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SUBSONIC PHASE TRANSITION WAVES IN BISTABLE LATTICE MODELS WITH SMALL SPINODAL REGION*

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Abstract. Although phase transition waves in atomic chains with double-well potential play a fundamental role in materials science, very little is known about their mathematical properties. In particular, the only available results about waves with large amplitudes concern chains with piecewise-quadratic pair potential. In this paper we consider perturbations of a bi-quadratic potential and prove that the corresponding three-parameter family of waves persists as long as the perturbation is small and localized with respect to the strain variable. As a standard Lyapunov–Schmidt reduction cannot be used due to the presence of an essential spectrum, we characterize the perturbation of the wave as a fixed point of a nonlinear and nonlocal operator and show that this operator is contractive on a small ball in a suitable function space. Moreover, we derive a uniqueness result for phase transition waves with certain properties and discuss the kinetic relations.

Key words. phase transitions in lattices, kinetic relations, heteroclinic traveling waves in Fermi–Pasta–Ulam chains

AMS subject classifications. 37K60, 47H10, 74J30, 82C26

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1. Introduction. Many standard models in one-dimensional discrete elasticity describe the motion in atomic chains with nearest neighbor interactions. The corresponding equation of motion reads

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

where Φ is the interaction potential and u_j denotes the displacement of particle j at time t .

Of particular importance is the case of nonconvex Φ , because then (1) provides a simple dynamical model for martensitic phase transitions. In this context, a propagating interface can be described by a *phase transition wave*, which is a traveling wave that moves with subsonic speed and is heteroclinic as it connects periodic oscillations in different wells of Φ . The interest in such waves is also motivated by the quest to derive selection criteria for the naive continuum limit of (1), which is the PDE $\partial_{tt}u = \partial_x\Phi'(\partial_x)$. For nonconvex Φ , this equation is ill-posed due to its elliptic-hyperbolic nature, and one proposal is to select solutions by so-called kinetic relations [AK91, Tru87] derived from traveling waves in atomistic models.

Combining the traveling wave ansatz $u_j(t) = U(j - ct)$ with (1) yields the delay-advance differential equation

$$(2) \quad c^2 R''(x) = \Delta_1 \Phi'(R(x)),$$

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where $R(x) := U(x + 1/2) - U(x - 1/2)$ is the (symmetrized) discrete strain profile and $\Delta_1 F(x) := F(x + 1) - 2F(x) + F(x - 1)$. Periodic and homoclinic traveling waves have been studied intensively; see [FW94, SW97, FP99, Pan05, EP05, Her10] and the references therein, but very little is known about heteroclinic waves. The authors are only aware of [HR10, Her11], which prove the existence of supersonic heteroclinic waves, and the small amplitude results from [Ioo00]. In particular, there seems to be no result that provides phase transition waves with large amplitudes for generic double-well potentials.

Phase transition waves with large amplitudes are only well understood for piecewise quadratic potentials, and there exists a rich body of literature on bi-quadratic potentials, starting with [BCS01a, BCS01b, TV05]. For the special case

$$(3) \quad \Phi(r) = \frac{1}{2}r^2 - |r|, \quad \Phi'(r) = r - \operatorname{sgn}(r),$$

the existence of phase transition waves has been established by two of the authors using rigorous Fourier methods. In [SZ09] they consider subsonic speeds c sufficiently close to 1, which is the speed of sound, and show that (2) admits for each c a two-parameter family of phase transition waves. These waves have exactly one interface and connect different periodic tail oscillations.

In this paper we allow for small perturbations of the potential (3) and show that the three-parameter family of phase transition waves from [SZ12] persists provided that the perturbation is sufficiently localized with respect to the strain variable r .

A related problem has been studied in [Vai10]. There, a piecewise quadratic family of potentials is considered such that the stress-strain relationship is continuous and trilinear, with a small spinodal region. Traveling wave solutions are shown to obey a relation of residuals in the Fourier representation, which is then approximately solved numerically. The regularity of the perturbed potential is lower than that of the class of perturbations considered here, so strictly speaking the results do not overlap. However, in spirit the settings are close and indeed the numerical evidence [Vai10, Figure 4, bottom right panel] is in good agreement with our findings: there is a one-sided asymptotically constant solution, and the tail behind the interface oscillates with slightly different amplitude than that related to (3). The range of velocities considered in [Vai10] is larger than the one studied here.

Our approach is in essence perturbative and reformulates the traveling wave equation with perturbed potential in terms of a corrector profile S , i.e., we write $R = R_0 + S$, where R_0 is a given wave in the chain with unperturbed potential. The resulting equation for the corrector S can be written as

$$(4) \quad \mathcal{M}S = \mathcal{A}^2\mathcal{G}(S) + \eta,$$

where η is a constant of integration and \mathcal{A} , \mathcal{M} , \mathcal{G} are operators to be identified below. More precisely, \mathcal{M} is a linear integral operator which depends on c and \mathcal{G} a nonlinear superposition operator involving R_0 . The analysis of (4) is rather delicate since the Fourier symbol of \mathcal{M} has real roots, which implies that 0 is an inner point of the continuous spectrum of \mathcal{M} . In particular, \mathcal{M} is not a Fredholm operator in the function spaces considered here, so a standard bifurcation analysis from $\delta = 0$ via a Lyapunov–Schmidt reduction is not possible.

In our existence proof, we first eliminate the corresponding singularities and derive an appropriate solution formula for the linear subproblem. Afterwards we introduce a class of admissible functions S and show that $\mathcal{A}^2\mathcal{G}(S)$ is compactly supported and

sufficiently small. These fine properties are illustrated in Figure 5 and allow us to define a nonlocal and nonlinear operator \mathcal{T} such that

$$\mathcal{M}\mathcal{T}(S) = \mathcal{A}^2\mathcal{G}(S) + \eta(S)$$

holds for all admissible S with some $\eta(S) \in \mathbb{R}$. This operator \mathcal{T} is contractive in some ball of an appropriately defined function space, so the existence of phase transition waves is granted by the contraction mapping principle; see Lemma 14. Moreover, the properties of \mathcal{M} and \mathcal{G} imply that our fixed point method for S yields all phase transition waves R that comply with certain requirements; see Proposition 17.

Our existence result yields—for each c from an interval of subsonic velocities—a genuine two-parameter family of solutions to (2) but it is not clear whether all these phase transition waves are physically reasonable. In the literature, one often employs selection criteria to single out a unique phase transition wave for each speed c . One selection criterion is the *causality principle*, which in our case selects waves with nonoscillatory tails in front of the interface; see [Sle01, Sle02, TV05] and Remark 5 following Theorem 3. These waves can also be observed in numerical simulations of atomistic Riemann problems with nonoscillatory initial data [HSZ12].

Below we tailor our perturbation method carefully in order to show the persistence of the amplitude of the tail oscillations in front of the interface. In particular, for each small δ and any given c we obtain exactly one wave that complies with the causality principle as it propagates towards an asymptotically constant state. The other solutions are oscillatory for both $x \rightarrow -\infty$ and $x \rightarrow +\infty$, and satisfy the *entropy principle*—which is less restrictive than the causality principle—as long as the oscillations in front of the interface have smaller amplitude than those behind; see [HSZ12] for more details and a discussion of the different versions of Sommerfeld’s *radiation condition*. It is not known whether waves with tail oscillations on both sides of the interface are dynamically stable or can be created by Riemann initial data. A related open question is whether such noncausality waves can be regarded as local building blocks for more complex solutions such as cascades of phase transition waves in chains with triple-well potential (where, for instance, a causality wave connecting two wells might be followed by a noncausality wave that connects to the third well). For phase transition waves in chains with piecewise quadratic potential Ψ_0 —which are computed in [TV05] by appropriately chosen contour integrals in the complex plane—the causality principle can be linked to the vanishing viscosity limit for the traveling wave equation as both favor the same indentation of the integral contour; see also [Sle01, Vai10]. We are, however, not aware of any mathematical result that establishes the causality principle for the solutions of initial value problems. It remains a challenging task to investigate the validity of selection criteria for phase transition waves, especially in cases with nondegenerate nonlinearities.

We also emphasize that phase transition waves satisfy Rankine–Hugoniot conditions for the macroscopic averages of mass, momentum, and total energy [HSZ12], which encode nontrivial restrictions between the wave speed and the tail oscillations on both sides of the interface. Although the jump conditions do not appear explicitly in our existence proof, they can be computed because the tail oscillations are given by harmonic waves; see Figure 2. For general double-well potentials, however, it is much harder to evaluate the Rankine–Hugoniot conditions and thus it remains unclear which tail oscillations can be connected by phase transition waves. Closely related to the jump condition for the total energy is the *kinetic relation*, which specifies the transfer between oscillatory and nonoscillatory energy at the interface and determines

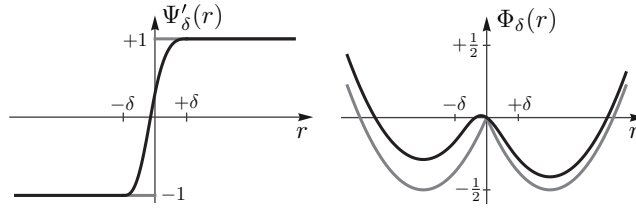


FIG. 1. Sketch of Ψ'_δ and Φ_δ for $\delta = 0$ (grey) and $\delta > 0$ (black). Since Φ_0 is symmetric, $-I_\delta$ is just half the energy difference between the two wells of Φ_δ .

the *configurational force* that drives the wave. In the final section we discuss how the kinetic relation changes to leading order under small perturbations of the potential (3).

We now present our main result in greater detail.

