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FRACTIONAL CONFORMAL LAPLACIANS AND FRACTIONAL YAMABE PROBLEMS

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Based on the relations between scattering operators of asymptotically hyperbolic metrics and Dirichlet-to-Neumann operators of uniformly degenerate elliptic boundary value problems observed by Chang and González, we formulate fractional Yamabe problems that include the boundary Yamabe problem studied by Escobar. We observe an interesting Hopf-type maximum principle together with interplay between analysis of weighted trace Sobolev inequalities and conformal structure of the underlying manifolds, which extends the phenomena displayed in the classic Yamabe problem and boundary Yamabe problem.

1. Introduction

In this paper, based on the relations between scattering operators of asymptotically hyperbolic metrics and Dirichlet-to-Neumann operators of uniformly degenerate elliptic boundary value problems observed in [Chang and González 2011], we formulate and solve fractional order Yamabe problems that include the boundary Yamabe problem studied in [Escobar 1992].

Suppose that X^{n+1} is a smooth manifold with smooth boundary M^n for $n \geq 3$. A function ρ is a defining function of the boundary M^n in X^{n+1} if

$$\rho > 0 \text{ in } X^{n+1} \quad \rho = 0 \text{ on } M^n, \quad d\rho \neq 0 \text{ on } M^n.$$

We say that g^+ is conformally compact if, for some defining function ρ, the metric $\bar{g} = \rho^2 g^+$ extends to $\overline{X}^{n+1}$ so that $(\overline{X}^{n+1}, \bar{g})$ is a compact Riemannian manifold. This induces a conformal class of metrics $\hat{h} = \bar{g}|_{TM^n}$ on M^n when defining functions vary. The conformal manifold $(M^n, [\hat{h}])$ is called the conformal infinity of (X^{n+1}, g^+). A metric g^+ is said to be asymptotically hyperbolic if it is conformally compact and the sectional curvature approaches -1 at infinity.

Graham and Zworski [2003] introduced the meromorphic family of scattering operators $S(s)$, which is a family of pseudodifferential operators, for a given asymptotically hyperbolic manifold (X^{n+1}, g^+) and a choice of the representative $\hat{h}$ of the conformal infinity $(M^n, [\hat{h}])$. Instead one often considers the normalized scattering operators

$$P_\gamma[g^+, \hat{h}] = 2^{2\gamma} \frac{\Gamma(\gamma)}{\Gamma(-\gamma)} S\Big(\frac{n}{2} + \gamma\Big).$$

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The normalized scattering operators $P_\gamma[g^+, \hat{h}]$ are conformally covariant,

$$P_\gamma[g^+, w^{4/(n-2\gamma)}\hat{h}]\phi = w^{-(n+2\gamma)/(n-2\gamma)} P_\gamma[g^+, \hat{h}](w\phi),$$

with principal symbol

$$\sigma(P_\gamma[g^+, \hat{h}]) = \sigma((-\Delta_{\hat{h}})^\gamma).$$

Hence they may be considered to be conformal fractional Laplacians for $\gamma \in (0, 1)$ for a given asymptotically hyperbolic metric g^+. As proven in [Graham and Zworski 2003; Fefferman and Graham 2012], when g^+ is Poincaré–Einstein, P_1 is the conformal Laplacian, P_2 is the Paneitz operator, and, in general, P_k for $k \in \mathbb{N}$ are the conformal powers of the Laplacian discovered in [Graham et al. 1992].

When g^+ is a fixed asymptotically hyperbolic metric, we may simply denote

$$P_\gamma^{\hat{h}} := P_\gamma[g^+, \hat{h}].$$

We will consider the associated "fractional order curvature"

$$Q_\gamma^{\hat{h}} = P_\gamma^{\hat{h}}(1)$$

and the normalized total curvature

$$I_\gamma[\hat{h}] = \frac{\int_{M^n} Q_\gamma^{\hat{h}} dv_{\hat{h}}}{\left(\int_{M^n} dv_{\hat{h}}\right)^{(n-2\gamma)/n}}.$$

When a background metric $\hat{h}$ is fixed, we may write

$$I_\gamma[w, \hat{h}] = I_\gamma[w^4/(n-2\gamma)\hat{h}] = \frac{\int_{M^n} w P_\gamma^{\hat{h}} w \, dv_{\hat{h}}}{\left(\int_{M^n} w^{2n/(n-2\gamma)} \, dv_{\hat{h}}\right)^{(n-2\gamma)/n}}.$$

This functional $I_\gamma[\hat{h}]$ is clearly an analogue to the Yamabe functional. Hence one may ask if there is a metric which is the minimizer of I_γ among metrics in the class $[\hat{h}]$ and whose curvature Q_γ is a constant. We will refer to that problem as a fractional Yamabe problem when $\gamma \in (0, 1)$. For the original Yamabe problem readers are referred to [Lee and Parker 1987; Schoen and Yau 1994]. A similar question was studied in [Qing and Raske 2006] for $\gamma > 1$ and g^+ being a Poincaré–Einstein metric. Because of the lack of a maximum principle, these generalized Yamabe problems are, in general, difficult to solve. Yet this new window to the analytic aspects of conformal geometry remains fascinating. For example, it was proven [Guillarmou and Qing 2010] that the location of the first scattering pole is dictated by the sign of the Yamabe constant and the Green's function of $P_\gamma^{\hat{h}}$ is positive for $\gamma \in (0, 1)$ when the Yamabe constant is positive, at least in the case where g^+ is conformally compact Einstein.

On the other hand, see [González 2012] for an interpretation of the fractional curvature Q_γ in relation to the first variation of some weighted volume. The singular version of the fractional Yamabe problem has been considered in [González et al. 2012], but there are still many open questions in this field.

It turns out that one may use the relations of scattering operators and the Dirichlet-to-Neumann operators to reformulate the above fractional Yamabe problems as degenerate elliptic boundary value problems. The correspondence between pseudodifferential equations and degenerate elliptic boundary value problems is inspired by [Caffarelli and Silvestre 2007]. Interestingly, the corresponding degenerate elliptic boundary value problem is a natural extension of the boundary Yamabe problem raised and studied in [Escobar 1992].

Recall from [Chang and González 2011] that, given an asymptotically hyperbolic manifold (X^{n+1}, g^+) and a representative $\hat{h}$ of the conformal infinity $(M^n, [\hat{h}])$, one can find a geodesic defining function ρ such that the compactified metric can be written as

$$\bar{g} := \rho^2 g^+ = d\rho^2 + h_\rho = d\rho^2 + \hat{h} + h^{(1)}\rho + h^{(2)}\rho^2 + o(\rho^2)$$

near infinity. One may consider the degenerate elliptic boundary value problem of $\bar{g}$ as follows:

$$\begin{cases} -\operatorname{div}(\rho^a \nabla U) + E(\rho)U = 0 & \text{in } (X^{n+1}, \bar{g}), \\ U|_{\rho=0} = f & \text{on } M^n, \end{cases} \tag{1-1}$$

where

$$E(\rho) = \rho^{-1-s}(-\Delta_{g^+} - s(n-s))\rho^{n-s},$$

$s = n/2 + \gamma$, and $a = 1 - 2\gamma$.

Lemma 1.1 [Chang and González 2011]. *Let (X^{n+1}, g^+) be an asymptotically hyperbolic manifold. Suppose that U is the solution to the boundary value problem (1-1). Then*

(1) *for $\gamma \in (0, 1/2)$ and $-n^2/4 + \gamma^2$ not an L^2-eigenvalue for the Laplacian of g^+,*

$$P_\gamma[g^+, \hat{h}]f = -d_\gamma^* \lim_{\rho \to 0} \rho^a \partial_\rho U, \tag{1-2}$$

where

$$d_\gamma^* = -\frac{2^{2\gamma-1}\Gamma(\gamma)}{\gamma\Gamma(-\gamma)}; \tag{1-3}$$

(2) *for $\gamma = 1/2$,*

$$P_{1/2}[g^+, \hat{h}]f = -\lim_{\rho \to 0} \partial_\rho U + \frac{n-1}{2} Hf,$$

where $H := (1/(2n)) \operatorname{Tr}_{\hat{h}}(h^{(1)})$ is the mean curvature of M;

(3) *for $\gamma \in (1/2, 1)$, (1-2) still holds if $H = 0$.*

In light of Lemma 1.1, consider, for $\gamma \in (0, 1)$,

$$I_\gamma^*[U, \bar{g}] = \frac{d_\gamma^* \int_{X^{n+1}} (\rho^a |\nabla U|^2 + E(\rho)U^2)\, dv_{\bar{g}}}{\int_{M^n} U^{2n/(n-2\gamma)}\, dv_{\hat{h}}}.$$

It is then a very natural variational problem for I_γ^*. For instance, right away one sees that a minimizer of I_γ^* is automatically nonnegative, which was a huge issue for the functional I_γ.

One key ingredient in our work here is the following Hopf-type maximum principle. We drew inspiration from some version of Hopf's lemma for the Euclidean half space case [Cabré and Sire 2010, Proposition 4.11].

Proposition 1.2. *Let $\gamma \in (0, 1)$. Suppose U is a nonnegative solution to (1-1) in X^{n+1}. Let $p_0 \in M^n = \partial X^{n+1}$ and B_r be a geodesic ball of radius r centered at p_0 in M^n. Then, for sufficiently small r_0, if*

$U(q_0) = 0$ for $q_0 \in B_{r_0} \setminus \overline{B_{1/2r_0}}$ and $U > 0$ on $\partial B_{1/2r_0}$,

$$y^a \partial_y U|_{q_0} > 0. \tag{1-4}$$

It seems weaker than the original one, but it suffices for our purposes. A nice and immediate consequence of the above maximum principle is that the first eigenfunction of the fractional conformal Laplacian $P_\gamma^{\hat{h}}$ is always positive, which has been a rather challenging question in general for the pseudodifferential operators $P_\gamma^{\hat{h}}$; see [Guillarmou and Qing 2010]. Hence one can produce a metric in the class $[\hat{h}]$ that has positive, negative, or zero Q_γ curvature when the first eigenvalue is positive, negative, or zero.

Our approach to solving the γ-Yamabe problem is very similar to that taken in [Escobar 1992], where one of the crucial steps is the understanding of a trace inequality. In our case, the relevant sharp weighted trace Sobolev inequality appears in [Lieb 1983; Cotsiolis and Tavoularis 2004; Nekvinda 1993].

Proposition 1.3. *Let $\gamma \in (0, 1)$ and $a = 1 - 2\gamma$. Suppose that $U \in W^{1,2}(\mathbb{R}^{n+1}_+, y^a)$ with trace $TU = w$. Then, for some constant $\bar{S}(n, \gamma)$,*

$$\|w\|^2_{L^{2^*}(\mathbb{R}^n)} \le \bar{S}(n, \gamma) \int_{\mathbb{R}^{n+1}_+} y^a |\nabla U|^2 \, dx \, dy, \tag{1-5}$$

where $2^* = 2n/(n - 2\gamma)$. Moreover the equality holds if and only if

$$w(x) = c\left(\frac{\mu}{|x - x_0|^2 + \mu^2}\right)^{(n-2\gamma)/2}, \quad x \in \mathbb{R}^n,$$

for $c \in \mathbb{R}$, $\mu > 0$ and $x_0 \in \mathbb{R}^n$ fixed, and U is its Poisson extension of w as given in (2-13).

As in the case of the original Yamabe problem, one can define the γ-Yamabe constant

$$\Lambda_\gamma(M^n, [\hat{h}]) = \inf_{h \in [\hat{h}]} I_\gamma[h].$$

It is then easily seen that

$$\Lambda_\gamma(S^n, [g_c]) = \frac{d^*_\gamma}{\bar{S}(n, \gamma)}$$

where $[g_c]$ is the canonical conformal class of metrics on the sphere S^n. Analogous to the cases of the original Yamabe problem, we obtain the following.

Theorem 1.4. *Suppose that (X^{n+1}, g^+) is an asymptotically hyperbolic manifold. Suppose, in addition, that $H = 0$ when $\gamma \in (1/2, 1)$. Then, if*

$$-\infty < \Lambda_\gamma(M, [\hat{h}]) < \Lambda_\gamma(S^n, [g_c]), \tag{1-6}$$

the γ-Yamabe problem is solvable for $\gamma \in (0, 1)$.

Remark. It is easily seen that $\Lambda_\gamma(M, [\hat{h}]) > -\infty$ in light of (1.4) in Theorems 1.1 and 1.2 of [Jin and Xiong 2013] when $\gamma \in (0, 1/2]$ or if some additional assumptions in Theorem 1.2 of [Jin and Xiong 2013] hold.

Based on computations similar to ones in [Escobar 1992], we have the following.

Theorem 1.5. *Suppose that (X^{n+1}, g^+) is an asymptotically hyperbolic manifold and that*

$$\rho^{-2}(R[g^+]-\mathrm{Ric}[g^+](\rho\partial_\rho)+n^2)\to 0 \quad \text{as } \rho\to 0. \tag{1-7}$$

If X^{n+1} has a nonumbilic point on ∂X^{n+1} and

$$\frac{n+a-3}{1-a}2^{2\gamma+1}\frac{\Gamma(\gamma)}{\Gamma(-\gamma)}+\frac{n-1+a}{a+1}<0, \tag{1-8}$$

then

$$\Lambda_\gamma(M,[\hat{h}])<\Lambda_\gamma(S^n,[g_c])$$

and hence the γ-Yamabe problem is solvable for $\gamma\in(0,1)$.

We remark now that the $1/2$-Yamabe problem introduced here reduces back to the boundary Yamabe problem considered in [Escobar 1992] in this way. Notice that, in this case, we have

$$I^*_{1/2}[U,\phi^{4/n-1}\bar{g}]=I^*_{1/2}[U\phi,\bar{g}] \tag{1-9}$$

for any positive function ϕ on $\overline{X}^{n+1}$, and therefore (1-7) is no longer needed. Also notice that the condition (1-8) becomes $n>5$ when $\gamma=1/2$, which agrees with the conclusion in [Escobar 1992].

Suppose we start with a compact Riemannian manifold $(X^{n+1},\bar{g})$ and its boundary $(M^n,\hat{h})$. Then one can construct an asymptotically hyperbolic manifold (X^{n+1},g^+) which is conformal to $(X^{n+1},\bar{g})$. For example, as observed in [Chang and González 2011], one may, according to [Mazzeo 1991; Andersson et al. 1992], require that

$$R[g^+]=-n(n+1). \tag{1-10}$$

Then the induced degenerate equation becomes

$$-\operatorname{div}(\rho^a\nabla U)+\frac{n-1+a}{4n}R[\bar{g}]\rho^a U=0 \quad \text{in } (X^{n+1},\bar{g}), \tag{1-11}$$

whose associated variational functional becomes

$$F[U]=\int_X \rho^a|\nabla U|^2_{\bar{g}}\,dv_{\bar{g}}+\frac{n-1+a}{4n}\int_X R[\bar{g}]\rho^a|U|^2\,dv_{\bar{g}}. \tag{1-12}$$

In Section 2 we recall [Chang and González 2011] to make possible the passage from pseudodifferential equations to second order elliptic boundary value problems as in [Caffarelli and Silvestre 2007]. In Section 3 we study regularity (L^∞ and Schauder estimates) for degenerate elliptic boundary value problems, and, more importantly, we establish the Hopf-type maximum principle. In Section 4 we formulate the fractional Yamabe problem and obtain some properties for the fractional case that are analogous to the original Yamabe problem with the help of the Hopf-type maximum principle. In Section 5 we analyze sharp weighted Sobolev trace inequalities. We define, on any conformal manifold, the fractional Yamabe constant associated with an asymptotically hyperbolic metric, and show that one of the standard round spheres associated to the standard hyperbolic metric is the largest. In Section 6 we take a subcritical approximation and prove Theorem 1.4. In Section 7 we adopt the calculation from [Escobar 1992] and prove Theorem 1.5 by choosing a suitable test function.

We finally mention the two related works [Barrios et al. 2012; Servadei 2013] on nonlinearities with critical exponents for the fractional Laplacian.

2. Conformal fractional Laplacians

In this section we introduce [Chang and González 2011] to relate two equivalent definitions of conformal fractional Laplacians. Conformal fractional Laplacians are defined via scattering theory on asymptotically hyperbolic manifolds [Graham and Zworski 2003; Fefferman and Graham 2012]. We have also seen fractional Laplacians defined as Dirichlet-to-Neumann operators for degenerate equations on compact manifolds with boundary [Caffarelli and Silvestre 2007]. It turns out that, in some way, these two fractional Laplacians are the same.

Let X^{n+1} be a smooth manifold of dimension $n+1$ with compact boundary $\partial X = M^n$. A function ρ is a *defining function* of ∂X in X if

$$\rho > 0 \text{ in } X, \quad \rho = 0 \text{ on } \partial X, \quad d\rho \neq 0 \text{ on } \partial X.$$

We say that g^+ is *conformally compact* if the metric $\bar{g} = \rho^2 g^+$ extends to $\bar{X}^{n+1}$ for a defining function ρ so that $(\bar{X}^{n+1}, \bar{g})$ is a compact Riemannian manifold. This induces a conformal class of metrics $\hat{h} = \bar{g}|_{TM^n}$ on M^n when the defining function varies, which is called the *conformal infinity* of (X^{n+1}, g^+). A metric g^+ is said to be *asymptotically hyperbolic* if it is conformally compact and the sectional curvature approaches -1 at infinity.

Given an asymptotically hyperbolic manifold (X^{n+1}, g^+) and a representative $\hat{h}$ of the conformal infinity $(M^n, [\hat{h}])$, there exists a uniquely geodesic defining function ρ such that, on a neighborhood $M \times (0, \delta)$ in X, g^+ has the normal form

$$g^+ = \rho^{-2}(d\rho^2 + h_\rho) \tag{2-1}$$

where h_ρ is a one parameter family of metrics on M such that

$$h_\rho = \hat{h} + h^{(1)}\rho + O(\rho^2). \tag{2-2}$$

From [Mazzeo and Melrose 1987; Graham and Zworski 2003] it follows that, given $f \in \mathscr{C}^\infty(M)$, $\mathrm{Re}(s) > n/2$ and $s(n-s)$ is not an L^2-eigenvalue for $-\Delta_{g^+}$, the generalized eigenvalue problem

$$-\Delta_{g^+}u - s(n-s)u = 0 \quad \text{in } X \tag{2-3}$$

has a solution of the form

$$u = F\rho^{n-s} + G\rho^s, \quad F, G \in \mathscr{C}^\infty(\bar{X}), \quad F|_{\rho=0} = f. \tag{2-4}$$

The *scattering operator* on M is then defined as

$$S(s)f = G|_M.$$

It is shown in [Graham and Zworski 2003] that, by a meromorphic continuation, $S(s)$ is a meromorphic family of pseudodifferential operators in the whole complex plane. Instead, it is often useful to consider the normalized scattering operators $P_\gamma[g^+, \hat{h}]$ defined as

$$P_\gamma[g^+, \hat{h}] := d_\gamma S\Big(\frac{n}{2}+\gamma\Big), \quad d_\gamma = 2^{2\gamma}\frac{\Gamma(\gamma)}{\Gamma(-\gamma)}. \tag{2-5}$$

Note that $s = n/2+\gamma$. With this regularization the principal symbol of $P_\gamma[g^*, \hat{h}]$ is exactly the principal symbol of the fractional Laplacian $(-\Delta_{\hat{h}})^\gamma$. Hence we will call (assuming implicitly the dependence on the extension metric g^+)

$$P_\gamma^{\hat{h}} := P_\gamma[g^+, \hat{h}]$$

a conformal fractional Laplacian for each $\gamma \in (0, 1)$ which is not a pole of the scattering operator, that is, $n^2/4-\gamma^2$ is not an L^2-eigenvalue for $-\Delta_{g^+}$. It is a conformally covariant operator, in the sense that it behaves like

$$P_\gamma^{\hat{h}_w}\varphi = w^{-(n+2\gamma)/(n-2\gamma)} P_\gamma^{\hat{h}}(w\varphi) \tag{2-6}$$

for a conformal change of metric $\hat{h}_w = w^{4/(n-2\gamma)}\hat{h}$. We will call

$$Q_\gamma^{\hat{h}} = P_\gamma^{\hat{h}}(1)$$

the fractional scalar curvature associated to the conformal fractional Laplacian $P_\gamma^{\hat{h}}$. From (2-6) we have

$$P_\gamma^{\hat{h}}(w) = Q_\gamma^{\hat{h}_w} w^{(n+2\gamma)/(n-2\gamma)}. \tag{2-7}$$

The familiar case is $\gamma = 1$, where

$$P_1^{\hat{h}} = -\Delta_{\hat{h}} + \frac{n-2}{4(n-1)}R[\hat{h}]$$

becomes the conformal Laplacian and the associated curvature is the scalar curvature

$$Q_1^{\hat{h}} = (n-2)/(4(n-1))R[\hat{h}]$$

of the metric $\hat{h}$ which undergoes the change

$$P_1^{\hat{h}} w = \frac{n-2}{4(n-1)}R[\hat{h}_w]w^{(n+2)/(n-2)}$$

when taking conformal change of metrics, provided that $(X^{n+1},\ g^+)$ is a Poincaré–Einstein as established in [Graham and Zworski 2003; Fefferman and Graham 2012]. The conformal fractional Laplacians and fractional scalar curvatures should also be compared to the higher order generalization of the conformal Laplacian and scalar curvature, the Paneitz operator $P_2^{\hat{h}}$ and its associated Q-curvature; see [Paneitz 2008; Branson 1995; Qing and Raske 2006].

It was observed in [Chang and González 2011] that the generalized eigenvalue problem (2-3) on a noncompact manifold (X^{n+1}, g^+) is equivalent to a linear degenerate elliptic problem on the compact manifold $(\overline{X}^{n+1}, \bar{g})$, for $\bar{g} = \rho^2 g^+$. Hence Chang and González reconciled the definition of the fractional Laplacians given above as normalized scattering operators and the one given in the spirit of the Dirichlet-to-Neumann operators by Caffarelli and Silvestre [2007]. This observation plays a fundamental role in this paper and provides an alternative way to study the fractional partial differential equation (2-7). First, we know by the conformal covariance that

$$P_1^{g^+}u = \rho^{(n+3)/2} P_1^{\bar{g}}(\rho^{-(n-1)/2}u).$$

Let $a = 1-2\gamma \in (-1, 1)$, $s = n/2+\gamma$, and $U = \rho^{s-n}u$. Then we may write (2-3) as

$$-\operatorname{div}(\rho^a \nabla_{\bar{g}} U) + E(\rho)U = 0 \quad \text{in } (X^{n+1}, \bar{g}),$$

where

$$E(\rho) := \rho^{a/2} P_1^{\bar{g}} \rho^{a/2} - \Big(s(n-s) + \frac{n-1}{4n} R[g^+]\Big)\rho^{a-2}, \tag{2-8}$$

or, writing everything back in the metric g^+,

$$E(\rho) = \rho^{-1-s}(-\Delta_{g^+} - s(n-s))\rho^{n-s}. \tag{2-9}$$

Notice that, in a neighborhood $M \times (0, \delta)$ where the metric g^+ is in the normal form

$$E(\rho) = \frac{n-1+a}{4n}\big(R[\bar{g}] - (n(n+1) + R[g^+])\rho^{-2}\big)\rho^a \quad \text{in } M \times (0, \delta). \tag{2-10}$$

Proposition 2.1 [Chang and González 2011]. *Let (X^{n+1}, g^+) be an asymptotically hyperbolic manifold. Then, given $f \in \mathscr{C}^\infty(M)$, the generalized eigenvalue problem (2-3) and (2-4) is equivalent to*

$$\begin{cases} -\operatorname{div}(\rho^a \nabla U) + E(\rho)U = 0 & \textit{in } (X, \bar{g}), \\ U|_{\rho=0} = f & \textit{on } M, \end{cases} \tag{2-11}$$

where $U = \rho^{n-s}u$ and U is the unique minimizer of the energy

$$F[V] = \int_X \rho^a |\nabla V|_{\bar{g}}^2 \, dv_{\bar{g}} + \int_X E(\rho)|V|^2 \, dv_{\bar{g}}$$

among all the functions $V \in W^{1,2}(X, \rho^a)$ with fixed trace $V|_{\rho=0} = f$. Moreover,

(1) *for $\gamma \in (0, 1/2)$,*

$$P_\gamma^{\hat{h}} f = -d_\gamma^* \lim_{\rho \to 0} \rho^a \partial_\rho U, \tag{2-12}$$

where the constant d_γ^* is given in (1-3);

(2) *for $\gamma = 1/2$, we have an extra term*

$$P_{1/2}^{\hat{h}} f = -\lim_{\rho \to 0} \partial_\rho U + \frac{n-1}{2} H f,$$

where $H := (1/(2n)) \operatorname{Tr}_{\hat{h}}(h^{(1)})$ is the mean curvature of M;

(3) *for $\gamma \in (1/2, 1)$, (2-12) still holds if and only if $H = 0$.*

Remark. It should be noted here that there are many asymptotically hyperbolic manifolds (X^{n+1}, g^+) whose conformal infinity is prescribed as $(M^n, [\hat{h}])$. If one insists on (X^{n+1}, g^+) being Poincaré–Einstein, then the normalized scattering operators $P_\gamma^{\hat{h}}$ are a bit more intrinsic, at least at positive integers as observed in [Graham and Zworski 2003; Fefferman and Graham 2012]. It should also be noted that one can simply start with a compact Riemannian manifold $(\overline{X}^{n+1}, \bar{g})$ with boundary $(M^n, \hat{h})$ and easily build an asymptotically hyperbolic manifold whose conformal infinity is given by $(M^n, [\hat{h}])$. Please see the details of this observation in [Chang and González 2011].

The simplest example of a conformally compact Einstein manifold is the hyperbolic space $(\mathbb{H}^{n+1}, g_{\mathbb{H}})$. It can be characterized as the upper half-space (with coordinates $x \in \mathbb{R}^n$, $y \in \mathbb{R}_+$), endowed with the metric

$$g^+ = \frac{dy^2 + |dx|^2}{y^2}.$$

Then (2-11) with Dirichlet condition w reduces to

$$\begin{cases} -\operatorname{div}(y^a \nabla U) = 0 & \text{in } \mathbb{R}^{n+1}_+, \\ U|_{y=0} = w & \text{on } \mathbb{R}^n, \end{cases}$$

and the fractional Laplacian at the boundary $\mathbb{R}^n$ is just

$$P_\gamma^{|dx|^2} w = (-\Delta_{|dx|^2})^\gamma w = -d_\gamma^* \lim_{y\to 0}(y^a \partial_y U).$$

This is precisely the Caffarelli–Silvestre extension [2007]. Note that this extension U can be written in terms of the Poisson kernel K_γ as follows:

$$U(x, y) = K_\gamma *_x w = C_{n,\gamma} \int_{\mathbb{R}^n} \frac{y^{1-a}}{(|x-\xi|^2 + |y|^2)^{(n+1-a)/2}} w(\xi)\, d\xi, \tag{2-13}$$

for some constant $C_{n,\gamma}$. Moreover, given $w \in H^\gamma(\mathbb{R}^n)$, U is the minimizer of the functional

$$F[V] = \int_{\mathbb{R}^{n+1}_+} y^a |\nabla V|^2\, dx\, dy$$

among all the possible extensions in the set

$$\left\{ V : \mathbb{R}^{n+1}_+ \to \mathbb{R} : \int_{\mathbb{R}^{n+1}_+} y^a |\nabla V|^2\, dx\, dy < \infty,\ V(\,\cdot\,, 0) = w \right\}.$$

Based on (2-9), it is observed in [Chang and González 2011] that one may use

$$\rho^* = v^{1/(n-s)}$$

as a defining function, where v solves

$$-\Delta_{g^+} v - s(n-s)v = 0$$

and $\rho^{s-n} v = 1$ on M, to eliminate $E(\rho^*)$ from (2-11). It suffices to show that v is strictly positive in the interior. But this is true because, away from the boundary, it is the solution of a uniformly elliptic equation in divergence form. Thus it cannot have a nonpositive minimum. Hence we arrive at an improvement of Proposition 2.1 as follows.

Proposition 2.2. *The function ρ^* is a defining function of M in X such that $E(\rho^*) \equiv 0$. Hence $U = (\rho^*)^{s-n} u$ solves*

$$\begin{cases} -\operatorname{div}((\rho^*)^a \nabla U) = 0 & \text{in } (X, \bar g^*), \\ U = w & \text{on } M, \end{cases} \tag{2-14}$$

with respect to the metric $\bar g^* = (\rho^*)^2 g^+$ and U is the unique minimizer of the energy

$$F[V] = \int_X (\rho^*)^a |\nabla V|^2_{\bar g^*} \, dv_{\bar g^*} \tag{2-15}$$

among all the extensions $V \in W^{1,2}(X, (\rho^*)^a)$ satisfying $V|_M = w$. Moreover,

$$\rho^*(\rho) = \rho \left[1 + \frac{Q_\gamma^{\hat h}}{(n-s)(-d_\gamma^*/(2\gamma))} \rho^{2\gamma} + O(\rho^2) \right]$$

near infinity and

$$P_\gamma^{\hat h} w = -d_\gamma^* \lim_{\rho^* \to 0} (\rho^*)^a \partial_{\rho^*} U + w Q_\gamma^{\hat h}, \tag{2-16}$$

provided that $H = 0$ when $\gamma \in (1/2, 1)$.

We will sometimes use the defining function ρ^*, denoted by y unless explicitly stated otherwise, because it allows us to work with a pure divergence equation with no lower order terms.

We end this section by discussing the assumption that $H = 0$ for an asymptotically hyperbolic metric g^+. It turns out that this indeed is an intrinsic condition.

Lemma 2.3. *Suppose that (X^{n+1}, g^+) is an asymptotically hyperbolic manifold and that ρ and $\tilde\rho$ are the geodesic defining functions of M in X associated with representatives $\hat h$ and $\tilde h$ of the conformal infinity $(M^n, [\hat h])$, respectively. Hence*

$$g^+ = \rho^{-2}(d\rho^2 + h_\rho) = \tilde\rho^{-2}(d\tilde\rho^2 + \tilde h_{\tilde\rho})$$

where

$$h_\rho = \hat h + \rho h^{(1)} + O(\rho^2) \quad \text{and} \quad \tilde h_{\tilde\rho} = \tilde h + \tilde\rho \tilde h^{(1)} + O(\tilde\rho^2)$$

near infinity. Then $\tilde h^{(1)} = h^{(1)}$ on M. In particular

$$H = \frac{\tilde\rho}{\rho}\Big|_{\rho=0} \widetilde H \quad \text{on } M.$$

Proof. This simply follows from the equations that define the geodesic defining functions. Let

$$\tilde\rho = e^w \rho$$

near infinity. Then

$$1 = |d(e^w \rho)|^2_{e^{2w}\rho^2 g^+} = |d\rho|^2_{\rho^2 g^+} + 2\rho \langle dw, d\rho \rangle_{\rho^2 g^+} + \rho^2 |dw|^2_{\rho^2 g^+},$$

which implies

$$2\frac{\partial w}{\partial \rho} + \rho \left[\left(\frac{\partial w}{\partial \rho} \right)^2 + |\nabla w|^2_{h_\rho} \right] = 0.$$

Hence it is rather obvious that $\partial w/\partial\rho = 0$ at $\rho = 0$. Therefore the proof is complete, since

$$\tilde g = \tilde\rho^2 g^+ = e^{2w}\rho^2 g^+ = e^{2w}\bar g. \qquad \square$$

3. Uniformly degenerate elliptic equations

Considering the fractional powers of the Laplacian as Dirichlet-to-Neumann operators in Proposition 2.2 allows us to relate the properties of nonlocal operators to those of uniformly degenerate elliptic equations in one more dimension. The same strategy has been used, for instance, in [Cabré and Sire 2010].

Fix $\gamma \in (0, 1)$. Let $y = \rho^*$ be the special defining function given in Proposition 2.2 and set $\bar g^* = y^2 g^+$. We are concerned with the uniformly degenerate elliptic equation

$$\begin{cases} -\operatorname{div}(y^a \nabla U) = 0 & \text{in } (X, \bar g^*), \\ U = w & \text{on } M. \end{cases} \tag{3-1}$$

For our purpose we concentrate on the local behaviors of the solutions to (3-1) near the boundary. First, we write our equation in local coordinates near a fixed boundary point $(p_0, 0)$. More precisely, for some $R > 0$, we set

$$\begin{aligned} B_R^+ &= \{(x, y) \in \mathbb{R}^{n+1} : y > 0, |(x, y)| < R\}, \\ \Gamma_R^0 &= \{(x, 0) \in \partial\mathbb{R}_+^{n+1} : |x| < R\}, \\ \Gamma_R^+ &= \{(x, y) \in \mathbb{R}^{n+1} : y \ge 0, |(x, y)| = R\}. \end{aligned}$$

In local coordinates on Γ_R^0 the metric $\hat h$ is of the form $|dx|^2(1 + O(|x|^2))$, where $x(p_0) = 0$. Consider the matrix

$$A(x, y) = \sqrt{|\det \bar g^*|}\, y^a (\bar g^*)^{-1}.$$

Then (3-1) is equivalent to

$$\sum_{i,j=1}^{n+1} \partial_i (A_{ij} \partial_j U) = 0. \tag{3-2}$$

Moreover, we know that

$$\frac{1}{c} y^a I \le A \le c y^a I. \tag{3-3}$$

This shows that (3-2) is a uniformly degenerate elliptic equation. For instance, the weight $\psi(y) = y^a$ is an $\mathcal{A}_2$ weight in the sense of [Muckenhoupt 1972]. Equation (3-2) has been well understood in a series of papers by Fabes, Jerison, Kenig, and Serapioni [Fabes et al. 1982b; Fabes et al. 1982a]. Let us state a regularity result that is relevant to us. We will concentrate on problems of the form

$$\begin{cases} \operatorname{Div}(A(DU)) = 0 & \text{in } B_R^+, \\ -y^a \partial_y U = F, & \text{on } \Gamma_R^0, \end{cases} \tag{3-4}$$

where, for the rest of the section, A satisfies the ellipticity condition (3-3) for $a \in (-1, 1)$, the derivatives are Euclidean, that is, $D := (\partial_{x_1}, \dots, \partial_{x_n}, y)$, and

$$\mathrm{Div}(A(DU)) := \sum_{i,j=1}^{n+1} \partial_i (A_{ij} \partial_j U).$$

Definition 3.1. Given $R > 0$ and a function $F \in L^1(\Gamma_R^0)$, we call U a weak solution of (3-4) if U satisfies

$$(DU)^t A(DU) \in L^1(B_R^+)$$

and

$$\int_{B_R^+} (D\phi)^t A(DU)\, dx\, dy - \int_{\Gamma_R^0} F\phi\, dx = 0$$

for all $\phi \in \mathscr{C}^1(\overline{B_R^+})$ such that $\phi \equiv 0$ on Γ_R^+ and $(D\xi)^t A(D\phi) \in L^1(B_R^+)$.

Hölder regularity for weak solutions was shown in [Fabes et al. 1982b, Lemma 2.3.12] for any A satisfying (3-3). Using this main result, regularity of weak solutions up to the boundary was carefully shown in [Cabré and Sire 2010, Lemma 4.3], at least when $A = y^a I$. However, their proof only depends on the divergence structure of the equation and the behavior of the weight. Hence we have the following.

Proposition 3.2. *Let $\gamma \in (0, 1)$, $\gamma = (1-a)/2$ and $\beta \in (0, \min\{1, 1-a\})$. Let $R > 0$ and*

$$U \in L^\infty(B_{2R^+}) \cap W^{1,2}(B_{2R}^+, y^a)$$

be a weak solution of

$$\begin{cases} \mathrm{Div}(A(DU)) = 0 & \text{in } B_{2R}^+, \\ -y^a \partial_y U = F(U) & \text{on } \Gamma_{2R}^0, \end{cases} \tag{3-5}$$

for A satisfying (3-3). If $F \in \mathscr{C}^{1,\beta}$, $U \in \mathscr{C}^{0,\tilde\beta}(\overline{B_R^+})$ and $\partial_{x_i} U \in \mathscr{C}^{0,\tilde\beta}(\overline{B_R^+})$, $i = 1, \dots, n$, for some $\tilde\beta \in (0, 1)$.

Particularly, when $F(x,t) = \alpha(x)t + \beta(x)t^{(n+2\gamma)/(n-2\gamma)}$, to get smoothness it is necessary to know the local boundedness of weak solutions U on $\overline{B_R^+}$. To get this local boundedness for weak solutions, we employ the usual Moser iteration scheme adapted to boundary valued problems (see Theorem 3.4). However, a new idea is required: we will perform two coupled iterations, one in the interior and one at the boundary, that need to be handled simultaneously. Note that in the linear case when $F \equiv 0$, local boundedness was shown in [Fabes et al. 1982b, Corollary 2.3.4], using the weighted Sobolev embeddings in the interior described in Proposition 3.3. However, when a nonlinearity $F(U)$ is present at the boundary term, instead we need to use weighted trace Sobolev embeddings. (For the half-Laplacian with some particular nonlinearlities, L^∞ estimates were shown in [González and Monneau 2012].)

First, we recall a weighted Sobolev embedding theorem in the interior (compare [Fabes et al. 1982b, Theorem 1.3]; see also [Chiarenza and Frasca 1985]).

Proposition 3.3. *Let Ω be an open bounded set in $\mathbb{R}^{n+1}$. Take $1 < p < \infty$. There exist positive constants C_Ω and δ such that for all $u \in \mathscr{C}_0^\infty(\Omega)$ and all k satisfying $1 \le k \le (n+1)/n + \delta$,*

$$\|u\|_{L^{kp}(\Omega, y^a)} \le C_\Omega \|\nabla u\|_{L^p(\Omega, y^a)}.$$

C_Ω may be taken to depend only on n, p, a, and the diameter of Ω.

Now we can state the theorem. Note that we actually prove it in the flat case but it is straightforward to generalize it to the manifold setting.

Theorem 3.4. *Let U be a weak solution of the problem*

$$\begin{cases} \operatorname{div}(y^a \nabla U) = 0 & \text{in } B_{2R}^+, \\ -y^a \partial_y U = F(U) & \text{on } \Gamma_{2R}^0, \end{cases} \tag{3-6}$$

where $F(z)$ satisfies

$$F(z) = O(|z|^{\beta-1}),$$

when $|z| \to \infty$ for some $2 < \beta < 2^*$. Assume, in addition, that $\int_{\Gamma_{2r_0}^0} |U|^{2^*}\, dx =: V < \infty$. Then, for each $\bar{p} > 1$, there exists a constant $C_{\bar{p}} = C(\bar{p}, V) > 0$ such that

$$\sup_{B_R^+} |U| + \sup_{\Gamma_R^0} |U| \leq C_{\bar{p}} \Big[\Big(\frac{1}{R^{n+1+a}} \Big)^{1/\bar{p}} \|U\|_{L^{\bar{p}}(B_{2R}, y^a)} + \Big(\frac{1}{R^n} \Big)^{1/\bar{p}} \|U\|_{L^{\bar{p}}(\Gamma_{2R}^0)} \Big].$$

Proof. Let $p \in \partial X$. Note that we can work with normal coordinates $x_1, \dots, x_n \in \mathbb{R}^n$, $y > 0$ near p. Without loss of generality, assume that $R = 1$. Then the general case is obtained by rescaling. Let $\eta = \eta(r)$, $r = (|x|^2 + y^2)^{1/2}$, be a smooth cutoff function such that $\eta = 1$ if $r < 1$, $\eta = 0$ if $r \geq 2$, $0 \leq \eta \leq 1$ if $r \in (1, 2)$. Next, by working with $U^+ := \max\{U, 0\}$, $U^- := \max\{-U, 0\}$ separately, we can assume that U is positive.

A good reference for Moser iteration arguments in divergence structure equations is [Gilbarg and Trudinger 1983, Chapter 8]. We generalize this method, considering a double iteration: one at the boundary, using Sobolev trace inequalities to handle the nonlinear term $F(U)$, the other in the interior domain.

The first step is to use that U is a weak solution of (3-6) by finding a good test function. Formally we can write the following: multiply (3-6) by $\eta^2 U^\alpha$ and integrate by parts:

$$0 = 2 \int_{B_2^+} y^a \eta U^\alpha \nabla \eta \nabla U \, dx\, dy + \alpha \int_{B_2^+} y^a \eta^2 U^{\alpha-1} |\nabla U|^2 \, dx\, dy + \int_{\Gamma_2^0} \eta^2 U^\alpha F(U)\, dx. \tag{3-7}$$

This implies, using Hölder estimates to handle the crossed term,

$$\int_{B_2^+} y^a \eta^2 U^{\alpha-1} |\nabla U|^2 \, dx\, dy \leq \frac{2}{\alpha} \int_{\Gamma_2^0} \eta^2 U^\alpha F(U)\, dx + \frac{4}{\alpha^2} \int_{B_2^+} y^a |\nabla \eta|^2 U^{\alpha+1} \, dx\, dy. \tag{3-8}$$

On the other hand, again using Hölder's inequality, we have

$$\int_{B_2^+} y^a |\nabla(\eta U^\delta)|^2 \, dx\, dy \leq 2\delta^2 \int_{B_2^+} y^a \eta^2 U^{2(\delta-1)} |\nabla U|^2 \, dx\, dy + 2 \int_{B_2^+} y^a U^{2\delta} |\nabla \eta|^2 \, dx\, dy.$$

If we insert formula (3-8) into the inequality above, for the choice $\alpha = 2\delta - 1$, we obtain

$$\begin{aligned} J &:= \int_{B_2^+} y^a |\nabla(\eta U^\delta)|^2 \,dx\,dy \\ &\le 2\Big(1 + \Big(\frac{\alpha+1}{\alpha}\Big)^2\Big) \int_{B_2^+} y^a |\nabla\eta|^2 U^{2\delta}\,dx\,dy + \frac{(\alpha+1)^2}{\alpha} \int_{\Gamma_2^0} \eta^2 U^\alpha F(U)\,dx \\ &=: I_1 + I_2. \end{aligned} \tag{3-9}$$

For the left hand side above, recall the trace Sobolev embedding (Corollary 5.3)

$$J = \int_{B_2^+} y^a |\nabla(\eta U^\delta)|^2 \,dx\,dy \gtrsim \Big(\int_{\Gamma_2^0} (\eta U^\delta)^{2^*} \,dx \Big)^{2/2^*}, \tag{3-10}$$

and the standard weighted Sobolev embedding from Proposition 3.3.

$$J = \int_{B_2^+} y^a |\nabla(\eta U^\delta)|^2 \,dx\,dy \gtrsim \Big(\int_{B_2^+} y^a (\eta U^\delta)^k \Big)^{2/k} \tag{3-11}$$

for some $1 < k < 2(n+1)/n$.

Next, we estimate from above the terms I_1, I_2 in (3-9). I_1 can be easily handled since $|\nabla\eta| \le C$:

$$I_1 = \int_{B_2^+} y^a |\nabla\eta|^2 U^{2\delta}\,dx\,dy \lesssim \int_{B_2^+} y^a U^{2\delta}\,dx\,dy. \tag{3-12}$$

Now we consider the second term. To estimate I_2, if we write $U^{2\delta-2+\beta} = U^{\beta-2} U^{2\delta}$, then, using Hölder's inequality with $p = 2^*/(\beta-2)$, $1/p + 1/q = 1$, we obtain

$$\int_{\Gamma_2^0} \eta^2 U^{2\delta-1} F(U)\,dx \le \Big[\int_{\Gamma_2^0} U^{2^*}\,dx \Big]^{1/p} \Big[\int_{\Gamma_2^0} \eta^{2q} U^{2\delta q}\,dx \Big]^{1/q} \le V^{1/p} \Big[\int_{\Gamma_2^0} \eta^{2q} U^{2\delta q}\,dx \Big]^{1/q}. \tag{3-13}$$

This last integral can be handled as follows. Call $\chi = 2^*/2$, for simplicity. Because our hypothesis on β, we know that $q \in (1, \chi)$. Then there exists $\lambda \in (0, 1)$ such that $q = \lambda + (1-\lambda)\chi$, and an interpolation inequality gives

$$\Big[\int f^q \Big]^{1/q} \le \Big[\int f \Big]^{\lambda/q} \Big[\int f^\chi \Big]^{(1-\lambda)/q} = \Big[\int f^\chi \Big]^{1/\chi} \Big(\Big[\int f \Big] \Big[\int f^\chi \Big]^{-1/\chi} \Big)^{\lambda/q}. \tag{3-14}$$

Since $\lambda/q < 1$, Young's inequality reads

$$z^{\lambda/q} \le C_\epsilon z + \epsilon,$$

for ϵ small. If we substitute $z = [\int f][\int f^\chi]^{-1/\chi}$ above, together with (3-14), we arrive at

$$\Big[\int f^q \Big]^{1/q} \le \epsilon \Big[\int f^\chi \Big]^{1/\chi} + C_\epsilon \int f.$$

Then from (3-13) it follows that

$$I_2 \le V^{1/p}\left\{\epsilon\left(\int_{\Gamma_2^0}(\eta U^\delta)^{2^*}\,dx\right)^{2/2^*}+C_\epsilon\int_{\Gamma_2^0}\eta^2U^{2\delta}\,dx\right\}, \tag{3-15}$$

where ϵ will be chosen later and will depend on the value of α, δ.

We go back now to the main iteration formula (3-9). It is clear from (3-10) that the first integral of the right hand side of the formula for I_2 (3-15) can be absorbed into the left hand side of (3-9), and, using (3-11) and (3-10), we get that

$$\left(\int_{\Gamma_1^0}U^{\delta 2^*}\,dx\right)^{2/2^*}+\left(\int_{B_1^+}U^{2k\delta}\,dx\,dy\right)^{1/k}\le C(\delta)\left[\int_{\Gamma_2^0}U^{2\delta}\,dx+\int_{B_2^+}U^{2\delta}\,dx\,dy\right],$$

for some suitable choice of ϵ. Or, switching notation from 2δ to δ,

$$\left(\int_{\Gamma_1^0}U^{\delta\chi}\,dx\right)^{1/\chi}+\left(\int_{B_1^0}U^{k\delta}\,dx\,dy\right)^{1/k}\le C(\delta)\left[\int_{\Gamma_2^0}U^{\delta}\,dx+\int_{B_2^0}U^{\delta}\,dx\,dy\right]. \tag{3-16}$$

Next, because we will always have $\delta>1$, we can use that

$$C_1(a^{1/\delta}+b^{1/\delta})\le(a+b)^{1/\delta}\le C_2(a^{1/\delta}+b^{1/\delta}),$$

so from (3-16) we get that

$$\|U\|_{L^{\chi\delta}(\Gamma_1^0)}+\|U\|_{L^{k\delta}(B_1^+,y^a)}\le\|U\|_{L^{\delta}(\Gamma_2^0)}+\|U\|_{L^{\delta}(B_2^+,y^a)}.$$

For simplicity, we set

$$\theta:=\min\{\chi,k\}>1,$$

and

$$\Phi(\delta,R):=\left(\frac{1}{R^n}\right)^{1/\delta}\|U\|_{L^\delta(\Gamma_1^0)}+\left(\frac{1}{R^{n+1+a}}\right)^{1/\delta}\|U\|_{L^\delta(B_1^+,y^a)}.$$

Then, after explicitly writing all the constants involved, formula (3-16) simply reduces to

$$\Phi(\theta\delta,1)\le[C(1+\delta)^\sigma]^{2/\delta}\Phi(\delta,2),$$

for some positive number σ. It is clear that the same proof works if we replace B_1, B_2 by B_{R_1}, B_{R_2}. The only difference is in (3-12), where we need to estimate $|\nabla\eta|\le C(R_2-R_1)^{-1}$. Thus we would obtain

$$\Phi(\theta\delta,R_1)\le\left[\frac{C(1+\delta)^\sigma}{R_2-R_1}\right]^{2/\delta}\Phi(\delta,R_2). \tag{3-17}$$

Now we iterate (3-17): set $R_m=1+1/2^m$ and $\theta_m=\theta^m\bar p$. Then

$$\Phi(\theta_m,1)\le\Phi(\theta_m,R_m)\le(c_1\theta)^{c_2\sum_{i=0}^{m-1}i/\theta^i}\Phi(\bar p,2)\le C\Phi(\bar p,2), \tag{3-18}$$

for some constant C, because the series $\sum_{i=0}^\infty i/\theta^i$ is convergent.

Finally, note that

$$\sup_{\Gamma_1^0}U=\lim_{\delta\to\infty}\|U\|_{L^\delta(\Gamma_1^0)},\qquad \sup_{B_1^+}U=\lim_{\delta\to\infty}\|U\|_{L^\delta(B_1^+,y^a)},$$

so that (3-18) is telling us that

$$\sup_{B_1^+} U + \sup_{\Gamma_1^0} U \le C[\|U\|_{L^{\bar p}(B_2, y^a)} + \|U\|_{L^{\bar p}(\Gamma_2^0)}].$$

Rescaling to a ball of radius R concludes the proof of the theorem. □

The next main ingredient is the proof of the positivity of a solution to (3-5). We observed that a Hopf lemma, some version of which was known for the Euclidean half space case [Cabré and Sire 2010, Proposition 4.10], can be obtained for the uniformly degenerate elliptic equation (3-1). This nice Hopf lemma turns out to be one of the keys for us in this paper. It is interesting to observe a different behavior between the cases $\gamma \in (0, 1/2)$ and $\gamma \in [1/2, 1)$ in our proof—this dichotomy does not seem to appear in the flat case in [Cabré and Sire 2010].

We continue to use the setting as in Proposition 2.2. Let $p_0 \in \partial X$ and (x, y) be the local coordinate at p_0 for $\overline{X}$ with $x(p_0) = 0$, where x is the normal coordinate at p_0 with respect to the metric $\hat h$ on the boundary M^n.

Theorem 3.5. *Suppose that U is a nonnegative solution to (3-1) in X^{n+1}. Then, for sufficiently small r_0, if $U(q_0) = 0$ for $q_0 \in \Gamma^0_{r_0} \setminus \overline{\Gamma^0_{1/2r_0}}$ and $U > 0$ on $\partial\Gamma^0_{1/2r_0}$ on the boundary M^n, then*

$$y^a \partial_y U|_{q_0} > 0. \tag{3-19}$$

Proof. First we assume that $\gamma \in [1/2, 1)$, that is, $a \in (-1, 0]$. We consider a positive function

$$W = y^{-a}(y + Ay^2)(e^{-B|x|} - e^{-Br_0}). \tag{3-20}$$

To calculate $\operatorname{div}(y^a \nabla W)$ in the metric $\bar g^*$, we first calculate from Proposition 2.2 that

$$\bar g^* = (1 + \alpha_1 y)dy^2 + (1 + \alpha_2 y)\hat h + o(y)$$

for some constants α_1, α_2 and

$$\det \bar g^* = \det \hat h(1 + \alpha_3 y) + o(y),$$

for some constant α_3. Then

$$\operatorname{div}(y^a \nabla W) = I_1 + I_2 + I_3 + I_4,$$

where

$$\begin{aligned} I_1 &= \frac{1}{\sqrt{\det \bar g^*}} \partial_y \big(\sqrt{\det \bar g^*}(\bar g^*)^{yy}((1-a) + (2-a)yA)(e^{-B|x|} - e^{-Br_0})\big) \\ &= (\alpha_4 + (2-a)A + o(1))(e^{-B|x|} - e^{-Br_0}), \\ I_2 &= \frac{1}{\sqrt{\det \bar g^*}} \partial_{x^k} \big(\sqrt{\det \bar g^*}(\bar g^*)^{ky}((1-a) + (2-a)yA)(e^{-B|x|} - e^{-Br_0})\big) \\ &= o(1)(e^{-B|x|} - e^{-Br_0}) + o(y)Be^{-Br}, \end{aligned}$$

for some constant α_4,

$$I_3 = \frac{1}{\sqrt{\det \bar g^*}} \partial_y \big(\sqrt{\det \bar g^*}(\bar g^*)^{yk}(y + y^2 A)\partial_{x^k}(e^{-B|x|} - e^{-Br_0})\big) = o(y)Be^{-Br},$$

and

$$
\begin{aligned}
I_4 &= \frac{y+y^2A}{\sqrt{\det \bar g^*}}\partial_{x^k}\big(\sqrt{\det \bar g^*}(\bar g^*)^{kj}\partial_{x^j}(e^{-B|x|}-e^{-Br_0})\big)\\
&= \frac{y+y^2A}{\sqrt{\det \bar g^*}}\partial_{x^k}\big(\sqrt{\det \bar g^*}(\bar g^*)^{kj}(-\frac{x_j}{r}Be^{-Br})\big)\\
&= yB^2e^{-Br}+o(y)B^2e^{-Br}+yB^2o(r^2)e^{-Br}+o(y)Be^{-Br}.
\end{aligned}
$$

Thus

$$\operatorname{div}(y^a\nabla W) = (\alpha_4+(2-a)A+o(1))(e^{-B|x|}-e^{-Br_0})+(B^2+o(1)B)ye^{-Br}.$$

We remark here that all α's can be explicit, but it would not be any more use. Take r_0 sufficiently small and A and B sufficiently large so that

$$\operatorname{div}(y^a\nabla W)\ge 0$$

provided that $a\le 0$. Now we know

$$\operatorname{div}(y^a\nabla(U-\epsilon W))\le 0$$

in $(\Gamma^0_{r_0}\setminus\overline{\Gamma^0_{1/2r_0}})\times(0,r_0)$ for all $\epsilon>0$, and, moreover,

$$U-\epsilon W\ge 0$$

on $\partial\{(\Gamma^0_{r_0}\setminus\overline{\Gamma^0_{1/2r_0}})\times(0,r_0)\}$, provided we choose ϵ appropriately small. Therefore, due to the maximum principle, we know that

$$U-\epsilon W>0$$

in $(\Gamma^0_{r_0}\setminus\overline{\Gamma^0_{1/2r_0}})\times(0,r_0)$. Thus, when $U(x(q_0),0)=0$, we have

$$y^a\partial_y(U-\epsilon W)|_{(x(q_0),0)}\ge 0,$$

which implies

$$y^a\partial_yU|_{(x(q_0),0)}\ge \epsilon y^a\partial_yW|_{(x(q_0),0)}=\epsilon(1-a)(e^{-B|x(q_0)|}-e^{-Br_0})>0,$$

as desired.

When $a\in(0,1)$, or equivalently, $\gamma\in(0,1/2)$, we instead use the function

$$W=y^{-a}(y+Ay^{2-a})(e^{-B|x|}-e^{-Br_0}).$$

Then a similar calculation will prove that the conclusion still holds. □

Positivity of solutions for (3-1) is now clear:

Corollary 3.6. *Suppose that $U\in\mathscr{C}^2(X)\cap\mathscr{C}(\overline{X})$ is a nonnegative solution to the equation*

$$
\begin{cases}
\operatorname{div}(y^a\nabla U)=0 & \text{in } (X,\bar g^*),\\
y^a\partial_yU=F(U) & \text{on } M,
\end{cases}
$$

where $F(0)=0$. Then $U>0$ on $\overline{X}$ unless $U\equiv 0$.

Proof. First, $U > 0$ in X, and U is not identically zero on the boundary if it is not identically zero on $\bar{X}$. Then, on the boundary, the set where U is positive is nonempty and open. Hence, if the set where U vanishes is not empty, then, for any small number r_0, there always exist points p_0 and q_0 as given in the assumptions of Theorem 3.5. Thus we would arrive at the contradiction from Theorem 3.5. □

4. The γ-Yamabe problem

Now we are ready to set up the fractional Yamabe problem for $\gamma \in (0, 1)$. On the conformal infinity $(M^n, [\hat{h}])$ of an asymptotically hyperbolic manifold (X^{n+1}, g^+), we consider a scale-free functional on metrics in the class $[\hat{h}]$ given by

$$I_\gamma[\hat{h}] = \frac{\int_M Q_\gamma^{\hat{h}}\, dv_{\hat{h}}}{(\int_M dv_{\hat{h}})^{(n-2\gamma)/n}}. \tag{4-1}$$

Or, if we set a base metric $\hat{h}$ and write a conformal metric

$$\hat{h}_w = w^{4/(n-2\gamma)}\hat{h},$$

then

$$I_\gamma[w, \hat{h}] = \frac{\int_M w P_\gamma^{\hat{h}}(w)\, dv_{\hat{h}}}{(\int_M w^{2^*}\, dv_{\hat{h}})^{2/2^*}} \tag{4-2}$$

where $2^* = 2n/(n-2\gamma)$. We call I_γ the γ-Yamabe functional.

The γ*-Yamabe problem* is to find a metric in the conformal class $[\hat{h}]$ that minimizes the γ-Yamabe functional I_γ. It is clear that a metric $\hat{h}_w$, where w is a minimizer of $I_\gamma[w, \hat{h}]$, has a constant fractional scalar curvature $Q_\gamma^{\hat{h}_w}$, that is,

$$P_\gamma^{\hat{h}}(w) = cw^{(n+2\gamma)/(n-2\gamma)}, \quad w > 0, \tag{4-3}$$

for some constant c on M.

This suggests that we define the γ-Yamabe constant

$$\Lambda_\gamma(M, [\hat{h}]) = \inf\{I_\gamma[h] : h \in [\hat{h}]\}. \tag{4-4}$$

It is then apparent that $\Lambda_\gamma(M, [\hat{h}])$ is an invariant on the conformal class $[\hat{h}]$ when g^+ is fixed.

In the mean time, based on Proposition 2.1, we set

$$I_\gamma^*[U, \bar{g}] = \frac{d_\gamma^* \int_X \rho^a |\nabla U|_{\bar{g}}^2\, dv_{\bar{g}} + \int_X E(\rho)|U|^2\, dv_{\bar{g}}}{(\int_M |U|^{2^*}\, dv_{\hat{h}})^{2/2^*}}, \tag{4-5}$$

or similarly, using Proposition 2.2, we may set

$$I_\gamma^*[U, \bar{g}^*] = \frac{d_\gamma^* \int_X y^a |\nabla U|_{\bar{g}^*}^2\, dv_{\bar{g}^*} + \int_M Q_\gamma^{\hat{h}}|U|^2\, dv_{\hat{h}}}{(\int_M |U|^{2^*}\, dv_{\hat{h}})^{2/2^*}}. \tag{4-6}$$

It is obvious that it is equivalent to solve the minimizing problems for I_γ and I_γ^*. But a very pleasant surprise is that this immediately tells us that

$$\Lambda_\gamma(X, [\hat{h}]) = \inf\{I_\gamma^*[U, \bar{g}] : U \in W^{1,2}(X, y^a)\}. \tag{4-7}$$

(Please see the definitions and discussions of the weighted Sobolev spaces in Section 5.) Note that one has that $I_\gamma^*[|U|] \le I_\gamma^*[U]$ to handle positivity issues. Therefore we have the following.

