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in bistable lattice models with small spinodal region**

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Subsonic phase transition waves in bistable lattice models with small spinodal region

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Abstract

Phase transitions waves in atomic chains with double-well potential play a fundamental role in materials science, but 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 localised with respect to the strain variable. More precisely, we introduce an anchor-corrector ansatz, characterise the corrector as a fixed point of a nonlinear and nonlocal operator, and show that this operator is contractive in a small ball of a certain function space.

Keywords: *phase transitions in lattices, heteroclinic travelling waves, FPU-type chains, kinetic relations*

MSC (2010): 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 neighbour interactions. The corresponding equation of motion reads

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

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 non-convex Φ , because then (1) provides a simple dynamical model for martensitic phase transitions. In this context, a propagating interface can be

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described by a *phase transition waves*, which is a travelling 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 naïve continuum limit of (1), which is the PDE $\partial_{tt}u = \partial_x \Phi'(\partial_x)$. This equation is ill-posed for nonconvex Φ due to its elliptic-hyperbolic nature, and one proposal is to select solutions by so-called kinetic relations [AK91, Tru87] derived from travelling waves in atomistic models.

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

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

where $R(x) := U(x + 1/2) - U(x - 1/2)$ the (symmetrised) discrete strain profile and $\Delta_1 F(x) := F(x + 1) - 2F(x) + F(x - 1)$. Periodic and homoclinic travelling waves have been studied intensively, see [FW94, SW97, FP99, Pan05, 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 transitions 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], or tri-quadratic potentials [Vai10]. For the special case

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

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 waves. These waves have exactly one interface and connect different periodic tail oscillations, see Figure 2 for an illustration.

In this paper we allow for small perturbations of the potential (3) and show that the phase transition waves from [SZ09] persist provided that the perturbation is sufficiently small and localised. Our approach is in essence perturbative and reformulates the travelling wave equation with perturbed potential in terms of a corrector profile S . The resulting equation can be written as

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

where η is a constant of integration. Moreover, \mathcal{M} and \mathcal{A} are linear integral operators and \mathcal{G} a nonlinear superposition operator to be identified below. The analysis of (4) is rather delicate since the Fourier symbol of \mathcal{M} has real roots. In our existence proof, we first eliminate the singularities and derive an appropriate inversion formula for \mathcal{M} . Afterwards we introduce a class of admissible functions S and show that the properties of \mathcal{A} and \mathcal{G} guarantee that $\mathcal{A}^2 \mathcal{G}(S)$ is compactly supported and sufficiently small. These fine properties are illustrated in Fig. 4 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 $\eta(S) \in \mathbb{R}$. In the final step, we show that \mathcal{T} is contractive in some ball of an appropriately defined function space.

We further remark that each phase transition wave satisfies Rankine-Hugoniot conditions for the macroscopic averages of mass, momentum, and total energy [HSZ12], which imply nontrivial restrictions between the wave speed and the tail oscillations on both sides of the interface. Although these conditions do not appear explicitly in our existence proof, they can (at least in principle) be computed because the tail oscillations are given by harmonic waves, see again Fig. 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 non-oscillatory energy at the interface and determines the *configurational*

force that drives the wave. In the final section we discuss how the kinetic relation changes to leading order under small perturbation 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 neighbourhood of 0. The travelling wave equation therefore reads

$$c^2 R'' = \triangle_1(R - \Psi'_\delta(R)) \quad (5)$$

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*

- (i) Ψ'_δ coincides with Ψ'_0 outside the interval $(-\delta, \delta)$,
- (ii) 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

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

As already mentioned, the case $\delta = 0$ has been solved in [SZ09]. The main result can be summarised as follows.

