} \right] \\ &= \sqrt{\frac{2}{\pi}} \frac{1}{\kappa} \left[ \frac{\alpha \left(1 + \frac{\kappa_0^2}{\beta^2}\right)}{\kappa_0^2} \frac{1}{\kappa(1 - x^2) \left(1 + \frac{\kappa^2}{\beta^2}\right)} - \frac{D(\kappa) + c^2 \kappa^2}{\kappa} \frac{1}{c^2 \kappa^2} - \frac{1 + c^2 \frac{\kappa^2}{D(\kappa)}}{\kappa} + \frac{\phi}{c^2} \right] \\ &= \sqrt{\frac{2}{\pi}} \left[ \frac{I}{(1 - c^2) \kappa^2 (1 - x^2)} + \frac{\phi}{c^2 \kappa} \right], \end{aligned} \quad (69)$$

where we abbreviate

$$I := \frac{1}{c^2} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} - (1 - c^2) (1 - x^2) \left( \frac{D(\kappa)}{c^2 \kappa^2} + 2 \right) - c^2 \frac{\kappa^2 (1 - c^2) (1 - x^2)}{D(\kappa)}. \quad (70)$$

We claim that  $I$  can be rewritten as

$$I = J_1 \kappa^2 + K_1 (\delta_1 - 1) \quad (71)$$

with

$$J_1 \kappa^2 := \frac{1}{c^2} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} - 2(1 - c^2) (1 - x^2) - \frac{(1 - c^2)^2 (1 - x^2)^2 \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)}{c^2} - \frac{c^2}{1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}} \quad (72)$$

and

$$K_1 := -\frac{(1-c^2)^2(1-x^2)^2\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)}{c^2} - \frac{c^2}{1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} \frac{1}{1+(\delta_1-1)}. \quad (73)$$

To see this, we expand (70) as follows. The first manipulations are to rewrite the expression in terms of  $\delta_1$  of Equation (67).

$$\begin{aligned} I &= \frac{1}{c^2} \frac{1}{1+\frac{\kappa^2}{\beta^2}} - 2(1-c^2)(1-x^2) \\ &\quad - \frac{(1-c^2)^2(1-x^2)^2\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)}{c^2} \frac{D(\kappa)}{(1-c^2)\kappa^2(1-x^2)\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)} \\ &\quad - \frac{c^2}{1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} \frac{(1-c^2)\kappa^2(1-x^2)\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)}{D(\kappa)} \\ &= \frac{1}{c^2} \frac{1}{1+\frac{\kappa^2}{\beta^2}} - 2(1-c^2)(1-x^2) \\ &\quad - \frac{(1-c^2)^2(1-x^2)^2\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)}{c^2} [(\delta_1-1)+1] - \frac{c^2}{1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} [(\delta_1^{-1}-1)+1] \\ &= \frac{1}{c^2} \frac{1}{1+\frac{\kappa^2}{\beta^2}} - 2(1-c^2)(1-x^2) - \frac{(1-c^2)^2(1-x^2)^2\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)}{c^2} - \frac{c^2}{1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} \\ &\quad - \frac{(1-c^2)^2(1-x^2)^2\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)}{c^2} (\delta_1-1) - \frac{c^2}{1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} (\delta_1^{-1}-1) \\ &= J_1\kappa^2 + K_1(\delta_1-1) \end{aligned}$$

as claimed; in the last step we used the identity

$$1 - \delta_1^{-1} = \frac{\delta_1 - 1}{1 + (\delta_1 - 1)}.$$

First, let us bound  $K_1$  by means of inequality (68). Since  $\kappa < 2$  in this lemma, it is easy to estimate

$$|K_1| \leq \frac{1}{c^2} \frac{(1-c^2)^2}{\kappa_0^4} \kappa_0^4 |1-x^2|^2 \cdot 1 + \frac{c^2}{1-\frac{2^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} \frac{1}{1-15\varepsilon_0\kappa_0^2\kappa^2\frac{(1+x^4)}{|1-x^2|}}. \quad (74)$$

Since the first factor in the second term depends only on  $\kappa_0$  and is monotonically decreasing for  $\kappa_0 \in (0, 1)$ , we bound it by

$$\frac{c^2}{1-\frac{2^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} \leq \frac{c^2}{1-\frac{2^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} \Bigg|_{\kappa_0=0} = \frac{15}{13}. \quad (75)$$

We observe

$$\frac{(1+x^4)}{|1-x^4|} \leq \begin{cases} \frac{5}{3} & \text{for } x^2 < \frac{1}{2}, \\ \frac{13}{5} & \text{for } x^2 > \frac{3}{2}, \end{cases} \quad (76)$$

and obtain thus for  $\kappa < 2$  and the global assumption  $\kappa_0^2 < \frac{1}{2}$  of (42)

$$15\varepsilon_0\kappa_0^2\kappa^2\frac{(1+x^4)}{|1-x^2|} = 15\varepsilon_0\kappa^2|\kappa_0^2+\kappa^2|\frac{(1+x^4)}{|1-x^4|} \leq 15\varepsilon_02^2\cdot(2^2+\frac{1}{2})\cdot\frac{13}{5} < \frac{1}{28}. \quad (77)$$

Thus, we can bound (74) with (59), (75), (77) and (58),

$$|K_1| \leq \frac{1}{c^2}\frac{1}{12^2}\kappa_0^4|1-x^2|^2 + \frac{15}{13}\frac{1}{1-\frac{1}{28}} \leq \frac{1}{c^2}\frac{2^4}{12^2} + \frac{15}{13}\frac{1}{1-\frac{1}{28}} < 1.32. \quad (78)$$

The combination of (69) and (71) shows that we need to bound  $\frac{|K_1|(\delta_1-1)}{(1-c^2)\kappa^2|1-x^2|}$ . To this end, we utilise the fact that the assumption  $|x^2-1| > \frac{1}{2}$  of this lemma implies

$$\frac{(1+x^2)}{|1-x^2|} \leq 5. \quad (79)$$

We use (68) for the second step; for the fourth bound, we collect the results from (60), the trivial bounds (76) and (79) and finally (78) to deduce the estimate

$$\begin{aligned} \left| \frac{|K_1|(\delta_1-1)}{(1-c^2)\kappa^2|1-x^2|} \right| &\leq \frac{|\delta_1-1|}{(1-c^2)\kappa^2|1-x^2|} |K_1| \leq \frac{15\varepsilon_0\kappa_0^2(1+x^4)}{(1-c^2)|1-x^2|^2} |K_1| \\ &\leq \frac{1}{c^2}15\varepsilon_0\frac{c^2\kappa_0^2}{(1-c^2)}\frac{(1+x^4)}{|1-x^4|}\frac{(1+x^2)}{|1-x^2|} |K_1| \\ &\leq \frac{15\varepsilon_0\cdot 12\cdot\frac{13}{5}\cdot 5\cdot 1.32}{c^2} < \frac{0.154}{c^2}. \end{aligned} \quad (80)$$

The equivalent estimate for  $J_1$  is (even) lengthier, but simpler. First, observe that there holds

$$\begin{aligned} 1-c^4 - \frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2} - c^4\frac{\kappa^2}{\beta^2} &= 1-c^4 - x^2\left(\frac{\frac{1}{30}\kappa_0^2}{1-\frac{1}{30}\kappa_0^2} + c^4\left(1+\frac{\kappa_0^2}{\beta^2}\right) - c^4\right) \\ &= (1-c^4)(1-x^2) - \frac{x^2}{1-\frac{1}{30}\kappa_0^2}T_1 \end{aligned}$$

where, using (20) in the last step,

$$\begin{aligned} T_1 &:= c^4\left(1+\frac{\kappa_0^2}{\beta^2}\right)\left(1-\frac{1}{30}\kappa_0^2\right) - \left(1-\frac{1}{15}\kappa_0^2\right) \\ &= \frac{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}{\frac{1}{12}\kappa_0^2}\left(\frac{\frac{1}{12}\kappa_0^2(1-\frac{1}{30}\kappa_0^2) - (1-c^2)}{(1-c^2)} + 1\right) - \left(1-\frac{1}{15}\kappa_0^2\right). \end{aligned}$$

Thus, we apply (31), (33) and (60) to obtain

$$|T_1| \leq \kappa_0^4\left(\frac{1}{420} + 12\varepsilon_0 + 12\kappa_0^2\varepsilon_1 + \frac{12\varepsilon_0}{c^2}\right). \quad (81)$$

Hence, we deduce

$$\frac{1}{c^2}\frac{1}{1+\frac{\kappa^2}{\beta^2}} - \frac{c^2}{1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}} = \frac{(1-c^4)(1-x^2)}{c^2\left(1+\frac{\kappa^2}{\beta^2}\right)\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)} - T_2\kappa_0^2\kappa^2, \quad (82)$$

where

$$T_2 := \frac{1}{\left(1+\frac{\kappa^2}{\beta^2}\right)\left(1-\frac{\kappa^2}{30}\frac{1}{1-\frac{1}{30}\kappa_0^2}\right)} \cdot \frac{T_1\kappa_0^{-4}}{c^2\left(1-\frac{1}{30}\kappa_0^2\right)}. \quad (83)$$

For  $\kappa \leq 2$  and  $\kappa_0^2 \leq \frac{1}{2}$ , it holds that

$$\left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right) \geq 1.$$

Thus, (81) implies, with (58), (79) and  $\kappa_0^2 \leq \frac{1}{2}$ , that

$$|T_2| \leq \frac{\frac{1}{420} + 12\varepsilon_0 + 12\kappa_0^2\varepsilon_1 + \frac{12\varepsilon_0}{c^2}}{c^2 \left(1 - \frac{1}{30}\kappa_0^2\right)} \cdot \frac{(1+x^2)}{|1-x^2|} \cdot \frac{|1-x^2|}{(1+x^2)} < \frac{0.24}{12} \frac{|1-x^2|}{(1+x^2)}. \quad (84)$$

We can now rewrite  $J_1$  given in (72), relying on (82) and (81) in the first equality below.

$$\begin{aligned} J_1 \kappa^2 &= -T_2 \kappa_0^2 \kappa^2 + \frac{(1-c^4)(1-x^2)}{c^2 \left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)} \\ &\quad - (1-c^2)(1-x^2) \left[2 + \frac{(1-c^2)(1-x^2)}{c^2} \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)\right] \\ &= -T_2 \kappa_0^2 \kappa^2 + \frac{(1-c^2)(1-x^2)}{c^2 \left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)} \left[1 + c^2 - 2c^2 \left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)\right] \\ &\quad - (1-c^2)(1-x^2) \left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)^2 \\ &= -T_2 \kappa_0^2 \kappa^2 + \frac{(1-c^2)\kappa^2(1-x^2)}{c^2} T_3, \end{aligned} \quad (85)$$

where we defined

$$T_3 := \frac{(1-c^2) \left(1 - (1-x^2) \left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)^2\right) - 2c^2 \left(\frac{\kappa^2}{\beta^2} - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2} - \frac{\kappa^4}{30\beta^2} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)}{\kappa^2 \left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2}\right)}.$$