Lemma 4.1. *Suppose that U is a minimizer of the functional $I_\gamma^*[\,\cdot\,, \bar{g}]$ in the weighted Sobolev space $W^{1,2}(X, y^a)$ with $\int_M |TU|^{2^*}\, dv_{\hat{h}} = 1$. Then its trace $w = TU \in H^\gamma(M)$ solves the equation*

$$P_\gamma^{\hat{h}}(w) = \Lambda_\gamma(X, [\hat{h}])w^{(n+2\gamma)/(n-2\gamma)}.$$

To resolve the γ-Yamabe problem is to verify I_γ has a minimizer w, which is positive and smooth. But before launching our resolution to the γ-Yamabe problem we are first due to discuss the sign of the γ-Yamabe constant. These statements are familiar and easy ones for the Yamabe problem but not so easy at all for the γ-Yamabe problem, where the conformal fractional Laplacians are just pseudodifferential operators. One knows that eigenvalues and eigenfunctions of the conformal fractional Laplacians are even more difficult to study than the differential operators. There are some affirmative results analogous to the conformal Laplacian proven in [Guillarmou and Qing 2010] when the Yamabe constant of the conformal infinity is assumed to be positive. Here we will take advantage of our Hopf lemma and the interpretation of conformal fractional Laplacians through extensions provided in Proposition 2.2.

For each $\gamma \in (0, 1)$ we know that each conformal fractional Laplacian is selfadjoint; see [Graham and Zworski 2003; Fefferman and Graham 2002]. Hence we may look for the first eigenvalue λ_1 by minimizing the quotient

$$\frac{\int_M w P_\gamma^{\hat{h}} w\, dv_{\hat{h}}}{\int_M w^2\, dv_{\hat{h}}}. \tag{4-8}$$

Moreover, again in light of Proposition 2.2, it is equivalent to minimizing

$$\frac{d_\gamma^* \int_X y^a |\nabla U|^2_{\bar{g}^*}\, dv_{\bar{g}^*} + \int_M Q_\gamma^{\hat{h}} |U|^2\, dv_{\hat{h}}}{\int_M |U|^2\, dv_{\hat{h}}}. \tag{4-9}$$

We arrive at the eigenvalue equation

$$P_\gamma^{\hat{h}} w = \lambda_1 w \quad \text{on } M.$$

Or, equivalently,

$$\begin{cases} \operatorname{div}(y^a \nabla U) = 0 & \text{in } (X, \bar{g}^*), \\ -d_\gamma^* \lim_{y\to 0} y^a \partial_y U + Q_\gamma^{\hat{h}} U = \lambda_1 U & \text{on } M, \end{cases} \tag{4-10}$$

As a consequence of Proposition 2.2 and Theorem 3.5 we have the following.

Theorem 4.2. *Suppose that (X^{n+1}, g^+) is an asymptotically hyperbolic manifold. For each $\gamma \in (0, 1)$ there is a smooth, positive first eigenfunction for $P_\gamma^{\hat{h}}$ and the first eigenspace is of dimension one, provided $H = 0$ when $\gamma \in (1/2, 1)$.*

Proof. We use the variational characterization (4-9) of the first eigenvalue. We first observe that one may always assume there is a nonnegative minimizer for (4-9). Then regularity and the maximum principle in

Section 3 insure that such a first eigenfunction is smooth and positive. To show that the first eigenspace is of dimension one, we suppose that ϕ and ψ are positive first eigenfunctions for $P_\gamma^{\hat{h}}$. Then

$$\begin{aligned} P_\gamma^{\hat{h}_\phi}\frac{\psi}{\phi} &= \phi^{-(n+2\gamma)/(n-2\gamma)}P_\gamma^{\hat{h}}\psi = \lambda_1\phi^{-(n+2\gamma)/(n-2\gamma)}\psi \\ &= (\phi^{-(n+2\gamma)/(n-2\gamma)}P_\gamma^{\hat{h}}\phi)\frac{\psi}{\phi} \\ &= Q_\gamma^{\hat{h}_\phi}\frac{\psi}{\phi}, \end{aligned}$$

where $\hat{h}_\phi = \phi^{4/(n-2\gamma)}\hat{h}$. That is, there is a function U satisfying

$$\begin{cases} \operatorname{div}(y_\phi^a \nabla U) = 0 & \text{in } (X, \bar{g}_\phi^*), \\ \lim_{y_\phi \to 0} y_\phi^a \dfrac{\partial U}{\partial y_\phi} U = 0 & \text{on } M, \end{cases}$$

and $U = \psi/\phi$ on M, where y_ϕ and $\bar{g}_\phi^*$ are associated with $\hat{h}_\phi$ as y and $\bar{g}^*$ are associated with $\hat{h}$ in Proposition 2.2, respectively. Replace U by $U - U_m$ for $U_m = \min_{\overline{X}} U$ and apply Theorem 3.5 and Corollary 3.6 to conclude that U has to be a constant. □

Consequently, we get the following.

Corollary 4.3. *Suppose (X^{n+1}, g^+) is an asymptotically hyperbolic manifold. Assume that $\gamma \in (0, 1)$ and that $H = 0$ when $\gamma \in (1/2, 1)$. Then there are three mutually exclusive possibilities for the conformal infinity $(M^n, [\hat{h}])$.*

(1) *The first eigenvalue of $P_\gamma^{\hat{h}}$ is positive, the γ-Yamabe constant is positive, and M admits a metric in $[\hat{h}]$ that has pointwise positive fractional scalar curvature.*

(2) *The first eigenvalue of $P_\gamma^{\hat{h}}$ is negative, the γ-Yamabe constant is negative, and M admits a metric in $[\hat{h}]$ that has pointwise negative fractional scalar curvature.*

(3) *The first eigenvalue of $P_\gamma^{\hat{h}}$ is zero, the γ-Yamabe constant is zero, and M admits a metric in $[\hat{h}]$ that has vanishing fractional scalar curvature.*

Proof. First, it is obvious that the sign of the first eigenvalue of the conformal fractional Laplacian $P_\gamma^{\hat{h}}$ does not change within the conformal class due to the conformal covariance property of the conformal fractional Laplacian. The three possibilities are distinguished by the sign of the first eigenvalue λ_1 of the conformal fractional Laplacian $P_\gamma^{\hat{h}}$. Because, if ϕ is the positive first eigenfunction of $P_\gamma^{\hat{h}}$, we have

$$Q_\gamma^{\hat{h}_\phi} = \lambda_1^{\hat{h}}\phi^{-4\gamma/(n-2\gamma)},$$

where $\hat{h}_\phi = \phi^{4/(n-2\gamma)}\hat{h}$. □

5. Weighted Sobolev trace inequalities

Let us continue in the setting provided by Proposition 2.2. On the compact manifold M^n, for $\gamma \in (0, 1)$, we recall the fractional order Sobolev space $H^\gamma(M)$, with its usual norm

$$\|w\|^2_{H^\gamma(M)} := \|w\|^2_{L^2(M)} + \int_M w(-\Delta_{\hat{h}})^\gamma w \, dv_{\hat{h}}.$$

An equivalent norm on this space is

$$\|w\|^2_{H^\gamma(M)} := A\|w\|^2_{L^2(M)} + \int_M w P^{\hat{h}}_\gamma w \, dv_{\hat{h}},$$

for some appropriately large number A, since $P^{\hat{h}}_\gamma$ is an elliptic pseudodifferential operator of order 2γ with its principal symbol being the same as that of $(-\Delta_{\hat{h}})^\gamma$.

Note that in $\mathbb{R}^n$, this Sobolev norm can be easily written in terms of the Fourier transform as

$$\|w\|^2_{H^\gamma(\mathbb{R}^n)} = \int_{\mathbb{R}^n} (1 + |\xi|^2)^\gamma \hat{w}^2(\xi) \, d\xi. \tag{5-1}$$

We would also like to recall the definition of the weighted Sobolev spaces. For $\gamma \in (0, 1)$ and $a = 1 - 2\gamma$, consider the norm

$$\|U\|^2_{W^{1,2}(X, y^a)} = \int_X y^a |\nabla U|^2_{\bar{g}^*} \, dv_{\bar{g}^*} + \int_X y^a U^2 \, dv_{\bar{g}^*}.$$

The following is then known.

Lemma 5.1. *There exists a unique linear bounded operator*

$$T : W^{1,2}(X, y^a) \to H^\gamma(M)$$

such that $TU = U|_M$ for all $U \in \mathscr{C}^\infty(\overline{X})$, which is called the trace operator.

Lemma 5.1 was explored by Nekvinda [1993] in the case when X is a subset of $\mathbb{R}^{n+1}$ and M^n a piece of its boundary; see also [Maz'ja 1985]. It then takes some standard argument to derive Lemma 5.1 from, for instance, [Nekvinda 1993].

The classical Sobolev trace inequality on Euclidean space is well known (see, for instance, [Escobar 1988]) and reads

$$\left(\int_{\mathbb{R}^n} |Tu|^{2n/(n-1)} \, dx\right)^{(n-1)/(2n)} \le C(n)\left(\int_{\mathbb{R}^{n+1}_+} |\nabla u|^2 \, dx \, dy\right)^{1/2} \tag{5-2}$$

where the constant $C(n)$ is sharp and the equality case is completely characterized. This corresponds to $a = 0$ for our cases. The same result is true for any other real $a \in (-1, 1)$. Indeed there are general weighted Sobolev trace inequalities. Let us first recall the well known fractional Sobolev inequalities. They were first considered in a remarkable paper by Lieb [1983]; see also [Frank and Lieb 2012; Cotsiolis and Tavoularis 2004] or the survey [Di Nezza et al. 2012].

Lemma 5.2. *Let $0 < \gamma < n/2$, $2^* = 2n/(n - 2\gamma)$. Then, for all $w \in H^\gamma(\mathbb{R}^n)$, we have*

$$\|w\|^2_{L^{2^*}(\mathbb{R}^n)} \le S(n, \gamma)\|(-\Delta)^{\gamma/2} w\|^2_{H^\gamma(\mathbb{R}^n)} = S(n, \gamma) \int_{\mathbb{R}^n} w(-\Delta)^\gamma w \, dx, \tag{5-3}$$

where

$$S(n,\gamma)=2^{-2\gamma}\pi^{-\gamma}\frac{\Gamma((n-2\gamma)/2)}{\Gamma((n+2\gamma)/2)}\left(\frac{\Gamma(n)}{\Gamma(n/2)}\right)^{2\gamma/n}=\frac{\Gamma((n-2\gamma)/2)}{\Gamma((n+2\gamma)/2)}|\mathrm{vol}(S^n)|^{-2\gamma/n}.$$

We have equality in (5-3) if and only if

$$w(x)=c\left(\frac{\mu}{|x-x_0|^2+\mu^2}\right)^{(n-2\gamma)/2},\qquad x\in\mathbb{R}^n,$$

for $c\in\mathbb{R}$, $\mu>0$ and $x_0\in\mathbb{R}^n$ fixed.

Note that we may interpret the above inequality as a calculation of the best γ-Yamabe constant on the standard sphere as the conformal infinity of the Hyperbolic space. Namely, if g_c is the standard round metric on the unit sphere,

$$\|w\|^2_{L^{2^*}(S^n)}\le S(n,\gamma)\int_{S^n} w P_\gamma^{g_c} w\, dv_{g_c}. \tag{5-4}$$

Such an inequality for the sphere case was also considered independently by Beckner [1993], Branson [1995], and Morpurgo [2002], in the setting of intertwining operators. Indeed, we have the following explicit expression for $P_\gamma^{S^n}$:

$$P_\gamma^{S^n}=\frac{\Gamma(B+\gamma+1/2)}{\Gamma(B-\gamma+1/2)},\quad \text{where}\quad B:=\sqrt{-\Delta_{S^n}+\left(\frac{n-1}{2}\right)^2}.$$

It is clear from (5-4) that

$$\Lambda_\gamma(S^n,[g_c])=\frac{1}{S(n,\gamma)}. \tag{5-5}$$

Sobolev trace inequalities can be obtained by the composition of the trace theorem and the Sobolev embedding theorem above. There have been some related works that deal with these types of energy inequalities, for instance, Nekvinda [1993], González [2009], and Cabré and Cinti [2012]. In particular, in light of the work of Caffarelli and Silvestre [2007] and Lemma 5.2, we easily see the more general form of (5-2) as follows.

Corollary 5.3. *Let $w\in H^\gamma(\mathbb{R}^n)$, $\gamma\in(0,1)$, $a=1-2\gamma$, and $U\in W^{1,2}(\mathbb{R}^{n+1}_+,y^a)$ with trace $TU=w$. Then*

$$\|w\|^2_{L^{2^*}(\mathbb{R}^n)}\le \bar S(n,\gamma)\int_{\mathbb{R}^{n+1}_+} y^a|\nabla U|^2\,dx\,dy, \tag{5-6}$$

where

$$\bar S(n,\gamma):=d^*_\gamma S(n,\gamma). \tag{5-7}$$

Equality holds if and only if

$$w(x)=c\left(\frac{\mu}{|x-x_0|^2+\mu^2}\right)^{(n-2\gamma)/2},\qquad x\in\mathbb{R}^n,$$

for $c\in\mathbb{R}$, $\mu>0$ and $x_0\in\mathbb{R}^n$ fixed, and U is its Poisson extension of w as given in (2-13).

In the following lines we take a closer look at the extremal functions that attain the best constant in the inequality above. On $\mathbb{R}^n$ we fix

$$w_\mu(x) := \Big(\frac{\mu}{|x|^2+\mu^2}\Big)^{(n-2\gamma)/2}. \tag{5-8}$$

These correspond to the conformal diffeomorphisms of the sphere. We set

$$U_\mu = K_\gamma *_x w_\mu \tag{5-9}$$

as given in (2-13). Then we have the equality

$$\|w_\mu\|^2_{L^{2^*}(\mathbb{R}^n)} = \bar{S}(n,\gamma)\int_{\mathbb{R}^{n+1}_+} y^a|\nabla U_\mu|^2\,dx\,dy.$$

It is clear that

$$w_\mu(x) = \frac{1}{\mu^{(n-2\gamma)/2}}w_1\Big(\frac{x}{\mu}\Big) \quad\text{and}\quad U_\mu(x,y) = \frac{1}{\mu^{(n-2\gamma)/2}}U_1\Big(\frac{x}{\mu},\frac{y}{\mu}\Big). \tag{5-10}$$

Moreover, U_μ is the (unique) solution of the problem

$$\begin{cases} \operatorname{div}(y^a\nabla U_\mu)=0 & \text{in } \mathbb{R}^{n+1}_+,\\ -\lim_{y\to 0} y^a\partial_y U_\mu = c_{n,\gamma}(w_\mu)^{(n+2\gamma)/(n-2\gamma)} & \text{on } \mathbb{R}^n. \end{cases} \tag{5-11}$$

On the other hand, if we multiply (5-11) by U_μ and integrate by parts,

$$\int_{\mathbb{R}^{n+1}_+} y^a|\nabla U_\mu|^2\,dx\,dy = c_{n,\gamma}\int_{\mathbb{R}^n}(w_\mu)^{2^*}\,dx. \tag{5-12}$$

Now we compare (5-12) with (5-6). Using (5-5), we arrive at

$$\Lambda(S^n,[g_c]) = c_{n,\gamma}d^*_\gamma\Big[\int_{\mathbb{R}^n}(w_\mu)^{2^*}\,dx\Big]^{2\gamma/n}. \tag{5-13}$$

Before the end of this section we calculate the general upper bound of the γ-Yamabe constants. Indeed there is a complete analogue to the case of the usual Yamabe problem (compare [Aubin 1982; Lee and Parker 1987]). Namely:

Proposition 5.4. *Let* $\gamma\in(0,1)$. *Then*

$$\Lambda_\gamma(M,[\hat{h}]) \le \Lambda_\gamma(S^n,[g_c]).$$

Proof. First, we instead use the functional (4-6) to estimate the γ-Yamabe constant for a good reason. The approach is rather the standard method of gluing a "bubble" (5-8) to the manifold M; see, for instance, Lemma 3.4 of [Lee and Parker 1987].

For any fixed $\epsilon>0$, let B_ϵ be the ball of radius ϵ centered at the origin in $\mathbb{R}^{n+1}$ and B^+_ϵ be the half ball of radius ϵ in $\mathbb{R}^{n+1}_+$. Choose a smooth radial cutoff function η, $0\le\eta\le 1$ supported on $B_{2\epsilon}$, and satisfying $\eta\equiv 1$ on B_ϵ. Then consider the function $V=\eta U_\mu$ with its trace $v=\eta w_\mu$ on $\mathbb{R}^n$. We have

$$\int_{\mathbb{R}^{n+1}_+} y^a|\nabla V|^2\,dx\,dy \le (1+\epsilon)\int_{\mathbb{R}^{n+1}_+} y^a|\nabla U_\mu|^2\,dx\,dy + C(\epsilon)\int_{B^+_{2\epsilon}\setminus B^+_\epsilon} U_\mu^2\,dx\,dy. \tag{5-14}$$

Note that $w_\mu = O(\mu^{(n-2\gamma)/2}|x|^{2\gamma-n})$ in the annulus $\epsilon \le |x| \le 2\epsilon$ and U_μ is $O(\mu^{(n-2\gamma)/2})$ in the annulus $B^+_{2\epsilon}\backslash B^+_\epsilon$. This allows us to estimate the second term in the right hand side of (5-14) by $O(\mu^{n-2\gamma})$ as $\mu \to 0$, for ϵ fixed. For the first term in the right hand side of (5-14) we first use the fact that w_μ attains the best constant in the Sobolev inequality, so

$$\bar S(n,\gamma)\int_{\mathbb{R}^{n+1}_+} y^a|\nabla U_\mu|^2\,dx\,dy = \left(\int_{\mathbb{R}^n} w_\mu^{2^*}\,dx\right)^{2/2^*} \le \left(\int_{\mathbb{R}^n} v^{2^*}\,dx\right)^{2/2^*} + O(\mu^n). \tag{5-15}$$

Now we need to transplant the function V to the manifold $(\bar X, \bar g^*)$. Fix a point on the boundary M and use normal coordinates $\{x_1,\dots,x_n,y\}$ around it, in a half ball $B^+_{2\epsilon}$ where V is supported. Two things must be modified: when $\epsilon \to 0$,

$$|\nabla V|^2_{\bar g^*} = |\nabla V|^2(1+O(\epsilon)),$$

and

$$dv_{\bar g^*} = (1+O(\epsilon))\,dx\,dy,$$

so that

$$\begin{aligned} I_{\epsilon,\mu} &:= d^*_\gamma \int_{B^+_{2\epsilon}} y^a|\nabla V|^2_{\bar g^*}\,dv_{\bar g^*} + \int_{|x|\le 2\epsilon} Q^{\hat h}_\gamma v^2\,dv_{\hat h} \\ &\le (1+O(\epsilon))\left(\int_{B^+_{2\epsilon}} y^a|\nabla V|^2\,dx\,dy + C\int_{|x|<2\epsilon} v^2\,dx\right). \end{aligned}$$

It is easily seen that

$$\int_{|x|<2\epsilon} w_\mu^2\,dx = o(1).$$

This is a small computation that can be found in Lemma 3.5 of [Lee and Parker 1987]. Then, from (5-15), fixing ϵ small and then μ small, we can get that

$$I_{\epsilon,\mu} \le (1+C\epsilon)\left(\frac{1}{S(n,\gamma)}\|v\|^2_{L^{2^*}(M)} + C\mu\right),$$

which implies

$$\Lambda_\gamma(M,[\hat h]) \le \frac{1}{S(n,\gamma)} = \Lambda_\gamma(S^n,[g_c]). \qquad \square$$

We end this section by remarking that, although most of the results mentioned here were already known in different contexts, it is certainly very interesting to put all the analysis and geometry together in the context of conformal fractional Laplacians and the associated γ-Yamabe problems in a way that is analogous to what has been done on the subject of the Yamabe problem, which becomes fundamental to the development of geometric analysis.

6. Subcritical approximations

In this section we take a well-known subcritical approximation method to solve the γ-Yamabe problem and prove Theorem 1.4. There does not seem to be any more difficulty than usual after our discussions in previous sections. But, for the convenience of the readers, we present a brief sketch of the proof. Similar to the case of the usual Yamabe problem we consider the following subcritical approximations to the functionals I_γ and I_γ^*, respectively. Set

$$I_\beta[w] = \frac{\int_M w P_\gamma^{\hat{h}} w \, dv_{\hat{h}}}{(\int_M w^\beta \, dv_{\hat{h}})^{2/\beta}}$$

and

$$I_\beta^*[U] = \frac{d_\gamma^* \int_X y^a |\nabla U|^2_{\bar{g}^*} \, dv_{\bar{g}} + \int_M Q_\gamma^{\hat{h}} U^2 \, dv_{\hat{h}}}{(\int_M U^\beta \, dv_{\hat{h}})^{2/\beta}}$$

for $\beta \in [2, 2^*)$, where $2^* = 2n/(n-2\gamma)$ and $\gamma \in (0, 1)$. These are subcritical problems and can be solved through standard variational methods. For clarity we state the following.

Proposition 6.1. *For each $2 \leq \beta < 2^*$, there exists a smooth positive minimizer U_β for $I_\beta^*[U]$ in $W^{1,2}(X, y^a)$, which satisfies the equations*

$$\begin{cases} \operatorname{div}(y^a \nabla U_\beta) = 0 & \text{in } (X, \bar{g}^*), \\ -d_\gamma^* \lim_{y\to 0} y^a U_\beta + Q_\gamma^{\hat{h}} U_\beta = c_\beta U_\beta^{\beta-1} & \text{on } M, \end{cases}$$

where the derivatives are taken with respect to the metric $\bar{g}^*$ in X and $c_\beta = I_\beta^*[U_\beta] = \min I_\beta^*$. And the boundary value w_β of U_β, which is a positive smooth minimizer for $I_\beta[w]$ in $H^\gamma(M)$, satisfies

$$P_\gamma^{\hat{h}} w_\beta = c_\beta w_\beta^{\beta-1}.$$

Using a similar argument as in the proof of Lemma 4.3 in [Lee and Parker 1987] (see also [Aubin 1982]), we have the following.

Lemma 6.2. *If $\operatorname{vol}(M, \hat{h}) = 1$, $|c_\beta|$ is nonincreasing as a function of $\beta \in [2, 2^*]$; and if $\Lambda_\gamma(M, [\hat{h}]) \geq 0$, c_β is continuous from the left at $\beta = 2^*$.*

Readers are referred to [Escobar 1992; Lee and Parker 1987; Schoen and Yau 1994] for more details.

Proof of Theorem 1.4. Instead of applying the standard Sobolev embedding in the Yamabe problem, we apply the weighted trace ones discussed in the previous section. To ensure that U_β as $\beta \to 2^*$ produces a minimizer for the γ-Yamabe problem, we want to establish the a priori estimates for U_β. In light of the discussions in Section 3, we only need to have a uniform L^∞ bound for w_β. We establish the L^∞ bound for w_β by the so-called blow-up method.

Otherwise, assume there exist sequences $\beta_k \to 2^*$, $w_k := w_{\beta_k}$ and $U_k := U_{\beta_k}$, $x_k \in M$ such that $w_k(x_k) = \max_M\{w_k\} = m_k \to \infty$ and $x_k \to x_0 \in M$ as $k \to \infty$. Take a normal coordinate system centered at x_0 and rescale

$$V_k(x, y) = m_k^{-1} U_k(\delta_k x + x_k, \delta_k y),$$

with the boundary value

$$v_k(x) = m_k^{-1} w_k(\delta_k x + x_k),$$

where $\delta_k = m_k^{(1-\beta_k)/2\gamma}$. Then V_k is defined in a half ball of radius $R_k = (1-|x_k|)/\delta_k$ and is a solution of

$$\begin{cases} \operatorname{div}(\rho^a \nabla V_k) = 0 & \text{in } B^+_{R_k}, \\ -d^*_\gamma \lim_{y\to 0} y^a \partial_y V_k + (Q^{\hat{h}}_\gamma)_k v_k = c_k v_k^{\beta-1} & \text{on } B_{R_k}, \end{cases} \tag{6-1}$$

with respect to the metric $\bar{g}^*(\delta_k x + x_k, \delta_k y)$, where

$$(Q^{\hat{h}}_\gamma)_k = \delta_k^{1-a} Q^{\hat{h}}_\gamma(\delta_k x + x_k) \to 0.$$

Due to, for example, $\mathscr{C}^{2,\alpha}$ a priori estimates for the rescaled solutions V_k, to extract a subsequence, if necessary, we have $V_k \to V_0$ in $C^{2,\alpha}_{\mathrm{loc}}$. Moreover the metrics $\bar{g}^*(\delta_k x + x_k, \delta_k y)$ converge to the Euclidean metric. Hence V_0 is a nontrivial, nonnegative solution of

$$\begin{cases} -\operatorname{div}(y^a \nabla V_0) = 0 & \text{in } \mathbb{R}^{n+1}_+, \\ -d^*_\gamma \lim_{y\to 0} y^a \partial_y V_0 = c_0 V_0^{(n+2\gamma)/(n-2\gamma)} & \text{on } \mathbb{R}^n. \end{cases} \tag{6-2}$$

Let $v_0 = T V_0$. It is easily seen that

$$\int_{\mathbb{R}^n} v_0^{2^*}(x)\, dx \le 1. \tag{6-3}$$

Theorem 3.5 and Corollary 3.6 then assure that $V_0 > 0$ on $\overline{\mathbb{R}^{n+1}_+}$. Therefore we can obtain

$$\int_{\mathbb{R}^{n+1}_+} y^a |\nabla V_0|^2\, dx\, dy = c_0 d^*_\gamma \int_{\mathbb{R}^n} v_0^{2^*}(x)\, dx. \tag{6-4}$$

It is then obvious that $c_0 > 0$, that is, $c_0 = \Lambda_\gamma(M, [\hat{h}])$ in light of Lemma 6.2. Moreover, by the trace inequalities from Corollary 5.3, we have

$$\left(\int_{\mathbb{R}^n} v_0^{2^*}(x)\, dx \right)^{2/2^*} \le \bar{S}(n,\gamma) \int_{\mathbb{R}^{n+1}_+} y^a |\nabla V_0|^2\, dx\, dy. \tag{6-5}$$

Then (6-3), (6-4), and (6-5), together with the definition of $\Lambda_\gamma(S^n, [g_c])$ in (5-5), contradict the initial hypothesis (1-6).

Once we have a uniform L^∞ estimate, by the regularity theorems in Section 3 we may extract a subsequence if necessary and pass to a limit U_0, whose boundary value w_0 satisfies

$$P^{\hat{h}}_\gamma w_0 = \Lambda w_0^{2^*-1}, \quad I_\gamma[w_0] = \Lambda, \quad \Lambda = \lim c_\beta. \tag{6-6}$$

Theorem 3.5 and Corollary 3.6 also ensure that $w_0 > 0$ on M. It remains to check that $\Lambda = \Lambda_\gamma(M, [\hat{h}])$. However, this is a direct consequence of Lemma 6.2 when $\Lambda_\gamma(M, [\hat{h}]) \ge 0$. Meanwhile it is easily seen that by the definition of the γ-Yamabe constants and (6-6) that Λ can not be less than $\Lambda_\gamma(M, [\hat{h}])$. Hence it is also implied that $\Lambda = \Lambda_\gamma(M, [\hat{h}])$ by Lemma 6.2 when $\Lambda_\gamma(M, [\hat{h}]) < 0$. Thus, in any case, w_0 is a minimizer of I_γ, as desired. □

7. A sufficient condition

In this section we give the proof of Theorem 1.5, which provides a sufficient condition for the resolution of the γ-Yamabe problem. Here the precise structure of the metric plays a crucial role, since a careful computation of the asymptotics is required, following the calculation in [Escobar 1992]. The section is divided into two parts: the first contains the necessary estimates on the Euclidean case, while in the second we go back to the geometry setting and finish the proof of the theorem.

Some preliminary results on $\mathbb{R}^{n+1}_+$. Here we consider the divergence equation (2-11) on $\mathbb{R}^{n+1}_+$, as understood in [Caffarelli and Silvestre 2007; González 2009]. The main point is that by using the Fourier transform, a solution to this problem can be written in terms on its trace value on $\mathbb{R}^n$ and the well-known Bessel functions. Indeed, let U be a solution of

$$\begin{cases} \operatorname{div}(y^a \nabla U) = 0 & \text{in } \mathbb{R}^{n+1}_+, \\ U(x,0) = w & \text{on } \mathbb{R}^n \times \{0\}, \end{cases} \tag{7-1}$$

or equivalently, $U = K_\gamma *_x w$, where K_γ is the Poisson kernel as given in (2-13).

The main idea is to reduce (7-1) to an ODE by taking the Fourier transform in x. We obtain

$$\begin{cases} -|\xi|^2 \hat{u}(\xi, y) + \dfrac{a}{y} \hat{u}_y(\xi, y) + \hat{u}_{yy}(\xi, y) = 0, \\ \widehat{U}(\xi, 0) = \hat{w}(\xi), \end{cases}$$

that is, an ODE for each fixed value of ξ.

On the other hand, consider the solution $\varphi : [0, +\infty) \to \mathbb{R}$ of the problem

$$-\varphi(y) + \frac{a}{y}\varphi_y(y) + \varphi_{yy}(y) = 0, \tag{7-2}$$

subject to the conditions $\varphi(0) = 1$ and $\lim_{t\to+\infty} \varphi(t) = 0$. This is a Bessel function and its properties are summarized in Lemma 7.1. Then we have that

$$\widehat{U}(\xi, y) = \hat{w}(\xi)\varphi(|\xi| y). \tag{7-3}$$

For a review of Bessel functions, see, for instance, Lemma 5.1 of [González 2009] or Section 9.6.1 of [Abramowitz and Stegun 1964].

Lemma 7.1. *Consider the following ODE in the variable $y > 0$:*

$$-\varphi(y) + \frac{a}{y}\varphi_y(y) + \varphi_{yy}(y) = 0,$$

with boundary conditions $\varphi(0) = 1$, $\varphi(\infty) = 0$. Its solution can be written in terms of Bessel functions:

$$\varphi(y) = c_1 y^\gamma \mathcal{K}_\gamma(y),$$

where $\mathcal{K}_\gamma$ is the modified Bessel function of the second kind that has asymptotic behavior

$$\mathcal{K}_\gamma(y) \sim \frac{\Gamma(\gamma)}{2}\Big(\frac{2}{y}\Big)^\gamma \quad \textit{when } y \to 0^+,$$

$$\mathcal{K}_\gamma(y) \sim \sqrt{\frac{\pi}{2y}}\, e^{-y} \quad \textit{when } y \to +\infty,$$

for a constant

$$c_1 = \frac{2^{1-\gamma}}{\Gamma(\gamma)}.$$

Now we are ready to prove the main technical lemmas in the proof of Theorem 1.5. More precisely, we will explicitly compute several energy terms through Fourier transforms, thanks to expression (7-3). Such precise computation is needed in order to obtain the exact value of the constant (1-8). For the rest of the section, we set

$$|\nabla U|^2 = (\partial_{x_1} U)^2 + \cdots + (\partial_{x_n} U)^2 + (\partial_y U)^2, \quad |\nabla_x U|^2 = (\partial_{x_1} U)^2 + \cdots + (\partial_{x_n} U)^2.$$

Lemma 7.2. *Given $w \in H^\gamma(\mathbb{R}^n)$, let $U = K_\gamma * w$ defined on $\mathbb{R}^{n+1}_+$. Then*

$$\mathcal{A}_1(w) := \int_{\mathbb{R}^{n+1}_+} y^{a+2}|\nabla U|^2\,dx\,dy = d_1 \int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{2(\gamma-1)}\,d\xi, \tag{7-4}$$

$$\mathcal{A}_2(w) := \int_{\mathbb{R}^{n+1}_+} y^{a+2}|\nabla_x U|^2\,dx\,dy = d_2 \int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{2(\gamma-1)}\,d\xi, \tag{7-5}$$

$$\mathcal{A}_3(w) := \int_{\mathbb{R}^{n+1}_+} y^{a} U^2\,dx\,dy = d_3 \int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{2(\gamma-1)}\,d\xi, \tag{7-6}$$

where

$$d_2 = \frac{-a+3}{6} d_1, \quad d_3 = \frac{1}{a+1} d_1.$$

Proof. We write $\mathcal{A}_i := \mathcal{A}_i(w)$, $i = 1, 2, 3$, for simplicity. Note that the integrals in the right hand side of (7-4), (7-5), (7-6) are finite because $w \in H^\gamma(\mathbb{R}^n) \hookrightarrow H^{\gamma-1}(\mathbb{R}^n)$ and because of the definition of the Sobolev norm (5-1).

Thanks to (7-3), we can easily compute, using the properties of the Fourier transform,

$$\begin{aligned}
\mathcal{A}_1 :&= \int_{\mathbb{R}^n_+} y^{a+2}|\nabla U|^2\,dx\,dy = \int_{\mathbb{R}^n_+} y^{a+2}(|\nabla_x U|^2 + |\partial_y U|^2)\,dx\,dy \\
&= \int_{\mathbb{R}^n}\int_0^\infty y^{a+2}(|\xi|^2|\widehat{U}|^2 + |\partial_y \hat{U}|^2)\,dy\,d\xi \\
&= \int_{\mathbb{R}^n}\int_0^\infty y^{a+2}|\hat{w}(\xi)|^2|\xi|^2(|\varphi(|\xi|y)|^2 + |\varphi'(|\xi|y)|^2)\,dy\,d\xi \\
&= \int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{-1-a}\int_0^\infty t^{a+2}(|\varphi(t)|^2 + |\varphi'(t)|^2)\,dt\,d\xi \\
&= d_1 \int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{-1-a} d\xi
\end{aligned} \tag{7-7}$$

for a constant

$$d_1 := \int_0^\infty t^{a+2}(|\varphi(t)|^2 + |\varphi'(t)|^2)\,dt. \tag{7-8}$$

Similarly,

$$\begin{aligned}\mathcal{A}_2 := \int_{\mathbb{R}^n_+} y^{a+2}|\nabla_x U|^2\,dx\,dy &= \int_{\mathbb{R}^n}\int_0^\infty y^{a+2}|\xi|^2|\widehat{U}|^2\,dy\,d\xi\\ &= \int_{\mathbb{R}^n}\int_0^\infty y^{a+2}|\hat{w}(\xi)|^2|\xi|^2|\varphi(|\xi|y)|^2\,dy\,d\xi\\ &= \int_{\mathbb{R}^n}|\hat{w}(\xi)|^2|\xi|^{-1-a}\int_0^\infty t^{a+2}|\varphi(t)|^2\,dt\,d\xi\\ &= d_2\int_{\mathbb{R}^n}|\hat{w}(\xi)|^2|\xi|^{-1-a}d\xi\end{aligned}$$

for

$$d_2 := \int_0^\infty t^{a+2}|\varphi(t)|^2\,dt. \tag{7-9}$$

And finally,

$$\begin{aligned}\mathcal{A}_3 := \int_{\mathbb{R}^{n+1}_+} y^a U^2\,dx\,dy &= \int_{\mathbb{R}^n}\int_0^\infty y^a|\widehat{U}|^2\,dy\,d\xi = \int_{\mathbb{R}^n}\int_0^\infty y^a|\hat{w}(\xi)|^2|\varphi(|\xi|y)|^2\,dy\,d\xi\\ &= \int_{\mathbb{R}^n}|\hat{w}(\xi)|^2|\xi|^{-1-a}\int_0^\infty t^a|\varphi(t)|^2\,dt\,d\xi = d_3\int_{\mathbb{R}^n}|\hat{w}(\xi)|^2|\xi|^{-1-a}\,d\xi,\end{aligned} \tag{7-10}$$

for

$$d_3 = \int_0^\infty t^a|\varphi(t)|^2\,dt.$$

In the next step, we find the relation between the constants d_1, d_2, d_3. All the integrals are evaluated between zero and infinity in the following. Multiply (7-2) by $\varphi_t t^{a+3}$ and integrate by parts:

$$-\int \varphi\varphi_t t^{a+3} + a\int \varphi_t^2 t^{a+2} + \int \varphi_{tt}\varphi_t t^{a+3} = 0. \tag{7-11}$$

In the above formula, we estimate the first term by

$$\int t^{a+3}\varphi\varphi_t = \tfrac{1}{2}\int t^{a+3}\partial_t(\varphi^2) = -\frac{a+3}{2}\int t^{a+2}\varphi^2,$$

and the last one by

$$\int t^{a+3}\varphi_{tt}\varphi_t = \tfrac{1}{2}\int t^{a+3}\partial_t(\varphi_t^2) = -\frac{a+3}{2}\int t^{a+2}\varphi_t^2,$$

so from (7-11) we obtain

$$(a+3)\int t^{a+2}\varphi^2 = (-a+3)\int t^{a+2}\varphi_t^2.$$

Together with (7-8) and (7-9) this gives

$$d_1 = \frac{6}{-a+3}d_2,$$

as desired.

Now, multiply (7-2) by φt^{a+2} and integrate:

$$-\int t^{a+2}\varphi\varphi_t + a\int t^{a+1}\varphi_t^2 + \int t^{a+2}\varphi_{tt}\varphi = 0. \tag{7-12}$$

The third term above is computed as

$$\int t^{a+2}\varphi_{tt}\varphi = -\int t^{a+2}\varphi_t^2 - (a+2)\int t^{a+1}\varphi_t\varphi,$$

so (7-12) becomes

$$d_1 = -2\int t^{a+1}\varphi_t\varphi = (a+1)\int t^a\varphi^2 = (a+1)d_3. \tag{7-13}$$

This completes the proof of the lemma. □

In the following, we continue the estimates of the different error terms, although now we only need the asymptotic behavior and not the precise constant.

Lemma 7.3. *Let w be defined on $\mathbb{R}^n$ and $U = K_\gamma *_x w$. Then*

(1) *for each $k \in \mathbb{N}$, if $w \in H^{\gamma-k/2}(\mathbb{R}^n)$,*

$$\mathscr{E}_k := \int_{\mathbb{R}^{n+1}_+} y^{a+k}|\nabla U|^2\,dx\,dy < \infty; \tag{7-14}$$

(2) *if $w \in H^{\gamma-3/2}(\mathbb{R}^n)$ and $(|x|w) \in H^{-1/2+\gamma}(\mathbb{R}^n)$,*

$$\tilde{\mathscr{E}}_3 := \int_{\mathbb{R}^{n+1}_+} y^a|(x,y)|^3|\nabla U|^2\,dx\,dy < \infty. \tag{7-15}$$

Proof. Taking into account (7-3), we can proceed as in the calculation for $\mathscr{A}_1$ in (7-7), easily arriving at

$$\mathscr{E}_k = c_k\int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{1-k-a}\,d\xi,$$

where

$$c_k := \int_0^\infty t^{a+k}(\varphi^2(t) + \varphi_t^2(t))\,dt < \infty,$$

and this last integral is finite for all $k \in \mathbb{N}$ because of the asymptotics of the Bessel functions from Lemma 7.1. The second conclusion of the lemma is a little more involved. To show that the integral (7-15) is finite, first note that (7-14) with $k = 3$ gives

$$\int_{\mathbb{R}^{n+1}_+} y^{a+3}|\nabla U|^2\,dx\,dy < \infty.$$

It is clear that it only remains to prove

$$\int_{\mathbb{R}^{n+1}_+} y^a|x|^3|\nabla U|^2\,dx\,dy < \infty.$$

Since the computation of the previous integral can be made component by component, it is clear that it is enough to restrict to the case $n=1$. Then we just need to show that

$$J := \int_0^\infty \int_{\mathbb{R}} y^a |x|^3 (\partial_x U)^2 \, dx \, dy < \infty. \tag{7-16}$$

This is an easy but tedious calculation using the Fourier transform. Without loss of generality, we drop all the constants 2π appearing in the Fourier transform. First notice that

$$\begin{aligned} \int_{\mathbb{R}} |x|^3 (\partial_x U)^2 \, dx &= \| \{ |x|^{3/2} \partial_x U \} \|^2_{L^2(\mathbb{R})} = \| D_\xi^{3/2} \widehat{\partial_x U} \|^2_{L^2(\mathbb{R})} = \| D^{3/2} (|\xi| \widehat{U}) \|^2_{L^2(\mathbb{R})} \\ &= \int_{\mathbb{R}} |\xi| \widehat{U} D_\xi^3 (|\xi| \widehat{U}) \, d\xi. \end{aligned} \tag{7-17}$$

At this point we go back to (7-3) to substitute the explicit expression for $\widehat{U}$. We need to compute

$$\begin{aligned} &D_\xi^3(|\xi| \hat{w}(\xi) \varphi(|\xi| y)) \\ &\qquad = \hat{w}'''[|\xi|\varphi] + \hat{w}''[3\varphi + 3|\xi|\varphi' y] + \hat{w}'[6\varphi' y + 3|\xi|\varphi'' y^2] + \hat{w}[|\xi|\varphi''' y^3 + 3\varphi'' y^2] \\ &\qquad = \hat{w}'''[|\xi|\varphi] + \hat{w}''[3\varphi + 3t\varphi'] + \hat{w}'[6|\xi|^{-1} t\varphi' + 3|\xi|^{-1} t^2 \varphi''] + \hat{w}[|\xi|^{-2} \varphi''' t^3 + 3|\xi|^{-2} t^2 \varphi''], \end{aligned}$$

after the change $|\xi| y = t$. When we substitute the above expression into (7-17) and then back into (7-16), taking into account the change of variables, we obtain

$$\begin{aligned} J &= \int_0^\infty t^a \varphi^2 \, dt \int_{\mathbb{R}} \hat{w}''' \hat{w} |\xi|^{1-a} \, d\xi + \int_0^\infty t^a [\varphi^2 + 3t\varphi\varphi'] \, dt \int_{\mathbb{R}} \hat{w}'' \hat{w} |\xi|^{-a} \, d\xi \\ &\quad + \int_0^\infty t^a [6t\varphi'\varphi + 3t^2 \varphi''\varphi] \, dt \int_{\mathbb{R}} \hat{w}' \hat{w} |\xi|^{-a-1} \, d\xi + \int_0^\infty t^a [t^3 \varphi''' \varphi + 3t^2 \varphi'' \varphi] dt \int_{\mathbb{R}} \hat{w}^2 |\xi|^{-a-2} \, d\xi \\ &\qquad =: c_1 J_1 + c_2 J_2 + c_3 J_3 + c_4 J_4. \end{aligned}$$

It is clear, looking at the asymptotic behavior of φ from Lemma 7.1 that the constants c_i, $i = 1, 2, 3, 4$, are finite. On the other hand, by a straightforward integration by parts argument, we can write each of the terms J_i, $i = 1, 2, 3, 4$, as a linear combination of just

$$\int_{\mathbb{R}} \hat{w}^2(\xi) |\xi|^{-a-2} \, d\xi \quad \text{and} \quad \int_{\mathbb{R}} \hat{w}'(\xi)^2 |\xi|^{-a} \, d\xi. \tag{7-18}$$

Finally, the proof is completed because the initial hypotheses show that both integrals in (7-18) are finite. In particular, these hypotheses show that all the derivations are rigorous. □

Lemma 7.4. *Let w be defined on $\mathbb{R}^n$ and $U = K_\gamma *_x w$.*

(1) *For each $k \in \mathbb{N}$, if $w \in H^{\gamma - k/2 - 1}(\mathbb{R}^n)$,*

$$\mathcal{F}_k := \int_{\mathbb{R}^{n+1}_+} y^{a+k} U^2 \, dx \, dy < \infty. \tag{7-19}$$

(2) *If $w \in H^{\gamma - 5/2}(\mathbb{R}^n)$ and $(|x| w) \in H^{\gamma - 3/2}(\mathbb{R}^n)$,*

$$\tilde{\mathcal{F}}_3 := \int_{\mathbb{R}^{n+1}_+} y^a |x|^3 U^2 \, dx \, dy < \infty. \tag{7-20}$$

Proof. The first assertion (7-19) follows as in (7-10):

$$\mathcal{F}_k := \int_{\mathbb{R}^{n+1}_+} y^{a+k} U^2\,dx\,dy = \int_{\mathbb{R}^n}\int_0^\infty y^{a+k}|\widehat{U}|^2\,dy\,d\xi = \int_{\mathbb{R}^n}\int_0^\infty y^{a+k}|\hat{w}(\xi)|^2|\varphi(|\xi|y)|^2\,dy\,d\xi$$
$$= \int_{\mathbb{R}^n} |\hat{w}(\xi)|^2|\xi|^{-1-a-k}\int_0^\infty |\varphi(t)|^2 t^{a+k}\,dt\,d\xi = c_k\int_{\mathbb{R}^n}|\hat{w}(\xi)|^2|\xi|^{-1-a-k}\,d\xi,$$

for

$$c_k := \int_0^\infty |\varphi(t)|^2 t^{a+k}\,dt < \infty.$$

For the second assertion, in light of our previous discussions, it is enough to show that, in the one-dimensional case,

$$\int_{\mathbb{R}} |x|^3 U^2\,dx = \|\{|x|^{3/2}U\}\|^2_{L^2(\mathbb{R})} = \|D^{3/2}\widehat{U}\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} \widehat{U} D^3_\xi(\widehat{U})\,d\xi.$$

Substitute the expression for $\widehat{U}$ from (7-3). Then

$$\int_{\mathbb{R}} |x|^3U^2\,dx = \int \hat{w}'''\hat{w}\varphi^2\,d\xi + 3\int \hat{w}''\hat{w}\varphi'\varphi y\,d\xi + 3\int \hat{w}'\hat{w}\varphi'\varphi y^2\,d\xi + \int \hat{w}^2\varphi'''\varphi y^3\,d\xi,$$

so when we change variables $t = |\xi|y$,

$$\int_0^\infty\int_{\mathbb{R}} y^a|x|^3U^2\,dx\,dy = \int_0^\infty t^a\varphi^2\,dt\int_{\mathbb{R}}\hat{w}'''\hat{w}|\xi|^{-1-a}\,d\xi + 3\int_0^\infty t^{1+a}\varphi'\varphi\,dt\int_{\mathbb{R}}\hat{w}''\hat{w}|\xi|^{-2-a}\,d\xi$$
$$+3\int_0^\infty t^{2+a}\varphi''\varphi\,dt\int_{\mathbb{R}}\hat{w}'\hat{w}|\xi|^{-3-a}\,d\xi + \int_0^\infty t^{3+a}\varphi'''\varphi dt\int_{\mathbb{R}}\hat{w}^2|\xi|^{-4-a}\,d\xi$$
$$= \tilde{c}_1\tilde{J}_1 + \tilde{c}_2\tilde{J}_2 + \tilde{c}_3\tilde{J}_3 + \tilde{c}_4\tilde{J}_4.$$

Clearly, from the asymptotics of the Bessel functions from Lemma 7.1, the constants $\tilde{c}_i$, $i = 1, 2, 3, 4$, are finite. At the same time, each of the integrals $\tilde{J}_i$, $i = 1, 2, 3, 4$, can be written as a linear combination of

$$\int (\hat{w}')^2|\xi|^{-2-a}\,d\xi \quad \text{and} \quad \int (\hat{w})^2|\xi|^{-4-a}\,d\xi,$$

which are finite because of the hypothesis on w. □

Next, we check what happens with the previous two lemmas under rescaling. Here $f = o(1)$ means

$$\lim_{\epsilon/\mu\to 0} f = 0.$$

Given any function w defined on $\mathbb{R}^n$, we consider its extension to $\mathbb{R}^{n+1}_+$ as $U = K_\gamma *_x w$, and the rescaling, for each $\mu > 0$,

$$U_\mu(x,y) := \frac{1}{\mu^{(n-2\gamma)/2}}U\Big(\frac{x}{\mu},\frac{y}{\mu}\Big). \tag{7-21}$$

Corollary 7.5. *Fix $\epsilon, \mu > 0$ and let the hypotheses be the as in Lemma 7.3 (in each of the two cases).*

(1) *For each* $k \in \mathbb{N}$,

$$\int_{B_\epsilon^+} y^{a+k}|\nabla U_\mu|^2 dx\,dy = \mu^k \int_{B_{\epsilon/\mu}^+} y^{a+k}|\nabla U|^2 dx\,dy = \mu^k[\mathscr{E}_k + o(1)]. \tag{7-22}$$

(2) *Moreover*,

$$\int_{B_\epsilon^+} y^a|(x,y)|^3|\nabla U_\mu|^2\,dx\,dy = \mu^3 \int_{B_{\epsilon/\mu}^+} y^{a+k}|\nabla U|^2\,dx\,dy = \mu^3[\tilde{\mathscr{E}}_3 + o(1)], \tag{7-23}$$

where U_μ *is the rescaling* (7-21), *and* $\mathscr{E}_k, \tilde{\mathscr{E}}_3 < \infty$ *are defined as in* Lemma 7.3.

Corollary 7.6. *Fix* $\epsilon, \mu > 0$ *and let the hypotheses be as in* Lemma 7.4 (*in each of the two cases*).

(1) *For each* $k \in \mathbb{N}$,

$$\int_{B_\epsilon^+} y^{a+k}(U_\mu)^2\,dx\,dy = \mu^{k+2} \int_{B_{\epsilon/\mu}^+} y^{a+k}U^2\,dx\,dy = \mu^{k+2}[\mathscr{F}_k + o(1)]. \tag{7-24}$$

(2) *Moreover*,

$$\int_{B_\epsilon^+} y^a|(x,y)|^3(U_\mu)^2\,dx\,dy = \mu^5 \int_{B_{\epsilon/\mu}^+} y^a|x|^3U^2\,dx\,dy = \mu^5[\tilde{\mathscr{F}}_3 + o(1)], \tag{7-25}$$

where U_μ *is the rescaling* (7-21), *and* $\mathscr{F}_k, \tilde{\mathscr{F}}_3 < \infty$ *are defined as in* Lemma 7.4.

Proof of Theorem 1.5. We first need to choose a very particular background metric for X near a nonumbilic point on M. We follow the same steps as in Lemmas 3.1–3.3 of [Escobar 1992]. But our situation is a little different. Our freedom of choice of metrics is restricted to the boundary. Hence we make some assumptions on the behavior of the asymptotically hyperbolic manifolds in order to allow us to see clearly what we can get for a good choice of representative from the conformal infinity.

Lemma 7.7. *Suppose that* (X^{n+1}, g^+) *is an asymptotically hyperbolic manifold and* ρ *is a geodesic defining function associated with a representative* $\hat{h}$ *of the conformal infinity* $(M^n, [\hat{h}])$. *Assume that*

$$\rho^{-2}(R[g^+] - \mathrm{Ric}[g^+](\rho\partial_\rho) + n^2) \to 0 \quad \text{as } \rho \to 0. \tag{7-26}$$

Then, at $\rho = 0$,

$$H := \mathrm{Tr}_{\hat{h}}\, h^{(1)} = 0 \tag{7-27}$$

and

$$\mathrm{Tr}_{\hat{h}}\, h^{(2)} = \tfrac{1}{2}\Big(\|h^{(1)}\|_{\hat{h}}^2 + \frac{1}{2(n-1)}R[\hat{h}]\Big), \tag{7-28}$$

where

$$g^+ = \frac{d\rho^2 + h_\rho}{\rho^2}, \qquad h_\rho = \hat{h} + h^{(1)}\rho + h^{(2)}\rho^2 + o(\rho^2).$$

Proof. This simply follows from the calculations in [Graham 2000]. Recall (2.5) from [Graham 2000]:

$$\rho h_{ij}'' + (1-n)h_{ij}' - h^{kl}h_{kl}'h_{ij} - \rho h^{kl}h_{ik}'h_{jl}' + \tfrac{1}{2}\rho h^{kl}h_{kl}'h_{ij}' - 2\rho R_{ij}[\hat{h}] = \rho(R_{ij}[g^+] + ng_{ij}^+), \tag{7-29}$$

where we use h to stand for h_ρ for simplicity. Taking its trace with respect to the metrics h, we have

$$\rho\,\mathrm{Tr}_h\,h'' + (1-2n)\,\mathrm{Tr}_h\,h' - \rho\|h'\|_h^2 + \tfrac{1}{2}\rho(\mathrm{Tr}_h\,h')^2 - 2\rho R[\hat{h}] = \rho^{-1}(R[g^+] - \mathrm{Ric}[g^+](x\partial_x) + n^2). \tag{7-30}$$

Immediately from (7-26) we see that

$$\mathrm{Tr}_h\,h' = 0 \quad \text{at } \rho = 0.$$

Then, dividing ρ in both sides of (7-30) and taking $\rho \to 0$, we have (7-28), under the assumption (7-26), because

$$(\mathrm{Tr}_h\,h')' = \mathrm{Tr}_{\hat{h}}\,h'' - \|h'\|_{\hat{h}}^2 \quad \text{at } \rho = 0. \qquad \square$$

Notice that (7-26) is an intrinsic curvature condition of an asymptotically hyperbolic manifold, which is independent of the choice of geodesic defining functions. Consequently we have the following.

Lemma 7.8. *Suppose that (X^{n+1}, g^+) is an asymptotically hyperbolic manifold and (7-26) holds. Then, given a point p on the boundary M, there exists a representative $\hat{h}$ of the conformal infinity such that*

(i) $H =: \mathrm{Tr}_{\hat{h}}\,h^{(1)} = 0$ *on* M,

(ii) $\mathrm{Ric}[\hat{h}](p) = 0$ *on* M,

(iii) $\mathrm{Ric}[\bar{g}](\partial_\rho)(p) = 0$ *on* M,

(iv) $R[\bar{g}](p) = \|h^{(1)}\|_{\hat{h}}^2$ *on* M.

Proof. The proof, like that of Lemma 3.3 in [Escobar 1992], uses Theorem 5.2 of [Lee and Parker 1987]. Therefore we may choose a representative of the conformal infinity whose Ricci curvature vanishes at any given point $p \in M$. In light of Lemma 7.7 we get *i.* and *ii.* right away. We then calculate

$$\mathrm{Ric}[\bar{g}](\partial_x) = -\tfrac{1}{2}\,\mathrm{Tr}_{\hat{h}}\,h^{(2)} + \tfrac{1}{4}\|h^{(1)}\|_{\hat{h}}^2 = 0$$

at $p \in M$ from (7-28). Finally we recall that

$$R[\bar{g}] = 2\,\mathrm{Ric}[\bar{g}](\partial_\rho) + R[\hat{h}] + \|h^{(1)}\|_{\hat{h}}^2 - (\mathrm{Tr}_{\hat{h}}\,h^{(1)})^2 = \|h^{(1)}\|_{\hat{h}}^2.$$

The proof is complete. $\square$

Assume that $0 \in M = \partial\overline{X}$ is a nonumbilic point. Choose normal coordinates $x_1, \ldots, x_n$ around 0 on M and let $(x_1, \ldots, x_n, \rho)$ be the Fermi coordinates on X around 0. In particular, we can write

$$g^+ = \rho^{-2}(d\rho^2 + h_{ij}(x, \rho)\,dx_i dx_j), \qquad \bar{g} = d\rho^2 + h_{ij}(x, \rho)\,dx_i dx_j.$$

In order to simplify the later notation, we denote the coordinate ρ by y. The only risk of confusion comes from the fact that we have previously used y for the special defining function ρ^* from Proposition 2.2, but we will not need it any longer. In the new notation we have

$$\bar{g} = dy^2 + h_{ij}(x, y)\,dx_i dx_j$$

for some functions $h_{ij}(x, y)$, $i, j = 1, \ldots, n$. From what we have in the above two lemmas, we get from Lemmas 3.1 and 3.2 of [Escobar 1992] the following.

Lemma 7.9. *Suppose that (X^{n+1}, g^+) is an asymptotically hyperbolic manifold satisfying (7-26). Given a nonumbilic point p on the boundary M, that is, one such $\|h^{(1)}\|_{\hat{h}}(p) \neq 0$ for $p \in M$, where $\hat{h}$ is chosen as in Lemma 7.8, we have*

(1) $\sqrt{|\bar{g}|} = 1 - \frac{1}{2}\|\pi\|^2 y^2 + O(|(x, y)|^3)$ *and*

(2) $\bar{g}^{ij} = \delta_{ij} + 2\pi^{ij} y - \frac{1}{3} R^{i\ \ j}_{\ kl}[\hat{h}]\, x_k x_l + \bar{g}^{ij}{}_{,ym}\, y x_m + (3\pi^{im}\pi_m{}^j + R^{i\ j}_{\ y\ y}[\bar{g}]) y^2 + O(|(x, y)|^3)$,

where, for simplicity, we set $\pi = h^{(1)}$.

As in Proposition 5.4, we try to find a good test function for the Sobolev quotient given by

$$I^*_\gamma[U, \bar{g}] = \frac{d^*_\gamma \int_X y^a |\nabla U|^2_{\bar{g}}\, dv_{\bar{g}} + \int_X E(y) U^2\, dv_{\bar{g}}}{(\int_M |U|^{2^*}\, dv_{\hat{h}})^{2/2^*}},$$

where $E(y)$ is given by (2-10), with respect to the metric $\bar{g}$:

$$E(y) = \frac{n-1+a}{4n}\big(R[\bar{g}] - (n(n+1) + R[g^+]) y^{-2}\big) y^a. \tag{7-31}$$

We need to perform a careful computation of the lower order terms in order to find an estimate for $\Lambda_\gamma(M, [\hat{h}])$. For simplicity, we introduce the following notation: for a subset $\Omega \subset \mathbb{R}^{n+1}_+$, we consider the energy functional restricted to Ω given by

$$\mathcal{K}(U, \Omega) := d^*_\gamma \int_\Omega y^a |\nabla U|^2_{\bar{g}}\, dv_{\bar{g}} + \int_\Omega E(y) U^2\, dv_{\bar{g}}.$$

Given any $\epsilon > 0$, let B_ϵ be the ball of radius ϵ centered at the origin in $\mathbb{R}^{n+1}$ and B^+_ϵ be the half ball of radius ϵ in $\mathbb{R}^{n+1}_+$. Choose a smooth radial cutoff function η, $0 \le \eta \le 1$, supported on $B_{2\epsilon}$, and satisfying $\eta = 1$ on B_ϵ. We recall here the conformal diffeomorphisms of the sphere w_μ given in (5-8) and their extension U_μ as in (5-9). Our test function is simply

$$V_\mu := \eta U_\mu.$$

Step 1: Computation of the energy in B^+_ϵ. It is clear that in the half ball B^+_ϵ, $V_\mu = U_\mu$, so that $\mathcal{K}(V_\mu, B^+_\epsilon) = \mathcal{K}(U_\mu, B^+_\epsilon)$. We compute the first term in the energy $\mathcal{K}(U_\mu, B^+_\epsilon)$. Using the asymptotics for $\bar{g}$ from Lemma 7.9, we have (here the indexes i, j run from 1 to n)

$$\begin{aligned}\int_{B^+_\epsilon} y^a |\nabla U_\mu|^2_{\bar{g}}\, dv_{\bar{g}} &= \int_{B^+_\epsilon} y^a [\bar{g}^{ij} (\partial_i U_\mu)(\partial_j U_\mu) + (\partial_y U_\mu)^2]\, dv_{\bar{g}} \\ &= J_1 + J_2 + J_3 + J_4 + J_5 + J_6,\end{aligned} \tag{7-32}$$

where

$$J_1 := \int_{B^+_\epsilon} y^a |\nabla U_\mu|^2\, dv_{\bar{g}},$$

$$J_2 := 2\pi^{ij} \int_{B^+_\epsilon} y^{a+1} (\partial_i U_\mu)(\partial_j U_\mu)\, dv_{\bar{g}},$$

$$J_3 := \int_{B^+_\epsilon} y^{a+2} (3\pi^{im}\pi_m{}^j + R^{i\ j}_{\ y\ y}[\bar{g}])(\partial_i U_\mu)(\partial_j U_\mu)\, dv_{\bar{g}},$$

$$J_4 := \int_{B_\epsilon^+} y^{a+1} \bar{g}^{ij}{}_{,tk} x_k (\partial_i U_\mu)(\partial_j U_\mu)\, dv_{\bar{g}}$$
$$J_5 := -\frac{1}{3} \int_{B_\epsilon^+} y^a R^i{}_{kl}{}^j [\bar{g}] x_k x_l (\partial_i U_\mu)(\partial_j U_\mu)\, dv_{\bar{g}}$$
$$J_6 := c \int_{B_\epsilon^+} y^a |(x, y)|^3 |\nabla U_\mu|^2\, dv_{\bar{g}}.$$

We estimate J_1 using the estimate for the volume element $\sqrt{|\bar{g}|}$ from Lemma 7.9:

$$\begin{aligned} J_1 &= \int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\, dv_{\bar{g}} \\ &\le \int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\, dx\, dy - \tfrac{1}{2}\|\pi\|^2 \int_{B_\epsilon^+} y^{2+a} |\nabla U_\mu|^2\, dx\, dy + c \int_{B_\epsilon^+} y^a |\nabla U_\mu|^2 |(x, y)|^3\, dx\, dy \\ &\le \int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\, dx\, dy - \tfrac{1}{2}\|\pi\|^2 \mu^2 \mathcal{A}_1 + \mu^2 o(1) + c\mu^3 [\tilde{\mathcal{E}}_3 + o(1)], \end{aligned} \tag{7-33}$$

if we take into account the notation from (7-4) and Corollary 7.5.

