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Existence of subsonic heteroclinic waves for the Frenkel-Kontorova model with piecewise quadratic on-site potential

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Abstract. We give an existence proof for heteroclinic wave solutions to the Frenkel-Kontorova model of dislocation dynamics. The on-site potential is assumed to be piecewise quadratic. The framework employed here allows us to determine explicitly a regime of subsonic velocities for which travelling waves exist.

AMS classification scheme numbers: 37K60, 34C37, 58F03, 70H05

1. Introduction

In 1938, Frenkel and Kontorova proposed a fundamental model for dislocation dynamics [1]. Namely, they describe the motion of a dislocation by the one-dimensional system

$$c^2u''(z) = u(z+1) - 2u(z) + u(z-1) - g'(u(z)) \qquad \text{a.e.,} \qquad z \in \mathbb{R}. \quad (1)$$

Here u is the deformation, and g is a periodic on-site potential.

In dislocation dynamics, a particular interest is in heteroclinic waves, that is, waves with asymptotic states in different wells of g as $z \to \pm\infty$. In 1963, Atkinson and Cabrera [2] gave a formal representation of a heteroclinic wave solution to (1) augmented by an additional external force acting on each atom. Atkinson and Cabrera consider the special case of a piecewise quadratic on-site potential

$$g(u) = \frac{1}{2}\alpha \, \min\{(u-1)^2, (u+1)^2\} \quad (2)$$

with $\alpha > 0$. Numerous papers have followed this approach for related models. However, it has been noted that a formal expression such as the one given in [2] is not necessarily a solution of the original equation (here (1), possibly augmented by external forcing) [3, 4]. This is not a mere mathematical issue; doubts about the existence of heteroclinic waves have been expressed for some time [5, 6]. In particular, Peyrard and Kruskal [6] give convincing numerical evidence that slow waves on a finite domain cannot travel with constant velocity, but have to slow down. It is likely that the (non-)existence of travelling heteroclinic waves depends sensitively on the wave speed c.

Given that the Frenkel-Kontorova model is the most fundamental model of dislocation dynamics, this situation requires a rigorous clarification. We give here what appears to be the first rigorous proof of the existence of heteroclinic waves for the classic model (1) with on-site potential g as in (2). As for the existing body of work in physics, a key step is to verify that a representation of a solution candidate in Fourier space has a sign (distribution); see Section 2 and in particular Equation (4) below for the precise formulation. The rational behind the argument is that (1) simplifies when one assumes a given distribution of the atoms into the wells of the on-site potential g. One then has to verify that the solution obtained from the simplified equation satisfies the assumed sign distribution, and this is what we call a sign condition. It is acknowledged in the physics literature that the verification of a sign condition is crucial [3, 4]; Earmme and Weiner write on the simplified equation "It is important to note that [this equation] is only valid under the assumption that, in the continued steady motion of the dislocation, the nth atom remains in the $(n+1)$st well for $t > 0$" [3].

In the framework of the established approach, we could not find any rigorous verification of such a sign distribution in the literature. A reason is that the traditional approach represents the solution candidate as a formal expression obtained from its Fourier or Laplace image. Since the Fourier / Laplace image of the solution candidate necessarily has singularities, distorted integration paths and a limit passage are used for the integration of the inverse transformations. The solution obtained in this way is then evaluated numerically to verify or disprove the sign condition. This evaluation is still nontrivial, and further approximations are made (e.g., all but two residues are ignored [3]).

We seek to present a mathematically rigorous analysis. To this behalf, we adopt a new approach [7], where the sign condition can be verified rigorously. We emphasise again that, while this may sound as a mere technical aspect, this step is essential for the analysis: if the sign condition is violated, then a solution candidate constructed with either approach cannot be a solution of (1). The approach employed here incorporates essential physical information, namely singularities in the Fourier image arising from the dispersion function, explicitly into account. This makes it possible to avoid the distortion and limit passage of integration paths of the traditional approach and may be of independent interest. It is noteworthy that while some technical aspects (collected in Section 5) are tedious to prove, the arguments are mathematically simple and natural.

The approach advocated here to find heteroclinic solutions (albeit at present only in special situations) is applicable in situations where common variational methods would be delicate to use, since the solution corresponds to a front connecting periodic orbits. Similarly, the solutions are not small, so local methods such as centre manifold reduction do not readily apply in the situation under consideration (cf. [8] and references therein).

Besides being rigorous, the approach taken here also has the advantage that, unlike the formal argument of [2], it allows us to explicitly quantify a parameter regime, in particular a regime of velocities c, for which such waves exist. The waves obtained here are rather fast, but subsonic. To be specific, we work in a regime of subsonic velocities where the dispersion relation has exactly one positive solution. This restriction is not of fundamental nature; an extension to lower velocities (possibly with several positive roots of the dispersion function) should be possible. However, it seems likely that travelling wave solutions may not exist at low velocities, as suggested by the analysis of Peyrard and Kruskal [6]. We remark that our analysis proving the existence of travelling waves is confined to high subsonic velocities, while the numerical investigation [6] questioning the existence of travelling waves focuses on the regime of slow waves. Thus, our findings are not in contradiction with the numerical investigation of [6].

This dichotomy of fast and slow subsonic velocities seems to merit a further investigation. The cited result for the Fermi-Pasta-Ulam chain with piecewise quadratic interaction potential [7] was shown for a range of velocities with only one resonant mode (phonon), as it is the case in the present paper. Recently, it has been proved [9] that at lower velocities, specifically in a situation with three resonant phonons, no travelling wave with a single interface can exist. We conjecture that a similar result holds true for the system studied here.

The precise analysis of the velocities intervals of existence and nonexistence of single-interface travelling waves is an open problem, both for the Frenkel-Kontorova and the Fermi-Pasta-Ulam chain. In particular, it is at present not known what the lower velocity bound for existence of travelling waves is. One would generically expect nonexistence to prevail at low velocities. But it is well possible that for suitably tuned settings travelling waves exist at low velocities. Indeed, Melvin, Champneys and Pelinovsky [10] proved the existence of slow non-radiating travelling solitons for suitable parameters in the structurally similar one-dimensional Salerno model.

While the focus in this article is on heteroclinic waves, since those waves represent in the context of this article moving dislocations, we would also like to mention the related seminal analysis of homoclinic solutions by MacKay and Aubry [11], where the first rigorous result on presence and stability of of coherent spatially localised temporally periodic solutions was obtained. Also, we should point out that the two-well nature (2) of the on-site potential chosen already by Atkinson and Cabrera [2] is not restrictive. While the on-site potential should be thought as periodic [1], solutions of the two-well problem are also solutions of a suitable periodic extension of the two-well setting. The framework employed here, unlike the formal setting, allows to make this statement rigorous; see Corollary 4.7.

For diffusive lattice models, comparable existence results for travelling fronts are available. In particular, the methods employed by Coutinho and Fernandez [12] are in spirit similar to the approach taken here. There, piecewise affine lattice models are studied, with the evolution being dissipative rather than conservative. There as here, the existence of travelling waves is obtained by verifying sign conditions. For this dissipative system, the fronts can under suitable assumptions also be shown to be nonlinearly stable.

2. Mathematical setup and solution strategy

We introduce the discrete Laplace operator $\Delta_{\mathrm{D}}\, u(z) := u(z+1) - 2u(z) + u(z-1)$ for $u\colon \mathbb{R} \to \mathbb{R}$ and rewrite (1) with (2) as

$$c^2 u''(z) - \Delta_{\mathrm{D}}\, u(z) + \alpha\, u(z) = \alpha\, \mathrm{sgn}(u(z)), \tag{3}$$

for $u(z) \neq 0$; here $\mathrm{sgn}(u)$ is the sign function.

We recall that by a *heteroclinic wave*, we mean here a wave with asymptotic states in different wells of g as $z \to \pm\infty$.

If one assumes that there is such a wave u with the property that

$$u(z) < 0 \text{ for } z < 0 \qquad \text{and} \qquad u(z) > 0 \text{ for } z > 0, \tag{4}$$

then the nonlinear equation (3) becomes inhomogeneous,

$$c^2 u''(z) - \Delta_{\mathrm{D}}\, u(z) + \alpha\, u(z) = \alpha\, \mathrm{sgn}((z)). \tag{5}$$

This equation is a forward-backward difference-differential equation. A natural approach is to employ the Fourier transform, which we define, whenever the integral exists, as

$$\mathscr{F}[f](\zeta) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x) e^{-i\zeta x} \mathrm{d}x.$$

We show in this article that a point-symmetric solution to (3) exists. Since it then suffices to consider odd f, this symmetry allows us to work with Fourier sine transform

$$\mathscr{F}_s\,[f]\,(\zeta) := \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} f(x) \sin(\zeta x) \mathrm{d}x$$

interchangeably with the Fourier transform, because $\mathscr{F}_s\,[f]\,(\zeta) = i\mathscr{F}[f]$ for odd f.

The Fourier image of (5) has singularities on the real axis, as spelt out below. Thus, a rigorous derivation of u as the inverse of the Fourier image is non-trivial. Atkinson and Cabrera consequently represent in [2] the solution of (5) as a formal Fourier sum. However, it is both trivial and crucial to observe that a solution of (5) is *not* a solution of the original simplified Frenkel-Kontorova model (3) we want to solve *unless* the sign condition (4) holds. Reading off a sign of a function where only the Fourier image is known is, however, a very hard problem, even more so if the Fourier expression is only formal. Given that the Frenkel-Kontorova model is the most fundamental model of dislocation dynamics, it seems desirable to have a clean derivation of the existence of a solution for an explicitly known parameter regime. We adopt a surprisingly simple approach, recently introduced in [7]. Namely, we split the solution in two parts by writing

$$u = u_p - r, \tag{6}$$

where u_p is an explicit *profile* given below in Equation (13) and $r \in L^2(\mathbb{R})$ is a *corrector*. The profile collects all contributions where the Fourier image of the solution is singular; this information can be read off from the dispersion function. The corrector and its

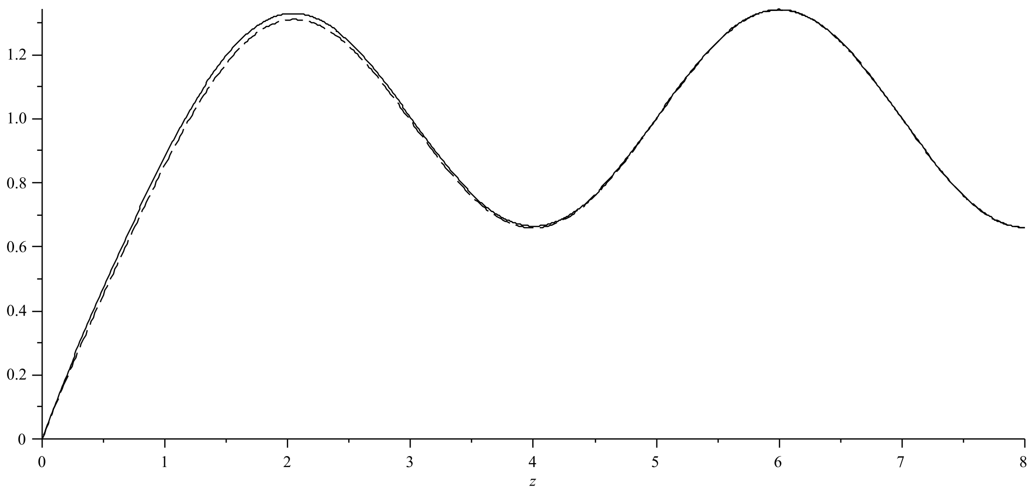

Figure 1. A plot of the profile $u_p(z)$ (dashed line) and of the solution $u = u_p - r$ (solid line) for $z > 0$, for the parameters $c^2 = 0.9$, $\alpha = c^2 \cdot \frac{\pi^2}{4} - 2$ and $k_0 = \frac{\pi}{2}$, the situation of Theorem 4.1. Shown is only the plot for $z > 0$; $u_p(z)$ is point symmetric with respect to the origin.

Fourier representation are then shown to be in $L^2(\mathbb{R})$. Specifically, Equation (3) shall be decomposed into

$$c^2 u_p''(z) - \Delta_{\mathrm{D}}\, u_p(z) + \alpha\, u_p(z) - \alpha \operatorname{sgn}(u_p(z)) = \Phi(z), \tag{7}$$

$$c^2 r''(z) - \Delta_{\mathrm{D}}\, r(z) + \alpha\, r(z) = \Phi(z). \tag{8}$$

Suppose for the moment that we are given a solution to (7)–(8). Then $u = u_p - r$ is a solution to (3) if and only if

$$\operatorname{sgn}(u_p(z)) \stackrel{!}{=} \operatorname{sgn}(u_p(z) - r(z)) = \operatorname{sgn}(u(z)) \stackrel{!}{=} \operatorname{sgn}(z). \tag{9}$$

Thus, the strategy is as follows: starting with a suitable profile u_p, Φ is determined via (7); we then show that there exists a solution r to (8) in $L^2(\mathbb{R})$. The main technical work is then to show that $\operatorname{sgn}(u_p(z)) = \operatorname{sgn}(u_p(z) - r(z))$ holds.