To analyse this term, it is convenient to denote

$$t_1 := \frac{1-c^2}{\kappa_0^2} \quad \xrightarrow{\kappa_0 \rightarrow 0} \quad \dot{t}_1 := \frac{1}{12},$$

and

$$t_2 := \frac{\frac{1}{15}}{1 - \frac{1}{30}\kappa_0^2} \quad \xrightarrow{\kappa_0 \rightarrow 0} \quad \dot{t}_2 := \frac{1}{15}. \quad (86)$$

Observe the identity  $1 - \frac{\kappa^2}{30} \frac{1}{1 - \frac{1}{30}\kappa_0^2} = 1 - \frac{t_2}{2} \kappa^2$ ; this enables us to rewrite  $T_3$  as

$$T_3 = \frac{1}{1 - \frac{t_2}{2} \kappa^2} \left[ -\frac{\frac{1+c^2}{\beta^2}}{\left(1 + \frac{\kappa^2}{\beta^2}\right)} + t_1 (1 - t_2 \kappa^2) + t_2 - \frac{1-c^2}{900} \frac{\kappa^2 (1-x^2)}{\left(1 - \frac{1}{30}\kappa_0^2\right)^2} \right]. \quad (87)$$

We define  $\dot{T}_3$  as the limit of  $T_3$  as  $\kappa_0 \rightarrow 0$ . Namely, with (45) and (86),

$$\dot{T}_3 := \frac{-\frac{1+c^2}{\beta^2} + \dot{t}_1 (1 - \dot{t}_2 \kappa^2) + \dot{t}_2}{1 - \frac{\dot{t}_2}{2} \kappa^2} = \frac{-\frac{4}{(1+\frac{2}{15}\kappa^2)} + \frac{1}{12} (1 - \frac{1}{15}\kappa^2) + \frac{1}{15}}{1 - \frac{1}{30}\kappa_0^2}. \quad (88)$$

Thus we can rewrite  $T_3$  from (87) as

$$\begin{aligned} T_3 &= \frac{1}{1 - \frac{t_2}{2}\kappa^2} \left[ -\frac{\frac{1+c^2}{\beta^2}}{\left(1 + \frac{\kappa^2}{\beta^2}\right)} + t_1(1 - t_2\kappa^2) + t_2 - \frac{\frac{1-c^2}{900}\kappa^2(1-x^2)}{\left(1 - \frac{1}{30}\kappa_0^2\right)^2} \right] \\ &= \frac{1}{1 - \frac{t_2}{2}\kappa^2} [II_1 + II_2 + II_3 + II_4] + \mathring{T}_3, \end{aligned} \quad (89)$$

where the error terms  $II_j$  with  $j = 1, \dots, 4$  are given by

$$\begin{aligned} II_1 &:= \frac{\frac{2}{\beta^2}}{\left(1 + \frac{\kappa^2}{\beta^2}\right)} - \frac{\frac{1+c^2}{\beta^2}}{\left(1 + \frac{\kappa^2}{\beta^2}\right)}, \\ II_2 &:= t_1(1 - t_2\kappa^2) + t_2 - \mathring{t}_1(1 - \mathring{t}_2\kappa^2) - \mathring{t}_2, \\ II_3 &:= -\frac{\frac{1-c^2}{900}\kappa^2(1-x^2)}{\left(1 - \frac{1}{30}\kappa_0^2\right)^2}, \\ II_4 &:= \mathring{T}_3 \frac{(t_2 - \mathring{t}_2)}{2} \kappa^2. \end{aligned}$$

The error terms are bounded as follows.

$$|II_1| = \left| \frac{-\left(\frac{1+c^2}{\beta^2} - \frac{2}{\beta^2}\right) + \frac{\kappa^2}{\beta^2\beta^2}(1-c^2)}{\left(1 + \frac{\kappa^2}{\beta^2}\right)\left(1 + \frac{\kappa^2}{\beta^2}\right)} \right| \leq \frac{1}{100} \frac{1 + \frac{\kappa^2}{\beta^2}}{\left(1 + \frac{\kappa^2}{\beta^2}\right)\left(1 + \frac{\kappa^2}{\beta^2}\right)} < \frac{1}{100},$$

since  $\kappa_0^2 < \frac{1}{2}$  implies

$$\left| \frac{1+c^2}{\beta^2} - \frac{2}{\beta^2} \right| < \frac{1}{100} \quad \text{and} \quad \frac{1-c^2}{\beta^2} < \frac{1}{100}.$$

To estimate  $|II_2|$ , we deduce from (31)

$$|t_1 - \mathring{t}_1| \leq \frac{1}{360}\kappa_0^2 + \varepsilon_0\kappa_0^4 < \frac{1}{700};$$

furthermore, we obtain for  $\kappa_0^2 < \frac{1}{2}$

$$|t_2 - \mathring{t}_2| \leq \frac{1}{15} \frac{\kappa_0^2}{30} \frac{1}{1 - \frac{1}{60}} < \frac{1}{885}. \quad (90)$$

Thus,

$$\begin{aligned} |II_2| &\leq \left| (t_1 - \mathring{t}_1) \left(1 - \kappa^2 \frac{t_2 + \mathring{t}_2}{2}\right) + (t_2 - \mathring{t}_2) \left(1 - \kappa^2 \frac{t_1 + \mathring{t}_1}{2}\right) \right| \\ &\leq |t_1 - \mathring{t}_1| + |t_2 - \mathring{t}_2| < \frac{1}{390}. \end{aligned}$$

For the third term  $II_3$ , we obtain from (59) for  $\kappa_0^2 \leq \frac{1}{2}$  and  $\kappa \leq 2$

$$\begin{aligned} |II_3| &\leq \frac{1}{900} \frac{1-c^2}{\kappa_0^2} \frac{1}{\left(1 - \frac{1}{30}\kappa_0^2\right)^2} \kappa^2 |\kappa^2 - \kappa_0^2| \\ &\leq \frac{1}{900} \frac{1}{12} \frac{1}{\left(1 - \frac{1}{60}\right)^2} \cdot 2^2 \cdot 2^2 < \frac{1}{650}. \end{aligned}$$

Finally, we observe in (88) that

$$\left| -\frac{\frac{4}{15}}{\left(1 + \frac{2}{15}\kappa^2\right)} + \frac{1}{12} \left(1 - \frac{1}{15}\kappa^2\right) + \frac{1}{15} \right| \leq \frac{4}{15} + \frac{1}{12} + \frac{1}{15} = \frac{5}{12}$$

and obtain for  $\kappa < 2$  with (86) and (90)

$$|II_4| = \left| \mathring{T}_3 \frac{(t_2 - \mathring{t}_2)}{2} \kappa^2 \right| \leq \frac{\frac{5}{12} \frac{1}{885}}{1 - \frac{2^2}{30}} \cdot 2^2 < \frac{1}{920}.$$

Also, let us remark that  $\mathring{T}_3$  is solely a function of  $\kappa$ , which is, for small  $\kappa$ , well approximated by the Fourier sine transform  $\phi$  of the chosen second order correction given in (36). That is,

$$\sup_{0 < \kappa < 2} \left| \mathring{T}_3 + \frac{\phi}{\kappa} \right| \leq 0.009. \quad (91)$$

Now we arrive at the key estimate for  $J_1 \kappa^2$ . Below, we employ (85) for the equality in the first line, and (84) for  $T_2$  in combination with (89) in the second bound, and finally use the bound (91),

$$\begin{aligned} & \left| \frac{J_1 \kappa^2}{(1-c^2)\kappa^2(1-x^2)} + \frac{\phi}{c^2 \kappa} \right| = \left| \frac{-T_2 \kappa_0^2 \kappa^2}{(1-c^2)\kappa^2(1-x^2)} + \frac{T_3}{c^2} + \frac{\phi}{c^2 \kappa} \right| \\ & \leq \frac{1}{c^2} \left( \frac{c^2 \kappa_0^2}{1-c^2} \frac{|T_2|}{|1-x^2|} + |T_3 - \mathring{T}_3| + \left| \mathring{T}_3 + \frac{\phi}{\kappa} \right| \right) \\ & \leq \frac{1}{c^2} \left( \frac{0.24}{1+x^2} + \frac{II_1 + II_2 + II_3 + II_4}{1 - \frac{t_2}{2} \kappa^2} + 0.009 \right) \\ & \leq \frac{1}{c^2} \left( \frac{0.24}{1+x^2} + \frac{\frac{1}{100} + \frac{1}{390} + \frac{1}{650} + \frac{1}{920}}{1 - \frac{\frac{2^2}{30}}{1 - \frac{1}{60}}} + 0.009 \right) \leq \frac{1}{c^2} \left( \frac{0.24}{1+x^2} + 0.027 \right). \end{aligned} \quad (92)$$

Let us recall (69) and (71) to bound  $F_s[\varepsilon_{\text{cor}}]$  as a combination of the estimates (80) and (92)

$$\begin{aligned} \sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| &= \frac{2}{\pi} \kappa \left| \frac{K_1(\delta_1 - 1) + J_1 \kappa^2}{(1-c^2)\kappa^2(1-x^2)} + \frac{\phi}{c^2 \kappa} \right| \\ &\leq \frac{2}{\pi} \kappa \left( \left| \frac{K_1(\delta_1 - 1)}{(1-c^2)\kappa^2(1-x^2)} \right| + \left| \frac{J_1 \kappa^2}{(1-c^2)\kappa^2(1-x^2)} + \frac{\phi}{c^2 \kappa} \right| \right) \\ &\leq \frac{2}{c^2} \left( \frac{0.24\kappa}{1+x^2} + 0.181\kappa \right). \end{aligned}$$

Thus, the claim of Lemma 3.6 is proved.  $\square$

## 4.2 Proof of Lemma 3.7

The proof of Lemma 3.7 is similar to the arguments in the proof of Lemma 3.6. However, we need to expand the integrand at the non-trivial zero  $\kappa_0$  of the dispersion relation (12) (or, in rescaled variables, at  $x = 1$ ) to deduce the desired estimate in  $I_2$ .