Now we look closely at the equation for U_μ. Multiply expression (5-11) by U_μ and integrate by parts:

$$\int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\, dx\, dy = c_{n,\gamma} \int_{\Gamma_\epsilon^0} w_\mu^{2^*}\, dx + \int_{\Gamma_\epsilon^+} U_\mu (\partial_\nu U_\mu)\, d\sigma \le c_{n,\gamma} \int_{\Gamma_\epsilon^0} w_\mu^{2^*}\, dx, \tag{7-34}$$

where ν is the exterior normal to B_ϵ^+. Here we have used the properties of the convolution with a radially symmetric, nonincreasing kernel K_γ. More precisely, since w_μ is radially symmetric and nonincreasing, $U_\mu = K_\gamma *_x w_\mu$ also satisfies $\partial_\nu U_\mu \le 0$ on Γ_ϵ^+; see [Cabré and Roquejoffre 2013, Lemma 2.3], for instance.

From (7-34), using (5-13), we arrive at

$$\int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\, dx\, dy \le \Lambda(S^m, [g_c])(d_\gamma^*)^{-1} \left[\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*}\, dx \right]^{(n-2\gamma)/n}. \tag{7-35}$$

For simplicity, we set $\Lambda_1 := \Lambda(S^m, [g_c])(d_\gamma^*)^{-1}$. Equations (7-33) and (7-35) tell us that

$$J_1 = \int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\, dv_{\bar{g}} \le \Lambda_1 \left[\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*}\, dx \right]^{2/2^*} - \tfrac{1}{2}\|\pi\|^2 \mu^2 \mathcal{A}_1 + \mu^2 o(1) + c\mu^3. \tag{7-36}$$

On the other hand, the asymptotics for the metric $\hat{h} = \bar{g}|_{y=0}$ near the origin are explicit. Indeed, from Lemma 7.8 we know that

$$\sqrt{|\hat{h}|} = 1 + O(|x|^3). \tag{7-37}$$

Moreover, we can compute from (5-10)

$$\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*} |x|^3\, dx = \mu^3 \int_{\Gamma_{\epsilon/\mu}^0} (w_1)^{2^*} |x|^3\, dx \le c\mu^3.$$

Consequently, from (7-37) we are able to relate the integrals in $dv_{\hat h}$ and dx:

$$\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*}\,dx \le \int_{\Gamma_\epsilon^0} (w_\mu)^{2^*}\,dv_{\hat h} + c\mu^3.$$

And substituting the above expression into (7-36) we get

$$J_1 = \int_{B_\epsilon^+} y^a |\nabla U_\mu|^2\,dv_{\bar g} \le \Lambda_1 \left[\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*}\,dv_{\hat h} \right]^{2/2^*} - \tfrac{1}{2}\|\pi\|^2\mu^2\mathcal{A}_1 + \mu^2 o(1) + c\mu^3.$$

Now we go back to (7-32) and try to estimate the second term J_2 in the right hand side. If we again use the asymptotics of the metric $\bar g$ given in Lemma 7.9,

$$\int_{B_\epsilon^+} y^{a+1}(\partial_i U_\mu)(\partial_j U_\mu)\,dv_{\bar g} \le \int_{B_\epsilon^+} y^{a+1}(\partial_i U_\mu)(\partial_j U_\mu)\,dx\,dy + \mathcal{B}, \tag{7-38}$$

for

$$\mathcal{B} \le c\int_{B_\epsilon^+} y^{a+3}|\nabla U_\mu|^2 dx\,dy + c\int_{B_\epsilon^+} y^{a+1}|\nabla U_\mu|^2 |(x,y)|^3\,dx\,dy.$$

We notice here that $\mathcal{B}$ can be easily estimated from Corollary 7.5:

$$\mathcal{B} \le c\mu^3(\mathcal{E}_3 + o(1)) + c\mu^3\epsilon(\tilde{\mathcal{E}}_3 + o(1)) \le c\mu^3 + \mu^3 o(1). \tag{7-39}$$

Let us look at the cross terms $(\partial_i U_\mu)(\partial_j U_\mu)$, $1 \le i, j \le n$ in (7-38). We note that $\partial_i U_\mu = K_\gamma *_x (\partial_i w_\mu)$, just by taking the derivatives in the convolution. This last derivative can be explicitly written, and in particular, $\partial_i w_\mu$ is an odd function in the variable x_i. By the properties of the convolution, we know that $\partial_i U_\mu$ is also an odd function in the variable x_i. Then, using the symmetries of the half ball, the integral

$$\int_{B_\epsilon^+} y^{a+1}(\partial_i U_\mu)(\partial_j U_\mu)\,dx\,dy$$

is zero if $i \ne j$. If $i = j$, we use that the mean curvature at the point vanishes, that is, $\pi_i^i = 0$ by Lemma 7.8. Then, when we substitute formula (7-38) in the expression for J_2, only the error term remains, and by (7-39) we conclude that

$$J_2 = 2\pi^{ij}\int_{B_\epsilon^+} y^{a+1}(\partial_i U_\mu)(\partial_j U_\mu)\,dv_{\bar g} \le \mathcal{B} \le \mu^3(c + o(1)). \tag{7-40}$$

Now we estimate the next term in (7-32), J_3. Again using the asymptotics for the volume element $dv_{\bar g}$ from Lemma 7.9, we have that

$$\int_{B_\epsilon^+} y^{a+2}(\partial_i U_\mu)(\partial_j U_\mu)\,dv_{\bar g} \le \int_{B_\epsilon^+} y^{a+2}(\partial_i U_\mu)(\partial_j U_\mu)\,dx\,dy + \mathcal{B}', \tag{7-41}$$

for

$$\begin{aligned}\mathcal{B}' &\le c\int_{B_\epsilon^+} y^{a+4}|\nabla U_\mu|^2 dx\,dy + c\int_{B_\epsilon^+} y^{a+2}|(x,y)|^3|\nabla U_\mu|^2 dx\,dy \\ &\le \mu^4(\mathcal{E}_4 + o(1)) + \mu^3\epsilon^2(\tilde{\mathcal{E}}_3 + o(1)) \le c\mu^3,\end{aligned}$$

where the last estimate follows again thanks to Corollary 7.5.

Notice that, again for $i \neq j$,, the first integral in the right hand side of (7-41) vanishes — thanks to the symmetries of the half ball and the discussion above on the oddness of the derivatives of U_μ. Then we recall the definition of $\mathcal{A}_2$ from (7-5) and the estimate (7-22). When we put all these ingredients together, we get

$$\begin{aligned} J_3 &= (3\pi^{im}\pi_m{}^j + R^i{}_y{}^j{}_y[\bar{g}]) \int_{B_\epsilon^+} y^{a+2}(\partial_i U_\mu)(\partial_j U_\mu)\, dv_{\bar{g}} \\ &= \frac{1}{n}[3\|\pi\|^2 + \mathrm{Ric}(\nu)]\mu^2 \mathcal{A}_2 + c\mu^3 \\ &= \frac{3}{n}\|\pi\|^2\mu^2\mathcal{A}_2 + \mu^2 o(1) + c\mu^3, \end{aligned}$$

if we take into account that $\mathrm{Ric}(\nu)(0)[\hat{h}] = 0$ because of Lemma 7.8.

Next, the calculation for J_4 is very similar to the previous one. Indeed,

$$\int_{B_\epsilon^+} y^{a+1} x_k (\partial_i U_\mu)(\partial_j U_\mu)\, dv_{\bar{g}} \leq \int_{B_\epsilon^+} y^{a+1} x_k (\partial_i U_\mu)(\partial_j U_\mu)\, dx\, dy + \mathcal{B}'',$$

and because of symmetries on the unit ball, the first integral in the right hand side above vanishes for all i, j, k, while $\mathcal{B}'' \leq c\mu^3$. Thus

$$J_4 = \bar{g}^{ij}{}_{,tk} \int_{B_\epsilon^+} y^{a+1} x_k (\partial_i V_\mu)(\partial_j V_\mu)\, dv_{\bar{g}} \leq c\mu^3.$$

And finally J_5, J_6 can be estimated in a similar manner.

Putting all the estimates together for the J_j, $j = 1, \ldots, 6$, we have shown that (7-32) reduces to

$$\int_{B_\epsilon^+} y^a |\nabla U_\mu|_{\bar{g}}^2\, dv_{\bar{g}} \leq \Lambda_1 \left[\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*}\, dv_{\hat{h}} \right]^{2/2^*} + \left[-\tfrac{1}{2}\mathcal{A}_1 + \frac{3}{n}\mathcal{A}_2 \right] \|\pi\|^2\mu^2 + \mu^2 o(1) + c\mu^3. \tag{7-42}$$

Finally, we are able to complete the computation of the energy $\mathcal{K}(U_\mu, B_\epsilon^+)$. Note that in the half ball B_ϵ^+, we have a very precise behavior for the lower order term (7-31). In particular, Lemma 7.8 gives that $R[\bar{g}](p) = \|\pi\|^2$, so

$$E(y) = \frac{n-1+a}{4n}\|\pi\|^2 y^a + O(y^{1+a}). \tag{7-43}$$

Then, again using the asymptotics for the volume element $dv_{\bar{g}}$,

$$\int_{B_\epsilon^+} E(y)(U_\mu)^2\, dv_{\bar{g}} = \frac{n-1+a}{4n}\|\pi\|^2 \int_{B_\epsilon^+} y^a (U_\mu)^2\, dx\, dy + \mathcal{B}''', \tag{7-44}$$

where

$$\mathcal{B}''' \leq c \int_{B_\epsilon^+} y^{a+1}(U_\mu)^2\, dx\, dy + c \int_{B_\epsilon^+} y^a |x|^3 (U_\mu)^3\, dx\, dy$$

can be estimated from Corollary 7.6 as

$$\mathcal{B}''' \leq c\mu^3 + o(1). \tag{7-45}$$

Summarizing, from (7-44) and (7-45), and using the scaling properties of U_μ as given in (5-10), we have

$$\begin{aligned}\int_{B_\epsilon^+} E(y)(U_\mu)^2\,dv_{\bar g} &\le \frac{n-1+a}{4n}\|\pi\|^2\mu^2\int_{B^+_{\epsilon/\mu}} y^a(U_1)^2\,dx\,dy + c\mu^3\\ &= \frac{n-1+a}{4n}\|\pi\|^2\mu^2\mathcal{A}_3 + c\mu^2 o(1) + c\mu^3,\end{aligned}\tag{7-46}$$

where for the last inequality we have used Corollary 7.6 and the definition of $\mathcal{A}_3$ from (7-6).

The energy of V_μ in the half ball B_ϵ^+ is computed from (7-42) and (7-46), noting the relation between $\mathcal{A}_1$, $\mathcal{A}_2$, $\mathcal{A}_3$ from Lemma 7.2 and that $\Lambda_1 = \Lambda(S^n, [g_c])d_\gamma^*$:

$$\begin{aligned}&\mathcal{K}(V_\mu, B_\epsilon^+)\\ &\quad= d_\gamma^*\int_{B_\epsilon^+} y^a|\nabla U_\mu|^2 dv_{\bar g} + \int_{B_\epsilon^+} E(y)(U_\mu)^2\,dv_{\bar g}\\ &\quad\le \Lambda(S^n,[g_c])\left[\int_{\Gamma_\epsilon^0}(w_\mu)^{2^*}dv_{\hat h}\right]^{2/2^*} + \left[d_\gamma^*\left(-\tfrac12\mathcal{A}_1 + \frac{3}{n}\mathcal{A}_2\right) + \frac{n-1+a}{4n}\mathcal{A}_3\right]\|\pi\|^2\mu^2 + \mu^2 o(1) + c\mu^3\\ &\quad\le \Lambda(S^n,[g_c])\left[\int_{\Gamma_\epsilon^0}(w_\mu)^{2^*}\,dv_{\hat h}\right]^{2/2^*} + \theta_{n,\gamma}\|\pi\|^2\mu^2\int_{\mathbb{R}^n}|\xi|^{2(\gamma-1)}|\hat w_1(\xi)|^2\,d\xi + \mu^2 o(1) + c\mu^3\end{aligned}$$

for

$$\theta_{n,\gamma} = \frac{1}{4n}\left[\frac{n+a-3}{1-a}2^{2\gamma+1}\frac{\Gamma(\gamma)}{\Gamma(-\gamma)} + \frac{n-1+a}{a+1}\right]d_1.\tag{7-47}$$

Finally, we note that $w_1 \in H^\gamma(\mathbb{R}^n)$ and $(|x|w) \in H^\gamma(\mathbb{R}^n)$, so that all our computations are well justified.

Step 2: Computation of the energy in the half-annulus $B_{2\epsilon}^+\backslash B_\epsilon^+$. To compute $\mathcal{K}(V_\mu, B_{2\epsilon}^+\backslash B_\epsilon^+)$, note that

$$|\nabla V_\mu|_{\bar g}^2 \le c|\nabla V_\mu|^2 \le c(\eta^2|\nabla U_\mu|^2 + (U_\mu)^2|\nabla\eta|^2)$$

so that, because of the structure of the cutoff function η,

$$|\nabla V_\mu|_{\bar g}^2 \le c|\nabla U_\mu|^2 + \frac{c}{\epsilon}(U_\mu)^2.\tag{7-48}$$

Moreover,

$$\int_{B_{2\epsilon}^+\backslash B_\epsilon^+} y^a(U_\mu)^2\,dx\,dy \le \mu^2\int_{B^+_{2\epsilon/\mu}\backslash B^+_{\epsilon/\mu}} y^a(U_1)^2\,dx\,dy = \mu^2 o(1),\tag{7-49}$$

because the integral $\int_{\mathbb{R}^n} y^a(U_1)^2\,dx\,dy$ is finite and $\epsilon/\mu \to \infty$. On the other hand, we know that

$$\left(\frac{\epsilon}{\mu}\right)^3\int_{B^+_{2\epsilon/\mu}\backslash B^+_{\epsilon/\mu}} y^a|\nabla U_1|^2\,dx\,dy \le \int_{B^+_{2\epsilon/\mu}\backslash B^+_{\epsilon/\mu}} y^a|(x,y)|^3|\nabla U_1|^2\,dx\,dy \le \tilde{\mathcal{E}}_3 < \infty$$

because of Lemma 7.4. As a consequence,

$$\int_{B_{2\epsilon}^+\backslash B_\epsilon^+} y^a|\nabla U_\mu|^2\,dx\,dy = \int_{B^+_{2\epsilon/\mu}\backslash B^+_{\epsilon/\mu}} y^a|\nabla U_1|^2\,dx\,dy \le \left(\frac{\mu}{\epsilon}\right)^3\tilde{\mathcal{E}}_3.\tag{7-50}$$

If we put together formulas (7-48), (7-49), and (7-50), we arrive at

$$\mathcal{K}(V_\mu, B_{2\epsilon}^+ \setminus B_\epsilon^+) = \int_{B_{2\epsilon}^+ \setminus B_\epsilon^+} y^a |\nabla U_\mu|^2 \, dx \, dy + \int_{B_{2\epsilon}^+ \setminus B_\epsilon^+} E(y)(U_\mu)^2 \, dx \, dy \le \mu^2 o(1)$$

when $\mu/\epsilon \to 0$.

Step 3: Completion of the proof. We have very carefully computed

$$\begin{aligned}\mathcal{K}(V_\mu, X) &= d_\gamma^* \int_X y^a |\nabla V_\mu|^2 \, d\mathrm{vol}_{\bar g} + \int_X E(y)(V_\mu)^2 \, d\mathrm{vol}_{\bar g} \\ &\le \Lambda(S^n, [g_c]) \left[\int_{\Gamma_\epsilon^0} (w_\mu)^{2^*} \, dv_{\hat h} \right]^{2/2^*} + \theta_{n,\gamma} \|\pi\|^2 \mu^2 \int_{\mathbb{R}^n} |\hat w_1(\xi)|^2 |\xi|^{2(\gamma-1)} \, d\xi + \mu^2 o(1) + c\mu^3,\end{aligned}$$

where $\theta_{n,\gamma}$ is given in (7-47).

If there is a nonumbilic point, $\|\pi\|^2 \neq 0$ at that point. In the case that $\theta_{n,\gamma} < 0$, we are done, because fixing ϵ small and then choosing μ much smaller,

$$\mathcal{K}(V_\mu, X) < \Lambda(S^n, [g_c]) \left[\int_M (w_\mu)^{2^*} \, dv_{\hat h} \right]^{2/2^*},$$

as desired. □

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L^p ESTIMATES FOR THE HILBERT TRANSFORMS ALONG A ONE-VARIABLE VECTOR FIELD

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Stein conjectured that the Hilbert transform in the direction of a vector field v is bounded on, say, L^2 whenever v is Lipschitz. We establish a wide range of L^p estimates for this operator when v is a measurable, nonvanishing, one-variable vector field in $\mathbb{R}^2$. Aside from an L^2 estimate following from a simple trick with Carleson's theorem, these estimates were unknown previously. This paper is closely related to a recent paper of the first author (*Rev. Mat. Iberoam.* **29**:3 (2013), 1021–1069).

1. Introduction

Given a nonvanishing measurable vector field $v\colon \mathbb{R}^2 \to \mathbb{R}^2$, define for $f : \mathbb{R}^2 \to \mathbb{R}^2$

$$H_v f(x, y) = \text{p.v.} \int \frac{f((x, y) - tv(x, y))}{t}\, dt. \tag{1-1}$$

In this paper we prove:

Theorem 1. *Suppose v is a nonvanishing measurable vector field such that for all $x, y \in \mathbb{R}$,*

$$v(x, y) = v(x, 0),$$

and suppose $p \in \left(\frac{3}{2}, \infty\right)$. Then

$$\|H_v f\|_p \lesssim \|f\|_p.$$

The estimate is understood as an a priori estimate for all f in an appropriate dense subclass of $L^p(\mathbb{R}^2)$, say the Schwartz class, on which the Hilbert transform H_v is initially defined. One can then use the estimate to extend H_v to all of $L^p(\mathbb{R}^2)$.

If the vector field is constant, then this follows from classical estimates for the one-dimensional Hilbert transform by evaluating the L^p norm as an iterated integral, with inner integration in the direction of the vector field. Theorem 1 follows from the special case for vector fields mapping to vectors of unit length, because the Hilbert transforms along v and $v/|v|$ are equal by a simple change of variables in (1-1). To prove the theorem for unit-length vector fields, it suffices to do so for vector fields with nonvanishing first component, because we can apply the result for constant vector fields to the restriction of H_v to the set where v takes the value $(0, 1)$ and the set where it takes the value $(0, -1)$. Dividing v by its first component, we may then assume it is of the form $(1, u(x))$; multiplying v by a negative number merely

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changes the sign of (1-1). We call u the slope of the vector field. The Hilbert transform (1-1) then takes the form

$$H_v f(x, y) = \text{p.v.} \int \frac{f(x-t, y-tu(x))}{t}\, dt. \tag{1-2}$$

1.1. ***Remarks and related work.*** The case $p = 2$ of Theorem 1 is equivalent to the Carleson–Hunt theorem in L^2. This observation is attributed (without reference) to Coifman in [Lacey and Li 2010] and to Coifman and El Kohen in [Carbery et al. 1999]. We briefly explain how to deduce Theorem 1 for $p = 2$ from the Carleson–Hunt theorem. Denote by $\mathcal{F}_2$ the Fourier transform in the second variable. Then we formally have for (1-2), ignoring principal value notation,

$$\int e^{2\pi i\eta y} \int \mathcal{F}_2 f(x-t, \eta) \frac{e^{-2\pi i u(x)\eta t}}{t}\, dt\, d\eta.$$

As the inner integral is independent of y, it suffices, by Plancherel, to prove

$$\left\| \int \mathcal{F}_2 f(x-t, \eta) \frac{e^{-2\pi i u(x)\eta t}}{t}\, dt \right\|_{L^2(x,\eta)} \lesssim \|\mathcal{F}_2 f\|_2.$$

For each fixed η, applying the Carleson–Hunt theorem in the form

$$\left\| \int g(x-t) \frac{e^{-2\pi i N(x)t}}{t}\, dt \right\|_2 \lesssim \|g\|_2$$

for $g \in L^2(\mathbb{R})$ and measurable function N, proves the desired estimate.

For any regular linear transformation of the plane, we have the identity

$$(H_{T\circ v\circ T^{-1}} f) \circ T = H(f \circ T).$$

The class of vector fields depending on the first variable is invariant under linear transformations that preserve the vertical direction. This symmetry group is generated by the isotropic dilations

$$(x, y) \to (\lambda x, \lambda y),$$

nonisotropic dilations

$$(x, y) \to (x, \lambda y),$$

and shearing transformations

$$(x, y) \to (x, y + \lambda x)$$

for $\lambda \neq 0$. By a simple limiting argument, it suffices to prove Theorem 1 under the assumption that $\|u\|_\infty$ is finite. By the above nonisotropic scaling, the operator norm is independent of $\|u\|_\infty$, and we may therefore assume without loss of generality that

$$\|u\|_\infty \leq 10^{-2}. \tag{1-3}$$

Following general principles of wave packet analysis, it is natural to decompose H_v into wave packet components, where the wave packets are obtained from a generating function ϕ via application of elements of the symmetry group of the operator. These wave packets can be visualized by acting with the same group element on the unit square in the plane. The shapes obtained under the above linear symmetry group of H_v are parallelograms with a pair of vertical edges. All parallelograms in this paper will be of this special type. Under the assumption (1-3), it suffices to consider parallelograms whose nonvertical edges are close to horizontal. Such parallelograms are well approximated by rectangles, which are used in [Bateman 2013b; Lacey and Li 2010].

Theorem 2 [Bateman 2013b]. *Assume* $\|u\|_\infty \le 1$ *and* $1 < p < \infty$. *Assume* $\hat{f}(\xi, \eta)$ *vanishes outside an annulus* $A < |(\xi, \eta)| \le 2A$ *for some* $A > 0$. *Then*

$$\|H_v f\|_p \lesssim \|f\|_p.$$

Actually, the theorem is stated in that reference for functions such that $\hat{f}$ vanishes outside a trapezoidal region inside an annulus, but this is inessential, as can be seen from the commentary below. This theorem is weaker than Theorem 1 in the region $p > \frac{3}{2}$, but holds in the full region $1 < p < \infty$. The width of the annulus can be altered by finite superposition of different annuli, at the expense of an implicit constant depending on the conformal width of the annulus. The case $p > 2$ and a weak-type endpoint at $p = 2$ of Theorem 2 are due to Lacey and Li [2006b], and hold for arbitrary measurable vector fields.

We reformulate Theorem 2 in a form invariant under the above linear transformation group. The adjoint linear transformations of this group leave the horizontal direction invariant.

Theorem 3. *Assume* $1 < p < \infty$. *Assume* $\hat{f}(\xi, \eta)$ *is supported in a horizontal pair of strips* $A < |\eta| < 2A$ *for some* $A > 0$. *Then*

$$\|H_v f\|_p \lesssim \|f\|_p.$$

To deduce Theorem 3 from Theorem 2, we use the nonisotropic dilation $(x, y) \to (\lambda x, y)$ to stretch the annulus in the ξ direction until in the limit it degenerates to a pair of strips $A < |\eta| < 2A$. The restriction $\|u\|_\infty \le \lambda^{-1}$ becomes void in the limit $\lambda \to 0$. This proves Theorem 3. For the converse direction, we use a bounded number of dilated strips to cover the annulus except for two thin annular sectors around the ξ-axis. It remains to prove bounds on functions supported in these sectors. For fixed constant vector v, the operator H_v is given by a Fourier multiplier that is constant on two half-planes separated by a line through the origin perpendicular to v. If $\|u\|_\infty \le 1$, then this line does not intersect the thin annular sectors, and we have, with the constant vector field $(1, 0)$,

$$H_v f(x, y) = H_{(1,0)} f(x, y). \tag{1-4}$$

But $H_{(1,0)}$ is trivially bounded, and this completes the deduction of Theorem 2 from Theorem 3.

Sharpness of the exponent $\frac{3}{2}$ in Theorem 1 is not known. In Remark 9 we mention a potential covering lemma that, when combined with the methods in this paper, would push the exponent down to $\frac{4}{3}$. The truth of this covering lemma is unknown, however. If f is an elementary tensor,

$$f(x, y) = g(x)h(y),$$

then a similar calculation to the above turns $H_v f$ into

$$\int \widehat{h}(\eta) e^{2\pi i \eta y} \int g(x-t) \frac{e^{-2\pi i u(x)\eta t}}{t} \, dt \, d\eta.$$

This expression can be read as a family of Fourier multipliers acting on h. Assuming the norm of h is normalized to $\|h\|_p = 1$, we can estimate the last display by

$$\left\| \left\| \int g(x-t) \frac{e^{-2\pi i u(x)\eta t}}{t} \, dt \right\|_{M^p(\eta)} \right\|_{L^p(x)},$$

where $M_p(\eta)$ denotes the operator norm of the Fourier multiplier acting on L^p. By scaling invariance of the multiplier norm, the factor $u(x)$ in the phase can be ignored. As shown in [Coifman et al. 1988], multiplier norms are controlled by variation norms. Hence we may estimate the last display by

$$\left\| \left\| \int g(x-t) \frac{e^{-2\pi i \eta t}}{t} \, dt \right\|_{V^r(\eta)} \right\|_{L^p(x)},$$

provided $\left|\frac{1}{2} - 1/p\right| \le 1/r$. The bounds on the variation norm Carleson operator in [Oberlin et al. 2012] imply that for $p > \frac{4}{3}$ and $r > p'$, the last display is bounded by a constant times $\|g\|_p$. Hence the exponent in Theorem 1 can be improved to $\frac{4}{3}$ under the additional assumption that the function f is an elementary tensor. The authors learned this argument from Ciprian Demeter. Related multiplier theorems in [Demeter et al. 2008; Demeter 2012] also show a phase transition at this exponent.

The Hilbert transform along a one-variable vector field was studied by Carbery, Seeger, Wainger, and Wright in [Carbery et al. 1999]. There, boundedness in L^p for $1 < p$ is proved under additional conditions on the vector field.

In a different direction, Stein conjectured that a truncation of H_v is bounded on L^2 under the assumption that the two-variable vector field v is Lipschitz with sufficiently small Lipschitz constant depending on the truncation. Stein's conjecture is related to a well-known conjecture of Zygmund on the differentiation of Lipschitz vector fields. Define

$$M_v f(x, y) = \sup_{0<L<1} \frac{1}{2L} \int_{-L}^{L} f\big((x, y) - v(x, y)t\big) \, dt.$$

Zygmund conjectured that M_v is (say) weak-type $(2, 2)$ if $\|v\|_\infty$ is bounded and the Lipschitz norm $\|\nabla v\|_\infty$ is small enough. Proving a weak-type estimate on this operator would yield corresponding differentiation results analogous to the Lebesgue differentiation theorem, except the averaging takes place over line segments instead of balls. Estimates on M_v are unknown on any L^p space, except for the trivial $p = \infty$ case, unless more stringent requirements are placed on v; for example, Bourgain [1989] proved M_v is bounded on L^p, $p > 1$, when v is real-analytic and the operator is restricted to a bounded domain. The corresponding result for the Hilbert transform was announced in [Stein and Street 2011], although the $p = 2$ case follows from work of Lacey and Li [2010]. Previously the Hilbert transform case in such a range of exponents was only known under the additional assumption that no integral curve of the vector field forms a straight line [Christ et al. 1999].

There is some history of using singular integral and time-frequency methods to control positive maximal operators. See Lacey's bilinear maximal theorem [2000] or the extension of Bourgain's return times theorem by Demeter, Lacey, Tao, and Thiele [Demeter et al. 2008].

This paper is structured as follows: Section 2 contains the main approach, a separation of frequency space into horizontal dyadic strips and application of Littlewood–Paley theory in the second variable to reduce to some vector-valued inequality; this step uses the one-variable property of the vector field to ensure that the strips are invariant under H_v. This fact was brought to our attention by Ciprian Demeter. The vector-valued inequality is proved by restricted weak-type interpolation, a tool that allows us to localize the operator to some benign sets G and H and prove strong L^2 bounds on these sets.

Section 3 gives the crucial construction of the sets G and H, relying on two covering lemmas. One is essentially an argument by Cordoba and R. Fefferman [1975], while the other is essentially an argument by Lacey and Li [2006a].

Section 4 outlines the proof of the L^2 bounds on the sets G and H, using time-frequency analysis as in [Bateman 2013b]. The operator that we estimate at this point is a refinement of the operator in that paper. We refer to the decomposition of this operator there without recalling details. The terms in this decomposition satisfy Estimates 16 through 20, which are also taken from the same paper. To complete the proof of Theorem 1, we need the additional Estimates 21 and 22, which depend on the sets G and H. These additional estimates are proved in Section 5, again with much reference to [Bateman 2013b].

Throughout the paper, we write $x \lesssim y$ to mean there is a universal constant C such that $x \le Cy$. We write $x \sim y$ to mean $x \lesssim y$ and $y \lesssim x$. We write $\mathbf{1}_E$ to denote the characteristic function of a set E.

2. Reduction to estimates for a single frequency band

We fix the vector field v with the normalization (1-2) and assume bounded slope as in (1-3). Let P_c be the Fourier restriction operator to a double cone:

$$\widehat{P_c f}(\xi, \eta) = \mathbf{1}_{10|\xi| \le |\eta|} \hat{f}(\xi, \eta).$$

It suffices to estimate $H_v P_c$ in place of H_v because, similarly to (1-4),

$$H_v(\mathbf{1} - P_c) f(\xi, \eta) = H_{(1,0)}(\mathbf{1} - P_c) f(\xi, \eta),$$

due to the restriction on the slope of v. Define the horizontal pair of bands

$$B_k := \{(\xi, \eta) \in \mathbb{R}^2 : |\eta| \in [2^k, 2^{k+1/100})\},$$

and define the corresponding Fourier restriction operator $\widehat{P_k f} = \mathbf{1}_{B_k} \hat{f}$. Since the Hilbert transform in a constant direction is given by a Fourier multiplier, and the vector field v is constant on vertical lines, we can formally write, for a family of multipliers parametrized by x,

$$H_v f(x, y) = \iint m_x(\xi, \eta) \hat{f}(\xi, \eta) e^{2\pi i (x\xi + y\eta)} \, d\xi \, d\eta.$$

Then it is clear that

$$H_v(P_k f)(x,y) = \int 1_{[2^k,2^{k+1/100})}(\eta) e^{2\pi i y\eta} \left[\int m_x(\xi,\eta) \hat{f}(\xi,\eta) e^{2\pi i x\xi}\, d\xi \right] d\eta = P_k(H_v f)(x,y).$$

Define

$$H_k := P_k H_v P_c = P_k H_v P_c P_k.$$

Littlewood–Paley theory implies

$$\|H_v P_c f\|_p \lesssim \left\| \left(\sum_{k\in\mathbb{Z}/100} |H_k f|^2 \right)^{1/2} \right\|_p,$$

where the summation is over integer multiples of $\frac{1}{100}$. Using Littlewood–Paley theory once more, it suffices to prove

$$\left\| \left(\sum_{k\in\mathbb{Z}/100} |H_k(P_k f)|^2 \right)^{1/2} \right\|_p \lesssim \left\| \left(\sum_{k\in\mathbb{Z}/100} |P_k f|^2 \right)^{1/2} \right\|_p,$$

which follows from the more general estimate

$$\left\| \left(\sum_{k\in\mathbb{Z}/100} |H_k f_k|^2 \right)^{1/2} \right\|_p \lesssim \left\| \left(\sum_{k\in\mathbb{Z}/100} |f_k|^2 \right)^{1/2} \right\|_p$$

for any sequence of functions $f_k \in L^p$. By a limiting argument, it suffices to prove, for all $k_0 > 0$,

$$\left\| \left(\sum_{|k|\le k_0} |H_k f_k|^2 \right)^{1/2} \right\|_p \lesssim \left\| \left(\sum_{|k|\le k_0} |f_k|^2 \right)^{1/2} \right\|_p, \tag{2-1}$$

with implicit constant independent of k_0, where it is understood that k runs through elements of $\mathbb{Z}/100$. Compare this inequality with a vector-valued Carleson inequality as in [Grafakos et al. 2005].

Theorem 3 implies that H_k is bounded in L^p for $1 < p < \infty$ for each k. In particular, (2-1) is true for $p = 2$ by interchanging the order of square summation and L^2 norm.

Note that H_k is defined a priori on all of L^p (by Theorem 3), and we may drop the assumption that f is in the Schwartz class. By Marcinkiewicz interpolation for l^2 vector valued functions, it suffices to prove, for $G, H \subseteq \mathbb{R}^2$ and $\sum_k |f_k|^2 \le \mathbf{1}_H$,

$$\left| \left\langle \left(\sum_{|k|\le k_0} |H_k f_k|^2 \right)^{1/2}, \mathbf{1}_G \right\rangle \right| \lesssim |H|^{1/p} |G|^{1-1/p}. \tag{2-2}$$

By Lebesgue's monotone convergence theorem, it suffices to prove this under the assumption that G is supported on a large square $[-N', N']^2$ as long as the implicit constant does not depend on N'. By another limiting argument using crude estimates in case the sets G and H have large distance, it suffices to prove this under the assumption that H is supported in a much larger square $[-N, N]$, again with bounds independent of N. Generalizing, we will only assume both G and H are supported on the larger square.

Since we already have (2-2) for $p = 2$, we immediately obtain this estimate for $p > 2$ provided $|H| \lesssim |G|$ and for $p < 2$ provided $|G| \lesssim |H|$. By a standard induction on the ratio of $|H|$ and $|G|$, it then suffices to prove the following lemma.

Lemma 4. *Let $G', H' \subset [-N, N]^2$ be measurable and let $\frac{3}{2} < p < \infty$.*

If $p > 2$ and $10|G'| < |H'|$, then there exists a subset $H \subset H'$ depending only on p, G', and H' with $|H| \geq |H'|/2$ such that (2-2) holds with $G = G'$ and any sequence of functions f_k with $\sum_{|k|\leq k_0} |f_k|^2 \leq \mathbf{1}_H$.

If $p < 2$ and $10|H'| < |G'|$, then there exists a subset $G \subset G'$ depending only on p, G', and H' with $|G| \geq |G'|/2$ such that (2-2) holds with $H = H'$ and any sequence of functions f_k with $\sum_{|k|\leq k_0} |f_k|^2 \leq \mathbf{1}_H$.

For example, in case $p > 2$ and $10|G'| < |H'|$, we split H' into H and $H' \setminus H$ and apply the triangle inequality. On $H' \setminus H$ we apply the induction hypothesis, which yields an estimate better than the desired one by a factor of $2^{-1/p}$ because of the size estimate for $H' \setminus H$. On H we use the conclusion of the lemma, which we may assume (by choosing the induction statement properly) to provide a bound no more than $1 - 2^{-1/p}$ times the desired bound.

By Cauchy–Schwarz, (2-2) follows from

$$\int \sum_{|k|\leq k_0} |H_k f_k|^2 \mathbf{1}_G \lesssim |H|^{2/p} |G|^{1-2/p}.$$

This in turn follows from

$$\int \sum_{|k|\leq k_0} |H_k f_k|^2 \mathbf{1}_G \lesssim \left(\frac{|G|}{|H|}\right)^{1-2/p} \int \sum_k |f_k|^2 \tag{2-3}$$

by the assumption on the sequence f_k. Now define the operator $H_{k,G,H}$ by

$$H_{k,G,H} f = \mathbf{1}_G H_k (\mathbf{1}_H f).$$

Then (2-3) follows from the estimate

$$\|H_{k,G,H} f\|_2 \lesssim \left(\frac{|G|}{|H|}\right)^{1/2-1/p} \|f\|_2$$

for any $f \in L^2$, and $|k| \leq k_0$, assuming the implicit constant does not depend on k or k_0. We will prove this L^2 estimate again by Marcinkiewicz interpolation between weak-type estimates. More precisely, we will prove:

Theorem 5. *Let p be as in Theorem 1 and let $G', H' \subseteq \mathbb{R}^2$ be as in Lemma 4. Then there are sets G, H as in Lemma 4 such that for any measurable sets $E, F \subset \mathbb{R}^2$ and each $|k| \leq k_0$, we have*

$$|\langle H_{k,G,H} \mathbf{1}_F, \mathbf{1}_E \rangle| \lesssim \left(\frac{|G|}{|H|}\right)^{1/2-1/p} |F|^{1/2} |E|^{1/2}. \tag{2-4}$$

Again, [Bateman 2013b] proves

$$|\langle H_{k,G,H} \mathbf{1}_F, \mathbf{1}_E \rangle| \lesssim |F|^{1/q} |E|^{1-1/q} \tag{2-5}$$

for all $1 < q < \infty$. The refinement we need here is the localization to G and H, with corresponding improvement in the estimate. The parameter k is irrelevant in proving (2-4), but it is crucial that the sets H and G be constructed independent of k. By interpolating Theorem 5 with (2-5) for q near 1 and ∞, we obtain strong-type estimates

$$|\langle H_{k,G,H} f, e\rangle| \lesssim \left(\frac{|G|}{|H|}\right)^{1/2-1/r} \|f\|_q \|e\|_{q'},$$

where r is as close to p as we wish and q is in a small punctured neighborhood of 2 whose size depends on r. Another interpolation allows q to be 2 as well, and we obtain (2-3) with power r instead of p, which is no harm since we seek an open range of exponents. We have thus reduced Theorem 1 to Theorem 5.

3. Construction of the sets G and H

In this section we present the sets G and H of Lemma 4 and prove the size estimates $|G| \geq |G'|/2$ and $|H| \geq |H'|/2$. Inequality (2-4) will be proved in subsequent sections.

We work with two shifted dyadic grids on the real line:

$$\mathcal{I}_1 = \left\{ \left[2^k \left(n + \frac{(-1)^k}{3} \right), 2^k \left(n + 1 + \frac{(-1)^k}{3} \right) \right) : k, n \in \mathbb{Z} \right\},$$
$$\mathcal{I}_2 = \left\{ \left[2^k \left(n - \frac{(-1)^k}{3} \right), 2^k \left(n + 1 - \frac{(-1)^k}{3} \right) \right) : k, n \in \mathbb{Z} \right\}.$$

The exceptional sets will be the union of two sets:

$$H' \setminus H = H_1 \cup H_2,$$
$$G' \setminus G = G_1 \cup G_2.$$

Fix $i \in \{1, 2\}$. The sets H_i and G_i will be constructed using the grid $\mathcal{I}_i$, and we will prove $4|H_i| \leq |H'|$ and $4|G_i| \leq |G'|$.

Given a parallelogram with two vertical edges, we define the height $H(R)$ of the parallelogram to be the common length of the two vertical edges. We define the shadow $I(R)$ to be the projection of R onto the x axis. The central line segment of R is the line segment that connects the midpoints of the two vertical edges. If a line segment can be written

$$\{(x, y) : x \in I(R) : y = ux + b\},$$

then we call u the slope of the line segment. For each parallelogram R, let $U(R)$ be the set of slopes of lines that intersect both vertical edges. Maximal and minimal slopes in $U(R)$ are attained by the diagonals of the parallelogram. Hence $U(R)$ is an interval of length $2H(R)/|I(R)|$ centered at the slope of the central line of R.

For an interval U and a positive number C, define CU to be the interval with the same center but length $C|U|$. If R is a parallelogram, define CR to be the parallelogram with the same central line segment as R but height $CH(R)$ (this definition of CR is used in Section 3 only). Note that $CU(R) = U(CR)$. For an interval $I \subset I(R)$, define

$$R_I = R \cap (I \times \mathbb{R}).$$

Given N and k_0 as in Lemma 4, we consider a finite set $\mathcal{R}_i$ of parallelograms R as follows: the projection of both vertical edges of R onto the y-axis are in $\mathcal{I}_1 \cup \mathcal{I}_2$, and $I(R) \in \mathcal{I}_i$. Further, the parallelogram is contained in the square $[-10^2N, 10^2N]^2$, the height is at least 2^{-k_0}, and the slope is at most 10^{-1}. These assumptions imply also that $|I(R)|$ is at least 2^{-k_0}.

We will use the following simple geometric observation:

Lemma 6. *Let R, R' be two parallelograms and assume $I(R) = I(R')$, $U(R) \cap U(R') \neq \varnothing$, $R \cap R' \neq \varnothing$, and without loss of generality $H(R) \leq H(R')$. Then we have $R \subseteq 7R'$. Moreover, if $7H(R) \leq H(R')$, then $7R \subseteq 7R'$.*

Proof. Since $U(R) \cap U(R') \neq \varnothing$, there exist two parallel lines, one intersecting both vertical edges of R and the other intersecting both vertical edges of R'. Since $R \cap R' \neq \varnothing$, the vertical displacement of these lines is less than $H(R) + H(R')$. If $H(R) \leq H(R')$, then the vertical edges of R have distance at most $2H(R')$ from the respective vertical edges of R' and are contained in the vertical edges of $7R'$. This proves the first statement of the lemma. The second statement follows similarly. $\square$

Let M_V denote the Hardy–Littlewood maximal operator in the vertical direction:

$$M_V f(x, y) = \sup_{y \in J} \frac{1}{|J|} \int_J |f(x, z)|\, dz,$$

where the supremum is taken over all intervals J containing y. For a measurable function $u : \mathbb{R} \to \mathbb{R}$ (which will be the slope function associated with the given vector field), define

$$E(R) := \{(x, y) \in R : u(x) \in U(R)\}.$$

3.1. ***Construction of the set H.*** With the sets G', H' as in Lemma 4, we define

$$H_i = \bigcup \{R \in \mathcal{R}_i : |E(R) \cap G'| \geq \delta |R|\},$$

with

$$\delta = C_\alpha \left(\frac{|G'|}{|H'|} \right)^{1-\alpha}$$

for some small α to be determined later through application of Estimate 22 and some constant C_α large enough that the desired estimate $4|H_i| \leq |H'|$ follows from the following lemma, applied with $G = G'$, $q = 1/(1-\alpha)$. We are essentially eliminating all rectangles R with large density parameter, where density has the meaning from [Bateman 2013b]. This will be used in the proof of Estimate 22 later in the paper. Essentially, trees with density $\geq \delta$ will have extremely small size, and will therefore be mostly negligible.

Lemma 7. *Let $\delta > 0$ and $q > 1$ and let $G \subset \mathbb{R}^2$ be a measurable set and $u : \mathbb{R} \to \mathbb{R}$ be a measurable function. Let $\mathcal{R}$ be a finite collection of parallelograms with vertical edges and dyadic shadow such that*

$$|E(R) \cap G| \geq \delta |R|$$

for each $R \in \mathcal{R}$. *Then*

$$\Big| \bigcup_{R \in \mathcal{R}} R \Big| \lesssim \delta^{-q} |G|.$$

Proof. We will find a subset $\mathcal{G} \subset \mathcal{R}$ such that

$$\Big| \bigcup_{R \in \mathcal{R}} R \Big| \lesssim \sum_{R \in \mathcal{G}} |R|, \tag{3-1}$$

$$\int \Big(\sum_{R \in \mathcal{G}} \mathbf{1}_{E(R)} \Big)^{q'} \lesssim \sum_{R \in \mathcal{G}} |R|. \tag{3-2}$$

Inequality (3-1) will complete the proof of Lemma 7, provided

$$\sum_{R \in \mathcal{G}} |R| \lesssim \delta^{-q} |G|. \tag{3-3}$$

But with the density assumption for the parallelograms in $\mathcal{R}$, we have

$$\sum_{R \in \mathcal{G}} |R| \le \sum_{R \in \mathcal{G}} \frac{1}{\delta} |E(R) \cap G| = \frac{1}{\delta} \Big\| \sum_{R \in \mathcal{G}} \mathbf{1}_{E(R)} \mathbf{1}_G \Big\|_1 \lesssim \frac{1}{\delta} \Big(\sum_{R \in \mathcal{G}} |R| \Big)^{1/q'} |G|^{1/q},$$

where in the last line we have used Hölder's inequality and (3-2). After division by the middle factor of the right hand side, we obtain (3-3).

The following argument is essentially the one used in [Cordoba and Fefferman 1975] to prove endpoint estimates for the strong maximal operator. We select parallelograms according to the following iterative procedure. Initialize

$$\mathrm{STOCK} \leftarrow \mathcal{R},$$
$$\mathcal{G} \leftarrow \varnothing,$$
$$\mathcal{B} \leftarrow \varnothing.$$

While $\mathrm{STOCK} \neq \varnothing$, choose an $R \in \mathrm{STOCK}$ with maximal $|I(R)|$. If

$$\sum_{R' \in \mathcal{G}:\ E(R) \cap E(R') \neq \varnothing} |7R \cap 7R'| \ge 10^{-2} |R|, \tag{3-4}$$

then update

$$\mathrm{STOCK} \leftarrow \mathrm{STOCK} \setminus R,$$
$$\mathcal{G} \leftarrow \mathcal{G},$$
$$\mathcal{B} \leftarrow \mathcal{B} \cup \{R\}.$$

Otherwise update

$$\mathrm{STOCK} \leftarrow \mathrm{STOCK} \setminus R,$$
$$\mathcal{G} \leftarrow \mathcal{G} \cup \{R\},$$
$$\mathcal{B} \leftarrow \mathcal{B}.$$

It is clear that this procedure yields a partition $\mathcal{R} = \mathcal{G} \sqcup \mathcal{B}$.

To prove (3-1), let $R \in \mathcal{B}$ and let R' be in the set $\mathcal{G}(R)$ of all elements in $\mathcal{G}$ that are chosen prior to R and satisfy $E(R) \cap E(R') \neq \varnothing$. The last property implies $U(R) \cap U(R') \neq \varnothing$ and $R \cap R' \neq \varnothing$. Also, $I(R) \subset I(R')$. By Lemma 6 applied to R and $R'_{I(R)}$, we have, for every vertical line L through the interval $I(R)$,

$$|L \cap 7R \cap 7R'| \geq \min(H(R), H(R')) \geq \frac{|7R \cap 7R'|}{7|I(R)|}.$$

Comparing for $(x, y) \in R$ and corresponding vertical line L the maximal function M_V with an average over the segment $L \cap 7R$, we obtain

$$M_V\Big(\sum_{R' \in \mathcal{G}(R)} \mathbf{1}_{7R'}\Big)(x, y) \geq 7^{-1} H(R)^{-1} \sum_{R' \in \mathcal{G}(R)} |L \cap 7R \cap 7R'| \geq 49^{-1}|R|^{-1} \sum_{R' \in \mathcal{G}(R)} |7R \cap 7R'| \geq 10^{-4},$$

where the last estimate follows from (3-4). Hence

$$\Big|\bigcup_{R \in \mathcal{B}} R\Big| \leq \Big|\Big\{x : M_V\Big(\sum_{r \in \mathcal{G}} \mathbf{1}_R\Big)(x) \geq 10^{-4}\Big\}\Big| \lesssim \sum_{R \in \mathcal{G}} |R|,$$

by the weak $(1, 1)$ inequality for M_V. This proves (3-1), because the corresponding estimate for the union of elements in $\mathcal{G}$ is trivial.

To prove (3-2), consider $R', R \in \mathcal{G}$ with $E(R) \cap E(R') \neq \varnothing$. If R' was selected first, then $H(R) > 7H(R')$, for otherwise we can use Lemma 6 as above to conclude, for $(x, y) \in R$,

$$M_V(\mathbf{1}_{7R'})(x, y) \geq 7^{-1}|H(R)|^{-1} \sum_{R' \in \mathcal{G}(R)} |L \cap 7R \cap 7R'| \geq 49^{-1},$$

and hence R would have been put into $\mathcal{B}$. Hence we have, by Lemma 6,

$$7R'_I \subset 7R_I \tag{3-5}$$

for every $I \subset I(R)$. Hence

$$\sum_{R' \in \mathcal{G}(R)} |7R'_I \cap 7R_I| = \sum_{R' \in \mathcal{G}(R)} |7R'_I|$$

is proportional to $|I|$ for $I \subset I(R)$. Hence we have, for all such I,

$$\sum_{R' \in \mathcal{G}(R)} |7R'_I \cap 7R_I| \lesssim |R_I|, \tag{3-6}$$

since for $I = I(R)$, this holds when condition (3-4) fails.

Let's say an n-tuple $(R^1, R^2, \ldots, R^n)$ of elements in $\mathcal{G}$ is *admissible* if R^j is selected after R^{j+1} for each j and $E(R^j) \cap E(R^{j+1}) \neq \varnothing$. Then we have

$$\begin{aligned}\int\Big(\sum_{R\in\mathcal{G}}\mathbf{1}_{E(R)}\Big)^n &\lesssim \sum_{R^1,\dots,R_n}\big|E(R^1)\cap E(R^2)\cap\cdots\cap E(R^n)\big|\\ &\lesssim \sum_{(R^1,R^2,\dots,R^n)\text{ adm.}}\big|E(R^1)\cap E(R^2)\cap\cdots\cap E(R^n)\big|\\ &\lesssim \sum_{(R^1,R^2,\dots,R^n)\text{ adm.}}\big|7R^1\cap 7R^2\cap\cdots\cap 7R^n\big|\\ &\lesssim \sum_{(R^1,R^2,\dots,R^n)\text{ adm.}}\big|7R^1\cap 7R^2_{I(R_1)}\cap\cdots\cap 7R^n_{I(R_1)}\big|.\end{aligned}$$

Using (3-5), which implies that the sets $7R^j_{I(R_1)}$ are nested, and the estimate (3-6) for the last pair of sets, we can estimate the last display by

$$\lesssim \sum_{(R^1,R^2,\dots,R^{n-1})\text{ adm.}}\big|7R^1\cap 7R^2_{I(R_1)}\cap\cdots\cap 7R^{n-1}_{I(R_1)}\big|. \tag{3-7}$$

Iterating the argument allows us to conclude (3-2) for q' an integer, which is clearly not a restriction, as the estimate is harder for larger q'. This completes the proof of Lemma 7. □

3.2. ***Construction of the set G.*** Let G', H', u be as in Lemma 4 and define

$$G_i=\bigcup_{k\in\mathbb{Z},k<0}\left\{R\in\mathcal{R}_i:\frac{|E(R)|}{|R|}\ge 2^k\text{ and }\frac{|H'\cap R|}{|R|}\ge C_\epsilon 2^{-(1/2+\epsilon)k}\left(\frac{|H'|}{|G'|}\right)^{1/2}\right\}$$

for some small $\epsilon>0$, to be determined later through application of Estimate 21, and some constant C_ϵ large enough that we obtain, with Theorem 8 below,

$$|G_i|\le\sum_{k\in\mathbb{Z},k<0}C2^{-k}\left(C_\epsilon 2^{-(1/2+\epsilon)k}\left(\frac{|H'|}{|G'|}\right)^{1/2}\right)^{-2}|H'|\le\frac{|G'|}{4}.$$

This construction essentially allows us to ignore trees with size and density both too large. This will be used in the proof of Estimate 21.

The following theorem is a variant of the result in [Lacey and Li 2006a]. The theorem there is valid for arbitrary Lipschitz vector fields. As stated here, the theorem is valid for vector fields depending on one variable. In fact, the theorem holds for vector fields that are Lipschitz in the vertical direction only. We recreate the proof given in [Lacey and Li 2006a] below in the one-variable case. The only use of the one-variable property comes in the proof of Lemma 12 below.

Theorem 8. *Let $0\le\delta,\sigma\le 1$, let H be a measurable set, and let $\mathcal{R}$ be a finite collection of parallelograms with vertical edges and dyadic shadow such that for each $R\in\mathcal{R}$, we have*

$$|E(R)|\ge\delta|R|,\qquad |H\cap R|\ge\sigma|R|.$$

Then

$$\Big|\bigcup_{R\in\mathcal{R}}R\Big|\lesssim\delta^{-1}\sigma^{-2}|H|.$$

Remark 9. It is of interest whether a result like Theorem 8 holds with σ-power less than 2. In the single height case, optimal results are already known with power all the way to $1+\epsilon$; see [Bateman 2009; Bateman 2013a]. However the important point is that the parallelograms in Theorem 8 can have arbitrary height, which is necessary for creating the exceptional sets needed in the current paper.

Proof. It is enough to find a subset $\mathcal{G} \subset \mathcal{R}$ such that

$$\Big|\bigcup_{R\in\mathcal{R}} R\Big| \lesssim \sum_{R\in\mathcal{G}} |R|, \tag{3-8}$$

$$\int \Big(\sum_{R\in\mathcal{G}} 1_R\Big)^2 \lesssim \delta^{-1} \sum_{R\in\mathcal{G}} |R|. \tag{3-9}$$

Namely, with (3-9) we have

$$\sum_{R\in\mathcal{G}} |R| \le \sigma^{-1} \int \sum_{R\in\mathcal{G}} \mathbf{1}_R(x)\mathbf{1}_H\,dx \le \sigma^{-1}\|H\|^{1/2}\bigg(\int \Big(\sum_{R\in\mathcal{G}} \mathbf{1}_R(x)\Big)^2 dx\bigg)^{1/2}$$
$$\lesssim \sigma^{-1}\delta^{-1/2}|H|^{1/2}\Big(\sum_{R\in\mathcal{G}} |R|\Big)^{1/2},$$

and the desired estimate follows from (3-8).

We define the set $\mathcal{G}$ by a recursive procedure. Initialize

$$\mathcal{G} \leftarrow \varnothing,$$
$$\mathrm{STOCK} \leftarrow \mathcal{R}.$$

While STOCK is not empty, select $R \in \mathrm{STOCK}$ such that $|I(R)|$ is maximal. Update

$$\mathcal{G} \leftarrow \mathcal{G} \cup \{R\},$$
$$\mathcal{B} \leftarrow \bigg\{R' \in \mathrm{STOCK} : R' \subset \bigg\{x : M_V\Big(\sum_{R\in\mathcal{G}} 1_R\Big)(x) \ge 10^{-3}\bigg\}\bigg\},$$
$$\mathrm{STOCK} \leftarrow \mathrm{STOCK} \setminus \mathcal{B}.$$

This loop will terminate, because the collection $\mathcal{R}$ is finite and we remove at each step at least the selected R from STOCK.

By the Hardy–Littlewood maximal bound, it is clear that (3-8) holds and it remains to show (3-9). By expanding the square in (3-9) and using symmetry, it suffices to show

$$\sum_{(R,R')\in\mathcal{P}} |R \cap R'| \lesssim \delta^{-1} \sum_{R\in\mathcal{G}} |R|,$$

where $\mathcal{P}$ is the set of all pairs $(R, R') \in \mathcal{G}\times\mathcal{G}$ with $R \cap R' \ne \varnothing$, and R is chosen prior to R'. We partition $\mathcal{P}$ into

$$\mathcal{P}' = \{(R, R') \in \mathcal{P} : U(R) \not\subset 10^2 U(R')\} \quad \text{and} \quad \mathcal{P}'' = \{(R, R') \in \mathcal{P} : U(R) \subset 10^2 U(R')\}.$$

Theorem 8 is reduced to the following two lemmas:

Lemma 10. *For fixed $R' \in \mathcal{G}$, we have*

$$\sum_{\substack{R \in \mathcal{R} \\ (R,R') \in \mathcal{P}''}} |R \cap R'| \lesssim |R'|.$$

Lemma 11. *For fixed $R \in \mathcal{G}$, we have*

$$\sum_{\substack{R' \in \mathcal{R} \\ (R,R') \in \mathcal{P}'}} |R \cap R'| \lesssim \delta^{-1} |R|.$$

Proof of Lemma 10. We first argue by contradiction that $\mathcal{P}''$ does not contain a pair (R, R') with $H(R') < H(R)$. By definition of $\mathcal{P}''$, we have $U(R) \cap U(100R') \neq \varnothing$. By Lemma 6 applied to $100R_{I(R')}$ and $100R'$, we conclude that R' is contained in $700R$. But then

$$R' \subset \left\{ M_V 1_R > \tfrac{1}{700} \right\},$$

which contradicts the selection of R' and completes the proof that we have $H(R) \leq H(R')$ for all $(R, R') \in \mathcal{P}''$.

Now we use Lemma 6 again to conclude that for each $(R, R') \in \mathcal{P}''$, we have $R_{I(R')} \subset 700R'$. Hence we have, for some point (x, y) in R',

$$10^{-3} \geq M_V \Bigg(\sum_{R \in \mathcal{G} : (R,R') \in \mathcal{P}''} 1_R \Bigg)(x, y) \geq \frac{1}{700 H(R')} \sum_{R : (R,R') \in \mathcal{P}''} H(R) \geq \frac{1}{700} \sum_{R : (R,R') \in \mathcal{P}''} |R \cap R'| / |R'|.$$

This proves Lemma 10. $\square$

There remains to give the proof of Lemma 11, which will occupy us through the end of the section. Fix $R \in \mathcal{G}$. We decompose $\{R' : (R, R') \in \mathcal{P}'\}$ by the following iterative procedure: Initialize

$$\text{STOCK} \leftarrow \{R' : (R, R') \in \mathcal{P}'\},$$
$$\mathcal{G}' \leftarrow \varnothing.$$

While STOCK is nonempty, select $R' \in \text{STOCK}$ with maximal $|I_{R'}|$. Update

$$\mathcal{G}' \leftarrow \mathcal{G}' \cup \{R'\},$$
$$\mathcal{B}(R') \leftarrow \{R'' \in \text{STOCK} : \Pi E(R'') \cap \Pi E(R') \neq \varnothing\},$$
$$\text{STOCK} \leftarrow \text{STOCK} \setminus \mathcal{B}(R'),$$

where Π denotes the projection onto the x axis. By construction, the sets $\Pi E(R')$ with $R' \in \mathcal{G}'$ are disjoint and we have

$$\sum_{R' \in \mathcal{G}'} |I_{R'}| \leq \delta^{-1} \sum_{R' \in \mathcal{G}'} |\Pi E(R')| \leq \delta^{-1} |I(R)|.$$

As the sets $\mathcal{B}(R')$ with $R' \in \mathcal{G}'$ partition the summation set of the left side of Lemma 11, it suffices to show that, for each $R' \in \mathcal{G}'$,

$$\sum_{R'' \in \mathcal{B}(R')} |R'' \cap R| \lesssim |R_{I(R')}|.$$

In what follows we fix $R' \in \mathcal{G}'$.