We claim that, if the Fourier transforms of r and Φ exist, Equation (8) reads in Fourier space

$$\mathscr{F}_s\left[c^2 r'' - \Delta_{\mathrm{D}}\, r + \alpha r\right](\zeta) = \left[-c^2\zeta^2 - 2\cos(\zeta) + (2+\alpha)\right] \mathscr{F}_s[r](\zeta) = \mathscr{F}_s[\Phi](\zeta),$$

or compactly

$$D(\zeta) \cdot \mathscr{F}_s[r](\zeta) = \mathscr{F}_s[\Phi](\zeta), \tag{10}$$

where

$$D(\zeta) = \alpha - c^2\zeta^2 + 2\left[1 - \cos(\zeta)\right] = \alpha - c^2\zeta^2 + 4\left[\sin\left(\frac{1}{2}\zeta\right)\right]^2 \tag{11}$$

is the *dispersion function*. The above calculation is elementary, using only integration by parts and the trigonometric identity $\sin(\varphi+\psi) + \sin(\varphi-\psi) = 2\sin(\varphi)\cos(\psi)$.

Thus, if the Fourier transform of r and Φ exists, then (8) is equivalent to (10). Oscillations of the solution will be represented in the profile; they can be read off as

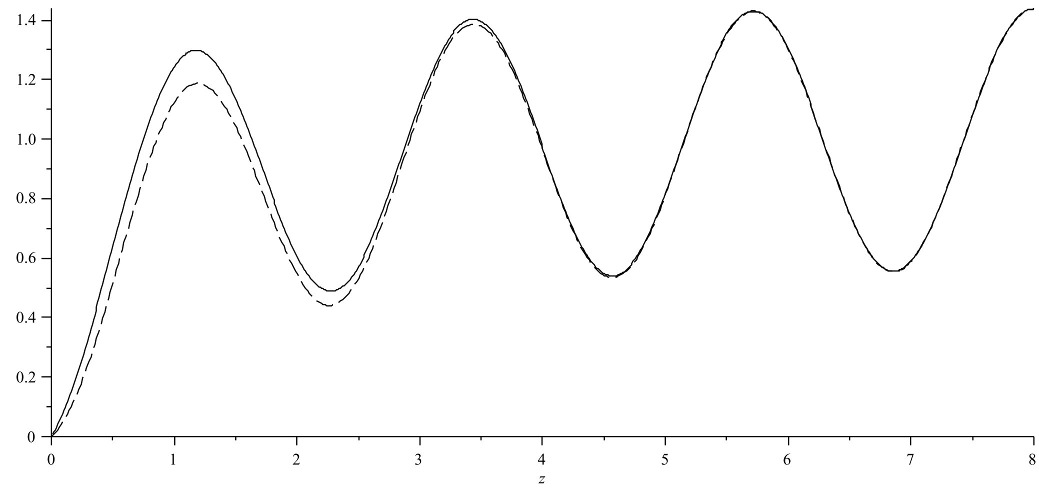

Figure 2. A plot of the profile $u_p(z)$ (dashed line) and of the solution $u = u_p - r$ (solid line) for $z > 0$, for $c^2 = 0.8$ and $\alpha = \frac{49}{80}\pi^2 - 2 - \sqrt{2 + \sqrt{2}} \approx 2.197$ ($u_p(z)$ is point symmetric with respect to the origin). The corresponding value for k_0 is $k_0 = \frac{7}{8}\pi$. We note that this is *not* in the range of parameters covered by Theorem 4.1 (i), and in fact far from that regime, where $k_0 = \frac{\pi}{2}$ is assumed. While the rigorous result may not directly applicable, an approximate solution can be computed by numerically inverting the Fourier transform of the corrector r. Then $u = u_p - r$ satisfies the crucial condition (9); u is a solution within numerical precision. Thus, the solution philosophy, splitting the solution as in (6), is applicable within a neighbourhood of the parameter choice yielding $k_0 = \frac{\pi}{2}$, as stated in Theorem 4.1 (ii).

solutions of the dispersion relation $D(\zeta) = 0$. As stated in the introduction, we choose the subsonic velocity c so large that only one frequency k_0 is supported, namely

$$c^2 k_0^2 - \alpha = 2\left(1 - \cos\left(k_0\right)\right). \tag{12}$$

It is immediate that for suitable fixed c and α, only one positive zero of D exists, namely $D(k) = 0$ for $k > 0$ if and only if $k = k_0$, where $k_0 = k_0(\alpha, c)$.

3. Profile and corrector

We now define the *profile* u_p by setting

$$u_p(z) := \operatorname{sgn}(z)\left[A\left(1 - e^{-\beta|z|}\right) + B\left(1 - \cos\left(k_0 z\right)\right)\right], \tag{13}$$

where A, B and β are initially free parameters. We note that the profile is symmetric with respect to the origin, and it thus suffices below to analyse the behaviour of u_p for positive values; the behaviour for negative values follows then by symmetry. We determine the values of A and B as follows. First, we ensure that the Fourier transform of $u(z) - \operatorname{sgn}(z)$ exists. To this behalf, we require that

$$\lim_{z\to\infty} \lim_{T\to\infty} \frac{1}{T} \int_z^{z+T} u_p(s)\,\mathrm{d}s = 1;$$

this implies

$$A + B = 1. \tag{14}$$

Second, we require that the right-hand side $c^2 u_p''(z) - \Delta_\mathrm{D}\, u_p(z) + \alpha\,(u_p(z) - \operatorname{sgn}(z))$ of (7) is continuous at 0. Since only the term $c^2 u_p''(z) - \alpha \operatorname{sgn}(z)$ jumps, we find the condition

$$\lim_{z \searrow 0} \left[c^2 \left(-A\beta^2 e^{-\beta z} + B k_0^2 \cos(k_0 z) \right) - \alpha \operatorname{sgn}(z) \right] = 0$$

and therefore from (14)

$$A = \frac{c^2 k_0^2 - \alpha}{c^2\,(\beta^2 + k_0^2)} \qquad \text{and} \qquad B = \frac{\alpha + \beta^2 c^2}{c^2\,(\beta^2 + k_0^2)}. \tag{15}$$

Lemma 3.1 *Suppose* $k_0 \in (0, \pi)$. *Let* $u_p(z) = \operatorname{sgn}(z) \left[A \left(1 - e^{-\beta |z|} \right) + B \left(1 - \cos(k_0 z) \right) \right]$, *as in (13), with parameters* A *and* B *as in (15) and* β *as defined by (18) below. Then the following holds.*

(i) The Fourier sine transform of the left-hand side of (7) exists.

(ii) If Φ *is defined through (7), then (8) can be solved for* $r \in L^2(0, \infty)$.

The assumption is actually stronger than required. For the conclusion of this lemma, it would suffice to require the right-hand side of (18) below to be positive.

Proof: We start by computing $\mathscr{F}_s[\Phi]$ with Φ from (7), i.e.,

$$\mathscr{F}_s \left[c^2 u_p'' - \Delta_\mathrm{D}\, u_p + \alpha (u_p - \operatorname{sgn}) \right].$$

Only $\Delta_\mathrm{D}\, u_p$ is slightly cumbersome to compute, and one finds

$$\begin{aligned} \left[\Delta_\mathrm{D}\, u_p(z) \right]\Big|_{z>0} &= -2A e^{-\beta z} \left[\cosh(\beta) - 1 \right] - 2B \cos(k_0 z) \left[\cos(k_0) - 1 \right] \\ &\quad - \mathbf{1}_{[0,1]} \Bigg(2A \left[1 - \cosh(\beta(z-1)) \right] + 2B \left[1 - \cos(k_0(z-1)) \right] \Bigg), \end{aligned}$$

where $\mathbf{1}_{[0,1]}$ is the indicator function of the interval $[0, 1]$.

A straightforward but lengthy calculation shows that for $z > 0$ (the second equality uses (14) for the constant terms and the dispersion function for the oscillatory parts in the profile)

$$\begin{aligned} \mathscr{F}_s[\Phi](\zeta) &= \mathscr{F}_s \left[c^2 u_p'' - \Delta_\mathrm{D}\, u_p + \alpha\,(u_p - \operatorname{sgn}) \right](\zeta) \\ &= \mathscr{F}_s \Big[A e^{-\beta z} \left(-\beta^2 c^2 - \alpha + 2 \left[\cosh(\beta) - 1 \right] \right) \\ &\qquad\quad + \mathbf{1}_{[0,1]} \left[2 - 2A \cosh(\beta(z-1)) - 2B \cos(k_0(z-1)) \right] \Big](\zeta) \\ &= A\, \frac{\zeta}{\beta^2 + \zeta^2} \left(-\beta^2 c^2 - \alpha + 2 \left[\cosh(\beta) - 1 \right] \right) \\ &\qquad + \Bigg[2 \cdot \frac{1 - \cos(\zeta)}{\zeta} - 2A\, \frac{\zeta}{\beta^2 + \zeta^2} \left[\cosh(\beta) - \cos(\zeta) \right] \\ &\qquad + 2B\zeta\, \frac{\cos(\zeta) - \cos(k_0)}{\zeta^2 - k_0^2} \Bigg] \\ &= 2 \cdot \frac{1 - \cos(\zeta)}{\zeta} - A\, \frac{\zeta}{\beta^2 + \zeta^2} \left[\beta^2 c^2 + \alpha + 2(1 - \cos(\zeta)) \right] \\ &\qquad + 2B\zeta\, \frac{\cos(\zeta) - \cos(k_0)}{\zeta^2 - k_0^2}. \end{aligned} \tag{16}$$

We rewrite this, using $A + B = 1$ from (14) and splitting the first term,

$$\begin{aligned}\mathscr{F}_s[\Phi](\zeta) &= -A\frac{\zeta}{\beta^2+\zeta^2}\left[\beta^2c^2+\alpha\right] \\ &\quad + 2A\frac{1-\cos(\zeta)}{\zeta}\left[1-\frac{\zeta^2}{\beta^2+\zeta^2}\right] + 2B\left[\zeta\,\frac{\cos(\zeta)-\cos(k_0)}{\zeta^2-k_0^2}+\frac{1-\cos(\zeta)}{\zeta}\right] \\ &= \frac{-A}{\beta^2+\zeta^2}\left[(\beta^2c^2+\alpha)\zeta - 2\frac{1-\cos(\zeta)}{\zeta}\cdot\beta^2\right] \\ &\quad + 2B\left[\zeta\,\frac{\cos(\zeta)-\cos(k_0)}{\zeta^2-k_0^2}+\frac{1-\cos(\zeta)}{\zeta}\right]. \qquad (17)\end{aligned}$$

We now show that β can be chosen such that $\mathscr{F}_s[\Phi](k_0) = 0$; this is a requirement to remove the singularity stemming from the dispersion function.

By de L'Hôpital's rule,

$$\lim_{\zeta\to k_0}\frac{2\zeta\left(\cos(\zeta)-\cos(k_0)\right)}{\zeta^2-k_0^2} = -\sin(k_0).$$

Thus inserting $\zeta = k_0$ into (16) and using (12) and the definitions of A and B from (15) in the second line yields

$$\begin{aligned}\mathscr{F}_s[\Phi](k_0) &= \frac{2(1-\cos(k_0))}{k_0} - A\frac{k_0}{\beta^2+k_0^2}\left[\beta^2c^2+\alpha+2\left(1-\cos(k_0)\right)\right] - B\sin(k_0) \\ &= \frac{c^2k_0^2-\alpha}{k_0} - \frac{c^2k_0^2-\alpha}{c^2\left(\beta^2+k_0^2\right)}\cdot\frac{k_0}{\beta^2+k_0^2}\left[\beta^2c^2+\alpha+c^2k_0^2-\alpha\right] \\ &\quad - \frac{\alpha+\beta^2c^2}{c^2\left(\beta^2+k_0^2\right)}\sin(k_0) \\ &= \frac{c^2k_0^2-\alpha}{k_0} - \frac{c^2k_0^2-\alpha}{c^2\left(\beta^2+k_0^2\right)}\cdot k_0\,c^2 - \frac{(\alpha+\beta^2c^2)\sin(k_0)}{c^2\left(\beta^2+k_0^2\right)} \\ &= \frac{(c^2k_0^2-\alpha)\,c^2\beta^2}{c^2(\beta^2+k_0^2)k_0} - \frac{(\alpha+\beta^2c^2)\,k_0\sin(k_0)}{c^2\left(\beta^2+k_0^2\right)k_0}.\end{aligned}$$

Setting this equal to zero we obtain

$$\beta^2\cdot c^2\left[\left(c^2k_0^2-\alpha\right)-k_0\sin(k_0)\right] = \alpha k_0\sin(k_0),$$

so that, employing (12) once more,

$$\beta^2 = \frac{\alpha}{c^2}\cdot\frac{k_0\sin(k_0)}{2-2\cos(k_0)-k_0\sin(k_0)}. \qquad (18)$$

The right-hand side of (18) is positive in particular for

$$0 < k_0 < \pi. \qquad (19)$$

To summarise, we have seen that while the condition (19) holds, there exists a $\beta > 0$ such that

$$\mathscr{F}_s[\Phi](k_0) = 0.$$

As the root of the dispersion function D at k_0 is simple, we find that the singularity of $D(\zeta)^{-1}\mathscr{F}_s[\Phi](\zeta)$ at $\zeta = k_0$ is removable. It is clear that this function decays for $\zeta \to \infty$

at least like ζ^{-3} (in fact it decays like ζ^{-5}, as we will see in the proof of Lemma 4.5). This shows that $D(\zeta)^{-1}\mathscr{F}_s[\Phi](\zeta)$ is continuous and in $L^1(0,\infty)$ and that its inverse Fourier sine transform exists. □

We remark that when varying k_0 in the range set in (19), the limits of β are

$$\beta \to 0 \quad \text{for} \quad k_0 \to \pi \qquad \text{and} \qquad \beta \to \infty \quad \text{for} \quad k_0 \to 0$$

(observe for the limit at 0 that the quadratic terms in the denominator cancel). In fact, β is a monotone function of k_0. (We should point out that k_0 is not an independent parameter but determined by the choices of α and c.)