1.1. Overview and main result. We study an atomic chain with interaction potential

$$\Phi_\delta(r) = \frac{1}{2}r^2 - \Psi_\delta(r), \quad \Psi_\delta(0) = 0,$$

where Ψ'_δ is a perturbation of $\Psi'_0 = \text{sgn}$ in a small neighborhood of 0. The traveling wave equation therefore reads

$$(5) \quad c^2 R'' = \Delta_1(R - \Psi'_\delta(R))$$

and depends on the parameters c and δ . In order to show that (5) admits solutions for small δ we rely on the following assumptions on Ψ'_δ ; see Figure 1 for an illustration.

Assumption 1. Let $(\Psi_\delta)_{\delta>0}$ be a one-parameter family of C^2 -potentials such that

1. Ψ'_δ coincides with Ψ'_0 outside the interval $(-\delta, \delta)$,
2. there is a constant C_Ψ independent of δ such that

$$|\Psi'_\delta(r)| \leq C_\Psi, \quad |\Psi''_\delta(r)| \leq \frac{C_\Psi}{\delta}$$

for all $r \in \mathbb{R}$.

The quantity

$$I_\delta := \frac{1}{2} \int_{\mathbb{R}} (\Psi'_\delta(r) - \Psi'_0(r)) \, dr$$

plays an important role in our perturbation result as it determines the leading order correction. Notice that our assumptions imply

$$(6) \quad I_\delta = \frac{1}{2} \int_{-\delta}^{\delta} \Psi'_\delta(r) \, dr = -\frac{1}{2}(\Phi_\delta(+1) - \Phi_\delta(-1)) \quad \text{and hence} \quad |I_\delta| \leq C_\Psi \delta.$$

As already mentioned, the case $\delta = 0$ has been solved in [SZ09]. We also refer to [TV05], which computes the causality wave \bar{R}_0 by means of contour integrals and the residue method. In this paper we rely on the following characterization of the waves in the unperturbed chain; see Figure 2 for an illustration.

PROPOSITION 2 ([SZ09], Proof of Theorem 3.11, and [SZ12, Theorem 1]). *There exists $0 < c_0 < 1$ such that for every $c \in [c_0, 1)$, there exists a two-parameter family of solutions $R_0 \in W^{2,\infty}(\mathbb{R})$ to the traveling wave equation (5) with $\delta = 0$. This family is normalized by $R_0(0) = 0$ and can be described as follows.*

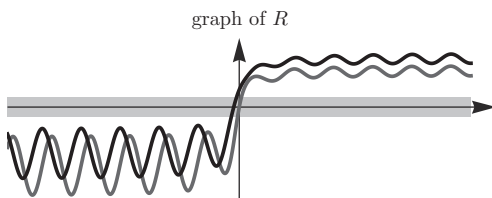


FIG. 2. Sketch of the waves for $\delta = 0$ (grey) and $\delta > 0$ (black) as provided by our perturbation result; the shaded region indicates the spinodal interval $[-\delta, +\delta]$, where Ψ'_δ differs from Ψ'_0 . Both waves differ by the constant $I_\delta = O(\delta)$ and a small corrector S of order $O(\delta^2)$, which is oscillatory for $x < 0$ but asymptotically constant as $x \rightarrow +\infty$. The tail oscillations of both waves do not penetrate the spinodal region and are generated by harmonic waves with wave number k_c . For each admissible δ and c there exists exactly one wave that satisfies the causality principle as it is nonoscillatory for $x \rightarrow +\infty$.

(i) There exists a unique traveling wave \bar{R}_0 such that

$$\begin{aligned} \bar{R}_0(x) &\xrightarrow{x \rightarrow +\infty} r_c^+, \\ \bar{R}_0(x) - \alpha_c^- (\cos(k_c x) - 1) - \beta_c^- \sin(k_c x) &\xrightarrow{x \rightarrow -\infty} \bar{r}_c^- \end{aligned}$$

for some constants r_c^\pm , k_c , α_c^- , and β_c^- depending on c .

(ii) There exists an open neighborhood U_c of 0 in \mathbb{R}^2 such that for any $(\alpha, \beta) \in U_c$ the function $R_0 = \bar{R}_0 + \alpha(\cos(k_c \cdot) - 1) + \beta \sin(k_c \cdot)$ is a traveling wave with

(a) $\|R_0\|_\infty \leq D_0(1 - c^2)^{-1}$,

(b) $R_0(x) > r_0$ for $x > x_0$ and $R_0(x) < -r_0$ for $x < -x_0$,

(c) $R'_0(x) > d_0$ for $|x| < x_0$

for some constants x_0 , r_0 , d_0 , and D_0 depending on c_0 .

The main result of this article can be described as follows.

THEOREM 3. For all $c_1 \in (c_0, 1)$ there exists $\delta_0 > 0$ such that for any $0 < \delta < \delta_0$, any speed $c_0 < c < c_1$, and any given wave R_0 as in Proposition 2 there exists a solution R to (5) with

$$R = R_0 - I_\delta + S.$$

Here $I_\delta = O(\delta)$ is defined in (6) and the corrector $S \in W^{2,\infty}(\mathbb{R})$

(i) vanishes at $x = 0$,

(ii) is nonoscillatory as $x \rightarrow +\infty$, i.e., the limit $\lim_{x \rightarrow +\infty} S(x)$ is well defined,

(iii) admits harmonic tail oscillations for $x \rightarrow -\infty$, that means there exists constants a_- and d_- such that $\lim_{x \rightarrow -\infty} S(x) - a_- R_0(x + d_-)$ is well defined,

(iv) is small in the sense of

$$\|S\|_\infty = O(\delta^2), \quad \|S'\|_\infty = O(\delta), \quad \|S''\|_\infty = O(1).$$

Moreover, the solution R with these properties is unique provided that δ is sufficiently small.

More detailed information about the existence and uniqueness part of our result is given in Propositions 15 and 17, respectively. We further mention

1. since the traveling wave equation is invariant under

$$c \rightsquigarrow -c, \quad R(x) \rightsquigarrow R(-x),$$

there exists an analogous result for $-1 < c \ll 0$;

2. different choices of c and R_0 provide different waves R ; see section 4;
3. the traveling wave equation (5) is, of course, invariant under shifts in x but fixing R_0 and S at 0 removes neutral directions in the contraction proof;
4. all constants derived below depend on c_1 and c_0 but for notational simplicity we do not write this dependence explicitly. It remains open whether δ_0 can be chosen independently of c_1 ;
5. the *causality principle* selects the solutions with $c_{\text{gr}} < c_{\text{ph}}$ and $c_{\text{gr}} > c_{\text{ph}}$ for all oscillatory harmonic modes ahead and behind the interface, respectively, where, c_{gr} and c_{ph} are the group and the phase velocity. For nearest neighbor chains with interaction potential Φ_0 and wave speed c sufficiently close to 1, the tail oscillations involve only a single harmonic mode and Proposition 2 yields

$$c_{\text{ph}} = c = a(k_c) = k_c^{-1}\Omega(k_c) > c_{\text{gr}} = \Omega'(k_c)$$

on *both* sides of the interface, where $\Omega(k) = 2|\sin(k/2)|$ is the dispersion relation [SCC05, TV05, HSZ12]. The causality principle therefore selects the solution \bar{R}_0 as it is the only wave having no tail oscillations ahead of the interface. Since our perturbative approach changes neither the wave speed c nor the wave number k_c in the oscillatory modes (but only the amplitude behind the interface and, of course, the behavior near the interface), we conclude that Theorem 3 provides for each δ and c exactly one wave that complies with the causality principle;

6. the surprisingly simple leading order effect, that is the addition of $-I_\delta$ to R_0 , implies that the kinetic relation does not change to order $O(\delta)$. Notice, however, that the kinetic relation depends on the choice of R_0 ; cf. [SZ12].

This paper is organized as follows. In section 2 we reformulate (5) in terms of integral operators \mathcal{A} and \mathcal{M} and show that it is sufficient to prove the existence of waves for the special case $I_\delta = 0$. Section 3 concerns the existence of correctors S . We first establish an inversion formula for \mathcal{M} which in turn enables us to define an appropriate solution operator \mathcal{L} to the affine subproblem $\mathcal{M}S = \mathcal{A}^2G + \eta$ with given G . Afterwards we investigate the properties of the nonlinear operator \mathcal{G} and prove the contractivity of the fixed point operator \mathcal{T} . In section 4 we establish our uniqueness result and conclude with a discussion of the kinetic relation in section 5.

2. Preliminaries and reformulation of the problem. In this section we reformulate the traveling wave equation (5) in terms of integral operators and show that elementary transformations allow us to assume that $I_\delta = 0$ holds for all $\delta > 0$.

2.1. Reformulation as integral equation. For our analysis it is convenient to reformulate the problem in terms of the convolution operator \mathcal{A} and the operator \mathcal{M} defined by

$$(\mathcal{A}F)(x) := \int_{x-1/2}^{x+1/2} F(s) \, ds, \quad \mathcal{M}F := \mathcal{A}^2F - c^2F.$$

In terms of these integral operators, the traveling wave equation can be stated as

$$(7) \quad \mathcal{M}R = \mathcal{A}^2\Psi'_\delta(R) + \mu,$$

where μ is some constant of integration; see [FV99, SW97, TV06, HR10, Her10] for similar reformulations of (5).

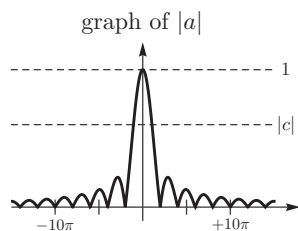


FIG. 3. The real roots of the symbol function m are the solutions to $|a(k)| = |c|$.