Proposition 2 ([SZ09], Proof of Theorem 3.11). *There exist $0 < c_0 < 1$ 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 travelling wave equation (5) with $\delta = 0$ such that*

- (i) $R_0(0) = 0$,
- (ii) $\|R_0\|_\infty \leq D_0(1 - c^2)^{-1}$,
- (iii) $R_0(x) > r_0$ for $x > x_0$ and $R_0(x) < -r_0$ for $x < -x_0$,
- (iv) $R'_0(x) > d_0$ for $|x| < x_0$,

for some constants x_0, r_0, d_0 and D_0 which depend only on c_0 . For any such profile R_0 there exists constants α_\pm and β_\pm such that

$$\lim_{x \rightarrow \pm\infty} |\pm r_c + \alpha_\pm(1 - \cos(k_c x)) + \beta_\pm \sin(k_c x) - R_0(x)| = 0,$$

where r_c and $k_c > 0$ are uniquely determined by c . Moreover, any two profiles R_0 and \tilde{R}_0 satisfy

$$R_0 - \tilde{R}_0 \in \text{span} \{ \sin(k_c \cdot), 1 - \cos(k_c \cdot) \}.$$

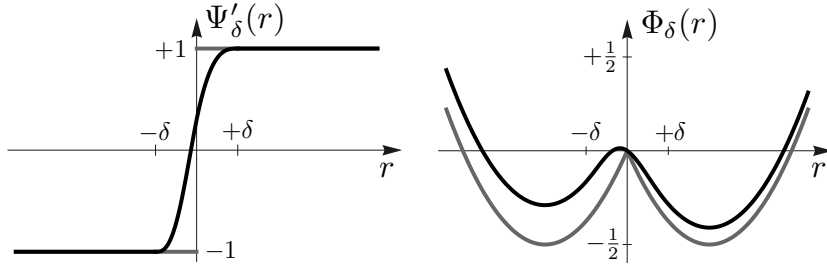


Figure 1: Sketch of Ψ'_δ and Φ_δ for $\delta = 0$ (grey) and $\delta > 0$ (black). Since Φ_0 is symmetric, $-I_\delta$ is just half the energy difference between the two wells of Φ_δ .

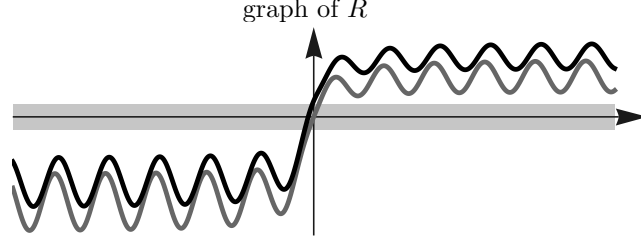


Figure 2: Sketch of the waves for $\delta = 0$ (grey) and $\delta > 0$ (black) as provided by our perturbation result; the shaded region indicates the spinodal interval $[-\delta, +\delta]$, where Ψ'_δ differs from Ψ'_0 . Both waves differ by the constant $I_\delta = O(\delta)$ and a small oscillatory corrector S of order $O(\delta^2)$. The tail oscillations of both waves do not penetrate the spinodal region and are generated by harmonic waves with wave number k_c . Notice that the phase shifts, amplitudes, and local averages are different on both sides of the interface and depend on δ .

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*

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

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

(i) vanishes at $x = 0$,

(ii) is small in the sense of

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

Moreover, for small δ there exists only one R with these properties.

Concerning these assertions, we emphasise that:

- (i) Our existence proof implies that different choices of R_0 provide different waves R , see Lemma 15.
- (ii) 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 .
- (iii) 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. [SZ].
- (iv) The travelling 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.

This paper is organised as follows. In §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 $I_\delta = 0$. In Section 3 we then study the equation for the corrector S . We first establish an inversion formula for \mathcal{M} and investigate afterwards the properties of the nonlinear \mathcal{G} . These result then allow us to establish the fixed point argument for the operator \mathcal{T} . Finally, we discuss the kinetic relation in §4.