*Proof:* It is convenient to write  $\Delta := \kappa - \kappa_0$ . We remark that

$$\begin{aligned} 4 \sin^2 \left( \frac{\kappa}{2} \right) - 4 \sin^2 \left( \frac{\kappa_0}{2} \right) &= 4 \sin \left( \frac{\kappa - \kappa_0}{2} \right) \sin \left( \frac{\kappa + \kappa_0}{2} \right), \\ &= 2 \sin(\kappa_0) \sin(\Delta) + \cos(\kappa_0) 4 \sin^2 \left( \frac{\Delta}{2} \right). \end{aligned}$$

This, together with  $\kappa = x\kappa_0$ ,  $D(\kappa_0) = 0$  and (12), yields with  $-\kappa_0^2 + \kappa^2 = -(2\kappa_0 + \Delta)\Delta$  that

$$\begin{aligned} \frac{D(\kappa)}{\kappa^2(1-x^2)} &= \frac{1}{x^2(1+x)} \frac{D(\kappa)}{\kappa_0^2(1-x)} = \frac{-1}{x^2(1+x)} \frac{D(\kappa) - D(\kappa_0)}{\kappa_0\Delta} \\ &= \frac{-1}{x^2(1+x)} \left( 2 \frac{\sin(\kappa_0)}{\kappa_0} \frac{\sin(\Delta)}{\Delta} + \frac{\Delta}{\kappa_0} \cos(\kappa_0) \frac{4\sin^2(\frac{\Delta}{2})}{\Delta^2} - c^2 \left( 2 + \frac{\Delta}{\kappa_0} \right) \right) \\ &= \frac{2}{x^2(1+x)} \left( \left( c^2 - \frac{\sin(\kappa_0)}{\kappa_0} \frac{\sin(\Delta)}{\Delta} \right) + \frac{\Delta}{2\kappa_0} \left( c^2 - \cos(\kappa_0) \frac{4\sin^2(\frac{\Delta}{2})}{\Delta^2} \right) \right). \end{aligned} \quad (93)$$

The obvious estimate

$$\left| \frac{\sin(\Delta)}{\Delta} - \left[ 1 - \frac{1}{6}\Delta^2 \left( 1 - \frac{1}{20}\Delta^2 \right) \right] \right| \leq \varepsilon_3 |\Delta|^6, \quad \text{with } \varepsilon_3 := \frac{1}{5040}, \quad (94)$$

combined with a division by  $\frac{1}{12}\kappa_0^2$  in (93), yields a bound for

$$\delta_2 := \frac{D(\kappa)}{\frac{1}{12}\kappa_0^2\kappa^2(1-x^2)}, \quad (95)$$

and

$$\begin{aligned} \tilde{\delta}_2 &:= \frac{2}{x^2(1+x)} \\ &\cdot \left( \left( \frac{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}{\frac{1}{12}\kappa_0^2} \right) + \frac{\Delta}{2\kappa_0} \left( \frac{c^2 - \cos(\kappa_0) \frac{4\sin^2(\frac{\Delta}{2})}{\Delta^2}}{\frac{1}{12}\kappa_0^2} \right) + 2 \left( \frac{\Delta}{\kappa_0} \right)^2 \frac{\sin(\kappa_0)}{\kappa_0} \left( 1 - \frac{\Delta^2}{20} \right) \right); \end{aligned} \quad (96)$$

namely, since  $\Delta = (x-1)\kappa_0$ ,

$$\left| \delta_2 - \tilde{\delta}_2 \right| \leq \frac{24\varepsilon_3}{x^2(1+x)} \kappa_0^4 \left( \frac{\Delta}{\kappa_0} \right)^6 \leq 24\varepsilon_3 \kappa_0^4 \frac{|1-x^2|^6}{x^2(1+x)^7} \leq \frac{\kappa_0^4}{12} |1-x^2| \varepsilon_4, \quad (97)$$

where, since  $|1-x^2| < \frac{1}{2}$  by assumption,

$$\varepsilon_4 := 2 \cdot 12^2 \cdot \varepsilon_3 \max_{x^2 \geq \frac{1}{2}} \left\{ \frac{\left(\frac{1}{2}\right)^5}{x^2(1+x)^7} \right\} < \frac{1}{11000}.$$

To proceed and formulate  $\tilde{\delta}_2$  as defined in (96) in a more suitable form, let us introduce

$$U_0 := \frac{c^2 - \frac{\sin(\kappa_0)}{\kappa_0}}{\frac{1}{12}\kappa_0^2}. \quad (98)$$

Since a short calculation reveals that

$$1 - \frac{x^2(1+x)}{2} = -\frac{5}{2} \frac{\Delta}{\kappa_0} - 2 \left( \frac{\Delta}{\kappa_0} \right)^2 - \frac{1}{2} \left( \frac{\Delta}{\kappa_0} \right)^3,$$

we can rewrite

$$\begin{aligned} \tilde{\delta}_2 &= \frac{2}{x^2(1+x)} \left[ U_0 \left( \frac{x^2(1+x)}{2} + 1 - \frac{x^2(1+x)}{2} \right) \right. \\ &\quad \left. + \frac{\Delta}{2\kappa_0} \left( \frac{c^2 - \cos(\kappa_0) \frac{4\sin^2(\frac{\Delta}{2})}{\Delta^2}}{\frac{1}{12}\kappa_0^2} \right) + 2 \left( \frac{\Delta}{\kappa_0} \right)^2 \frac{\sin(\kappa_0)}{\kappa_0} \left( 1 - \frac{\Delta^2}{20} \right) \right] \\ &= U_0 + \frac{\Delta}{\kappa_0} \frac{c^2 - \cos(\kappa_0) \frac{4\sin^2(\frac{\Delta}{2})}{\Delta^2}}{x^2(1+x)} - \left( 5 + \left( \frac{\Delta}{\kappa_0} \right)^2 \right) U_0 + 4 \left( \frac{\Delta}{\kappa_0} \right)^2 \frac{\sin(\kappa_0)}{\kappa_0} \frac{\left( 1 - \frac{\Delta^2}{20} \right) - U_0}{x^2(1+x)}. \end{aligned} \quad (99)$$

We also recall from Subsection 3.2 the following three estimates (30), (31) and (33),

$$\left| \frac{4 \sin^2\left(\frac{\Delta}{2}\right)}{\Delta^2} - \left(1 - \frac{1}{12} \Delta^2 \left(1 - \frac{1}{30} \Delta^2\right)\right) \right| \leq \varepsilon_0 |\Delta|^6 \quad (100)$$

$$\left| c^2 - \left(1 - \frac{1}{12} \kappa_0^2 \left(1 - \frac{\kappa_0^2}{30}\right)\right) \right| \leq \varepsilon_0 \kappa_0^6, \quad (101)$$

$$\left| \frac{\sin(\kappa_0)}{\kappa_0} - \left(1 - \frac{1}{6} \kappa_0^2 \left(1 - \frac{1}{20} \kappa_0^2 \left(1 - \frac{1}{42} \kappa_0^2\right)\right)\right) \right| \leq \varepsilon_1 \kappa_0^8. \quad (102)$$

We also notice that for  $U_0$  in (98), estimate (34) implies, with the natural definition

$$U_1 := 1 - \frac{1}{15} \kappa_0^2 + \frac{1}{420} \kappa_0^4,$$

that

$$|U_0 - U_1| < \varepsilon_5 \kappa_0^4, \text{ with } \varepsilon_5 := \frac{1}{1600}. \quad (103)$$

Also, the trigonometric identity  $2(1 - \cos(\kappa_0)) = 4 \sin^2\left(\frac{\kappa_0}{2}\right)$  allows us to deduce from (100) (with  $\Delta$  replaced by  $\kappa_0$ ) that

$$\left| \cos(\kappa_0) - \left(1 - \frac{\kappa_0^2}{2} \left(1 - \frac{1}{12} \kappa_0^2 \left(1 - \frac{\kappa_0^2}{30}\right)\right)\right) \right| \leq \frac{\varepsilon_0}{2} \kappa_0^8. \quad (104)$$

To obtain a bound for the second term in parentheses in (96), we introduce the abbreviation  $y := \frac{\Delta}{\kappa_0} = x - 1$ . Therefore we can show similarly that with

$$U_2 := 5 + y^2 - \kappa_0^2 \left(\frac{7}{15} + \frac{1}{2} y^2 + \frac{1}{30} y^4\right) + \kappa_0^4 \left(\frac{1}{60} + \frac{1}{24} y^2 + \frac{1}{60} y^4\right)$$

the following bound is valid,

$$\left| \frac{c^2 - \cos(\kappa_0) \frac{4 \sin^2\left(\frac{\Delta}{2}\right)}{\Delta^2}}{\frac{1}{12} \kappa_0^2} - U_2 \right| \leq \kappa_0^4 \varepsilon_6, \text{ with } \varepsilon_6 := \frac{1}{1200}. \quad (105)$$

Finally we deduce for the third term in parentheses in (96)

$$\left| \frac{\sin(\kappa_0)}{\kappa_0} \left(1 - \frac{\Delta^2}{20}\right) - U_3 \right| \leq \kappa_0^6 \varepsilon_7, \text{ with } \varepsilon_7 := \frac{1}{4200}, \quad (106)$$

where

$$U_3 := 1 - \kappa_0^2 \left(\frac{1}{6} + \frac{1}{20} y^2\right) + \frac{\kappa_0^4}{120} (1 + y^2).$$

Let us state the following algebraic identity,

$$\begin{aligned} & U_2 - (5 + y^2) U_1 + 4y(U_3 - U_1) \\ &= -\kappa_0^2 \left(\frac{2}{15} + \frac{11}{280} y^2 + \frac{1}{60} y^4 + \frac{1}{5} y(2 + y^2)\right) + \kappa_0^4 \left(\frac{1}{210} + \frac{13}{30} y^2 + \frac{1}{30} y^4 + \frac{1}{42} y \left(1 + \frac{7}{5} y^2\right)\right) \\ &= \frac{\kappa_0^2}{30} \left(-x^2(1+x)^2 \left(1 - \frac{\kappa_0^2}{28}\right) + \kappa_0^2 \left(\frac{5}{7} y^2 + \frac{13}{28} y^4 + \frac{1}{14} y(4 + 11y^2)\right)\right). \end{aligned} \quad (107)$$

Thus, we can estimate as follows (the first equality is (99) divided by  $1 - x^2 = -(1+x)\frac{\Delta}{\kappa_0}$ , with  $U_1$ ,  $U_2$  and  $U_3$  each added and subtracted; the first inequality relies on (105), (106), (103)

and (107) divided by  $x^2(1+x^2)$ .

$$\begin{aligned}
& \left| \frac{\tilde{\delta}_2 - U_0}{(1-x^2)} + \frac{\kappa_0^2}{30} \left(1 - \frac{1}{28}\kappa_0^2\right) \right| \\
&= \left| \frac{1}{x^2(1+x)^2} \left( \left[ \frac{c^2 - \cos \kappa_0 \frac{4 \sin^2(\frac{\Delta}{2})}{\Delta^2}}{\frac{1}{12}\kappa_0^2} - U_2 \right] + 4y \left[ \frac{\sin(\kappa_0)}{\kappa_0} \left(1 - \frac{\Delta^2}{20}\right) - U_3 \right] \right. \right. \\
&\quad \left. \left. - (5 + y^2 + 4y) [U_0 - U_1] \right) \right. \\
&\quad \left. + \frac{U_2 - (5 + y^2)U_1 + 4y(U_3 - U_1)}{x^2(1+x)^2} + \frac{\kappa_0^2}{30} \left(1 - \frac{1}{28}\kappa_0^2\right) \right| \\
&\leq \frac{\kappa_0^4}{x^2(1+x)^2} \left( \varepsilon_6 + 4|y|\kappa_0^2\varepsilon_7 + (5 + |y|^2 + 4|y|)\varepsilon_5 + \frac{1}{30} \left| \frac{5}{7}y^2 + \frac{13}{28}y^4 + \frac{1}{14}y(4 + 11y^2) \right| \right) \\
&\leq \frac{\kappa_0^4}{x^2(1+x)^2} \cdot \frac{0.13}{12}. \tag{108}
\end{aligned}$$