LEMMA 4. A function $R \in W^{2,\infty}(\mathbb{R})$ solves the traveling wave equation (5) if and only if there exists a constant $\mu \in \mathbb{R}$ such that (R, μ) solves (7).

Proof. By the definition of \mathcal{A} , we have $\frac{d^2}{dx^2}\mathcal{A}^2 = \Delta_1$. Equation (5) is therefore, and due to the definition of \mathcal{M} , equivalent to

$$(8) \quad (\mathcal{M}R)'' = P'', \quad P := \mathcal{A}^2\Psi'_\delta(R).$$

The implication (7) \implies (5) now follows immediately. Towards the reversed statement, we integrate (8)₁ twice with respect to x and obtain $\mathcal{M}R = P + \lambda x + \mu$, where λ and μ denote constants of integration. The condition $R \in L^\infty(\mathbb{R})$ implies $\mathcal{M}R, \Psi'_\delta(R), P \in L^\infty(\mathbb{R})$, and we conclude that $\lambda = 0$. \square

2.2. Properties of the operators \mathcal{A} and \mathcal{M} . Some of our arguments rely on the Fourier transform, which we normalize as follows:

$$\widehat{F}(k) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{ikx} F(x) dx, \quad F(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ikx} \widehat{F}(k) dk.$$

Using standard techniques for the Fourier transform in the space of tempered distributions we readily verify the following assertions.

Remark 5. The operators \mathcal{A} and \mathcal{M} diagonalize in Fourier space and have symbols

$$a(k) = \frac{\sin(k/2)}{k/2} \quad \text{and} \quad m(k) = a(k)^2 - c^2,$$

respectively. In particular, we have

$$\mathcal{M} \cos(k_c \cdot) = 0, \quad \mathcal{M} \sin(k_c \cdot) = 0, \quad \mathcal{M}1 = 1 - c^2$$

for any real root k_c of m , and

$$F \in \text{span} \{ \cos(k_c \cdot), \sin(k_c \cdot) : m(k_c) = 0, \quad k_c > 0 \}$$

for any tempered distribution F with $\mathcal{M}F = 0$.

The set of real roots of m depends strongly on the value of c ; see Figure 3. In what follows we only deal with positive and near sonic speed c , that means $c \lesssim 1$, for which m has two simple real roots.

We next summarize further properties of the operator \mathcal{A} and recall that the Sobolev space $W^{1,p}(\mathbb{R})$ is for any $1 \leq p \leq \infty$ continuously embedded into $BC(\mathbb{R})$.

LEMMA 6. For any $1 \leq p \leq \infty$ we have $\mathcal{A}: L^p(\mathbb{R}) \rightarrow W^{1,p}(\mathbb{R}) \subset BC(\mathbb{R})$ with

$$(9) \quad \|\mathcal{A}F\|_p \leq \|F\|_p, \quad \|(\mathcal{A}F)'\|_p \leq 2\|F\|_p, \quad \|\mathcal{A}F\|_\infty \leq \|F\|_p$$

for all $F \in L^p(\mathbb{R})$, where $(\mathcal{A}F)' = \nabla F := F(\cdot + \frac{1}{2}) - F(\cdot - \frac{1}{2})$. Moreover, $\text{supp } F \subseteq [x_1, x_2]$ implies $\text{supp } \mathcal{A}F \subseteq [x_1 - \frac{1}{2}, x_2 + \frac{1}{2}]$.

Proof. Let $1 \leq p < \infty$ and $F \in L^p(\mathbb{R})$ be fixed. The definition of \mathcal{A} ensures that $\mathcal{A}F$ has in fact the weak derivative ∇F , and this implies the estimate (9)₂ via $\|\nabla F\|_p \leq 2\|F\|_p$. Using Hölder’s inequality we find

$$|(\mathcal{A}F)(x)|^p \leq \int_{x-1/2}^{x+1/2} |F(s)|^p ds$$

and integration with respect to x yields (9)₁. We also infer that $|(\mathcal{A}F)(x)| \leq \|F\|_p$ holds for all $x \in \mathbb{R}$, and this gives (9)₃. Finally, the arguments for $p = \infty$ are similar and the claimed relation between $\text{supp } F$ and $\text{supp } \mathcal{A}F$ is a direct consequence of the definition of \mathcal{A} . \square

2.3. Transformation to the special case $I_\delta = 0$. The key observation that traces the general case $I_\delta \neq 0$ back to the special case $I_\delta = 0$ is that any shift in Ψ'_δ can be compensated for by adding a constant to R .

LEMMA 7. *The family $(\tilde{\Psi}_\delta)_{\tilde{\delta}>0}$ defined by*

$$\tilde{\delta} = \delta(1 + C_\Psi), \quad \tilde{\Psi}'_\delta(r) = \Psi'_\delta(r - I_\delta)$$

satisfies Assumption 1 with constant $\tilde{C}_\Psi = C_\Psi(1 + C_\Psi)$ as well as

$$\tilde{I}_\delta = \frac{1}{2} \int_{\mathbb{R}} \tilde{\Psi}'_\delta(r) - \Psi'_0(r) dr = 0 \quad \text{for all } \tilde{\delta} > 0.$$

Moreover, each solution $(\tilde{R}, \tilde{\mu})$ to the modified traveling wave equation

$$(10) \quad \mathcal{M}\tilde{R} = \mathcal{A}^2\tilde{\Psi}'_\delta(\tilde{R}) + \tilde{\mu}$$

defines a solution (R, μ) to (7) via $R = \tilde{R} - I_\delta$ and $\mu = \tilde{\mu} - (c^2 - 1)I_\delta$ and vice versa.

Proof. Due to $|I_\delta| \leq C_\Psi\delta$ and our definitions we find $\tilde{\Psi}'_\delta(r) = \Psi'_0(r)$ at least for all r with $|r| \geq \tilde{\delta}$, as well as

$$\left| \tilde{\Psi}'_\delta(r) \right| \leq C_\Psi \leq \tilde{C}_\Psi, \quad \left| \tilde{\Psi}''_\delta(r) \right| \leq \frac{C_\Psi}{\delta} = \frac{C_\Psi}{\delta} \frac{1 + C_\Psi}{1 + C_\Psi} = \frac{\tilde{C}_\Psi}{\tilde{\delta}} \quad \text{for all } r \in \mathbb{R}.$$

We also have

$$\begin{aligned} \tilde{I}_\delta &= \frac{1}{2} \int_{\mathbb{R}} (\Psi'_\delta(r - I_\delta) - \Psi'_0(r)) dr = \frac{1}{2} \int_{\mathbb{R}} (\Psi'_\delta(r) - \Psi'_0(r + I_\delta)) dr \\ &= \frac{1}{2} \int_{\mathbb{R}} (\Psi'_\delta(r) - \Psi'_0(r)) dr + \frac{1}{2} \int_{\mathbb{R}} (\Psi'_0(r) - \Psi'_0(r + I_\delta)) dr = I_\delta - I_\delta = 0. \end{aligned}$$

Finally, the equivalence of (7) and (10) is obvious. \square

3. Existence of phase transition waves. In this section, we show that each phase transition wave for Ψ_0 persists under the perturbation $\Psi_0 \rightsquigarrow \Psi_\delta$, provided that δ is sufficiently small. To this end we proceed as follows.

1. We fix $c \in [c_0, c_1]$ with $0 < c_0 < c_1 < 1$ as in Proposition 2 and Theorem 3. Then there exists a unique solution $k_c > 0$ to $a(k_c) = c$, and this implies $m(\pm k_c) = 0$, $m'(\pm k_c) \neq 0$, and $m(k) \neq 0$ for $k \neq \pm k_c$. All constants derived below can be chosen independently of c but are allowed to depend on c_0 and c_1 .

2. Thanks to Proposition 2 and Lemma 4, we fix (R_0, μ_0) from the two-parameter family of solutions to the integrated traveling wave equation (7) for $\delta = 0$ and given c . Recall that R_0 is normalized by $R_0(0) = 0$.
3. In view of Lemma 7, we assume that $I_\delta = 0$ holds for all $\delta > 0$. To avoid unnecessary technicalities we also assume from now on that δ is sufficiently small.

In order to find a solution (R, μ) to the integrated traveling wave equation (7) for $\delta > 0$, we further make the ansatz

$$R = R_0 + S, \quad \mu = \mu_0 + \eta,$$

and seek correctors (S, η) such that

$$(11) \quad \mathcal{M}S = \mathcal{A}^2G + \eta, \quad G = \mathcal{G}(S).$$

Here, the nonlinear operator \mathcal{G} is defined by

$$(12) \quad \mathcal{G}(S)(x) = \Psi'_\delta(R_0(x) + S(x)) - \Psi'_0(R_0(x)).$$

In order to identify a natural ansatz space X for S , we first remark that the smoothing properties of \mathcal{A} (see Lemma 6) imply $S \in W^{2,\infty}(\mathbb{R})$. Notice, however, that $R = R_0 + S$ is in general more regular due to the smoothness of Ψ_δ . More precisely, (7) combined with $\Psi_\delta \in C^k(\mathbb{R})$ yields $R \in C^{k+1}(\mathbb{R})$. We also impose the normalization condition $S(0) = 0$ in order to eliminate the nonuniqueness that results from the shift invariance of the traveling wave equation (7). In fact, without this constraint any corrector S provides a whole family of other possible correctors via $\tilde{S} = S(\cdot + x_0) + R_0(\cdot + x_0) - R_0$ with $x_0 = O(\delta^2)$.