2 Preliminaries and reformulation of the problem

In this section we reformulate the travelling 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

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

The travelling wave equation can then be stated as

$$\mathcal{M}R = \mathcal{A}^2 \Psi'_\delta(R) + \mu. \quad (6)$$

Lemma 4. *A function $W \in W^{2,\infty}(\mathbb{R})$ solves the travelling wave equation (5) if and only if there exists a constant $\mu \in \mathbb{R}$ such that (R, μ) solves (6).*

Proof. By 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

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

The implication (6) \implies (5) now follows immediately. Towards the reversed statement, we integrate (7)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

We next summarize some properties of the operator \mathcal{A} .

Lemma 5. *For any $1 \leq p \leq \infty$ we have $\mathcal{A}: L^p(\mathbb{R}) \rightarrow W^{1,p}(\mathbb{R}) \cap BC(\mathbb{R})$ with*

$$\|\mathcal{A}F\|_{L^p(\mathbb{R})} \leq \|F\|_{L^p(\mathbb{R})}, \quad \|(\mathcal{A}F)'\|_{L^p(\mathbb{R})} \leq 2\|F\|_{L^p(\mathbb{R})}, \quad \|\mathcal{A}F\|_{BC(\mathbb{R})} \leq \|F\|_{L^p(\mathbb{R})}$$

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, $\text{supp } F \subset [x_1, x_2]$ implies $\text{supp } \mathcal{A}F \subset [x_1 - \frac{1}{2}, x_2 + \frac{1}{2}]$.

Proof. All assertions follow immediately from the definition of \mathcal{A} and Hölder's inequality. \square

Some of the arguments in our existence proof rely on Fourier transform (in the space of tempered distributions), which we normalise as follows

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

In particular, the operators \mathcal{A} and \mathcal{M} diagonalise 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.

2.2 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 by adding a constant to R .

Lemma 6. *The family $(\tilde{\Psi}_\delta)_{\delta>0}$ 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 travelling wave equation

$$\mathcal{M}\tilde{R} = \mathcal{A}^2 \tilde{\Psi}'_\delta(\tilde{R}) + \tilde{\mu} \tag{8}$$

defines a solution (R, μ) to (6) 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 (6) and (8) is obvious. \square

3 Proof of the existence and uniqueness result

We now show that for fixed c the two-parameter family of phase transitions for $\delta = 0$ persists under the perturbation $\Psi_0 \rightsquigarrow \Psi_\delta$ provided that δ is sufficiently small. To this end we proceed as follows.

- (i) We fix c with $c_0 < c < c_1 < 1$ with c_0 and c_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 $k \neq \pm k_c$. We emphasise again that all constants derived below can be chosen independently of c but are allowed to depend on c_0 and c_1 .
- (ii) Thanks to Proposition 2 and Lemma 4, we fix (R_0, μ_0) from the two-parameter family of solutions to the integrated travelling wave equation (6) for $\delta = 0$ and given c . Recall that R_0 is normalised by $R_0(0) = 0$.
- (iii) In view of Lemma 6, 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 travelling wave equation (6) for $\delta > 0$, we further make the anchor-corrector ansatz

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

and seek correctors (S, η) such that

$$\mathcal{M}S = \mathcal{A}^2G + \eta, \quad G = \mathcal{G}(S). \quad (9)$$

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

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

A natural ansatz space for S is given by

$$\mathbf{X} := \{S \in W^{2,\infty}(\mathbb{R}) : S(0) = 0\},$$

where we impose the constraint $S(0) = 0$ in order to eliminate the non-uniqueness resulting from the shift invariance of the travelling wave equation (6). In fact, without this normalisation condition 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 $x_0 = O(\delta^2)$.

3.1 Inversion formula for \mathcal{M}

Our first task is to construct for given G a solution (S, η) to the affine equation $(9)_1$. In a preparatory step, we therefore derive an appropriate inversion formula for the operator \mathcal{M} . Recall that there does not exist a unique inverse of \mathcal{M} as the corresponding Fourier symbol, which is the function m , has real roots at $k = \pm k_c$.