In particular, since (103) implies

$$|U_0 - 1| \leq \frac{\kappa_0^2}{15},$$

we obtain easily from (108) for  $|1-x^2| \leq \frac{1}{2}$  the bound

$$\begin{aligned}
|\tilde{\delta}_2 - 1| &\leq \frac{\kappa_0^2}{15} + \frac{\kappa_0^2}{30}(1-x^2) \left(1 - \frac{1}{28}\kappa_0^2\right) + \frac{\kappa_0^4}{12}(1-x^2) \frac{0.13}{x^2(1+x)^2} \\
&\leq \kappa_0^2 \left( \frac{1}{15} + |1-x^2| \left( \frac{1}{30} + 0.01 \cdot \kappa_0^2 \right) \right) \\
&\leq \kappa_0^2 \left( \frac{1}{12} + 0.005 \cdot \kappa_0^2 \right) < \frac{\kappa_0^2}{11}. \tag{109}
\end{aligned}$$

Then we can rewrite  $I$  as given in (70); the second equality relies on the definition (95) of  $\delta_2$ .

$$\begin{aligned}
I &= \frac{1}{c^2} \frac{1}{1 + \frac{\kappa_0^2}{\beta^2}} - (1-c^2)(1-x^2) \left( \frac{D(\kappa)}{c^2\kappa^2} + 2 \right) - c^2 \frac{\kappa^2(1-c^2)(1-x^2)}{D(\kappa)} \\
&= \frac{1}{c^2} \left[ \frac{1}{1 + \frac{\kappa_0^2}{\beta^2}x^2} - (1-c^2)(1-x^2) \left( \delta_2 \cdot \frac{1}{12}\kappa_0^2(1-x^2) + 2c^2 \right) - \frac{c^4(1-c^2)}{\frac{1}{12}\kappa_0^2} \frac{1}{\delta_2} \right] \\
&= \frac{1}{c^2} [J_2 + K_2]; \tag{110}
\end{aligned}$$

in the last step, we use the identity  $\frac{1}{1+t} = 1 - t + \frac{t^2}{1+t}$ , for  $t := \frac{\frac{\kappa_0^2}{\beta^2}}{1 + \frac{\kappa_0^2}{\beta^2}}(x^2 - 1)$ , since then  $1 + \frac{\kappa_0^2}{\beta^2}x^2 =$

$1 + \frac{\kappa_0^2}{\beta^2} + \frac{\kappa_0^2}{\beta^2} (x^2 - 1)$  and  $1 + t = 1 + \frac{\kappa^2}{\beta^2}$ , and thus obtain

$$\begin{aligned}
J_2 &:= \frac{1 - \frac{\kappa_0^2}{\beta^2} (x^2 - 1)}{1 + \frac{\kappa_0^2}{\beta^2}} + \left( \frac{\kappa_0^2}{\beta^2} (x^2 - 1) \right)^2 - \frac{c^4 (1 - c^2)}{\frac{1}{12} \kappa_0^2} \frac{1}{\tilde{\delta}_2} \\
&\quad - (1 - c^2) (1 - x^2) \left( \frac{1}{12} \kappa_0^2 (1 - x^2) + 2c^2 \right), \\
K_2 &:= \left( \frac{\kappa_0^2}{\beta^2} (x^2 - 1) \right)^2 \left( \frac{1}{1 + \frac{\kappa^2}{\beta^2}} - 1 \right) - (1 - c^2) (1 - x^2) (\delta_2 - 1) \cdot \frac{1}{12} \kappa_0^2 (1 - x^2) \\
&\quad + \frac{c^4 (1 - c^2)}{\frac{1}{12} \kappa_0^2} \frac{\delta_2 - \tilde{\delta}_2}{\delta_2 \tilde{\delta}_2}.
\end{aligned}$$

Estimate (97) together with  $\frac{|1-x^2|}{x^2} \leq 1$ , (60) and (109) can be employed to bound  $K_2$  in the third inequality to come, whereas the first inequality relies again on  $\kappa = x\kappa_0$  and (59).

$$\begin{aligned}
&\left| \frac{K_2}{(1 - c^2) \kappa^2 (1 - x^2)} \right| \\
&\leq \frac{\left( \frac{\kappa_0^2}{\beta^2} (x^2 - 1) \right)^2}{(1 - c^2) \kappa^2 (1 - x^2)} \cdot \left| \frac{1}{1 + \frac{\kappa^2}{\beta^2}} - 1 \right| + \left| \frac{(\delta_2 - 1) (1 - x^2)}{12x^2} \right| + \left| \frac{c^4}{\delta_2 \tilde{\delta}_2} \frac{\delta_2 - \tilde{\delta}_2}{(1 - c^2) \kappa^2 (1 - x^2)} \right| \\
&\leq \frac{\frac{\kappa_0^2}{(1 - c^2)}}{\beta^4} \frac{|1 - x^2|}{x^2} \cdot \frac{\kappa^2}{1 + \frac{\kappa^2}{\beta^2}} + \frac{\left( |\tilde{\delta}_2 - 1| + |\delta_2 - \tilde{\delta}_2| \right)}{12} \cdot \frac{|1 - x^2|}{x^2} \\
&\quad + \left| \frac{c^4}{\tilde{\delta}_2 \left( \tilde{\delta}_2 - |\delta_2 - \tilde{\delta}_2| \right)} \frac{\delta_2 - \tilde{\delta}_2}{(1 - c^2) \kappa^2 (1 - x^2)} \right| \\
&\leq \frac{12}{c^2 \beta^4} \frac{\frac{3}{4}}{\beta^2} + \frac{1}{12} \left( \frac{\kappa_0^2}{11} + \frac{\kappa_0^4 \varepsilon_4}{12 \cdot 2} \right) + \frac{c^2}{\left( 1 - \frac{\kappa_0^2}{11} \right) \left( 1 - \frac{\kappa_0^2}{11} - \frac{\kappa_0^4 \varepsilon_4}{12 \cdot 2} \right)} \cdot \frac{\frac{1}{12} c^2 \kappa_0^2 \varepsilon_4}{(1 - c^2) x^2} \\
&\leq \frac{9}{c^2 \beta^6} + \frac{1}{12} \left( \frac{\kappa_0^2}{11} + \frac{\kappa_0^4 \varepsilon_4}{12 \cdot 2} \right) + \frac{c^2}{\left( 1 - \frac{\kappa_0^2}{11} \right) \left( 1 - \frac{\kappa_0^2}{11} - \frac{\kappa_0^4 \varepsilon_4}{12 \cdot 2} \right)} \cdot 2 \cdot \varepsilon_4 < 0.005. \tag{111}
\end{aligned}$$

Now we turn to the estimates for  $J_2$ . Observe that (20) combined with (98) implies that  $\frac{c^4(1-c^2)}{\frac{1}{12}\kappa_0^2} \left( 1 + \frac{\kappa_0^2}{\beta^2} \right) = U_0$ ; thus, we can conclude that

$$\frac{J_2}{\kappa_0^2 (1 - x^2)} = \frac{\frac{\tilde{\delta}_2 - U_0}{\kappa_0^2 (1 - x^2)}}{\tilde{\delta}_2 \left( 1 + \frac{\kappa_0^2}{\beta^2} \right)} + \frac{\frac{1}{\beta^2}}{\left( 1 + \frac{\kappa_0^2}{\beta^2} \right)^2} + \frac{\frac{\kappa_0^2}{\beta^4} (1 - x^2)}{\left( 1 + \frac{\kappa_0^2}{\beta^2} \right)^2} - \frac{(1 - c^2)}{\kappa_0^2} \left( 2c^2 + \frac{1}{12} \kappa_0^2 (1 - x^2) \right). \tag{112}$$

In order to estimate  $J_2$  we introduce in an intermediate step the term

$$\begin{aligned}
U_4 &:= \frac{1}{30} \left(1 - \frac{1}{28} \kappa_0^2\right) \left(1 - \frac{\kappa_0^2}{\beta^2} + \frac{67}{8400} \kappa_0^4\right) + \left(\frac{1}{\beta^2} + \frac{1}{\beta^4} k_0^2 (1-x^2)\right) \left(1 - 2\frac{\kappa_0^2}{\beta^2} + \frac{17}{504} \kappa_0^4\right) \\
&\quad - \frac{(1-c^2)}{\kappa_0^2} \left(\frac{1}{12} \kappa_0^2 (1-x^2) + 2c^2\right) + \frac{7}{60} (1-c^2) x^2 + \frac{1}{900} \kappa_0^2 (1+x^2) \\
&= \frac{1}{30} \left(1 - \frac{1}{28} \kappa_0^2\right) \left(1 - \frac{\kappa_0^2}{\beta^2} + \frac{67}{8400} \kappa_0^4\right) + \left(\frac{1}{\beta^2} + \frac{1}{\beta^4} k_0^2 (1-x^2)\right) \left(1 - 2\frac{\kappa_0^2}{\beta^2} + \frac{17}{504} \kappa_0^4\right) \\
&\quad - \frac{1-c^2}{\frac{1}{12} k_0^2} \left(\frac{1}{6} + \frac{\kappa_0^2}{12^2} \left(-2\frac{1-c^2}{\frac{1}{12} k_0^2} - \frac{7}{5} + \frac{12}{5} (1-x^2)\right)\right) + \frac{\kappa_0^2}{900} (2 - (1-x^2)).
\end{aligned}$$

We can estimate this term as follows, using (32) twice in the second line as well as (29) in combination with (45).