A key property of our existence and uniqueness result is that the tail oscillations of R are harmonic with wave number k_c and that both R and R_0 share the same tail oscillations for $x \rightarrow +\infty$. The corrector S is therefore nonoscillatory in the sense that $S(x)$ converges as $x \rightarrow +\infty$ to some well-defined limit σ . In summary, we seek solutions (S, η) to (11) with $S \in \mathsf{X}$ and $\eta \in \mathbb{R}$, where

$$\mathsf{X} := \left\{ S \in W^{2,\infty}(\mathbb{R}) : S(0) = 0, \quad \sigma = \lim_{x \rightarrow +\infty} S(x) \text{ exists} \right\}$$

is a closed subspace of $W^{2,\infty}(\mathbb{R})$ and hence a Banach space.

3.1. Inversion formula for \mathcal{M} . Our first task is to construct for given G a solution (S, η) to the affine equation (11)₁. In a preparatory step, we therefore study the solvability of the equation

$$(13) \quad \mathcal{M}F = Q$$

using the Fourier transform for tempered distributions, where $Q \in L^\infty(\mathbb{R})$ is some given function. This problem is not trivial because the symbol function m has two simple roots at $\pm k_c$, or, equivalently, because 0 is an element of the continuous spectrum of \mathcal{M} corresponding to a two-dimensional space of generalized eigenfunctions. We are therefore confronted with the following two issues in Fourier space:

1. \hat{F} is uniquely determined only up to elements from the space

$$\text{span} \{ \delta_{-k_c}(k), \delta_{+k_c}(k) \},$$

which contains the Fourier transforms of all bounded kernel functions of \mathcal{M} ;

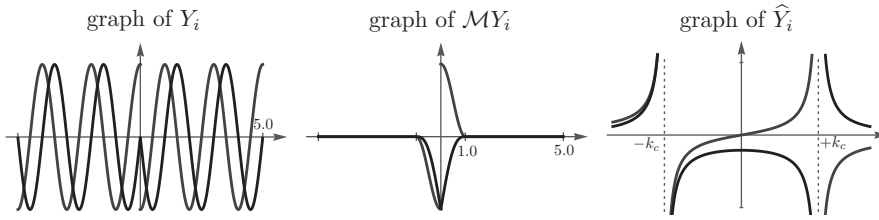


FIG. 4. Properties of Y_1 (grey) and Y_2 (black).

- 2. \widehat{F} exhibits—for generic Q with $\widehat{Q}(\pm k_c) \neq 0$ —two poles at $\pm k_c$ and is hence not Lebesgue integrable in the vicinity of $\pm k_c$. In particular, the dual pairing between \widehat{F} and a Schwartz function is defined in the sense of Cauchy principal values only.

The nonuniqueness is actually an advantage because it allows us to select solutions with particular properties; see the proof of Lemma 10, where we add an appropriately chosen kernel function to ensure nonoscillatory behavior for $x \rightarrow +\infty$. Concerning the nonintegrable poles at $\pm k_c$, we split \widehat{F} into a two-dimensional singular part and a remaining regular part, and show that any solution F to (13) belongs to some Lebesgue space provided that \widehat{Q} is sufficiently regular.

As illustrated in Figure 4, we introduce two functions $Y_1, Y_2 \in L^\infty(\mathbb{R})$ with

$$Y_1(x) := \frac{\sqrt{2\pi}}{m'(k_c)} \cos(k_c x) \operatorname{sgn}(x), \quad Y_2(x) := \frac{\sqrt{2\pi}}{m'(k_c)} \sin(k_c x) \operatorname{sgn}(x),$$

and verify by direct computations the following assertions.

Remark 8. We have

- 1. $\mathcal{M}Y_i \in L^\infty(\mathbb{R})$ with $\operatorname{supp} \mathcal{M}Y_i \subseteq [-1, 1]$,
- 2. $\widehat{Y}_1(k) = +\frac{2i}{m'(k_c)} \frac{k}{k^2 - k_c^2}$ and $\widehat{Y}_2(k) = -\frac{2}{m'(k_c)} \frac{k_c}{k^2 - k_c^2}$,
- 3. $m\widehat{Y}_i \in L^2(\mathbb{R}) \cap BC^1(\mathbb{R})$ with

$$\lim_{k \rightarrow \pm k_c} m(k)\widehat{Y}_1(k) = \pm i, \quad \lim_{k \rightarrow \pm k_c} m(k)\widehat{Y}_2(k) = -1.$$

In particular, \widehat{Y}_1 and \widehat{Y}_2 have normalized poles at $\pm k_c$, and this allows us to derive the following linear and continuous inversion formula for \mathcal{M} .

LEMMA 9. Let Q be given with $\widehat{Q} \in L^2(\mathbb{R}) \cap BC^1(\mathbb{R})$. Then there exists a unique $Z \in L^2(\mathbb{R})$ such that

$$(14) \quad \mathcal{M} \left(Z - i \frac{\widehat{Q}(+k_c) - \widehat{Q}(-k_c)}{2} Y_1 - \frac{\widehat{Q}(+k_c) + \widehat{Q}(-k_c)}{2} Y_2 \right) = Q,$$

Moreover, Z depends linearly on Q and satisfies

$$\|Z\|_2 \leq C \left(\|\widehat{Q}\|_2 + \|\widehat{Q}\|_{1, \infty} \right)$$

for some constant C independent of Q .

Proof. The function \widehat{Z} with

$$(15) \quad \widehat{Z}(k) := \frac{\widehat{Q}(k) + i \frac{\widehat{Q}(+k_c) - \widehat{Q}(-k_c)}{2} m(k)\widehat{Y}_1(k) + \frac{\widehat{Q}(+k_c) + \widehat{Q}(-k_c)}{2} m(k)\widehat{Y}_2(k)}{m(k)}$$

is well defined and continuously differentiable for $k \neq \pm k_c$. Moreover, Remark 8 and l'Hôpital's rule ensure that the limits $\lim_{k \rightarrow -k_c} \widehat{Z}(k)$ and $\lim_{k \rightarrow +k_c} \widehat{Z}(k)$ do exist, and combining this with the integrability properties of m and \widehat{Q} we find $\widehat{Z} \in L^2(\mathbb{R})$. The inverse Fourier transform $Z \in L^2(\mathbb{R})$ is therefore well defined by Parseval's theorem, depends linearly on Q , and satisfies (14) by construction. With $J := [-2k_c, +2k_c]$ we readily verify the estimates

$$\begin{aligned} \|\widehat{Z}\|_{L^2(\mathbb{R} \setminus J)} &\leq \|m^{-1}\|_{L^\infty(\mathbb{R} \setminus J)} \|\widehat{Q}\|_{L^2(\mathbb{R} \setminus J)} \\ &\quad + \left(|\widehat{Q}(+k_c)| + |\widehat{Q}(-k_c)| \right) \left(\|\widehat{Y}_1\|_{L^2(\mathbb{R} \setminus J)} + \|\widehat{Y}_2\|_{L^2(\mathbb{R} \setminus J)} \right) \\ &\leq C \left(\|\widehat{Q}\|_{L^2(\mathbb{R})} + \|\widehat{Q}\|_{L^\infty(\mathbb{R})} \right), \end{aligned}$$

and Taylor expanding both the numerator and the denominator of the right-hand side in (15) at $k = \pm k_c$ we get

$$\|\widehat{Z}\|_{L^2(J)} \leq C \|\widehat{Z}\|_{C^0(J)} \leq C \|\widehat{Q}\|_{C^1(J)}.$$

The desired estimate for $\|Z\|_2$ now follows from $\|Z\|_{L^2(\mathbb{R})}^2 = \|\widehat{Z}\|_{L^2(\mathbb{R} \setminus J)}^2 + \|\widehat{Z}\|_{L^2(J)}^2$. Finally, Z is the unique solution in $L^2(\mathbb{R})$ since any other solution to (14) differs from Z by a linear combination of $\cos(k_c \cdot)$ and $\sin(k_c \cdot)$; see Remark 5. \square

Lemma 9 implies that the linear operator \mathcal{M} admits a linear and continuous inverse

$$\mathcal{M}^{-1} : \mathcal{F}^{-1}(L^2(\mathbb{R}) \cap BC^1(\mathbb{R})) \rightarrow L^2(\mathbb{R}) \oplus \text{span} \{Y_1, Y_2\},$$

where \mathcal{F}^{-1} denotes the inverse Fourier transform. The proof of Lemma 9 also reveals that \mathcal{M}^{-1} can be extended to a larger space since one only needs that \widehat{Q} is continuously differentiable in some neighborhood of $\pm k_c$. For our purpose, however, it is sufficient to assume that $\widehat{Q} \in BC^1(\mathbb{R})$. We also mention that the constant C in Lemma 9, which is the Lipschitz constant of \mathcal{M}^{-1} , is uniform in $c_0 < c < c_1$ but will grow with $c_1 \rightarrow 1$, due to the definition of Y_1 and Y_2 and the properties of m .

3.2. Solution operator to the affine subproblem. We are now able to prove that the affine problem (11)₁ admits a solution operator

$$\mathcal{L} : G \in \mathcal{Y} \mapsto (S, \eta) \in X \times \mathbb{R},$$

where

$$\mathcal{Y} := \left\{ G \in L^\infty(\mathbb{R}) : \text{supp } G \subseteq [-1, 1] \right\}.$$

The existence of \mathcal{L} is a consequence of the following result.