With the expression (18) for β at hand, some expressions can be reformulated so that future calculations simplify. For immediate use, we will also derive an explicit expression for $\mathscr{F}_s[r](\zeta)$. We start by computing the terms for B defined in (15),

$$\alpha + \beta^2 c^2 = \alpha\left(1 + \frac{k_0 \sin(k_0)}{2 - 2\cos(k_0) - k_0\sin(k_0)}\right) = \frac{\alpha\,(2 - 2\cos(k_0))}{2 - 2\cos(k_0) - k_0 \sin(k_0)}$$

and

$$\begin{aligned} c^2\left(\beta^2 + k_0^2\right) &= c^2 k_0^2 + \frac{\alpha \cdot k_0 \sin(k_0)}{2 - 2\cos(k_0) - k_0\sin(k_0)} \\ &= \frac{c^2k_0^2\,(2 - 2\cos(k_0) - k_0\sin(k_0)) + \alpha k_0 \sin(k_0)}{2 - 2\cos(k_0) - k_0\sin(k_0)} \\ &= \frac{c^2k_0^2\,(2 - 2\cos(k_0)) + k_0\sin(k_0)\,(\alpha - c^2k_0^2)}{2 - 2\cos(k_0) - k_0\sin(k_0)} \\ &= \frac{(2 - 2\cos(k_0))\,(c^2k_0^2 - k_0\sin(k_0))}{2 - 2\cos(k_0) - k_0\sin(k_0)}. \end{aligned}$$

Combining the two, we obtain

$$B = \frac{\alpha}{c^2k_0^2 - k_0\sin(k_0)}. \tag{20}$$

This implies an alternative representation of A via (14). Indeed, one sees immediately with (12) that

$$A = 1 - \frac{\alpha}{c^2k_0^2 - k_0\sin(k_0)} = \frac{2 - 2\cos(k_0) - k_0\sin(k_0)}{c^2k_0^2 - k_0\sin(k_0)}. \tag{21}$$

(This shows $A \to 0$ for $k_0 \to 0$ and $A \to \frac{4}{4+\alpha}$ for $k_0 \to \pi$.) Also, again with (12) and then (21),

$$\begin{aligned} \beta^2 + k_0^2 &= \frac{\alpha k_0 \sin(k_0)}{c^2\,(2 - 2\cos(k_0) - k_0\sin(k_0))} + k_0^2 \\ &= \frac{c^2k_0^2\,(2 - 2\cos(k_0)) - (c^2k_0^2 - \alpha)\,k_0\sin(k_0)}{c^2\,(2 - 2\cos(k_0) - k_0\sin(k_0))} \\ &= (2 - 2\cos(k_0))\,\frac{c^2k_0^2 - k_0\sin(k_0)}{c^2\,(2 - 2\cos(k_0) - k_0\sin(k_0))} = \frac{2 - 2\cos(k_0)}{c^2 \cdot A}. \end{aligned}$$

Altogether, we obtain from (8) the following expression for the corrector in Fourier space.

Corollary 3.2 *In the situation of Lemma 3.1, the Fourier transform of the corrector r is given by*

$$\mathscr{F}_s\left[r\right](\zeta) = \frac{1}{D(\zeta)} \cdot \frac{2\alpha}{\alpha k_0 \sin\left(k_0\right) + c^2\zeta^2 \left(2 - 2\cos\left(k_0\right) - k_0 \sin\left(k_0\right)\right)} \cdot \cdot \left[\left(2 - 2\cos\left(k_0\right)\right) \cdot \zeta \frac{\cos(\zeta) - \cos\left(k_0\right)}{\zeta^2 - k_0^2} + k_0 \sin\left(k_0\right) \frac{\left(1 - \cos(\zeta)\right)}{\zeta}\right]. \tag{22}$$

4. The main result

The expressions simplify considerably for $k_0 = \frac{\pi}{2}$, the midpoint of the interval for k_0 of (19) and Lemma 3.1. We thus restrict the detailed analysis to this case and write $p := \frac{\pi}{2}$. For this one-parameter family, the relation (12) shows

$$\alpha = c^2 k_0^2 - 2\left(1 - \cos\left(k_0\right)\right) = c^2 p^2 - 2, \tag{23}$$

so c is now the only free parameter. To ensure $\alpha > 0$ we can therefore consider only velocities c with $c^2 p^2 - 2 > 0$, i.e., $c^2 > 2p^{-2} \approx 0.81057$. The upper bound is the sound speed $c_0 = 1$. We remark that the continuous dependence on the parameters implies that the existence results of Theorem 4.1 below can be extended to nearby values of the chosen parameters.

We obtain from (21) and (20) combined with (23)

$$A = \frac{2 - p}{c^2 p^2 - p} \qquad \text{and} \qquad B = \frac{c^2 p^2 - 2}{c^2 p^2 - p}. \tag{24}$$

The profile u_p from (13) thus has in this special case the form

$$u_p(z) = \operatorname{sgn}(z) \left\{ \frac{2 - p}{c^2 p^2 - p} \left[1 - \exp\left(-|z| \sqrt{\frac{p\left(c^2 p^2 - 2\right)}{c^2(2 - p)}}\right)\right] + \frac{c^2 p^2 - 2}{c^2 p^2 - p} \left[1 - \cos(pz)\right] \right\}, \tag{25}$$

and the dispersion function (11) reduces to

$$D(\zeta) = -c^2\left(\zeta^2 - p^2\right) - 2\cos(\zeta). \tag{26}$$

We then find from (22)

$$\mathscr{F}_s\left[r\right](\zeta) = \frac{1}{D(\zeta)} \cdot \frac{2\left(c^2 p^2 - 2\right)}{p\left(c^2 p^2 - 2\right) + c^2 \zeta^2 (2 - p)} \left[\frac{2\zeta \cos(\zeta)}{\zeta^2 - p^2} + \frac{p(1 - \cos(\zeta))}{\zeta}\right]. \tag{27}$$

The main result of this article is as follows.

Theorem 4.1 *(i) For $k_0 = \frac{\pi}{2}$, let $c^2 \in [0.83, 1]$ and $\alpha > 0$ such that $\alpha = c^2 \frac{\pi^2}{4} - 2$. Then (3) has a solution $u = u_p - r$ with u_p given by (25) and r as in (27) and (30).*

(ii) There exists an open neighbourhood $N \subset \mathbb{R}_+^2$ of the compact set

$$\left\{ \left(c^2, \alpha\right) \in \mathbb{R}_+^2 : c^2 \in [0.83, 1],\ \alpha = \frac{c^2 \pi^2}{4} - 2 \right\},$$

such that for every choice $(c^2, \alpha) \in N$ of parameters, (3) has a solution $u = u_p - r$, with u_p as in Lemma 3.1 and r as in Corollary 3.2.

See Fig. 1 for a plot for item (i) and Fig. 2 for a plot illustrating item (ii). Shown is in both cases the profile u_p and a numerical approximation to the full solution. Fig. 2 shows the situation for $k_0 = \frac{7}{8}\pi$. For this choice of parameters, no analytical proof is available that $u = u_p - r$ satisfies the sign condition (9) and is thus a solution for this relatively large deviation of the parameters (the neighbourhood could be so small that $k_0 = \frac{7}{8}\pi$ is excluded). Yet, a numerical inversion of the Fourier image of r suggests that the sign condition holds even for the choice of parameters made in the plot; thus u can be seen as a solution up to numerical precision.

Before stating the idea of the proof of Theorem 4.1, we mention a direct consequence.

Corollary 4.2 *In the situation of Theorem 4.1, let u be the solution for fixed wave speed c. Then $u(z) + A\sin(k_0 z)$ is also a solution for A small enough.*

So in fact, there is a two-parameter family of solutions, where one parameter is the wave speed c. The proof of this corollary is an immediate consequence of the point symmetry of sin with respect to the origin and the fact that the condition to be verified, sign condition (9), is open.

The idea of the proof of Theorem 4.1 has already been outlined after Equations (7)–(8). Namely, Lemma 3.1 affirms that r from (27) and (30) is well-defined. It thus only remains to see that r is small enough so that the sign condition (9) holds. The proof is rather technical but, in terms of mathematics, completely elementary. It relies on four technical lemmata, which are proved in the following section. The idea is always simple; the arguments rely on good approximations of (components of) the Fourier image of the solution candidate in terms of elementary functions, which can be bounded explicitly.

Lemma 4.3 *Let $I_1 := \left[0, \frac{p}{2}\right]$. Then*

$$\int_{I_1} |\mathscr{F}_s[r](\zeta)| \, \mathrm{d}\zeta \quad \leq \begin{cases} 0.043, & \text{for } c^2 \in [0.9, 1], \\ 0.125, & \text{for } c^2 \in [0.83, 0.9], \end{cases} \tag{28}$$

$$\int_{I_1} \zeta \, |\mathscr{F}_s[r](\zeta)| \, \mathrm{d}\zeta \leq \begin{cases} 0.017, & \text{for } c^2 \in [0.9, 1], \\ 0.035, & \text{for } c^2 \in [0.83, 0.9]. \end{cases} \tag{29}$$

Lemma 4.4 *Let $I_2 := \left[\frac{p}{2}, \frac{3p}{2}\right]$. Then for $c^2 \in [0.83, 1]$*

$$\int_{I_2} |\mathscr{F}_s[r](\zeta)| \, \mathrm{d}\zeta \leq 0.056 \qquad \textit{and} \qquad \int_{I_2} \zeta \, |\mathscr{F}_s[r](\zeta)| \, \mathrm{d}\zeta \leq 0.073.$$

Lemma 4.5 *Let $I_3 := \left[\frac{3p}{2}, \infty\right)$. Then*

$$\int_{I_3} |\mathscr{F}_s[r](\zeta)| \, \mathrm{d}\zeta \quad \leq 0.158 \qquad \text{for } c^2 \in [0.83, 1],$$

$$\int_{I_3} \zeta \, |\mathscr{F}_s[r](\zeta)| \, \mathrm{d}\zeta \leq \begin{cases} 0.34, & \text{for } c^2 \in [0.9, 1], \\ 0.232, & \text{for } c^2 \in [0.83, 0.9]. \end{cases}$$

Lemma 4.6 *For $c^2 \in [0.9, 1]$ and $z \geq 1$, the profile u_p satisfies*

$$u_p(z) \geq 0.34926.$$

For $c^2 \in [0.83, 0.9]$ and $z \geq \frac{3}{2}$, the profile u_p satisfies

$$u_p(z) \geq 0.41139.$$

With these auxiliary statements at hand, it is not hard to prove Theorem 4.1.

Proof of Theorem 4.1: (i) Lemma 3.1 affirms that r from (27) and (30) below is well-defined, so it only remains to see that r is small enough so that the sign condition (9) holds. By definition of the inverse Fourier sine transform,

$$r(z) = \sqrt{\frac{2}{\pi}} \int_0^\infty \mathscr{F}_s[r](\zeta) \sin(\zeta z)\, \mathrm{d}\zeta \quad \text{and} \quad r'(z) = \sqrt{\frac{2}{\pi}} \int_0^\infty \zeta \cdot \mathscr{F}_s[r](\zeta) \sin(\zeta z)\, \mathrm{d}\zeta. \tag{30}$$

Thus, it follows from Lemmata 4.3–4.5,

$$\begin{aligned} \sqrt{\frac{\pi}{2}}\, |r(z)| &\leq \int_0^\infty \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \\ &\leq \begin{cases} 0.043 + 0.056 + 0.158 = 0.257, & c^2 \in [0.9, 1], \\ 0.125 + 0.056 + 0.158 = 0.339, & c^2 \in [0.83, 0.9], \end{cases} \end{aligned} \tag{31}$$

and

$$\begin{aligned} \sqrt{\frac{\pi}{2}}\, |r'(z)| &\leq \int_0^\infty \zeta \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \\ &\leq \begin{cases} 0.017 + 0.073 + 0.34 = 0.43, & c^2 \in [0.9, 1], \\ 0.035 + 0.073 + 0.232 = 0.34, & c^2 \in [0.83, 0.9]. \end{cases} \end{aligned} \tag{32}$$

We consider first the case $c \in [0.9, 1]$. Since $0.257\sqrt{\frac{2}{\pi}} \leq 0.206 < 0.34926$, Lemma 4.6 shows $|r(z)| < u_p(z)$ for $z \geq 1$. On the other hand, u_p is obviously concave on $[0, 1]$, hence $u_p(z) > 0.34926z$ for $z \in [0, 1]$. But $|r'(z)| < 0.43\sqrt{\frac{2}{\pi}} \leq 0.344$ implies $|r(z)| < 0.344z$, therefore $|r(z)| < u_p(z)$ for all $z \in \mathbb{R}^+$. This establishes the sign condition (9) for this case.