$$\begin{aligned}
|U_4| &\leq \frac{\kappa_0^2}{900} (2 - (1-x^2)) + \frac{1}{30} \left(1 - \frac{1}{28} \kappa_0^2\right) \left(1 - \frac{\kappa_0^2}{\beta^2} + \frac{67}{8400} \kappa_0^4\right) \\
&\quad + \left(\frac{1}{\beta^2} + \frac{247}{25200} \kappa_0^2 + \varepsilon_2 \kappa_0^4 + \frac{1}{\beta^4} k_0^2 (1-x^2)\right) \left(1 - 2\frac{\kappa_0^2}{\beta^2} + \frac{17}{504} \kappa_0^4\right) \\
&\quad + \left(1 - \frac{1}{30} \kappa_0^2 + 12\varepsilon_0 \kappa_0^4\right) \left(\frac{1}{6} + \frac{\kappa_0^2}{12^2} \left(-2 \left(1 - \frac{1}{30} \kappa_0^2 + 12\varepsilon_0 \kappa_0^4\right) - \frac{7}{5} + \frac{12}{5} (1-x^2)\right)\right) \\
&\leq \frac{1}{12} k_0^4 \left(\frac{4}{315} \left(1 + \frac{1781}{5600} \kappa_0^2\right) + \frac{113}{2250} (1-x^2) \left(-1 + \frac{340}{2373} \kappa_0^2\right)\right) \\
&\quad + (24\varepsilon_0 + 12\varepsilon_2) + ((27 + 12|1-x^2|) \varepsilon_0 + 16\varepsilon_2) \frac{\kappa_0^2}{5} + \left(\frac{2}{15} \varepsilon_0 + \frac{17}{42} \varepsilon_2\right) \kappa_0^4 + 24\varepsilon_0^2 \kappa_0^6.
\end{aligned}$$

Thus, since  $\kappa_0^2 < \frac{1}{2}$  and  $|1-x^2| < \frac{1}{2}$ , we can conclude that

$$|U_4| \leq \frac{1}{12} k_0^4 \cdot \varepsilon_8, \text{ with } \varepsilon_8 := 0.057. \quad (113)$$

We continue to estimate the term involving  $J_2$  given in (112). To this behalf, we combine the well-known bounds  $\kappa_0^2 \leq \frac{1}{2}$  with (109); the first inequality employs (113), while the last estimate

utilises the fact that  $\frac{1}{\left(1 - \frac{\kappa_0^2}{11}\right)\left(1 + \frac{\kappa_0^2}{\beta^2}\right)} \leq 1$ .

$$\begin{aligned}
& \left| \frac{J_2}{\kappa_0^2(1-x^2)} + \frac{7}{60}(1-c^2)x^2 + \frac{\kappa_0^2}{900}(1+x^2) \right| \leq |U_4| + \frac{\left| \frac{\tilde{\delta}_2 - U_0}{\kappa_0^2(1-x^2)} - \frac{1}{30} \left(1 - \frac{\kappa_0^2}{28}\right) \right|}{\tilde{\delta}_2 \left(1 + \frac{\kappa_0^2}{\beta^2}\right)} \\
& + \frac{\frac{1}{30} \left(1 - \frac{\kappa_0^2}{28}\right)}{1 + \frac{\kappa_0^2}{\beta^2}} \left| \frac{1}{\tilde{\delta}_2} - 1 \right| + \frac{1}{30} \left(1 - \frac{\kappa_0^2}{28}\right) \left| \frac{1}{1 + \frac{\kappa_0^2}{\beta^2}} - \left(1 - \frac{\kappa_0^2}{\beta^2} + \frac{67}{8400} \kappa_0^4\right) \right| \\
& + \frac{k_0^2(1-x^2) \left| \frac{1}{\beta^4} - \frac{1}{\beta^4} \right|}{\left(1 + \frac{\kappa_0^2}{\beta^2}\right)^2} \\
& + \left( \frac{1}{\beta^2} + \frac{1}{\beta^4} k_0^2(1-x^2) \right) \left| \frac{1}{\left(1 + \frac{\kappa_0^2}{\beta^2}\right)^2} - \left(1 - 2\frac{\kappa_0^2}{\beta^2} + \frac{17}{504} \kappa_0^4\right) \right| \\
& \leq \frac{k_0^4}{12} \varepsilon_8 + \left( \frac{k_0^2}{12} \frac{0.13}{x^2(1+x)^2} + \frac{1}{30} \frac{k_0^2}{11} \right) \frac{1}{\tilde{\delta}_2 \left(1 + \frac{\kappa_0^2}{\beta^2}\right)} + \frac{1}{30} (1.4 \cdot \varepsilon_2 \kappa_0^6) \\
& + k_0^2(1-x^2) \frac{1}{\beta^4} \left( \left( \frac{21}{20} \right)^2 - 1 \right) + \frac{1}{\beta^2} \left( \frac{21}{20} + \frac{1}{\beta^2} k_0^2(1-x^2) \right) (4.2 \cdot \varepsilon_2 \kappa_0^6) \\
& \leq \frac{k_0^4}{12} \varepsilon_8 + \left( \frac{k_0^2}{12} \frac{0.13}{x^2(1+x)^2} + \frac{1}{30} \frac{k_0^2}{11} \right) \frac{1}{\left(1 - \frac{\kappa_0^2}{11}\right) \left(1 + \frac{\kappa_0^2}{\beta^2}\right)} \\
& + \frac{\kappa_0^2}{2} \frac{1}{\beta^4} \left( \left( \frac{21}{20} \right)^2 - 1 \right) + \varepsilon_2 \kappa_0^6 \left( \frac{1.4}{30} + \frac{4.2}{\beta^2} \left( \frac{21}{20} + \frac{1}{\beta^2} \right) \right) \\
& < \frac{k_0^2}{12} \left( \frac{0.13}{x^2(1+x)^2} + 0.076 \right). \tag{114}
\end{aligned}$$

We are finally in a position to conclude by combining the last result with (69), (110) in the identity; (111) and (114) enter in the second estimate, while (58) and (60) are employed in the third step. We obtain

$$\begin{aligned}
& \sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| = \frac{2}{c^2} \kappa \left| \frac{J_2 + K_2}{(1-c^2)\kappa^2(1-x^2)} + \frac{\phi}{\kappa} \right| \\
& \leq \frac{2}{c^2} \kappa \left[ \frac{\left| \frac{J_2}{\kappa_0^2(1-x^2)} + \frac{7}{60}(1-c^2)x^2 + \frac{\kappa_0^2}{900}(1+x^2) \right|}{(1-c^2)x^2} + \left| \frac{K_2}{(1-c^2)\kappa^2(1-x^2)} \right| \right. \\
& \quad \left. + \left| -\frac{7}{60} + \frac{\phi}{\kappa} \right| + \frac{1}{900} \frac{\kappa_0^2}{1-c^2} \left(1 + \frac{1}{x^2}\right) \right] \\
& \leq \frac{2}{c^2} \kappa \left[ \frac{\frac{1}{12} c^2 \kappa_0^2}{(1-c^2)} \frac{1}{c^2 x^2} \left( \frac{0.13}{x^2(1+x)^2} + 0.076 \right) + 0.005 + \left| \frac{\phi}{\kappa} - \frac{7}{60} \right| + \frac{12}{900 c^2} \cdot \frac{\frac{1}{12} c^2 \kappa_0^2}{1-c^2} \cdot 3 \right] \\
& \leq \frac{2}{c^2} \left[ \frac{1}{c^2} \cdot \frac{0.13}{x^4(1+x)^2} \cdot \kappa + \kappa \left( \frac{2}{c^2} \cdot 0.076 + 0.005 + \frac{7}{60} \cdot 0.14 \left( \sqrt{\frac{3}{2}} \kappa_0 \right)^2 + \frac{1}{25 c^2} \right) \right] \\
& \leq \frac{2}{c^2} \left[ \frac{1}{c^2} \cdot \frac{0.13}{x^4(1+x)^2} \cdot \kappa + 0.219 \kappa \right],
\end{aligned}$$

which finally is the claimed result of Lemma 3.7.  $\square$

### 4.3 Proof of Lemma 3.8

The proof of Lemma 3.8 is shorter than those of the two previous statements.

*Proof:* Here we start with the representation in (39), and then employ Formula (19) and the identity  $-\frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{c^2 \kappa^2} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{D(\kappa)} = -\frac{(4 \sin^2(\frac{\kappa}{2}))^2}{\kappa^3 c^2 D(\kappa)}$  in the second equality.

$$\begin{aligned} F_s[\varepsilon_{\text{cor}}](\kappa) &= \sqrt{\frac{2}{\pi}} \left[ \frac{\alpha}{\kappa (\kappa_0^2 - \kappa^2)} \frac{\beta^2 + \kappa_0^2}{\beta^2 + \kappa^2} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{c^2 \kappa^2} - \frac{4 \sin^2(\frac{\kappa}{2})}{\kappa} \frac{1}{D(\kappa)} + \frac{\phi}{c^2} \right] \\ &= \frac{\sqrt{\frac{2}{\pi}}}{c^2} \left[ \frac{1}{\kappa^3} \frac{\kappa_0^2}{\kappa^2 - \kappa_0^2} \left( -\frac{\kappa^2}{1 + \frac{\kappa^2}{\beta^2}} + \frac{1 - c^2}{\kappa_0^2} \frac{(\kappa^2 - \kappa_0^2)}{-D(\kappa)} \left( 4 \sin^2\left(\frac{\kappa}{2}\right) \right)^2 \right) + \phi \right], \end{aligned} \quad (115)$$

$$= \frac{\sqrt{\frac{2}{\pi}}}{c^2} \left[ \frac{1}{\kappa^5} t_3 \left( -\frac{\kappa^2}{1 + \frac{\kappa^2}{\beta^2}} + \frac{1}{\delta_3} \left( 4 \sin^2\left(\frac{\kappa}{2}\right) \right)^2 \right) + \phi \right], \quad (116)$$

where we introduced in the last step

$$t_3 := \frac{\frac{\kappa_0^2}{1 - c^2}}{1 - \frac{\kappa_0^2}{\kappa^2}} \quad (117)$$

and

$$\delta_3 := \frac{-D(\kappa)}{\frac{1 - c^2}{\kappa_0^2} (\kappa^2 - \kappa_0^2)}.$$

Note that, since  $\kappa_0 \rightarrow 0$  implies  $c^2 \rightarrow 1$ , while the denominator can be determined by (59),

$$\delta_3 \xrightarrow{\kappa_0 \rightarrow 0} \delta_3^\circ := \frac{\kappa^2 - 4 \sin^2\left(\frac{\kappa}{2}\right)}{\frac{1}{12} \kappa^2}.$$

With these preparations in place, it follows easily from (116) that

$$F_s[\varepsilon_{\text{cor}}](\kappa) = \frac{\sqrt{\frac{2}{\pi}}}{c^2} \left[ \frac{1}{\kappa^5} t_3 (V_1 + V_2 + V_3) + \phi \right] \quad (118)$$

with

$$\begin{aligned} V_1 &:= -\frac{\kappa^2}{1 + \frac{\kappa^2}{\beta^2}} + \frac{1}{12} \frac{\kappa^2}{\kappa^2 - 4 \sin^2\left(\frac{\kappa}{2}\right)} \left( 4 \sin^2\left(\frac{\kappa}{2}\right) \right)^2, \\ V_2 &:= \frac{\kappa^2}{1 + \frac{\kappa^2}{\beta^2}} - \frac{\kappa^2}{1 + \frac{\kappa^2}{\beta^2}}, \\ V_3 &:= -\frac{\delta_3 - \delta_3^\circ}{\delta_3^\circ} \left( 4 \sin^2\left(\frac{\kappa}{2}\right) \right)^2, \end{aligned}$$