LEMMA 10. *For each $G \in \mathcal{Y}$ there exists a unique $(S, \eta) \in X \times \mathbb{R}$ such that*

$$(16) \quad \mathcal{M}S = \mathcal{A}^2G + \eta.$$

Moreover, S and η depend linearly on G and we have

1. $|\eta| \leq C_{\mathcal{M}} \|\mathcal{A}^2G\|_\infty,$
2. $\|S\|_\infty \leq C_{\mathcal{M}} \|\mathcal{A}^2G\|_\infty,$
3. $\|S'\|_\infty \leq C_{\mathcal{M}} \|\mathcal{A}G\|_\infty,$
4. $\|S''\|_\infty \leq C_{\mathcal{M}} \|G\|_\infty$

for some constant $C_{\mathcal{M}} > 0$ independent of G .

Proof. The function $Q := \mathcal{A}^2G$ satisfies $\text{supp } Q \subseteq [-2, 2]$, and using

$$\left| \widehat{Q}(k) \right| + \left| \frac{d}{dk} \widehat{Q}(k) \right| \leq C \int_{-2}^2 (1 + |x|) |Q(x)| \, dx \leq C \|Q\|_\infty \quad \text{for all } k \in \mathbb{R}$$

as well as $\|\widehat{Q}\|_2 = \|Q\|_2$, we easily verify that

$$\|\widehat{Q}\|_2 + \|\widehat{Q}\|_{1, \infty} \leq C \|Q\|_\infty.$$

By Lemma 9, the function $\tilde{S} := \mathcal{M}^{-1} \mathcal{A}^2G$ takes the form $\tilde{S} = Z + f_1 Y_1 + f_2 Y_2$, where $Z \in L^2(\mathbb{R})$ and $f_1, f_2 \in \mathbb{R}$ satisfy

$$(17) \quad \|Z\|_2 + |f_1| + |f_2| \leq C \|Q\|_\infty = C \|\mathcal{A}^2G\|_\infty.$$

In particular, we have $\mathcal{M}\tilde{S} = \mathcal{A}^2G$ and hence

$$c^2 Z = \mathcal{A}^2 Z - \mathcal{A}^2 G + f_1 \mathcal{M}Y_1 + f_2 \mathcal{M}Y_2.$$

The functions $\mathcal{M}Y_1, \mathcal{M}Y_2$ are supported in $[-1, +1]$ (see Remark 8) and $G \in \mathbf{Y}$ combined with Lemma 6 implies that \mathcal{A}^2G vanishes outside of $[-2, +2]$. For $|x| \geq 2$ we therefore find

$$c^2 |Z(x)| = |(\mathcal{A}^2 Z)(z)| \leq \left(\int_{x-1/2}^{x+1/2} ((\mathcal{A}Z)(s))^2 \, ds \right)^{1/2} \xrightarrow{x \rightarrow \pm\infty} 0,$$

thanks to Hölder’s inequality and since Lemma 6 implies $\mathcal{A}Z \in L^2(\mathbb{R})$. By definition of \mathcal{M}, Q , and \tilde{S} we also have

$$(18) \quad c^2 \tilde{S} = -\mathcal{A}^2 G + \mathcal{A}^2 \tilde{S} = -\mathcal{A}^2 G + \mathcal{A}^2 (Z + f_1 Y_1 + f_2 Y_2),$$

and Lemma 6 ensures that

$$\|\mathcal{A}^2 Z\|_\infty \leq \|Z\|_2, \quad \|\mathcal{A}^2 Y_i\|_\infty \leq \|Y_i\|_\infty.$$

Combining these estimates with (17) and (18), we arrive at $\tilde{S} \in L^\infty(\mathbb{R})$ with

$$\|\tilde{S}\|_\infty \leq C \|\mathcal{A}^2 G\|_\infty.$$

Moreover, differentiating the first identity in (18) with respect to x , we get

$$c^2 \tilde{S}' = \nabla(-\mathcal{A}G + \mathcal{A}\tilde{S}), \quad c^2 \tilde{S}'' = \nabla \nabla(-G + \tilde{S}),$$

where the discrete differential operator ∇ is defined as $\nabla U = U(\cdot + \frac{1}{2}) - U(\cdot - \frac{1}{2})$, cf. Lemma 6. This implies

$$\|\tilde{S}'\|_\infty \leq C \|\mathcal{A}G\|_\infty, \quad \|\tilde{S}''\|_\infty \leq C \|G\|_\infty$$

thanks to $\|\mathcal{A}^2 G\|_\infty \leq \|\mathcal{A}G\|_\infty \leq \|G\|_\infty$ and $\|\mathcal{A}\tilde{S}\|_\infty \leq \|\tilde{S}\|_\infty$. Since \tilde{S} does not belong to \mathbf{X} , we now define

$$(19) \quad S(x) := \tilde{S}(x) - \tilde{S}(0) - f_1 \frac{\sqrt{2\pi}}{m'(k_c)} (\cos(k_c x) - 1) - f_2 \frac{\sqrt{2\pi}}{m'(k_c)} \sin(k_c x)$$

as well as

$$(20) \quad \eta := (1 - c^2) \left(f_1 \frac{\sqrt{2\pi}}{m'(k_c)} - \tilde{S}(0) \right),$$

and observe that $S \in X$ and (16) hold by construction and due to $\lim_{x \rightarrow \infty} Z(x) = 0$. Moreover, S and η depend linearly on G and the above estimates for f_1 and f_2 and \tilde{S} provide the desired estimates for both S and η . Finally, the uniqueness of (S, η) is a direct consequence of $S \in X$ and Lemma 5. \square

Notice that the solution (S, η) to (11)₁ is unique only in the space $X \times \mathbb{R}$ and that further solution branches exist due to the nontrivial kernel functions of \mathcal{M} . For instance, replacing (19) and (20) by

$$S(x) := \tilde{S} - \tilde{S}(0), \quad \eta := -(1 - c^2)\tilde{S}(0)$$

we can define an operator

$$(21) \quad \bar{\mathcal{L}}: G \in Y \rightarrow (\bar{S}, \bar{\eta}) \in \bar{X} \times \mathbb{R}, \quad \bar{X} := \{ \bar{S} \in W^{2,\infty}(\mathbb{R}) : S(0) = 0 \},$$

which provides another solution to the affine problem (11)₁. The corresponding corrector \bar{S} , however, does in general not belong to X as it is oscillatory for both $x \rightarrow -\infty$ and $x \rightarrow +\infty$.

We emphasize that the three-parameter family of traveling waves $R = R_0 + S$, which we construct below by fixed points arguments involving \mathcal{L} , is—at least for sufficiently small δ —independent of the details in the definition of \mathcal{L} . The reason is, roughly speaking, that changing \mathcal{L} is equivalent to changing R_0 ; see the discussion at the end of section 4. However, choosing $X \times \mathbb{R}$ as the image space for \mathcal{L} provides more information on the resulting family of traveling waves: The existence of $\lim_{x \rightarrow +\infty} S(x)$ reveals that for each c there exists precisely one wave $R = R_0 + S$ that complies with the causality principle as it is nonoscillatory for $x \rightarrow +\infty$.

3.3. Properties of the nonlinear operator \mathcal{G} . In order to investigate the properties of the nonlinear superposition operator \mathcal{G} , we introduce a class of admissible perturbations S . More precisely, we say that $S \in X$ is δ -admissible if there exist two numbers $x_- < 0 < x_+$, which both depend on S and δ , such that

1. $R_0(x_\pm) + S(x_\pm) = \pm\delta$,
2. $R_0(x) + S(x) < -\delta$ for $x < x_-$,
3. $R_0(x) + S(x) > +\delta$ for $x > x_+$,
4. $\frac{1}{2}R'_0(0) < R'_0(x) + S'(x) < 2R'_0(0)$ for $x_- < x < x_+$,

where R_0 is the chosen wave for $\delta = 0$. Below we show that each sufficiently small ball in X consists entirely of δ -admissible functions, and this enables us to find traveling waves by the contraction mapping principle.

We are now able to derive the second key argument for our fixed point argument.

LEMMA 11. *Let $S \in X$ be δ -admissible and $G = \mathcal{G}(S)$ as in (12). Then we have*

$$(22) \quad \|G\|_\infty \leq C, \quad \text{supp } G \subseteq [-C\delta, C\delta], \quad \int_{\mathbb{R}} G(x) \, dx \leq C(1 + \|S''\|_\infty)\delta^2$$

for some constant C independent of S and δ , and hence $G \in Y$ for $0 < \delta < 1/C$.