Similarly, for $c^2 \in [0.83, 0.9]$, the estimate $0.339\sqrt{\frac{2}{\pi}} \leq 0.271 < 0.41139$ implies by Lemma 4.6 that $|r(z)| < u_p(z)$ for $z \geq \frac{3}{2}$. For $z \in \left[0, \frac{3}{2}\right]$, the trivial concavity of u_p shows $u_p(z) > \frac{2}{3} \cdot 0.41139z \geq 0.274z$, and the sign condition (9) holds for $z \in \left[0, \frac{3}{2}\right]$ due to $|r(z)| \leq |r'(z)|\, z \leq 0.34\sqrt{\frac{2}{\pi}}z < 0.272z$. This concludes the proof of (i).

To prove (ii), it suffices to observe that, in the proof of (i), the inequalities $|r(z)| < u_p(z)$, $z > 0$, are strict and that r and u_p depend continuously on the parameters (c^2, α). □

The proof also validates the claim we stated at the end of the introduction in Section 1, namely that the proof carries over to a periodic piecewise quadratic on-site potential. Indeed, at the core of our argument is a strong quantitative control over the solution. This differentiates the approach presented here from formal methods [2], where no such control is available. Indeed, Atkinson and Cabrera work exclusively with a non-periodic potential [2], while the model of Frenkel and Kontorova is characterised by a periodic potential.

Corollary 4.7 *Define*

$$\tilde{g}(u) = \frac{1}{2}\alpha \, \min\{(u - 2m + 1)^2 : m \in \mathbb{Z}\}$$

and let $u = u_p - r$ as in Theorem 4.1, i.e., with u_p be given by (25) and r by (30) and (27). Then, under the conditions of Theorem 4.1 on c^2 and α, u solves (3) with $\tilde{g}$ instead of g.

Proof: By definition of the profile u_p, we have for all $z \in \mathbb{R}$

$$|u_p(z)| \le A + 2B = \frac{2c^2p^2 - 2 - p}{c^2p^2 - p},$$

and from (14), (24) and the monotonicity of the fraction as a function of c^2

$$|(A + 2B) - 1| = B = \frac{c^2p^2 - 2}{c^2p^2 - p} \le \frac{p^2 - 2}{p^2 - p} \le 0.522.$$

From (31), $|r(z)| \le 0.339$ for $c^2 \in [0.83, 1]$. This shows $|u(z)| < 2$ for all $z \in \mathbb{R}$ and $c^2 \in [0.83, 1]$. The corollary follows from the fact that $g(u) = \tilde{g}(u)$ for all $|u| < 2$. □

5. Auxiliary statements

In this section, we prove Lemmata 4.3–4.6. In the following, (27) will be written as

$$\mathscr{F}_s[r](\zeta) = \frac{f_3(\zeta)}{D(\zeta)}[f_1(\zeta) + f_2(\zeta)] \tag{33}$$

with the dispersion function $D(\zeta) = -c^2(\zeta^2 - p^2) - 2\cos(\zeta)$ as in (26), and

$$f_1(\zeta) := \frac{2\zeta\cos(\zeta)}{\zeta^2 - p^2}, \qquad f_2(\zeta) := \frac{p(1 - \cos(\zeta))}{\zeta}, \tag{34}$$

$$f_3(\zeta) := \frac{2(c^2p^2 - 2)}{p(c^2p^2 - 2) + c^2\zeta^2(2 - p)} = \frac{2}{p + q\zeta^2}, \tag{35}$$

where $p = \frac{\pi}{2}$ and $q := \frac{c^2(2-p)}{c^2p^2-2}$.

Proof of Lemma 4.3: Expanding f_1 and f_2 at 0, we get

$$f_1(\zeta) = \frac{2\zeta\cos(\zeta)}{\zeta^2 - p^2} = \frac{-2\zeta}{p^2} \cdot \frac{1}{-\left(\frac{\zeta}{p}\right)^2 + 1}\cos(\zeta)$$

$$= \frac{-2\zeta}{p^2}\left(\sum_{n=0}^{\infty}\frac{1}{p^{2n}}\zeta^{2n}\right)\left(\sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}\zeta^{2n}\right) = -\frac{2\zeta}{p^2}\sum_{n=0}^{\infty}\left[\sum_{k=0}^{n}\frac{(-1)^k}{(2k)!}p^{-2(n-k)}\right]\zeta^{2n} \tag{36}$$

and

$$f_2(\zeta) = p\frac{1-\cos(\zeta)}{\zeta} = p\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{(2n)!}\zeta^{2n-1};$$

both are alternating and decreasing series. Indeed, this is obvious for f_2; for f_1, observe that for each $n \in \mathbb{N}$, the (finite) sum $\sum_{k=0}^{n}(-1)^k\frac{1}{(2k)!}p^{-2(n-k)}$ is alternating because

$$\frac{1}{(2k)!}p^{-2(n-k)} = \frac{1}{(2k-2)!}\frac{p}{(2k)(2k-1)}p^{-2(n-k-1)} < \frac{1}{(2k-2)!}p^{-2(n-k-1)},$$

thus the sign of this sum is determined by the first and largest summand.

Denoting the Taylor polynomial of degree one of a function f with $T_1 f$, we may write

$$T_1 f_1(\zeta) = -\frac{2}{p^2}\zeta \qquad \text{and} \qquad T_1 f_2(\zeta) = \frac{1}{2}p\zeta,$$

and from the above it is easy to see that $T_1 f_1(\zeta) \le f_1(\zeta) \le 0$ and $T_1 f_2(\zeta) \ge f_2(\zeta) \ge 0$. Also $f_1(\zeta) + f_2(\zeta) \le 0$, so that (since $|T_1 f_1 + T_1 f_2| = -|T_1 f_1| + |T_1 f_2| \ge -|f_1| + |f_2| = |f_1 + f_2|$)

$$|f_1(\zeta) + f_2(\zeta)| \le |T_1 f_1(\zeta) + T_1 f_2(\zeta)| = \left(\frac{2}{p^2} - \frac{p}{2}\right)\zeta. \tag{37}$$

Note that none of these expressions depends on c^2.

The strictly positive function f_3 will be approximated by

$$\tilde{f}_3(\zeta) := -\frac{8q}{p^2(4+qp)}\zeta^2 + \frac{2}{p}.$$

The equation $f_3(\zeta) = \tilde{f}_3(\zeta)$ has only the three distinct solutions 0 and $\pm\frac{p}{2}$. Hence the sign of $f_3 - \tilde{f}_3$ does not change on I_1. A direct calculation shows that

$$f_3(\zeta) - \tilde{f}_3(\zeta) = -\frac{2q}{p^2}\cdot\frac{qp}{4+qp}\zeta^2 + \frac{2}{p}\sum_{n=2}^{\infty}\left(\frac{-q\zeta^2}{p}\right)^n.$$

The leading coefficient is negative, so $f_3(\zeta) \le \tilde{f}_3(\zeta)$ in a neighbourhood of 0, hence on all of I_1.

As for the dispersion function (26), note first that, for all $\zeta \in I_1$,

$$\cos(z) \le -\frac{4-2\sqrt{2}}{p^2}\zeta^2 + 1 =: f_{\cos}(\zeta),$$

with equality at 0 and $\frac{p}{2}$. This inequality is proved by observing that $f'_{\cos}(\zeta)+\sin(\zeta)$ has exactly one zero on $\left(0, \frac{p}{2}\right)$ because $f'_{\cos}(\zeta)$ is a linear function with slope $\frac{4\sqrt{2}-8}{p^2} > -1$. Hence Rolle's theorem shows that the function $f_{\cos}(\zeta) - \cos(\zeta)$ cannot have any zero in $\left(0, \frac{p}{2}\right)$. Moreover, in a neighbourhood of 0, $f_{\cos}(\zeta) - \cos(\zeta)$ is positive because the leading coefficient in

$$\begin{aligned} f_{\cos}(\zeta) - \cos(\zeta) &= -\frac{4-2\sqrt{2}}{p^2}\zeta^2 + 1 - \sum_{n=0}^{\infty}\frac{(-1)^n}{(2n)!}\zeta^{2n} \\ &= \left[-\frac{4-2\sqrt{2}}{p^2} + \frac{1}{2}\right]\zeta^2 - \sum_{n=2}^{\infty}\frac{(-1)^n}{(2n)!}\zeta^{2n} \end{aligned}$$

is positive ($-\frac{4-2\sqrt{2}}{p^2}+\frac{1}{2}\approx 0.025$). Therefore, from (26),

$$\begin{aligned} D(\zeta) &= -c^2\left(\zeta^2-p^2\right)-2\cos(\zeta) \geq -c^2\left(\zeta^2-p^2\right)-2f_{\cos}(\zeta) \\ &= \zeta^2\left(\frac{8-4\sqrt{2}}{p^2}-c^2\right)+c^2p^2-2. \end{aligned} \tag{38}$$

Thus

$$\begin{aligned} \left|\mathscr{F}_s\left[r\right](\zeta)\right| &\leq \frac{\tilde{f}_3(\zeta)}{-c^2\left(\zeta^2-p^2\right)-2f_{\cos}(\zeta)}\left|T_1f_1(\zeta)+T_1f_2(\zeta)\right| \qquad (39)\\ &= \left(-\frac{8q}{p^2(4+qp)}\zeta^2+\frac{2}{p}\right)\frac{1}{\zeta^2\left(\frac{8-4\sqrt{2}}{p^2}-c^2\right)+c^2p^2-2}\left(\frac{2}{p^2}-\frac{p}{2}\right)\zeta \\ &= \frac{2}{p}\left(\frac{2}{p^2}-\frac{p}{2}\right)\frac{1}{c^2p^2-2}\cdot\frac{-\frac{4q}{p(4+qp)}\zeta^3+\zeta}{\zeta^2\cdot\frac{8-4\sqrt{2}-c^2p^2}{p^2(c^2p^2-2)}+1}. \end{aligned}$$

The right-hand side is, apart from a constant factor, of the form $\frac{a\zeta^3+\zeta}{b\zeta^2+1}$, with $a := -\frac{4q}{p(4+qp)} = \frac{-4c^2(2-p)}{p(3c^2p^2+2c^2p-8)}$ and $b := \frac{8-4\sqrt{2}-c^2p^2}{p^2(c^2p^2-2)}$. The integral of this expression can be calculated explicitly, and one finds (for convenience, we write $b_2 := b\frac{p^2}{4}$)

$$\begin{aligned} \int_0^{\frac{p}{2}}\frac{a\zeta^3+\zeta}{b\zeta^2+1}\,\mathrm{d}\zeta &= \left[\frac{a}{b}\zeta^2+\frac{b-a}{b^2}\ln\left(b\zeta^2+1\right)\right]_0^{\frac{p}{2}} \\ &= \frac{a}{b}\cdot\frac{p^2}{8}\left[1-\frac{\ln(b_2+1)}{b_2}\right]+\frac{p^2}{8}\cdot\frac{\ln(b_2+1)}{b_2}. \end{aligned}$$

(As a function of c^2, b vanishes at one point in the relevant parameter interval, but the expression above shows that this is a removable singularity, since $\lim_{x\to 0}\frac{\ln(1+x)}{x}=1$.) Thus

$$\begin{aligned} \int_0^{\frac{p}{2}}\left|\mathscr{F}_s\left[r\right](\zeta)\right|\mathrm{d}\zeta &\leq \frac{2}{p}\left(\frac{2}{p^2}-\frac{p}{2}\right)\frac{1}{c^2p^2-2}\left[\frac{a}{b}\cdot\frac{p^2}{8}\left(1-\frac{\ln(b_2+1)}{b_2}\right)+\frac{p^2}{8}\cdot\frac{\ln(b_2+1)}{b_2}\right] \\ &= \frac{\frac{p}{4}\left(\frac{2}{p^2}-\frac{p}{2}\right)}{c^2p^2-2}\left[-\frac{a}{b}\left(\frac{\ln(b_2+1)}{b_2}-1\right)+\frac{\ln(b_2+1)}{b_2}\right] \\ &= \frac{q\left(2-\frac{p^3}{2}\right)}{(4+qp)\left(8-4\sqrt{2}-c^2p^2\right)}\left(\frac{\ln(b_2+1)}{b_2}-1\right) \\ &\quad+\left(\frac{2}{p}-\frac{p^2}{2}\right)\frac{\ln(b_2+1)}{8-4\sqrt{2}-c^2p^2}. \end{aligned} \tag{40}$$

The first summand of (40),

$$\frac{q\left(2-\frac{p^3}{2}\right)}{(4+qp)\left(8-4\sqrt{2}-c^2p^2\right)}\left(\frac{\ln(b_2+1)}{b_2}-1\right),$$

is negative for c^2 in the parameter interval in question. Indeed, the factor $\frac{q\left(2-\frac{1}{2}p^3\right)}{4+qp}$ is positive (because q is positive), while the expression in brackets and $\frac{1}{8-4\sqrt{2}-c^2p^2}$ both switch signs at the removable singularity of the latter (at $c^2 \approx 0.94964$). We estimate this term from above by 0.