Lemma 12. *There is an interval U of slopes (depending on R and R') with*

$$5|U(R)| \le |U|, \tag{3-10}$$

$$U(R) \cap 5U = \varnothing, \tag{3-11}$$

$$U(R) \subset 6U, \tag{3-12}$$

$$U(R'') \subset U \tag{3-13}$$

for all $R'' \subset \mathcal{B}(R')$.

Proof. We distinguish two cases: $|U(R)| \le |U(R')|$ and $|U(R)| > |U(R')|$.

First case: $|U(R)| \le |U(R')|$. In the first case we use the definition of $\mathcal{P}'$ to conclude

$$U(R) \cap 25U(R') = \varnothing.$$

We then define $U = KU(R')$, where $K \ge 5$ is the largest number (or very close to that) such that $U(R) \cap 5KU(R') = \varnothing$. Then we have immediately (3-10), (3-11) and (3-12). To see (3-13), assume $U(R'') \not\subset U$ to get a contradiction.

By the construction of $\mathcal{B}(R')$, we know that $\Pi(E(R''))$ and $\Pi(E(R'))$ intersect, which implies that $U(R'') \cap U(R') \neq \varnothing$, since the underlying vector field v is constant along vertical lines. Since $U(R')$ is contained in the middle fifth of the interval U, we conclude $|U| \le 3|U(R'')|$ and $U \subset 7U(R'')$. But then $U(R) \subset 10^2 U(R'')$, a contradiction to $(R, R'') \in \mathcal{P}'$.

Second case: $|U(R)| > |U(R')|$. Then $H(R) > H(R')$ because $|I(R')| \le |I(R)|$. Since R' is not contained in the set $\{M_V 1_R > 10^{-3}\}$ and thus not in $10^3 R$, we conclude that $U(R')$ contains an element not in $400U(R)$. Hence

$$25\frac{|U(R)|}{|U(R')|}U(R')$$

does not intersect $U(R)$. From there we may proceed as before, with $U(R')$ replaced by this bigger interval. This completes the proof of Lemma 12. □

Lemma 13. *Let I be a dyadic interval contained in $I_{R'}$. Then for all $R'' \in \mathcal{B}(R')$ with $H(R'') \le 20|U|\,|I|$, we have that*

$$R_I \cap R'' \neq \varnothing \implies R''_I \subset 50\big(1 + |U|\,|I| H(R)^{-1}\big) R \tag{3-14}$$

and

$$|R_I \cap R''| \le 10|U|^{-1} H(R'') H(R). \tag{3-15}$$

Proof. By a shearing transformation and translation we may assume that the central line segment of R is on the x axis.

Statement (3-14) follows immediately from the central slope of R'' being less than $10|U|$ and $H(R'') \le 20|U|\,|I|$, and hence the vertical distance of any point in R'' from R is at most $50|U|\,|I|$. To see the second statement, note that the central slope u_0 of R'' is at least $2|U|$. Hence (3-15) follows, because $R \cap R''$ is contained in a parallelogram of height $H(R)$ and base $H(R'')u_0^{-1}$. This proves Lemma 13. □

Lemma 14. *Let I be a dyadic interval contained in $I_{R'}$. If*

$$\sum_{\substack{R''\in\mathcal{B}(R')\\ \text{s.t. } I\subset I_{R''}}} |R_I\cap R''| > 10^{-1}|R_I|,$$

then there does not exist $R'''\in\mathcal{B}(R')$ with $I_{R'''}\subset I$, $I_{R'''}\neq I$.

Proof. For every $R'''\in\mathcal{B}(R')$, we have $U(R''')\subset U$, and thus

$$H(R''')\leq 10U|I_{R'''}|.$$

Hence if $I_{R'''}\subset I$, then $H(R''')\leq 20U|I|$. The parallelogram R''' has been selected for $\mathcal{G}$ after the parallelogram R and the parallelograms $R''\in\mathcal{B}(R')$ with $I\subset I_{R''}$. By Lemma 13, it suffices to show that the maximal function

$$M_V\Bigg(1_R+\sum_{\substack{R''\in\mathcal{B}(R')\\ \text{s.t. } I\subset I_{R''}}} 1_{R''}\Bigg)$$

is larger than 10^{-3} on the parallelogram

$$\tilde{R}:=50\big(1+|U|\,|I|H(R)^{-1}\big)R.$$

First assume there exists $R''\in\mathcal{B}(R')$ with $I\subset I_{R''}$ and $R_I\cap R''\neq\varnothing$ and $H(R'')\geq 20\,|U|\,|I|$. Note that $U(R'')$ and $U(\tilde{R})$ have nonempty intersection because $U(R'')\subset U\subset U(\tilde{R})$. Applying Lemma 6 to the rectangles R''_I and $\tilde{R}_I$, we obtain similarly as before

$$M_V(1_{R''}+1_R)\geq 7^{-1}H(\tilde{R})^{-1}\big(\min(H(R''),H(\tilde{R}))+H(R)\big)>10^{-3}$$

on $\tilde{R}_I$, which proves Lemma 14 in the given case.

Hence we may assume

$$H(R'')\leq 20\,|U|\,|I|$$

for every $R''\in\mathcal{B}(R')$ with $I\subset I_{R''}$ and $R_I\cap R''\neq\varnothing$. We then have on $\tilde{R}_I$, by Lemma 13,

$$\begin{aligned}
M_V\Bigg(1_R+\sum_{\substack{R''\in\mathcal{B}(R')\\ \text{s.t. } I\subset I_{R''}}} \mathbf{1}_{R''}\Bigg) &\geq H(\tilde{R})^{-1}\Bigg(H(R)+\sum_{\substack{R''\in\mathcal{B}(R')\\ \text{s.t. } I\subset I_{R''}}} H(R'')\Bigg)\\
&\geq H(\tilde{R})^{-1}\Bigg(H(R)+\sum_{\substack{R''\in\mathcal{B}(R')\\ \text{s.t. } I\subset I_{R''}}} |R_I\cap R''|\,|U|H(R)^{-1}\Bigg)\\
&\geq H(\tilde{R})\big(H(R)+|U|H(R)^{-1}10^{-1}|R_I|\big)\geq 500^{-1}.
\end{aligned}$$

This completes the proof of Lemma 14. □

We have used the hypothesis $I_{R'''}\neq I$ of Lemma 14 only to conclude that R''' has been selected last to $\mathcal{G}$. Consider the collection of all $R''\in\mathcal{B}(R')$ with $I=I_{R''}$ and let R''' be the parallelogram chosen last in this collection. Since $|R_I\cap R'''|\leq|R_I|$, the proof of the previous lemma also gives:

Lemma 15. *For every $I \subset I_{R'}$,*

$$\sum_{R'' \in \mathcal{B}(R'): I = I_{R''}} |R_I \cap R''| \le 2|R_I|.$$

Now let $\mathcal{J}$ be the set of maximal dyadic intervals contained in $I_{R'}$ such that

$$\sum_{\substack{R'' \in \mathcal{B}(R') \\ \text{s.t. } I \subset I_{R''}}} |R_I \cap R''| > 2|R_I|.$$

By Lemma 15, we have $I_{R'} \notin \mathcal{J}$. Let $I \in \mathcal{J}$ and denote the parent of I by $\tilde{I}$. By Lemma 14 and by maximality of I and Lemma 15, we have

$$\sum_{R'' \in \mathcal{B}(R')} |R_I \cap R''| = \sum_{R'' \in \mathcal{B}(R'): \tilde{I} \subset I_{R''}} |R_I \cap R''| + \sum_{R'' \in \mathcal{B}(R'): I = I_{R''}} |R_I \cap R''| \le 2|R_{\tilde{I}}| + 2|R_I| \le 6|R_I|.$$

By adding over all $I \in \mathcal{J}$, we obtain

$$\sum_{I \in \mathcal{J}'} \sum_{R'' \in \mathcal{B}(R')} |R_I \cap R''| \le 6|R_{I(R')}|. \tag{3-16}$$

Now let $\mathcal{J}'$ be the set of maximal dyadic intervals that are contained in $I_{R'}$, disjoint from any interval in $\mathcal{J}$, and do not contain any $I(R'')$ with $R'' \in \mathcal{R}(R')$. By construction of $\mathcal{J}$, we have for each $I \in \mathcal{J}'$

$$\sum_{R'' \in \mathcal{R}(R')} |R_I \cap R''| = \sum_{R'' \in \mathcal{R}(R'): I \subset I_{R''}} |R_I \cap R''| \le 2|R_I|.$$

Summing over all intervals in $\mathcal{J}'$ gives

$$\sum_{I \in \mathcal{J}'} \sum_{R'' \in \mathcal{R}(R')} |R_I \cap R''| \le 2|R_{I(R')}|. \tag{3-17}$$

Together with (3-16) this completes the proof of Lemma 11, because $\mathcal{J}$ and $\mathcal{J}'$ form a partition of $I(R')$. □

4. Outline of the proof of Theorem 5

Recall that we need to prove, for each $|k| \le k_0$, the inequality

$$|\langle H_{k,G,H} \mathbf{1}_F, \mathbf{1}_E \rangle| \lesssim \left(\frac{|G|}{|H|} \right)^{1/2 - 1/p} |F|^{1/2} |E|^{1/2}. \tag{4-1}$$

We assume without loss of generality that $E \subset G$ and $F \subset H$. Recall also that Theorem 2 implies, for $1 < q < \infty$,

$$|\langle H_k \mathbf{1}_F, \mathbf{1}_E \rangle| \lesssim \left(\frac{|E|}{|F|} \right)^{1/2 - 1/q} |F|^{1/2} |E|^{1/2}. \tag{4-2}$$

The left sides of (4-1) and (4-2) are identical. Hence our task is to strengthen the proof of Theorem 2 in [Bateman 2013b] in case the factor involving G and H in (4-1) is less than the corresponding factor involving E and F in (4-2).

We recall some details about the proof in [Bateman 2013b]. The form $\langle H_k \mathbf{1}_F, \mathbf{1}_E\rangle$ is written as a linear combination of a bounded number of model forms

$$\sum_{s\in\mathcal{U}_k} \langle \mathbf{C}_{s,k}\mathbf{1}_F, \mathbf{1}_E\rangle,$$

where the index set $\mathcal{U}_k$ is a set of parallelograms with vertical edges and constant height (depending on k). The paper proves the bound analogous to (4-2) for the absolute sum

$$\sum_{s\in\mathcal{U}'_k} |\langle \mathbf{C}_{s,k}\mathbf{1}_F, \mathbf{1}_E\rangle|, \tag{4-3}$$

where $\mathcal{U}'_k$ is an arbitrary finite subset of $\mathcal{U}_k$ and the bound is independent of the choice of subset, which may be assumed to only account for nonzero summands.

To estimate (4-3), one first proves estimates for the sum over certain subsets of $\mathcal{U}'_k$ called trees. Each tree T is assigned a parallelogram $\mathbf{top}(T)$. It is also assigned a density $\delta(T)$, which measures the contribution of E to the tree, and a size $\sigma(T)$, which measures the contribution of F to the tree. One obtains, for each tree T,

$$\sum_{s\in T} |\langle \mathbf{C}_s\mathbf{1}_F, \mathbf{1}_E\rangle| \lesssim \delta(T)\sigma(T)|\mathbf{top}(T)|.$$

The collection $\mathcal{U}'_k$ is then written as a disjoint union of subcollections $\mathcal{U}_{\delta,\sigma}$, where δ and σ run through the set of integer powers of two. Each $\mathcal{U}_{\delta,\sigma}$ is written as a disjoint union of a collection $\mathcal{T}_{\delta,\sigma}$ of trees with density at most δ and size at most σ. With the above tree estimate, it remains to estimate $\sum_{\delta,\sigma} S_{\delta,\sigma}$ with

$$S_{\delta,\sigma} := \sum_{T\in\mathcal{T}_{\delta,\sigma}} \delta\sigma|\mathbf{top}(T)|.$$

We list the estimates on $S_{\delta,\sigma}$ used in [Bateman 2013b]; we include an additional factor of $\delta\sigma$ relative to the corresponding expressions in [Bateman 2013b].

Estimate 16 (orthogonality). $S_{\delta,\sigma} \lesssim |F|\delta\sigma^{-1}$.

Estimate 17 (density). $S_{\delta,\sigma} \lesssim |E|\sigma$.

Estimate 18 (maximal). *For any* $\epsilon > 0$, $S_{\delta,\sigma} \lesssim |F|^{1-\epsilon}|E|^{\epsilon}\sigma^{-\epsilon}$.

Estimate 19 (trivial density restriction). *If* $\delta > 1$, *then* $S_{\delta,\sigma} = 0$.

Estimate 20 (trivial size restriction). *There is a universal* σ_0 *such that if* $\sigma > \sigma_0$, *then* $S_{\delta,\sigma} = 0$.

Our improvement comes through two additional estimates depending on G and H that will be proved in Section 5.

Estimate 21 (second maximal). *If* $p < 2$ *and* G, H *are as in Theorem 5, then for every* $\epsilon > 0$,

$$S_{\delta,\sigma} \lesssim |E|\left(\frac{|H|}{|G|}\right)^{1/2}\sigma^{-\epsilon}\delta^{-1/2-\epsilon}.$$

Estimate 22 (size restriction). *Let $p > 2$ and let G, H be as in Theorem 5. Let $n > 2$ be a large integer and $\alpha = 1/n$ and C_α be some constant. Then there is a constant σ_1 such that if*

$$\sigma \geq \sigma_1 \left(\frac{\tilde{\delta}}{\delta}\right)^n$$

with

$$\tilde{\delta} = C_\alpha \left(\frac{|G|}{|H|}\right)^{1-\alpha},$$

then we have $S_{\delta,\sigma} = 0$.

To obtain summability for small σ, it is convenient to take weighted geometric averages of Estimates 16, 18, and 21 with Estimate 17 to obtain positive powers of σ. We record these modified estimates, where we simplify exponents using that we may assume universal upper bounds on δ and σ. We have, for any $\epsilon > 0$:

Estimate 23 (modified orthogonality). $S_{\delta,\sigma} \lesssim |E|^{1/2+\epsilon}|F|^{1/2-\epsilon}\delta^{1/2-\epsilon}\sigma^{2\epsilon}$.

Estimate 24 (modified maximal). $S_{\delta,\sigma} \lesssim |F|^{1-4\epsilon}|E|^{4\epsilon}\sigma^{\epsilon}$.

Estimate 25 (modified second maximal). *Under the assumptions of Estimate 21,*

$$S_{\delta,\sigma} \lesssim |E| \left(\frac{|H|}{|G|}\right)^{1/2-\epsilon} \sigma^{\epsilon}\delta^{-1/2}.$$

In the rest of this section we show how these estimates are used to estimate $\sum_{\delta,\sigma} S_{\delta,\sigma}$, and thereby complete the proof of Theorem 5.

4.1. ***Case $p < 2$ and $|H| \leq |G|$.*** Inequality (4-1) for $\frac{3}{2} < p < 2$ follows from inequality (4-2) for $1 < q < 2$ unless

$$\left(\frac{|H|}{|G|}\right)^{1/3} \leq \frac{|F|}{|E|}, \tag{4-4}$$

which we shall therefore assume.

Pick $\epsilon > 0$ small compared to the distance of p to $\frac{3}{2}$. We split the sum over δ at

$$\delta_0 = \left(\frac{|H|}{|G|}\frac{|E|}{|F|}\right)^{1/2}.$$

For $\delta \leq \delta_0$, we use Estimate 23 together with Estimate 20 to obtain

$$\sum_{\delta \leq \delta_0} \sum_{\sigma} S_{\delta,\sigma} \lesssim \delta_0^{1/2-\epsilon}|E|^{1/2+\epsilon}|F|^{1/2-\epsilon} = |E|^{3/4+\epsilon/2}|F|^{1/4-\epsilon/2}\left(\frac{|H|}{|G|}\right)^{1/4-\epsilon/2}.$$

For $\delta \geq \delta_0$ we use Estimate 25 together with Estimate 20 to obtain

$$\sum_{\delta \geq \delta_0} \sum_{\sigma} S_{\delta,\sigma} \lesssim \delta_0^{-1/2}|E|\left(\frac{|H|}{|G|}\right)^{1/2-\epsilon} = |E|^{3/4}|F|^{1/4}\left(\frac{|H|}{|G|}\right)^{1/4-\epsilon}.$$

Using (4-4) and $|H| \le |G|$, we may estimate both partial sums by

$$\lesssim |E|^{1/2}|F|^{1/2}\left(\frac{|H|}{|G|}\right)^{1/6-3\epsilon}.$$

This completes the proof of (4-1) in case $p < 2$.

4.2. *Case $p > 2$ and $|G| \le |H|$.* Pick ϵ very small compared to $1/p$. Inequality (4-1) for $2 < p < \infty$ follows from inequality (4-2) unless

$$\frac{|G|}{|H|} \le \left(\frac{|E|}{|F|}\right)^{1+\epsilon}, \tag{4-5}$$

which we shall therefore assume. Let α and $1/n$ be very small compared to ϵ, let C_α be as in the construction of the set H, and let $\tilde{\delta}$ be as in Estimate 22. We split the sum over δ at

$$\delta_1 := \tilde{\delta}\left(\frac{1}{\tilde{\delta}}\frac{|E|}{|F|}\right)^{1/n}.$$

For $\delta \le \delta_1$ we use a weighted geometric mean of Estimates 23 and 24 together with Estimate 20 to obtain

$$\sum_{\delta\le\delta_1}\sum_{\sigma} S_{\delta,\sigma} \lesssim \delta_1^{1/2-4\epsilon}|E|^{1/2-\epsilon}|F|^{1/2+\epsilon} \lesssim \tilde{\delta}^{(1-1/n)(1/2-4\epsilon)}|E|^{1/2}|F|^{1/2}\left(\frac{|G|}{|H|}\right)^{-2\epsilon},$$

where in the last line we have used (4-5) and $|G| \le |H|$. Using the definition of $\tilde{\delta}$ in Estimate 22, we may estimate the last display by

$$\lesssim |E|^{1/2}|F|^{1/2}\left(\frac{|G|}{|H|}\right)^{1/2-10\epsilon}. \tag{4-6}$$

For $\delta \ge \delta_1$ we use Estimate 17 together with Estimate 22 to obtain

$$\sum_{\delta\ge\delta_1}\sum_{\sigma} S_{\delta,\sigma} \lesssim \sum_{\delta\ge\delta_1}(\tilde{\delta}/\delta)^n|E| \lesssim (\tilde{\delta}/\delta_1)^n|E| \lesssim \tilde{\delta}|F| \lesssim |F|^{1/2}|E|^{1/2}\left(\frac{|G|}{|H|}\right)^{1/2-10\epsilon},$$

where in the last line we have used (4-5) and $|G| \le |H|$. This completes the proof of (4-1) in case $p > 2$.

5. Proof of the additional Estimates 21 and 22

In this section we deviate from the notation in Section 3 as follows: for a parallelogram R we denote by CR the isotropically scaled parallelogram with the same center and slope as R but with height $H(CR) = CH(R)$ and shadow $I(CR) = CI(R)$.

We say that a set is approximated by a parallelogram R if it is contained in the parallelogram and the parallelogram has at most one hundred times the area of the set. Any parallelogram R can be approximated by a parallelogram R' with $I(R') \in \mathcal{I}_1 \cup \mathcal{I}_2$ and both vertical edges of R' in $\mathcal{I}_1 \cup \mathcal{I}_2$. To see this, first identify an interval I in $\mathcal{I}_1 \cup \mathcal{I}_2$ that contains $I(R)$ and has at most three times the length; this interval I will be the shadow of R'. Consider the extension of R that has same central line and height as R but shadow I. Then find two intervals in $\mathcal{I}_1 \cup \mathcal{I}_2$ that have mutually equal length at most three times the height of R and that contain the respective vertical edges of the extended parallelogram. These intervals define the vertical edges of R'.

We recall some details of the proof of Estimate 17 in [Bateman 2013b]. Given δ, σ, one constructs a collection $\mathcal{R}_{\delta,\sigma}$ of parallelograms of the same height as the parallelograms in $\mathcal{U}'_k$ such that each tree T in $T_{\delta,\sigma}$ is assigned a parallelogram R in $\mathcal{R}_{\delta,\sigma}$ with $\mathbf{top}(T) \subset C_0 R$ and $\mathbf{top}(T') \subset C_0 R$ for every subtree T' of T, for some constant C_0. If $\mathcal{T}(R)$ denotes the trees in $\mathcal{T}_{\delta,\sigma}$ that are assigned a given parallelogram $R \in \mathcal{R}_{\delta,\sigma}$, then we have

$$\sum_{T \in \mathcal{T}(R)} |\mathbf{top}(T)| \le C_1 |R|$$

for some constant C_1. Estimate 17 is then deduced from the inequality

$$\sum_{R \in \mathcal{R}_{\sigma,\delta}} |R| \lesssim |E| \delta^{-1}, \tag{5-1}$$

which follows essentially from pairwise incomparability of the parallelograms in $\mathcal{R}_{\delta,\sigma}$. (In other words, if two parallelograms P_1, P_2 overlap, then they are pointed in different directions, resulting in disjointness of the sets $E(P_1)$ and $E(P_2)$.) All parallelograms in $\mathcal{R}_{\delta,\sigma}$ have height at least 2^{-k_0}, length of shadow at least 2^{-k_0}, and slope at most 10^{-1}.

Let $Q = [-N, N]^2$ be the large square with N as in Lemma 4. We claim that every set $Q \cap 2^k R$ with $R \in \mathcal{R}_{\delta,\sigma}$ and $k \ge 0$ can be approximated by a parallelogram in $\mathcal{R}_1 \cup \mathcal{R}_2$. If $Q \cap 2^k R$ is a parallelogram, then this is clear by the remarks above. If $Q \cap 2^k R$ is not a parallelogram, then we first extend it to the minimal parallelogram containing it, which thanks to the bounded slope of R is not much larger than $Q \cap 2^k R$, and then approximate the extension by a parallelogram in $\mathcal{R}_1 \cup \mathcal{R}_2$.

5.1. ***Proof of Estimate 21.*** We partition $\mathcal{R}_{\delta,\sigma}$ into subset $\mathcal{R}_{\delta,\sigma,j}$ consisting of all parallelograms in $\mathcal{R}_{\delta,\sigma}$ such that

$$C_1 2^{-j-1} |R| \le \sum_{T \in \mathcal{T}(R)} |\mathbf{top}(T)| < C_1 2^{-j} |R|.$$

We claim that $\mathcal{R}_{\delta,\sigma,j}$ is empty unless j satisfies (5-3) below. Specifically, the number j_0 used in the following display is implicitly defined in (5-3); our present claim justifies that the summation immediately below should only be over $j \gtrsim j_0$. This claim together with (5-1) will prove Estimate 21:

$$S_{\delta,\sigma} \lesssim \delta\sigma \sum_{j_0 \lesssim j} \sum_{\mathcal{R}_{\delta,\sigma,j}} 2^{-j} |R| \lesssim \sum_{j_0 \lesssim j} 2^{-j} |E| \sigma \lesssim |E| \sigma^{-\epsilon} \delta^{-1/2\epsilon} \left(\frac{|H|}{|G|} \right)^{1/2}.$$

It remains to prove the claim. Suppose there is a parallelogram R in $R \in \mathcal{R}_{\sigma,\delta,j}$. It has large density as defined and discussed in [Bateman 2013b], which implies that there is a $k \ge 0$ with

$$|E(2^k R) \cap G| \ge 2^{20k} \delta |2^k R|.$$

Since G is contained in Q, we may approximate $Q \cap 2^k R$ by a parallelogram R' of $\mathcal{R}_1 \cup \mathcal{R}_2$ and obtain

$$|E(R')| \ge |E(R') \cap G| \gtrsim 2^{20k} \delta |R'|. \tag{5-2}$$

Now suppose first that $2^k \geq \sigma^{-\epsilon}$. By Claim 18 in [Bateman 2013b], and using $F \subset Q$, we obtain

$$\frac{|F \cap H \cap R'|}{|R'|} \gtrsim \frac{|F \cap H \cap 2^k R|}{|2^k R|} \gtrsim 2^{-2k} 2^{-j} \sigma^{1+\epsilon}.$$

On the other hand, (5-2) implies in particular $R' \cap G \neq \varnothing$, which by construction of G (see Section 3) implies, using $k \geq 1$,

$$2^{-2k} 2^{-j} \sigma^{1+\epsilon} \lesssim (2^{20k}\delta)^{-(1/2+\epsilon)} \left(\frac{|H|}{|G|}\right)^{1/2},$$
$$2^{-j} \lesssim 2^{-j_0} := \sigma^{-1-\epsilon} \delta^{-1/2-\epsilon} \left(\frac{|H|}{|G|}\right)^{1/2}. \tag{5-3}$$

If $2^k \leq \sigma^{-\epsilon}$, we use the variant

$$\frac{|F \cap H \cap \sigma^{-\epsilon} R|}{|\sigma^{-\epsilon} R|} \geq 2^{-j} \sigma^{1+3\epsilon}$$

of Claim 18 in [Bateman 2013b] to obtain the same conclusion.

5.2. ***Proof of Estimate 22.*** By Estimates 19 and 20, we may assume $C_0 \tilde{\delta} \leq \delta$ with C_0 as above. Suppose $T_{\delta,\sigma}$ is nonempty. Consider a tree T in $\mathcal{T}_{\delta,\sigma}$ and let $R \in \mathcal{R}_{\delta,\sigma}$ be the associated parallelogram as above. As above, for some $k \geq 0$ we have

$$|E(2^k R) \cap G| \geq 2^{20k} \delta |2^k R|.$$

Define m so that δ is within a factor of two of $C_0^2 2^m \tilde{\delta}$ and note that $m \geq 0$. Let $R' \in \mathcal{R}_1 \cup \mathcal{R}_2$ be an approximation of $Q \cap \max(2^k, C_0 2^m) R$. We then have

$$|E(R') \cap G| \geq \tilde{\delta} |R'|.$$

By construction, R' is disjoint from H. Since $\mathbf{top}(T)$ is contained in $C_0 R$, we have that $2^m \mathbf{top}(T)$ is contained in $R' \cup Q^c$, and the same holds with T replaced by any subtree T' of T.

But by Lemma 29 of [Bateman 2013b] with $f = \mathbf{1}_{F \cap H}$, we obtain, with the notation in that lemma for every subtree T' of T,

$$\sum_{s \in T'} |\langle f, \phi_s \rangle|^2 = \sum_{m' \geq m} \sum_{s \in T'} \left|\left\langle f \mathbf{1}_{2^{m'+1}\mathbf{top}(T') \setminus 2^{m'}\mathbf{top}(T')}, \phi_s \right\rangle\right|^2$$
$$\lesssim \sum_{m' \geq m} 2^{-4nm'} \left\| f 1_{2^{m'+1}\mathbf{top}(T')} \right\|_2^2 \lesssim 2^{-2nm} |\mathbf{top}(T')|.$$

By the definition of $\sigma(T)$, this implies

$$\sigma(T) \leq 2^{-nm},$$

which in turn implies Estimate 22.

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CARLEMAN ESTIMATES FOR ANISOTROPIC ELLIPTIC OPERATORS WITH JUMPS AT AN INTERFACE

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We consider a second-order self-adjoint elliptic operator with an anisotropic diffusion matrix having a jump across a smooth hypersurface. We prove the existence of a weight function such that a Carleman estimate holds true. We also prove that the conditions imposed on the weight function are sharp.

1. Introduction

1A. *Carleman estimates.* Let $P(x, D_x)$ be a differential operator defined on some open subset of $\mathbb{R}^n$. A *Carleman estimate* for this operator is the weighted a priori inequality

$$\|e^{\tau\varphi} P w\|_{L^2(\mathbb{R}^n)} \gtrsim \|e^{\tau\varphi} w\|_{L^2(\mathbb{R}^n)}, \tag{1-1}$$

where the weight function φ is real-valued with a nonvanishing gradient, τ is a large positive parameter, and w is any smooth compactly supported function. This type of estimate was used for the first time by T. Carleman [1939] to handle uniqueness properties for the Cauchy problem for nonhyperbolic operators. To this day, it remains essentially the only method to prove unique continuation properties for ill-posed problems,[1] and in particular to handle uniqueness of the Cauchy problem for elliptic operators with nonanalytic coefficients.[2] This tool has been refined, polished and generalized by manifold authors.

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[1] F. John [1960] showed that, although the Hadamard well-posedness property is a privilege of hyperbolic operators, a weaker type of continuous dependence, which he called *Hölder continuous well-behavior*, could occur. Strong connections between the well-behavior property and Carleman estimates can be found in an article by H. Bahouri [1987].

[2] For analytic operators, Holmgren's theorem provides uniqueness for the noncharacteristic Cauchy problem, but that analytical result falls short of giving a control of the solution from the data.

A. P. Calderón [1958] gave a very important development of the Carleman method with a proof of an estimate of the form (1-1) using a pseudodifferential factorization of the operator, giving a new start to singular-integral methods in local analysis. L. Hörmander [1958; 1963, Chapter VIII] showed that local methods could provide the same estimates, with weaker assumptions on the regularity of the coefficients of the operator.

For instance, for second-order elliptic operators with real coefficients[3] in the principal part, Lipschitz continuity of the coefficients suffices for a Carleman estimate to hold and thus for unique continuation across a $\mathscr{C}^1$ hypersurface. Naturally, pseudodifferential methods require more derivatives, at least tangentially, that is, essentially on each level surface of the weight function φ. Chapters 17 and 28 in [Hörmander 1985b] contain more references and results.

Furthermore, it was shown by A. Pliś [1963] that Hölder continuity is not enough to get unique continuation: he constructed a real homogeneous linear differential equation of second order and of elliptic type on $\mathbb{R}^3$ without the unique continuation property, although the coefficients are Hölder-continuous with any exponent less than one. The constructions by K. Miller [1974] and later by N. Mandache [1998] and N. Filonov [2001] showed that Hölder continuity is not sufficient to obtain unique continuation for second-order elliptic operators, even in divergence form (see also [Buonocore and Manselli 2000; Schulz 1998] for the particular two-dimensional case where boundedness is essentially enough to get unique continuation for elliptic equations in the case of $W^{1,2}$ solutions).

The results cited above are related to the regularity of the principal part of the second-order operator. For strong unique continuation properties for second-order operators with Lipschitz-continuous coefficients, many results are also available for differential inequalities with singular potentials, originating with the seminal work of D. Jerison and C. Kenig [1985]. The reader is also referred to the work of C. Sogge [1989] and some of the most recent and general results of H. Koch and D. Tataru [2001; 2002].

In more recent years, the field of applications of Carleman estimates has gone beyond the original domain. They are also used in the study of inverse problems (see, for example, [Bukhgeim and Klibanov 1981; Isakov 1998; Imanuvilov et al. 2003; Kenig et al. 2007]) and control theory for PDEs. Through unique continuation properties, they are used for the exact controllability of hyperbolic equations [Bardos et al. 1992]. They also yield the null controllability of linear parabolic equations [Lebeau and Robbiano 1995] and the null controllability of classes of semilinear parabolic equations [Fursikov and Imanuvilov 1996; Barbu 2000; Fernández-Cara and Zuazua 2000].

1B. ***Jump discontinuities.*** Although the situation seems to be almost completely clarified by the previous results, with a minimal and somewhat necessary condition on Lipschitz continuity, we are interested in the following second-order elliptic operator $\mathcal{L}$:

$$\mathcal{L}w = -\operatorname{div}(A(x)\nabla w), \quad A(x) = (a_{jk}(x))_{1\le j,k\le n} = A^T(x), \quad \inf_{\|\xi\|_{\mathbb{R}^n}=1} \langle A(x)\xi, \xi\rangle > 0, \tag{1-2}$$

[3] S. Alinhac [1980] showed the nonunique continuation property for second-order elliptic operators with nonconjugate roots; of course, if the coefficients of the principal part are real, this is excluded.

in which the matrix A has a jump discontinuity across a smooth hypersurface. However, we shall impose some stringent — yet natural — restrictions on the domain of functions w, which will be required to satisfy some homogeneous *transmission conditions*, detailed in the next sections. Roughly speaking, this means that w must belong to the domain of the operator, with continuity at the interface, so that ∇w remains bounded, and continuity of the flux across the interface, so that $\operatorname{div}(A\nabla w)$ remains bounded, avoiding in particular the occurrence of a simple or multiple layer at the interface.[4]

A. Doubova, A. Osses, and J.-P. Puel [Doubova et al. 2002] tackled that problem in the isotropic case (the matrix A is $c\,\mathrm{Id}$ for scalar c) with a monotonicity assumption: the observation takes place in the region where the diffusion coefficient c is the "lowest". (The work of Doubova et al. [2002] concerns the case of a parabolic operator, but an adaptation to an elliptic operator is straightforward.) In the one-dimensional case, the monotonicity assumption was relaxed for general piecewise $\mathscr{C}^1$ coefficients by A. Benabdallah, Y. Dermenjian, and J. Le Rousseau [Benabdallah et al. 2007] and for coefficients with bounded variations [Le Rousseau 2007]. The case of an arbitrary dimension without any monotonicity condition in the elliptic case was solved by J. Le Rousseau and L. Robbiano [2010]: there the isotropic case is treated, as well as a particular case of anisotropic medium. An extension of their approach to the case of parabolic operators can be found in [Le Rousseau and Robbiano 2011]. A. Benabdallah, Y. Dermenjian, and J. Le Rousseau [Benabdallah et al. 2011] also tackled the situation in which the interface meets the boundary, a case that is typical of stratified media. They treat particular forms of anisotropic coefficients.

The purpose of the present article is to show that a Carleman estimate can be proven for any operator of type (1-2) without an isotropy assumption: $A(x)$ is a symmetric positive-definite matrix with a jump discontinuity across a smooth hypersurface. We also provide conditions on the Carleman weight function that are rather simple to handle, and we prove that they are sharp.

The approach we follow differs from that of [Le Rousseau and Robbiano 2010], where the authors base their analysis on the usual Carleman method for certain microlocal regions and on Calderón projectors for others. The regions they introduce are determined by the ellipticity or nonellipticity of the conjugated operator. The method in [Benabdallah et al. 2011] exploits a particular structure of the anisotropy that allows one to use Fourier series. The analysis is then close to that of [Le Rousseau and Robbiano 2010; 2011] in the sense that second-order operators are inverted in some frequency ranges. Here, our approach is somewhat closer to A. Calderón's original work [1958] on unique continuation: the conjugated operator is factored out in first-order (pseudodifferential) operators, for which estimates are derived. Naturally, the quality of these estimates depends on their elliptic or nonelliptic nature; we thus recover microlocal regions that correspond to those of [Le Rousseau and Robbiano 2010]. Such a factorization is also used in [Imanuvilov and Puel 2003] to address nonhomogeneous boundary conditions.

1C. ***Notation and statement of the main result.*** Let Ω be an open subset of $\mathbb{R}^n$ and let Σ be a $\mathscr{C}^\infty$ oriented hypersurface of Ω; we have the partition

$$\Omega = \Omega_+ \cup \Sigma \cup \Omega_-, \quad \overline{\Omega_\pm} = \Omega_\pm \cup \Sigma, \quad \Omega_\pm \text{ open subsets of } \mathbb{R}^n, \tag{1-3}$$

[4] In the sections below, we shall also consider nonhomogeneous boundary conditions.

and we introduce the Heaviside-type functions

$$H_\pm = \mathbf{1}_{\Omega_\pm}. \tag{1-4}$$

We consider the elliptic second-order operator

$$\mathcal{L} = D \cdot AD = -\operatorname{div}(A(x)\nabla) \quad (D = -i\nabla), \tag{1-5}$$

where $A(x)$ is a symmetric positive-definite $n \times n$ matrix such that

$$A = H_- A_- + H_+ A_+, \quad A_\pm \in \mathscr{C}^\infty(\Omega). \tag{1-6}$$

We shall consider functions w of the type

$$w = H_- w_- + H_+ w_+, \quad w_\pm \in \mathscr{C}^\infty(\Omega). \tag{1-7}$$

We have $dw = H_- dw_- + H_+ dw_+ + (w_+ - w_-)\delta_\Sigma \nu$, where δ_Σ is the Euclidean hypersurface measure on Σ and ν is the unit conormal vector field to Σ pointing into Ω_+. To remove the singular term, we assume

$$w_+ = w_- \quad \text{at } \Sigma, \tag{1-8}$$

so that $A\,dw = H_- A_- dw_- + H_+ A_+ dw_+$ and

$$\operatorname{div}(A\,dw) = H_- \operatorname{div}(A_- dw_-) + H_+ \operatorname{div}(A_+ dw_+) + \langle A_+ dw_+ - A_- dw_-, \nu\rangle \delta_\Sigma.$$

Also, we shall assume that

$$\langle A_+ dw_+ - A_- dw_-, \nu\rangle = 0 \quad \text{at } \Sigma, \text{ that is, } \langle dw_+, A_+\nu\rangle = \langle dw_-, A_-\nu\rangle, \tag{1-9}$$

so that

$$\operatorname{div}(A\,dw) = H_- \operatorname{div}(A_- dw_-) + H_+ \operatorname{div}(A_+ dw_+). \tag{1-10}$$

Conditions (1-8)–(1-9) will be called *transmission conditions* on the function w, and we define the vector space

$$\mathcal{W} = \{H_- w_- + H_+ w_+\}_{w_\pm \in \mathscr{C}^\infty(\Omega)}, \quad w_\pm \text{ satisfying (1-8)–(1-9)}. \tag{1-11}$$

Note that (1-8) is a continuity condition of w across Σ and (1-9) is concerned with the continuity of $\langle A\,dw, \nu\rangle$ across Σ, that is, the continuity of the flux of the vector field $A\,dw$ across Σ. A weight function *suitable for observation from* Ω_+ is defined as a Lipschitz continuous function φ on Ω such that

$$\varphi = H_- \varphi_- + H_+ \varphi_+, \quad \varphi_\pm \in \mathscr{C}^\infty(\Omega), \quad \varphi_+ = \varphi_-, \quad \langle d\varphi_\pm, X\rangle > 0 \quad \text{at } \Sigma, \tag{1-12}$$

for any positively transverse vector field X to Σ (that is, $\langle \nu, X\rangle > 0$).

Theorem 1.1. *Let $\Omega, \Sigma, \mathcal{L}, \mathcal{W}$ be as in (1-3), (1-5), and (1-11). Then for any compact subset K of Ω, there exist a weight function φ satisfying (1-12) and positive constants C, τ_1 such that for all $\tau \geq \tau_1$ and* *all* $w \in \mathcal{W}$ *with* $\operatorname{supp} w \subset K$,

$$C\|e^{\tau\varphi}\mathcal{L}w\|_{L^2(\mathbb{R}^n)} \geq \tau^{3/2}\|e^{\tau\varphi}w\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\big\|H_+e^{\tau\varphi}\nabla w_+\big\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\big\|H_-e^{\tau\varphi}\nabla w_-\big\|_{L^2(\mathbb{R}^n)} + \tau^{3/2}\big|(e^{\tau\varphi}w)_{|\Sigma}\big|_{L^2(\Sigma)} + \tau^{1/2}\big|(e^{\tau\varphi}\nabla w_+)_{|\Sigma}\big|_{L^2(\Sigma)} + \tau^{1/2}\big|(e^{\tau\varphi}\nabla w_-)_{|\Sigma}\big|_{L^2(\Sigma)}. \quad (1\text{-}13)$$

Remark 1.2. The proof of Theorem 1.1 provides an explicit construction of the weight function φ. The precise properties of φ are given in Section 2D, specifically (2-22), (2-24), and (2-26). The weight function is at first constructed only depending on x_n. Dependency upon the other variables, that is, convexification with respect to $\{x_n = 0\}$, is introduced in Section 4E.

Remark 1.3. It is important to notice that whenever a true discontinuity occurs for the vector field $A\nu$, the space $\mathcal{W}$ does *not* contain $\mathscr{C}^\infty(\Omega)$: the inclusion $\mathscr{C}^\infty(\Omega) \subset \mathcal{W}$ implies by (1-9) that for all $w \in \mathscr{C}^\infty(\Omega)$, $\langle dw, A_+\nu - A_-\nu\rangle = 0$ at Σ, so that $A_+\nu = A_-\nu$ at Σ, which is continuity for $A\nu$. The Carleman estimate which is proven in the present paper naturally takes into account these transmission conditions on the function w, and it is important to keep in mind that the occurrence of a jump excludes many smooth functions from the space $\mathcal{W}$. On the other hand, we have $\mathcal{W} \subset \operatorname{Lip}(\Omega)$.

Remark 1.4. We also point out the geometric content of our assumptions, which do not depend on the choice of a coordinate system. For each $x \in \Omega$, the matrix $A(x)$ is a positive-definite symmetric mapping from $T_x(\Omega)^*$ onto $T_x(\Omega)$, so that $A(x)dw(x)$ belongs indeed to $T_x(\Omega)$ and $A\,dw$ is a vector field with an L^2 divergence (inequality (1-13) yields the L^2 bound by density).

1D. *Examples of applications.* We mention some applications of the Carleman estimate of Theorem 1.1, namely, controllability for parabolic equations and stabilization for hyperbolic equations.

Following [Lebeau and Robbiano 1995; Lebeau and Zuazua 1998] (see also [Le Rousseau and Robbiano 2010]), we first deduce the following interpolation inequality. With $\alpha \in (0, X_0/2)$, we set $X = (0, X_0)\times\Omega$, $Y = (\alpha, X_0-\alpha)\times\Omega$.

Theorem 1.5. *There exist* $C \geq 0$ *and* $\delta \in (0,1)$ *such that for* $u \in H^1(X)$ *that satisfies* $u_\pm = u|_{(0,X_0)\times\Omega_\pm} \in H^2((0,X_0)\times\Omega_\pm)$,

$$u_+ = u_- \quad \textit{and} \quad \langle du_+, A_+\nu\rangle = \langle du_-, A_-\nu\rangle \quad \textit{at } (0,X_0)\times\Sigma,$$

and

$$u(x_0,x)|_{x\in\partial\Omega} = 0, \quad x_0 \in (0,X_0), \quad \textit{and} \quad u(0,x) = 0,\ x \in \Omega,$$

we have

$$\|u\|_{H^1(Y)} \leq C\|u\|^{\delta}_{H^1(X)}\Big(\big\|(D^2_{x_0}+\mathcal{L})u\big\|_{L^2(X)} + \big\|\partial_{x_0}u(0,x)\big\|_{L^2(\omega)}\Big)^{1-\delta}.$$

This interpolation inequality was first proven in [Lebeau and Robbiano 1995; Lebeau and Zuazua 1998] for second-order elliptic operators with smooth coefficients and in [Le Rousseau and Robbiano 2010] in the case of an isotropic diffusion coefficient with a jump at an interface. Here, a jump for the whole diffusion matrix is permitted.

Remark 1.6. In fact, the interpolation inequality of Theorem 1.5 rather follows from the nonhomogeneous version of Theorem 1.1 stated in Theorem 2.2 below.

From Theorem 1.5 we can prove an estimation of the loss of orthogonality for the eigenfunctions $\phi_j(x)$, $j \in \mathbb{N}$, of the operator $\mathcal{L}$, with Dirichlet boundary conditions, when these eigenfunctions are restricted to some subset ω of Ω (see [Lebeau and Zuazua 1998; Jerison and Lebeau 1999] and also [Le Rousseau and Lebeau 2012]). We denote by μ_j, $j \in \mathbb{N}$, the associated eigenvalues, sorted in an increasing sequence.

Theorem 1.7. *There exists $C > 0$ such that for any $(a_j)_{j\in\mathbb{N}} \subset \mathbb{C}$, we have*

$$\Big(\sum_{\mu_j\le\mu} |a_j|^2\Big)^{1/2} = \Big\|\sum_{\mu_j\le\mu} a_j\phi_j\Big\|_{L^2(\Omega)} \le Ce^{C\sqrt{\mu}}\Big\|\sum_{\mu_j\le\mu} a_j\phi_j\Big\|_{L^2(\omega)}, \quad \mu > 0. \tag{1-14}$$

In turn, this yields the following null-controllability result for the associated anisotropic parabolic equation with jumps in the coefficients across Σ (see [Lebeau and Robbiano 1995; Lebeau and Zuazua 1998; Le Rousseau and Robbiano 2010] and also [Le Rousseau and Lebeau 2012]).

Theorem 1.8. *For an arbitrary time $T > 0$, an arbitrary nonempty open subset $\omega \subset \Omega$, and an initial condition $y_0 \in L^2(\Omega)$, there exists $v \in L^2((0, T) \times \Omega)$ such that the solution y of*

$$\begin{cases} \partial_t y + \mathcal{L}y = 1_\omega u & \text{in } (0,T)\times\Omega, \\ y(t,x) = 0 & \text{on } (0,T)\times\partial\Omega, \\ y(0,x) = y_0(x) & \text{in } \Omega \end{cases} \tag{1-15}$$

satisfies $y(T) = 0$ almost everywhere in Ω.

The interpolation inequality of Theorem 1.5 also yields the stabilization of the hyperbolic equation

$$\begin{cases} \partial_{tt} y + \mathcal{L}y + a(x)\partial_t y = 0 & \text{in } (0,T)\times\Omega, \\ y(t,x) = 0 & \text{on } (0,T)\times\partial\Omega, \end{cases} \tag{1-16}$$

where a is a nonvanishing nonnegative smooth function. From [Lebeau 1996; Lebeau and Robbiano 1997], we can obtain a resolvent estimate which in turn yields the following energy decay estimate.

Theorem 1.9 [Burq 1998, Theorem 3]. *For all $k \in \mathbb{N}$, there exists $C > 0$ such that*

$$\|\partial_t y(t)\|_{L^2(\Omega)} + \|y(t)\|_{H^1(\Omega)} \le \frac{C}{[\log(2+t)]^k}\big(\|\partial_t y_{|t=0}\|_{D(\mathcal{L}^{k/2})} + \|y_{|t=0}\|_{D(\mathcal{L}^{(k+1)/2})}\big), \quad t > 0,$$

for y a solution to (1-16).

The same decay can also be obtained in the case of a boundary damping (see [Lebeau and Robbiano 1997]).

Remark 1.10. Exponential decay cannot be achieved if the set $\mathcal{O} = \{a > 0\}$ does not satisfy the geometrical control condition of [Rauch and Taylor 1974; Bardos et al. 1992]. Because of the jump in the matrix coefficient $A(x)$ here, some bicharacteristics of the hyperbolic operators $\partial_{tt} + \mathcal{L}$ can be trapped in Ω_+ or Ω_- and may remain away from the stabilization region $\mathcal{O}$.

1E. ***Sketch of the proof.*** We provide in this subsection an outline of the main arguments used in our proof. To avoid technicalities, we somewhat simplify the geometric data and the weight function, keeping of course the anisotropy. We consider the operator

$$\mathcal{L}_0 = \sum_{1\le j\le n} D_j c_j D_j, \quad c_j(x) = H_+ c_j^+ + H_- c_j^-, \quad c_j^\pm > 0 \text{ constants}, \quad H_\pm = \mathbf{1}_{\{\pm x_n > 0\}}, \tag{1-17}$$

with $D_j = \dfrac{\partial}{i\,\partial x_j}$, and the vector space $\mathcal{W}_0$ of functions $H_+w_+ + H_-w_-$, $w_\pm \in \mathscr{C}_c^\infty(\mathbb{R}^n)$, such that

$$\text{at } x_n = 0, \quad w_+ = w_-, \quad c_n^+\partial_n w_+ = c_n^-\partial_n w_- \text{ (transmission conditions across } x_n = 0). \tag{1-18}$$

As a result, for $w \in \mathcal{W}_0$, we have $D_n w = H_+ D_n w_+ + H_- D_n w_-$ and

$$\mathcal{L}_0 w = \sum_j \bigl(H_+ c_j^+ D_j^2 w_+ + H_- c_j^- D_j^2 w_-\bigr). \tag{1-19}$$

We also consider a weight function[5]

$$\varphi = \underbrace{\left(\alpha_+ x_n + \frac{\beta x_n^2}{2}\right)}_{\varphi_+} H_+ + \underbrace{\left(\alpha_- x_n + \frac{\beta x_n^2}{2}\right)}_{\varphi_-} H_-, \quad \alpha_\pm > 0, \quad \beta > 0, \tag{1-20}$$

a positive parameter τ, and the vector space $\mathcal{W}_\tau$ of functions $H_+v_+ + H_-v_-$, $v_\pm \in \mathscr{C}_c^\infty(\mathbb{R}^n)$, such that at $x_n = 0$,

$$v_+ = v_-, \tag{1-21}$$

$$c_n^+(D_n v_+ + i\tau\alpha_+ v_+) = c_n^-(D_n v_- + i\tau\alpha_- v_-). \tag{1-22}$$

Observe that $w \in \mathcal{W}_0$ is equivalent to $v = e^{\tau\varphi} w \in W_\tau$. We have

$$e^{\tau\varphi}\mathcal{L}_0 w = \underbrace{e^{\tau\varphi}\mathcal{L}_0 e^{-\tau\varphi}}_{\mathcal{L}_\tau}(e^{\tau\varphi} w),$$

so that proving a weighted a priori estimate $\|e^{\tau\varphi}\mathcal{L}_0 w\|_{L^2(\mathbb{R}^n)} \gtrsim \|e^{\tau\varphi} w\|_{L^2(\mathbb{R}^n)}$ for $w \in \mathcal{W}_0$ amounts to getting $\|\mathcal{L}_\tau v\|_{L^2(\mathbb{R}^n)} \gtrsim \|v\|_{L^2(\mathbb{R}^n)}$ for $v \in \mathcal{W}_\tau$.

Step 1 (pseudodifferential factorization). We have, using the Einstein convention on repeated indices $j \in \{1, \dots, n-1\}$,

$$\mathcal{L}_\tau = (D_n + i\tau\varphi')c_n(D_n + i\tau\varphi') + D_j c_j D_j,$$

and for $v \in \mathcal{W}_\tau$, by (1-19), with $m_\pm = m_\pm(D') = (c_n^\pm)^{-1/2}(c_j^\pm D_j^2)^{1/2}$,

$$\mathcal{L}_\tau v = H_+ c_n^+\bigl((D_n + i\tau\varphi_+')^2 + m_+^2\bigr)v_+ + H_- c_n^-\bigl((D_n + i\tau\varphi_-')^2 + m_-^2\bigr)v_-,$$

[5] In the main text, we shall introduce some minimal requirements on the weight function and suggest other possible choices.

so that

$$\mathcal{L}_\tau v = H_+ c_n^+ \big(D_n + i\,(\overbrace{\tau\varphi'_+ + m_+}^{e_+})\big)\big(D_n + i\,(\overbrace{\tau\varphi'_+ - m_+}^{f_+})\big)v_+ \\ + H_- c_n^- \big(D_n + i\,(\underbrace{\tau\varphi'_- - m_-}_{f_-})\big)\big(D_n + i\,(\underbrace{\tau\varphi'_- + m_-}_{e_-})\big)v_-. \tag{1-23}$$

Note that $e_\pm$ are elliptic positive in the sense that $e_\pm = \tau\alpha_\pm + m_\pm \gtrsim \tau + |D'|$. At this point, we want to use certain natural estimates for first-order factors on the half-lines $\mathbb{R}_\pm$. Let us, for instance, check on $t > 0$ for $\omega \in \mathscr{C}_c^\infty(\mathbb{R})$, λ, γ positive:

$$\begin{aligned} &\big\|D_t\omega + i(\lambda+\gamma t)\omega\big\|^2_{L^2(\mathbb{R}_+)} \\ &\qquad = \|D_t\omega\|^2_{L^2(\mathbb{R}_+)} + \|(\lambda+\gamma t)\omega\|^2_{L^2(\mathbb{R}_+)} + 2\operatorname{Re}\big\langle D_t\omega, iH(t)(\lambda+\gamma t)\omega\big\rangle \\ &\qquad \geq \int_0^{+\infty} \big((\lambda+\gamma t)^2 + \gamma\big)|\omega(t)|^2\,dt + \lambda|\omega(0)|^2 \geq (\lambda^2+\gamma)\|\omega\|^2_{L^2(\mathbb{R}_+)} + \lambda|\omega(0)|^2, \end{aligned} \tag{1-24}$$

which is in a sense a perfect estimate of elliptic type, suggesting that the first-order factor containing e_+ should be easy to handle. Changing λ in $-\lambda$ gives

$$\big\|D_t\omega + i(-\lambda+\gamma t)\omega\big\|^2_{L^2(\mathbb{R}_+)} \geq 2\operatorname{Re}\big\langle D_t\omega, iH(t)(-\lambda+\gamma t)\omega\big\rangle = \int_0^{+\infty} \gamma|\omega(t)|^2\,dt - \lambda|\omega(0)|^2,$$

so that $\|D_t\omega + i(-\lambda+\gamma t)\omega\|^2_{L^2(\mathbb{R}_+)} + \lambda|\omega(0)|^2 \geq \gamma\|\omega\|^2_{L^2(\mathbb{R}_+)}$, an estimate of lesser quality, because we need to secure a control of $\omega(0)$ to handle this type of factor.

Step 2 (case $f_+ \geq 0$). Looking at formula (1-23), since the factor containing e_+ is elliptic in the sense given above, we have to discuss the sign of f_+. Identifying the operator with its symbol, we have $f_+ = \tau(\alpha_+ + \beta x_n) - m_+(\xi')$, and thus $\tau\alpha_+ \geq m_+(\xi')$, yielding a nonnegative f_+. Iterating the method outlined above on the half-line $\mathbb{R}_+$, we get a nice estimate of the form of (1-24) on $\mathbb{R}_+$; in particular, we obtain a control[6] of $v_+(0)$ and $D_n v_+(0)$. From the transmission condition, we have $v_+(0) = v_-(0)$, and hence this amounts to also controlling $v_-(0)$. That control, along with the natural estimates on $\mathbb{R}_-$, is enough to prove an inequality of the form of the Carleman estimate we seek.

Step 3 (case $f_+ < 0$). Here we assume that $\tau\alpha_+ < m_+(\xi')$. On $\mathbb{R}_+$ we can still use the factor containing e_+, and by (1-23) and (1-24) we can control the quantity

$$c_n^+(D_n + if_+)v_+(0) = \overbrace{c_n^+(D_n v_+ + i\tau\alpha_+)v_+(0)}^{=\mathcal{V}_+} - c_n^+ i m_+ v_+(0). \tag{1-25}$$

[6]In the case $f_+(0) = 0$, one needs to consider the estimation of

$$\big\|(D_n + ie_+)(D_n + if_+)v_+\big\|_{L^2(\mathbb{R}^+)} + \big\|(D_n + if_+)(D_n + ie_+)v_+\big\|_{L^2(\mathbb{R}^+)}$$

from below to obtain a control of $v_+(0)$ and $D_n v_+(0)$ with the previous estimates used in cascade. Indeed, the first term will give an estimate of $D_n v_+(0)$, and the second term one of $v_+(0)$.

Our key assumption is

$$f_+(0) < 0 \implies f_-(0) \leq 0. \tag{1-26}$$

Under that hypothesis, we can use the negative factor f_- on $\mathbb{R}_-$ (note that f_- is increasing with x_n, so that $f_-(0) \leq 0 \implies f_-(x_n) < 0$ for $x_n < 0$). We then control

$$c_n^-(D_n + ie_-)v_-(0) = \underbrace{c_n^-(D_n v_- + i\tau\alpha_-)v_-(0)}_{=\mathcal{V}_-} + c_n^- i m_- v_-(0). \tag{1-27}$$

Nothing more can be achieved with inequalities on each side of the interface. At this point, however, we notice that the second transmission condition in (1-22) implies $\mathcal{V}_- = \mathcal{V}_+$, yielding the control of the difference of (1-27) and (1-25), that is, of

$$c_n^- i m_- v_-(0) + c_n^+ i m_+ v_+(0) = i\big(c_n^- m_- + c_n^+ m_+\big)v(0).$$

Now, as $c_n^- m_- + c_n^+ m_+$ is elliptic positive, this gives a control of $v(0)$ in (tangential) H^1-norm, which is enough to then get an estimate on both sides that leads to the Carleman estimates we seek.

Step 4 (patching estimates together). The analysis we have sketched here relies on a separation into two zones in the (τ, ξ') space. Patching the estimates of the form of (1-13) in each zone together allows us to conclude the proof of the Carleman estimate.

1F. *Explaining the key assumption.* Our key assumption, condition (1-26), can be reformulated as

$$\text{for all } \xi' \in \mathbb{S}^{n-2}, \quad \frac{\alpha_+}{\alpha_-} \geq \frac{m_+(\xi')}{m_-(\xi')}. \tag{1-28}$$

In fact,[7] (1-26) means $\tau\alpha_+ < m_+(\xi') \implies \tau\alpha_- \leq m_-(\xi')$, and since $\alpha_\pm, m_\pm$ are all positive, this is equivalent to having $m_+(\xi')/\alpha_+ \leq m_-(\xi')/\alpha_-$, which is (1-28). An analogy with an estimate for a first-order factor may shed some light on this condition. With

$$f(t) = H(t)(\tau\alpha_+ + \beta t - m_+) + H(-t)(\tau\alpha_- + \beta t - m_-), \quad \tau, \alpha_\pm, \beta, m_\pm \text{ positive constants,}$$

we want to prove an injectivity estimate of the type $\|D_t v + if(t)v\|_{L^2(\mathbb{R})} \gtrsim \|v\|_{L^2(\mathbb{R})}$, say for $v \in \mathscr{C}_c^\infty(\mathbb{R})$. It is a classical fact (see, for example, Lemma 3.1.1 in [Lerner 2010]) that such an estimate (for a smooth f) is equivalent to the condition that $t \mapsto f(t)$ does not change sign from $+$ to $-$ while t increases: it means that the adjoint operator $D_t - if(t)$ satisfies the so-called condition (Ψ). Looking at the function f, we see that it increases on each half-line $\mathbb{R}_\pm$, so that the only place to get a "forbidden" change of sign from

[7] For the main theorem, we shall in fact require the stronger strict inequality

$$\frac{\alpha_+}{\alpha_-} > \frac{m_+(\xi')}{m_-(\xi')}. \tag{1-29}$$

This condition is then stable under perturbations, whereas (1-28) is not. This gives us the freedom to introduce microlocal cutoff in the analysis below.

However, we shall see in Section 5 that in the particular case presented here, where the matrix A is piecewise constant and the weight function φ depends solely on x_n, the inequality (1-28) is actually a *necessary and sufficient* condition to obtain a Carleman estimate with weight φ.