Proof. The estimate (22)₁ is a consequence of $\|G\|_\infty \leq 1 + C_\Psi$. Since S is δ -admissible, we also have

$$\text{supp } G = [x_-, x_+], \quad \pm\delta = \pm \int_0^{x_\pm} (R'_0(x) + S'(x)) \, dx$$

with x_{\pm} as above, and this implies

$$(23) \quad \frac{1}{2R'_0(0)}\delta \leq |x_{\pm}| \leq \frac{2}{R'_0(0)}\delta, \quad \text{supp } G \subseteq \frac{2}{R'_0(0)}[-\delta, \delta].$$

Using the Taylor estimate

$$(24) \quad |R'_0(x) + S'(x) - R'_0(0) - S'(0)| \leq (\|R''_0\|_{\infty} + \|S''\|_{\infty})|x|,$$

we also verify that

$$(25) \quad \left| x_{\pm} \mp \frac{\delta}{R'_0(0) + S'(0)} \right| \leq \frac{|x_{\pm}|^2 \|R''_0\|_{\infty} + \|S''\|_{\infty}}{2 R'_0(0) + S'(0)} \leq 4\delta^2 \frac{\|R''_0\|_{\infty} + \|S''\|_{\infty}}{R'_0(0)^3}.$$

A direct computation now yields

$$(26) \quad \begin{aligned} \int_{\mathbb{R}} G(x) dx &= \int_{x_-}^{x_+} \Psi'_\delta(R_0(x) + S(x)) dx - \int_{x_-}^{x_+} \text{sgn}(R_0(x)) dx \\ &= \int_{-\delta}^{\delta} \Psi'_\delta(r) \frac{dr}{z(r)} - |x_+ + x_-|, \end{aligned}$$

due to $\text{sgn}(R_0(x)) = \text{sgn}(x)$. Here, the function z with $z(R_0(x) + S(x)) = R'_0(x) + S'(x)$ for all $x \in [x_-, x_+]$ is well defined since $R + S_0$ is strictly increasing on $[x_-, x_+]$. Thanks to (24), our assumption $I_\delta = \int_{-\delta}^{+\delta} \Psi'_\delta(r) dr = 0$, and the estimate $z(r), z(0) \geq \frac{1}{2}R'_0(0)$ we get

$$\begin{aligned} \left| \int_{-\delta}^{\delta} \Psi'_\delta(r) \frac{dr}{z(r)} \right| &= \left| \int_{-\delta}^{\delta} \Psi'_\delta(r) \left(\frac{1}{z(r)} - \frac{1}{z(0)} \right) dr \right| \leq \int_{-\delta}^{\delta} |\Psi'_\delta(r)| \frac{|z(r) - z(0)|}{z(r)z(0)} dr \\ &\leq C\delta \frac{(|x_+| + |x_-|)(\|R''_0\|_{\infty} + \|S''\|_{\infty})}{R'_0(0)^2}, \end{aligned}$$

and combining this with (23), (25), and (26) gives

$$(27) \quad \begin{aligned} \left| \int_{\mathbb{R}} G(x) dx \right| &\leq |x_- + x_+| + C\delta(|x_-| + |x_+|) \frac{\|R''_0\|_{\infty} + \|S''\|_{\infty}}{R'_0(0)^2} \\ &\leq C\delta^2 \frac{\|R''_0\|_{\infty} + \|S''\|_{\infty}}{R'_0(0)^3}. \end{aligned}$$

By Proposition 2, item (ii)(c), the value $R'_0(0)$ is bounded from below. Moreover, combining item (ii)(a) of Proposition 2 with the equation for R''_0 , that is,

$$c^2 R''_0 = \Delta_1 R_0 - \Delta_1 \text{sgn},$$

we find a constant C , which depends only on c_0 and c_1 , such that $\|R''_0\|_{\infty} \leq C$. The claims (22)₂ and (22)₃ are now direct consequences of these observations and the estimates (25) and (27). Moreover, $G = \mathcal{G}(S) \in \mathcal{Y}$ follows with $\delta \leq 1/C$ from (23)₂. \square

COROLLARY 12. *There exists a constant $C_{\mathcal{G}}$, which is independent of δ , such that*

$$(28) \quad \|\mathcal{A}G\|_{\infty} \leq C_{\mathcal{G}}\delta, \quad \|\mathcal{A}^2G\|_{\infty} \leq C_{\mathcal{G}}(1 + \|S''\|_{\infty})\delta^2,$$

hold with $G = \mathcal{G}(S)$ for all δ -admissible S .

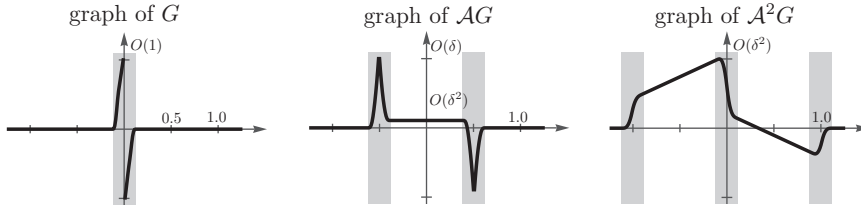


FIG. 5. Properties of $G = \mathcal{G}(S)$ for δ -admissible S . The shaded regions indicate intervals with length of order $O(\delta)$.

Proof. Thanks to Lemma 11 and since \mathcal{A} is the convolution with the characteristic function of the interval $[-\frac{1}{2}, +\frac{1}{2}]$, there exists a constant C such that

$$\begin{aligned} |\mathcal{A}G(x)| &\leq C\delta && \text{for } |x \pm \frac{1}{2}| \leq C\delta, \\ \mathcal{A}G(x) &= \int_{\mathbb{R}} G(x) dx && \text{for } |x| \leq \frac{1}{2} - C\delta, \\ \mathcal{A}G(x) &= 0 && \text{for } |x| \geq \frac{1}{2} + C\delta; \end{aligned}$$

see Figure 5 for an illustration. The first bound in (28) is now a consequence of the trivial estimate $|\int_{\mathbb{R}} G(x) dx| \leq |\text{supp } G| \|G\|_{\infty} \leq C\delta$, whereas the second one follows from

$$|(\mathcal{A}^2G)(x)| \leq C\delta^2 + \left| \int_{\mathbb{R}} G(x) dx \right| \quad \text{for all } x \in \mathbb{R}$$

and the refined estimate $|\int_{\mathbb{R}} G(x) dx| \leq C(1 + \|S\|''_{\infty})\delta^2$. \square

In the general case $I_{\delta} \neq 0$, one finds—due to $\int_{\mathbb{R}} G(x) dx = 2I_{\delta} + O(\delta^2)$ —the weaker estimate $\|\mathcal{A}^2G\|_{\infty} \leq C(1 + \|S''_{\infty}\|)\delta$. This bound is still sufficient to establish the fixed point argument but provides a corrector S of order $O(\delta)$ only. Recall, however, that Lemma 7 shows that shifting Ψ_{δ} and changing R_0 allows us to find correctors of order $O(\delta^2)$ even in the case $I_{\delta} \neq 0$.

We finally derive continuity estimates for \mathcal{G} .

LEMMA 13. *There exists a constant C_L independent of δ such that*

$$\|\mathcal{A}^2G_2 - \mathcal{A}^2G_1\|_{\infty} + \|\mathcal{A}G_2 - \mathcal{A}G_1\|_{\infty} + \delta\|G_2 - G_1\|_{\infty} \leq C_L\delta\|S'_2 - S'_1\|_{\infty}$$

holds for all δ -admissible correctors S_1 and S_2 with $G_{\ell} = \mathcal{G}(S_{\ell})$.

Proof. According to Lemma 11, there exists a constant C , such that $G_{\ell}(x) = 0$ for all x with $|x| \geq C\delta$. For $|x| \leq C\delta$, we use Taylor expansions for $S_1 - S_2$ at $x = 0$ to find

$$|S_2(x) - S_1(x)| \leq \|S'_2 - S'_1\|_{\infty} |x|,$$

where we used that $S_2(0) - S_1(0) = 0$. Combining this estimate with the upper bound for Ψ''_{δ} gives

$$|G_2(x) - G_1(x)| \leq \frac{C}{\delta} |S_2(x) - S_1(x)| \leq C\|S'_2 - S'_1\|_{\infty}$$

for all $|x| \leq C\delta$, and this implies the desired estimate for $\|G_2 - G_1\|_{\infty}$. We also have

$$\begin{aligned} \|\mathcal{A}^2G_2 - \mathcal{A}^2G_1\|_{\infty} &\leq \|\mathcal{A}G_2 - \mathcal{A}G_1\|_{\infty} \\ &\leq |\text{supp } (G_2 - G_1)| \|G_2 - G_1\|_{\infty} \leq C\delta\|G_2 - G_1\|_{\infty}, \end{aligned}$$

which completes the proof. \square

3.4. Fixed point argument. Now we have prepared all the ingredients to prove that the operator

$$\mathcal{T} := \mathcal{P}_S \circ \mathcal{L} \circ \mathcal{G}$$

admits a unique fixed point in the space

$$\mathbf{X}_\delta := \left\{ S \in \mathbf{X} : \|S\|_\infty \leq C_0\delta^2, \quad \|S'\|_\infty \leq C_1\delta, \quad \|S''\|_\infty \leq C_2 \right\}.$$

Here, \mathcal{P}_S denotes the projector on the first component, that means $\mathcal{P}_S(S, \eta) = S$, and the constants C_i are defined by

$$C_2 := C_{\mathcal{M}}(1 + C_\Psi), \quad C_1 := C_{\mathcal{M}}C_{\mathcal{G}}, \quad C_0 := C_{\mathcal{M}}C_{\mathcal{G}}(1 + C_2).$$

Notice that any fixed point of \mathcal{T} provides a solution to (11) and vice versa.