The remaining summand is, apart from the constant $\left(\frac{2}{p} - \frac{p^2}{2}\right)$,

$$g(c^2) := \frac{\ln(b_2+1)}{8-4\sqrt{2}-c^2p^2} = \frac{\ln\left(\frac{8-4\sqrt{2}-c^2p^2+4c^2p^2-8}{4c^2p^2-8}\right)}{8-4\sqrt{2}-c^2p^2} = \frac{\ln\left(\frac{3c^2p^2-4\sqrt{2}}{4c^2p^2-8}\right)}{8-4\sqrt{2}-c^2p^2},$$

and its derivative is given by

$$\begin{aligned} g'(c^2) &= \frac{\left(8-4\sqrt{2}-c^2p^2\right)\frac{4c^2p^2-8}{3c^2p^2-4\sqrt{2}}\cdot\frac{3\left(4c^2p^2-8\right)-4\left(3c^2p^2-4\sqrt{2}\right)}{4c^2p^2-8} + \ln\left(\frac{3c^2p^2-4\sqrt{2}}{4c^2p^2-8}\right)}{\left(8-4\sqrt{2}-c^2p^2\right)^2} \\ &= \frac{1}{8-4\sqrt{2}-c^2p^2}\left[\frac{16\sqrt{2}-24}{(4c^2p^2-8)(3c^2p^2-4\sqrt{2})} + \frac{\ln\left(\frac{3c^2p^2-4\sqrt{2}}{4c^2p^2-8}\right)}{8-4\sqrt{2}-c^2p^2}\right]. \end{aligned}$$

The expression in square brackets vanishes for $c^2p^2 = 8-4\sqrt{2}$ (by de L'Hôpital's rule) and changes sign at this point in opposite direction from the factor $\frac{1}{8-4\sqrt{2}-c^2p^2}$. Thus the product is negative and we conclude that g is a decreasing function in c^2.

Hence the first claim (28) follows from

$$\left(\frac{2}{p} - \frac{p^2}{2}\right) g(0.9) < 0.043 \qquad \text{and} \qquad \left(\frac{2}{p} - \frac{p^2}{2}\right) g(0.83) < 0.125.$$

The proof of the estimate of the second integral (29) resembles the preceding arguments. From (33) and (34), we obtain with (37) and (38) (i.e., applying the same estimates as in (39) except that f_3 is kept)

$$\begin{aligned} |\zeta \mathscr{F}_s[r](\zeta)| &\le \zeta \cdot \frac{2}{(p+q\zeta^2)\left(\zeta^2\left(\frac{8-4\sqrt{2}}{p^2} - c^2\right) + c^2p^2 - 2\right)} \left(\frac{2}{p^2} - \frac{p}{2}\right)\zeta \\ &= \frac{\left(\frac{4}{p^2} - p\right)}{q\left(\frac{8-4\sqrt{2}-c^2p^2}{p^2}\right)} \cdot \frac{\zeta^2}{\zeta^4 + \zeta^2\left(\frac{p}{q} + \frac{p^2(c^2p^2-2)}{8-4\sqrt{2}-c^2p^2}\right) + \frac{p}{q}\cdot\frac{p^2(c^2p^2-2)}{8-4\sqrt{2}-c^2p^2}} \\ &\le \frac{p\left(\frac{4}{p^2} - p\right)}{q\left(\frac{8-4\sqrt{2}-c^2p^2}{p}\right)} \cdot \frac{\zeta^2}{\zeta^2\left(p\,\frac{1}{q} + p\,\frac{p(c^2p^2-2)}{8-4\sqrt{2}-c^2p^2}\right) + p\,\frac{p^2(c^2p^2-2)}{q\left(8-4\sqrt{2}-c^2p^2\right)}} \\ &= \left(\frac{4}{p} - p^2\right) \cdot \frac{\zeta^2}{\zeta^2\left(8-4\sqrt{2}-c^2p^2+qp\left(c^2p^2-2\right)\right) + p^2\left(c^2p^2-2\right)}. \end{aligned}$$

The coefficient of ζ^2 in the denominator is strictly positive for $c^2 \in [0.83, 1]$. We note that the integral of this expression is of the type $\int_0^x \frac{\zeta^2}{a^2\zeta^2+b^2}\,\mathrm{d}\zeta = \frac{1}{a^2}\left[x - \frac{b}{a}\arctan\left(\frac{ax}{b}\right)\right]$. Thus, using $q(c^2p^2-2) = \frac{c^2(2-p)}{c^2p^2-2}(c^2p^2-2) = c^2(2-p)$ from (35), we find, writing $y\left(c^2\right) := \sqrt{\frac{p^2(c^2p^2-2)}{8-4\sqrt{2}-c^2p^2+c^2p(2-p)}}$ for convenience,

$$\int_{I_1} \zeta\left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \le \frac{\frac{4}{p} - p^2}{8-4\sqrt{2}-c^2p^2+c^2p(2-p)} \cdot \left[\frac{p}{2} - y(c^2)\arctan\left(\frac{\frac{p}{2}}{y(c^2)}\right)\right]. \quad (41)$$

The right-hand side is an increasing function of c^2 on $[0.83, 1]$. The function $y \mapsto y \arctan\left(\frac{1}{y}\right)$ is concave, thus the expression in square brackets is a convex function of c^2. Therefore

$$\int_{I_1} \zeta \left|\mathscr{F}_s\left[r\right](\zeta)\right| \mathrm{d}\zeta \leq \frac{\frac{4}{p} - p^2}{8 - 4\sqrt{2} - 2c^2 p(p-1)} \cdot h\big(c^2\big)\,, \tag{42}$$

where h is the affine function which agrees with the expression in square brackets of (41) for $c^2 = 0.83$ and $c^2 = 1$. The right-hand side of (42) is of the form $\frac{ac^2+b}{dc^2+e}$, and it is elementary to check that it is decreasing on $[0.83, 1]$. Thus we can estimate the right-hand side of (41) for all $c^2 \in [0.83, 1]$ by its value for $c^2 = 0.83$ which is below 0.035, i.e.,

$$\int_{I_1} \zeta \left|\mathscr{F}_s\left[r\right](\zeta)\right| \mathrm{d}\zeta \leq \frac{\frac{4}{p} - p^2}{8 - 4\sqrt{2} - 2p(p-1)\cdot 0.83} \cdot h(0.83) \leq 0.035.$$

Now let $\overline{h}$ be the affine function which agrees with the expression in square brackets of (41) for $c^2 = 0.9$ and $c^2 = 1$. We find for $c^2 \in [0.9, 1]$ the sharper estimate

$$\int_{I_1} \zeta \left|\mathscr{F}_s\left[r\right](\zeta)\right| \mathrm{d}\zeta \leq \frac{\frac{4}{p} - p^2}{8 - 4\sqrt{2} - 2p(p-1)\cdot 0.9} \cdot \overline{h}(0.9) \leq 0.017.$$

Thus Lemma 4.3 is proved. □

We turn to Lemma 4.4. The interval $I_2 = \left[\frac{p}{2}, \frac{3p}{2}\right]$ is tricky due to the removable singularity in the integrand at p. Several statements rely on the fact that certain functions are convex or concave. We give one proof of each statement in detail; the other proofs are similar.

Lemma 5.1 *Let*

$$f_{3D}(\zeta) := (\zeta - p)\frac{f_3(\zeta)}{D(\zeta)} = \frac{2}{(p + q\zeta^2)\left(-c^2(\zeta + p) + 2\frac{\sin(\zeta - p)}{\zeta - p}\right)}.$$

This function f_{3D} is nonpositive and concave on I_2.

Proof: We have $f_{3D}(\zeta) \leq 0$ because $f_3(\zeta) > 0$ for all $\zeta \in \mathbb{R}^+$ and $D(\zeta) \gtrless 0$ for $\zeta \lessgtr p$. Consider

$$f_{3D}''(\zeta) = f_3(\zeta)\left(\frac{\zeta - p}{D(\zeta)}\right)'' + 2f_3'(\zeta)\left(\frac{\zeta - p}{D(\zeta)}\right)' + f_3''(\zeta)\left(\frac{\zeta - p}{D(\zeta)}\right);$$

we will see that each summand is negative. The derivatives of f_3 are

$$f_3'(\zeta) = \frac{-4q\zeta}{(p + q\zeta^2)^2} \qquad \text{and} \qquad f_3''(\zeta) = \frac{-4q\left(p - 3q\zeta^2\right)}{(p + q\zeta^2)^3}.$$

While f_3' is obviously negative, it is easy to see that f_3'' is positive for $|\zeta| > \sqrt{\frac{p}{3q}} = \sqrt{\frac{p(c^2p^2-2)}{3c^2(2-p)}}$, which is less than $\frac{p}{2}$ for all $c < 1$ (it is increasing in c^2 and $\sqrt{\frac{p(p^2-2)}{3(2-p)}} \approx 0.755$).

As indicated above, $(\zeta-p)(D(\zeta))^{-1}\le 0$. Using $\frac{\sin(x)}{x}=\sum_{n=0}^\infty \frac{(-1)^n}{(2n+1)!}x^{2n}$, we obtain

$$\left(\frac{\zeta-p}{D(\zeta)}\right)'=\frac{c^2-2\sum_{n=1}^\infty(-1)^n\frac{2n}{(2n+1)!}(\zeta-p)^{2n-1}}{\left(-c^2(\zeta+p)+2\frac{\sin(\zeta-p)}{\zeta-p}\right)^2}>0$$

because $\left|\sum_{n=1}^\infty(-1)^n\frac{2n}{(2n+1)!}(\zeta-p)^{2n-1}\right|\le\frac{1}{6}p<c^2$ for $|\zeta-p|\le\frac{1}{2}p<1$. Also, one can see similarly that

$$\left(\frac{\zeta-p}{D(\zeta)}\right)''<0$$

so that we may conclude that f_{3D} is indeed concave on I_2. □

Lemma 5.2 *The function*

$$\zeta\mapsto-\frac{\sin(\zeta-p)-(\zeta-p)}{(\zeta-p)^2}\cdot\frac{\zeta}{\zeta+p}$$

is positive and convex on $\left[p,\frac{3p}{2}\right]$.

Proof: The positivity is obvious. To see the convexity, we re-write the two factors in terms of $x:=\zeta-p$,

$$\left(-\sum_{n=1}^\infty\frac{(-1)^n}{(2n+1)!}x^{2n-1}\right)\frac{x+p}{x+2p}=:\varphi(x).$$

We calculate $\varphi(x+\varepsilon)+\varphi(x-\varepsilon)=$

$$\begin{aligned}
&=\left(\sum_{n=1}^\infty\frac{(-1)^{n+1}}{(2n+1)!}(x+\varepsilon)^{2n-1}\right)\frac{x+\varepsilon+p}{x+2p+\varepsilon}\\
&\quad+\left(\sum_{n=1}^\infty\frac{(-1)^{n+1}}{(2n+1)!}(x-\varepsilon)^{2n-1}\right)\frac{x-\varepsilon+p}{x+2p-\varepsilon}\\
&=\sum_{n=1}^\infty\frac{(-1)^{n+1}}{(2n+1)!}\frac{(x+\varepsilon)^{2n-1}(x+p+\varepsilon)(x+2p-\varepsilon)+(x-\varepsilon)^{2n-1}(x+p-\varepsilon)(x+2p+\varepsilon)}{(x+2p)^2-\varepsilon^2}\\
&=\sum_{n=1}^\infty\frac{(-1)^{n+1}}{(2n+1)!}\left[(x+p)(x+2p)-\varepsilon^2\right]\\
&\quad\cdot\frac{\left[(x+\varepsilon)^{2n-1}+(x-\varepsilon)^{2n-1}\right]+\varepsilon p\left[(x+\varepsilon)^{2n-1}-(x-\varepsilon)^{2n-1}\right]}{(x+2p)^2-\varepsilon^2}\\
&=\frac{2}{(x+2p)^2-\varepsilon^2}\sum_{n=1}^\infty\frac{(-1)^{n+1}}{(2n+1)!}\left[\frac{(x+p)(x+2p)^2}{x+2p}\cdot\right.\\
&\quad\left.\cdot\left(x^{2n-1}+\varepsilon^2\binom{2n-1}{2}x^{2n-3}\right)-\varepsilon^2x^{2n-1}+\varepsilon p\cdot(2n-1)\varepsilon x^{2n-2}\right]\\
&\quad+O\left(\varepsilon^4\right)\\
&=2\frac{(x+2p)^2}{(x+2p)^2-\varepsilon^2}\left[\varphi(x)+\frac{\varepsilon^2}{(x+2p)^2}\sum_{n=1}^\infty\frac{(-1)^{n+1}}{(2n+1)!}\cdot\right.
\end{aligned}$$

$$\cdot\left(\left(x^2+3px+2p^2\right)\binom{2n-1}{2}x^{2n-3}p(2n-1)x^{2n-2}-x^{2n-1}\right)\Bigg]$$
$$+O\left(\varepsilon^4\right).$$

Now since for all $n\in\mathbb{N}$ and for $x\in\left[0,\frac{1}{2}p\right]$

$$\left(\left(x^2+3px+2p^2\right)\binom{2n-1}{2}x^{2n-3}+p(2n-1)x^{2n-2}-x^{2n-1}\right)\geq 0$$

and $\frac{(x+2p)^2}{(x+2p)^2-\varepsilon^2}\geq 1$, we obtain that $\varphi(x+\varepsilon)+\varphi(x-\varepsilon)\geq 2\varphi(x)$ for $\varepsilon>0$ small enough. This shows that

$$\varphi(x)=\varphi(\zeta-p)=-\frac{\sin(\zeta-p)-(\zeta-p)}{(\zeta-p)^2}\cdot\frac{\zeta}{\zeta+p}$$

is convex for $\zeta\in\left[p,\frac{3}{2}p\right]$, as claimed. □

We are now in a position to prove Lemma 4.4.