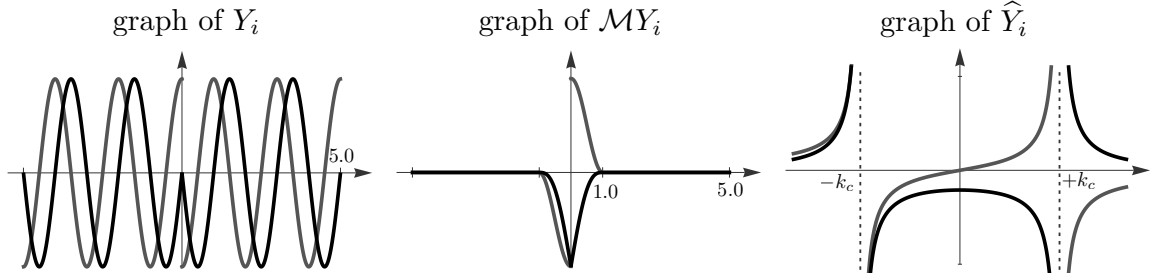


Figure 3: Properties of Y_1 (grey) and Y_2 (black).

As illustrated in Figure 3, we introduce two functions $Y_1, Y_2 \in L^\infty(\mathbb{R})$ by

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

and verify by direct computations the following assertions.

Remark 7. *We have*

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

Using Y_1 and Y_2 , we can establish the following linear and continuous inversion formula for \mathcal{M} .

Lemma 8. *Let Q be given with $\hat{Q} \in L^2(\mathbb{R}) \cap BC^1(\mathbb{R})$. Then there exists $Z \in L^2(\mathbb{R})$, which depends linearly on Q , such that*

$$\mathcal{M}\left(Z - i \frac{\hat{Q}(+k_c) - \hat{Q}(-k_c)}{2} Y_1 - \frac{\hat{Q}(+k_c) + \hat{Q}(-k_c)}{2} Y_2\right) = Q, \quad (10)$$

and

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

for some constant D independent of Q .

Proof. Thanks to our assumptions on Q and the properties of m and $Y_{1,2}$, the function $Z \in \mathbf{L}^2(\mathbb{R})$ is well defined by

$$\widehat{Z}(k) := \frac{\widehat{Q}(k) + i \frac{\widehat{Q}(+k_c) - \widehat{Q}(-k_c)}{2} m(k) \widehat{Y}_1(k) + \frac{\widehat{Q}(+k_c) + \widehat{Q}(-k_c)}{2} m(k) \widehat{Y}_2(k)}{m(k)} \in \mathbf{L}^2(\mathbb{R}) \cap \mathbf{BC}(\mathbb{R})$$

and satisfies (10) by construction. Moreover, with $J := [-2k_c, +2k_c]$ we readily verify the estimates

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

and $\|\widehat{Z}\|_{\mathbf{C}(J)} \leq D \|\widehat{Q}\|_{\mathbf{C}^1(J)}$. □

We note that the constant D in Lemma 8 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 linear subproblem

We are now able to prove that the affine problem $(9)_1$ has a nice solution operator on the space of all compactly supported functions G .

Lemma 9. *Let $G \in \mathbf{L}^\infty(\mathbb{R})$ be given, with $\text{supp } G \subseteq [-1, 1]$. Then there exist $\mathcal{S} \in \mathbf{X}$ and $\eta \in \mathbb{R}$, both depending linearly on G , such that*

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

Moreover, we have

- (i) $|\eta| \leq C_{\mathcal{M}} \|\mathcal{A}^2 G\|_\infty$,
- (ii) $\|\mathcal{S}\|_\infty \leq C_{\mathcal{M}} \|\mathcal{A}^2 G\|_\infty$,
- (iii) $\|\mathcal{S}'\|_\infty \leq C_{\mathcal{M}} \|\mathcal{A} G\|_\infty$,
- (iv) $\|\mathcal{S}''\|_\infty \leq C_{\mathcal{M}} \|G\|_\infty$.