LEMMA 14. *For all sufficiently small δ , the operator \mathcal{T} has a unique fixed point in \mathbf{X}_δ .*

Proof. Step 1. We first show that each $S \in \mathbf{X}_\delta$ is δ -admissible provided that δ is sufficiently small. According to Proposition 2, there exist positive constants r_0 , x_0 , and d_0 such that

$$|R_0(x)| \geq r_0 \quad \text{for } |x| > x_0, \quad d_0 < R'_0(x) \quad \text{for } |x| < x_0,$$

and combining the upper estimate for $\|R_0\|_\infty$ with the equation for R_0 we find $\|R''_0\|_\infty \leq D_2$ for some constant D_2 . We now set

$$\delta_0 := \frac{1}{2} \min \left\{ \frac{d_0}{2\frac{D_2}{d_0} + C_1}, x_0d_0, \sqrt{\frac{r_0}{C_0}}, r_0 \right\}, \quad x_\delta := \frac{2}{d_0}\delta,$$

and assume that $\delta \leq \delta_0$. For any x with $|x| \leq x_\delta \leq x_0$, we then estimate

$$|R'_0(x) + S'(x) - R'_0(0)| \leq D_2x_\delta + C_1\delta \leq \left(2\frac{D_2}{d_0} + C_1\right)\delta \leq \frac{1}{2}d_0 < \frac{1}{2}R'_0(0),$$

and this gives $\frac{1}{2}R'_0(0) \leq R'_0(x) + S'(x) \leq \frac{3}{2}R'_0(0)$. Moreover, $x_\delta \leq |x| \leq x_0$ implies

$$|R_0(x) + S(x)| \geq \left| \int_0^x R'_0(s) \, ds \right| - \|S'\|_\infty |x| \geq (d_0 - C_1\delta) |x| > \frac{1}{2}d_0 \cdot \frac{2}{d_0}\delta = \delta,$$

whereas for $|x| > x_0$ we find

$$|R_0(x) + S(x)| \geq r_0 - C_1\delta^2 \geq \frac{1}{2}r_0 \geq \delta.$$

Using

$$x_- := \max\{x : R_0(x) + S(x) \leq -\delta\}, \quad x_+ := \min\{x : R_0(x) + S(x) \geq +\delta\},$$

we now verify that S is δ -admissible provided that $\delta \leq \delta_0$. Moreover, making δ_0 smaller (if necessary) we can also guarantee that $\mathcal{G}(S) \in \mathbf{Y}$ holds for all $S \in \mathbf{X}_\delta$ and $\delta \leq \delta_0$; see Lemma 11.

Step 2. We next show that $\mathcal{T}(\mathbf{X}_\delta) \subset \mathbf{X}_\delta$ holds for all $\delta \leq \delta_0$. Since each $S \in \mathbf{X}_\delta$ is δ -admissible, Corollary 12 yields

$$\|\mathcal{A}\mathcal{G}(S)\|_\infty \leq C_{\mathcal{G}}\delta, \quad \|\mathcal{A}^2\mathcal{G}(S)\|_\infty \leq C_{\mathcal{G}}(1 + C_2)\delta^2,$$

and $\|\mathcal{G}(S)\|_\infty \leq 1 + C_\Psi$ holds by definition of \mathcal{G} and Assumption 1. Lemma 10 now provides

$$\begin{aligned} \|\mathcal{T}(S)\|_\infty &\leq C_{\mathcal{M}}C_{\mathcal{G}}(1 + C_2)\delta^2 = C_0\delta^2, \\ \|\mathcal{T}(S)'\|_\infty &\leq C_{\mathcal{M}}C_{\mathcal{G}}\delta = C_1\delta, \\ \|\mathcal{T}(S)''\|_\infty &\leq C_{\mathcal{M}}(1 + C_\Psi) = C_2, \end{aligned}$$

and hence $\mathcal{T}(S) \in X_\delta$.

Step 3. We equip X_δ with the norm $\|S\|_\# = \|S\|_\infty + \|S'\|_\infty + \delta\|S''\|_\infty$, which is, for any fixed δ , equivalent to the standard norm. For given $S_1, S_2 \in X_\delta$, we now employ the estimates from Lemmas 10 and 13 for $S = S_2 - S_1$ and $G = \mathcal{G}(S_2) - \mathcal{G}(S_1) \in Y$. This gives

$$\begin{aligned} \|\mathcal{T}(S_2) - \mathcal{T}(S_1)\|_\# &\leq C_{\mathcal{M}}\|\mathcal{A}^2\mathcal{G}(S_2) - \mathcal{A}^2\mathcal{G}(S_1)\|_\infty + C_{\mathcal{M}}\|\mathcal{A}\mathcal{G}(S_2) - \mathcal{A}\mathcal{G}(S_1)\|_\infty \\ &\quad + \delta C_{\mathcal{M}}\|\mathcal{G}(S_2) - \mathcal{G}(S_1)\|_\infty \\ &\leq C_{\mathcal{M}}C_L\delta\|S_2' - S_1'\|_\infty \leq C_{\mathcal{M}}C_L\delta\|S_2 - S_1\|_\#, \end{aligned}$$

and we conclude that \mathcal{T} is contractive with respect to $\|\cdot\|_\#$ provided that $\delta < 1/(C_{\mathcal{M}}C_L)$. The claim is now a direct consequence of the Banach fixed point theorem. \square

The previous result implies the existence of a three-parameter family of waves that is parametrized by the speed $c \in [c_0, c_1]$ and by R_0 , where R_0 can be regarded as a parameter in the two-dimensional L^∞ -kernel of \mathcal{M} .

PROPOSITION 15. *Suppose that $I_\delta = 0$ for all δ . Then there exists $\delta_0 > 0$ with the following property: For any $\delta < \delta_0$, each $c \in [c_0, c_1]$, and any R_0 as in Proposition 2 there exists a δ -admissible corrector*

$$S \in X_\delta \cap \left(L^2(\mathbb{R}) \oplus \text{span} \left\{ 1, Y_1 - \frac{\sqrt{2\pi}}{m'(k_c)} \cos(k_c \cdot), Y_2 - \frac{\sqrt{2\pi}}{m'(k_c)} \sin(k_c \cdot) \right\} \right)$$

such that $R = R_0 + S$ solves the traveling wave equation (7) for some μ . In particular, we have $R(0) = 0$, the limits

$$\lim_{x \rightarrow -\infty} (R(x) - \alpha_- \cos(k_c x) - \beta_- \sin(k_c x)) \quad \text{and} \quad \lim_{x \rightarrow +\infty} (R(x) - R_0(x))$$

are well defined for some constants α_-, β_- depending on c and R_0 , and the estimates

$$(29) \quad R(x) \leq -\delta \quad \text{for } x \leq -C\delta, \quad R(x) \geq +\delta \quad \text{for } x \geq +C\delta$$

hold for some constant $C > 0$ independent of c and R_0 .

Proof. For given c and R_0 , Lemma 14 provides a unique fixed point $S \in X_\delta$ of \mathcal{T} , which solves

$$\mathcal{M}S = \mathcal{A}^2\mathcal{G}(S) + \eta$$

for some $\eta \in \mathbb{R}$, and this implies that $R = R_0 + S$ is in fact a traveling wave. Moreover, by construction—see the proof of Lemma 10—we also have

$$S = Z + \lambda + f_1 \left(Y_1 - \frac{\sqrt{2\pi}}{m'(k_c)} \cos(k_c \cdot) \right) + f_2 \left(Y_2 - \frac{\sqrt{2\pi}}{m'(k_c)} \sin(k_c \cdot) \right)$$

for some constants f_1, f_2 , and λ and a function $Z \in L^2(\mathbb{R})$ with $Z(x) \rightarrow 0$ as $x \rightarrow \pm\infty$. The claims on the asymptotic behavior as $x \rightarrow \pm\infty$ now follow immediately since R_0 has harmonic tail oscillations with wave number k_c . Finally, the fixed point S is δ -admissible—see the proof of Lemma 14—and this implies the validity of (29) due to $0 \leq x_+, -x_- \leq C\delta$. \square

Notice that Proposition 15 yields a genuine three-parameter family in the sense that different choices of the parameters c and R_0 correspond to different tail oscillations for $x \rightarrow +\infty$ and hence to different waves $R = R_0 + S$. This finishes the existence proof of Theorem 3.

4. Uniqueness of phase transition waves. In this section we establish the uniqueness result of Theorem 3 by showing that the family provided by Proposition 17 contains all phase transition waves that have harmonic tail oscillations for $x \rightarrow +\infty$ and penetrate the spinodal region in a small interval only.

LEMMA 16. *Let $\kappa > \frac{1}{2}$ be given and suppose that $I_\delta = 0$ for all δ . Then there exists $\delta_\kappa > 0$ such that the following statement holds for all $0 < \delta < \delta_\kappa$: Let (R_1, μ_1) and (R_2, μ_2) be two solutions to the traveling wave equation (7) with speed $c \in [c_0, c_1]$ such that*

$$R_i \in W^{2,\infty}(\mathbb{R}), \quad \mu_i \in \mathbb{R}, \quad R_i(0) = 0$$

and

$$R_i(x) \leq -\delta \quad \text{for } x \leq -\delta^\kappa, \quad R_i(x) \geq +\delta \quad \text{for } x \geq +\delta^\kappa$$

for both $i = 1$ and $i = 2$. Then, R_1 and R_2 are either identical or satisfy

$$R_1(x) - R_2(x) - \alpha_+(\cos(k_c x) - 1) - \beta_+ \sin(k_c x) - \gamma_+ \xrightarrow{x \rightarrow +\infty} 0$$

for some constants γ_+ and $(\alpha_+, \beta_+) \neq (0, 0)$.