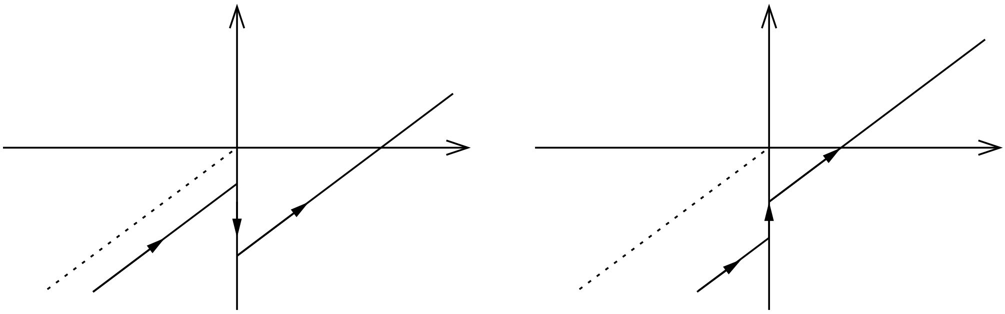

Figure 1. $f(0^-) \le 0$; $f(0^+) < 0$.

$+$ to $-$ is at $t = 0$: to get an injectivity estimate, we have to avoid the situation where $f(0^+) < 0$ and $f(0^-) > 0$, that is, we have to make sure that $f(0^+) < 0 \implies f(0^-) \le 0$, which is indeed the condition (1-28). The function f is increasing affine on $\mathbb{R}_\pm$ with the same slope β on both sides, with a possible discontinuity at 0; see Figure 1.

In Figure 1, when $f(0^+) < 0$, we should have $f(0^-) \le 0$, and the line on the left cannot go above the dotted line, in such a way that the discontinuous zigzag curve with the arrows has only a change of sign from $-$ to $+$.

When $f(0^+) \ge 0$, there is no other constraint on $f(0^-)$: even with a discontinuity, the change of sign can only occur from $-$ to $+$; see Figure 2.

We prove below (Section 5) that condition (1-28) is relevant to our problem in the sense that it is indeed necessary to have a Carleman estimate with this weight: if (1-28) is violated, we are able, for this model, to construct a quasimode for $\mathcal{L}_\tau$, that is, a τ-family of functions v with L^2-norm 1 such that $\|\mathcal{L}_\tau v\|_{L^2} \ll \|v\|_{L^2}$, as τ goes to ∞, ruining any hope of proving a Carleman estimate. As usual for this type of construction, it uses a certain complex geometrical optics method, which is easy in this case to implement directly, due to the simplicity of the expression of the operator.

Remark 1.11. A very particular case of anisotropic medium was tackled in [Le Rousseau and Robbiano 2010] for the purpose of proving a controllability result for linear parabolic equations. The condition

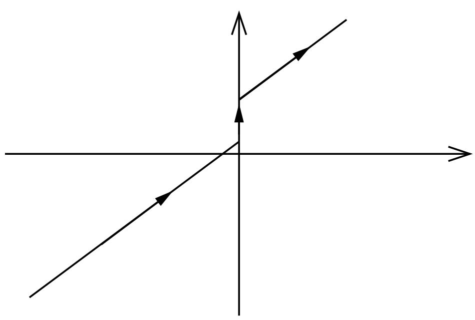

Figure 2. $f(0^-) \gtrless 0$; $f(0^+) \ge 0$.

imposed on the weight function in [Le Rousseau and Robbiano 2010, Assumption 2.1] is much more demanding than what we impose here. In the isotropic case, $c_j^{\pm} = c_{\pm}$ for all $j \in \{1, \dots, n\}$, we have $m_+ = m_- = |\xi'|$ and our condition (1-29) reads $\alpha_+ > \alpha_-$. Note also that the isotropic case $c_- \geq c_+$ was already considered in [Doubova et al. 2002].

In [Le Rousseau and Robbiano 2010], the controllability result concerns an isotropic parabolic equation. The Carleman estimate we derive here extends this result to an anisotropic parabolic equation.

2. Framework

2A. ***Presentation.*** Let Ω, Σ be as in (1-3). With

$$\Xi = \{\text{positive-definite } n \times n \text{ matrices}\},$$

we consider $A_\pm \in \mathscr{C}^\infty(\Omega; \Xi)$ and let $\mathcal{L}, \varphi$ be as in (1-5) and (1-12). We set

$$\mathcal{L}_\pm = D \cdot A_\pm D = -\operatorname{div}(A_\pm \nabla).$$

Here, we generalize our analysis to nonhomogeneous transmission conditions: for θ and Θ smooth functions of the interface Σ, we set

$$w_+ - w_- = \theta \quad \text{and} \quad \langle A_+ dw_+ - A_- dw_-, \nu \rangle = \Theta \quad \text{at } \Sigma \tag{2-1}$$

(compare with (1-8)-(1-9)) and introduce

$$\mathcal{W}_0^{\theta,\Theta} = \{H_- w_- + H_+ w_+\}_{w_\pm \in \mathscr{C}_c^\infty(\Omega)}, \qquad w_\pm \text{ satisfying (2-1)}. \tag{2-2}$$

For $\tau \geq 0$, we define the affine space

$$\mathcal{W}_\tau^{\theta,\Theta} = \{e^{\tau\varphi} w\}_{w \in \mathcal{W}_0^{\theta,\Theta}}. \tag{2-3}$$

For $v \in \mathcal{W}_\tau^{\theta,\Theta}$, we have $v = e^{\tau\varphi} w$ with $w \in \mathcal{W}_0^{\theta,\Theta}$, so that using the notation introduced in (1-4), (1-7), with $v_\pm = e^{\tau\varphi_\pm} w_\pm$, we have

$$v = H_- v_- + H_+ v_+, \tag{2-4}$$

and we see that the transmission conditions (2-1) on w read for v as

$$v_+ - v_- = \theta_\varphi, \quad \big\langle dv_+ - \tau v_+ d\varphi_+, A_+ \nu \big\rangle - \big\langle dv_- - \tau v_- d\varphi_-, A_- \nu \big\rangle = \Theta_\varphi \quad \text{at } \Sigma, \tag{2-5}$$

with

$$\theta_\varphi = e^{\tau\varphi_{|\Sigma}} \theta, \qquad \Theta_\varphi = e^{\tau\varphi_{|\Sigma}} \Theta. \tag{2-6}$$

Observing that $e^{\tau\varphi_\pm} D e^{-\tau\varphi_\pm} = D + i\tau d\varphi_\pm$ for $w \in \mathcal{W}^{\theta,\Theta}$, we obtain

$$e^{\tau\varphi_\pm} \mathcal{L}_\pm w_\pm = e^{\tau\varphi_\pm} D \cdot A_\pm D e^{-\tau\varphi_\pm} v_\pm = (D + i\tau d\varphi_\pm) \cdot A_\pm (D + i\tau d\varphi_\pm) v_\pm.$$

We define

$$\mathcal{P}_\pm = (D + i\tau d\varphi_\pm) \cdot A_\pm (D + i\tau d\varphi_\pm). \tag{2-7}$$

Proposition 2.1. *Let Ω, Σ, $\mathcal{L}$, $\mathcal{W}_\tau^{\theta,\Theta}$ be as in (1-3), (1-5), and (2-3). Then for any compact subset K of Ω, there exist a weight function φ satisfying (1-12) and positive constants C, τ_1 such that for all $\tau \geq \tau_1$ and all $v \in \mathcal{W}_\tau$ with* supp $v \subset K$,

$$C\big(\|H_-\mathcal{P}_-v_-\|_{L^2(\mathbb{R}^n)} + \|H_+\mathcal{P}_+v_+\|_{L^2(\mathbb{R}^n)} + \mathcal{T}_{\theta,\Theta}\big)$$
$$\geq \tau^{3/2}|v_\pm|_{L^2(\Sigma)} + \tau^{1/2}|(\nabla v_\pm)|_{L^2(\Sigma)} + \tau^{3/2}\|v\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\|H_+\nabla v_+\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\|H_-\nabla v_-\|_{L^2(\mathbb{R}^n)},$$

where $\mathcal{T}_{\theta,\Theta} = \tau^{3/2}|\theta_\varphi|_{L^2(\Sigma)} + \tau^{1/2}|\nabla_\Sigma\theta_\varphi|_{L^2(\Sigma)} + \tau^{1/2}|\Theta_\varphi|_{L^2(\Sigma)}$.

Here, ∇_Σ denotes the tangential gradient to Σ. The proof of this proposition will occupy a large part of the remainder of the article (Sections 3 and 4), as it implies the result of the following theorem, a nonhomogeneous version of Theorem 1.1.

Theorem 2.2. *Let Ω, Σ, $\mathcal{L}$, $\mathcal{W}_0^{\theta,\Theta}$ be as in (1-3), (1-5), and (2-2). Then for any compact subset K of Ω, there exist a weight function φ satisfying (1-12) and positive constants C, τ_1 such that for all $\tau \geq \tau_1$ and all $w \in \mathcal{W}$ with* supp $w \subset K$,

$$\begin{aligned} C\Big(\big\|H_-e^{\tau\varphi_-}\mathcal{L}_-w_-\big\|_{L^2(\mathbb{R}^n)} + \big\|H_+e^{\tau\varphi_+}\mathcal{L}_+w_+\big\|_{L^2(\mathbb{R}^n)} + T_{\theta,\Theta}\Big) \\ \geq \tau^{3/2}\|e^{\tau\varphi}w\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\Big(\big\|H_+e^{\tau\varphi}\nabla w_+\big\|_{L^2(\mathbb{R}^n)} + \big\|H_-e^{\tau\varphi}\nabla w_-\big\|_{L^2(\mathbb{R}^n)}\Big) \\ + \tau^{3/2}|e^{\tau\varphi}w_\pm|_{L^2(\Sigma)} + \tau^{1/2}|e^{\tau\varphi}\nabla w_\pm|_{L^2(\Sigma)}, \end{aligned} \tag{2-8}$$

where $T_{\theta,\Theta} = \tau^{3/2}|e^{\tau\varphi_{|\Sigma}}\theta|_{L^2(\Sigma)} + \tau^{1/2}|e^{\tau\varphi_{|\Sigma}}\nabla_\Sigma\theta|_{L^2(\Sigma)} + \tau^{1/2}|e^{\tau\varphi_{|\Sigma}}\Theta|_{L^2(\Sigma)}$.

Theorem 1.1 corresponds to the case $\theta = \Theta = 0$, since by (1-10), we then have

$$\|e^{\tau\varphi}\mathcal{L}w\|_{L^2(\mathbb{R}^n)} = \big\|H_-e^{\tau\varphi_-}\mathcal{L}_-w_-\big\|_{L^2(\mathbb{R}^n)} + \big\|H_+e^{\tau\varphi_+}\mathcal{L}_+w_+\big\|_{L^2(\mathbb{R}^n)}.$$

Remark 2.3. It is often useful to have such a Carleman estimate at hand for the case of nonhomogeneous transmission conditions, for example when one tries to patch such local estimates together in the neighborhood of the interface.

Here we derive local Carleman estimates. We can in fact consider a similar geometrical situation on a Riemannian manifold (with or without boundary) with a metric exhibiting jump discontinuities across interfaces. For the associated Laplace–Beltrami operator, the local estimates we derive can be patched together to yield a global estimate. We refer to [Le Rousseau and Robbiano 2011, Section 5] for such questions.

Proof that Proposition 2.1 implies Theorem 2.2. Replacing v by $e^{\tau\varphi}w$, we get

$$\begin{aligned} \|H_-e^{\tau\varphi_-}\mathcal{L}_-w_-\|_{L^2(\mathbb{R}^n)} + \|H_+e^{\tau\varphi_+}\mathcal{L}_+w_+\|_{L^2(\mathbb{R}^n)} + T_{\theta,\Theta} \\ \gtrsim \tau^{3/2}\|e^{\tau\varphi}w\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\big(\|H_+\nabla e^{\tau\varphi}w_+\|_{L^2(\mathbb{R}^n)} + \|H_-\nabla e^{\tau\varphi}w_-\|_{L^2(\mathbb{R}^n)}\big) \\ + \tau^{3/2}|e^{\tau\varphi}w_\pm|_{L^2(\Sigma)} + \tau^{1/2}|\nabla e^{\tau\varphi}w_\pm|_{L^2(\Sigma)}. \end{aligned} \tag{2-9}$$

Commuting ∇ with $e^{\tau\varphi}$ produces

$$\begin{aligned} C\big(\big\| H_- e^{\tau\varphi_-}\mathcal{L}_- w_-\big\|_{L^2(\mathbb{R}^n)} + \big\| H_+ e^{\tau\varphi_+}\mathcal{L}_+ w_+\big\|_{L^2(\mathbb{R}^n)} + T_{\theta,\Theta}\big) \\ + C_1\tau^{3/2}\|e^{\tau\varphi} w\|_{L^2(\mathbb{R}^n)} + C_2\tau^{3/2}\big(|e^{\tau\varphi} w_{\pm|\Sigma}|_{L^2(\Sigma)}\big) \\ \geq \tau^{1/2}\big\| H_- e^{\tau\varphi} D w_-\big\|_{L^2(\mathbb{R}^n)} + \tau^{1/2}\big\| H_+ e^{\tau\varphi} D w_+\big\|_{L^2(\mathbb{R}^n)} + \tau^{3/2}\|e^{\tau\varphi} w\|_{L^2(\mathbb{R}^n)} \\ + \tau^{1/2}|e^{\tau\varphi} D w_\pm|_{L^2(\Sigma)} + \tau^{3/2}|e^{\tau\varphi} w_\pm|_{L^2(\Sigma)}, \end{aligned}$$

but by (2-9), we have

$$\begin{aligned} C_1\tau^{3/2}\|e^{\tau\varphi} w\| + C_2\tau^{3/2}|e^{\tau\varphi} w| \\ \leq C\max(C_1, C_2)\big(\big\| H_- e^{\tau\varphi_-}\mathcal{L}_- w_-\big\|_{L^2(\mathbb{R}^n)} + \big\| H_+ e^{\tau\varphi_+}\mathcal{L}_+ w_+\big\|_{L^2(\mathbb{R}^n)} + T_{\theta,\Theta}\big), \end{aligned}$$

proving the implication. □

2B. ***Description in local coordinates.*** Carleman estimates of types (1-13) and (2-8) can be handled locally, as they can be patched together. Assuming, as we may, that the hypersurface Σ is given locally by the equation $\{x_n = 0\}$, we have, using the Einstein convention on repeated indices $j \in \{1, \dots, n-1\}$, and noting from the ellipticity condition that $a_{nn} > 0$ (the matrix $A(x) = (a_{jk}(x))_{1\leq j,k\leq n}$),

$$\begin{aligned} \mathcal{L} &= D_n a_{nn} D_n + D_n a_{nj} D_j + D_j a_{jn} D_n + D_j a_{jk} D_k \\ &= D_n a_{nn}\big(D_n + a_{nn}^{-1} a_{nj} D_j\big) + D_j a_{jn} D_n + D_j a_{jk} D_k. \end{aligned}$$

With $T = a_{nn}^{-1} a_{nj} D_j$, we have

$$\mathcal{L} = (D_n + T^*) a_{nn} (D_n + T) - T^* a_{nn} D_n - T^* a_{nn} T + D_j a_{jn} D_n + D_j a_{jk} D_k;$$

and since $T^* = D_j a_{nn}^{-1} a_{nj}$, we have $T^* a_{nn} D_n = D_j a_{nj} D_n = D_j a_{jn} D_n$ and

$$\mathcal{L} = (D_n + T^*) a_{nn} (D_n + T) + D_j b_{jk} D_k, \tag{2-10}$$

where the $(n-1)\times(n-1)$ matrix (b_{jk}) is positive-definite, since with $\xi' = (\xi_1, \dots, \xi_{n-1})$ and $\xi = (\xi', \xi_n)$,

$$\langle B\xi', \xi'\rangle = \sum_{1\leq j,k\leq n-1} b_{jk}\xi_j\xi_k = \langle A\xi, \xi\rangle,$$

where $a_{nn}\xi_n = -\sum_{1\leq j\leq n-1} a_{nj}\xi_j$. Note also that $b_{jk} = a_{jk} - (a_{nj}a_{nk}/a_{nn})$.

Remark 2.4. The positive-definite quadratic form B is the restriction of $\langle A\xi, \xi\rangle$ to the hyperplane $\mathcal{H}$ defined by $\{\langle A\xi, \xi\rangle, x_n\} = \partial_{\xi_n}\big(\langle A\xi, \xi\rangle\big) = 0$, where $\{\cdot, \cdot\}$ stands for the Poisson bracket. In fact, the principal symbol of $\mathcal{L}$ is $\langle A(x)\xi, \xi\rangle$, and if Σ is defined by the equation $\psi(x) = 0$ with $d\psi \neq 0$ at Σ, we have

$$\tfrac{1}{2}\big\{\langle A(x)\xi, \xi\rangle, \psi\big\} = \langle A(x)\xi, d\psi(x)\rangle,$$

so that $\mathcal{H}_x = (A(x)d\psi(x))^\perp = \big\{\xi \in T_x^*(\Omega), \langle \xi, A(x)d\psi(x)\rangle_{T_x^*(\Omega), T_x(\Omega)} = 0\big\}$. When $x \in \Sigma$, that set does not depend on the choice of the defining function ψ of Σ, and we simply have

$$\mathcal{H}_x = (A(x)\nu(x))^\perp = \big\{\xi \in T_x^*(\Omega), \langle \xi, A(x)\nu(x)\rangle_{T_x^*(\Omega), T_x(\Omega)} = 0\big\},$$

where $\nu(x)$ is the conormal vector to Σ at x (recall that from Remark 1.4, $\nu(x)$ is a cotangent vector at x, and $A(x)\nu(x)$ is a tangent vector at x). Now, for $x \in \Sigma$, we can restrict the quadratic form $A(x)$ to $\mathcal{H}_x$: this is the positive-definite quadratic form $B(x)$, providing a coordinate-free definition.

For $w \in \mathcal{W}_0^{\theta,\Theta}$, we have

$$\mathcal{L}_\pm w_\pm = (D_n + T_\pm^*) a_{nn}^\pm (D_n + T_\pm) w_\pm + D_j b_{jk}^\pm D_k w_\pm, \tag{2-11}$$

and the nonhomogeneous transmission conditions (2-1) read

$$w_+ - w_- = \theta, \quad a_{nn}^+ (D_n + T_+) w_+ - a_{nn}^- (D_n + T_-) w_- = \Theta \quad \text{at } \Sigma. \tag{2-12}$$

2C. *Pseudodifferential factorization on each side.* At first, we consider the weight function $\varphi = H_+\varphi_+ + H_-\varphi_-$, with $\varphi_\pm$ that solely depend on x_n. Later on, we shall allow for some dependency upon the tangential variables x' (see Section 4E). We define, for $m \in \mathbb{R}$, the class of tangential standard symbols $\mathcal{S}^m$ as the smooth functions on $\mathbb{R}^n \times \mathbb{R}^{n-1}$ such that for all $(\alpha, \beta) \in \mathbb{N}^n \times \mathbb{N}^{n-1}$,

$$\sup_{(x,\xi')\in\mathbb{R}^n\times\mathbb{R}^{n-1}} \langle \xi' \rangle^{-m+|\beta|} \left| \left(\partial_x^\alpha \partial_{\xi'}^\beta a \right)(x, \xi') \right| < \infty, \tag{2-13}$$

with $\langle \xi' \rangle = (1 + |\xi'|^2)^{1/2}$. Some basic properties of standard pseudodifferential operators are recalled in Section AA. Section 2B and formulae (2-7), (2-11) give

$$\mathcal{P}_\pm = \left(D_n + i\tau\varphi'_\pm + T_\pm^* \right) a_{nn}^\pm \left(D_n + i\tau\varphi'_\pm + T_\pm \right) + D_j b_{jk}^\pm D_k. \tag{2-14}$$

We define $m_\pm \in \mathcal{S}^1$ such that

$$\text{for } |\xi'| \geq 1, \quad m_\pm = \left(\frac{b_{jk}^\pm}{a_{nn}^\pm} \xi_j \xi_k \right)^{1/2}, \quad m_\pm \geq C \langle \xi' \rangle, \quad M_\pm = \mathrm{op}^w(m_\pm). \tag{2-15}$$

We then have $M_\pm^2 \equiv D_j b_{jk}^\pm D_k \mod \mathrm{op}(\mathcal{S}^1)$.

We define

$$\Psi^1 = \mathrm{op}(\mathcal{S}^1) + \tau \mathrm{op}(\mathcal{S}^0) + \mathrm{op}(\mathcal{S}^0) D_n. \tag{2-16}$$

Modulo the operator class Ψ^1, we may write

$$\mathcal{P}_+ \equiv \mathcal{P}_{E+} a_{nn}^+ \mathcal{P}_{F+}, \quad \mathcal{P}_- \equiv \mathcal{P}_{F-} a_{nn}^- \mathcal{P}_{E-}, \tag{2-17}$$

where

$$\mathcal{P}_{E\pm} = D_n + S_\pm + i\underbrace{(\tau\varphi'_\pm + M_\pm)}_{E_\pm}, \quad \mathcal{P}_{F\pm} = D_n + S_\pm + i\underbrace{(\tau\varphi'_\pm - M_\pm)}_{F_\pm}, \tag{2-18}$$

with

$$S_\pm = s^w(x, D'), \quad s_\pm = \sum_{1\leq j\leq n-1} \frac{a_{nj}^\pm}{a_{nn}^\pm} \xi_j, \quad \text{so that } S_\pm^* = S_\pm, \quad S_\pm = T_\pm + \tfrac{1}{2} \operatorname{div} T_\pm, \tag{2-19}$$

where

$$T_\pm \text{ is the vector field } \sum_{1\le j\le n-1} \frac{a^\pm_{nj}}{i a^\pm_{nn}} \partial_j. \tag{2-20}$$

We denote by $f_\pm$ and $e_\pm$ the homogeneous principal symbols of $F_\pm$ and $E_\pm$, respectively, determined modulo the symbol class $\mathcal{S}^1 + \tau\mathcal{S}^0$. The transmission conditions (2-12) with our choice of coordinates read, at $x_n = 0$,

$$\begin{cases} v_+ - v_- = \theta_\varphi = e^{\tau\varphi_{|x_n=0}}\theta, \\ a^+_{nn}(D_n + T_+ + i\tau\varphi'_+)v_+ - a^-_{nn}(D_n + T_- + i\tau\varphi'_-)v_- = \Theta_\varphi = e^{\tau\varphi_{|x_n=0}}\Theta. \end{cases} \tag{2-21}$$

Remark 2.5. The Carleman estimate we shall prove is insensitive to terms in Ψ^1 in the conjugated operator $\mathcal{P}$. Formulae (2-17) and (2-18) for $\mathcal{P}_+$ and $\mathcal{P}_-$ will thus be the base of our analysis.

Remark 2.6. In [Le Rousseau and Robbiano 2010; 2011], the zero crossing of the roots of the symbol of $\mathcal{P}_\pm$, as seen as a polynomial in ξ_n, is analyzed. Here the factorization into first-order operators isolates each root. In fact, $f_\pm$ changes sign, and we shall impose a condition on the weight function at the interface to obtain a certain scheme for this change of sign; see Section 4.

2D. *Choice of weight function.* The weight function can be taken of the form

$$\varphi_\pm(x_n) = \alpha_\pm x_n + \frac{\beta x_n^2}{2}, \quad \alpha_\pm > 0, \quad \beta > 0. \tag{2-22}$$

The choice of the parameters $\alpha_\pm$ and β will be done below and will take into account the geometric data of our problem: $\alpha_\pm$ will be chosen to fulfill a geometric condition at the interface, and $\beta > 0$ will be chosen large. Here, we shall require $\varphi' \ge 0$, that is, we choose an "observation" region on the right-hand side of Σ. As we shall need β large, this amounts to working in a small neighborhood of the interface, that is, $|x_n|$ small. Also, we shall see below (Section 4E) that this weight can be perturbed by any smooth function with a small gradient.

Other choices for the weight functions are possible. In fact, two sufficient conditions can be put forward. We shall describe them now.

The operators $M_\pm$ have a principal symbol $m_\pm(x,\xi')$ in $\mathcal{S}^1$, which is positively homogeneous[8] of degree 1 and elliptic, that is, there exist $\lambda_0^\pm, \lambda_1^\pm$ positive such that for $|\xi'| \ge 1, x \in \mathbb{R}^n$,

$$\lambda_0^\pm|\xi'| \le m_\pm(x,\xi') \le \lambda_1^\pm|\xi'|. \tag{2-23}$$

We choose $\varphi'_{|x_n=0^\pm} = \alpha_\pm$ such that

$$\frac{\alpha_+}{\alpha_-} > \sup_{\substack{x',\xi' \\ |\xi'|\ge 1}} \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}}. \tag{2-24}$$

[8]The homogeneity property means, as usual, $m_\pm(x,\rho\xi') = \rho m_\pm(x,\xi')$ for $\rho \ge 1$, $|\xi'| \ge 1$.

The consequence of this condition will be made clear in Section 4. We shall also prove that this condition is sharp in Section 5: a strong violation of this condition, namely, $\alpha_+/\alpha_- < \sup(m_+/m_-)_{|x_n=0}$, ruins any possibility of deriving a Carleman estimate of the form of Theorem 1.1.

Condition (2-24) concerns the behavior of the weight function at the interface. Conditions away from the interface are also needed. These conditions are more classical. From (2-14), the symbols of $\mathcal{P}_\pm$, modulo the symbol class $\mathcal{S}^1 + \tau\mathcal{S}^0 + \mathcal{S}^0\xi_n$, are given by $p_\pm(x,\xi,\tau) = a^\pm_{nn}\big(q_2^\pm + 2iq_1^\pm\big)$, with

$$q_2^\pm = (\xi_n + s_\pm)^2 + \frac{b^\pm_{jk}}{a^\pm_{nn}}\xi_j\xi_k - \tau^2(\varphi'_\pm)^2, \quad q_1^\pm = \tau\varphi'_\pm(\xi_n + s_\pm),$$

for φ solely depending on x_n, and from the construction of $m_\pm$, for $|\xi'| \geq 1$, we have

$$q_2^\pm = (\xi_n + s_\pm)^2 + m_\pm^2 - (\tau\varphi'_\pm)^2 = (\xi_n + s_\pm)^2 - f_\pm e_\pm. \tag{2-25}$$

We can then formulate the usual *subellipticity* condition, with *loss of a half-derivative*:

$$q_2^\pm = 0 \text{ and } q_1^\pm = 0 \implies \{q_2^\pm, q_1^\pm\} > 0, \tag{2-26}$$

which can be achieved by choosing β sufficiently large. It is important to note that this property is coordinate-free. For second-order elliptic operators with real smooth coefficients, this property is necessary and sufficient for a Carleman estimate such as that of Theorem 1.1 to hold (see [Hörmander 1963], or, for example, [Le Rousseau and Lebeau 2012]).

With the weight functions provided in (2-22), we choose $\alpha_\pm$ according to condition (2-24) and $\beta > 0$ large enough, and we restrict ourselves to a small neighborhood of Σ, that is, $|x_n|$ small, to have $\varphi' > 0$ and so that (2-26) is fulfilled.

Remark 2.7. Other "classical" forms for the weight function φ are also possible. For instance, one may use $\varphi(x_n) = e^{\beta\phi(x_n)}$ with the function ϕ depending solely on x_n of the form

$$\phi = H_-\phi_- + H_+\phi_+, \quad \phi_\pm \in \mathscr{C}_c^\infty(\mathbb{R}),$$

such that ϕ is *continuous* and $|\phi'_\pm| \geq C > 0$. In this case, property (2-24) can be fulfilled by properly choosing $\phi'_{|x_n=0^\pm}$, and (2-26) by choosing β sufficiently large.

Property (2-26) concerns the conjugated second-order operator. We show now that this condition concerns, in fact, only one of the first-order terms in the pseudodifferential factorization that we put forward above, namely, $\mathcal{P}_{F\pm}$.

Lemma 2.8. *There exist $C > 0$, $\tau_1 > 1$, and $\delta > 0$ such that for $\tau \geq \tau_1$,*

$$|f_\pm| \leq \delta\lambda \implies C^{-1}\tau \leq |\xi'| \leq C\tau \text{ and } \{\xi_n + s_\pm, f_\pm\} \geq C'\lambda,$$

with $\lambda^2 = \tau^2 + |\xi'|^2$.

See Appendix AB.1 for a proof. This is the form of the subellipticity condition, with loss of a half-derivative, that we shall use. This will be further highlighted by the estimates we derive in Section 3 and by the proof of the main theorem.

3. Estimates for first-order factors

Unless otherwise specified, the notation $\|\cdot\|$ will stand for the $L^2(\mathbb{R}^n)$-norm and $|\cdot|$ for the $L^2(\mathbb{R}^{n-1})$-norm. The $L^2(\mathbb{R}^n)$ and $L^2(\mathbb{R}^{n-1})$ dot-products will be both denoted by $\langle\cdot,\cdot\rangle$.

In this section, we shall use the function space

$$\mathscr{S}_c(\mathbb{R}^n) = \{u \in \mathscr{S}(\mathbb{R}^n) : \operatorname{supp}(u) \subset \mathbb{R}^{n-1} \times (-L, L) \text{ for some } L > 0\}.$$

3A. *Preliminary estimates.* Most of our pseudodifferential arguments concern a calculus with large parameter $\tau \geq 1$: with

$$\lambda^2 = \tau^2 + |\xi'|^2, \tag{3-1}$$

we define for $m \in \mathbb{R}$ the class of tangential symbols $\mathcal{S}^m_\tau$ as the smooth functions on $\mathbb{R}^n \times \mathbb{R}^{n-1}$, depending on the parameter $\tau \geq 1$, such that, for all $(\alpha, \beta) \in \mathbb{N}^n \times \mathbb{N}^{n-1}$,

$$\sup_{(x,\xi')\in\mathbb{R}^n\times\mathbb{R}^{n-1}} \lambda^{-m+|\beta|} \big|(\partial_x^\alpha \partial_{\xi'}^\beta a)(x, \xi', \tau)\big| < \infty. \tag{3-2}$$

Some basic properties of the calculus of the associated pseudodifferential operators are recalled in Section AA.2. We shall refer to this calculus as the semiclassical calculus (with a large parameter). In particular, we introduce the Sobolev norms

$$\|u\|_{\mathcal{H}^s} := \|\Lambda^s u\|_{L^2(\mathbb{R}^{n-1})}, \quad \text{with } \Lambda^s := \operatorname{op}(\lambda^s). \tag{3-3}$$

For $s \geq 0$, note that we have $\|u\|_{\mathcal{H}^s} \sim \tau^s \|u\|_{L^2(\mathbb{R}^{n-1})} + \|\langle D'\rangle^s u\|_{L^2(\mathbb{R}^{n-1})}$. Observe also that we have

$$\|u\|_{\mathcal{H}^s} \leq C\tau^{s-s'} \|u\|_{\mathcal{H}^{s'}}, \quad s \leq s'.$$

In what follows, we shall often refer implicitly to this inequality when invoking a large value for the parameter τ.

The operator $M_\pm$ is of pseudodifferential nature in the standard calculus. Observe, however, that in any region where $\tau \gtrsim |\xi'|$ the symbol, $m_\pm$ does not satisfy the estimates of $\mathcal{S}^1_\tau$. We shall circumvent this technical point by introducing a cut-off procedure.

Let $C_0, C_1 > 0$ be such that $\varphi' \geq C_0$ and

$$(M_\pm u, H^+ u) \leq C_1 \|H^+ u\|^2_{L^2(\mathbb{R}; H^{1/2}(\mathbb{R}^{n-1}))}. \tag{3-4}$$

We choose $\psi \in \mathscr{C}^\infty(\mathbb{R}^+)$ nonnegative such that $\psi = 0$ in $[0, 1]$ and $\psi = 1$ in $[2, +\infty)$. We introduce the Fourier multiplier

$$\psi_\epsilon(\tau, \xi') = \psi\left(\frac{\epsilon\tau}{\langle\xi\rangle}\right) \in \mathcal{S}^0_\tau, \quad \text{with } 0 < \epsilon \leq \epsilon_0, \tag{3-5}$$

such that $\tau \gtrsim \langle\xi'\rangle/\epsilon$ in its support. We choose ϵ_0 sufficiently small that $\operatorname{supp}(\psi_\epsilon)$ is disjoint from a conic neighborhood (for $|\xi'| \geq 1$) of the sets $\{f_\pm = 0\}$ (see Figure 3).

The following lemma states that we can obtain very natural estimates on both sides of the interface in the region $|\xi'| \ll \tau$, that is, for ϵ small. We refer to Section AB.2 for a proof.

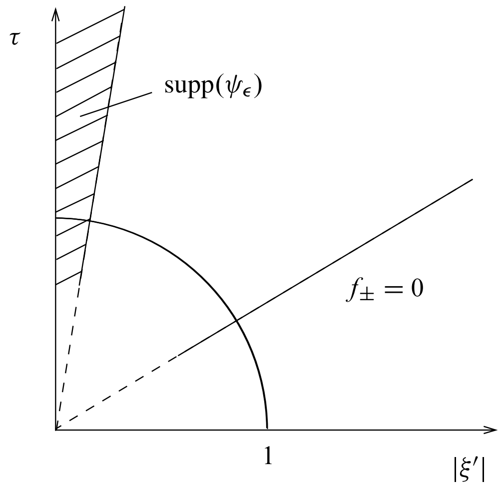

Figure 3. Relative positions of $\operatorname{supp}(\psi_\epsilon)$ and the sets $\{f_\pm = 0\}$.

Lemma 3.1. *Let $\ell \in \mathbb{R}$. There exist $\tau_1 \geq 1$ and $0 < \epsilon_1 \leq \epsilon_0$ and $C > 0$ such that*

$$C\big\| H_+\mathcal{A}_+\operatorname{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \geq \big|\operatorname{op}(\psi_\epsilon)\omega_{|x_n=0^+}\big|_{\mathcal{H}^{\ell+1/2}} + \big\| H_+\operatorname{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})},$$
$$C\big(\big\| H_-\mathcal{A}_-\operatorname{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \big|\operatorname{op}(\psi_\epsilon)\omega_{|x_n=0^-}\big|_{\mathcal{H}^{\ell+1/2}}\big) \geq \big\| H_-\operatorname{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}$$

for $0 < \epsilon \leq \epsilon_1$, with $A_+ = \mathcal{P}_{E+}$ or $\mathcal{P}_{F+}$, $\mathcal{A}_- = \mathcal{P}_{E-}$ or $\mathcal{P}_{F-}$, for $\tau \geq \tau_1$ and $\omega \in \mathscr{S}_c(\mathbb{R}^n)$.

3B. *Positive imaginary part on a half-line.* We have the following estimates for the operators $\mathcal{P}_{E+}$ and $\mathcal{P}_{E-}$.

Lemma 3.2. *Let $\ell \in \mathbb{R}$. There exist $\tau_1 \geq 1$ and $C > 0$ such that*

$$C\| H_+\mathcal{P}_{E_+}\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \geq |\omega_{|x_n=0^+}|_{\mathcal{H}^{\ell+1/2}} + \|H_+\omega\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})} + \|H_+D_n\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \tag{3-6}$$

and

$$C\big(\|H_-\mathcal{P}_{E_-}\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + |\omega_{|x_n=0^-}|_{\mathcal{H}^{\ell+1/2}}\big) \geq \|H_-\omega\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})} + \|H_+D_n\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \tag{3-7}$$

for $\tau \geq \tau_1$ and $\omega \in \mathscr{S}_c(\mathbb{R}^n)$.

The first estimate, in $\mathbb{R}_+$, is of very good quality, as both the trace and the volume norms are dominated: we have a perfect elliptic estimate. In $\mathbb{R}_-$, we obtain an estimate of lesser quality. Observe also that no assumption on the weight function, apart from the positivity of φ', is used in the proof below.

Proof. Let ψ_ϵ be defined as in Section 3A. We let $\tilde{\psi} \in \mathscr{C}^\infty(\mathbb{R}^+)$ be nonnegative and such that $\tilde{\psi} = 1$ in $[4, +\infty)$ and $\tilde{\psi} = 0$ in $[0, 3]$. We then define $\tilde{\psi}_\epsilon$ according to (3-5), and we have $\tau \lesssim \langle \xi' \rangle$ in $\operatorname{supp}(1 - \tilde{\psi}_\epsilon)$ and $\operatorname{supp}(1 - \psi_\epsilon) \cap \operatorname{supp}(\tilde{\psi}_\epsilon) = \varnothing$. We set $\tilde{m}_\pm = m_\pm(1 - \tilde{\psi}_\epsilon)$ and observe that $\tilde{m}_\pm \in \mathcal{S}^1_\tau$. We define

$$\tilde{e}_\pm = \tau\varphi' + \tilde{m}_\pm \in \mathcal{S}^1_\tau, \quad \tilde{E}_\pm = \operatorname{op}^w(\tilde{e}_\pm).$$

From the definition of $\tilde{\psi}_\epsilon$, we have

$$\tilde{e}_\pm \geq C\lambda. \tag{3-8}$$

Next,

$$M_\pm \mathrm{op}(1-\psi_\epsilon)\omega = \mathrm{op}^w(\tilde{m}_\pm)\mathrm{op}(1-\psi_\epsilon)\omega + \mathrm{op}^w(m_\pm\tilde{\psi}_\epsilon)\mathrm{op}(1-\psi_\epsilon)\omega,$$

and since $m_\pm\tilde{\psi}_\epsilon \in \mathcal{S}^1$ and $1-\psi_\epsilon \in \mathcal{S}^0_\tau$, with the latter vanishing in a region $\langle\xi'\rangle \leq C\tau$, Lemma A.4 yields

$$M_\pm \mathrm{op}(1-\psi_\epsilon)\omega = \mathrm{op}^w(\tilde{m}_\pm)\mathrm{op}(1-\psi_\epsilon)\omega + R_1\omega, \quad \text{with } R_1 \in \mathrm{op}(\mathcal{S}^{-\infty}_\tau). \tag{3-9}$$

We set $u = \mathrm{op}(1-\psi_\epsilon)\omega$. For $s = 2\ell+1$, we compute

$$\begin{aligned} 2\,\mathrm{Re}\langle \mathcal{P}_{E_+}u, iH_+\Lambda^s u\rangle &= \langle i[D_n, H_+]u, \Lambda^s u\rangle + \langle i[S_+, \Lambda^s]u, H_+u\rangle + 2\,\mathrm{Re}\langle E_+u, H_+\Lambda^s u\rangle \\ &\geq |u_{|x_n=0^+}|^2_{\mathcal{H}^{\ell+1/2}} + 2\,\mathrm{Re}\langle E_+u, H_+\Lambda^s u\rangle - C\|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})}. \end{aligned} \tag{3-10}$$

By (3-9), we have $E_+u = \tilde{E}_+u + R_1\omega$. This yields

$$\mathrm{Re}\langle E_+u, H_+\Lambda^s u\rangle + \|H_+\omega\|^2 \gtrsim \mathrm{Re}\langle \tilde{E}_+u, H_+\Lambda^s u\rangle \gtrsim \|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})},$$

for τ sufficiently large, by (3-8) and Lemma A.2. We thus obtain

$$\mathrm{Re}\langle \mathcal{P}_{E_+}u, iH_+\Lambda^s u\rangle + \|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})} + \|H_+\omega\|^2 \gtrsim |u_{|x_n=0^+}|^2_{\mathcal{H}^{\ell+1/2}} + \|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

With the Young inequality and taking τ sufficiently large, we then find

$$\|H_+\mathcal{P}_{E_+}u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\| \gtrsim |u_{|x_n=0^+}|_{\mathcal{H}^{\ell+1/2}} + \|H_+u\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

We now invoke the corresponding estimate provided by Lemma 3.1,

$$\big\|H_+\mathcal{P}_{E+}\mathrm{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \gtrsim \big|\mathrm{op}(\psi_\epsilon)\omega_{|x_n=0^+}\big|_{\mathcal{H}^{\ell+1/2}} + \|H_+\mathrm{op}(\psi_\epsilon)\omega\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

Adding the two estimates, with the triangle inequality we obtain

$$\begin{aligned} \big\|H_+\mathcal{P}_{E_+}\mathrm{op}(1-\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\mathcal{P}_{E+}\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\| \\ \gtrsim |\omega_{|x_n=0^+}|_{\mathcal{H}^{\ell+1/2}} + \|H_+\omega\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}. \end{aligned}$$

Lemma A.4 gives $\big[\mathcal{P}_{E_+}, \mathrm{op}(1-\psi_\epsilon)\big] \in \mathrm{op}(\mathcal{S}^0_\tau)$. We thus have

$$\begin{aligned} \big\|H_+\mathcal{P}_{E_+}\mathrm{op}(1-\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} &\lesssim \big\|H_+\mathrm{op}(1-\psi_\epsilon)\mathcal{P}_{E_+}\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \\ &\lesssim \|H_+\mathcal{P}_{E_+}\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)}. \end{aligned}$$

By taking τ sufficiently large, we thus obtain

$$\|H_+\mathcal{P}_{E_+}\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \gtrsim |\omega_{|x_n=0^+}|_{\mathcal{H}^{\ell+1/2}} + \|H_+\omega\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}. \tag{3-11}$$

The term $\|H_+D_n\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)}$ can simply be introduced on the right-hand side of this estimate to yield (3-6), thanks to the form of the first-order operator $\mathcal{P}_{E_+}$. To obtain estimate (3-7), we compute $2\,\mathrm{Re}\langle \mathcal{P}_{E\_}\omega, iH_-\omega\rangle$. The argument is similar, but the trace term comes out with the opposite sign. ☐

For the operator $\mathcal{P}_{F+}$, we can also obtain a microlocal estimate. We place ourselves in a microlocal region where $f_+ = \tau\varphi^+ - m_+$ is positive. More precisely, let $\chi(x,\tau,\xi') \in \mathcal{S}^0_\tau$ be such that $|\xi'| \le C\tau$ and $f_+ \ge C_1\lambda$ in $\operatorname{supp}(\chi)$, $C_1 > 0$, and $|\xi'| \ge C'\tau$ in $\operatorname{supp}(1-\chi)$.

Lemma 3.3. *Let $\ell \in \mathbb{R}$. There exist $\tau_1 \ge 1$ and $C > 0$ such that*

$$C\big(\big\| H_+\mathcal{P}_{F+}\mathrm{op}^w(\chi)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\|\big) \\ \ge \big|\mathrm{op}^w(\chi)\omega_{|x_n=0^+}\big|_{\mathcal{H}^{\ell+1/2}} + \big\|H_+\mathrm{op}^w(\chi)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})} + \big\|H_+D_n\mathrm{op}^w(\chi)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)},$$

for $\tau \ge \tau_1$ and $\omega \in \mathscr{S}_c(\mathbb{R}^n)$.

As for (3-6) of Lemma 3.2, up to a harmless remainder term, we obtain an elliptic estimate in this microlocal region.

Proof. Let ψ_ϵ be as defined in Section 3A, and let $\tilde\psi_\epsilon$ be as in the proof of Lemma 3.2. We set

$$\tilde f_\pm = \tau\varphi' - \tilde m_\pm \in \mathcal{S}^1_\tau, \quad \tilde F_\pm = \mathrm{op}^w(\tilde f_\pm). \tag{3-12}$$

We have

$$\tilde f_\pm = \tau\varphi' - \tilde m_\pm = \tau\varphi' - m_\pm(1-\tilde\psi_\epsilon) = f_\pm + \tilde\psi_\epsilon m_\pm \ge f_\pm.$$

This gives $\tilde f_+ \ge C\lambda$ in $\operatorname{supp}(\chi)$.

We set $u = \mathrm{op}(1-\psi_\epsilon)\mathrm{op}^w(\chi)\omega$. Following the proof of Lemma 3.2, for $s = 2\ell+1$, we obtain

$$\mathrm{Re}\langle\mathcal{P}_{F+}u, iH_+\Lambda^s u\rangle + \|H_+\omega\|^2 + \|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})} \gtrsim |u_{|x_n=0^+}|^2_{\mathcal{H}^{\ell+1/2}} + \mathrm{Re}\langle\tilde F_+u, H_+\Lambda^s u\rangle.$$

Let now $\tilde\chi \in \mathcal{S}^0_\tau$ satisfy the same properties as χ, with $\tilde\chi = 1$ on a neighborhood of $\operatorname{supp}(\chi)$. We then write

$$\tilde f_+ = \check f_+ + r, \quad \text{with } \check f_+ = \tilde f_+\tilde\chi + \lambda(1-\tilde\chi) \in \mathcal{S}^1_\tau, \quad r = (\tilde f_+ - \lambda)(1-\tilde\chi) \in \mathcal{S}^1_\tau.$$

As $\operatorname{supp}(1-\tilde\chi)\cap\operatorname{supp}(\chi) = \varnothing$, we find $r\sharp(1-\psi_\epsilon)\sharp\chi \in \mathcal{S}^{-\infty}_\tau$. Since $\check f_+ \ge C\lambda$ by construction, with Lemma A.2 we obtain

$$\mathrm{Re}\langle\mathcal{P}_{F+}u, iH_+\Lambda^s u\rangle + \|H_+\omega\|^2 + \|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})} \gtrsim |u_{|x_n=0^+}|^2_{\mathcal{H}^{\ell+1/2}} + \|H_+u\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

With the Young inequality, taking τ sufficiently large, we obtain

$$\|H_+\mathcal{P}_{F+}u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\| \gtrsim |u_{|x_n=0^+}|_{\mathcal{H}^{\ell+1/2}} + \|H_+u\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

Invoking the corresponding estimate provided by Lemma 3.1 for $\mathrm{op}^w(\chi)\omega$,

$$\big\|H_+\mathcal{P}_{F+}\mathrm{op}(\psi_\epsilon)\mathrm{op}^w(\chi)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \\ \gtrsim \big|\mathrm{op}(\psi_\epsilon)\mathrm{op}^w(\chi)\omega_{|x_n=0^+}\big|_{\mathcal{H}^{\ell+1/2}} + \big\|H_+\mathrm{op}(\psi_\epsilon)\mathrm{op}^w(\chi)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})},$$

and arguing as in the end of the proof of Lemma 3.2, we obtain the result. □

For the operator $\mathcal{P}_{F-}$ we can also obtain a microlocal estimate. We place ourselves in a microlocal region where $f_- = \tau\varphi^- - m_-$ is positive. More precisely, let $\chi(x,\tau,\xi') \in \mathcal{S}^0_\tau$ be such that $|\xi'| \le C\tau$ and $f_- \ge C_1\lambda$ in $\operatorname{supp}(\chi)$, $C_1 > 0$, and $|\xi'| \ge C'\tau$ in $\operatorname{supp}(1-\chi)$.

Lemma 3.4. *Let $\ell \in \mathbb{R}$. There exist $\tau_1 \geq 1$ and $C > 0$ such that*

$$C\big(\|H_-\mathcal{P}_{F_-}u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_-\omega\| + \|H_-D_n\omega\| + |u_{|x_n=0^-}|_{\mathcal{H}^{\ell+1/2}}\big) \geq \|H_-u\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}, \tag{3-13}$$

for $\tau \geq \tau_1$ and $u = a_{nn}^- \mathcal{P}_{E-}\mathrm{op}^w(\chi)\omega$ with $\omega \in \mathscr{S}_c(\mathbb{R}^n)$.

Proof. Let ψ_ϵ be defined as in Section 3A. We define $\tilde{f}_-$ and $\tilde{F}_-$ as in (3-12). We have $\tilde{f}_- \geq f_- \geq C\lambda$ in $\mathrm{supp}(\chi)$. We set $z = \mathrm{op}(1-\psi_\epsilon)u$ and for $s = 2\ell+1$, we compute

$$\begin{aligned}2\,\mathrm{Re}\langle \mathcal{P}_{F_-}z, iH_-\Lambda^s z\rangle &= \langle i[D_n, H_-]z, \Lambda^s z\rangle + i\langle [S_-, \Lambda^s]z, H_-z\rangle + 2\,\mathrm{Re}\langle F_-z, H_-\Lambda^s z\rangle \\ &\geq -|z_{|x_n=0^-}|^2_{\mathcal{H}^{\ell+1/2}} + 2\,\mathrm{Re}\langle F_-z, H_-\Lambda^s z\rangle - C\|H_-z\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})}.\end{aligned}$$

Arguing as in the proof of Lemma 3.2 (see (3-9) and (3-10)), we obtain

$$2\,\mathrm{Re}\langle \mathcal{P}_{F_-}z, iH_-\Lambda^s z\rangle + C\|H_-u\|^2 + |z_{|x_n=0^-}|^2_{\mathcal{H}^{\ell+1/2}} + C\|H_-z\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})} \geq 2\,\mathrm{Re}\langle \tilde{F}_-z, H_-\Lambda^s z\rangle.$$

Let now $\tilde{\chi} \in \mathcal{S}^0_\tau$ satisfy the same properties as χ, with $\tilde{\chi} = 1$ on a neighborhood of $\mathrm{supp}(\chi)$. We then write

$$\tilde{f}_- = \check{f}_- + r, \quad \text{with } \check{f}_- = \tilde{f}_-\tilde{\chi} + \lambda(1-\tilde{\chi}) \in \mathcal{S}^1_\tau, \quad r = (\tilde{f}_- - \lambda)(1-\tilde{\chi}) \in \mathcal{S}^1_\tau.$$

As $\check{f}_- \geq C\lambda$ and $\mathrm{supp}(1-\tilde{\chi}) \cap \mathrm{supp}(\chi) = \varnothing$, with Lemma A.2 we obtain, for τ large,

$$\begin{aligned}2\,\mathrm{Re}\langle \mathcal{P}_{F_-}z, iH_-\Lambda^s z\rangle + C\|H_-u\|^2 + |z_{|x_n=0^-}|^2_{\mathcal{H}^{\ell+1/2}} + C\|H_-z\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1/2})} + \|H_-\omega\|^2 + \|H_-D_n\omega\|^2 \\ \geq C'\|H_-z\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.\end{aligned}$$

With the Young inequality and taking τ sufficiently large, we then find

$$\|H_-\mathcal{P}_{F_-}z\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_-u\| + |z_{|x_n=0^-}|_{\mathcal{H}^{\ell+1/2}} + \|H_-\omega\| + \|H_-D_n\omega\| \gtrsim \|H_-z\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

Invoking the corresponding estimate provided by Lemma 3.1 for u yields

$$\big\|H_-\mathcal{P}_{F_-}\mathrm{op}(\psi_\epsilon)u\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \big|\mathrm{op}(\psi_\epsilon)u_{|x_n=0^-}\big|_{\mathcal{H}^{\ell+1/2}} \gtrsim \big\|H_-\mathrm{op}(\psi_\epsilon)u\big\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})},$$

and arguing as in the end of Lemma 3.2, we obtain the result. ☐

3C. *Negative imaginary part on the negative half-line.* Here we place ourselves in a microlocal region where $f_- = \tau\varphi^- - m_-$ is negative. More precisely, let $\chi(x,\tau,\xi') \in \mathcal{S}^0_\tau$ be such that $|\xi'| \geq C\tau$ and $f_- \leq -C_1\lambda$ in $\mathrm{supp}(\chi)$, $C_1 > 0$. We have the following lemma, whose form is adapted to our needs in the next section. Up to harmless remainder terms, this can also be considered as a good elliptic estimate.

Lemma 3.5. *There exist $\tau_1 \geq 1$ and $C > 0$ such that*

$$C\big(\|H_-\mathcal{P}_{F_-}u\| + \|H_-\omega\| + \|H_-D_n\omega\|\big) \geq |u_{|x_n=0^-}|_{\mathcal{H}^{1/2}} + \|H_-u\|_{L^2(\mathbb{R};\mathcal{H}^1)}, \tag{3-14}$$

for $\tau \geq \tau_1$ and $u = a_{nn}^- \mathcal{P}_{E-}\mathrm{op}^w(\chi)\omega$ with $\omega \in \mathscr{S}_c(\mathbb{R}^n)$.

Proof. We compute

$$2\,\mathrm{Re}\langle \mathcal{P}_{F\_}u, -iH_-\Lambda^1 u\rangle = \langle i[D_n, -H_-]u, \Lambda^1 u\rangle - i\langle [S_-, \Lambda^1]u, H_-u\rangle + 2\,\mathrm{Re}\langle -F_-u, H_-\Lambda^1 u\rangle$$
$$\geq |u_{|x_n=0^-}|^2_{\mathcal{H}^{1/2}} + 2\,\mathrm{Re}\langle -F_-u, H_-\Lambda^1 u\rangle - C\|H_-u\|^2_{L^2(\mathbb{R};\mathcal{H}^{1/2})}.$$

Let now $\tilde{\chi} \in \mathcal{S}^0_\tau$ satisfy the same properties as χ, with $\tilde{\chi} = 1$ on a neighborhood of $\mathrm{supp}(\chi)$. We then write

$$f_- = \check{f}_- + r, \quad \text{with } \check{f}_- = f_-\tilde{\chi} - \lambda(1-\tilde{\chi}), \quad r = (f_- + \lambda)(1-\tilde{\chi}).$$

Observe that $f_-\tilde{\chi} \in \mathcal{S}^1_\tau$ because of the support of $\tilde{\chi}$. Hence $\check{f}_- \in \mathcal{S}^1_\tau$. As $-\check{f}_- \geq C\lambda$, with Lemma A.2 we obtain, for τ large, $\mathrm{Re}\langle -\mathrm{op}^w(\check{f}_-)u, H_-\Lambda^1 u\rangle \gtrsim \|H_-u\|^2_{L^2(\mathbb{R};\mathcal{H}^1)}$. Note that r does not satisfy the estimates of the semiclassical calculus because of the term $m_-(1-\tilde{\chi})$. However, we have

$$\mathrm{op}^w(r)u = \mathrm{op}^w(r)a^-_{nn}\mathrm{op}^w(\chi)D_n\omega + \mathrm{op}^w(r)a^-_{nn}S_-\mathrm{op}^w(\chi)\omega + i\,\mathrm{op}^w(r)a^-_{nn}E_-\mathrm{op}^w(\chi)\omega.$$

Applying Lemma A.4 and using that $1-\tilde{\chi} \in \mathcal{S}^0_\tau \subset \mathcal{S}^0$ yields

$$\mathrm{op}^w(r)u = R\omega \qquad \text{with } R \in \mathrm{op}(\mathcal{S}^1_\tau)D_n + \mathrm{op}(\mathcal{S}^2_\tau).$$

As $\mathrm{supp}(1-\tilde{\chi}) \cap \mathrm{supp}(\chi) = \varnothing$, the composition formula (A-7) (which is valid in this case — see Lemma A.4) yields $R \in \mathrm{op}(\mathcal{S}^{-\infty}_\tau)D_n + \mathrm{op}(\mathcal{S}^{-\infty}_\tau)$. We thus find, for τ sufficiently large,

$$\mathrm{Re}\langle \mathcal{P}_{F\_}u, -iH_-\Lambda^1 u\rangle + \|H_-\omega\|^2 + \|H_-D_n\omega\|^2 \gtrsim |u_{|x_n=0^-}|^2_{\mathcal{H}^{1/2}} + \|H_-u\|^2_{L^2(\mathbb{R};\mathcal{H}^1)},$$

and we conclude with the Young inequality. □

3D. *Increasing imaginary part on a half-line.* Here we allow the symbols $f_\pm$ to change sign. For the first-order factor $\mathcal{P}_{F_\pm}$, this will lead to an estimate that exhibits a loss of a half-derivative, as can be expected.

Let ψ_ϵ be as defined in Section 3A, and let $\tilde{\psi}_\epsilon$ be as in the proof of Lemma 3.2. We define $\tilde{f}_\pm$ and $\tilde{F}_\pm$ as in (3-12), and set $\tilde{\mathcal{P}}_{F_\pm} = D_n + S_\pm + i\tilde{F}_\pm$.

As $\mathrm{supp}(\tilde{\psi}_\epsilon)$ remains away from the sets $\{f_\pm = 0\}$, the subellipticity property of Lemma 2.8 is preserved for $\tilde{f}_\pm$ in place of $f_\pm$. We shall use the following inequality.

Lemma 3.6. *There exist $C > 0$ such that for $\mu > 0$ sufficiently large, we have*

$$\rho_\pm = \mu\tilde{f}^2_\pm + \tau\{\xi_n + s_\pm, \tilde{f}_\pm\} \geq C\lambda^2,$$

with $\lambda^2 = \tau^2 + |\xi'|^2$.

Proof. If $|\tilde{f}_\pm| \leq \delta\lambda$, for δ small, then $\tilde{f}_\pm = f_\pm$ and $\tau\{\xi_n + s_\pm, \tilde{f}_\pm\} \geq C\lambda^2$, by Lemma 2.8.

If $|\tilde{f}_\pm| \geq \delta\lambda$, observing that $\tau\{\xi_n + s_\pm, \tilde{f}_\pm\} \in \tau\mathcal{S}^1_\tau \subset \mathcal{S}^2_\tau$, we obtain $\rho_\pm \geq C\lambda^2$, by choosing μ sufficiently large. □

We now prove the following estimate for $\mathcal{P}_{F_\pm}$.

Lemma 3.7. *Let $\ell \in \mathbb{R}$. There exist $\tau_1 \geq 1$ and $C > 0$ such that*

$$C\big(\|H_\pm \mathcal{P}_{F_\pm}\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + |\omega_{|x_n=0^\pm}|_{\mathcal{H}^{\ell+1/2}}\big) \geq \tau^{-1/2}\big(\|H_\pm\omega\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})} + \|H_\pm D_n\omega\|_{L^2(\mathbb{R};\mathcal{H}^\ell)}\big),$$

for $\tau \geq \tau_1$ and $\omega \in \mathscr{S}_c(\mathbb{R}^n)$.

Proof. We set $u = \mathrm{op}(1-\psi_\epsilon)\omega$. We start by invoking (3-9), and the fact that $[\tilde{\mathcal{P}}_{F+}, \Lambda^\ell] \in \mathrm{op}(\mathcal{S}^\ell_\tau)$, and write

$$\begin{aligned}\|H_+\tilde{\mathcal{P}}_{F+}\Lambda^\ell u\| &\lesssim \|H_+\Lambda^\ell\tilde{\mathcal{P}}_{F+}u\| + \|H_+[\tilde{\mathcal{P}}_{F+}, \Lambda^\ell]u\| \\ &\lesssim \|H_+\tilde{\mathcal{P}}_{F+}u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \\ &\lesssim \|H_+\mathcal{P}_{F+}u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\| + \|H_+u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)}.\end{aligned} \tag{3-15}$$

We set $u_\ell = \Lambda^\ell u$. We then have

$$\begin{aligned}\|H_+\tilde{\mathcal{P}}_{F+}u_\ell\|^2 &= \big\|H_+(D_n+S_+)u_\ell\big\|^2 + \|H_+\tilde{F}_+u_\ell\|^2 + 2\,\mathrm{Re}\big\langle (D_n+S_+)u_\ell, iH_+\tilde{F}_+u_\ell\big\rangle \\ &\geq \tau^{-1}\,\mathrm{Re}\big\langle\big(\mu\tilde{F}_+^2 + i\tau\big[D_n+S_+, \tilde{F}_+\big]\big)u_\ell, H_+u_\ell\big\rangle + \langle i[D_n, H_+]u_\ell, \tilde{F}_+u_\ell\rangle,\end{aligned}$$

if $\mu\tau^{-1} \leq 1$. As the principal symbol (in the semiclassical calculus) of $\mu\tilde{F}_+^2 + i\tau\big[D_n+S_+, \tilde{F}_+\big]$ is $\rho_+ = \mu\tilde{f}_+^2 + \tau\{\xi_n + s_+, \tilde{f}_+\}$, Lemmata 3.6 and A.2 yield

$$\|H_+\tilde{\mathcal{P}}_{F+}u_\ell\|^2 + |u_\ell|^2_{\mathcal{H}^{1/2}} \gtrsim \tau^{-1}\|H_+u_\ell\|^2_{L^2(\mathbb{R};\mathcal{H}^1)},$$

for μ large, that is, τ large. With (3-15) we obtain, for τ sufficiently large,

$$\|H_+\mathcal{P}_{F+}u\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} + \|H_+\omega\| + |u|_{\mathcal{H}^{\ell+1/2}} \gtrsim \tau^{-1/2}\|H_+u\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.$$

We now invoke the corresponding estimate provided by Lemma 3.1,

$$\big\|H_+\mathcal{P}_{F+}\mathrm{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^\ell)} \gtrsim \big|\mathrm{op}(\psi_\epsilon)\omega_{|x_n=0^+}\big|_{\mathcal{H}^{\ell+1/2}} + \big\|H_+\mathrm{op}(\psi_\epsilon)\omega\big\|_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})},$$

and we proceed as in the end of the proof of Lemma 3.2 to obtain the result for $\mathcal{P}_{F+}$. The same computation and arguments, *mutatis mutandis*, give the result for $\mathcal{P}_{F-}$. □

4. Proof of the Carleman estimate

With the estimates for the first-order factors obtained in Section 3, we shall now prove Proposition 2.1, which gives the result of Theorems 1.1 and 2.2 (see the end of Section 2A).