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

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

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

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

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

Using Lemma 8, we now define $\tilde{S} := Z + f_1 Y_1 + f_2 Y_2$ such that $\mathcal{M}\tilde{S} = Q$, where $Z \in \mathbf{L}^2(\mathbb{R})$, and

$$\|Z\|_2 + |f_1| + |f_2| \leq C \|Q\|_\infty = C \|\mathcal{A}^2 G\|_\infty. \quad (11)$$

By definition of \mathcal{M} , Q , and \tilde{S} we have

$$c^2 \tilde{S} = -\mathcal{A}^2 G + \mathcal{A}^2 \tilde{S} = -\mathcal{A}^2 G + \mathcal{A}^2 (Z + f_1 Y_1 + f_2 Y_2), \quad (12)$$

and the properties of \mathcal{A} imply

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

Combining these estimates with (11) and (12), we arrive at $\tilde{S} \in \mathbf{L}^\infty(\mathbb{R})$ with

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

Moreover, differentiating the first identity in (11) 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 5. 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 $\|\mathcal{A}\tilde{S}\|_\infty \leq \|\tilde{S}\|_\infty$. We finally define $S(x) = \tilde{S}(x) - \tilde{S}(0)$ and $\eta = (1 - c^2)\tilde{S}(0)$. All assertions now follow by taking $C_{\mathcal{M}}$ as the maximum of all constants C in this proof. \square

While we will work in a subset of $W^{2,\infty}$, we remark that the regularity of the equation (Lemma 9 (iv)) would allow us to start the iteration with $S \in W^{1,\infty}$.

3.3 Properties of the nonlinear operator \mathcal{G}

We say that $S \in \mathbf{X}$ is δ -admissible if there exist two number $x_- < 0 < x_+$, which both depend on S and δ , such that

- (i) $R_0(x_\pm) + S(x_\pm) = \pm\delta$,
- (ii) $R_0(x) + S(x) < -\delta$ for $x < x_-$,
- (iii) $R_0(x) + S(x) > +\delta$ for $x > x_+$,
- (iv) $\frac{1}{2}R'_0(0) < R'_0(x) + S'(x) < 2R'_0(0)$ for $x_- < x < x_+$,

Notice that the properties of R_0 implies that the set of admissible correctors is not empty for all sufficiently small δ .

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

Lemma 10. *Let S be δ -admissible and $G = \mathcal{G}(S)$. Then we have*

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

for some constant D independent of S and δ .

Proof. The first assertion is a consequence of $\|G\|_\infty \leq 1 + C_\Psi$. Since S is δ -admissible, we 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

$$\frac{1}{2R'_0(0)}\delta \leq |x_{\pm}| \leq \frac{2}{R'_0(0)}\delta, \quad \text{supp } G \subseteq \frac{2}{R'_0(0)}[-\delta, \delta]. \quad (13)$$

Using the Taylor estimate

$$|R'_0(x) + S'(x) - R'_0(0) - S'(0)| \leq (\|R''_0\|_{\infty} + \|S''\|_{\infty})|x|, \quad (14)$$

we also verify that

$$\left| x_{\pm} \mp \frac{\delta}{R'_0(0) + S'(0)} \right| \leq \frac{|x_{\pm}|^2}{2} \frac{\|R''_0\|_{\infty} + \|S''\|_{\infty}}{R'_0(0) + S'(0)} \leq 4\delta^2 \frac{\|R''_0\|_{\infty} + \|S''\|_{\infty}}{R'_0(0)^3}. \quad (15)$$