Proof of Lemma 4.4: In this proof, we will frequently use linear interpolation. Obviously, an affine function of the form $\overline{g}(\zeta)=a\zeta+b$ with $\overline{g}\left(\frac{p}{2}\right)=\alpha$ and $\overline{g}(p)=\beta$ has the coefficients

$$a=\frac{2(\beta-\alpha)}{p}\qquad\text{and}\qquad b=2\alpha-\beta,$$

and an affine function of the form $\overline{h}(\zeta)=d\zeta+e$ with $\overline{h}(p)=\beta$ and $\overline{h}\left(\frac{3p}{2}\right)=\gamma$ has the coefficients

$$d=\frac{2(\gamma-\beta)}{p}\qquad\text{and}\qquad e=3\beta-2\gamma.$$

We again use the decomposition (33). To do so, it is here convenient to write

$$f_{3D}:=(\zeta-p)\frac{f_3(\zeta)}{D(\zeta)},\ f_{12}(\zeta):=\frac{f_1(\zeta)+f_2(\zeta)}{\zeta-p}=\frac{1}{\zeta-p}\left(\frac{2\zeta\cos(\zeta)}{\zeta^2-p^2}+\frac{p(1-\cos(\zeta))}{\zeta}\right).\quad(43)$$

This split is motivated by the facts that neither of these functions has a pole at $\zeta=p$ and that f_{12} is independent of c.

We consider first f_{3D}. By Lemma 5.1, f_{3D} is nonpositive and concave on I_2. Hence a linear interpolation of f_{3D} increases its absolute value. So

$$|f_{3D}(\zeta)|\leq\left|\frac{2}{p}\left[f_{3D}(p)-f_{3D}\left(\frac{p}{2}\right)\right]\cdot\zeta+2f_{3D}\left(\frac{p}{2}\right)-f_{3D}(p)\right|,\qquad\zeta\in\left[\frac{p}{2},p\right],\quad(44)$$

$$|f_{3D}(\zeta)|\leq\left|\frac{2}{p}\left[f_{3D}\left(\frac{3p}{2}\right)-f_{3D}(p)\right]\cdot\zeta+3f_{3D}(p)-2f_{3D}\left(\frac{3p}{2}\right)\right|,\qquad\zeta\in\left[p,\frac{3p}{2}\right],(45)$$

where $f_{3D}\left(\frac{p}{2}\right)=\frac{16}{(4+qp)\left(4\sqrt{2}-3p^2c^2\right)}$, $f_{3D}(p)=\frac{1}{p(1+qp)(1-c^2p)}$ and $f_{3D}\left(\frac{3p}{2}\right)=\frac{16}{(4+9qp)\left(4\sqrt{2}-5p^2c^2\right)}$.

We turn to the terms that do not depend on c (see (43)),

$$f_{12}(\zeta)=\frac{f_1(\zeta)+f_2(\zeta)}{\zeta-p}=\frac{1}{\zeta-p}\left(\frac{2\zeta\cos(\zeta)}{\zeta^2-p^2}+\frac{p(1-\cos(\zeta))}{\zeta}\right)$$

$$= \frac{1}{\zeta - p}\left(\frac{-2\zeta\sin(\zeta-p)}{\zeta^2-p^2} + \frac{p}{\zeta} + \frac{p\sin(\zeta-p)}{\zeta}\right)$$
$$= \frac{1}{\zeta-p}\cdot\frac{p}{\zeta} + \frac{\sin(\zeta-p)}{(\zeta-p)^2}\cdot\frac{-2\zeta}{\zeta+p} + \frac{\sin(\zeta-p)}{\zeta-p}\cdot\frac{p}{\zeta}$$
$$= -\left[\frac{1}{\zeta} + \frac{1}{\zeta+p}\right] + \left[\frac{\sin(\zeta-p)-(\zeta-p)}{(\zeta-p)^2}\right]\frac{-2\zeta}{\zeta+p} + \frac{\sin(\zeta-p)}{\zeta-p}\cdot\frac{p}{\zeta}, \tag{46}$$

where the identity

$$\frac{p}{\zeta} + \frac{-2\zeta}{\zeta+p} = \frac{\zeta p + p^2 - 2\zeta^2}{\zeta(\zeta+p)} = -(\zeta-p)\frac{2\zeta+p}{\zeta(\zeta+p)} = -(\zeta-p)\left[\frac{1}{\zeta}+\frac{1}{\zeta+p}\right]$$

was used in the last line.

On $\left[\frac{p}{2}, p\right]$, the function f_{12} is convex in ζ. Linear interpolation shows, with $f_{12}\left(\frac{p}{2}\right) = \frac{4\sqrt{2}}{3p^2} + \frac{1}{p}\left(2\sqrt{2}-4\right)$ and $f_{12}(p) = 1 - \frac{3}{2p}$,

$$f_{12}(\zeta) \le \frac{2}{p}\left[f_{12}(p) - f_{12}\left(\frac{p}{2}\right)\right]\cdot\zeta + 2f_{12}\left(\frac{p}{2}\right) - f_{12}(p)$$

for all $\zeta \in \left[\frac{p}{2}, p\right]$.

Integrating, we obtain for $\mathscr{F}_s[r](\zeta)$ defined in (33), since $\mathscr{F}_s[r](\zeta) = f_{3D}(\zeta)\cdot f_{12}(\zeta)$,

$$\int_{\frac{p}{2}}^{p} \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \le \frac{a_1 + a_2c^2 + a_3q + a_4c^2q}{36p^2(1+qp)\left(1-c^2p\right)(4+qp)\left(4\sqrt{2}-3p^2c^2\right)}$$

where we abbreviate

$$a_1 := 48p^3 + \left(288\sqrt{2}-456\right)p^2 + \left(192 - 208\sqrt{2}\right)p + 128 \approx 33.392$$
$$a_2 := -120p^4 + \left(708 - 264\sqrt{2}\right)p^3 - 176p^2\sqrt{2} \approx -47.686$$
$$a_3 := 48p^4 + \left(216\sqrt{2}-456\right)p^3 + \left(48+44\sqrt{2}\right)p^2 + 32p \approx 31.042$$
$$a_4 := -66p^5 + \left(519 - 210\sqrt{2}\right)p^4 - 140p^3\sqrt{2} \approx -46.888$$

Substituting the definition of q and expanding the expressions into partial fractions, we get

$$\int_{\frac{p}{2}}^{p} \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \le \frac{a_5}{\left(1-pc^2\right)^2} + \frac{a_6}{1-pc^2} + \frac{a_7}{1-a_9c^2} + \frac{a_8}{1-a_{10}c^2}, \tag{47}$$

with

$$a_5 \approx -0.00194, \qquad a_6 \approx -0.00710,$$
$$a_7 \approx -0.06761, \qquad a_8 \approx 0.05998,$$
$$a_9 \approx 1.31797, \qquad a_{10} \approx 1.30854$$

(the algebraic expressions for $a_5, \ldots, a_{10}$ are rather lengthy and not very instructive). We will estimate this expression in a moment.

The situation is a bit more delicate on $\left[p, \frac{3p}{2}\right]$ because the function f_{12} becomes concave at about $1.75 \approx \frac{10}{9}p$. Continuing from (46), note that

$$-\left[\frac{1}{\zeta} + \frac{1}{\zeta+p}\right] + \frac{\sin(\zeta-p)}{\zeta-p}\cdot\frac{p}{\zeta} \le \frac{p-1}{\zeta} - \frac{1}{\zeta+p} =: f_{12,a}(\zeta)$$

because obviously $\frac{\sin(x)}{x} \le 1$. This function $f_{12,a}$ is convex. Indeed,

$$\frac{\mathrm{d}^2}{\mathrm{d}\zeta^2} f_{12,a}(\zeta) = \frac{2(p-1)}{\zeta^3} - \frac{2}{(\zeta+p)^3}$$

is positive because $\frac{1}{\left(\frac{3}{2}p\right)^3} = \frac{8}{27p^3} > \frac{1}{4p^3} = \frac{2}{(p+p)^3}$ implies, since $\frac{2(p-1)}{\zeta^3}$ and $\frac{2}{(\zeta+p)^3}$ are both decreasing functions in ζ,

$$\min_{\zeta\in\left[p,\frac{3p}{2}\right]} \frac{2(p-1)}{\zeta^3} > \max_{\zeta\in\left[p,\frac{3p}{2}\right]} \frac{2}{(\zeta+p)^3}.$$

Linear interpolation of $f_{12,a}$ yields (with $f_{12,a}(p) = 1 - \frac{3}{2p}$ and $f_{12,a}\left(\frac{3p}{2}\right) = \frac{2}{3} - \frac{16}{15p}$) the affine function $\overline{f}_{12,a}(\zeta) := -\frac{1}{30p^3}\left[(20p^2 - 26p)\,\zeta + 71p^2 - 50p^3\right]$.

The remaining summand $f_{12,b}(\zeta) := -\left[\frac{\sin(\zeta-p)-(\zeta-p)}{(\zeta-p)^2}\right]\frac{2\zeta}{\zeta+p}$ of (46) is positive and convex by Lemma 5.2. Linear interpolation of $f_{12,b}(\zeta)$ yields (with $f_{12,b}(p) = 0$ and $f_{12,b}\left(\frac{3p}{2}\right) = \frac{12}{5p^2}\left(p-\sqrt{2}\right)$) the affine function $\overline{f}_{12,b}(\zeta) := \frac{24}{5p^3}\left(p-\sqrt{2}\right)(\zeta - p)$.

Thus altogether

$$\begin{aligned} f_{12}(\zeta) &\le \overline{f}_{12,a}(\zeta) + \overline{f}_{12,b}(\zeta) \\ &= \frac{1}{30p^3}\left[\left(170p - 20p^2 - 144\sqrt{2}\right)\zeta + \left(50p^3 - 215p^2 + 144\sqrt{2}p\right)\right] \end{aligned}$$

on $[p, \frac{3p}{2}]$. Integrating, we obtain

$$\int_p^{\frac{3p}{2}} \left|\mathscr{F}_s\left[r\right](\zeta)\right| \mathrm{d}\zeta \le \frac{b_1 + b_2c^2 + b_3q + b_4c^2q}{45p^2(1+qp)\left(1-c^2p\right)(4+9qp)\left(4\sqrt{2} - 5p^2c^2\right)},$$

where we abbreviate

$$\begin{aligned} b_1 &:= -220p^3 + (610 + 640\sqrt{2})p^2 - 1948p\sqrt{2} + 1440 \approx -1.6894 \\ b_2 &:= -580p^4 + 1465p^3 - 612p^2\sqrt{2} \approx 11.412 \\ b_3 &:= -220p^4 + (610 + 1440\sqrt{2})p^3 - 4023p^2\sqrt{2} + 3240p \approx -30.842 \\ b_4 &:= -1580p^5 + \frac{16235}{4}p^4 - 1737p^3\sqrt{2} \approx 79.403 \end{aligned}$$

Expanding the right-hand side into partial fractions, we find

$$\int_p^{\frac{3p}{2}} \left|\mathscr{F}_s\left[r\right](\zeta)\right| \mathrm{d}\zeta \le \frac{b_5}{\left(1-pc^2\right)^2} + \frac{b_6}{1-pc^2} + \frac{b_7}{1-b_9c^2} + \frac{b_8}{1-b_{10}c^2}, \qquad (48)$$

where

$$\begin{aligned} b_5 &\approx -0.00411, & b_6 &\approx -0.01506, \\ b_7 &\approx 0.12085, & b_8 &\approx -0.15093, \\ b_9 &\approx 1.99217, & b_{10} &\approx 2.18090 \end{aligned}$$

(again, the algebraic expressions for $b_5, \ldots, b_{10}$ do not carry significant information).