Proof. For given R_1, R_2 , there exist constant $\mu_1, \mu_2 \in \mathbb{R}$ such that

$$\mathcal{M}(R_2 - R_1) = \mathcal{A}^2 G + \mu_2 - \mu_1, \quad G := \Psi'_\delta(R_2) - \Psi'_\delta(R_1).$$

By assumption and due to the bounds of Ψ''_δ we also find $G(x) = 0$ for $|x| \geq \delta^\kappa$ as well as

$$|G(x)| \leq \frac{C}{\delta} |R_2(x) - R_1(x)| \leq C\delta^{\kappa-1} \|R'_2 - R'_1\|_\infty \quad \text{for } |x| \leq \delta^\kappa,$$

and this implies

$$\|\mathcal{A}G\|_\infty \leq |\text{supp } G| \|G\|_\infty \leq C\delta^{2\kappa-1} \|R'_2 - R'_1\|_\infty.$$

Moreover, Lemma 10 provides $S \in \mathbf{X}$ as well as $\eta \in \mathbb{R}$ such that

$$\mathcal{M}S = \mathcal{A}^2 G + \eta, \quad \|S'\|_\infty \leq C\delta^{2\kappa-1} \|R'_2 - R'_1\|_\infty.$$

In particular, we have

$$\mathcal{A}^2 G = \mathcal{M}(R_2 - R_1 - (1 - c^2)^{-1}(\mu_2 - \mu_1)) = \mathcal{M}(S - (1 - c^2)^{-1}\eta).$$

Since the space of bounded kernel functions for \mathcal{M} is spanned by $\sin(k_c \cdot)$ and $\cos(k_c \cdot)$, we conclude that there exist constants α_+ and β_+ such that

$$R_2(x) - R_1(x) = S(x) - \sigma + \alpha_+(1 - \cos(k_c x)) + \beta_+ \sin(k_c x) + \gamma_+,$$

where $\sigma := \lim_{x \rightarrow +\infty} S(x)$ and $\gamma_+ := (1 - c^2)^{-1}(\mu_2 - \mu_1 - \eta) + \sigma - \alpha_+$. In the case of $\alpha_+ = \beta_+ = 0$ we therefore find

$$\|R'_2 - R'_1\|_\infty = \|S'\|_\infty \leq C\delta^{2\kappa-1}\|R'_2 - R'_1\|_\infty,$$

and combining this with $R_1(0) = R_2(0)$ we get $R_2 = R_1$ for all sufficiently small δ . \square

PROPOSITION 17. *Suppose that $I_\delta = 0$ for all δ and that κ with $\frac{1}{2} < \kappa < 1$ is fixed. Then there exists δ_κ with $0 < \delta_\kappa \leq \delta_0$ such that the following statement holds for all $0 < \delta < \delta_\kappa$: Let R be a traveling wave with speed $c \in [c_0, c_1]$ such that the limit*

$$\lim_{x \rightarrow +\infty} (R(x) - R_0(x))$$

is well defined for some R_0 from Proposition 2 and such that

$$R(x) \leq -\delta \quad \text{for } x \leq -\delta^\kappa, \quad R(x) \geq +\delta \quad \text{for } x \geq +\delta^\kappa.$$

Then R belongs to the family of waves provided by Proposition 15.

Proof. Let $R_0 + S$ be the traveling wave from Proposition 15. By construction, $R - R_0 - S$ converges as $x \rightarrow +\infty$ and for all sufficiently small δ we also have $C\delta \leq \delta^\kappa$. Lemma 16 applied with $R_1 = R$ and $R_2 = R_0 + S$ therefore implies $R = R_0 + S$. \square

With Propositions 15 and 17 we have established our existence and uniqueness result in the special case that $I_\delta = 0$ holds for all δ . The corresponding result for the general case is then provided by Lemma 7.

We finally mention a particular consequence of our uniqueness result, namely, that the family from Proposition 15 does not depend on the particular choice of the solution operator \mathcal{L} to the affine problem (11)₁. At a first glance, this might be surprising since the operator \mathcal{T} and hence each fixed point surely depend on \mathcal{L} . We can, however, argue as follows (a similar idea is used in the theory of Lyapunov–Schmidt reduction in order to show that different projections on the kernel and cokernel yield the same solutions): Suppose we would choose in the proof of Lemma 10 another reasonable solution operator $\bar{\mathcal{L}}$ (for instance, the operator from (21) that does not involve any kernel function of \mathcal{M}). Repeating all arguments from section 3 we then find—for any given δ , c , and R_0 —a different corrector $\bar{S} \in W^{2,\infty}(\mathbb{R})$. In general, this corrector \bar{S} does not converge as $x \rightarrow +\infty$ but satisfies

$$\bar{S}(0) = 0, \quad \|\bar{S}\|_\infty \leq \bar{C}\delta^2, \quad \|\bar{S}'\|_\infty \leq \bar{C}\delta, \quad \|\bar{S}''\|_\infty \leq \bar{C}$$

for some constant \bar{C} that is independent of c , R_0 , and δ . Moreover, we also have

$$\bar{S} \in L^2(\mathbb{R}) \oplus \text{span} \{1, Y_1, Y_2, \cos(k_c \cdot), \sin(k_c \cdot)\}$$

that means the tail oscillations of \bar{S} for both $x \rightarrow -\infty$ and $x \rightarrow +\infty$ are again harmonic waves with wave number k_c . Adding a suitable linear combination of $1 - \cos(k_c \cdot)$ and $\sin(k_c \cdot)$ to R_0 we can construct another wave \bar{R}_0 such that \bar{R}_0 and $R_0 + \bar{S}$ have the same tail oscillations as $x \rightarrow +\infty$. This function \bar{R}_0 is, at least for small δ , also a traveling wave for the unperturbed problem and hence among the family of waves provided by Proposition 2. We can therefore use \bar{R}_0 instead of R_0 in order to define the operator \mathcal{G} . Theorem 10, which relies on the oscillation-preserving operator \mathcal{L} , then provides a corrector S that converges as $x \rightarrow +\infty$, and from Lemma 16 we finally infer that $\bar{R}_0 + S = R_0 + \bar{S}$ because both waves have, by construction, the same tail oscillations for $x \rightarrow +\infty$. We therefore conclude, at least for small δ , that changing \mathcal{L} does not alter the family of traveling waves but only its parametrization by R_0 .

5. Kinetic relations. We finally show that the kinetic relation does not change to order $O(\delta)$. To this end we denote by R_δ a traveling wave solution to (2) as provided by Theorem 3. The corresponding *configurational force* (cf. [TV05, HSZ12]) is then defined by $\Upsilon_\delta := \Upsilon_{e,\delta} - \Upsilon_{f,\delta}$ with

$$\Upsilon_{e,\delta} := \Phi_\delta(\bar{r}_{\delta,+}) - \Phi_\delta(\bar{r}_{\delta,-}), \quad \Upsilon_{f,\delta} := \frac{\Phi'_\delta(\bar{r}_{\delta,+}) + \Phi'_\delta(\bar{r}_{\delta,-})}{2} (\bar{r}_{\delta,+} - \bar{r}_{\delta,-}),$$

where the *macroscopic* strains $\bar{r}_{\delta,\pm}$ on both sides of the interface can be computed from R_δ via

$$\bar{r}_{\delta,\pm} = \lim_{L \rightarrow \infty} \frac{1}{L} \int_0^{+L} R_\delta(\pm x) \, dx.$$

LEMMA 18. *Let R_δ be a traveling wave from Theorem 3, and R_0 the corresponding wave for $\delta = 0$. Then we have $\Upsilon_\delta = \Upsilon_0 + O(\delta^2)$.*

Proof. By construction, we know that the only asymptotic contributions to the profile R_δ are due to $R_0 - I_\delta$ plus a small asymptotic corrector of order $O(\delta^2)$ from $\text{span}\{1, Y_1, Y_2\}$. This implies

$$\bar{r}_{\delta,\pm} = \bar{r}_{0,\pm} - I_\delta + O(\delta^2).$$

As $\bar{r}_{0,\pm}$ and $\bar{r}_{\delta,\pm}$ are both larger than δ we know that

$$\Psi'_\delta(\bar{r}_{\delta,\pm}) = \mp 1 = \Psi'_0(\bar{r}_{\delta,\pm}).$$

Thus, we conclude

$$\Phi'_\delta(\bar{r}_{\delta,\pm}) = \bar{r}_{\delta,\pm} \mp 1 = \Phi'_0(\bar{r}_{0,\pm}) - I_\delta + O(\delta^2),$$

and hence

$$\Upsilon_{f,\delta} = \Upsilon_{f,0} - I_\delta(\bar{r}_{0,+} - \bar{r}_{0,-}) + O(\delta^2).$$

Moreover, we calculate

$$\begin{aligned} \Upsilon_{e,\delta} &= \int_{\bar{r}_{\delta,-}}^{\bar{r}_{\delta,+}} \Phi'_\delta(r) \, dr = \int_{\bar{r}_{\delta,-}}^{\bar{r}_{\delta,+}} (r - \Psi'_\delta(r) - \Psi'_0(r) + \Psi'_0(r)) \, dr \\ &= \int_{\bar{r}_{\delta,-}}^{\bar{r}_{\delta,+}} \Phi'_0(r) \, dr - \int_{\bar{r}_{\delta,-}}^{\bar{r}_{\delta,+}} (\Psi'_\delta(r) - \Psi'_0(r)) \, dr \\ &= \Phi_0(\bar{r}_{\delta,+}) - \Phi_0(\bar{r}_{\delta,-}) - 2I_\delta = \frac{1}{2}(\bar{r}_{\delta,+} - 1)^2 - \frac{1}{2}(\bar{r}_{\delta,-} + 1)^2 - 2I_\delta \\ &= \frac{1}{2}(\bar{r}_{0,+} - I_\delta - 1)^2 - \frac{1}{2}(\bar{r}_{0,-} - I_\delta + 1)^2 - 2I_\delta + O(\delta^2) \\ &= \frac{1}{2}(\bar{r}_{0,+} - 1)^2 - \frac{1}{2}(\bar{r}_{0,-} + 1)^2 - I_\delta(\bar{r}_{0,+} - 1 - \bar{r}_{0,-} - 1) - 2I_\delta + O(\delta^2) \\ &= \Upsilon_{e,0} - I_\delta(\bar{r}_{0,+} - \bar{r}_{0,-}) + O(\delta^2). \end{aligned}$$

Subtracting both results gives $\Upsilon_\delta = \Upsilon_0 + O(\delta^2)$, the desired result. □

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