A direct computation now yields

$$\int_{\mathbb{R}} G(x) dx = \int_{x_-}^{x_+} \Psi'_\delta(R_0(x) + S(x)) dx - \int_{x_-}^{x_+} \text{sgn}(x) dx = \int_{-\delta}^{\delta} \Psi'_\delta(r) \frac{dr}{z(r)} - |x_+ + x_-|, \quad (16)$$

where $z(R_0(x) + S(x)) = R'_0(x) + S'(x)$ for all $x \in [x_-, x_+]$. Thanks to (14), 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

$$\left| \int_{-\delta}^{\delta} \Psi'_\delta(r) \frac{dr}{z(r)} \right| \leq \int_{-\delta}^{\delta} |\Psi'_\delta(r)| \frac{|z(r) - z(0)|}{z(r)z(0)} dr \leq D\delta \frac{(|x_+| + |x_-|)(\|R''_0\|_{\infty} + \|S''\|_{\infty})}{R'_0(0)^2}.$$

and combining this with (13), (15) and (16) gives

$$\left| \int_{\mathbb{R}} G(x) dx \right| \leq D\delta^2 \frac{\|R''_0\|_{\infty} + \|S''\|_{\infty}}{R'_0(0)^3}. \quad (17)$$

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

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

we find a constant D , which depends only on c_0 and c_1 , such that $\|R''_0\|_{\infty} \leq D$. The second and third assertion are now direct consequences of these observations and the estimates (15) and (17). \square

Corollary 11. *There exists a constant $C_{\mathcal{G}}$, which is independent of δ , such that*

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

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

Proof. Thanks to Lemma 10 and the properties of \mathcal{A} , we find some constant D such that

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

see Figure 4 for an illustration. The first estimate is now a consequence of the trivial estimate $|\int_{\mathbb{R}} G(x) dx| \leq |\text{supp } G| \|G\|_{\infty} \leq D\delta$, whereas the second one follows from

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

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

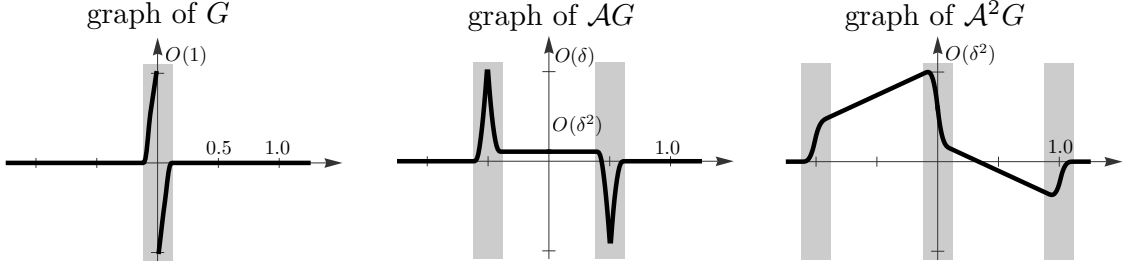


Figure 4: Properties of $G = \mathcal{G}(S)$ for δ -admissible S . The shaded regions indicate intervals with length of order $O(\delta)$.

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 $\|\mathcal{A}^2 G\|_\infty \leq D(1 + \|S''_\infty\|)\delta$. This bound is still sufficient to establish a fixed point argument, but provides only a corrector S of order $O(\delta)$. Recall, however, that Lemma 6 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 12. *There exists a constant C_L independent of δ such that*

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

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

Proof. According to Lemma 10, there exists a constant D , such that $G_\ell(x) = 0$ for all x with $|x| \geq D\delta$. For $|x| \leq D\delta$, we use Taylor expansions for $S_1 - S_2$ at $x = 0$ to find

$$|S_2(x) - S_1(x)| \leq \|S'_2 - S'_1\|_\infty |x| + \|S''_2 - S''_1\|_\infty |x|^2,$$

where we used that $S_2(0) - S_1(0) = 0$. Combining this estimate with the upper bounds for $|\Psi''_\delta|$ gives

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

and hence the desired estimate for $\|G_2 - G_1\|_\infty$. We also have

$$\|\mathcal{A}^2 G_1 - \mathcal{A}^2 G_2\|_\infty \leq \|\mathcal{A} G_1 - \mathcal{A} G_2\|_\infty \leq |\text{supp}(G_2 - G_1)| \|G_2 - G_1\|_\infty \leq D\delta \|G_2 - G_1\|_\infty,$$

and this completes the proof. \square

3.4 Fixed point argument

Now we have prepared all ingredients to establish a suitable fixed point argument in the space

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

with constants

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

Lemma 13. *For all sufficiently small δ there exists an operator*

$$\mathcal{T} : \mathbf{X}_\delta \rightarrow \mathbf{X}_\delta$$

such that for any $S \in \mathbf{X}_\delta$ we have

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

for some $\eta(S) \in \mathbb{R}$ with $|\eta(S)| \leq C_0 \delta^2$.