The Carleman estimates we prove are well known away from the interface $\{x_n = 0\}$. Since local Carleman estimates can be patched together, we may thus assume that the compact set K in the statements of Theorems 1.1 and 2.2 is such that $|x_n|$ is sufficiently small for the arguments below to be carried out. Hence, we shall assume the functions $w_\pm$ in Theorem 2.2 (resp. $v_\pm$ in Proposition 2.1) have small supports near 0 in the x_n-direction.

4A. ***The geometric hypothesis.*** In Section 2D, we chose a weight function φ that satisfies the condition

$$\frac{\alpha_+}{\alpha_-} > \sup_{\substack{x',\xi' \\ |\xi'|\geq 1}} \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}}, \quad \alpha_\pm = \partial_{x_n}\varphi_{\pm|x_n=0^\pm}. \tag{4-1}$$

Let us explain the immediate consequences of that assumption. First of all, we can reformulate it by saying that

$$\frac{\alpha_+}{\alpha_-} = \sigma^2 \sup_{\substack{x',\xi' \\ |\xi'|\geq 1}} \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}} \quad \text{for some } \sigma > 1. \tag{4-2}$$

Let $1 < \sigma_0 < \sigma$.

Consider $(x',\xi',\tau) \in \mathbb{R}^{n-1} \times \mathbb{R}^{n-1} \times \mathbb{R}^{+,*}$, $|\xi'| \geq 1$, such that

$$\tau\alpha_+ \geq \sigma_0 m_+(x',\xi')_{|x_n=0^+}. \tag{4-3}$$

We then have

$$\tau\alpha_+ - m_+(x',\xi')_{|x_n=0^+} \geq \tau\alpha_+(1-\sigma_0^{-1}) \geq \frac{\sigma_0 - 1}{2\sigma_0}\tau\alpha_+ + \frac{\sigma_0-1}{2} m_+(x',\xi')_{|x_n=0^+} \geq C\lambda. \tag{4-4}$$

We choose τ sufficiently large, say $\tau \geq \tau_2 > 0$, that this inequality remains true for $0 \leq |\xi'| \leq 2$. It also remains true for $x_n > 0$ small. As $f_+ = \tau(\varphi' - \alpha_+) + \tau\alpha_+ - m_+(x,\xi')$, for $|x_n|$ small, we obtain $f_+ \geq C\lambda$, which means that f_+ is elliptic positive in that region.

Second, if we now have $|\xi'| \geq 1$ and

$$\tau\alpha_+ \leq \sigma m_+(x',\xi')_{|x_n=0^+}, \tag{4-5}$$

we get that $\tau\alpha_- \leq \sigma^{-1} m_-(x',\xi')_{|x_n=0^-}$: otherwise we would have $\tau\alpha_- > \sigma^{-1} m_-(x',\xi')_{|x_n=0^-}$ and thus

$$\frac{m_-(x',\xi')_{|x_n=0^-}}{\sigma\alpha_-} < \tau \leq \frac{\sigma m_+(x',\xi')_{|x_n=0^+}}{\alpha_+},$$

implying

$$\frac{\alpha_+}{\alpha_-} < \sigma^2 \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}} \leq \sigma^2 \sup_{\substack{x',\xi' \\ |\xi'|\geq 1}} \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}} = \frac{\alpha_+}{\alpha_-}, \quad \text{which is impossible.}$$

As a consequence, we have

$$\begin{aligned} \tau\alpha_- - m_-(x',\xi')_{|x_n=0^-} &\leq -m_-(x',\xi')_{|x_n=0^-}\frac{(\sigma-1)}{\sigma} \\ &\leq -m_-(x',\xi')_{|x_n=0^-}\frac{(\sigma-1)}{2\sigma} - \frac{(\sigma-1)}{2}\tau\alpha_- \leq -C\lambda. \end{aligned} \tag{4-6}$$

With $f_- = \tau(\varphi' - \alpha_-) + \tau\alpha_- - m_-(x,\xi')$, for $|x_n|$ sufficiently small, we obtain $f_- \leq -C\lambda$, which means that f_- is elliptic negative in that region.

We have thus proven the following result.

Lemma 4.1. *Let $\sigma > \sigma_0 > 1$ and $\alpha_\pm$ be positive numbers such that (4-2) holds. For $s > 0$, we define the following "cones" in $\mathbb{R}^{n-1}_{x'} \times \mathbb{R}^{n-1}_{\xi'} \times \mathbb{R}^*_+$:*

$$\Gamma_s = \big\{(x', \tau, \xi') : |\xi'| < 2 \text{ or } \tau\alpha_+ > s m_+(x', \xi')_{|x_n=0^+}\big\},$$
$$\widetilde{\Gamma}_s = \big\{(x', \tau, \xi') : |\xi'| > 1 \text{ and } \tau\alpha_+ < s m_+(x', \xi')_{|x_n=0^+}\big\}.$$

For $|x_n|$ sufficiently small and τ sufficiently large, we have $\mathbb{R}^{n-1} \times \mathbb{R}^{n-1} \times \mathbb{R}^*_+ = \Gamma_{\sigma_0} \cup \widetilde{\Gamma}_\sigma$ and

$$\Gamma_{\sigma_0} \subset \big\{(x', \xi', \tau) \in \mathbb{R}^{n-1} \times \mathbb{R}^{n-1} \times \mathbb{R}^*_+ : \ f_+(x, \xi') \geq C\lambda, \ \text{if } 0 \leq x_n \text{ small}\big\},$$
$$\widetilde{\Gamma}_\sigma \subset \big\{(x', \xi', \tau) \in \mathbb{R}^{n-1} \times \mathbb{R}^{n-1} \times \mathbb{R}^*_+ : \ f_-(x, \xi') \leq -C\lambda, \ \text{if } |x_n| \text{ small}, \ x_n \leq 0\big\}.$$

N.B. The key result for the sequel is that property (4-1) is securing the fact that the overlapping open regions Γ_{σ_0} and $\widetilde{\Gamma}_\sigma$ are such that on Γ_{σ_0}, f_+ is elliptic positive and on $\widetilde{\Gamma}_\sigma$, f_- is elliptic negative. Using a partition of unity and symbolic calculus, we shall be able to assume that either F_+ is elliptic positive, or F_- is elliptic negative.

N.B. Note that we can keep the preliminary cut-off region of Section 3A away from the overlap of Γ_{σ_0} and $\widetilde{\Gamma}_\sigma$ by choosing ϵ sufficiently small (see (3-5) and Lemma 3.1). This is illustrated in Figure 4.

With the two overlapping "cones", for $\tau \geq \tau_2$, we introduce a homogeneous partition of unity

$$1 = \chi_0(x', \xi', \tau) + \chi_1(x', \xi', \tau), \qquad \underbrace{\operatorname{supp}(\chi_0) \subset \Gamma_{\sigma_0}}_{|\xi'| \lesssim \tau, \ f_+ \text{ elliptic} > 0}, \qquad \underbrace{\operatorname{supp}(\chi_1) \subset \widetilde{\Gamma}_\sigma}_{|\xi'| \gtrsim \tau, \ f_- \text{ elliptic} < 0}. \tag{4-7}$$

Note that χ_j', $j = 0, 1$, are supported at the overlap of the regions Γ_{σ_0} and $\widetilde{\Gamma}_\sigma$, where $\tau \lesssim |\xi'|$. Hence, χ_0 and χ_1 satisfy the estimates of the semiclassical calculus and we have $\chi_0, \chi_1 \in \mathcal{S}^0_\tau$. With these symbols

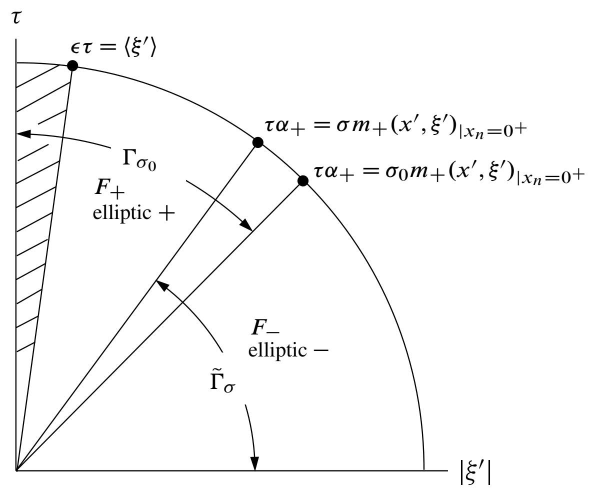

Figure 4. The overlapping microlocal regions Γ_{σ_0} and $\widetilde{\Gamma}_\sigma$ in the $\tau, |\xi'|$ plane above a point x'. Dashed is the region used in Section 3A, which is kept away from the overlap of Γ_{σ_0} and $\widetilde{\Gamma}_\sigma$.

we associate the operators

$$\Xi_j = \mathrm{op}^w(\chi_j), \; j = 0, 1, \quad \text{and we have } \Xi_0 + \Xi_1 = \mathrm{Id}. \tag{4-8}$$

Remark 4.2. Here we have chosen to let χ_0 and χ_1 (resp. Ξ_0 and Ξ_1) be independent of x_n. As the functions $v_\pm$ have supports in which $|x_n|$ is small (see the introductory paragraph of this section), we can further introduce a cut-off in the x_n direction. The lemmata of Section 3 can then be applied directly.

By the transmission conditions (2-21), we find

$$\Xi_j v_{+|x_n=0^+} - \Xi_j v_{-|x_n=0^-} = \Xi_j \theta_\varphi \tag{4-9}$$

and

$$\begin{aligned} a_{nn}^+\big(D_n + T_+ + i\tau\varphi'_+\big)\Xi_j v_{+|x_n=0^+} - a_{nn}^-\big(D_n + T_- + i\tau\varphi'_-\big)\Xi_j v_{-|x_n=0^-} \\ = \Xi_j \Theta_\varphi + \mathrm{op}^w(\kappa_0) v_{|x_n=0^+} + \mathrm{op}^w(\tilde\kappa_0)\theta_\varphi, \quad j = 0, 1, \end{aligned}$$

with $\kappa_0, \tilde\kappa_0 \in \mathcal{S}_\tau^0$ that originate from commutators and (4-9). Defining

$$\mathcal{V}_{j,\pm} = a_{nn}^\pm\big(D_n + S_\pm + i\tau\varphi'_\pm\big)\Xi_j v_{\pm|x_n=0^\pm} \tag{4-10}$$

and recalling (2-19), we find

$$\mathcal{V}_{j,+} - \mathcal{V}_{j,-} = \Xi_j \Theta_\varphi + \mathrm{op}^w(\kappa_1) v_{|x_n=0^+} + \mathrm{op}^w(\tilde\kappa_1)\theta_\varphi, \quad \kappa_1, \tilde\kappa_1 \in \mathcal{S}_\tau^0. \tag{4-11}$$

We shall now prove microlocal Carleman estimates in the regions Γ_{σ_0} and $\widetilde\Gamma_\sigma$.

4B. ***Region Γ_{σ_0}: both roots are positive on the positive half-line.*** On the one hand, by Lemma 3.2, we have

$$\big\| H_+ \mathcal{P}_+ \Xi_0 v_+ \big\| \gtrsim \big| \mathcal{V}_{0,+} - i a_{nn}^+ M_+ \Xi_0 v_{+|x_n=0^+} \big|_{\mathcal{H}^{1/2}} + \big\| H_+ \mathcal{P}_{F+} \Xi_0 v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^1)}, \tag{4-12}$$

where the operator $\mathcal{P}_+$ is defined in (2-7) (see also (2-17)). The positive ellipticity of F_+ on the $\operatorname{supp}\chi_0 \cap \operatorname{supp}(v_+)$ allows us to reiterate the estimate by Lemma 3.3 to obtain

$$\begin{aligned} \big\| H_+ \mathcal{P}_+ \Xi_0 v_+ \big\| + \| H_+ v_+ \| \gtrsim \big| \mathcal{V}_{0,+} - i a_{nn}^+ M_+ \Xi_0 v_{+|x_n=0^+} \big|_{\mathcal{H}^{1/2}} + \big| \Xi_0 v_{+|x_n=0^+} \big|_{\mathcal{H}^{3/2}} \\ + \big\| H_+ \Xi_0 v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^2)} + \big\| H_+ D_n \Xi_0 v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^1)}. \end{aligned}$$

Since we also have

$$|\mathcal{V}_{0,+}|_{\mathcal{H}^{1/2}} \lesssim \big| \mathcal{V}_{0,+} - i a_{nn}^+ M_+ \Xi_0 v_{+|x_n=0^+} \big|_{\mathcal{H}^{1/2}} + \big| \Xi_0 v_{+|x_n=0^+} \big|_{\mathcal{H}^{3/2}}, \tag{4-13}$$

writing the $\mathcal{H}^{1/2}$ norm as $|\,.\,|_{\mathcal{H}^{1/2}} \sim \tau^{1/2}|\,.\,|_{L^2} + |\,.\,|_{H^{1/2}}$ and using the regularity of $M_+ \in \mathrm{op}(\mathcal{S}^1)$ in the standard calculus, we obtain

$$\begin{aligned} \big\| H_+ \mathcal{P}_+ \Xi_0 v_+ \big\| + \| H_+ v_+ \| \gtrsim |\mathcal{V}_{0,+}|_{\mathcal{H}^{1/2}} + \big| \Xi_0 v_{+|x_n=0^+} \big|_{\mathcal{H}^{3/2}} \\ + \big\| H_+ \Xi_0 v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^2)} + \big\| H_+ \Xi_0 D_n v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^1)}. \end{aligned} \tag{4-14}$$

On the other hand, with Lemma 3.7, we have, for $k=0$ or $k=\frac{1}{2}$,

$$\big\| H_-\mathcal{P}_-\Xi_0 v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{-k})}+\big|\mathcal{V}_{0,-}+ia_{nn}^- M_-\Xi_0 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}}\gtrsim \tau^{-1/2}\big\| H_-\mathcal{P}_{E-}\Xi_0 v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}.$$

This gives

$$\big\| H_-\mathcal{P}_-\Xi_0 v_-\big\| +\tau^k\big|\mathcal{V}_{0,-}+ia_{nn}^- M_-\Xi_0 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}}\gtrsim \tau^{k-1/2}\big\| H_-\mathcal{P}_{E-}\Xi_0 v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})},$$

which with Lemma 3.2 yields

$$\begin{aligned}\big\| H_-\mathcal{P}_-\Xi_0 v_-\big\| +\tau^k\big|\mathcal{V}_{0,-}+ia_{nn}^- M_-\Xi_0 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}}+\tau^{k-1/2}\big|\Xi_0 v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}}&\\ \gtrsim \tau^{k-1/2}\big(\big\| H_-\Xi_0 v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})}+\big\| H_-\Xi_0 D_n v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\big).&\end{aligned}$$

Arguing as for (4-13), we find

$$\begin{aligned}\big\| H_-\mathcal{P}_-\Xi_0 v_-\big\| +\tau^k|\mathcal{V}_{0,-}|_{\mathcal{H}^{1/2-k}}+\tau^{k}\big|\Xi_0 v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}}&\\ \gtrsim \tau^{k-1/2}\big(\big\| H_-\Xi_0 v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})}+\big\| H_-\Xi_0 D_n v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\big).&\end{aligned}\tag{4-15}$$

Now, from the transmission conditions (4-9)–(4-11), by adding ε(4-15) + (4-14), we obtain

$$\begin{aligned}\big\| H_-\mathcal{P}_-\Xi_0 v_-\big\| +\big\| H_+\mathcal{P}_+\Xi_0 v_+\big\| +\tau^k\big(|\theta_\varphi|_{\mathcal{H}^{3/2-k}}+|\Theta_\varphi|_{\mathcal{H}^{1/2-k}}+|v_{|x_n=0^+}|_{\mathcal{H}^{1/2-k}}\big)+\|H_+v_+\|&\\ \gtrsim \tau^k\big(|\mathcal{V}_{0,-}|_{\mathcal{H}^{1/2-k}}+|\mathcal{V}_{0,+}|_{\mathcal{H}^{1/2-k}}+\big|\Xi_0 v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}}+\big|\Xi_0 v_{+|x_n=0^+}\big|_{\mathcal{H}^{3/2-k}}\big)&\\ +\tau^{k-1/2}\big(\|\Xi_0 v\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})}+\big\| H_-\Xi_0 D_n v_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}+\big\| H_+\Xi_0 D_n v_+\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\big),&\end{aligned}$$

by choosing $\varepsilon>0$ sufficiently small and τ sufficiently large. Finally, recalling the form of $\mathcal{V}_{0,\pm}$ and arguing as for (4-13), we obtain

$$\begin{aligned}\|H_-\mathcal{P}_-\Xi_0 v_-\|+\|H_+\mathcal{P}_+\Xi_0 v_+\|+\tau^k\big(|\theta_\varphi|_{\mathcal{H}^{\frac{3}{2}-k}}+|\Theta_\varphi|_{\mathcal{H}^{\frac{1}{2}-k}}+|v_{|x_n=0^+}|_{\mathcal{H}^{\frac{1}{2}-k}}\big)+\|H_+v_+\|&\\ \gtrsim\tau^k\Big(|\Xi_0 D_n v_{-|x_n=0^-}|_{\mathcal{H}^{\frac{1}{2}-k}}+|\Xi_0 D_n v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{1}{2}-k}}+|\Xi_0 v_{-|x_n=0^-}|_{\mathcal{H}^{\frac{3}{2}-k}}+|\Xi_0 v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{3}{2}-k}}\Big)&\\ +\tau^{k-\frac{1}{2}}\Big(\|\Xi_0 v\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})}+\|H_-\Xi_0 D_n v_-\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}+\|H_+\Xi_0 D_n v_+\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big),&\end{aligned}\tag{4-16}$$

for $k=0$ or $k=\frac{1}{2}$.

Remark 4.3. In the case $k=0$, recalling the form of the second-order operators $\mathcal{P}_\pm$, we can estimate the additional terms $\tau^{-1/2}\big\| H_\pm\Xi_0 D_n^2 v_\pm\big\|$.

4C. ***Region $\tilde{\Gamma}_\sigma$: only one root is positive on the positive half-line.*** This case is more difficult a priori, since we cannot expect to control $v_{|x_n=0^+}$ directly from the estimates of the first-order factors. Nevertheless, when the positive ellipticity of F_+ is violated, F_- is elliptic negative: this is the result of our main geometric assumption in Lemma 4.1.

As in (4-12), we have

$$\big\| H_+\mathcal{P}_+\Xi_1 v_+\big\| \gtrsim \big|\mathcal{V}_{1,+}-ia_{nn}^+ M_+\Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2}}+\big\| H_+\mathcal{P}_{F+}\Xi_1 v_+\big\|_{L^2(\mathbb{R};\mathcal{H}^1)},$$

and using Lemma 3.5 for the negative half-line, we have

$$\|H_-\mathcal{P}_-\Xi_1 v_-\| + \|H_- v_-\| + \|H_- D_n v_-\| \\ \gtrsim \big|\mathcal{V}_{1,-} + i a_{nn}^- M_- \Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2}} + \|H_-\mathcal{P}_{E-}\Xi_1 v_-\|_{L^2(\mathbb{R};\mathcal{H}^1)}.$$

A quick glance at the above estimates shows that none could be iterated in a favorable manner, since F_+ could be negative on the positive half-line and E_- is indeed positive on the negative half-line. We have to use the additional information given by the transmission conditions. From the above inequalities, we control

$$\tau^k\Big(\big|\mathcal{V}_{1,-} + i a_{nn}^- M_- \Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}} + \big|-\mathcal{V}_{1,+} + i a_{nn}^+ M_+ \Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}}\Big)$$

for $k = 0$ or $\frac{1}{2}$, which, by the transmission conditions (4-9)–(4-11), implies the control of

$$\tau^k\Big|\mathcal{V}_{1,-} - \mathcal{V}_{1,+} + i a_{nn}^- M_- \Xi_1 v_{-|x_n=0^-} + i a_{nn}^+ M_+ \Xi_1 v_{+|x_n=0^+}\Big|_{\mathcal{H}^{1/2-k}} \\ \geq \tau^k\big|(a_{nn}^- M_- + a_{nn}^+ M_+)\Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}} - C\tau^k\big(|\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |\theta_\varphi|_{\mathcal{H}^{3/2-k}} + \big|v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}}\big).$$

Let now $\tilde{\chi}_1 \in \mathcal{S}_\tau^0$ satisfy the same properties as χ_1, with $\tilde{\chi}_1 = 1$ on a neighborhood of $\operatorname{supp}(\chi_1)$. We then write

$$m_\pm = \check{m}_\pm + r, \quad \text{with } \check{m}_\pm = m_\pm\tilde{\chi}_1 + \lambda(1-\tilde{\chi}_1), \quad r = (m_\pm + \lambda)(1-\tilde{\chi}_1).$$

We have $\check{m}_\pm \geq C\lambda$ and $\check{m}_\pm \in \mathcal{S}_\tau^1$ because of the support of $\tilde{\chi}_1$. Because of the supports of $1-\tilde{\chi}_1$ and χ_1, in particular $\tau \lesssim |\xi'|$ in $\operatorname{supp}(\chi_1)$, Lemma A.4 yields $r \sharp \chi_1 \in \mathcal{S}_\tau^{-\infty}$. With Lemma A.2 and (4-9), we thus obtain

$$\big|\mathcal{V}_{1,-} + i a_{nn}^- M_- \Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}} + \big|-\mathcal{V}_{1,+} + i a_{nn}^+ M_+ \Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}} \\ + |\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |\theta_\varphi|_{\mathcal{H}^{3/2-k}} + \big|v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}} \gtrsim \big|\Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}} + \big|\Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{3/2-k}}.$$

From the form of $\mathcal{V}_{1,+}$ we obtain

$$\big|\mathcal{V}_{1,-} + i a_{nn}^- M_- \Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}} + \big|-\mathcal{V}_{1,+} + i a_{nn}^+ M_+ \Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}} \\ + |\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |\theta_\varphi|_{\mathcal{H}^{3/2-k}} + \big|v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}} \\ \gtrsim \big|\Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}} + \big|\Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{3/2-k}} + \big|\Xi_1 D_n v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}} + \big|\Xi_1 D_n v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}}.$$

We thus have

$$\|H_-\mathcal{P}_-\Xi_1 v_-\| + \|H_+\mathcal{P}_+\Xi_1 v_+\| \\ + \tau^k\Big(|\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |\theta_\varphi|_{\mathcal{H}^{3/2-k}} + \big|v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}}\Big) + \|H_- v_-\| + \|H_- D_n v_-\| \\ \gtrsim \tau^k\Big(\big|\Xi_1 v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}} + \big|\Xi_1 v_{+|x_n=0^+}\big|_{\mathcal{H}^{3/2-k}} + \big|\Xi_1 D_n v_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}} \\ + \big|\Xi_1 D_n v_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}} + \|H_-\mathcal{P}_{E-}\Xi_1 v_-\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} + \|H_+\mathcal{P}_{F+}\Xi_1 v_+\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big),$$

for $k = 0$ or $\frac{1}{2}$. The remaining part of the discussion is very similar to the last part of the argument in the previous subsection. By Lemmata 3.2 and 3.7, we have

$$\begin{aligned}\left\| H_-\mathcal{P}_{E_-}\Xi_1 v_-\right\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} &+ \left|\Xi_1 v_{-|x_n=0^-}\right|_{\mathcal{H}^{3/2-k}} \\ &\gtrsim \left\| H_-\Xi_1 v_-\right\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \left\| H_-\Xi_1 D_n v_-\right\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\end{aligned}$$

and

$$\begin{aligned}\left\| H_+\mathcal{P}_{F_+}\Xi_1 v_+\right\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} &+ \left|\Xi_1 v_{+|x_n=0^+}\right|_{\mathcal{H}^{3/2-k}} \\ &\gtrsim \tau^{-1/2}\Big(\left\| H_+\Xi_1 v_+\right\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \left\| H_+\Xi_1 D_n v_+\right\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big).\end{aligned}$$

Since $\left|\Xi_1 v_{\pm|x_n=0^\pm}\right|_{\mathcal{H}^{3/2-k}}$ are already controlled, we also control the right-hand side of the above inequalities and have

$$\begin{aligned}&\|H_-\mathcal{P}_-\Xi_1 v_-\| + \|H_+\mathcal{P}_+\Xi_1 v_+\| + \tau^k\Big(|\Theta_\varphi|_{\mathcal{H}^{\frac{1}{2}-k}} + |\theta_\varphi|_{\mathcal{H}^{\frac{3}{2}-k}} + |v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{1}{2}-k}}\Big) \\ &\quad + \|H_- v_-\| + \|H_- D_n v_-\| \\ &\quad \gtrsim \tau^k\Big(|\Xi_1 v_{-|x_n=0^-}|_{\mathcal{H}^{\frac{3}{2}-k}} + |\Xi_1 v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{3}{2}-k}} + |\Xi_1 D_n v_{-|x_n=0^-}|_{\mathcal{H}^{\frac{1}{2}-k}} + |\Xi_1 D_n v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{1}{2}-k}}\Big) \\ &\qquad + \tau^{k-\frac{1}{2}}\Big(\|\Xi_1 v\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \|H_-\Xi_1 D_n v_-\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} + \|H_+\Xi_1 D_n v_+\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big). \qquad (4\text{-}17)\end{aligned}$$

Remark 4.4. In the case $k = 0$, recalling the form of the second-order operators $\mathcal{P}_\pm$, we can estimate the additional terms $\tau^{-1/2}\left\| H_\pm\Xi_1 D_n^2 v_\pm\right\|$.

4D. ***Patching together microlocal estimates.*** We now sum estimates (4-16) and (4-17) together. By the triangle inequality, this gives, for $k = 0$ or $\frac{1}{2}$,

$$\begin{aligned}&\sum_{j=0,1}\big(\|H_-\mathcal{P}_-\Xi_j v_-\| + \|H_+\mathcal{P}_+\Xi_j v_+\|\big) + \tau^k\Big(|\Theta_\varphi|_{\mathcal{H}^{\frac{1}{2}-k}} + |\theta_\varphi|_{\mathcal{H}^{\frac{3}{2}-k}} + |v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{1}{2}-k}}\Big) \\ &\qquad + \|H_+ v_+\| + \|H_- v_-\| + \|H_- D_n v_-\| \\ &\qquad\qquad \gtrsim \tau^k\Big(|v_{-|x_n=0^-}|_{\mathcal{H}^{\frac{3}{2}-k}} + |v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{3}{2}-k}} + |D_n v_{-|x_n=0^-}|_{\mathcal{H}^{\frac{1}{2}-k}} + |D_n v_{+|x_n=0^+}|_{\mathcal{H}^{\frac{1}{2}-k}}\Big) \\ &\qquad\qquad\qquad + \tau^{k-\frac{1}{2}}\Big(\|v\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \|H_- D_n v_-\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} + \|H_+ D_n v_+\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big).\end{aligned}$$

For τ sufficiently large, we now obtain

$$\begin{aligned}&\sum_{j=0,1}\Big(\left\| H_-\mathcal{P}_-\Xi_j v_-\right\| + \left\| H_+\mathcal{P}_+\Xi_j v_+\right\|\Big) + \tau^k\big(|\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |\theta_\varphi|_{\mathcal{H}^{3/2-k}}\big) \\ &\quad \gtrsim \tau^k\Big(\left|v_{-|x_n=0^-}\right|_{\mathcal{H}^{3/2-k}} + \left|v_{+|x_n=0^+}\right|_{\mathcal{H}^{3/2-k}} + \left|D_n v_{-|x_n=0^-}\right|_{\mathcal{H}^{1/2-k}} + \left|D_n v_{+|x_n=0^+}\right|_{\mathcal{H}^{1/2-k}}\Big) \\ &\qquad + \tau^{k-1/2}\Big(\|v\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \left\| H_- D_n v_-\right\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} + \left\| H_+ D_n v_+\right\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big).\end{aligned}$$

Arguing with commutators, as in the end of Lemma 3.2, noting here that the second-order operators $\mathcal{P}_\pm$ belong to the semiclassical calculus, that is, $\mathcal{P}_\pm \in \mathcal{S}^2_\tau$, we obtain, for τ sufficiently large,

$$\begin{aligned}\|H_-\mathcal{P}_-v_-\| + \|H_+\mathcal{P}_+v_+\| &+ \tau^k\big(|\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |\theta_\varphi|_{\mathcal{H}^{3/2-k}}\big)\\ &\gtrsim \tau^k\Big(\big|v_{-|x_n=0^-}\big|_{\mathcal{H}^{3/2-k}} + \big|v_{+|x_n=0^+}\big|_{\mathcal{H}^{3/2-k}} + \big|D_nv_{-|x_n=0^-}\big|_{\mathcal{H}^{1/2-k}} + \big|D_nv_{+|x_n=0^+}\big|_{\mathcal{H}^{1/2-k}}\Big)\\ &\qquad + \tau^{k-1/2}\Big(\|v\|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \big\|H_-D_nv_-\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} + \big\|H_+D_nv_+\big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}\Big).\end{aligned}$$

In particular, this estimate allows us to absorb the perturbation in Ψ^1 as defined by (2-16) by taking τ large enough. For $k = \frac{1}{2}$, we obtain the result of Proposition 2.1, which concludes the proof of the Carleman estimate.

N.B. The case $k = 0$ gives higher Sobolev norm estimates of the trace terms $v_{\pm|x_n=0^\pm}$ and $D_nv_{\pm|x_n=0^\pm}$. It also allows one to estimate $\tau^{-1/2}\|H_\pm D_n^2 v_\pm\|$, as noted in Remarks 4.3 and 4.4. These estimates are obtained at the price of higher requirements (one additional tangential half-derivative) on the nonhomogeneous transmission condition functions θ and Θ.

4E. ***Convexification.*** We want now to slightly modify the weight function φ, for instance to allow some convexification. We started with $\varphi = H_+\varphi_+ + H_-\varphi_-$, where $\varphi_\pm$ were given by (2-22) and our proof relied heavily on a smooth factorization in first-order factors. We modify $\varphi_\pm$ into

$$\Phi_\pm(x', x_n) = \underbrace{\alpha_\pm x_n + \tfrac{1}{2}\beta x_n^2}_{\varphi_\pm(x_n)} + \kappa(x', x_n), \quad \kappa \in \mathscr{C}^\infty(\Omega;\mathbb{R}), \quad |d\kappa| \text{ bounded on } \Omega.$$

We shall prove below that the Carleman estimates of Theorems 1.1 and 2.2 also hold in this case if we choose $\|\kappa'\|_{L^\infty}$ sufficiently small.

We start by inspecting what survives in our factorization argument. We have from (2-7) $\mathcal{P}_\pm = (D + i\tau d\Phi_\pm)\cdot A_\pm(D + i\tau d\Phi_\pm)$, so that, modulo Ψ^1,

$$\mathcal{P}_\pm \equiv a^\pm_{nn}\Big(\big[D_n + S_\pm(x, D') + i\tau\big(\partial_n\Phi_\pm + S_\pm(x, \partial_{x'}\Phi_\pm)\big)\big]^2 + \frac{b^\pm_{jk}}{a^\pm_{nn}}\big(D_j + i\tau\partial_j\Phi_\pm\big)\big(D_k + i\tau\partial_k\Phi_\pm\big)\Big). \tag{4-18}$$

(See also (2-10).) The new difficulty comes from the fact that the roots in the variable D_n are not necessarily smooth: when Φ does not depend on x', the symbol of the term $b^\pm_{jk}(D_j + i\tau\partial_j\Phi_\pm)(D_k + i\tau\partial_k\Phi_\pm)$ equals $b^\pm_{jk}\xi_j\xi_k$ and thus is positive elliptic with a smooth positive square root. It is no longer the case when we have an actual dependence of Φ upon the variable x'; nevertheless, we have, as $\partial_{x'}\Phi_\pm = \partial_{x'}\kappa$,

$$\begin{aligned}\operatorname{Re}\Big(\frac{b^\pm_{jk}}{a^\pm_{nn}}(\xi_j + i\tau\partial_j\kappa)(\xi_k + i\tau\partial_k\kappa)\Big) &= \frac{b^\pm_{jk}}{a^\pm_{nn}}\xi_j\xi_k - \tau^2\frac{b^\pm_{jk}}{a^\pm_{nn}}\partial_j\kappa\partial_k\kappa \geq (\lambda^\pm_0)^2|\xi'|^2 - \tau^2(\lambda^\pm_1)^2|\partial_{x'}\kappa|^2\\ &\geq \frac{3}{4}(\lambda^\pm_0)^2|\xi'|^2 \quad \text{if } \tau\|\partial_{x'}\kappa\|_{L^\infty} \leq \frac{\lambda^\pm_0}{2\lambda^\pm_1}|\xi'|,\end{aligned}$$

where

$$\lambda_0^\pm = \inf_{\substack{x',\xi \\ |\xi'|=1}} \left(\frac{b_{jk}^\pm}{a_{nn}^\pm} \xi_j \xi_k \right)^{1/2}_{|x_n=0^\pm}, \quad \lambda_1^\pm = \sup_{\substack{x',\xi \\ |\xi'|=1}} \left(\frac{b_{jk}^\pm}{a_{nn}^\pm} \xi_j \xi_k \right)^{1/2}_{|x_n=0^\pm}.$$

As a result, the roots are smooth when $\tau \|\partial_{x'}\kappa\|_{L^\infty} \leq \dfrac{\lambda_0^\pm}{2\lambda_1^\pm}|\xi'|$.

In this case, we define $\mathfrak{m}_\pm \in \mathcal{S}^1$ such that

$$\text{for } |\xi'| \geq 1, \quad \mathfrak{m}_\pm(x,\xi') = \left(\frac{b_{jk}^\pm}{a_{nn}^\pm} (\xi_j + i\tau\partial_j\kappa)(\xi_k + i\tau\partial_k\kappa) \right)^{1/2}, \quad \mathfrak{m}_\pm(x,\xi') \geq C\langle\xi'\rangle.$$

Here we use the principal value of the square root function for complex numbers.

Introducing

$$\mathfrak{e}_\pm = \tau\big(\partial_n\Phi_\pm + S_\pm(x,\partial_{x'}\kappa)\big) + \operatorname{Re}\mathfrak{m}_\pm(x,\xi'), \mathfrak{f}_\pm = \tau\big(\partial_n\Phi_\pm + S_\pm(x,\partial_{x'}\kappa)\big) - \operatorname{Re}\mathfrak{m}_\pm(x,\xi'),$$

we set $\mathfrak{E}_\pm = \operatorname{op}(\mathfrak{e}_\pm)$ and $\mathfrak{F}_\pm = \operatorname{op}(\mathfrak{f}_\pm)$ and

$$\mathcal{P}_{\mathfrak{E}\pm} = D_n + S_\pm(x,D') - \operatorname{op}^w(\operatorname{Im}\mathfrak{m}_\pm) + i\mathfrak{E}_\pm,$$
$$\mathcal{P}_{\mathfrak{F}\pm} = D_n + S_\pm(x,D') + \operatorname{op}^w(\operatorname{Im}\mathfrak{m}_\pm) + i\mathfrak{F}_\pm.$$

Modulo the operator class Ψ^1, as in Section 2C, we may write

$$\mathcal{P}_+ \equiv \mathcal{P}_{\mathfrak{E}+} a_{nn}^+ \mathcal{P}_{\mathfrak{F}+}, \quad \mathcal{P}_- \equiv \mathcal{P}_{\mathfrak{F}-} a_{nn}^- \mathcal{P}_{\mathfrak{E}-}.$$

We keep the notation $m_\pm$ for the symbols that correspond to the previous sections, that is, if κ vanishes:

$$m_\pm(x,\xi') = \left(\frac{b_{jk}^\pm}{a_{nn}^\pm} \xi_j \xi_k \right)^{1/2}, \quad |\xi'| \geq 1.$$

As above, see (4-1), we choose the weight function such that the following property is fulfilled:

$$\frac{\alpha_+}{\alpha_-} > \sup_{\substack{x',\xi' \\ |\xi'|\geq 1}} \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}}, \quad \alpha_\pm = \partial_{x_n}\varphi_{\pm|x_n=0^\pm};$$

and we let $\sigma > 1$ be such that

$$\frac{\alpha_+}{\alpha_-} = \sigma^2 \sup_{\substack{x',\xi' \\ |\xi'|\geq 1}} \frac{m_+(x',\xi')_{|x_n=0^+}}{m_-(x',\xi')_{|x_n=0^-}}.$$

We also introduce $1 < \sigma_0 < \sigma$. As in Section 2C, we set $f_\pm = \tau\varphi'_\pm - m_\pm$ (compare with $\mathfrak{f}_\pm$ above).

We can choose $\alpha_+/\|\partial_{x'}\kappa\|_{L^\infty}$ large enough that

$$\frac{\sigma m^+_{|x_n=0^+}}{\alpha_+} < \frac{\lambda_0^+|\xi'|}{4\lambda_1^+\|\partial_{x'}\kappa\|_{L^\infty}}$$

and

$$f_\pm \geq C\lambda \quad \text{if } \tau \geq |\xi'| \frac{\lambda_0^+}{4\lambda_1^+ \|\partial_{x'}\kappa\|_{L^\infty}} \text{ for } |x_n| \text{ sufficiently small.} \tag{4-19}$$

We may then consider the following cases.

(1) When $\tau\alpha_+ \leq \sigma m^+(x',\xi')_{|x_n=0^+}$, arguing as in (4-5)–(4-6), we find that

$$\tau(\alpha_- + \beta x_n) - m_-(x',\xi')_{|x_n=0^-} \leq -C\lambda,$$

if $|x_n|$ is sufficiently small. It follows that $\mathfrak{F}_-$ is elliptic negative if $\alpha_+/\|\kappa'\|_{L^\infty}$ is sufficiently large. In this region we may thus argue as we did in Section 4C.

(2) When

$$\frac{\lambda_0^+|\xi'|}{2\lambda_1^+\|\partial_{x'}\kappa\|_{L^\infty}} \geq \tau \geq \frac{\sigma_0 m_+(x',\xi')}{\alpha_+},$$

the factorization is valid. Arguing as in (4-3)–(4-4), we find that

$$\tau(\alpha_+ + \beta x_n) - m_+(x',\xi') \geq C\lambda,$$

if $|x_n|$ is sufficiently small. It follows that $\mathfrak{F}_+$ is elliptic positive if $\alpha_+/\|\kappa'\|_{L^\infty}$ is sufficiently large. In this region we may thus argue as we did in Section 4B.

It is important to note that for β large and $\|\kappa'\|_{L^\infty}$ and $\|\kappa''\|_{L^\infty}$ sufficiently small, the weight functions $\Phi_\pm$ satisfy the (necessary and sufficient) subellipticity condition (2-26) with a loss of a half-derivative. Then the counterpart of Lemma 2.8 becomes, for $\|\kappa'\|_{L^\infty}$ sufficiently small,

$$|\mathfrak{f}_\pm| \leq \delta\lambda \implies C^{-1}\tau \leq |\xi'| \leq C\tau \text{ and } \{\xi_n + s_\pm + \operatorname{Im}(\mathfrak{m}_\pm), \mathfrak{f}_\pm\} \geq C'\lambda,$$

for some $\delta > 0$ chosen sufficiently small. This allows us to then obtain the same results as those of Lemma 3.7 for the first-order factors $\mathcal{P}_{\mathfrak{F}\pm}$.

(3) Finally we consider the region

$$\tau \geq |\xi'| \frac{\lambda_0^+}{4\lambda_1^+\|\partial_{x'}\kappa\|_{L^\infty}}.$$

There the roots are no longer smooth, but we are well inside an elliptic region; with a perturbation argument, we may in fact disregard the contribution of κ.

By (4-18), we may write

$$\mathcal{P}_\pm \equiv \underbrace{a_{nn}^\pm\left(\left[D_n + S_\pm(x,D') + i\tau\partial_n\varphi_\pm\right]^2 + \frac{b_{jk}^\pm}{a_{nn}^\pm} D_j D_k\right)}_{P_\pm^0} + R_\pm, \tag{4-20}$$

with $R_\pm = R_{1,\pm}(x,D',\tau)D_n + R_{2,\pm}(x,D',\tau)$, where $R_{j,\pm} \in \operatorname{op}^w(\mathcal{S}_\tau^j)$, with $j = 1,2$, satisfy

$$\left\| R_{j,\pm}(x,D',\tau)u \right\| \leq C\|\kappa'\|_{L^\infty}\|u\|_{L^2(\mathbb{R};\mathcal{H}^j)}. \tag{4-21}$$

The first term $P^0_\pm$ in (4-20) corresponds to the conjugated operator in the sections above, where the weight function only depends on the x_n variable. This term can be factored into two pseudodifferential first-order terms,

$$\mathcal{P}^0_+ \equiv \mathcal{P}_{E+} a^+_{nn} \mathcal{P}_{F+}, \quad \mathcal{P}^0_- \equiv \mathcal{P}_{F-} a^-_{nn} \mathcal{P}_{E-}, \tag{4-22}$$

with the notation we introduced in Section 2C. In this third region we have $f_\pm \geq C\lambda$, by (4-19). Let $\chi_2 \in \mathcal{S}^0_\tau$ be a symbol that localizes in this region and set $\Xi_2 = \mathrm{op}^w(\chi_2)$.

For $\|\kappa'\|_{L^\infty}$ bounded with (4-23), we have

$$\big\| H_\pm R_{1,\pm} D_n \Xi_2 v_\pm \big\| \lesssim \tau^k \|\kappa'\|_{L^\infty} \big\| H_\pm D_n \Xi_2 v_\pm \big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k}} + C(\kappa) \| H_\pm D_n v_\pm \|, \tag{4-23}$$

$$\big\| H_\pm R_{2,\pm} D_n \Xi_2 v_\pm \big\| \lesssim \tau^k \|\kappa'\|_{L^\infty} \| H_\pm \Xi_2 v_\pm \|_{L^2(\mathbb{R};\mathcal{H}^{2-k}} + C(\kappa) \| H_\pm v_\pm \|, \tag{4-24}$$

for $k = 0$ or $\frac{1}{2}$.

On the one hand, arguing as in Section 4B, we have (see (4-14))

$$\begin{aligned} &\big\| H_+ \mathcal{P}^0_+ \Xi_2 v_+ \big\| + \| H_+ v_+ \| \\ &\qquad \gtrsim |\mathcal{V}_{2,+}|_{\mathcal{H}^{1/2}} + \big| \Xi_2 v_{+|x_n=0^+} \big|_{\mathcal{H}^{3/2}} + \| H_+ \Xi_2 v_+ \|_{L^2(\mathbb{R};\mathcal{H}^2)} + \big\| H_+ \Xi_2 D_n v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^1)}, \end{aligned} \tag{4-25}$$

where $\mathcal{V}_{2,\pm}$ is given as in (4-10).

On the other hand, with Lemma 3.4, we have

$$\begin{aligned} \big\| H_- \mathcal{P}^0_- \Xi_2 v_- \big\|_{L^2(\mathbb{R};\mathcal{H}^{-k})} + \| H_- v_- \| + \| H_- D_n v_- \| + \big| \mathcal{V}_{2,-} + i a^-_{nn} M_- \Xi_2 v_{-|x_n=0^-} \big|_{\mathcal{H}^{1/2-k}} \\ \gtrsim \big\| H_- \mathcal{P}_{E-} \Xi_2 v_- \big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}, \end{aligned}$$

for $k = 0$ or $\frac{1}{2}$, which gives

$$\begin{aligned} \big\| H_- \mathcal{P}^0_- \Xi_2 v_- \big\| + \tau^k \| H_- v_- \| + \tau^k \| H_- D_n v_- \| + \tau^k \big| \mathcal{V}_{2,-} + i a^-_{nn} M_- \Xi_2 v_{-|x_n=0^-} \big|_{\mathcal{H}^{1/2-k}} \\ \gtrsim \tau^k \big\| H_- \mathcal{P}_{E-} \Xi_2 v_- \big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}. \end{aligned}$$

Combining this with Lemma 3.2, we obtain

$$\begin{aligned} \big\| H_- \mathcal{P}^0_- \Xi_2 v_- \big\| + \tau^k \Big(\| H_- v_- \| + \| H_- D_n v_- \| + |\mathcal{V}_{2,-}|_{\mathcal{H}^{1/2-k}} + \big| \Xi_2 v_{-|x_n=0^-} \big|_{\mathcal{H}^{3/2-k}} \Big) \\ \gtrsim \tau^k \| H_- \Xi_2 v_- \|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} + \tau^k \big\| H_+ \Xi_2 D_n v_- \big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})}. \end{aligned} \tag{4-26}$$

Now, from the transmission conditions (4-9)–(4-11), by adding ε(4-26) + (4-25) we obtain, for ε small,

$$\begin{aligned} &\big\| H_+ \mathcal{P}^0_+ \Xi_2 v_+ \big\| + \big\| H_- \mathcal{P}^0_- \Xi_2 v_- \big\| + \tau^k \big(|\theta_\varphi|_{\mathcal{H}^{3/2-k}} + |\Theta_\varphi|_{\mathcal{H}^{1/2-k}} + |v_{|x_n=0^+}|_{\mathcal{H}^{1/2-k}} \big) \\ &\quad + \tau^k \big(\| H_- v_- \| + \| H_- D_n v_- \| \big) + \| H_+ v_+ \| + \| H_+ D_n v_+ \| \\ &\quad \gtrsim \tau^k \Big(\big| \Xi_2 D_n v_{-|x_n=0^-} \big|_{\mathcal{H}^{1/2-k}} + \big| \Xi_2 D_n v_{+|x_n=0^+} \big|_{\mathcal{H}^{1/2-k}} \\ &\qquad\qquad + \big| \Xi_2 v_{-|x_n=0^-} \big|_{\mathcal{H}^{3/2-k}} + \big| \Xi_2 v_{+|x_n=0^+} \big|_{\mathcal{H}^{3/2-k}} + \| \Xi_2 v \|_{L^2(\mathbb{R};\mathcal{H}^{2-k})} \\ &\qquad\qquad + \big\| H_- \Xi_2 D_n v_- \big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} + \big\| H_+ \Xi_2 D_n v_+ \big\|_{L^2(\mathbb{R};\mathcal{H}^{1-k})} \Big). \end{aligned} \tag{4-27}$$

With (4-23)–(4-24), we see that the same estimate holds for $\mathcal{P}_\pm$ in place of $\mathcal{P}^0_\pm$ for $\|\kappa'\|_{L^\infty}$ chosen sufficiently small. This estimate is of the same quality as those obtained in the two other regions.

Summing up, we have obtained three microlocal overlapping regions and estimates in each of them. The three regions are illustrated in Figure 5. As we did above, we make sure that the preliminary cut-off region of Section 3A does not interact with the overlapping zones by choosing ϵ sufficiently small (see (3-5) and Lemma 3.1).

The overlap of the regions allows us to use a partition of unity argument, and we can conclude as in Section 4D.

5. Necessity of the geometric assumption on the weight function

Considering the operator $\mathcal{L}_\tau$ given by (1-23), we may wonder about the relevance of conditions (1-28) to derive a Carleman estimate. In the simple model and weight used here, it turns out that we can show that condition (1-28) is necessary for an estimate to hold. For simplicity, we consider a *piecewise constant* case $c = H_+c_+ + H_-c_-$ as in Section 1E.

Theorem 5.1. *Let us assume that* (1-29) *is violated, that is,*

$$\frac{\alpha_+}{\alpha_-} < \frac{m_+(\xi'_0)}{m_-(\xi'_0)} \text{ for some } \xi'_0 \in \mathbb{R}^{n-1} \setminus 0. \tag{5-1}$$

Then, for any neighborhood V of the origin, $C > 0$, and $\tau_0 > 0$, there exist

$$v = H_+v_+ + H_-v_-, \quad v_\pm \in \mathscr{C}^\infty_c(\mathbb{R}^n),$$

satisfying the transmission conditions (1-21)–(1-22) *at $x_n = 0$, and $\tau \geq \tau_0$ such that*

$$\operatorname{supp}(v) \subset V \quad \textit{and} \quad C\|\mathcal{L}_\tau v\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \leq \|v\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})}.$$

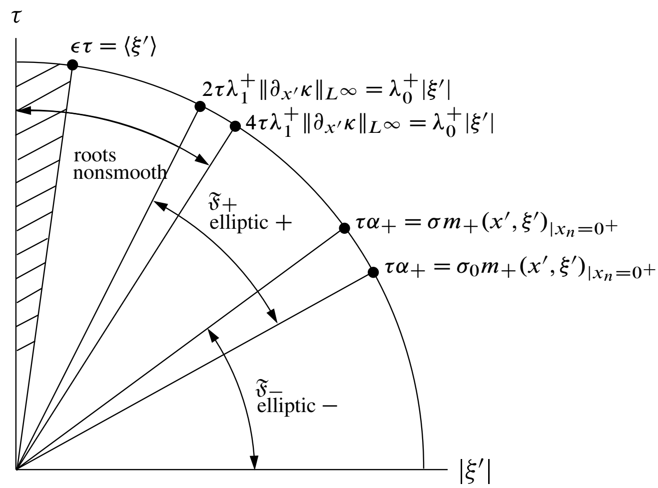

Figure 5. The overlapping microlocal regions in the case of a convex weight function.

To prove Theorem 5.1, we wish to construct a function v, depending on the parameter τ, such that $\|\mathcal{L}_\tau v\|_{L^2} \ll \|v\|_{L^2}$ as τ becomes large. The existence of such a quasimode v obviously ruins any hope of obtaining a Carleman estimate for the operator $\mathcal{L}$ with a weight function satisfying (5-1). The remainder of this section is devoted to this construction.

We set

$$(\mathcal{M}_\tau u)(\xi', x_n) = H_+(x_n) c_n^+ (D_n + ie_+)(D_n + if_+) u_+ + H_-(x_n) c_n^- (D_n + ie_-)(D_n + if_-) u_-, \quad (5\text{-}2)$$

that is, the action of the operator $\mathcal{L}_\tau$ given in (1-23) in the Fourier domain with respect to x'. Observe that the terms in each product commute here. We start by constructing a quasimode for $\mathcal{M}_\tau$, that is, functions $u_\pm(\xi', x_n)$ compactly supported in the x_n variable and in a conic neighborhood of ξ'_0 in the variable ξ' with $\|\mathcal{M}_\tau u\|_{L^2} \ll \|u\|_{L^2}$, so that u is nearly an eigenvector of $\mathcal{M}_\tau$ for the eigenvalue 0.

Condition (5-1) implies that there exists $\tau_0 > 0$ such that

$$\frac{m_-(\xi'_0)}{\alpha_-} < \tau_0 < \frac{m_+(\xi'_0)}{\alpha_+} \implies \tau_0 \alpha_+ - m_+(\xi'_0) < 0 < \tau_0 \alpha_- - m_-(\xi'_0).$$

By homogeneity, we may in fact choose (τ_0, ξ'_0) such that $\tau_0^2 + |\xi'_0|^2 = 1$. We thus have, using the notation in (1-23),

$$f_+(x_n = 0) = \tau\alpha_+ - m_+(\xi') < 0 < f_-(x_n = 0) = \tau\alpha_- - m_-(\xi'),$$

for (τ, ξ') in a conic neighborhood Γ of (τ_0, ξ'_0) in $\mathbb{R} \times \mathbb{R}^{n-1}$. Let $\chi_1 \in \mathscr{C}_c^\infty(\mathbb{R})$, $0 \le \chi_1 \le 1$, with $\chi_1 \equiv 1$ in a neighborhood of 0, such that $\operatorname{supp}(\psi) \subset \Gamma$ with

$$\psi(\tau, \xi') = \chi_1\left(\frac{\tau}{(\tau^2 + |\xi'|^2)^{1/2}} - \tau_0\right) \chi_1\left(\left|\frac{\xi'}{(\tau^2 + |\xi'|^2)^{1/2}} - \xi'_0\right|\right).$$

We thus have

$$f_+(x_n = 0) \le -C\tau, \quad C'\tau \le f_-(x_n = 0) \quad \text{in } \operatorname{supp}(\psi).$$

Let $(\tau, \xi') \in \operatorname{supp}(\psi)$. We can solve the equations

$$\begin{aligned}
\big(D_n + if_+(x_n, \xi')\big) q_+ &= 0 \quad \text{on } \mathbb{R}_+, & f_+(x_n, \xi') &= \tau\varphi'(x_n) - m_+(\xi') = f_+(0) + \tau\beta x_n,\\
\big(D_n + if_-(x_n, \xi')\big) q_- &= 0 \quad \text{on } \mathbb{R}_-, & f_-(x_n, \xi') &= \tau\varphi'(x_n) - m_-(\xi') = f_-(0) + \tau\beta x_n,\\
\big(D_n + ie_-(x_n, \xi')\big) \tilde{q}_- &= 0 \quad \text{on } \mathbb{R}_-, & e_-(x_n, \xi') &= \tau\varphi'(x_n) + m_-(\xi') = e_-(0) + \tau\beta x_n,
\end{aligned}$$

that is,

$$\begin{aligned}
q_+(\xi', x_n) &= Q_+(\xi', x_n) q_+(\xi', 0), & Q_+(\xi', x_n) &= e^{x_n(f_+(0) + \tau\beta x_n/2)},\\
q_-(\xi', x_n) &= Q_-(\xi', x_n) q_-(\xi', 0), & Q_-(\xi', x_n) &= e^{x_n(f_-(0) + \tau\beta x_n/2)},\\
\tilde{q}_-(\xi', x_n) &= \tilde{Q}_-(\xi', x_n) \tilde{q}_-(\xi', 0), & \tilde{Q}_-(\xi', x_n) &= e^{x_n(e_-(0) + \tau\beta x_n/2)}.
\end{aligned}$$

Since $f_+(0) < 0$, a solution of the form of q_+ is a good idea on $x_n \ge 0$ as long as $\tau\beta x_n + 2f_+(0) \le 0$, that is, $x_n \le 2|f_+(0)|/\tau\beta$. Similarly, as $f_-(0) > 0$ (resp. $e_-(0) > 0$), a solution of the form of q_- (resp.

$\tilde{q}_-$) is a good idea on $x_n \le 0$ as long as $\tau\beta x_n + 2f_-(0) \ge 0$ (resp. $\tau\beta x_n + 2e_-(0) \ge 0$). To secure this, we introduce a cut-off function $\chi_0 \in \mathscr{C}_c^\infty((-1,1);[0,1])$, equal to 1 on $\left[-\frac{1}{2}, \frac{1}{2}\right]$, and for $\gamma \ge 1$ we define

$$u_+(\xi', x_n) = Q_+(\xi', x_n)\psi(\tau, \xi')\chi_0\left(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\right) \tag{5-3}$$

and

$$u_-(\xi', x_n) = aQ_-(\xi', x_n)\psi(\tau, \xi')\chi_0\left(\frac{\tau\beta\gamma x_n}{f_-(0)}\right) + b\tilde{Q}_-(\xi', x_n)\psi(\tau, \xi')\chi_0\left(\frac{\tau\beta\gamma x_n}{e_-(0)}\right), \tag{5-4}$$

with $a, b \in \mathbb{R}$ and

$$u(\xi', x_n) = H_+(x_n)u_+(\xi', x_n) + H_-(x_n)u_-(\xi', x_n).$$

The factor γ is introduced to control the size of the support in the x_n direction. Observe that we can satisfy the transmission condition (1-21)–(1-22) by choosing the coefficients a and b. Transmission condition (1-21) implies

$$a + b = 1. \tag{5-5}$$

Transmission condition (1-22) and the equations satisfied by Q_+, Q_- and $\tilde{Q}_-$ imply

$$c_+m_+ = c_-(a-b)m_-. \tag{5-6}$$

In particular, note that $a - b \ge 0$, which gives $a \ge \frac{1}{2}$.

Lemma 5.2. *For τ sufficiently large, we have*

$$\|\mathcal{M}_\tau u\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \le C(\gamma^2 + \tau^2)\gamma\tau^{n-1}e^{-C'\tau/\gamma}$$

and

$$\|u\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \ge C\tau^{n-2}\left(1 - e^{-C'\tau/\gamma}\right).$$

See Section AB.3 for a proof.

We now introduce

$$v_\pm(x', x_n) = (2\pi)^{-(n-1)}\chi_0\left(\left|\tau^{1/2}x'\right|\right)\check{\hat{u}}_\pm(x', x_n) = (2\pi)^{-(n-1)}\chi_0\left(\left|\tau^{1/2}x'\right|\right)\hat{u}_\pm(-x', x_n),$$

that is, a localized version of the inverse Fourier transform (in x') of $u_\pm$. The functions $v_\pm$ are smooth and compactly supported in $\mathbb{R}^{n-1}_\pm \times \mathbb{R}$ and they satisfy transmission conditions (1-21)–(1-22). We set $v(x', x_n) = H_+(x_n)v_+(x', x_n) + H_-(x_n)v_-(x', x_n)$. In fact, we have the following estimates.

Lemma 5.3. *Let $N \in \mathbb{N}$. For τ sufficiently large, we have*

$$\|\mathcal{L}_\tau v\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \le C(\gamma^2 + \tau^2)\gamma\tau^{n-1}e^{-C'\tau/\gamma} + C_{\gamma,N}\tau^{-N}$$

and

$$\|v\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \ge C\tau^{n-2}\left(1 - e^{-C'\tau/\gamma}\right) - C_{\gamma,N}\tau^{-N}.$$

See Section AB.4 for a proof.