We now return to (47). The last two terms of (47) are

$$\frac{a_7}{1-a_9c^2} + \frac{a_8}{1-a_{10}c^2} = \frac{a_7 + a_8 - \left(a_7a_{10} + a_8a_9\right)c^2}{\left(1-a_9c^2\right)\left(1-a_{10}c^2\right)}$$

and the latter expression, considered as a function of $c^2 \in [0.83, 1]$ (here for $a_7, \dots a_{10}$ and in all future analogous calculations, we work with the algebraic expressions, rather than their numerical approximations), is a simple rational function. It is elementary to verify that it takes a maximum near $c^2 = 0.8596$, with a value there of less than 0.029, so

$$\frac{a_7}{1 - a_9 c^2} + \frac{a_8}{1 - a_{10} c^2} \leq 0.029. \tag{49}$$

The last two terms of (48) are estimated as

$$\begin{aligned} \frac{b_7}{1 - b_9 c^2} + \frac{b_8}{1 - b_{10} c^2} &= \frac{b_7 + b_8 - (b_7 b_{10} + b_8 b_9)\, c^2}{(1 - b_9 c^2)(1 - b_{10} c^2)} \\ &\leq \frac{b_7 + b_8 - (b_7 b_{10} + b_8 b_9) \cdot 1}{(1 - b_9 \cdot 1)(1 - b_{10} \cdot 1)} \leq 0.006 \end{aligned} \tag{50}$$

because the expression in the first line is again a rational function and it is elementary to check that it is increasing as a function of $c^2 \in [0.83, 1]$. The sum of the four other terms of (47) and (48),

$$\frac{a_5}{(1 - pc^2)^2} + \frac{a_6}{1 - pc^2} + \frac{b_5}{(1 - pc^2)^2} + \frac{b_6}{1 - pc^2}$$

takes a maximum as a function of $c^2 \in [0.83, 1]$; the maximum is attained near $c^2 = 0.9842$ and its value there is smaller than 0.021, so

$$\frac{a_5}{(1 - pc^2)^2} + \frac{a_6}{1 - pc^2} + \frac{b_5}{(1 - pc^2)^2} + \frac{b_6}{1 - pc^2} \leq 0.021. \tag{51}$$

Thus, adding up (49)–(51),

$$\int_{\frac{1}{2}p}^{\frac{3}{2}p} |\mathscr{F}_s[r](\zeta)| \,\mathrm{d}\zeta \leq 0.056.$$

We come to the integral of $\zeta\, |\mathscr{F}_s[r]\, \zeta|$. The function $f_{12\zeta}(\zeta) := \zeta f_{12}(\zeta)$ is, unlike f_{12}, convex on all of I_2. As before, we use linear interpolation, with $f_{12\zeta}(\frac{p}{2}) = \frac{2\sqrt{2}}{3p} + \sqrt{2} - 2$, $f_{12\zeta}(p) = p - \frac{3}{2}$ and $f_{12\zeta}(\frac{3p}{2}) = 2 + \sqrt{2} - \frac{18\sqrt{2}}{5p}$. Thus

$$\begin{aligned} f_{12\zeta}(\zeta) &\leq \left(2 + \tfrac{1 - 2\sqrt{2}}{p} - \tfrac{4\sqrt{2}}{3p^2}\right)\zeta + \left(2\sqrt{2} - \tfrac{5}{2} + \tfrac{4\sqrt{2}}{3p} - p\right) && \text{for } \zeta \in \left[\frac{p}{2}, p\right], \\ f_{12\zeta}(\zeta) &\leq \left(-2 + \tfrac{7 + 2\sqrt{2}}{p} - \tfrac{36\sqrt{2}}{5p^2}\right)\zeta + \left(-2\sqrt{2} - \tfrac{17}{2} + \tfrac{36\sqrt{2}}{5p} + 3p\right) && \text{for } \zeta \in \left[p, \frac{3p}{2}\right]. \end{aligned}$$

Using the same estimates (44) and (45) for f_{3D} as before and integrating, we find

$$\int_{\frac{p}{2}}^{p} \zeta \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \leq \frac{d_{1,1} + d_{1,2}c^2 + d_{1,3}q + d_{1,4}c^2 q}{36p(1 + qp)(1 - c^2 p)(4 + qp)\left(4\sqrt{2} - 3p^2 c^2\right)}$$

and

$$\int_{p}^{\frac{3p}{2}} \zeta \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \leq \frac{d_{2,1} + d_{2,2}c^2 + d_{2,3}q + d_{2,4}c^2 q}{p^2(1 + qp)(1 - c^2 p)(4 + 9qp)\left(4\sqrt{2} - 5p^2 c^2\right)},$$

with the abbreviations

$d_{1,1} := -48p^3 + (264 - 192\sqrt{2})p^2 - (96 - 176\sqrt{2})p - 64 \approx -28.437$
$d_{1,2} := 120p^4 - (444 - 132\sqrt{2})p^3 + 88p^2\sqrt{2} \approx 40.307$
$d_{1,3} := -48p^4 + (264 - 120\sqrt{2})p^3 - (24 + 4\sqrt{2})p^2 - 16p \approx -25.071$
$d_{1,4} := 66p^5 - (309 - 105\sqrt{2})p^4 + 70p^3\sqrt{2} \approx 37.668$
$d_{2,1} := -80p^3 - (200 + 320\sqrt{2})p^2 - (160 - 656\sqrt{2})p + 576 \approx -138.22$
$d_{2,2} := 280p^4 + (100 + 260\sqrt{2})p^3 - 936p^2\sqrt{2} \approx 251.24$
$d_{2,3} := -80p^4 - (200 + 520\sqrt{2})p^3 - (360 - 756\sqrt{2})p^2 + 1296p \approx -326.92$
$d_{2,4} := 530p^5 - (25 - 385\sqrt{2})p^4 - 1386p^3\sqrt{2} \approx 634.11$

The partial fraction decomposition of the estimates above is

$$\int_{I_2} \zeta \left|\mathscr{F}_s[r](\zeta)\right| \,\mathrm{d}\zeta \leq \frac{d_3}{(1-pc^2)^2} + \frac{d_4}{1-pc^2} + \frac{d_5}{1-d_{11}c^2} + \frac{d_6}{1-d_{12}c^2} + \frac{d_7}{(1-pc^2)^2} + \frac{d_8}{1-pc^2} + \frac{d_9}{1-d_{13}c^2} + \frac{d_{10}}{1-d_{14}c^2} \tag{52}$$

with

$d_3 \approx -0.00279,\qquad d_4 \approx -0.01021,$
$d_5 \approx -0.08236,\qquad d_6 \approx 0.07314$
$d_7 \approx -0.00563,\qquad d_8 \approx -0.02059,$
$d_9 \approx 0.15510,\qquad d_{10} \approx -0.19369,$
$d_{11} \approx 1.31797,\qquad d_{12} \approx 1.30854,$
$d_{13} \approx 1.99217,\qquad d_{14} \approx 2.18090.$

The last two terms of the first line of (52) are

$$\frac{d_5}{1-d_{11}c^2} + \frac{d_6}{1-d_{12}c^2} = \frac{d_5 + d_6 - (d_5 d_{12} + d_6 d_{11})\,c^2}{(1-d_{11}c^2)\,(1-d_{12}c^2)},$$

and this simple function (with the algebraic expressions for d_j, $j \in \{5, 6, 11, 12\}$, not the approximate values) takes its maximum for $c^2 \in [0.83, 1]$ near $c^2 = 0.8595$, with a value there well below 0.035. The last two terms of the second line of (52) are

$$\frac{d_9}{1-d_{13}c^2} + \frac{d_{10}}{1-d_{14}c^2} = \frac{d_9 + d_{10} - (d_9 d_{14} + d_{10} d_{13})\,c^2}{(1-d_{13}c^2)\,(1-d_{14}c^2)} \leq \frac{d_9 + d_{10} - (d_9 d_{14} + d_{10} d_{13})\cdot 1}{(1-d_{13}\cdot 1)\,(1-d_{14}\cdot 1)} = 0.00770;$$

the function in the first line is increasing for $c^2 \in [0.83, 1]$, as in the previous argument for (50). The sum of the four other terms of (52) is

$$\frac{d_3}{(1-pc^2)^2} + \frac{d_4}{1-pc^2} + \frac{d_7}{(1-pc^2)^2} + \frac{d_8}{1-pc^2} = \frac{d_{15} + d_{16}c^2}{(1-pc^2)^2}$$

with

$d_{15} \approx -0.03922 \qquad \text{and} \qquad d_{16} \approx 0.04839,$

and this function attains its maximum on $c^2 \in [0.83, 1]$ near $c^2 = 0.9845$, with a value there below 0.03. Thus altogether

$$\int_{I_2} \zeta \left|\mathscr{F}_s\left[r\right](\zeta)\right| \,\mathrm{d}\zeta \le 0.035 + 0.0077 + 0.03 < 0.073,$$

as claimed. □

The proof of Lemma 4.5 is less demanding.

Proof of Lemma 4.5: Here, f_1 and f_2 are considered together,

$$\begin{aligned}|f_1(\zeta) + f_2(\zeta)| &= \left|\frac{2\zeta^2\cos(\zeta) + p(\zeta^2 - p^2)(1 - \cos(\zeta))}{\zeta(\zeta^2 - p^2)}\right| = \left|\frac{p}{\zeta} + \cos(\zeta)\,\frac{\zeta^2(2-p) + p^3}{\zeta(\zeta^2 - p^2)}\right| \\ &\le \frac{p}{\zeta} + \frac{\zeta^2(2-p) + p^3}{\zeta(\zeta^2 - p^2)} = \frac{p(\zeta^2 - p^2) + 2\zeta^2 - \zeta^2 p + p^3}{\zeta(\zeta^2 - p^2)} = \frac{2\zeta}{\zeta^2 - p^2}\end{aligned}$$

The dispersion function is strictly negative and may be estimated as

$$|D(\zeta)| = -D(\zeta) = c^2(\zeta^2 - p^2) + 2\cos(\zeta) \ge c^2(\zeta^2 - p^2) - 2,$$

so from (33) and (35)

$$\begin{aligned}\int_{\frac{3}{2}p}^{\infty} \left|\mathscr{F}_s\left[r\right](\zeta)\right| \,\mathrm{d}\zeta &\le \int_{\frac{3}{2}p}^{\infty} \frac{2}{p + \zeta^2 q} \cdot \frac{1}{c^2\zeta^2 - (c^2p^2 + 2)} \cdot \frac{2\zeta}{\zeta^2 - p^2}\,\mathrm{d}\zeta \\ &= \frac{4}{qc^2}\int_{\frac{3}{2}p}^{\infty} \frac{1}{\zeta^2 + \frac{p}{q}} \cdot \frac{1}{\zeta^2 - \left[\frac{c^2p^2+2}{c^2}\right]} \cdot \frac{\zeta}{\zeta^2 - p^2}\,\mathrm{d}\zeta. \qquad (53)\end{aligned}$$

Integrating, we get

$$\begin{aligned}&\int_{\frac{3}{2}p}^{\infty} \left|\mathscr{F}_s\left[r\right](\zeta)\right| \,\mathrm{d}\zeta \\ &\le -\frac{2}{qc^2}\left[\frac{\ln\left((\frac{3}{2}p)^2 - p^2\right)}{p\,\frac{2c^2p-2}{c^2(2-p)} \cdot \frac{-2}{c^2}} - \frac{\ln\left((\frac{3}{2}p)^2 - \frac{c^2p^2+2}{c^2}\right)}{\frac{2c^2p^2-4p+4}{c^2(2-p)} \cdot \frac{-2}{c^2}} + \frac{\ln\left((\frac{3}{2}p)^2 + \frac{p(c^2p^2-2)}{c^2(2-p)}\right)}{\frac{2c^2p^2-4p+4}{c^2(2-p)} \cdot p\,\frac{2c^2p-2}{c^2(2-p)}}\right] \\ &= -\frac{2}{\frac{c^2(2-p)}{c^2p^2-2}\,c^2}\left[-\frac{\ln\left(\frac{9}{4}p^2 - p^2\right)}{4p\,\frac{c^2p-1}{c^4(2-p)}} + \frac{\ln\left(\frac{9}{4}p^2 - p^2 - \frac{2}{c^2}\right)}{4\,\frac{c^2p^2-2p+2}{c^4(2-p)}} + \frac{\ln\left(\frac{9}{4}p^2 + \frac{p(c^2p^2-2)}{c^2(2-p)}\right)}{4\,\frac{c^2p^2-2p+2}{c^2(2-p)} \cdot p\,\frac{c^2p-1}{c^2(2-p)}}\right] \\ &= \frac{c^2p^2 - 2}{2}\left[\frac{\ln\left(\frac{5}{4}p^2\right)}{p(c^2p-1)} - \frac{\ln\left(\frac{5}{4}p^2 - \frac{2}{c^2}\right)}{c^2p^2 - 2p + 2} - \frac{(2-p)\,\ln\left(\frac{9}{4}p^2 + \frac{p(c^2p^2-2)}{c^2(2-p)}\right)}{(c^2p^2 - 2p + 2)(c^2p^2 - p)}\right]\end{aligned}$$

The first and the third term of the square bracket satisfy

$$\begin{aligned}&\frac{\ln\left(\frac{5}{4}p^2\right)}{(c^2p^2 - p)} - \frac{(2-p)\,\ln\left(\frac{9}{4}p^2 + \frac{p(c^2p^2-2)}{c^2(2-p)}\right)}{(c^2p^2 - 2p + 2)(c^2p^2 - p)} \\ &\qquad\le \frac{1}{(c^2p^2 - p)}\left(\ln\left(\frac{5}{4}p^2\right) - \frac{(2-p)\,\ln\left(\frac{9}{4}p^2\right)}{p^2 - 2p + 2}\right)\end{aligned}$$

because $\frac{p(c^2p^2-2)}{c^2(2-p)}$ is increasing in c^2; we write e_1 for the bracket on the right-hand side, which is independent of c; $e_1 \approx 0.57141$. Further, the function $c^2 \mapsto -\ln\left(\frac{5}{4}p^2 - \frac{2}{c^2}\right)$ is decreasing and convex and has a zero on $(0.83, 1)$. Therefore $-\ln\left(\frac{5}{4}p^2 - \frac{2}{c^2}\right) \le 5(c^2-1)\ln\left(\frac{5}{4}p^2 - \frac{2}{0.8}\right)$ on the interval $[0.80, 1]$ (with equality at its endpoints 0.80 and 1) and, observing $c^2 > \frac{1}{2}p$,

$$-\frac{\ln\left(\frac{5}{4}p^2 - \frac{2}{c^2}\right)}{c^2p^2 - 2p + 2} \le \frac{5(c^2-1)\ln\left(\frac{5}{4}p^2 - \frac{2}{0.8}\right)}{\frac{1}{2}p^3 - 2p + 2} \le (1-c^2)\cdot e_2$$

with $e_2 := -\frac{5\ln\left(\frac{5}{4}p^2 - \frac{2}{0.8}\right)}{\frac{1}{2}p^3 - 2p + 2} \approx 3.37451$. Hence altogether

$$\frac{c^2p^2-2}{2}\left[\frac{\ln\left(\frac{5}{4}p^2\right)}{(c^2p^2-p)} - \frac{\ln\left(\frac{5}{4}p^2 - \frac{2}{c^2}\right)}{c^2p^2-2p+2} - \frac{(2-p)\,\ln\left(\frac{9}{4}p^2 + \frac{p(c^2p^2-2)}{c^2(2-p)}\right)}{(c^2p^2-2p+2)(c^2p^2-p)}\right]$$
$$\le \frac{1}{2}\left[\frac{c^2p^2-2}{c^2p^2-p}\,e_1 + (c^2p^2-2)(1-c^2)\,e_2\right]$$

This elementary function takes a maximum on $(0.83, 1)$, near 0.962; its value there is less than 0.158. This finishes the proof of the first claim.