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

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

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

$$\delta_0 := \frac{1}{2} \min \left\{ \frac{d_0}{2\frac{D_2}{d_0} + C_1}, x_0 d_0, \sqrt{\frac{r_0}{C_0}}, r_0 \right\}, \quad x_\delta := \frac{2}{d_0} \delta$$

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

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

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 easily verify that S is δ -admissible.

Step 2: We next show that \mathbf{X}_δ is invariant under \mathcal{T} for $\delta < \delta_0$. Since each $S \in \mathbf{X}_\delta$ is δ -admissible, Corollary 11 yields

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

and $\|\mathcal{G}(S)\|_\infty \leq 1 + C_\Psi$ holds by definition of \mathcal{G} and Assumption 1. Lemma 9 now provides $\mathcal{T}(S)$ and $\eta(S)$, as well as the estimates

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

and $|\eta(S)| \leq C_0 \delta^2$. In particular, we have $\mathcal{T}(S) \in \mathbf{X}_\delta$. □

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

Proof. We equip \mathbf{X}_δ with the norm $\|S\|_\# = \|S\|_\infty + \|S'\|_\infty + \delta \|S''\|_\infty$, which is, for fixed δ , equivalent to the standard norm. For given $S_1, S_2 \in \mathbf{X}_\delta$, we now employ the estimates from Lemma 9 and Lemma 12. This gives

$$\begin{aligned} \|\mathcal{T}(S_2) - \mathcal{T}(S_1)\|_\# &\leq C_M \left(\|\mathcal{A}^2 \mathcal{G}(S_2) - \mathcal{A}^2 \mathcal{G}(S_1)\|_\infty + \|\mathcal{AG}(S_2) - \mathcal{AG}(S_1)\|_\infty + \delta \|\mathcal{G}(S_2) - \mathcal{G}(S_1)\|_\infty \right) \\ &\leq C_M C_L \delta \|S_2 - S_1\|_\#, \end{aligned}$$

and we conclude that \mathcal{T} is contractive with respect to $\|\cdot\|_\#$ provided that $\delta < 1/(C_M C_L)$. The claim is now a direct consequence of the Banach Fixed Point Theorem. □

We now show that different anchors provide different waves.

Lemma 15. *Let (R_0, μ_0) and $(\tilde{R}_0, \tilde{\mu}_0)$ be two different travelling waves for $\delta = 0$ and the same value of c , and (S, η) and $(\tilde{S}, \tilde{\eta})$ be the corresponding correctors provided by Theorem 14. Then $R_0 + S_0$ and $\tilde{R}_0 + \tilde{S}$ are different.*

Proof. By construction, we have

$$S, \tilde{S} \in \mathcal{U}_1 := \text{span}\{Y_1, Y_2, 1\} \oplus \mathcal{L}^2(\mathbb{R}),$$

while Proposition 2 guarantees that

$$R_0 - \tilde{R}_0 \in \mathcal{U}_2 := \text{span}\{\sin(k_c \cdot), 1 - \cos(k_c \cdot)\}.$$

The claim now follows since $\mathcal{U}_1 \cap \mathcal{U}_2 = \{0\}$. □

4 Change in the kinetic relation

In this final section we show that the kinetic relation does not change to order $O(\delta)$. To this end we denote by R_δ a travelling wave solution to (2) as provided by Theorem 3. The corresponding *configurational force*, cf. [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 16. *Let R_δ be a travelling 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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