We may now conclude the proof of Theorem 5.1. In fact, if V is an arbitrary neighborhood of the origin, we choose τ and γ sufficiently large that $\operatorname{supp}(v) \subset V$. We then keep γ fixed. The estimates of Lemma 5.3 show that

$$\|\mathcal{L}_\tau v\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \|v\|^{-1}_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \xrightarrow[\tau\to\infty]{} 0.$$

Remark 5.4. As opposed to the analogy we give at the beginning of Section 1F, the construction of this quasimode does not simply rely on one of the first-order factors. The transmission conditions are responsible for this fact. The construction relies on the factor $D_n + if_+$ in $x_n \geq 0$, that is, a one-dimensional space of solutions (see (5-3)), and on both factors $D_n + if_-$ and $D_n + ie_-$ in $x_n \geq 0$, that is, a two-dimensional space of solutions (see (5-4)). See also (5-5) and (5-6).

Appendix

AA. *A few facts on pseudodifferential operators.*

AA.1. *Standard classes and Weyl quantization.* We define for $m \in \mathbb{R}$ the class of tangential symbols $\mathcal{S}^m$ as the smooth functions on $\mathbb{R}^n \times \mathbb{R}^{n-1}$ such that for all $(\alpha, \beta) \in \mathbb{N}^n \times \mathbb{N}^{n-1}$,

$$N_{\alpha\beta}(a) = \sup_{(x,\xi')\in\mathbb{R}^n\times\mathbb{R}^{n-1}} \langle\xi'\rangle^{-m+|\beta|} \left|(\partial_x^\alpha \partial_{\xi'}^\beta a)(x,\xi')\right| < \infty, \tag{A-1}$$

with $\langle\xi'\rangle^2 = 1 + |\xi'|^2$. The quantities on the left-hand side are called the seminorms of the symbol a. For $a \in \mathcal{S}^m$, let $\operatorname{op}(a)$ be the operator defined on $\mathscr{S}(\mathbb{R}^n)$ by

$$(\operatorname{op}(a)u)(x', x_n) = a(x, D')u(x', x_n) = \int_{\mathbb{R}^{n-1}} e^{ix'\cdot\xi'} a(x', x_n, \xi')\hat{u}(\xi', x_n)\, d\xi' (2\pi)^{1-n}, \tag{A-2}$$

with $(x', x_n) \in \mathbb{R}^{n-1} \times \mathbb{R}$, where $\hat{u}$ is the partial Fourier transform of u with respect to the variable x'. For all $(k, s) \in \mathbb{Z} \times \mathbb{R}$, we have

$$\operatorname{op}(a) : H^k\big(\mathbb{R}_{x_n}; H^{s+m}(\mathbb{R}^{n-1}_{x'})\big) \to H^k\big(\mathbb{R}_{x_n}; H^{s}(\mathbb{R}^{n-1}_{x'})\big) \quad \text{continuously}, \tag{A-3}$$

and the norm of this mapping depends only on $\{N_{\alpha\beta}(a)\}_{|\alpha|+|\beta|\leq\mu(k,s,m,n)}$, where $\mu : \mathbb{Z}\times\mathbb{R}\times\mathbb{R}\times\mathbb{N} \to \mathbb{N}$.

We shall also use the *Weyl quantization* of a, denoted by $\operatorname{op}^w(a)$ and given by the formula

$$\begin{aligned}(\operatorname{op}^w(a)u)(x', x_n) &= a^w(x, D')u(x', x_n)\\ &= \iint_{\mathbb{R}^{2n-2}} e^{i(x'-y')\cdot\xi'} a\Big(\frac{x'+y'}{2}, x_n, \xi'\Big) u(y', x_n)\, dy'\, d\xi' (2\pi)^{1-n}.\end{aligned} \tag{A-4}$$

Property (A-3) holds as well for $\operatorname{op}^w(a)$. A nice feature of the Weyl quantization that we use in this article is the simple relationship with adjoint operators with the formula

$$(\operatorname{op}^w(a))^* = \operatorname{op}^w(\bar{a}), \tag{A-5}$$

so that for a real-valued symbol $a \in \mathcal{S}^m$, we have $(\mathrm{op}^w(a))^* = \mathrm{op}^w(a)$. We have also, for $a_j \in \mathcal{S}^{m_j}$, $j = 1, 2$,

$$\mathrm{op}^w(a_1)\mathrm{op}^w(a_2) = \mathrm{op}^w(a_1 \sharp a_2), \quad a_1 \sharp a_2 \in \mathcal{S}^{m_1+m_2}, \tag{A-6}$$

with, for any $N \in \mathbb{N}$,

$$(a_1 \sharp a_2)(x,\xi) - \sum_{j<N} \left(\frac{i\sigma(D_{x'}, D_{\xi'}; D_{y'}, D_{\eta'})}{2} \right)^j \frac{a_1(x,\xi)a_2(y,\eta)}{j!} \Big|_{(y,\eta)=(x,\xi)} \in \mathcal{S}^{m-N}, \tag{A-7}$$

where σ is the symplectic two-form, that is, $\sigma(x,\xi; y,\eta) = y \cdot \xi - x \cdot \eta$. In particular,

$$\mathrm{op}^w(a_1)\mathrm{op}^w(a_2) = \mathrm{op}^w(a_1 a_2) + \mathrm{op}^w(r_1), \qquad r_1 \in \mathcal{S}^{m_1+m_2-1}, \tag{A-8}$$

$$\text{with } r_1 = \frac{1}{2i}\{a_1, a_2\} + r_2, \qquad r_2 \in \mathcal{S}^{m_1+m_2-2}, \tag{A-9}$$

$$\big[\mathrm{op}^w(a_1), \mathrm{op}^w(a_2)\big] = \mathrm{op}^w\left(\frac{1}{i}\{a_1, a_2\}\right) + \mathrm{op}^w(r_3), \qquad r_3 \in \mathcal{S}^{m_1+m_2-3}, \tag{A-10}$$

where $\{a_1, a_2\}$ is the Poisson bracket. Also, for $b_j \in \mathcal{S}^{m_j}$, $j = 1, 2$, both real-valued, we have

$$\big[\mathrm{op}^w(b_1), i\,\mathrm{op}^w(b_2)\big] = \mathrm{op}^w(\{b_1, b_2\}) + \mathrm{op}^w(s_3), \quad s_3 \text{ real-valued} \in \mathcal{S}^{m_1+m_2-3}. \tag{A-11}$$

Lemma A.1. *Let $a \in \mathcal{S}^1$ be such that $a(x,\xi') \geq \mu\langle\xi'\rangle$, with $\mu \geq 0$. Then there exists $C > 0$ such that*

$$\mathrm{op}^w(a) + C \geq \mu\langle D'\rangle, \quad (\mathrm{op}^w(a))^2 + C \geq \mu^2\langle D'\rangle^2.$$

Proof. The first statement follows from the sharp Gårding inequality [Hörmander 1985a, Chapters 18.1,18.5] applied to the nonnegative first-order symbol $a(x,\xi') - \mu\langle\xi'\rangle$; also, $(\mathrm{op}^w(a))^2 = \mathrm{op}^w(a^2) + \mathrm{op}^w(r)$ with $r \in \mathcal{S}^0$, so that the Fefferman–Phong inequality [Hörmander 1985a, Chapter 18.5] applied to the second-order $a^2 - \mu^2\langle\xi'\rangle^2$ implies the result. ☐

AA.2. *Semiclassical pseudodifferential calculus with a large parameter.* We let $\tau \in \mathbb{R}$ be such that $\tau \geq \tau_0 \geq 1$. We set $\lambda^2 = 1 + \tau^2 + |\xi'|^2$. We define, for $m \in \mathbb{R}$, the class of symbols $\mathcal{S}^m_\tau$ as the smooth functions on $\mathbb{R}^n \times \mathbb{R}^{n-1}$ depending on the parameter τ such that for all $(\alpha, \beta) \in \mathbb{N}^n \times \mathbb{N}^{n-1}$,

$$N_{\alpha\beta}(a) = \sup_{\substack{(x,\xi')\in\mathbb{R}^n\times\mathbb{R}^{n-1} \\ \tau\geq\tau_0}} \lambda^{-m+|\beta|} \big|(\partial_x^\alpha \partial_{\xi'}^\beta a)(x,\xi',\tau)\big| < \infty. \tag{A-12}$$

Note that $\mathcal{S}^0_\tau \subset \mathcal{S}^0$. The associated operators are defined by (A-2). We can introduce Sobolev spaces and Sobolev norms which are adapted to the scaling large parameter τ. Let $s \in \mathbb{R}$; we set

$$\|u\|_{\mathcal{H}^s} := \|\Lambda^s u\|_{L^2(\mathbb{R}^{n-1})}, \quad \text{with } \Lambda^s := \mathrm{op}(\lambda^s),$$

and

$$\mathcal{H}^s = \mathcal{H}^s(\mathbb{R}^{n-1}) := \big\{u \in \mathcal{S}'(\mathbb{R}^{n-1}) : \|u\|_{\mathcal{H}^s} < \infty\big\}.$$

The space $\mathcal{H}^s$ is algebraically equal to the classical Sobolev space $H^s(\mathbb{R}^{n-1})$, whose norm is denoted by $\| \,.\, \|_{H^s}$. For $s \geq 0$, we have

$$\|u\|_{\mathcal{H}^s} \sim \tau^s \|u\|_{L^2(\mathbb{R}^{n-1})} + \|\langle D' \rangle^s u\|_{L^2(\mathbb{R}^{n-1})}.$$

If $a \in \mathcal{S}^m_\tau$ then, for all $(k, s) \in \mathbb{Z} \times \mathbb{R}$, we have

$$\operatorname{op}(a) : H^k\big(\mathbb{R}_{x_n}; \mathcal{H}^{s+m}\big) \to H^k\big(\mathbb{R}_{x_n}; \mathcal{H}^s\big(\mathbb{R}^{n-1}_{x'}\big)\big) \quad \text{continuously}, \tag{A-13}$$

and the norm of this mapping depends only on $\{N_{\alpha\beta}(a)\}_{|\alpha|+|\beta| \leq \mu(k,s,m,n)}$, where $\mu : \mathbb{Z} \times \mathbb{R} \times \mathbb{R} \times \mathbb{N} \to \mathbb{N}$.

For the calculus with a large parameter, we shall also use the Weyl quantization of (A-4). The formulae (A-5)–(A-11) hold as well, with $\mathcal{S}^m$ everywhere replaced by $\mathcal{S}^m_\tau$. We shall often use the Gårding inequality as stated in the following lemma.

Lemma A.2. *Let $a \in \mathcal{S}^m_\tau$ such that $\operatorname{Re} a \geq C\lambda^m$. Then*

$$\operatorname{Re}\big(\operatorname{op}^w(a)u, u\big) \gtrsim \|u\|^2_{L^2(\mathbb{R}; \mathcal{H}^{m/2})},$$

for τ sufficiently large.

Proof. The proof follows from the sharp Gårding inequality [Hörmander 1985a, Chapters 18.1 and 18.5] applied to the nonnegative symbol $a - C\lambda^m$. □

Definition A.3. The essential support of a symbol $a \in \mathcal{S}^m_\tau$, denoted by $\operatorname{esssupp}(a)$, is the complement of the largest open set of $\mathbb{R} \times \mathbb{R}^{n-1} \times \{\tau \geq 1\}$ where the estimates for $\mathcal{S}^{-\infty}_\tau = \cap_{m \in \mathbb{R}} \mathcal{S}^m_\tau$ hold.

For technical reasons we shall often need the following result.

Lemma A.4. *Let $m, m' \in \mathbb{R}$ and $a_1(x, \xi') \in \mathcal{S}^m$ and $a_2(x, \xi', \tau) \in \mathcal{S}^{m'}_\tau$ such that the essential support of a_2 is contained in a region where $\langle \xi' \rangle \gtrsim \tau$. Then*

$$\operatorname{op}^w(a_1)\operatorname{op}^w(a_2) = \operatorname{op}^w(b_1), \quad \operatorname{op}^w(a_2)\operatorname{op}^w(a_1) = \operatorname{op}^w(b_2),$$

with $b_1, b_2 \in \mathcal{S}^{m+m'}_\tau$. Moreover, the asympotic series of (A-7) is also valid for these cases (with $\mathcal{S}^m$ replaced by $\mathcal{S}^m_\tau$).

Proof. As the essential support is invariant when we change quantization, we may simply use the standard quantization in the proof. With a_1 and a_2 satisfying the assumption listed above, we thus consider $\operatorname{op}(a_1)\operatorname{op}(a_2)$. For fixed τ, the standard composition formula applies, and we have (see [Hörmander 1985a, Section 18.1] or [Alinhac and Gérard 2007])

$$(a_1 \circ a_2)(x, \xi', \tau) = (2\pi)^{1-n} \iint e^{-iy' \cdot \eta'} a_1(x, \xi' - \eta') a_2\big(x' - y', x_n, \xi', \tau\big)\, dy'\, d\eta'.$$

Properties of oscillatory integrals (see, for example, [Alinhac and Gérard 2007, Appendices I.8.1 and I.8.2]) give, for some $k \in \mathbb{N}$,

$$\big|(a_1 \circ a_2)(x, \xi', \tau)\big| \leq C \sup_{\substack{|\alpha|+|\beta| \leq k \\ (y', \eta') \in R^{2n-2}}} \langle (y', \eta') \rangle^{-|m|} \big|\partial^\alpha_{y'} \partial^\beta_{\eta'} a_1(x, \xi' - \eta') a_2\big(x' - y', x_n, \xi', \tau\big)\big|.$$

In a region $\langle\xi'\rangle \gtrsim \tau$ that contains the essential support of a_2, we have $\langle\xi'\rangle \sim \lambda$. With the Peetre inequality, we thus obtain

$$\big|(a_1 \circ a_2)(x, \xi', \tau)\big| \lesssim \langle\eta'\rangle^{-|m|}\langle\xi' - \eta'\rangle^m \lambda^{m'} \lesssim \langle\xi'\rangle^m \lambda^{m'} \lesssim \lambda^{m+m'}.$$

In a region $\langle\xi'\rangle \lesssim \tau$ outside of the essential support of a_2, we find, for any $\ell \in \mathbb{N}$,

$$\big|(a_1 \circ a_2)(x, \xi', \tau)\big| \lesssim \langle\eta'\rangle^{-|m|}\langle\xi' - \eta'\rangle^m \lambda^{-\ell} \lesssim \langle\xi'\rangle^m \lambda^{-\ell} \lesssim \lambda^{m-\ell}.$$

In the whole phase space we thus obtain $\big|(a_1 \circ a_2)(x, \xi')\big| \lesssim \lambda^{m+m'}$. The estimation of

$$\big|\partial_x^\alpha \partial_{\xi'}^\beta (a_1 \circ a_2)(x, \xi', \tau)\big|$$

can be done similarly to give

$$\big|\partial_x^\alpha \partial_\xi^\beta (a_1 \circ a_2)(x, \xi', \tau)\big| \lesssim \lambda^{m+m'-|\beta|}.$$

Hence $a_1 \circ a_2 \in \mathcal{S}_\tau^{m+m'}$. We also obtain the asymptotic series (following the references cited above)

$$(a_1 \circ a_2)(x, \xi', \tau) - \sum_{j<N} \frac{(iD_\xi \cdot D_y)^j a_1(x, \xi) a_2(y, \eta, \tau)}{j!}\Big|_{(y,\eta)=(x,\xi)} \in \mathcal{S}_\tau^{m+m'-N},$$

where each term is respectively in $\mathcal{S}_\tau^{m+m'-j}$ by the arguments given above. From this series, the corresponding Weyl quantization series follows.

For the second result, considering the adjoint operator $\big(\mathrm{op}(a_2)\mathrm{op}(a_1)\big)^*$ yields a composition of operators as in the first case. The second result thus follows from the first one. □

Remark A.5. The symbol class and calculus we have introduced in this section can be written as $\mathcal{S}_\tau^m = \mathcal{S}(\lambda^m, g)$ in the sense of the Weyl–Hörmander calculus [Hörmander 1985a, Sections 18.4–18.6] with the phase-space metric $g = |dx|^2 + |d\xi|^2/\lambda^2$.

AB. *Proofs of some intermediate results.*

AB.1. *Proof of Lemma 2.8.* For simplicity we remove the $\pm$ notation here. We first prove that there exist $C > 0$ and $\eta > 0$ such that

$$|q_2| \leq \eta\tau^2 \text{ and } |q_1| \leq \eta\tau^2 \implies \{q_2, q_1\} \geq C\tau^3. \tag{A-14}$$

We set

$$\tilde{q}_2 = (\xi_n + s)^2 + \frac{b_{jk}}{a_{nn}}\xi_j\xi_k - (\varphi')^2, \quad \tilde{q}_1 = \varphi'(\xi_n + s).$$

We have $q_j(x, \xi) = \tau^2 \tilde{q}_j(x, \xi/\tau)$. Observe next that we have $\{q_2, q_1\}(x, \xi) = \tau^3\{\tilde{q}_2, \tilde{q}_1\}(x, \xi/\tau)$. We thus have $\tilde{q}_2 = 0$ and $\tilde{q}_1 = 0 \implies \{\tilde{q}_2, \tilde{q}_1\} > 0$. As $\tilde{q}_2(x, \xi) = 0$ and $\tilde{q}_1(x, \xi) = 0$ yield a compact set for (x, ξ) (recall that x lies in a compact set K here), for some $C > 0$, we have

$$\tilde{q}_2 = 0 \text{ and } \tilde{q}_1 = 0 \implies \{\tilde{q}_2, \tilde{q}_1\} > C.$$

This remains true locally, that is, for some $C' > 0$ and $\eta > 0$,

$$|\tilde{q}_2| \le \eta \text{ and } |\tilde{q}_1| \le \eta \implies \{\tilde{q}_2, \tilde{q}_1\} > C'.$$

Then (A-14) follows.

We note that $q_2^{\pm} = 0$ and $q_1^{\pm} = 0$ imply $\tau \sim |\xi'|$. Hence, for τ sufficiently large, we have (2-25). We thus obtain

$$q_2^{\pm} = 0 \text{ and } q_1^{\pm} = 0 \iff \xi_n + s_{\pm} = 0 \text{ and } \tau\varphi'_{\pm} = m_{\pm}.$$

Let us assume that $|f| \le \delta\lambda$ with δ small and $\lambda^2 = 1 + \tau^2 + |\xi'|^2$. Then

$$\tau \lesssim |\xi'| \lesssim \tau. \tag{A-15}$$

We set $\xi_n = -s$, that is, we choose $q_1 = 0$. A direct computation yields

$$\{q_2, q_1\} = \tau e\varphi'\{\xi_n + s, f\} + \tau f\varphi'\{\xi_n + s, e\} \quad \text{if } \xi_n + s = 0.$$

With (2-25), we have $|q_2| \le C\delta\tau^2$. For δ small, by (A-14) we have $\{q_2, q_1\} \ge C\tau^3$. Since $f\tau\varphi'\{\xi_n+s, e\} \le C\delta\tau^3$, we obtain $e\tau\varphi'\{\xi_n + s, f\} \ge C\tau^3$, with $C > 0$, for δ sufficiently small. With (A-15), we have $\tau \lesssim e \lesssim \tau$ and the result follows. □

AB.2. *Proof of Lemma 3.1.* We set $s = 2\ell + 1$ and $\omega_1 = \mathrm{op}(\psi_\epsilon)\omega$. We write

$$\begin{aligned}
2\,\mathrm{Re}\big(\mathcal{P}_{F+}\omega_1, iH_+\tau^s\omega_1\big) &= \big(i[D_n, H_+]\omega_1, \tau^s\omega_1\big) + 2\big(F_+\omega_1, H_+\tau^s\omega_1\big) \\
&= \tau^s\big|\omega_{1|x_n=0^+}\big|^2_{L^2(\mathbb{R}^{n-1})} + 2\big(\tau^{s+1}\varphi'\omega_1, H_+\omega_1\big) - 2\big(\tau^s M_+\omega_1, H_+\omega_1\big) \\
&\ge \tau^s\big|\omega_{1|x_n=0^+}\big|^2_{L^2(\mathbb{R}^{n-1})} + 2\big(\tau^{s+1}C_0\omega_1, H_+\omega_1\big) - 2C_1\tau^s\|H_+\omega_1\|^2_{L^2(\mathbb{R};H^{1/2}(\mathbb{R}^{n-1}))},
\end{aligned}$$

by (3-4). We have

$$\begin{aligned}
&2\big(\tau^{s+1}C_0\omega_1, H_+\omega_1\big) - 2C_1\tau^s\|H_+\omega_1\|^2_{L^2(\mathbb{R};H^{1/2}(\mathbb{R}^{n-1}))} \\
&\qquad = 2\tau^s(2\pi)^{1-n}\int_0^\infty\int_{\mathbb{R}^{n-1}}\big(C_0\tau - C_1\langle\xi'\rangle\big)\big|\psi_\epsilon(\tau,\xi')\hat{\omega}(\xi', x_n)\big|^2\,d\xi'\,dx_n.
\end{aligned}$$

As $\tau \ge C\langle\xi\rangle/\epsilon$ in $\mathrm{supp}(\psi_\epsilon)$, for ϵ sufficiently small we have

$$\begin{aligned}
&2\big(\tau^{s+1}C_0\omega_1, H_+\omega_1\big) - 2C_1\tau^s\|H_+\omega_1\|^2_{L^2(\mathbb{R};H^{1/2}(\mathbb{R}^{n-1}))} \\
&\qquad \gtrsim \int_0^\infty\int_{\mathbb{R}^{n-1}}\lambda^{s+1}\big|\psi_\epsilon(\tau,\xi')\hat{\omega}(\xi', x_n)\big|^2\,d\xi'\,dx_n \gtrsim \|H_+\omega_1\|^2_{L^2(\mathbb{R};\mathcal{H}^{\ell+1})}.
\end{aligned}$$

Similarly, we find $\tau^s\big|\omega_{1|x_n=0^+}\big|^2_{L^2(\mathbb{R}^{n-1})} \gtrsim \big|\omega_{1|x_n=0^+}\big|^2_{\mathcal{H}^{\ell+1/2}}$. The result for $\mathcal{P}_{E+}$ follows from the Young inequality. The proof is identical for $\mathcal{P}_{F+}$.

On the other side of the interface we write

$$\begin{aligned}
2\,\mathrm{Re}\big(H_-\mathcal{P}_{F-}\omega_1, iH_-\tau^s\omega_1\big) &= \big(i[D_n, H_-]\omega_1, \tau^s\omega_1\big) + 2\big(F_-\omega_1, H_-\tau^s\omega_1\big) \\
&= -\tau^s\big|\omega_{1|x_n=0^-}\big|^2_{L^2(\mathbb{R}^{n-1})} + 2\big(\tau^{s+1}\varphi'\omega_1, H_-\omega_1\big) - 2\big(\tau^s M_-\omega_1, H_-\omega_1\big),
\end{aligned}$$

which yields a boundary contribution with the opposite sign. □

AB.3. *Proof of Lemma 5.2.* Let $(\tau,\xi')\in\operatorname{supp}(\psi)$. We choose τ sufficiently large that, through $\operatorname{supp}(\psi)$, $|\xi'|$ is itself sufficiently large that the symbol $m_\pm$ is homogeneous — see (2-15).

We set

$$y_+(\xi',x_n)=Q_+(\xi',x_n)\chi_0\Big(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\Big),$$
$$y_-(\xi',x_n)=aQ_-(\xi',x_n)\chi_0\Big(\frac{\tau\beta\gamma x_n}{f_-(0)}\Big)+b\tilde Q_-(\xi',x_n)\chi_0\Big(\frac{\tau\beta\gamma x_n}{e_-(0)}\Big).$$

On the one hand, we have $i(D_n+if_+)y_+=\dfrac{\tau\beta\gamma}{|f_+(0)|}Q_+(\xi',x_n)\chi_0'\Big(\dfrac{\tau\beta\gamma x_n}{|f_+(0)|}\Big)$ and

$$(\mathcal{M}_\tau y_+)(\xi',x_n)=2\tau\beta\gamma c_+m_+\frac{Q_+(\xi',x_n)}{|f_+(0)|}\chi_0'\Big(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\Big)-(\tau\beta\gamma)^2c_+\frac{Q_+(\xi',x_n)}{|f_+(0)|^2}\chi_0''\Big(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\Big),$$

as $D_n+ie_+=D_n+i(f_++2m_+)$, so that

$$\int_0^{+\infty}\big|(\mathcal{M}_\tau y_+)(\xi',x_n)\big|^2\,dx_n\le 8c_+^2m_+^2\Big(\frac{\tau\beta\gamma}{f_+(0)}\Big)^2\int_0^{+\infty}\chi_0'\Big(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\Big)^2e^{x_n(2f_+(0)+\tau\beta x_n)}\,dx_n$$
$$+2c_+^2\Big(\frac{\tau\beta\gamma}{f_+(0)}\Big)^4\int_0^{+\infty}\chi_0''\Big(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\Big)^2e^{x_n(2f_+(0)+\tau\beta x_n)}\,dx_n.$$

On the support of $\chi_0^{(j)}(\tau\beta\gamma x_n/|f_+(0)|)$, $j=1,2$, we have $|f_+(0)|/(2\tau\beta\gamma)\le x_n\le|f_+(0)|/(\tau\beta\gamma)$, and in particular $2f_+(0)+\tau\beta\gamma x_n\le-|f_+(0)|$, which gives

$$\int_0^{+\infty}\big|(\mathcal{M}_\tau y_+)(\xi',x_n)\big|^2\,dx_n$$
$$\le c_+^2\Big(\frac{\tau\beta\gamma}{f_+(0)}\Big)^2\Big(8m_+^2\|\chi_0'\|_{L^\infty}^2+2\Big(\frac{\tau\beta\gamma}{f_+(0)}\Big)^2\|\chi_0''\|_{L^\infty}^2\Big)\int_{\frac{|f_+(0)|}{2\tau\beta\gamma}\le x_n\le\frac{|f_+(0)|}{\tau\beta\gamma}}e^{-|f_+(0)|x_n}\,dx_n$$
$$\le c_+^2\frac{\tau\beta\gamma}{|f_+(0)|}\Big(4m_+^2\|\chi_0'\|_{L^\infty}^2+\Big(\frac{\tau\beta\gamma}{f_+(0)}\Big)^2\|\chi_0''\|_{L^\infty}^2\Big)e^{-\frac{f_+(0)^2}{2\tau\beta\gamma}}.$$

Similarly, we have

$$(\mathcal{M}_\tau y_-)(\xi',x_n)=2\tau\beta\gamma c_-m_-\Big(\frac{aQ_-(\xi',x_n)}{f_-(0)}\chi_0'\Big(\frac{\tau\beta\gamma x_n}{f_-(0)}\Big)-b\frac{\tilde Q_-(\xi',x_n)}{e_-(0)}\chi_0'\Big(\frac{\tau\beta\gamma x_n}{e_-(0)}\Big)\Big)$$
$$-c_-(\tau\beta\gamma)^2\Big(a\frac{Q_-(\xi',x_n)}{f_-(0)^2}\chi_0''\Big(\frac{\tau\beta\gamma x_n}{f_-(0)}\Big)+b\frac{\tilde Q_-(\xi',x_n)}{e_-(0)^2}\chi_0''\Big(\frac{\tau\beta\gamma x_n}{e_-(0)}\Big)\Big),$$

and because of the support of $\chi_0^{(j)}\Big(\dfrac{\tau\beta\gamma x_n}{f_-(0)}\Big)$, resp. $\chi_0^{(j)}\Big(\dfrac{\tau\beta\gamma x_n}{e_-(0)}\Big)$, $j=1,2$, for $x_n\le0$, we obtain

$$\int_{-\infty}^0\big|(\mathcal{M}_\tau y_-)(\xi',x_n)\big|^2\,dx_n\le2c_-^2\frac{\tau\beta\gamma a^2}{f_-(0)}\Big(4m_-^2\|\chi_0'\|_{L^\infty}^2+\|\chi_0''\|_{L^\infty}^2\Big(\frac{\tau\beta\gamma}{f_-(0)}\Big)^2\Big)e^{-\frac{f_-(0)^2}{2\tau\beta\gamma}}$$
$$+2c_-^2\frac{\tau\beta\gamma b^2}{e_-(0)}\Big(4m_-^2\|\chi_0'\|_{L^\infty}^2+\|\chi_0''\|_{L^\infty}^2\Big(\frac{\tau\beta\gamma}{e_-(0)}\Big)^2\Big)e^{-\frac{e_-(0)^2}{2\tau\beta\gamma}}.$$

Now we have $(\mathcal{M}_\tau u)(\xi', x_n) = \psi(\tau, \xi')(\mathcal{M}_\tau y)(\xi', x_n)$. As $|\xi'| \sim \tau$ in $\operatorname{supp}(\psi)$, we obtain

$$\|\mathcal{M}_\tau u\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \le C(\gamma^2+\tau^2)\gamma e^{-C'\tau/\gamma} \int_{\mathbb{R}^{n-1}} \psi(\tau,\xi')^2\, d\xi'.$$

With the change of variable $\xi' = \tau\eta$, we find

$$\int_{\mathbb{R}^{n-1}} \psi(\tau,\xi')^2\, d\xi' = C\tau^{n-1}, \tag{A-16}$$

which gives the first result.

On the other hand, observe now that

$$\begin{aligned}
\|y_+\|^2_{L^2(\mathbb{R}_+)} &= \int_0^{+\infty} Q_+(\xi', x_n)^2 \chi_0\Big(\frac{\tau\beta\gamma x_n}{|f_+(0)|}\Big)^2\, dx_n \\
&\ge \int_{0\le \frac{\tau\beta\gamma x_n}{|f_+(0)|}\le 1/2} e^{x_n(2f_+(0)+\tau\beta x_n)}\, dx_n = \frac{|f_+(0)|}{\tau\beta\gamma}\int_0^{1/2} e^{2t\frac{|f_+(0)|}{\tau\beta\gamma}\left(f_+(0)+t\frac{|f_+(0)|}{2\gamma}\right)} dt \\
&\ge \frac{|f_+(0)|}{\tau\beta\gamma}\int_0^{1/2} e^{-2t\frac{|f_+(0)|^2}{\tau\beta\gamma}}\, dt = \frac{1}{2|f_+(0)|}\Big(1-e^{-\frac{|f_+(0)|^2}{\tau\beta\gamma}}\Big).
\end{aligned}$$

We also have

$$\begin{aligned}
\|y_-\|^2_{L^2(\mathbb{R}_-)} &= \int_{-\infty}^0 \Big(aQ_-(\xi',x_n)\chi_0\Big(\frac{\tau\beta\gamma x_n}{f_-(0)}\Big) + b\tilde{Q}_-(\xi',x_n)\chi_0\Big(\frac{\tau\beta\gamma x_n}{e_-(0)}\Big)\Big)^2\, dx_n \\
&\ge \int_{-1/2\le\frac{\tau\beta\gamma x_n}{f_-(0)}\le 0} e^{x_n(2f_-(0)+\tau\beta x_n)}\big(a+be^{x_n(e_-(0)-f_-(0))}\big)^2\, dx_n,
\end{aligned}$$

and as $e_-(0)-f_-(0) = 2m_- \ge 0$ and $a+b=1$ and $a\ge\frac12$, we have $a+be^{x_n(e_-(0)-f_-(0))}\ge\frac12$, and thus obtain

$$\|y_-\|^2_{L^2(\mathbb{R}_-)} \ge \frac14\int_{-1/2\le\frac{\tau\beta\gamma x_n}{f_-(0)}\le 0} e^{x_n(2f_-(0)+\tau\beta x_n)}\, dx_n \ge \frac{1}{8f_-(0)}\Big(1-e^{-\frac{|f_-(0)|^2}{\tau\beta\gamma}}\Big),$$

arguing as above. As a result, using (A-16), we have

$$\|u\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R})} \ge C\tau^{n-2}\big(1-e^{-C'\tau/\gamma}\big). \qquad \square$$

AB.4. *Proof of Lemma 5.3*. We start with the second result. We set

$$z_+ = \big(1-\chi_0\big(|\tau^{1/2}x'|\big)\big)\check{\hat{u}}_+(x',x_n), \quad \text{for } x_n\ge 0.$$

We shall prove that for all $N\in\mathbb{N}$, we have $\|z_+\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R}_+)} \le C_{\gamma,N}\tau^{-N}$.

From the definition of χ_0, we find

$$\|z_+\|^2_{L^2(\mathbb{R}^{n-1}\times\mathbb{R}_+)} \le \int_{|\tau^{1/2}x'|\ge 1/2}\int_{\mathbb{R}_+} |\hat{u}_+(x',x_n)|^2\, dx'\, dx_n.$$

Recalling the definition of u_+ and performing the change of variable $\xi' = \tau\eta$, we obtain

$$\hat{u}_+(x', x_n) = \tau^{n-1} \int_{\mathbb{R}^{n-1}} e^{i\tau\phi} \tilde{\psi}(\eta) \chi_0\Big(\frac{\beta\gamma x_n}{|\tilde{f}_+(\eta)|}\Big) d\eta,$$

where the complex phase function is given by

$$\phi = -x' \cdot \eta - i x_n \Big(\tilde{f}_+(\eta) + \frac{\beta x_n}{2}\Big), \quad \text{with } \tilde{f}_+(\eta) = \alpha_+ - m_+(\eta)$$

and

$$\tilde{\psi}(\eta) = \chi_1\Big(\frac{1}{(1+|\eta|^2)^{1/2}} - \tau_0\Big) \chi_1\Big(\Big|\frac{\eta}{(1+|\eta|^2)^{1/2}} - \xi_0'\Big|\Big).$$

Here τ is chosen sufficiently large that m_+ is homogeneous. Observe that $\tilde{\psi}$ has a compact support independent of τ and that $\tilde{f}_+(\eta) + \beta x_n/2 \le -C < 0$ in the support of the integrand.

We place ourselves in the neighborhood of a point x' such that $|\tau^{1/2} x'| \ge \frac{1}{2}$. Up to a permutation of the variables, we may assume that $|\tau^{1/2} x_1| \ge C$. We then introduce the differential operator

$$L = \tau^{-1} \frac{\partial_{\eta_1}}{-i x_1 - x_n \partial_{\eta_1} m_+(\eta)},$$

which satisfies $L e^{i\tau\phi} = e^{i\tau\phi}$. We thus have

$$\hat{u}_+(x', x_n) = \tau^{n-1} \int_{\mathbb{R}^{n-1}} e^{i\tau\phi} (L^t)^N \Big(\tilde{\psi}(\eta) \chi_0\Big(\frac{\beta\gamma x_n}{|\tilde{f}_+(\eta)|}\Big)\Big) d\eta,$$

and we find

$$\big|\hat{u}_+(x', x_n)\big| \le C_N \frac{\tau^{n-1}\gamma^N}{|\tau x_1|^N} e^{-C\tau x_n}.$$

More generally, for $|\tau^{1/2} x'| \ge \frac{1}{2}$ we have

$$\big|\hat{u}_+(x', x_n)\big| \le C_N \frac{\tau^{n-1}\gamma^N}{|\tau x'|^N} e^{-C\tau x_n}.$$

Then we obtain

$$\begin{aligned}
\int_{|\tau^{1/2}x'| \ge 1/2} \int_{\mathbb{R}_+} &\big|\hat{u}_+(x', x_n)\big|^2 \, dx' \, dx_n \\
&\le C_N^2 \gamma^{2N} \tau^{2n-2} \Big(\int_{|\tau^{1/2}x'| \ge 1/2} \frac{1}{|\tau x'|^{2N}} \, dx'\Big)\Big(\int_{\mathbb{R}_+} e^{-2C\tau x_n} \, dx_n\Big) \\
&\le C_N' \gamma^{2N} \tau^{(3/2)n - N - 5/2} \int_{|x'| \ge 1/2} \frac{1}{|x'|^{2N}} \, dx'.
\end{aligned}$$

Similarly, setting $z_- = \big(1 - \chi_0\big(|\tau^{1/2} x'|\big)\big)\check{\hat{u}}_-(x', x_n)$ for $x_n \le 0$, we get $\|z_-\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R}_-)} \le C_{\gamma,N} \tau^{-N}$. The second result thus follows from Lemma 5.2.

For the first result we write

$$\mathcal{L}_\tau v_\pm = (2\pi)^{-(n-1)} \chi_0\big(|\tau^{1/2} x'|\big) \mathcal{L}_\tau \check{\hat{u}}_\pm + (2\pi)^{-(n-1)} \big[\mathcal{L}_\tau, \chi_0\big(|\tau^{1/2} x'|\big)\big] \check{\hat{u}}_\pm.$$

The first term is estimated, using Lemma 5.2, as

$$(2\pi)^{-(n-1)/2}\|\mathcal{L}_\tau \check{\hat{u}}_\pm\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R}_\pm)} = \|\mathcal{M}_\tau u_\pm\|_{L^2(\mathbb{R}^{n-1}\times\mathbb{R}_\pm)}.$$

Observe that $\mathcal{L}_\tau$ is a *differential* operator; the commutator is thus a first-order differential operator in x' with support in a region $|\tau^{1/2}x'| \geq C$, because of the behavior of χ_1 near 0. The coefficients of this operator depend on τ polynomially. The zero-order terms can be estimated as we did for z_+ above with an additional $\tau^{3/2}$ factor.

For the first-order term, observe that we have

$$\partial_{x'_j}\check{\hat{u}}_+(x',\tau) = \tau^n \int_{\mathbb{R}^{n-1}} \eta_j e^{i\tau\left(x'\cdot\eta - i x_n\left(\tilde{f}_+(\eta)+\frac{\beta x_n}{2}\right)\right)}\tilde{\psi}(\eta)\chi_0\left(\frac{\beta\gamma x_n}{|\tilde{f}_+(\eta)|}\right)d\eta.$$

We thus obtain similar estimates as above with an additional $\tau^{3/2}$ factor. This concludes the proof. □

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THE SEMICLASSICAL LIMIT OF THE TIME DEPENDENT HARTREE–FOCK EQUATION: THE WEYL SYMBOL OF THE SOLUTION

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For a family of solutions to the time dependent Hartree–Fock equation, depending on the semiclassical parameter h, we prove that if at the initial time the Weyl symbol of the solution is in $L^1(\mathbb{R}^{2n})$ as well as all its derivatives, then this property is true for all time, and we give an asymptotic expansion in powers of h of this Weyl symbol. The main term of the asymptotic expansion is a solution to the Vlasov equation, and the error term is estimated in the norm of $L^1(\mathbb{R}^{2n})$.

1. Introduction

The essential goal of this work is a semiclassical analysis of the solutions of the time dependent Hartree–Fock equation (TDHF) in the framework of trace class h-pseudodifferential operators. This equation describes the time evolution of the density operator of a quantum system in the mean field approximation, in other words, when the number N of particles tends to infinity, the interaction between two particles being of order $1/N$. (See, for instance, [Ammari and Nier 2008; 2009; Bardos et al. 2003; Erdős and Schlein 2009; Fröhlich et al. 2009; Rodnianski and Schlein 2009; Spohn 1980].)

A solution to the TDHF equation is a nonnegative self-adjoint trace class operator $\rho_h(t)$ in $\mathscr{H} = L^2(\mathbb{R}^n)$ (for particles moving in $\mathbb{R}^n$), of trace equal to 1, evolving as a function of t. This operator is usually called the density operator. Its evolution depends on a parameter $h > 0$, and on two potentials V and W, which are here C^∞ real valued functions on $\mathbb{R}^n$, bounded as well as all their derivatives: the first one is the external potential, interacting with all the particles, and the second one describes the interaction between two particles. Then the density operator obeys the equation

$$ih\frac{\partial}{\partial t}\rho_h(t) = -h^2[\Delta, \rho_h(t)] + [V_q(\rho_h(t)), \rho_h(t)], \tag{1-1}$$

where Δ is the Laplacian and $V_q(\rho_h(t))$ is the multiplication operator by the mean quantum potential, defined at each point $x \in \mathbb{R}^n$, and for each time t, according to the principles of quantum mechanics, by

$$V_q(x, \rho_h(t)) = V(x) + \mathrm{Tr}(W_x \rho_h(t)), \tag{1-2}$$

where W_x is the multiplication operator by the function $y \to W(x-y)$. We shall see later the meaning of the commutators in the equation, and the other hypotheses which are needed.

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Using semiclassical analysis, we want to make precise the relationship with the Vlasov equation, which plays the role of TDHF in classical mechanics. A solution of this equation is a nonnegative real-valued function $v(\cdot, t)$ in $L^1(\mathbb{R}^n)$, depending on $t \in \mathbb{R}$. This function defines the particle density at the point x and at the time t in classical mechanics. Then the mean classical potential at (x, t) is

$$V_{\rm cl}(x, v(\cdot, t)) = V(x) + \int_{\mathbb{R}^{2n}} W(x-y)v(y, \eta, t)\, dy\, d\eta. \tag{1-3}$$

Then the density function $v(\cdot, t)$ satisfies the Vlasov equation, which is the Liouville equation with the mean potential

$$\frac{\partial v}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial v}{\partial x_j} - \sum_{j=1}^{n} \frac{\partial V_{\rm cl}(x, v(\cdot, t))}{\partial x_j} \frac{\partial v}{\partial \xi_j} = 0. \tag{1-4}$$

The asymptotic relationship, when h tends to 0, between a density operator $\rho_h(t)$ (that is, a nonnegative self-adjoint trace class operator, with trace 1) satisfying the TDHF equation and a density function $v(x, t)$ (a nonnegative real-valued function in $L^1(\mathbb{R}^n)$, with integral 1) satisfying the Vlasov equation will be provided by the semiclassical quantization. We can use either the semiclassical Weyl calculus or the semiclassical Wick symbol. This paper is devoted to the approach by the Weyl calculus. The Wick symbol, which needs weaker hypotheses, will be studied elsewhere (see [Amour et al. 2011]). In this work we also use the semiclassical anti-Wick calculus in Section 2, only to give examples.

The semiclassical Weyl calculus associates to a suitable function F on $\mathbb{R}^{2n}$ an operator, in our case in $L^2(\mathbb{R}^n)$, depending on the parameter $h > 0$, formally defined for $f \in L^2(\mathbb{R}^n)$ by

$$\big(\mathrm{Op}_h^{\rm weyl}(F) f\big)(x) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{(i/h)(x-y)\cdot\xi} F\left(\frac{x+y}{2}, \xi\right) f(y)\, dy\, d\xi. \tag{1-5}$$

This operator can also be written $F^w(x, hD)$. Let us denote by $W^{m,p}(\mathbb{R}^{2n})$ the Sobolev space of functions which are in $L^p(\mathbb{R}^{2n})$ together with all their derivatives up to the order m ($1 \le p \le +\infty$, $m \ge 0$). In the oldest results on the Weyl calculus, the function F is in $W^{\infty,\infty}(\mathbb{R}^{2n})$ and the operator $\mathrm{Op}_h^{\rm weyl}(F)$ is a bounded operator in $L^2(\mathbb{R}^n)$. See [Calderón and Vaillancourt 1972; Hörmander 1985a, Chapter 18; Lerner 2010; Taylor 1981] and, in the semiclassical context, [Robert 1987; 1998; Zworski 2012; Dimassi and Sjöstrand 1999; Helffer 1997; Martinez 2002], for example. These results cannot be directly applied to our problem, since our function $v(\cdot, t)$ is in $L^1(\mathbb{R}^{2n})$, and the operator $\rho_h(t)$ has to be not only bounded, but also trace class. Rather, we shall use, in definition (1-5), symbols F in $W^{\infty,1}(\mathbb{R}^{2n})$. It was proved by C. Rondeaux [1984] that for each function F in $W^{m,1}(\mathbb{R}^{2n})$ (m large enough), the operator $\mathrm{Op}_h^{\rm weyl}(F)$ formally defined by (1-5) is trace class. This result is very useful for the study of solutions of the TDHF equation. However, in [Rondeaux 1984], there was no parameter h, and the Weyl calculus was not semiclassical, but we need only standard modifications for that.

We want to prove that if at the initial time $t = 0$ the density operator $\rho_h(0)$ is associated by the semiclassical Weyl calculus to a function in $W^{\infty,1}(\mathbb{R}^{2n})$, then for each $t \in \mathbb{R}$, the operator $\rho_h(t)$ is also associated in the same way to another function in $W^{\infty,1}(\mathbb{R}^n)$, and we shall make precise the time evolution of this function. Before giving the precise statement, we recall the standard formula

$$\mathrm{Tr}\big(\mathrm{Op}_h^{\mathrm{weyl}}(F)\big) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(x,\xi)\,dx\,d\xi, \qquad F \in W^{\infty,1}(\mathbb{R}^{2n}). \tag{1-6}$$

Let us recall also that if F is real-valued, then $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is self-adjoint. By [Rondeaux 1984], we can associate to each nonnegative function F in $W^{\infty,1}(\mathbb{R}^{2n})$ with integral equal to 1 a self-adjoint trace class operator $\rho_h(0)$ with trace 1, in the following way:

$$\rho_h(0) = (2\pi h)^n \,\mathrm{Op}_h^{\mathrm{weyl}}(F). \tag{1-7}$$

However, the positivity of F does not imply the positivity of the operator, which will be another hypothesis. We shall prove that, for a solution $\rho_h(t)$ of the TDHF equation, if a relation like (1-7) exists for $t=0$, it will exist at each time.

Before the statements of the results, we have to explain the meaning of the TDHF equation and recall the notion of a *classical solution* of TDHF introduced by Bove, Da Prato and Fano [Bove et al. 1974; 1976] (see also [Chadam and Glassey 1975]). Let us denote by $\mathcal{L}^1(\mathcal{H})$ the space of trace class operators $\mathcal{H} = L^2(\mathbb{R}^n)$. Denote by $\mathfrak{D}$ the space of operators A in $\mathcal{L}^1(\mathcal{H})$ such that the limit

$$\lim_{t\to 0} \frac{e^{it\Delta} A e^{-it\Delta} - A}{t}$$

exists in $\mathcal{L}^1(\mathcal{H})$. This limit is denoted by $i[\Delta, A]$. It can be easily proved that a trace class operator A is in $\mathfrak{D}$ if and only if its commutator with the Laplacian Δ (a priori defined as an operator from $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$) can be extended as a trace class operator in $\mathcal{H} = L^2(\mathbb{R}^n)$. A *classical solution* of TDHF (for a fixed $h > 0$) is a map $t \to \rho_h(t)$ in $C^1(\mathbb{R}, \mathcal{L}^1(\mathcal{H})) \bigcap C(\mathbb{R}, \mathfrak{D})$ satisfying (1-1). The Cauchy for the TDHF equation was also studied in [Bove et al. 1974; 1976], where it is proved that for each nonnegative self-adjoint operator A in $\mathfrak{D}$, and for each $h > 0$, there is a unique classical solution $\rho_h(t)$ of the TDHF equation such that $\rho_h(0) = A$. Moreover, $\rho_h(t)$ is also self-adjoint and nonnegative, and its trace is constant. We have similar properties for the Vlasov equation. If v is a solution of (1-4), and if at an initial time the data $v(\,\cdot\,,0)$ is in $L^1(\mathbb{R}^{2n})$, and if it is nonnegative, these two properties remain true for all $t \in \mathbb{R}$, and the integral over $\mathbb{R}^{2n}$ of $v(\,\cdot\,,t)$ is constant (see, for instance, [Braun and Hepp 1977]).

Theorem 1.1. *Let $(\rho_h(t))_{(h>0)}$ be a family of classical solutions of the TDHF equation (1-1), with V and W real-valued functions in $W^{\infty,\infty}(\mathbb{R}^n)$. We assume that, for every $h > 0$, the operator $\rho_h(0)$ can be written*

$$\rho_h(0) = (2\pi h)^n \,\mathrm{Op}_h^{\mathrm{weyl}}(F_h), \tag{1-8}$$

where F_h is in $W^{\infty,1}(\mathbb{R}^{2n})$, real-valued, and bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h in $(0,1]$. We also assume that the operator $\rho_h(0)$ is nonnegative, and that

$$\int_{\mathbb{R}^{2n}} F_h(x,\xi)\,dx\,d\xi = 1. \tag{1-9}$$

Then for every $t \in \mathbb{R}$, the operator $\rho_h(t)$ can be written in the form

$$\rho_h(t) = (2\pi h)^n \,\mathrm{Op}_h^{\mathrm{weyl}}(u_h(\,\cdot\,,t)), \tag{1-10}$$

where $u_h(\cdot\,, t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h in $(0, 1]$ and of t in a compact set of $\mathbb{R}$. We have, for all $t \in \mathbb{R}$,

$$\int_{\mathbb{R}^{2n}} u_h(x, \xi, t)\, dx\, d\xi = 1. \tag{1-11}$$

The positivity of the operator $\rho_h(t)$ is needed. Then by [Bove et al. 1976], we have $\rho_h(t) \geq 0$ and $\mathrm{Tr}(\rho_h(t)) = 1$ for all t. The condition $\rho_h(0) \geq 0$ is verified if $\rho_h(0) = (2\pi h)^n \mathrm{Op}_h^{\mathrm{AW}}(G)$, with $G \geq 0$ in $L^1(\mathbb{R}^{2n})$, where $\mathrm{Op}_h^{\mathrm{AW}}(G)$ is the anti-Wick operator associated to G (see Section 2).

If there was no interaction between the particles ($W = 0$), the evolution equation (1-1) would be linear, and then we would have

$$\rho_h(t) = e^{-(it/h)H(h)} \rho_h(0) e^{(it/h)H(h)}, \qquad H(h) = -h^2\Delta + V(x). \tag{1-12}$$

In this particular case, the Egorov theorem could be applied. The earliest version of the Egorov theorem says that if A is a pseudodifferential operator and U an invertible Fourier integral operator, then $U^{-1}AU$ is a pseudodifferential operator (see [Hörmander 1985b, Chapter 25]). In the case of an evolution equation like (1-12), it can be proved, without the Fourier integral operators, that if $\rho_h(0)$ is a pseudodifferential operator with a symbol F in $W^{\infty,\infty}(\mathbb{R}^{2n})$, then it is the same for the right-hand side of (1-12). The proof was given (in the semiclassical context) by D. Robert [1987] and M. Zworski [2012], who proved that the error term in the asymptotic expansion is itself a pseudodifferential operator. For this last point, the characterization theorem of R. Beals [1977] is needed.

For our problem, we need an extension of the above Egorov theorem for two reasons: this theorem will be applied for symbols in $W^{\infty,1}(\mathbb{R}^{2n})$ (the Rondeaux class), and for time dependent Hamiltonians. In the proof, we shall use the Beals type characterization of operators with symbols in $W^{\infty,1}(\mathbb{R}^{2n})$, also given by Rondeaux, but with some modifications.

Now we shall give an asymptotic expansion of the function u_h of Theorem 1.1. The first term will be a solution of the Vlasov equation, and the rest will be majorized in the $L^1(\mathbb{R}^{2n})$ norm. One can see in [Domps et al. 1997] a formulation of the physics of this problem.

Theorem 1.2. *Let $(\rho_h(t))_{(h>0)}$ be a family of classical solutions of the TDHF equation (1-1) satisfying the hypotheses of Theorem 1.1. Then there exists a sequence of functions $(X, t) \to u_j(X, t, h)$ on $\mathbb{R}^{2n} \times \mathbb{R}$ $(j \geq 0)$ such that:*

- *The function $t \to u_j(\cdot\,, t, h)$ is C^∞ from $\mathbb{R}$ into $W^{\infty,1}(\mathbb{R}^{2n})$. For every multi-index (α, β), there exists a function $C_{\alpha\beta}(t)$, bounded on every compact set of $\mathbb{R}$, such that*

$$\left\| \partial_x^\alpha \partial_\xi^\beta u_j(\cdot\,, t, h) \right\|_{L^1(\mathbb{R}^{2n})} \leq C_{\alpha\beta}(t) \tag{1-13}$$

for all $t \in \mathbb{R}$ and $h \in (0, 1]$.

- *If F_h is the function of (1-8),*

$$u_0(X, 0, h) = F_h(X) \quad \textit{and} \quad u_j(X, 0, h) = 0, \qquad j \geq 1. \tag{1-14}$$

- *The function $u_0(X,t,h)$ verifies the Vlasov equation*

$$\frac{\partial u_0}{\partial t}+2\sum_{j=1}^{n}\xi_j\frac{\partial u_0}{\partial x_j}=\sum_{j=1}^{n}\frac{\partial}{\partial x_j}V_{\mathrm{cl}}\big(u_0(\,\cdot\,,t)\big)\frac{\partial u_0(\,\cdot\,,t)}{\partial \xi_j}. \tag{1-15}$$

- *For every $N\geq 1$, the function $u_h(\,\cdot\,,t)$ defined by (1-10) and the function $F^{(N)}(\,\cdot\,,t,h)$ defined by*

$$F^{(N)}(X,t,h)=\sum_{k=0}^{N-1}h^j u_j(X,t,h) \tag{1-16}$$

satisfy, for all $h\in(0,1]$,

$$\big\|u_h(\,\cdot\,,t)-F^{(N)}(\,\cdot\,,t,h)\big\|_{L^1(\mathbb{R}^{2n})}\leq C_N(t)h^N, \tag{1-17}$$

where C_N is a function on $\mathbb{R}$ which is bounded on the compact sets of $\mathbb{R}$.

- *For every $N\geq 1$, the operator $\rho_h^{(N)}(t)$ defined by*

$$\rho_h^{(N)}(t)=(2\pi h)^n\,\mathrm{Op}_h^{\mathrm{weyl}}\big(F^{(N)}(\,\cdot\,,t,h)\big) \tag{1-18}$$

(where $F^{(N)}(\,\cdot\,,t,h)$ is the function of (1-16)) verifies

$$\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}\leq C(t)h^{N+1}. \tag{1-19}$$

In Section 5, we will make precise the construction of the $u_j(X,t,h)$ ($j\geq 1$), and we will prove the theorem. The successive terms $u_j(X,t,h)$ depend on the initial data F_h. If F_h depends on h, without admitting an asymptotic expansion in powers of h, the $u_j(X,t,h)$ will depend on h.

In [Amour et al. 2011], we study the case where $\rho_h(0)$ is trace class but not necessarily a pseudodifferential operator. In this case, the Weyl symbol is not available. It is defined as a function in $L^2(\mathbb{R}^{2n})$ but not necessarily in $L^1(\mathbb{R}^{2n})$, which is the natural space here. Therefore, in this other paper, we shall use the Wick symbol instead of the Weyl symbol, and a relation with the Vlasov equation will appear also.

Since the TDHF appears as a limiting process when the number N of particles tends to infinity, a natural question is the one of the interchange of the two limits, where N tends to infinity and the semiclassical parameter h tends to 0. It is the subject of [Pezzotti and Pulvirenti 2009], where it is shown that the Weyl symbol of the marginal density operator associated to a particle in a system of N particles admits an asymptotic expansion in powers of h; that when N tends to infinity, the Weyl symbol of the marginal density operator tends towards the symbol of a solution of TDHF; that the coefficient of h^j in the asymptotic expansion of the symbol has a limit; and that, for $j=0$, this limit is a solution of the Vlasov equation. See also [Pezzotti 2009; Graffi et al. 2003; Gasser et al. 1998]. We observe that in [Pezzotti and Pulvirenti 2009], the limits are in the sense of $\mathscr{S}'(\mathbb{R}^{2n})$, while in this work and in [Amour et al. 2011], they are in the sense of $L^1(\mathbb{R}^{2n})$.

In Section 2, we will recall some standard results on h-pseudodifferential operators, particularly the semiclassical analogue of the results of [Rondeaux 1984], which need only standard modifications in order to be applied in the semiclassical context. However, we give a different proof of the Beals type characterization theorem for this class, in order to give precisely the number of derivatives which are needed. The results on the composition of operators and the Moyal bracket for the class of Rondeaux operators are stated in Section 3, since, surprisingly, these results are not in [Rondeaux 1984]. Section 4 is devoted to the proofs of Theorem 1.1 and, first, of the analogue of the Egorov theorem for the Rondeaux class and for time dependent Hamiltonians. In Section 5, we prove Theorem 1.2. The results stated in Sections 2 and 3 are proved in Appendices A and B. For Section 2 and Appendix A, we use a technique of A. Unterberger [1980].

2. Weyl calculus and trace class operators

We define $\mathscr{H} = L^2(\mathbb{R}^n)$ and denote by $\mathscr{L}^1(\mathscr{H})$ the set of trace class operators in $\mathscr{H}$. This space is a normed space with the norm defined by

$$\|A\|_{\mathscr{L}^1(\mathscr{H})} = \mathrm{Tr}\big((A^\star A)^{1/2}\big). \tag{2-1}$$

We will denote by $W^{m,p}(\mathbb{R}^{2n})$ (where $1 \le p \le +\infty$, and m is an integer ≥ 0 or $+\infty$) the space of functions F which are in $L^p(\mathbb{R}^{2n})$, as well as all their derivatives up to order m.

Since $W^{m,p}(\mathbb{R}^{2n})$ may be considered as an exotic class of symbols, let us explain why definition (1-5) makes sense for such symbols. The semiclassical Weyl calculus sets a bijection between operators from $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}'(\mathbb{R}^n)$, thus admitting a distribution kernel in $\mathscr{S}'(\mathbb{R}^{2n})$ and tempered distributions on $\mathbb{R}^{2n}$ (symbols). This bijection depends on a parameter $h > 0$. For every F in $\mathscr{S}'(\mathbb{R}^{2n})$, we set $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ the operator A defined by (1-5), or equivalently the operator $A : \mathscr{S}(\mathbb{R}^n) \to \mathscr{S}'(\mathbb{R}^n)$ whose distribution kernel is

$$K_A(x, y) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F\left(\frac{x+y}{2}, \xi\right) e^{(i/h)(x-y).\xi}\, d\xi. \tag{2-2}$$

This relationship is understood in the sense of distributions and may be inverted. We will denote by $\sigma_h^{\mathrm{weyl}}(A)$ the distribution F (Weyl symbol of A) such that $A = \mathrm{Op}_h^{\mathrm{weyl}}(F)$:

$$F = \sigma_h^{\mathrm{weyl}}(A) \iff A = \mathrm{Op}_h^{\mathrm{weyl}}(F).$$

In view of applications to trace class operators, we can rewrite (1-5) equivalently when F is in $L^1(\mathbb{R}^{2n})$ as

$$\mathrm{Op}_h^{\mathrm{weyl}}(F) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X)\Sigma_{Xh}\, dX, \tag{2-3}$$

where for $X = (x, \xi)$ in $\mathbb{R}^{2n}$, Σ_{Xh} is the "symmetry" operator defined by

$$(\Sigma_{Xh} f)(u) = e^{(2i/h)(u-x)\xi} f(2x-u), \qquad X = (x, \xi) \in \mathbb{R}^{2n}. \tag{2-4}$$

If A is trace class, one has

$$\sigma_h^{\mathrm{weyl}}(A)(X) = 2^n\, \mathrm{Tr}(A \circ \Sigma_{Xh}), \qquad X \in \mathbb{R}^{2n}. \tag{2-5}$$

It is shown in [Rondeaux 1984] that if F is in $W^{m,p}(\mathbb{R}^{2n})$ ($1 \le p < \infty$, m large enough), the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is in the Schatten class $\mathscr{L}^p(\mathscr{H})$. For $p = +\infty$, this is the classical result of Calderón and Vaillancourt [1972] (see also [Hörmander 1985a]). If F is in $W^{\infty,1}(\mathbb{R}^{2n})$, one has

$$\operatorname{Tr}\bigl(\mathrm{Op}_h^{\mathrm{weyl}}(F)\bigr) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X)\,dX. \tag{2-6}$$

If F is in $W^{\infty,p}(\mathbb{R}^{2n})$ and G in $W^{\infty,q}(\mathbb{R}^{2n})$ ($p \geq 1$, $q \geq 1$, $\frac{1}{p}+\frac{1}{q}=1$), one has

$$\operatorname{Tr}\bigl(\mathrm{Op}_h^{\mathrm{weyl}}(F)\circ \mathrm{Op}_h^{\mathrm{weyl}}(G)\bigr) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X)G(X)\,dX. \tag{2-7}$$

The left-hand side makes sense, since from [Rondeaux 1984], the two operators under composition are respectively $\mathcal{L}^p(\mathcal{H})$ and $\mathcal{L}^q(\mathcal{H})$, and therefore their composition is trace class.