Observe that  $t_3$  is monotonically increasing in  $\kappa_0$  and decreasing in  $\kappa$ , so that in  $I_3$

$$12 \leq t_3 \leq t_3|_{\substack{\kappa_0^2 = \frac{1}{2} \\ \kappa = 2}} < 14. \quad (119)$$

Relying on (31), we estimate for  $2 \leq \kappa \leq 4$ ,

$$\left| \frac{(\kappa^2 - 4 \sin^2\left(\frac{\kappa}{2}\right)) \kappa^2}{30} - \left( \frac{1}{12} \kappa^4 - (\kappa^2 - 4 \sin^2\left(\frac{\kappa}{2}\right)) \right) \right| \leq 1.9.$$

Hence, as a step towards bounding  $|\delta_3 - \mathring{\delta}_3|$ , two applications of (31) for the terms involving  $1 - c^2$  yield

$$\begin{aligned}
& \left| \left( \frac{1}{12} - \frac{1-c^2}{\kappa_0^2} \right) (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \kappa^2 - (1-c^2) \left( \frac{1}{12} \kappa^4 - (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \right) \right| \\
& \leq \frac{\kappa_0^2}{12} \left| \frac{(\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \kappa^2}{30} - \left( \frac{1}{12} \kappa^4 - (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \right) \right| \\
& \quad + \varepsilon_0 \kappa_0^4 \left| (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \kappa^2 \right| + \left( \frac{\kappa_0^4}{360} + \varepsilon_0 \kappa_0^6 \right) \left| \left( \frac{1}{12} \kappa^4 - (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \right) \right| \\
& \leq \frac{\kappa_0^2}{12} \cdot 1.9 + \frac{1}{100} \leq \frac{1}{12} 1.9 + \frac{1}{100} < \frac{9}{100}. \tag{120}
\end{aligned}$$

Below, we deduce with (120) for the first, (60) for the second, and (58) for the third inequality that

$$\begin{aligned}
|\delta_3 - \mathring{\delta}_3| &= \frac{\left| \left( \frac{1}{12} - \frac{1-c^2}{\kappa_0^2} \right) (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \kappa^2 - (1-c^2) \left( \frac{1}{12} \kappa^4 - (\kappa^2 - 4 \sin^2 \left( \frac{\kappa}{2} \right)) \right) \right|}{\frac{1}{12} \frac{1-c^2}{\kappa_0^2} \kappa^2 (\kappa^2 - \kappa_0^2)} \\
&\leq \frac{\frac{9}{100}}{c^2 \frac{1}{12} \frac{1-c^2}{\kappa_0^2} \kappa^2 (\kappa^2 - \kappa_0^2)} \\
&\leq \frac{9}{100} \frac{12^2}{c^2} \frac{1}{2^2 (2^2 - \frac{1}{2})} < \frac{1}{10}
\end{aligned}$$

holds true since  $\kappa \geq 2$ .

Further, (45) implies

$$0 \leq V_2 < \frac{\kappa^4}{\left(1 + \frac{\kappa^2}{\beta^2}\right) \left(1 + \frac{\kappa^2}{\mathring{\beta}^2}\right)} \left( \frac{1}{\beta^2} - \frac{1}{\mathring{\beta}^2} \right) < \max_{\kappa \leq 4} \left\{ \frac{\kappa^4}{\left(1 + \frac{\kappa^2}{\beta^2}\right)^2} \right\} \frac{1}{\mathring{\beta}^2} \frac{1}{20} < 0.18. \tag{121}$$

Also, note that  $\mathring{\delta}_3$  as the limit of  $\delta_3$  as  $\kappa_0 \rightarrow 0$  is independent of  $\kappa_0$ . Since  $\frac{\mathring{\delta}_3}{\kappa} \geq \frac{7}{4}$  for  $2 \leq \kappa \leq 4$ , we find for  $\kappa \geq 2$  that

$$\begin{aligned}
|V_3| &\leq 16 \frac{|\delta_3 - \mathring{\delta}_3|}{\kappa^2} \frac{1}{\frac{\mathring{\delta}_3}{\kappa} \left( \frac{\mathring{\delta}_3}{\kappa} - \frac{|\delta_3 - \mathring{\delta}_3|}{2} \right)} \\
&\leq 16 \frac{\frac{1}{10}}{\kappa^2} \frac{1}{\frac{7}{4} \left( \frac{7}{4} - \frac{1}{20} \right)} < \frac{0.54}{\kappa^2}. \tag{122}
\end{aligned}$$

Finally, since  $V_1$  and  $\phi$  are solely functions of  $\kappa$ , we observe for  $2 \leq \kappa \leq 4$  that there holds

$$\left| \frac{V_1}{\kappa^5} \right| \leq 0.01$$

and

$$\left| 12 \frac{V_1}{\kappa^5} + \phi \right| \leq 0.012.$$

We combine these two estimates with (119), (121) and (122) in the second inequality below; the identity relies on the representation (118).

$$\begin{aligned}\sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| &= \frac{\frac{2}{\pi}}{c^2} \left| \frac{1}{\kappa^5} t_3 (V_1 + V_2 + V_3) + \phi \right| \\ &\leq \frac{\frac{2}{\pi}}{c^2} \left( \frac{t_3}{\kappa^5} (|V_2| + |V_3|) + (t_3 - 12) \frac{V_1}{\kappa^5} + \left| 12 \frac{V_1}{\kappa^5} + \phi \right| \right) \\ &\leq \frac{\frac{2}{\pi}}{c^2} \left( 14 \left( \frac{0.18}{\kappa^5} + \frac{0.54}{\kappa^7} \right) + 2 \cdot 0.01 + 0.012 \right).\end{aligned}$$

This proves the claim of Lemma 3.8.  $\square$

#### 4.4 Proof of Lemma 3.9

We now turn our attention to the proof of Lemma 3.9.

*Proof:* Here we rewrite the representation (115),

$$F_s[\varepsilon_{\text{cor}}](\kappa) = \frac{\sqrt{\frac{2}{\pi}}}{c^2} \left[ \frac{1}{\kappa^3} \left( -\frac{t_3}{1 + \frac{\kappa^2}{\beta^2}} + \frac{(4 \sin^2(\frac{\kappa}{2}))^2}{-D(\kappa)} \right) + \phi \right],$$

where we used, as in the proof of Lemma 3.8,

$$t_3 = \frac{\frac{\kappa_0^2}{1-c^2}}{1 - \frac{\kappa_0^2}{\kappa^2}}.$$

Now, however,  $\kappa > 4$  implies for  $I_4$  the estimate

$$12 \leq t_3 \leq t_3 \Big|_{\substack{\kappa_0^2 = \frac{1}{2} \\ \kappa = 4}} < 12.6.$$

Thus, due to (45) and the fact that  $-D(\kappa) > 0$  for  $\kappa > 4 > \kappa_0$ , and  $\phi > 0$ ,

$$\sqrt{\frac{2}{\pi}} F_s[\varepsilon_{\text{cor}}] \geq -\frac{\frac{2}{\pi}}{c^2} \frac{1}{\kappa^3} \frac{t_3}{1 + \frac{\kappa^2}{\beta^2}} \geq -\frac{\frac{2}{\pi}}{c^2} \frac{1}{\kappa^3} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \cdot 12.6.$$

On the other hand,  $\kappa > 4$  implies

$$\begin{aligned}-\frac{t_3}{1 + \frac{\kappa^2}{\beta^2}} + \frac{(4 \sin^2(\frac{\kappa}{2}))^2}{-D(\kappa)} &\leq \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \left( -t_3 + 16 \frac{1 + \frac{\kappa^2}{\beta^2}}{-D(\kappa)} \right) \\ &\leq \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \left( -[t_3]_{\kappa_0=0} + 16 \left[ \frac{1 + \frac{\kappa^2}{\beta^2}}{-D(\kappa)} \right]_{\kappa_0^2 = \frac{1}{2}} \right) \leq 0.\end{aligned}$$

Hence, by (36) and (45),

$$\sqrt{\frac{2}{\pi}} F_s[\varepsilon_{\text{cor}}] \leq \frac{\frac{2}{\pi}}{c^2} \phi = \frac{\frac{2}{\pi}}{c^2} \frac{1}{\kappa^3} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \left( \frac{7}{60} \kappa^4 \frac{1 + \frac{44}{100} \kappa^2}{\left(1 + \frac{\kappa^2}{\beta^2}\right)^3} \right) \leq \frac{\frac{2}{\pi}}{c^2} \frac{1}{\kappa^3} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \cdot 22.$$

In summary, the absolute value is bounded by

$$\sqrt{\frac{2}{\pi}} |F_s[\varepsilon_{\text{cor}}]| \leq \frac{\frac{2}{\pi}}{c^2} \frac{1}{\kappa^3} \frac{1}{1 + \frac{\kappa^2}{\beta^2}} \cdot 22,$$

hence the claim of Lemma 3.9 is proved.  $\square$

## 5 The Rankine-Hugoniot condition and the kinetic relation

From an applied point of view, one object of interest is the kinetic relation of a travelling wave. We sketch the derivation for the wave discussed in Section 3. All the arguments in this section rely on macroscopic definitions of the relevant quantities. The discussion is greatly simplified by the fact that throughout Section 3,  $\varepsilon(x) = \varepsilon_{\text{pr}}(x) - \varepsilon_{\text{cor}}(x)$  with  $\varepsilon_{\text{cor}} \in L^2(\mathbb{R})$ . It thus follows that the relevant macroscopic quantities can be directly read off from the profile function  $\varepsilon_{\text{pr}}$ , which is explicitly known.

We first show that the Rankine-Hugoniot conditions are satisfied. We write  $\llbracket f \rrbracket$  for  $f(s(t)+, t) - f(s(t)-, t)$ , that is, the difference of the limiting values from the right and from the left of the interface, which has position  $s(t)$ . In continuum mechanical limit of (1), for an interface moving with velocity  $c$ , either the strain  $u_x$  or the velocity  $\dot{u}$  may be discontinuous at the interface, but must satisfy the *Rankine-Hugoniot* conditions [1, Equations (2.6) and (2.7)]

$$\begin{aligned}\llbracket \sigma(u_x) \rrbracket &= -\rho c \llbracket \dot{u} \rrbracket, \\ c \llbracket u_x \rrbracket &= -\llbracket \dot{u} \rrbracket.\end{aligned}$$

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

$$\rho c^2 \llbracket \varepsilon \rrbracket = \llbracket \sigma(\varepsilon) \rrbracket. \quad (123)$$

Here, one has  $\rho \equiv 1$  and, thanks to (3),  $\llbracket \sigma(\varepsilon) \rrbracket = \llbracket \varepsilon \rrbracket - 2$ , so (123) is equivalent to

$$\llbracket \varepsilon \rrbracket = \frac{2}{1 - c^2}. \quad (124)$$

Although the strain is continuous, it oscillates at  $\pm\infty$ . Thus, the jump in  $\varepsilon$  in (124) needs to be understood in the sense

$$\llbracket \varepsilon \rrbracket = \bar{\varepsilon}_+ - \bar{\varepsilon}_-, \quad (125)$$

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

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

and

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

By construction, only  $\varepsilon_{\text{pr}}$  contributes to the asymptotic strains  $\bar{\varepsilon}_{\pm}$ . A direct calculation shows that

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

Analogously

$$\bar{\varepsilon}_- = -\bar{\varepsilon}_+. \quad (126)$$

Thus,

$$\bar{\varepsilon}_+ - \bar{\varepsilon}_- = 2 \frac{1}{1 - c^2},$$

and, via (125), we have verified the Rankine-Hugoniot condition (124).