We address the second claim. A multiplication of both sides of (53) by ζ yields

$$\int_{\frac{3p}{2}}^{\infty} \zeta\,|\mathscr{F}_s[r](\zeta)|\,\mathrm{d}\zeta \le \frac{4}{qc^2}\cdot\frac{1}{\zeta^2+\frac{p}{q}}\cdot\frac{1}{\zeta^2-\left(\frac{c^2p^2+2}{c^2}\right)}\cdot\frac{\zeta^2}{\zeta^2-p^2}.$$

We observe that

$$\left(\zeta^2+\frac{p}{q}\right)(\zeta^2-p^2) = \zeta^4 - \zeta^2\left(p^2-\frac{p}{q}\right) - \frac{4p}{9q}\cdot\frac{9}{4}p^2$$
$$\ge \zeta^4 - \zeta^2\left(p^2-\frac{p}{q}\right) - \frac{4p}{9q}\zeta^2 = \zeta^4 - \zeta^2\left(p^2 - \frac{5p}{9q}\right)$$

and obtain

$$\int_{\frac{3}{2}p}^{\infty} |\mathscr{F}_s[r](\zeta)|\,\mathrm{d}\zeta \le \frac{4}{qc^2}\int_{\frac{3}{2}p}^{\infty}\frac{1}{\zeta^2-\left(\frac{c^2p^2+2}{c^2}\right)}\cdot\frac{1}{\zeta^2-\left(p^2-\frac{5p}{9q}\right)}\,\mathrm{d}\zeta$$
$$= \frac{1}{\frac{1}{2}qc^2\left(\frac{2}{c^2}+\frac{5p}{9q}\right)}\left[\frac{1}{\sqrt{\frac{c^2p^2+2}{c^2}}}\ln\left(\frac{\frac{3}{2}p+\sqrt{\frac{c^2p^2+2}{c^2}}}{\frac{3}{2}p-\sqrt{\frac{c^2p^2+2}{c^2}}}\right) - \frac{1}{\sqrt{p^2-\frac{5p}{9q}}}\ln\left(\frac{\frac{3}{2}p+\sqrt{p^2-\frac{5p}{9q}}}{\frac{3}{2}p-\sqrt{p^2-\frac{5p}{9q}}}\right)\right]$$
$$=: \frac{1}{q+\frac{5}{18}pc^2}\left[\varphi_1(\zeta)-\varphi_2(\zeta)\right] \tag{54}$$

with

$$\varphi_1(\zeta) := \frac{1}{\sqrt{\frac{c^2p^2+2}{c^2}}}\cdot\ln\left(\frac{\frac{3}{2}p+\sqrt{\frac{c^2p^2+2}{c^2}}}{\frac{3}{2}p-\sqrt{\frac{c^2p^2+2}{c^2}}}\right)$$

and

$$\varphi_2(\zeta) := \frac{1}{\sqrt{p^2 - \frac{5p}{9q}}} \cdot \ln\left(\frac{\frac{3}{2}p + \sqrt{p^2 - \frac{5p}{9q}}}{\frac{3}{2}p - \sqrt{p^2 - \frac{5p}{9q}}}\right).$$

The first factor of φ_1 is obviously increasing in c^2 and may therefore be estimated as

$$\frac{1}{\sqrt{\frac{c^2p^2+2}{c^2}}} = \sqrt{\frac{c^2}{c^2p^2+2}} \le \begin{cases} \sqrt{\dfrac{1}{p^2+2}} \le 0.47313, & c^2 \in [0.9, 1], \\ \sqrt{\dfrac{0.9}{0.9p^2+2}} \le 0.46178, & c^2 \in [0.83, 0.9]. \end{cases} \tag{55}$$

The second (logarithmic) factor of φ_1,

$$\varphi_{1,a} := \ln\left(\frac{\frac{3}{2}p + \sqrt{\frac{c^2p^2+2}{c^2}}}{\frac{3}{2}p - \sqrt{\frac{c^2p^2+2}{c^2}}}\right) \tag{56}$$

is decreasing because the derivative of

$$x \mapsto \frac{ax + \sqrt{x^2p^2+2}}{ax - \sqrt{x^2p^2+2}} \qquad \text{is} \qquad x \mapsto \frac{-4a}{\left(ax - \sqrt{x^2p^2+2}\right)^2 \sqrt{x^2p^2+2}} \qquad (a = \frac{3}{2}p),$$

which shows that the argument of the monotone function $\ln(\cdot)$ is decreasing. Moreover, the function $c^2 \mapsto \sqrt{\frac{c^2p^2+2}{c^2}}$ is convex, and both the first and the second derivative of $x \mapsto \ln\left(\frac{1+x}{1-x}\right)$ are positive. Thus the trivial formula $f(g(x))'' = f'(g(x))g''(x) + f''(g(x))\left[g'(x)\right]^2$ shows that the second factor $\varphi_{1,a}$ of φ_1 is altogether convex, and we may replace it by its linear interpolation on each of the intervals $[0.9, 1]$ and $[0.83, 0.9]$.

We turn to φ_2 and calculate, using (35) for q,

$$\begin{aligned} p^2 - \frac{5p}{9q} &= p\left[p - \frac{5(c^2p^2-2)}{9c^2(2-p)}\right] = \frac{2p}{9(2-p)} \cdot \left[\frac{9}{2}(2-p)\,p - \frac{5}{2}p^2 + \frac{5}{c^2}\right] \\ &= \frac{2p}{9(2-p)} \cdot \left[9p - 7p^2 + \frac{5}{c^2}\right]. \end{aligned}$$

This is obviously a decreasing function of c^2. The function $x \mapsto \frac{1}{x}\ln\left(\frac{1+x}{1-x}\right)$ is positive for $x \in (0, 1)$, and so is its first derivative. Thus the chain rule implies that φ_2 is decreasing in c^2 for $c^2 \in [0.83, 1]$. Below we will use $\varphi_2(1) \ge 0.94197$ and $\varphi_2(0.9) \ge 0.97804$.

We now use two interpolations and first consider the interval $[0.9, 1]$. Let $\overline{\varphi}_{1,a}$ be the affine function which agrees with the second factor $\varphi_{1,a}$ of φ_1 at $c^2 = 0.9$ and $c^2 = 1$. Then we have from (55)

$$\varphi_1 - \varphi_2 \le 0.47313 \cdot \overline{\varphi}_{1,a} - \varphi_2(1) \le 0.47313 \cdot \overline{\varphi}_{1,a} - 0.94197 = g_1 - g_2c^2$$

with

$$g_1 \approx 1.63104 \qquad \text{and} \qquad g_2 \approx 1.19443,$$

so that, with (35) and (54),

$$\int_{\frac{3}{2}p}^{\infty} \zeta \left|\mathscr{F}_s[r](\zeta)\right| \mathrm{d}\zeta \le \frac{g_1 - g_2c^2}{\frac{c^2(2-p)}{c^2p^2-2} + \frac{5}{18}pc^2} = \frac{18\,(c^2p^2-2)\,(g_1 - g_2c^2)}{c^2\,(5p^3c^2 + 36 - 28p)}.$$

The right-hand side attains its maximum for $c^2 \in [0.9, 1]$ near 0.99510, with a value there well below 0.34.

Similarly, for the second interval $[0.83, 0.9]$, let $\underline{\varphi}_{1,a}$ be the affine function which agrees with the second factor of φ_1 at $c^2 = 0.83$ and $c^2 = 0.9$. Then we have

$$\varphi_1 - \varphi_2 \leq 0.46178 \cdot \underline{\varphi}_{1,a} - \varphi_2(0.9) \leq 0.46178 \cdot \underline{\varphi}_{1,a} - 0.97804 = g_3 - g_4 c^2$$

with

$$g_3 \approx 2.05153 \qquad \text{and} \qquad g_4 \approx 1.74164,$$

and

$$\int_{\frac{3}{2}p}^{\infty} \zeta \left|\mathscr{F}_s\left[r\right](\zeta)\right| \mathrm{d}\zeta \leq \frac{g_3 - g_4 c^2}{\frac{c^2(2-p)}{c^2p^2-2} + \frac{5}{18}pc^2} = \frac{18\left(c^2p^2-2\right)\left(g_3 - g_4c^2\right)}{c^2\left(5p^3c^2 + 36 - 28p\right)}.$$

The right-hand side is increasing in $c^2 \in [0.83, 0.9]$ and therefore attains its maximum at 0.9, with a value there below 0.232. □

It remains to prove Lemma 4.6.

Proof of Lemma 4.6: By the form of the profile, for all $z \geq z_0 > 0$,

$$u_p(z) \geq \frac{2-p}{c^2p^2-p}\left[1 - \exp\left(-z_0\sqrt{\frac{p\left(c^2p^2-2\right)}{c^2(2-p)}}\right)\right]. \tag{57}$$

It is not hard to see that the factor in the square brackets is concave as function of c^2. Indeed, the fraction under the square root is, by elementary calculations, increasing, thus the argument of the exponential is decreasing, thus the exponential alone is convex, thus the expression in the square brackets is concave. We replace the square brackets by a linear interpolation to estimate this function from below.

First, we use this interpolation for $c^2 \in [0.9, 1]$ and $z_0 = 1$. We obtain by linear interpolation between $c^2 = 0.9$ and $c^2 = 1$

$$1 - \exp\left(-z_0\sqrt{\frac{p(c^2p^2-2)}{c^2(2-p)}}\right) \geq h_1 + h_2c^2$$

with

$$h_1 \approx -0.44452 \qquad \text{and} \qquad h_2 \approx 1.17413.$$

The factor $\frac{2-p}{c^2p^2-p}$ in (57) is decreasing in c^2 and positive. Since

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{t_1 + t_2x}{px - 1}\right) = \frac{(px-1)t_2 - (t_1 + t_2x)p}{(px-1)^2} = \frac{-t_1p - t_2}{(px-1)^2}$$

and $-h_1p - h_2 < 0$, we find that (57) with $z_0 = 1$ is decreasing as a function of $c^2 \in [0.9, 1]$. Thus for $c^2 \in [0.9, 1]$ and $z \geq 1$,

$$u(z) \geq \frac{2-p}{p^2-p}\left[1 - \exp\left(-\sqrt{\frac{p\left(p^2-2\right)}{2-p}}\right)\right] \geq 0.34926. \tag{58}$$

The argument for $z_0 = \frac{3}{2}$ is similar. It suffices to interpolate the square brackets in (57) linearly on the entire interval $c^2 \in [0.83, 1]$, and we obtain

$$1 - \exp\left(-\frac{3}{2}\sqrt{\frac{p(c^2p^2-2)}{c^2(2-p)}}\right) \geq h_3 + h_4 c^2$$

with

$$h_3 \approx -1.26496 \qquad \text{and} \qquad h_4 \approx 2.12436.$$

Now, by the same argument as above, $-h_3 p - h_4 < 0$ shows that (57) with $z_0 = \frac{3}{2}$ is decreasing in c^2 for $c^2 \in [0.83, 1]$. Thus we find for $c^2 \in [0.83, 0.9]$ and $z \geq \frac{3}{2}$,

$$u_p(z) \geq \frac{2-p}{p^2-p}\left[1 - \exp\left(-\frac{3}{2}\sqrt{\frac{p(p^2-2)}{2-p}}\right)\right] \geq 0.41139, \tag{59}$$

as claimed. □

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