We now turn our attention to the kinetic relation. We start with the definition. A moving interface can dissipate energy, and the amount of dissipation is measured by the *configurational force* (or *driving force*). To define it, we let  $\{\sigma\} := \frac{1}{2} (\sigma(s(t)+, t) + \sigma(s(t)-, t))$  denote the average stress across the discontinuity. Furthermore, suppose for the moment that the strain on both sides

of the interface is constant; we write  $\varepsilon_l$  respectively  $\varepsilon_r$  for the strain on the left respectively on the right. Then, the *configurational force* acting on an interface is

$$f := \int_{\varepsilon_l}^{\varepsilon_r} \sigma(\varepsilon) d\varepsilon - \{\sigma\} [[\varepsilon]] \quad (127)$$

(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,

$$R(c) := cf(c) \quad (128)$$

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

Here, we interpret Equation (127) in an averaged sense by setting  $\varepsilon_l := \bar{\varepsilon}_-$  and analogously  $\varepsilon_r := \bar{\varepsilon}_+$ . By symmetry (see (3) and (126)), the integral on the right-hand side of (127) vanishes, and  $\{\sigma\} = \{\varepsilon\} = 0$ . Thus, the driving force is zero, that is, the interface moves freely. We point out that this is due to the symmetry of the configuration; the configuration is force-free since  $\bar{\varepsilon}_+ + \bar{\varepsilon}_- = 0$ . Solutions with  $\bar{\varepsilon}_+ + \bar{\varepsilon}_- \neq 0$  have a non-vanishing kinetic relation. For the solution considered here, the entropy inequality is trivially satisfied.

We close this section by mentioning that the vanishing kinetic relation can be explained from microscopic considerations. Though only a trivial kinetic relation is derived, the argument demonstrates the ease with which the analysis of the kinetic relation can be performed.

To determine the kinetic relation, we need to consider the energy transport due to lattice waves which disappear in the continuum limit. The energy carried by these waves is “lost” in the continuous setting and thus perceived as dissipation. It suffices to study the energy associated with the mode  $\pm\kappa_0$ . The contribution to these modes is in  $\varepsilon_{\text{pr}}$  in Equation (21). Since the asymptotic average strains agree, the average energy density  $\langle G_{\pm\kappa_0} \rangle$  carried by the waves with wave number  $\pm\kappa_0$  agree. Then, if  $V_g$  is the *group velocity*, the associated *energy flux*  $R$  is

$$R_{\pm\kappa_0}(c) = \pm \langle G_{\pm\kappa_0} \rangle (V_g - c);$$

see [10, Equation (6.4)]. We remark that

$$V_g - c = \frac{D'(\kappa_0)}{2c\kappa_0} = \frac{1}{c} \left( \frac{\sin(\kappa_0)}{\kappa_0} - c^2 \right).$$

Finally, the *kinetic relation*  $f$  is the one determined by (128), where  $R$  is obtained by summing over the individual contributions  $R_k$ . Since only  $R_{-\kappa_0}$  and  $R_{\kappa_0}$  contribute, we find again that  $R(c) = 0$  and thus  $f(c) = 0$ .

## 6 Inclusion of further nonlinearities: numerical investigations

So far, we considered a specific nonlinear problem and introduced a new decomposition method, which splits the solution  $\varepsilon$  into a profile and a corrector, and enables us to solve the problem with linear (Fourier) methods.

A natural question is then whether the idea developed here extends to problems with more general nonlinearities. Clearly, the Fourier analysis is restricted to the linear part of the problem studied in the previous sections. However, the decomposition strategy may be well suited for a wider class of interaction potentials, and in this section, we investigate its feasibility numerically. We simulate solutions with phase transition wave character, where one interface moves over along period of time essentially with constant velocity  $c$ . Obviously, the travelling wave solution of Theorem 3.1 is such a wave for the special interaction potential  $V$  of (2) for arbitrarily long time, with constant speed. We consider the initial value problem for (1) with different interaction

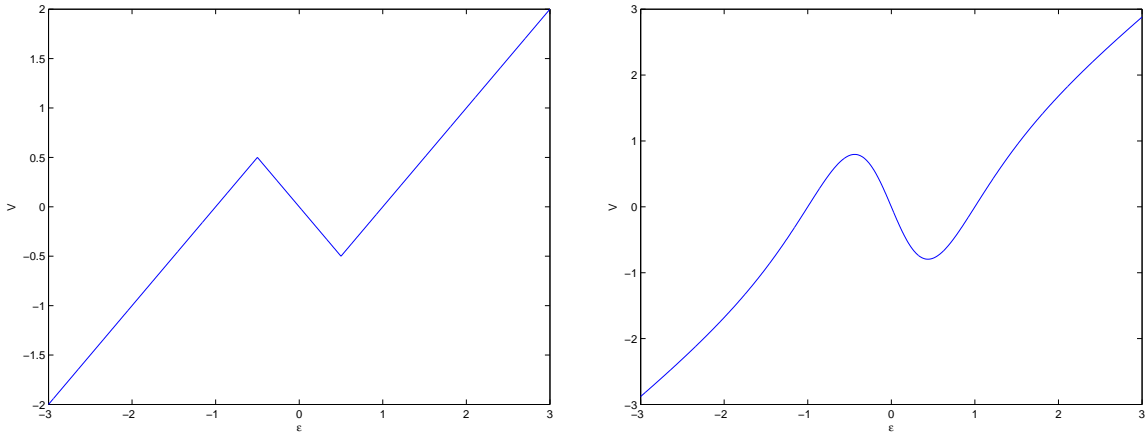


Figure 5: The stress-strain relationship for the interaction potential  $V_{\varepsilon_0}$  for  $\varepsilon_0 = \frac{1}{2}$  (left panel) and the potential  $V$  of Equation (131) Shown is the stress  $V'$  plotted versus the strain  $\varepsilon$ .

potentials  $V$ . We take the profile (21) as initial value. The numerical scheme is a simple explicit Euler method. As discussed below, the travelling phase transition character is observed for a wide range of choices for  $V$ . This shows that for a wider range of nonlinearities trajectories with phase transition character are well approximated by the special travelling wave obtained in this article. The persistence of the wave character is so strong that it seems promising to apply a suitable extension of the decomposition approach, coupled with fix point arguments, to establish the existence of travelling waves for more general  $V$  rigorously.

### 6.1 Simulation of moving phase boundaries

We solve numerically the initial boundary value problem for (1) in the discrete strain  $\varepsilon_j(t) := u_{j+1}(t) - u_j(t)$ ,

$$\ddot{\varepsilon}_j(t) = V'(\varepsilon_{j+1}(t)) - 2V'(\varepsilon_j(t)) + V'(\varepsilon_{j-1}(t)) \quad (129)$$

for 201 particles. The profile  $\varepsilon_{\text{pr}}$  moving with velocity  $c$  induces our initial and boundary conditions, that is,

$$\begin{pmatrix} \varepsilon_j \\ \dot{\varepsilon}_j \end{pmatrix} (0) := \begin{pmatrix} \varepsilon_{\text{pr}}(j) \\ -c\varepsilon'_{\text{pr}}(j) \end{pmatrix} \text{ for } j = -100, \dots, 100$$

and

$$\varepsilon_{\pm 100}(t) := \varepsilon_{\text{pr}}(\pm 100 - ct).$$

The profile  $\varepsilon_{\text{pr}}$  and the speed  $c$  are both taken for  $\kappa_0 = 0.7$ . The simulations are carried out for various interaction potentials  $V$ . We use the explicit Euler method for a time step  $\Delta t = 0.0002$ .

While the specific  $V$  of (2) is analysed in a number of physical papers, it is a common assumption that the interaction potential  $V$  contains a spinodal region, that is, two wells joined by a concave segment. We choose  $\varepsilon_0 > 0$  and define

$$V(\varepsilon) = V_{\varepsilon_0}(\varepsilon) := \frac{1}{2} \begin{cases} (\varepsilon + 1)^2 & \text{for } \varepsilon < -\varepsilon_0, \\ 1 - \varepsilon_0 - \left(\frac{1}{\varepsilon_0} - 1\right) \varepsilon^2 & \text{for } |\varepsilon| \leq \varepsilon_0, \\ (\varepsilon - 1)^2 & \text{for } \varepsilon > \varepsilon_0, \end{cases} \quad (130)$$

see Fig 5. This one-parameter family has been shown to capture all the qualitative features of general bi-stable models [6]. We remark that the stress-strain relation of this family is continuous.

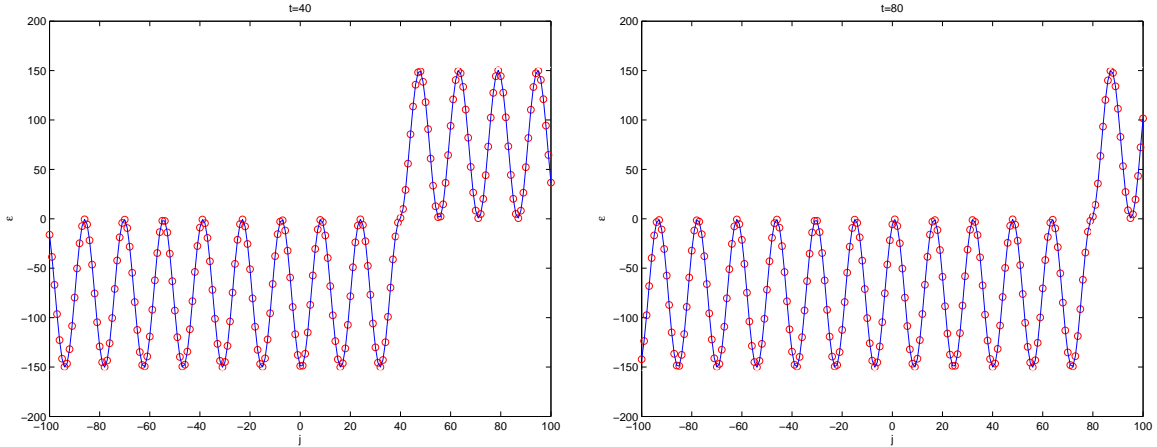


Figure 6: The numerical long-time integration for (129) for  $V = V_{\varepsilon_0}$  with  $\varepsilon_0 = \frac{1}{100}$ . The plots are taken at  $t = 40$  (left) and  $t = 80$  (right); circles denote the positions of the particles and we superimpose the shifted profile  $\varepsilon_{\text{pr}}(\cdot - ct)$ .

In Fig. 6, we show a simulations for  $\varepsilon_0 = \frac{1}{100}$ . We show the numerical solution at times  $t = 40$  and  $t = 80$ . This means the phase transition should have advanced 40 particles respectively 80 particles; the latter can be interpreted as the interface approaching the boundary of the computational domain. The two plots show the positions of the particles as circles superimposed to the profile  $\varepsilon_{\text{pr}}$  propagated with speed  $c$ . Since the quantitative agreement is very good, we turn now to a different form of representation, and plot the relative deviation, that is, the difference of the snapshot positions of the particles to the shifted profile  $\varepsilon_{\text{pr}}(\cdot - ct)$  divided by the maximal amplitude. This is done in Fig. 7 for solutions at time  $t = 80$ .

We remark that smaller values of  $\kappa_0$  improve the quality of the approximation, due to the increased amplitude of the wave profile. This is surprising, as the absolute deviation remains small despite the growth of the solution's amplitude as  $\kappa_0 \rightarrow 0$ .

Finally, we consider an interaction potential  $V$  that is nowhere quadratic, but has quadratic asymptotic growth. For the simulation, we choose

$$V(\varepsilon) := \frac{1}{2} \frac{(\varepsilon^2 - 1)^2}{\varepsilon^2 + 1}, \quad (131)$$

see Fig 5. Again, the quality is particularly good for smaller values of  $\kappa_0$ . In Fig. 8, we plot the numerical solution and the relative difference for  $\kappa_0 = \frac{1}{2}$ . It is noteworthy that for this choice of  $V$ , the difference is maximal for particles near or at the interface.

## 7 Discussion

Our knowledge of travelling waves in atomistic models with nonlinear interactions is not nearly as good as we would like it to be; this is even more the case for nonconvex problems such as springs with non-monotone stress-strain relationships as investigated here, or periodic on-site potentials as in the Frenkel-Kontorova model [4].

The philosophy behind this article is a straightforward one. Namely, we choose the simplest possible setting, a piecewise quadratic energy, and seek to prove the existence of waves representing phase transitions on the real line.

To us, the appeal of the approach presented here is that there is relatively little choice along the flow of the argument. The main choice is the strain distribution. Here, with the symmetric distribution (8), the heteroclinic wave is symmetric, which in turn implies that the kinetic relation is trivial. Additional freedom is obviously given by the choice of the profile (see Subsection 3.1).

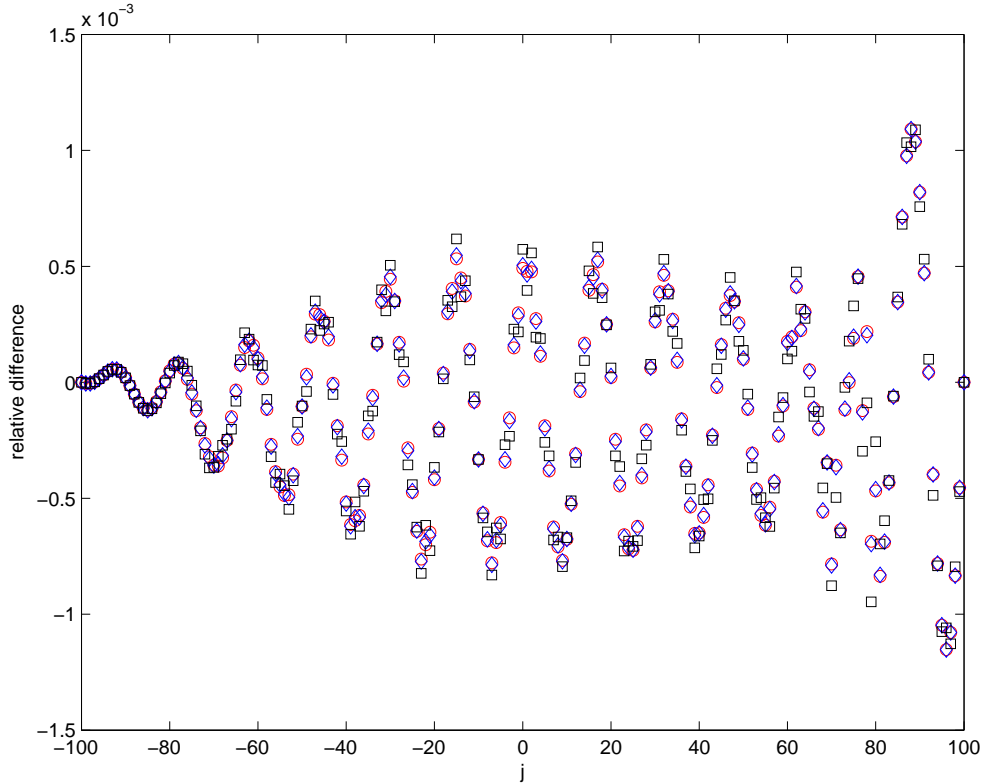


Figure 7: For the potentials  $V = V_{\varepsilon_0}$ , we show is the relative difference between the position of the particles from the shifted profile  $\varepsilon_{\text{pr}}(\cdot - ct)$  as  $t = 80$ . Plots are taken for  $\varepsilon_0 = \frac{1}{100}$  (circles),  $\varepsilon_0 = \frac{1}{10}$  (diamonds),  $\varepsilon_0 = \frac{1}{2}$  (squares). The vertical scale is  $10^{-3}$ .

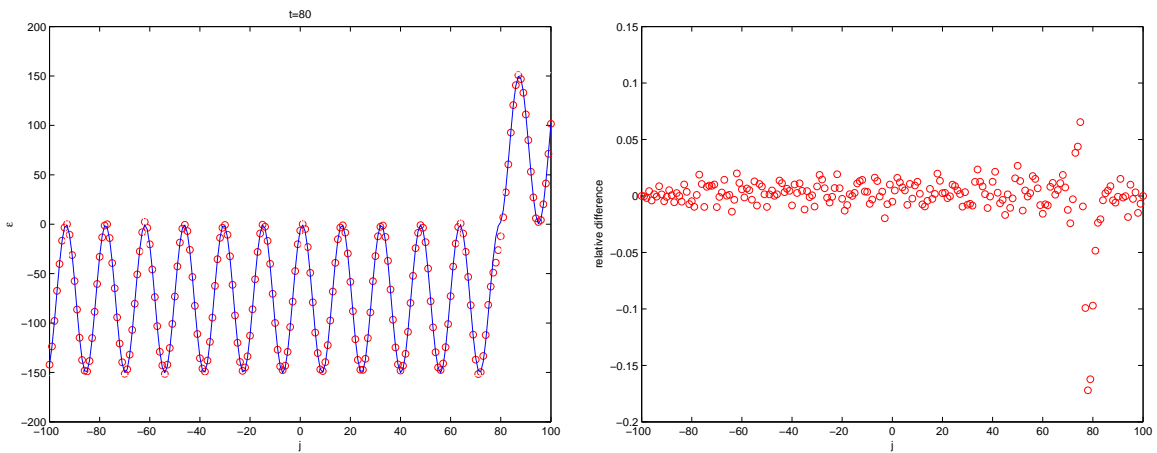


Figure 8: The numerical long-time integration for (129) with  $V$  as in (131). On the left, we plot the solution at  $t = 80$ . On the right we show the corresponding relative deviation from the shifted profile.

Yet, different choices mainly influence the ease of the argument showing that the sign condition (8) is satisfied (Subsection 3.4 and Section 4). The advantage of the choice made here is that the distance between the profile (21) and the real axis can be read off immediately due to the explicit nature of the profile. The control of the magnitude of the corrector in relation to this distance is then the crucial step in the argument.

Sections 2–5 concern the rigorous analysis for a nonharmonic (and nonconvex) interaction potential without a spinodal segment. As shown in Section 6, the profile used in the proof continues to be a good approximation for further interaction potentials  $V$  with a non-vanishing spinodal region. The numerical investigations of the shape of the solution in this section suggest that a suitable adaptation of the decomposition technique developed in this article is promising for a rigorous existence proof via a fixed-point argument. Therefore, we see the method developed here as a crucial step toward the understanding of structural properties of travelling wave solutions traversing a spinodal region.

## Acknowledgements

Both authors acknowledge the support of the Max Planck Institute for Mathematics in the Sciences, where this work started. JZ gratefully acknowledges the financial support of the EPSRC through an Advanced Research Fellowship (GR/S99037/1).

## References

- [1] Rohan Abeyaratne and James K. Knowles. Kinetic relations and the propagation of phase boundaries in solids. *Arch. Rational Mech. Anal.*, 114(2):119–154, 1991.
- [2] Alexander M. Balk, Andrej V. Cherkaev, and Leonid I. Slepyan. Dynamics of chains with non-monotone stress-strain relations. I. Model and numerical experiments. *J. Mech. Phys. Solids*, 49(1):131–148, 2001.
- [3] Alexander M. Balk, Andrej V. Cherkaev, and Leonid I. Slepyan. Dynamics of chains with non-monotone stress-strain relations. II. Nonlinear waves and waves of phase transition. *J. Mech. Phys. Solids*, 49(1):149–171, 2001.
- [4] J. Frenkel and T. Kontorova. On the theory of plastic deformation and twinning. *Acad. Sci. U.S.S.R. J. Phys.*, 1:137–149, 1939.
- [5] Ingo Müller and Piero Villaggio. A model for an elastic-plastic body. *Arch. Rational Mech. Anal.*, 67:25–46, 1977.
- [6] G. Puglisi and L. Truskinovsky. Mechanics of a discrete chain with bi-stable elements. *J. Mech. Phys. Solids*, 48(1):1–27, 2000.
- [7] Leonid Slepyan, Andrej Cherkaev, and Elena Cherkaev. Transition waves in bistable structures. II. Analytical solution: wave speed and energy dissipation. *J. Mech. Phys. Solids*, 53(2):407–436, 2005.
- [8] Leonid I. Slepyan. *Models and phenomena in fracture mechanics*. Foundations of Engineering Mechanics. Springer-Verlag, Berlin, 2002.
- [9] L. M. Truskinovskii. Dynamics of nonequilibrium phase boundaries in a heat conducting non-linearly elastic medium. *Prikl. Mat. Mekh.*, 51(6):1009–1019, 1987.
- [10] Lev Truskinovsky and Anna Vainchtein. Kinetics of martensitic phase transitions: lattice model. *SIAM J. Appl. Math.*, 66(2):533–553 (electronic), 2005.
- [11] Lev Truskinovsky and Anna Vainchtein. Quasicontinuum models of dynamic phase transitions. *Contin. Mech. Thermodyn.*, 18(1-2):1–21, 2006.