A characterization of the set of operators whose Weyl symbol is in $W^{\infty,1}(\mathbb{R}^{2n})$ is given in [Rondeaux 1984]. This is the analogue of the Beals characterization [1977], which concerns the symbols in $W^{\infty,\infty}(\mathbb{R}^{2n})$. In the next proposition, we recall the results of [Rondeaux 1984], taking into account of the semiclassical parameter h. We denote by $P_j(h) = (h/i)(\partial/\partial x_j)$ the momentum operators and by $Q_j(h)$ the multiplication by x_j. For each operator P, we denote by $(\mathrm{ad}\,P)$ the mapping $Q \to (\mathrm{ad}\,P)(Q) = [P, Q] = PQ - QP$. For every operator A of $\mathcal{S}(\mathbb{R}^n)$ in $\mathcal{S}'(\mathbb{R}^n)$, and for every multi-index (α,β), we set

$$(\mathrm{ad}\,P(h))^{\alpha}(\mathrm{ad}\,Q(h))^{\beta}A = (\mathrm{ad}\,P_1(h))^{\alpha_1}\dots(\mathrm{ad}\,Q_n(h))^{\beta_n}A. \tag{2-8}$$

Proposition 2.1. (a) *If F is in $W^{2n+2,1}(\mathbb{R}^{2n})$, then for all $h > 0$, the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is trace class and*

$$\bigl\|\mathrm{Op}_h^{\mathrm{weyl}}(F)\bigr\|_{\mathcal{L}^1(\mathcal{H})} \leq Ch^{-n} \sum_{|\alpha|+|\beta|\leq 2n+2} h^{(|\alpha|+|\beta|)/2}\|\partial_x^{\alpha}\partial_{\xi}^{\beta}F\|_{L^1(\mathbb{R}^{2n})}. \tag{2-9}$$

(b) *If A is a trace class operator and if for every multi-index (α,β) such that $|\alpha|+|\beta|\leq 2n+2$ the operator $(\mathrm{ad}\,P(h))^{\alpha}(\mathrm{ad}\,Q(h))^{\beta}A$ is trace class, then the Weyl symbol of A is in $L^1(\mathbb{R}^{2n})$ and*

$$(2\pi h)^{-n}\|\sigma_h^{\mathrm{weyl}}(A)\|_{L^1(\mathbb{R}^{2n})} \leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{-(|\alpha|+|\beta|)/2}\bigl\|(\mathrm{ad}\,P(h))^{\alpha}(\mathrm{ad}\,Q(h))^{\beta}A\bigr\|_{\mathcal{L}^1(\mathcal{H})}, \tag{2-10}$$

where the constant C depends only on n.

(c) *The following are equivalent*:

(i) *A family of operators $(A_h)_{0<h\leq 1}$ is of the form $A_h = \mathrm{Op}_h^{\mathrm{weyl}}(F_h)$, where (F_h) is a bounded family of functions in $W^{\infty,1}(\mathbb{R}^{2n})$.*

(ii) *For every $h > 0$, the operator A_h is trace class as well as all iterated commutators of A_h with the operators $P_j(h)$ and $Q_j(h)$, and for every (α,β), the family of norms*

$$h^{n-|\alpha|-|\beta|}\bigl\|(\mathrm{ad}\,P(h))^{\alpha}(\mathrm{ad}\,Q(h))^{\beta}A\bigr\|_{\mathcal{L}^1(\mathcal{H})} \tag{2-11}$$

stays bounded when h varies in $(0, 1]$.

Part (a) is proved in [Rondeaux 1984], without the parameter h, and needs only standard modifications to introduce this parameter. In the same paper, part (c) is proved without the precise estimation (b), which is needed for applications to our nonlinear problem and proved in Appendix A.

For the sake of clarity, it might be useful to recall the well known analogue of Proposition 2.1 for bounded operators and symbols in $W^{\infty,\infty}(\mathbb{R}^{2n})$, that is to say, the Calderón–Vaillancourt and the Beals characterization.

Proposition 2.2. (a) *If F is in $L^\infty(\mathbb{R}^{2n})$ as well as all derivatives up to order $2n+2$, then for all $h>0$, the operator $\mathrm{Op}_h^{\mathrm{weyl}}(F)$ is bounded in $\mathcal{H}=L^2(\mathbb{R}^n)$ and*

$$\left\|\mathrm{Op}_h^{\mathrm{weyl}}(F)\right\|_{\mathcal{L}(\mathcal{H})} \leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{(|\alpha|+|\beta|)/2} \|\partial_x^\alpha \partial_\xi^\beta F\|_{L^\infty(\mathbb{R}^{2n})}. \tag{2-12}$$

(b) *If A is a bounded operator and if, for all multi-indices (α,β) such that $|\alpha|+|\beta|\leq 2n+2$, the operator $(\mathrm{ad}\, P(h))^\alpha(\mathrm{ad}\, Q(h))^\beta A$ is bounded, then the Weyl symbol of A is in $L^\infty(\mathbb{R}^{2n})$, and one has*

$$\|\sigma_h^{\mathrm{weyl}}(A)\|_{L^\infty(\mathbb{R}^{2n})} \leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{-(|\alpha|+|\beta|)/2} \left\|(\mathrm{ad}\, P(h))^\alpha(\mathrm{ad}\, Q(h))^\beta A\right\|_{\mathcal{L}(\mathcal{H})}. \tag{2-13}$$

Anti-Wick calculus. The definition of this calculus uses coherent states, in other words the family of functions Ψ_{Xh} in $L^2(\mathbb{R}^n)$, indexed by the parameter $X=(x,\xi)$ in $\mathbb{R}^{2n}$ and depending on $h>0$, defined by

$$\Psi_{X,h}(u) = (\pi h)^{-n/4} e^{-|u-x|^2/2h} e^{(i/h)u.\xi-(i/2h)x.\xi}, \quad X=(x,\xi)\in\mathbb{R}^{2n}. \tag{2-14}$$

These functions will be used, with the anti-Wick calculus recalled below, to give examples of operators satisfying the hypotheses of Theorem 1.1. They will be also helpful in proving Proposition 2.1 in Appendix A. Their two fundamental properties are that

$$|\langle \Psi_{Xh}, \Psi_{Yh}\rangle| = e^{-(1/4h)|X-Y|^2}, \quad \|\Psi_{Xh}\|=1, \tag{2-15}$$

and that for all f and g in $\mathcal{H}$,

$$\langle f, g\rangle = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \langle f, \Psi_{Xh}\rangle\langle \Psi_{Xh}, g\rangle\, dX. \tag{2-16}$$

For every function F in $L^1(\mathbb{R}^{2n})$ and for every $h>0$, the operator $\mathrm{Op}_h^{\mathrm{AW}}(F)$ associated to F by the anti-Wick calculus is the bounded operator in $L^2(\mathbb{R}^n)$ such that for all f and g in $\mathcal{H}$,

$$\langle \mathrm{Op}_h^{\mathrm{AW}}(F) f, g\rangle = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} a(X)\langle f, \Psi_{Xh}\rangle\langle \Psi_{Xh}, g\rangle\, dX. \tag{2-17}$$

If F is in $L^1(\mathbb{R}^{2n})$, we see that $\mathrm{Op}_h^{\mathrm{AW}}(F)$ is indeed trace class in $\mathcal{H}$, and that

$$\left\|\mathrm{Op}_h^{\mathrm{AW}}(F)\right\|_{\mathcal{L}^1(\mathcal{H})} \leq (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} |F(X)|\, dX. \tag{2-18}$$

Moreover, one has

$$\mathrm{Tr}\big(\mathrm{Op}_h^{\mathrm{AW}}(F)\big) = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} F(X)\, dX. \tag{2-19}$$

If $F\geq 0$, the operator $\mathrm{Op}_h^{\mathrm{AW}}(F)$ is self-adjoint and nonnegative. The Weyl symbol of the operator $\mathrm{Op}_h^{\mathrm{AW}}(F)$ is given by

$$\sigma_h^{\mathrm{weyl}}\big(\mathrm{Op}_h^{\mathrm{AW}}(F)\big) = e^{(h/4)\Delta} F, \tag{2-20}$$

where Δ is the Laplacian on $\mathbb{R}^{2n}$. In fact, the operator Σ_{Yh} defined in (2-4) and the operator P_{Xh} of orthogonal projection on $\mathrm{Vect}(\Psi_{Xh})$ satisfy

$$\mathrm{Tr}(P_{Xh}\Sigma_{Yh}) = e^{-|X-Y|^2/h}. \tag{2-21}$$

3. Basic facts on the Moyal bracket

The composition of symbols in the Weyl calculus is a very classical field (see [Hörmander 1985a] or [Robert 1987] for the dependence on the semiclassical parameter h). We need to adapt that to the classes of Rondeaux symbols, and to make precise the dependence on the parameter h.

We define a differential operator $\sigma(\nabla_1, \nabla_2)$ on $\mathbb{R}^{2n}\times\mathbb{R}^{2n}$ by

$$\sigma(\nabla_1, \nabla_2) = \sum_{j=1}^{n} \frac{\partial^2}{\partial y_j \partial \xi_j} - \frac{\partial^2}{\partial x_j \partial \eta_j}, \tag{3-1}$$

where (x, ξ, y, η) denotes the variable of $\mathbb{R}^{2n}\times\mathbb{R}^{2n}$.

Theorem 3.1. *For all functions F in $W^{\infty,p}(\mathbb{R}^{2n})$ and G in $W^{\infty,q}(\mathbb{R}^{2n})$ ($p \geq 1$, $q \geq 1$, $1/p + 1/q = 1$), for all $h > 0$, there exists a function $M_h(F, G, \cdot)$ in $W^{\infty,1}(\mathbb{R}^{2n})$ (Moyal bracket) such that*

$$\Big[\mathrm{Op}_h^{\mathrm{weyl}}(F), \mathrm{Op}_h^{\mathrm{weyl}}(G)\Big] = \mathrm{Op}_h^{\mathrm{weyl}}\big(M_h(F, G, \cdot)\big). \tag{3-2}$$

For all integers $N \geq 2$, one has

$$M_h(F, G, X) = \sum_{k=1}^{N-1} h^k C_k(F, G, X) + R_h^{(N)}(F, G, X), \tag{3-3}$$

where the function $C_k(F, G, X)$ is defined by

$$C_k(F, G, X) = \frac{1}{(2i)^k k!}\big[\sigma(\nabla_1, \nabla_2)^k (F\otimes G)(X, X) - \sigma(\nabla_1, \nabla_2)^k (G\otimes F)(X, X)\big], \tag{3-4}$$

and where the function $R_h^{(N)}(F, G, \cdot)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$. For every integer ℓ, there exists a constant C such that

$$h^{\ell/2}\big\|\nabla^\ell R_h^{(N)}(F, G, \cdot)\big\|_{L^1(\mathbb{R}^{2n})} \leq C \sum_{\substack{|\alpha|+|\beta|\leq \ell+4n+2+2N \\ |\alpha|\geq N, |\beta|\geq N}} h^{(\alpha+\beta)/2} \|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\, \|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}. \tag{3-5}$$

The operator $\widehat{R}_h^{(N)}(F, G) = \mathrm{Op}_h^{\mathrm{weyl}}\big(R_h^{(N)}(F, G, \cdot)\big)$ verifies

$$\|\widehat{R}_h^{(N)}(F, G)\|_{\mathscr{L}^1(\mathscr{H})} \leq C h^{-n} \sum_{\substack{|\alpha|+|\beta|\leq 6n+4+2N \\ |\alpha|\geq N, |\beta|\geq N}} h^{(\alpha+\beta)/2} \|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})} \|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}. \tag{3-6}$$

This theorem will be proved in Appendix B. It is also used in [Amour et al. 2011]. We shall also use the well-known analogue of Theorem 3.1, which we recall here in order to be used when needed.

Theorem 3.2. *With the notations of Theorem 3.1, if the functions F and G are in $W^{\infty,\infty}(\mathbb{R}^{2n})$, the function $R_h^{(N)}(F, G, \cdot)$ defined by the equality (3-3) verifies, for any $\ell \geq 0$,*

$$h^{\ell/2}\big\|\nabla^\ell R_h^{(N)}(F,G,\cdot)\big\|_{L^\infty(\mathbb{R}^{2n})} \leq C \sum_{\substack{j\geq N,\, k\geq N\\ \ell+2N\leq j+k\leq \ell+2N+4n+2}} h^{(j+k)/2}\|\nabla^j F\|_{L^\infty(\mathbb{R}^{2n})}\|\nabla^k G\|_{L^\infty(\mathbb{R}^{2n})}. \tag{3-7}$$

The operator $\widehat{R}_h^{(N)}(F, G)$ verifies

$$\|\widehat{R}_h^{(N)}(F,G)\|_{\mathcal{L}(\mathcal{H})} \leq C \sum_{\substack{j\geq N,\, k\geq N\\ 2N\leq j+k\leq 2N+6n+4}} h^{(j+k)/2}\|\nabla^j F\|_{L^\infty(\mathbb{R}^{2n})}\|\nabla^k G\|_{L^\infty(\mathbb{R}^{2n})}. \tag{3-8}$$

4. The Egorov theorem for trace class operators and proof of Theorem 1.1

We are going to adapt to the case of symbols in $L^1(\mathbb{R}^{2n})$ and trace class operators the idea of the proof of the Egorov theorem contained in [Robert 1987]. The difference with [Robert 1987] comes from the fact that the classes of operators considered here are the classes introduced by Rondeaux and that Hamiltonians are time dependent.

We consider a function $(x, t) \to V(x, t)$ on $\mathbb{R}^n \times \mathbb{R}$, which is real valued, depending in a C^∞ way on x, and continuously on t. We suppose that, for every α, there exists $C_\alpha > 0$ such that

$$|\partial_x^\alpha V(x,t)| \leq C_\alpha, \quad (x,t) \in \mathbb{R}^n \times \mathbb{R}. \tag{4-1}$$

We set

$$H(x,\xi,t) = |\xi|^2 + V(x,t). \tag{4-2}$$

We denote by $V(t)$ the multiplication by $V(\cdot\,, t)$. We set

$$\widehat{H}_h(t) = -h^2\Delta + V(t). \tag{4-3}$$

Therefore, $\widehat{H}_h(t) = \mathrm{Op}_h^{\mathrm{weyl}}(H(\cdot\,,t))$. Let us now recall some facts on unitary propagators (see [Reed and Simon 1975, Section X.12]).

Proposition 4.1. *For all $t \in \mathbb{R}$, let $V(\cdot\,, t)$ be a C^∞ function on $\mathbb{R}^n$ satisfying (4-1) and depending in a C^1 way on $t \in \mathbb{R}$. Let $\widehat{H}_h(t)$ be the operator defined in (4-3). For every f in $\mathcal{S}(\mathbb{R}^n)$ and every s in $\mathbb{R}$, there exists a function denoted by $t \to U_h(t, s)f$ that verifies*

$$ih\frac{\partial}{\partial t}U_h(t,s)f = (\widehat{H}_h(t))U_h(t,s)f, \quad U_h(s,s)f = f. \tag{4-4}$$

The operator $U_h(t, s)$ maps $\mathcal{S}(\mathbb{R}^n)$ into itself and, by duality, $\mathcal{S}'(\mathbb{R}^n)$ into itself. One has $U_h(s, t) = U_h(t, s)^{-1}$. One also has

$$ih\frac{\partial}{\partial s}U_h(t,s) = -U_h(t,s)(\widehat{H}_h(s)). \tag{4-5}$$

For every operator A from $\mathcal{S}(\mathbb{R}^n)$ into $\mathcal{S}'(\mathbb{R}^n)$, let us set

$$G_h(t,s)(A) = U_h(t,s)\circ A\circ U_h(s,t). \tag{4-6}$$

One has

$$ih\frac{\partial}{\partial t}G_h(t,s)(A)=\big[\widehat{H}_h(t),G_h(t,s)(A)\big],\quad G_h(s,s)(A)=A. \tag{4-7}$$

Let us state the analogue of the Egorov theorem for the class of Rondeaux operators [1984].

Theorem 4.2. *Let F be a function defined on $W^{\infty,1}(\mathbb{R}^{2n})$. Let $A_h=\mathrm{Op}_h^{\mathrm{weyl}}(A)$. Then for every $t\in\mathbb{R}$, there exists a function F_{ht} in $W^{\infty,1}(\mathbb{R}^{2n})$ such that*

$$G_h(t,0)(A_h)=\mathrm{Op}_h^{\mathrm{weyl}}(F_{ht}). \tag{4-8}$$

If the function F and the potential $V(\,\cdot\,,t)$ depend on a parameter λ, while staying bounded respectively in $W^{\infty,1}(\mathbb{R}^{2n})$ and in $W^{\infty,\infty}(\mathbb{R}^{2n})$ independently of λ, then the function F_{ht} remains bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of λ, of h in $(0,1]$, and of t in a compact set of $\mathbb{R}$.

Following the idea of Robert [1987], which is related in some sense to Dyson series, we will express our solution $G_h(t,0)(A_h)$ in the form

$$G_h(t,0)(A_h)=\sum_{k=0}^{N-1}\mathrm{Op}_h^{\mathrm{weyl}}\big(D_k(\,\cdot\,,t)\big)+h^N E_N(t,h), \tag{4-9}$$

where the functions $D_k(\,\cdot\,,t)$ will be in $W^{\infty,1}(\mathbb{R}^{2n})$ and $E_N(t,h)$ will be a trace class operator with bounded trace norm. In a second step, we will show that the commutators of $E_N(t,h)$ with the position and momentum operators are also trace class operators, and we will estimate their traces. Finally, we will rely on the characterization recalled in Proposition 2.1 to show that $G_h(t,0)(A_h)$ is itself a pseudodifferential operator, with a symbol in $W^{\infty,1}(\mathbb{R}^{2n})$.

The construction of the terms $D_k(\,\cdot\,,t)$ will use the Hamiltonian flow of $H(\,\cdot\,,t)$. For every function G in $W^{\infty,1}(\mathbb{R}^{2n})$, we call $\Phi_{ts}(G)$ the function on $\mathbb{R}^{2n}$ defined by

$$\frac{\partial\Phi_{t,s}(G)}{\partial t}=\{H(\,\cdot\,,t),\Phi_{ts}(G)\},\quad \Phi_{s,s}(G)=G. \tag{4-10}$$

Under hypothesis (4-1), one knows that if $(G_\lambda)_{\lambda\in E}$ is a family of bounded functions in $W^{\infty,1}(\mathbb{R}^{2n})$, then $\Phi_{ts}(G_\lambda)$ stays bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ when (t,s) varies in a compact set of $\mathbb{R}^2$ and λ in E.

Lemma 4.3. *For every function G in $W^{\infty,1}(\mathbb{R}^{2n})$ and for (t,s) in $\mathbb{R}^2$, one has*

$$G_h(t,s)\big(\mathrm{OP}_h^{\mathrm{weyl}}(G)\big)=\mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{ts}(G))+h\int_s^t G_h(t,t_1)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R(\,\cdot\,,t_1,s,h))\big)\,dt_1, \tag{4-11}$$

where the function $R(\,\cdot\,,t_1,s,h)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$. If G depends on some parameter and is bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of this parameter, then the function $R(\,\cdot\,,t_1,s,h)$ associated to G is also bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of this parameter and of (t_1,s) in a compact set of $\mathbb{R}^2$ and of h in $(0,1]$.

Proof of the lemma. From definition (4-10),

$$\frac{\partial}{\partial t} \mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{ts}(G)) = \mathrm{Op}_h^{\mathrm{weyl}}\big(\{H(\cdot\,,t), \Phi_{ts}(G)\}\big).$$

With the notations of Theorem 3.1 and with $N = 2$, one may write

$$\big[\widehat{H}_h(t), \mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{tsh}(G))\big] = \frac{h}{i}\,\mathrm{Op}_h^{\mathrm{weyl}}\big(\{H(\cdot\,,t), \Phi_{ts}(G)\}\big) + \mathrm{OP}_h^{\mathrm{weyl}}\big(R_h^{(2)}(H(\cdot\,,t), \Phi_{ts}(G))\big).$$

Consequently,

$$\frac{\partial}{\partial t} \mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{ts}(G)) - \frac{i}{h}\big[\widehat{H}_h(t), \mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{ts}(G))\big] = -\frac{i}{h}\,\mathrm{OP}_h^{\mathrm{weyl}}\big(R_h^{(2)}(H(\cdot\,,t), \Phi_{ts}(G))\big).$$

On the other hand,

$$\frac{\partial}{\partial t} G_h(t,s)(\mathrm{OP}_h^{\mathrm{weyl}}(G)) - \frac{i}{h}\big[\widehat{H}_h(t), G_h(t,s)(\mathrm{OP}_h^{\mathrm{weyl}}(G))\big] = 0.$$

By combining these two equalities, noting that for $t = s$ the two operators $G_h(s,s)(\mathrm{Op}_h^{\mathrm{weyl}}(G))$ and $\mathrm{Op}_h^{\mathrm{weyl}}(\Phi_{ss}(G))$ are equal, and using Duhamel's principle, we obtain (4-11), with

$$R(\cdot\,,t_1,s,h) = -\frac{i}{h} R_h^{(2)}\big(H(\cdot\,,t_1), \Phi_{t_1 s}(G)\big).$$

It is well known that when $F(x,\xi) = |\xi|^2$, one has $R_h^{(2)}(F,G) = 0$ for every function G. Hence

$$R(\cdot\,,t_1,s,h) = -\frac{i}{h^2} R_h^{(2)}\big(V(\cdot\,,t_1), \Phi_{t_1 s}(G)\big).$$

By hypothesis, $V(\cdot\,,t_1)$ is in $W^{\infty,\infty}(\mathbb{R}^n)$ and is bounded independently of t_1. We have seen that $\Phi_{t_1 s}(G)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t_1 and of s when (t_1,s) varies in a compact set of $\mathbb{R}^2$. According to Theorem 3.1 applied to the case $N = 2$, it follows that $R(\cdot\,,t_1,s,h)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t_1 and of s when (t_1,s) varies in a compact set of $\mathbb{R}^2$ and h in $(0,1]$. □

Proof of Theorem 4.2, first step. Let F be a function in $W^{\infty,1}(\mathbb{R}^{2n})$. Let $A_h = \mathrm{Op}_h^{\mathrm{weyl}}(F)$. Let $\Phi_{ts}(G)$ be the function satisfying (4-10). For every $t \in \mathbb{R}$, we define a function $D_0(\cdot\,,t)$ in $W^{\infty,1}(\mathbb{R}^{2n})$ by

$$D_0(\cdot\,,t) = \Phi_{t,0}(F). \tag{4-12}$$

We have seen that this function is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t on every compact set of $\mathbb{R}$. By Lemma 4.3 applied to $G = F$ and $s = 0$, and from (4-12), one has

$$G_h(t,0)(A_h) = \mathrm{Op}_h^{\mathrm{weyl}}(D_0(t)) + h\int_0^t G_h(t,t_1)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_1(\cdot\,,t_1,h))\big)\,dt_1,$$

where $R_1(\cdot\,,t_1,h)$ stays bounded in $W^{\infty,1(\mathbb{R}^{2n})}$ when t_1 belongs to a compact set of $\mathbb{R}$ and h is in $(0,1]$. We iterate by applying Lemma 4.3 with $s = t_1$ and $G = R_1(\cdot\,,t_1,h)$. We obtain

$$G_h(t,t_1)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_1(\cdot\,,t_1,h))\big) = \mathrm{Op}_h^{\mathrm{weyl}}\big(\Phi(t,t_1)(R_1(\cdot\,,t_1,h))\big) + h\int_{t_1}^t G_h(t,t_2)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_2(\cdot\,,t_2,t_1,h))\big)\,dt_2,$$

where $R_2(\,\cdot\,, t_2, t_1, h)$ stays bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ when (t_1, t_2) belongs to a compact set of $\mathbb{R}^2$ and h is in $(0, 1]$. We define a function $D_1(\,\cdot\,, t)$ in $W^{\infty,1}(\mathbb{R}^{2n})$ by

$$D_1(\,\cdot\,, t) = \int_0^t \Phi(t, t_1)\big(R_1(\,\cdot\,, t_1, h)\big)\, dt_1.$$

This function is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of t on every compact set of $\mathbb{R}$. We have, if $t > 0$,

$$G_h(t, 0)(A_h) = \mathrm{Op}_h^{\mathrm{weyl}}\big(D_0(t) + h D_1(t)\big) + h^2 \int_{0<t_1<t_2<t} G_h(t, t_2)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_2(\,\cdot\,, t_2, t_1, h))\big)\, dt_1\, dt_2.$$

Iterating this process, we obtain, for every N, the equality (4-9), with

$$E_N(t, h) = \int_{\Delta_N(t,0)} G_h(t, t_N)\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,, t_N, \dots, t_1, h))\big)\, dt_1 \dots dt_N, \tag{4-13}$$

where $\Delta_N(t, s)$ is the set defined, if $s < t$, by

$$\Delta_N(t, s) = \big\{(t_1, \dots, t_N) \in \mathbb{R}^N,\ s < t_1 < \cdots < t_N < t\big\}, \tag{4-14}$$

and in a symmetric way if $s > t$. In (4-9), the $D_j(\,\cdot\,, t, h)$ $(j \geq 0)$ and $R_N(\,\cdot\,, t_N, \dots, t_1, h)$ are in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded independently of h in $(0, 1]$, of $(t_1, \dots, t_N)$ in $\Delta_N(t, 0)$, and of t in a compact set of $\mathbb{R}$.

It remains to prove that $E_N(t, h)$ is also a pseudodifferential operator. For that, we shall give in the second step upper bounds for trace norms of iterated commutators of $E_N(t, h)$ with the position and momentum operators. In order to do that, we will use the following lemma, also used in Section 5 and in [Amour et al. 2011]. If an operator A is bounded in $L^2(\mathbb{R}^n)$, as well as all its iterated commutators up to order m, we set

$$I_h^{m\infty}(A) = \sum_{|\alpha|+|\beta|\leq m} \big\|(\mathrm{ad}\, Q(h))^\beta (\mathrm{ad}\, P(h))^\alpha A\big\|_{\mathcal{L}(\mathcal{H})}. \tag{4-15}$$

If an operator A in $L^2(\mathbb{R}^n)$ is trace class, as well as all its iterated commutators up to order m, we set

$$I_h^{m,\mathrm{tr}}(A) = \sum_{|\alpha|+|\beta|\leq m} \big\|(\mathrm{ad}\, Q(h))^\beta (\mathrm{ad}\, P(h))^\alpha A\big\|_{\mathcal{L}^1(\mathcal{H})}. \tag{4-16}$$

The aim of the next lemma is to show that these properties are preserved by the mapping $G_h(t, s)$.

Lemma 4.4. *Let $\widehat{H}_h(t)$ be the operator defined in (4-3), where $V(\,\cdot\,, t)$ verifies (4-1). Let $U_h(t, s)$ denote the unitary propagator and $G_h(t, s)$ the map of Proposition 4.1. Let A be a trace class operator in $\mathcal{H} = L^2(\mathbb{R}^n)$, as well as all iterated commutators $(\mathrm{ad}\, Q(h))^\beta (\mathrm{ad}\, P(h))^\alpha A$ for $|\alpha| + |\beta| \leq m$. Then, for all s and t in $\mathbb{R}$, the operator $G_h(t, s)(A)$ is also trace class, as well as all iterated commutators with the $P_j(h)$ and $Q_j(h)$ up to order m. Moreover, for every compact set K of $\mathbb{R}$, there exists $C_K > 0$ such that*

$$I_h^{m,\mathrm{tr}}(G_h(t, s)(A)) \leq C_K I_h^{m,\mathrm{tr}}(A), \quad (s, t) \in K^2,\ h \in (0, 1]. \tag{4-17}$$

An identical result holds for bounded operators and for the norms $I_h^{m,\infty}$.

Proof of the lemma. By (4-7), one checks that, for every operator A satisfying the hypothesis of the lemma, and for each of the momentum operators $P_j(h)$, the following equality is valid:

$$\frac{\partial}{\partial t}[P_j(h), G_h(t,s)(A)] - \frac{1}{ih}\big[\widehat{H}_h(t), [P_j(h), G_h(t,s)(A)]\big] = \frac{1}{ih}\big[[P_j(h), \widehat{H}_h(t)], G_h(t,s)(A)\big].$$

Then the following equality results by the Duhamel principle:

$$\big[P_j(h), G_h(t,s)(A)\big] = G_h(t,s)\big([P_j(h), A]\big) + \frac{1}{ih}\int_s^t G_h(t,t_1)\big(\big[[P_j(h), \widehat{H}_h(t_1)], G_h(t_1,s)(A)\big]\big)\,dt_1.$$

We have an analogous equality for the position operators $Q_j(h)$. One has

$$[P_j(h), \widehat{H}_h(t)] = \frac{h}{i}\frac{\partial V(\,\cdot\,,t)}{\partial x_j}, \qquad [Q_j(h), \widehat{H}_h(t)] = 2ihP_j(h).$$

We therefore deduce

$$\big[P_j(h), G_h(t,s)(A)\big] = G_h(t,s)\big([P_j(h), A]\big) - \int_s^t G_h(t,t_1)\bigg(\bigg[\frac{\partial V(\,\cdot\,,t_1)}{\partial x_j}, G_h(t_1,s)(A)\bigg]\bigg)\,dt_1,$$

$$\big[Q_j(h), G_h(t,s)(A)\big] = G_h(t,s)\big([Q_j(h), A]\big) + 2\int_s^t G_h(t,t_1)\big(\big[P_j(h), G_h(t_1,s)(A)\big]\big)\,dt_1.$$

If A and its commutators with $P_j(h)$ and $Q_j(h)$ are trace class, we first observe that $[P_j(h), G_h(t,s)(A)]$ is a trace class operator since $G_h(t,s)$ maps $\mathscr{L}^1(\mathscr{H})$ into itself. Using the second equality, we see that $[Q_j(h), G_h(t,s)(A)]$ is also a trace class operator, and that the upper bound (4-17) is proved for $m = 1$. We pursue the same reasoning to prove (4-17), by induction, for every m. The analogue of (4-17) for the bounded operators is proved similarly. □

Proof of Theorem 4.2, second step. Following Proposition 2.1, it suffices to show that, for every multi-index (α,β) and for every compact set K of $\mathbb{R}$, there exists $C_{\alpha\beta K} > 0$ such that

$$h^{n-(|\alpha|+|\beta|)}\big\|(\mathrm{ad}\,P(h))^\alpha(\mathrm{ad}\,Q(h))^\beta G_h(t,0)(A_h)\big\|_{\mathscr{L}^1(\mathscr{H})} \le C_{\alpha\beta K} \tag{4-18}$$

for all $t \in K$ and $h \in (0,1]$. In order to achieve this, one will use the asymptotic expansion (4-9) up to an order N that will depend on α and β. Since from the first step, the $D_j(\,\cdot\,,t,h)$ $(j \ge 0)$ of the equality (4-9) belong to $W^{\infty,1}(\mathbb{R}^{2n})$ and are bounded independently of h in $(0,1]$ and of t in a compact set of $\mathbb{R}$, Proposition 2.1 shows that

$$h^{n-(|\alpha|+|\beta|)}\big\|(\mathrm{ad}\,P(h))^\alpha(\mathrm{ad}\,Q(h))^\beta\,\mathrm{Op}_h^{\mathrm{weyl}}(D_j(\,\cdot\,,t,h))\big\|_{\mathscr{L}^1(\mathscr{H})} \le C_{\alpha\beta K}$$

for all $t \in K$ and $h \in (0,1]$. Let us now derive an analogous upper bound for the term $E_N(t,s,h)$. For that, we use the expression (4-13) of $E_N(t,s,h)$, and we apply Lemma 4.4 with (t,s) replaced by (t,t_N) and A by $\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,,t_N,\dots,t_1,h))$. Since $R_N(\,\cdot\,,t_N,\dots,t_1,h)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$ and is bounded independently of h in $(0,1]$, of $(t_1,\dots t_N)$ in $\Delta_N(0,t)$, and of t in a compact set of $\mathbb{R}$, Proposition 2.1 shows that, for every integer $m \ge 0$ and every compact set K of $\mathbb{R}$, there exists $C > 0$ such that

$$h^n I_h^{m,\mathrm{tr}}\big(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\,\cdot\,,t_N,\dots,t_1,h))\big) \le C_{mK}$$

for all $h \in (0, 1]$, $(t_1, \dots, t_N) \in \Delta_N(0, t)$, and $t \in K$. Hence by Lemma 4.4, we deduce that the iterated commutators of $G_h(t, t_N)(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\cdot, t_N, \dots, t_1, h)))$ with the position and momentum operators are themselves trace class, and that there exists another constant C_{mK} such that

$$h^n I_h^{m,\mathrm{tr}}\big(G_h(t, t_N)(\mathrm{Op}_h^{\mathrm{weyl}}(R_N(\cdot, t_N, \dots, t_1, h)))\big) \le C_{mK}.$$

We can therefore write, if $A_h = \mathrm{Op}_h^{\mathrm{weyl}}(F)$, for every multi-index (α, β) and every integer N,

$$h^n \big\| (\mathrm{ad}\, Q(h))^\beta (\mathrm{ad}\, P(h))^\alpha E_N(t, h) \big\|_{\mathscr{L}^1(\mathscr{H})} \le C_{\alpha\beta N}.$$

By reporting this in (4-9), and by choosing $N = |\alpha| + |\beta|$, one deduces (4-18). Using the characterization of Proposition 2.1, Theorem 4.2 follows.

Proof of Theorem 1.1. Let $\rho_h(t)$ be a classical solution of TDHF satisfying the hypotheses of Theorem 1.1. Let us denote by $V_h(t)$ the operator of multiplication by the function

$$x \to V_q(x, \rho_h(t)) = V(x) + \mathrm{Tr}(W_x \circ \rho_h(t)), \qquad W_x(y) = W(x - y). \tag{4-19}$$

Under the hypotheses of Theorem 1.1, we have $\rho_h(t) \ge 0$ and $\mathrm{Tr}(\rho_h(t)) = 1$ for all t, and therefore the trace norm of $\rho_h(t)$ is constant. Since all the derivatives of V and W are bounded, it follows that

$$|\partial_x^\alpha V_q(\rho_h(t))(x)| \le C_\alpha, \qquad (x, t) \in \mathbb{R}^n \times \mathbb{R}. \tag{4-20}$$

Let $\widehat{H}_h(t)$ denote the operator defined in (4-3), where $V(t)$ is the multiplication by $V_q(x, \rho_h(t))$. With these notations, the TDHF equation can be written

$$ih \frac{d\rho_h(t)}{dt} = [\widehat{H}_h(t), \rho_h(t)]. \tag{4-21}$$

We note that $V_h(t)$ depends on h, but in Theorem 4.2, the potential $V(t)$ may depend on a parameter that could be h. The only requirement is that $V_q(\cdot, \rho_h(t))$ should be bounded in $W^{\infty,\infty}(\mathbb{R}^n)$ independently of h, which is the case. Denoting by $G_h(t, s)$ the unitary propagator associated to the Hamiltonian $H_h(t)$ as in Proposition 4.1, one therefore has

$$\rho_h(t) = G_h(t, 0)(\rho_h(0)) = G_h(t, 0)(\mathrm{Op}_h^{\mathrm{weyl}}(F_h)).$$

Theorem 1.1 is therefore a particular case of Theorem 4.2. □

5. Proof of Theorem 1.2

We are going to state precisely the explicit construction of an approximate solution of order N, denoted by $\rho_h^{(N)}(t)$, of the TDHF equation. The exact solution $\rho_h(t)$ is determined by the interaction potentials V and W, which belong to $W^{\infty,\infty}(\mathbb{R}^n)$, and the initial data $\rho_h(0)$. We look for an approximate solution with the ansatz (1-18), where $F^{(N)}(t, h)$ is a function $\mathbb{R}^{2n}$ of the form (1-16). The functions $u_j(\cdot, t)$ in the sum (1-16) will be determined in Proposition 5.1. They will be in $W^{\infty,1}(\mathbb{R}^{2n})$, and they can depend also on h. We will associate to this solution the average quantum potential, like in (1-2):

$$V_q(x, \rho_h^{(N)}(t)) = V(x) + \mathrm{Tr}\big(W_x \rho_h^{(N)}(t)\big). \tag{5-1}$$

By (2-7), if F is in $W^{\infty,1}(\mathbb{R}^{2n})$ and G in $W^{\infty,\infty}(\mathbb{R}^{2n})$, one has

$$\operatorname{Tr}\big(\operatorname{Op}_h^{\mathrm{weyl}}(F)\circ\operatorname{Op}_h^{\mathrm{weyl}}(G)\big)=(2\pi h)^{-n}\int_{\mathbb{R}^{2n}}F(X)G(X)\,dX.$$

Therefore, if $\rho_h^{(N)}(t)$ is defined by (1-18) and $F^{(N)}(t,h)$ by (1-16), we have

$$V_q(x,\rho_h^{(N)}(t))=V_{\mathrm{cl}}\big(x,F^{(N)}(\,\cdot\,,t,h)\big),\tag{5-2}$$

where, for every function v in $L^1(\mathbb{R}^{2n})$, the function $V_{\mathrm{cl}}(\,\cdot\,,v)$ is defined as in (1-3). One similarly shows that

$$V_q(x,\rho_h^{(N)}(t))=V_{\mathrm{cl}}\big(x,F^{(N)}(\,\cdot\,,t,h)\big).\tag{5-3}$$

With these notations, the function $u_h(\,\cdot\,,t)$ defined in (1-10) should satisfy

$$\frac{\partial u_h(\,\cdot\,,t)}{\partial t}+2\sum_{j=1}^{n}\xi_j\frac{\partial u_h(\,\cdot\,,t)}{\partial\xi_j}=\frac{1}{ih}M_h\big(V_{\mathrm{cl}}(u_h(\,\cdot\,,t)),u_h(\,\cdot\,,t)\big),\tag{5-4}$$

where for all suitable functions A and B, $M_h(A,B)$ denotes the Moyal bracket of A and B, defined in (3-2). For all functions A and B in $C^\infty(\mathbb{R}^{2n})$, and for every integer $k\ge 0$, let $C_k(A,B,\cdot)$ be the function defined in (3-4). We set $C_0(A,B)=0$. One has $C_1(A,B)=(1/i)\{A,B\}$. Now we will choose the u_j in a such a way that Equation (5-4) is approximatively verified. The construction of the functions u_j of Theorem 1.2 is detailed in the following proposition.

Proposition 5.1. *There exists a sequence of functions $(X,t)\to u_j(X,t)$ on $\mathbb{R}^{2n}\times\mathbb{R}$ $(j\ge 0)$ such that*:

(a) *The function $t\to u_j(\,\cdot\,,t,h)$ is C^∞ from $\mathbb{R}$ into $W^{\infty,1}(\mathbb{R}^{2n})$. The function $u_j(\,\cdot\,,t,h)$ is bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h in $(0,1]$ and of t in every compact set of $\mathbb{R}$.*

(b) *One has*

$$u_0(X,0)=F_h(X)\quad\textit{and}\quad u_j(X,0,h)=0,\qquad j\ge 1.$$

(c) *For every N, the function $u_N(X,t,h)$ verifies*

$$\frac{\partial u_N}{\partial t}+2\sum_{j=1}^{n}\xi_j\frac{\partial u_N}{\partial x_j}=\frac{1}{i}\sum_{j+k+\ell=N+1}C_k\big(V_{\mathrm{cl}}(\,\cdot\,,u_j(\,\cdot\,,t,h)),u_\ell(\,\cdot\,,t,h)\big).\tag{5-5}$$

In the sum (5-5), the indices j and ℓ are ≥ 0 and k is ≥ 1.

Determination of u_0. For $N=0$, Equation (5-5) reduces to the Vlasov equation,

$$\frac{\partial u_0}{\partial t}+2\sum_{j=1}^{n}\xi_j\frac{\partial u_0}{\partial x_j}=\sum_{j=1}^{n}\frac{\partial}{\partial x_j}V_{\mathrm{cl}}\big(u_0(\,\cdot\,,t)\big)\frac{\partial u_0(\,\cdot\,,t)}{\partial\xi_j},$$

and we want that $u_0(\,\cdot\,,0)=F_h$, where F_h is the function of (1-6), which is in $W^{\infty,1}(\mathbb{R}^{2n})$. It is well known (see [Braun and Hepp 1977]) that there exists a unique solution u_0 of this Cauchy problem, and that the function u_0 is continuous from $\mathbb{R}$ into $W^{\infty,1}(\mathbb{R}^{2n})$. If F_h stays bounded in $W^{\infty,1}(\mathbb{R}^{2n})$ independently of h, it is also the case for $u_0(\,\cdot\,,t,h)$.

Determination of u_N ($N \geq 1$). For every $N \geq 1$, Equation (5-5) can be written as

$$\begin{aligned}\frac{\partial u_N}{\partial t} + 2\sum_{j=1}^n \xi_j \frac{\partial u_N}{\partial x_j} &= \sum_{j=1}^n \frac{\partial}{\partial x_j} V_{\mathrm{cl}}\big(u_0(\,\cdot\,,t,h)\big)\frac{\partial u_N(\,\cdot\,,t)}{\partial \xi_j}\\ &\quad + \sum_{j=1}^n \frac{\partial}{\partial x_j} V_{\mathrm{cl}}\big(u_N(\,\cdot\,,t,h)\big)\frac{\partial u_0(\,\cdot\,,t,h)}{\partial \xi_j} + G_N(X,t,h),\\ G_N &= \frac{1}{i}\sum_{\substack{j+k+\ell=N+1\\ j<N,\,\ell<N}} C_k\big(V_{\mathrm{cl}}(u_j(\,\cdot\,,t,h)), u_\ell(\,\cdot\,,t,h)\big).\end{aligned}$$

One also requires that $u_N(X,0,h)=0$. To solve this equation, dropping the parameter h for the sake of simplifying notations, let us denote by $X \to \varphi_t(X) = (q(t,X), p(t,X))$ the Hamiltonian flow that is the solution of

$$q'(t,X) = 2p(t,X), \qquad p'(t,X) = -\nabla V(q(t,X)) - \int_{\mathbb{R}^{2n}} \nabla W(q(t,X)-y)u_0(y,\eta,t)\,dy\,d\eta$$

satisfying

$$q(0,X)=x, \qquad p(0,X)=\xi, \qquad X=(x,\xi).$$

The function v_N defined by $v_N(X,t) = u_N(\varphi_t(X),t)$ should satisfy

$$\frac{\partial v_N}{\partial t} = \sum_{j=1}^n \frac{\partial u_0}{\partial \xi_j}(\varphi_t(X),t)\int_{\mathbb{R}^{2n}} \frac{\partial W}{\partial x_j}\big(q_t(X)-y\big)\,u_N(y,\eta,t)\,dy\,d\eta + \widetilde{G}_N(X,t),$$

where $\widetilde{G}_N(X,t) = G_N(\varphi_t(X),t)$. By using in the integral the change of variables $(y,\eta) = \varphi_t(z,\zeta)$, whose jacobian equals 1, we see that v_N should satisfy

$$\begin{aligned}\frac{\partial v_N}{\partial t}(X,t) &= \widetilde{G}_N(X,t) + \int_{\mathbb{R}^{2n}} A(X,Y,t)v_N(Y,t)\,dY,\\ A(X,Y,t) &= \sum_{j=1}^n \frac{\partial u_0}{\partial \xi_j}\big(\varphi_t(X),t\big)\frac{\partial W}{\partial x_j}\big(q_t(X)-q_t(Y)\big).\end{aligned}$$

Moreover, one must have $v_N(\,\cdot\,,0)=0$. According to standard results on the Vlasov equation, one knows that $\nabla u_0(\,\cdot\,,t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded when t varies in a compact set. The same is true for $\nabla\varphi_t$. If the u_j ($0 \leq j < N$) have been built with the properties of Proposition 5.1, one sees that $G_N(\,\cdot\,,t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$, bounded when t varies in a compact set. It is also the case for $\widetilde{G}_N(\,\cdot\,,t)$. Then the Cauchy problem verified by v_N and the one verified by u_N can be solved in a standard way.

To prove Theorem 1.2, we will show that the functions $F^{(N)}(t,h)(X)$ defined in (1-16) starting from the $u_j(\,\cdot\,,t,h)$ of Proposition 5.1 and the operators $\rho_h^{(N)}(t)$ defined in (1-18) satisfy (1-17) and (1-19). The next proposition is an intermediate step.

Proposition 5.2. *Let $\rho_h(t)$ be an exact solution of TDHF satisfying the hypotheses of Theorems 1.1 and 1.2. Let $\widehat{H}_h(t)$ be the operator defined in (4-3), where $V(t)$ is the multiplication by $V_q(x,\rho_h(t))$. Let u_j*

($j \geq 0$) be the functions of Proposition 5.1, and, for each integer N, let $F^{(N)}$ be the function defined by (1-16) and $\rho_h^{(N)}(t)$ defined in (1-18). Then we can write

$$ih \frac{d\rho_h^{(N)}(t)}{dt} = [\widehat{H}_h(t), \rho_h^{(N)}(t)] + \mathrm{Op}_h^{\mathrm{weyl}}\big(S_h^{(N)}(\,\cdot\,, t)\big), \tag{5-6}$$

where $S_h^{(N)}(\,\cdot\,, t)$ is in $W^{\infty,1}(\mathbb{R}^{2n})$ and verifies, for every multi-index α,

$$\big\| \nabla^\alpha S_h^{(N)}(\,\cdot\,, t) \big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\alpha N}(t)\big[h^{N+2} + h \big\| \rho_h(t) - \rho_h^{(N)}(t) \big\|_{\mathcal{L}^1(\mathcal{H})}\big], \tag{5-7}$$

where $C_{\alpha N}(t)$ is a function on $\mathbb{R}$ which is bounded on every compact set.

Proof. By (5-5), we have

$$\frac{\partial F^{(N)}}{\partial t} + 2\sum_{j=1}^{n} \xi_j \frac{\partial F^{(N)}}{\partial x_j} = \frac{1}{h} \sum_{k=1}^{N+1} h^k C_k\big(V_{\mathrm{cl}}(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)), F^{(N)}(\,\cdot\,, t, h)\big) + \Phi^{(N)}(\,\cdot\,, t, h), \tag{5-8}$$

where $\Phi^{(N)}(\,\cdot\,, t, h)$ is a function in $W^{\infty,1}(\mathbb{R}^{2n})$, such that

$$\big\| \nabla^\alpha \Phi^{(N)}(\,\cdot\,, t, h) \big\|_{L^1(\mathbb{R}^{2n})} \leq h^{N+1} C_{\alpha N}(t). \tag{5-9}$$

We define an approximation of the operator $\widehat{H}_h(t)$ by setting

$$\widehat{H}_h^{\mathrm{APP}}(t) = -h^2 \Delta + V_{\mathrm{cl}}\big(F^{(N)}(\,\cdot\,, t, h)\big). \tag{5-10}$$

Since $F^{(N)}$ verifies (5-8), we may write

$$ih \frac{d\rho_h^{(N)}(t)}{dt} = \big[\widehat{H}_h^{\mathrm{APP}}(t), \rho_h^{(N)}(t)\big] + \mathrm{Op}_h^{\mathrm{weyl}}\big(T_h^{(N)}(\,\cdot\,, t)\big), \tag{5-11}$$

where the function $T_h^{(N)}(\,\cdot\,, t)$ is defined by

$$T_h^{(N)}(\,\cdot\,, t) = h\Phi^{(N)}(\,\cdot\,, t, h) + R_h^{(N+2)}\big(V_{\mathrm{cl}}(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)), F^{(N)}(\,\cdot\,, t, h)\big).$$

(For all functions A and B satisfying the hypotheses of Theorem 3.1, we denote by $R_h^{(N)}(A, B, \cdot)$ the function associated by Theorem 3.1 to such functions.) Then by the definition (5-3) of the map V_{cl}, and Proposition 5.1(a), we can write

$$\big\| \nabla_x^\alpha V_{\mathrm{cl}}\big(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)\big) \big\|_{L^\infty(\mathbb{R}^{2n})} \leq C_{\alpha N}(t), \quad \big\| \nabla^\beta F^{(N)}(\,\cdot\,, t, h)) \big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\beta N}(t). \tag{5-12}$$

Using these upper bounds and following Theorem 3.1 on the Moyal bracket, we may write

$$\big\| \nabla^\ell R_h^{(N+2)}\big(V_{\mathrm{cl}}(\,\cdot\,, F^{(N)}(\,\cdot\,, t, h)), F^{(N)}(\,\cdot\,, t, h)\big) \big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\ell N}(t) h^{N+2}.$$

According to these upper bound estimates, and the estimates (5-9) of the derivatives of $\Phi^{(N)}(\,\cdot\,, t, h)$, one has

$$\big\| \nabla^\alpha T_h^{(N)}(\,\cdot\,, t) \big\|_{L^1(\mathbb{R}^{2n})} \leq C_{\alpha N}(t) h^{N+2}. \tag{5-13}$$

According to (5-11), and since

$$\widehat{H}_h^{\mathrm{APP}}(t)-\widehat{H}_h(t)=V_q(\,\cdot\,,\rho_h(t))-V_q(\,\cdot\,,\rho_h^{(N)}(t)),$$

we can write the equality (5-6) with

$$S_h^{(N)}(\,\cdot\,,t)=T_h^{(N)}(\,\cdot\,,t)+M_h\big(V_q(\,\cdot\,,\rho_h(t))-V_q(\,\cdot\,,\rho_h^{(N)}(t)),\,F^{(N)}(\,\cdot\,,t,h)\big). \tag{5-14}$$

One has

$$\big\|\nabla_x^\alpha\big(V_q(\,\cdot\,,\rho_h(t))-V_q(\,\cdot\,,\rho_h^{(N)}(t))\big)\big\|_{L^\infty(\mathbb{R}^{2n})}\le C_\alpha\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}.$$

Using all of these estimates and the L^1 norm estimates (5-12) of $F^{(N)}(\,\cdot\,,t,h)$, and using Theorem 3.1 on the Moyal bracket, it results that

$$\big\|\nabla^\alpha M_h\big(V_q(\rho_h(t))-V_q(\rho_h^{(N)}(t)),\,F^{(N)}(\,\cdot\,,t,h)\big)\big\|_{L^1(\mathbb{R}^{2n})}\le C(t)h\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}. \tag{5-15}$$

The norm upper bound estimate (5-7) of $S_h^{(N)}(\,\cdot\,,t)$ results from (5-14), (5-13) and (5-15).

End of the proof of Theorem 1.2. Let $U_h(t,s)$ and $G_h(t,s)$ be the unitary propagator and the mapping defined in Proposition 4.1, associated to the operator $\widehat{H}_h(t)$ of Proposition 5.2. The comparison of equalities (4-21) (verified by the exact solution) and (5-6) (verified by the approximate solution) and the Duhamel principle allow us to write

$$\rho_h(t)-\rho_h^{(N)}(t)=\frac{i}{h}\int_0^t G_h(t,s)\big(\mathrm{Op}_h^{\mathrm{weyl}}(S_h^{(N)}(\,\cdot\,,s))\big)\,ds. \tag{5-16}$$

Since $U_h(t,s)$ is unitary, the map $G_h(t,s)$ preserves the trace norm, and from that we may deduce that

$$\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}\le\frac{1}{h}\int_0^t\big\|\mathrm{Op}_h^{\mathrm{weyl}}(S_h^{(N)}(\,\cdot\,,s))\big\|_{\mathscr{L}^1(\mathscr{H})}\,ds.$$

Using Proposition 2.1 and the upper bounds (5-7) of Proposition 5.2, we obtain

$$\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}\le\frac{1}{h}\int_0^t C(s)\big[h^{N+2}+h\big\|\rho_h(s)-\rho_h^{(N)}(s)\big\|_{\mathscr{L}^1(\mathscr{H})}\big]\,ds.$$

By the Gronwall lemma, we deduce that, with another constant,

$$\big\|\rho_h(t)-\rho_h^{(N)}(t)\big\|_{\mathscr{L}^1(\mathscr{H})}\le C(t)h^{N+1}.$$

Therefore the Theorem 1.2(1-19) is proved. We deduce from this inequality and from (5-7) that

$$\big\|\nabla^\alpha S_h^{(N)}(\,\cdot\,,t)\big\|_{L^1(\mathbb{R}^{2n})}\le C_{\alpha N}(t)h^{N+2},$$

where $C_{\alpha N}(t)$ is a function on $\mathbb{R}$, bounded on every compact set. From Proposition 2.1 and Lemma 4.4, for every multi-index (α,β), the operators

$$h^{-N-2}(\mathrm{ad}\,Q(h))^\beta(\mathrm{ad}\,P(h))^\alpha G_h(t,s)\big(\mathrm{Op}_h^{\mathrm{weyl}}(S_h^{(N)}(\,\cdot\,,s)\big)$$

are trace class, and their trace norm is bounded, independently of (t, s) in a compact set of $\mathbb{R}$, and of h in $(0, 1]$. By (5-16), for every multi-index (α, β), and for every $N > 0$, there exists a function $C_{\alpha N}(t) > 0$, bounded on every compact set of $\mathbb{R}$, such that

$$\left\| (\operatorname{ad} Q(h))^{\beta} (\operatorname{ad} P(h))^{\alpha} \left(\rho_h(t) - \rho_h^{(N)}(t) \right) \right\|_{\mathcal{L}^1(\mathcal{H})} \leq C_{\alpha N}(t) h^{N+1}.$$

Using Proposition 2.1(b), we deduce

$$(2\pi h)^{-n} \left\| \sigma_h^{\text{weyl}} \left(\rho_h(t) - \rho_h^{(N)}(t) \right) \right\|_{L^1(\mathbb{R}^{2n})} \leq C(t) h^{(N+1)-(2n+2)/2}.$$

In other words, with the notations of Theorem 1.2,

$$\left\| u_h(\,\cdot\,, t) - F^{(N)}(\,\cdot\,, t, h) \right\|_{L^1(\mathbb{R}^{2n})} \leq C(t) h^N.$$

This is the Theorem 1.2(1-17), which is proved now. □

Appendix A: Proof of Proposition 2.1

The proof of Proposition 2.1 calls upon a different notion of symbol. One can associate to every bounded operator A in $\mathcal{H}$ a function $S_h(A)$ on $\mathbb{R}^{2n} \times \mathbb{R}^{2n}$ defined by

$$S_h(A)(X, Y) = \frac{\langle A \Psi_{Xh}, \Psi_{Yh} \rangle}{\langle \Psi_{Xh}, \Psi_{Yh} \rangle}, \tag{A-1}$$

where the Ψ_{Xh} are defined in (2-14). An explicit computation of integrals shows that

$$|\langle \Psi_{Xh}, \Psi_{Yh} \rangle| = e^{-(1/4h)|X-Y|^2}, \qquad \|\Psi_{Xh}\| = 1. \tag{A-2}$$

Consequently,

$$|S_h(A)(X, Y)| = e^{(1/4h)|X-Y|^2} |\langle A \Psi_{Xh}, \Psi_{Yh} \rangle|. \tag{A-3}$$

The function $S_h(A)$ is, up to a slight modification, what G. B. Folland [1989] calls the Wick symbol. The following proposition shows that $S_h(A)$ and the Weyl symbol $\sigma_h^{\text{weyl}}(A)$ are related to each other by an integral operator. (By contrast, the Weyl symbol cannot be calculated from what is commonly called the Wick symbol, namely the restriction of $S_h(A)$ to the diagonal.) The function $S_h(A)$ can be majorized (in some norm) and minorized (in another norm) by the trace norm of A (Proposition A.2).

Proposition A.1. *The Weyl symbol of an operator A is related to the function $S_h(A)$ by*

$$S_h(A)(X, Y) = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} e^{-(1/h)(Z-X).(\overline{Z}-\overline{Y})} \sigma_h^{\text{weyl}}(A)(Z)\, dZ, \tag{A-4}$$

$$\sigma_h^{\text{weyl}}(A)(Z) = 2^n (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} S_h(A)(X, Y) K_h(X, Y, Z)\, dX\, dY, \tag{A-5}$$

$$K_h(X, Y, Z) = e^{-(1/h)(\overline{Z}-\overline{X})(Z-Y)-(1/2h)|X-Y|^2}. \tag{A-6}$$

Proof. By the definition (2-3) of the Weyl calculus, one has

$$A = (\pi h)^{-n} \int_{\mathbb{R}^{2n}} \Sigma_{Zh} \sigma_h^{\text{weyl}}(A)(Z)\, dZ,$$

where Σ_{Zh} is the operator defined in (2-4). An explicit computation shows that

$$\frac{\langle \Sigma_{Zh}\Psi_{Xh}, \Psi_{Yh}\rangle}{\langle \Psi_{Xh}, \Psi_{Yh}\rangle} = e^{-(1/h)(Z-X).(\overline{Z}-\overline{Y})}. \tag{A-7}$$

The equality (A-4) follows. By the fundamental formula (2-16) of coherent states, one has

$$A = (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \langle A\Psi_{Xh}, \Psi_{Yh}\rangle P_{XYh}\, dX\, dY, \tag{A-8}$$

where P_{XYh} is the operator defined by

$$P_{XYh} f = \langle f, \Psi_{Xh}\rangle \Psi_{Yh}. \tag{A-9}$$

One knows from (2-5) that

$$\sigma_h^{\text{weyl}}(P_{XYh})(Z) = 2^n \operatorname{Tr}(P_{XYh}\circ \Sigma_Z) = 2^n \langle \Sigma_{Zh}\Psi_{Yh}, \Psi_{Xh}\rangle.$$

By the computation leading to (A-7) (where X and Y are permuted), we may deduce

$$\sigma_h^{\text{weyl}}(A)(Z) = 2^n (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} S_h(A)(X, Y) \big|\langle \Psi_{Xh}, \Psi_{Yh}\rangle\big|^2 e^{-(1/h)(\overline{Z}-\overline{X})(Z-Y)}\, dX\, dY.$$

Using the equality (2-15) on the scalar product of coherent states, we obtain (A-5). □

Proposition A.2. *Let A be a trace class operator and G a function in $L^1(\mathbb{R}^{2n})$. Then one has*

$$(2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \left| \langle A\Psi_{Xh}, \Psi_{Yh}\rangle G\left(\frac{X-Y}{\sqrt{h}}\right)\right| dX\, dY \le (2\pi)^{-n} \|G\|_{L^1(\mathbb{R}^{2n})} \|A\|_{\mathcal{L}^1(\mathcal{H})}, \tag{A-10}$$

$$\|A\|_{\mathcal{L}^1(\mathcal{H})} \le (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \big|\langle A\Psi_{Xh}, \Psi_{Yh}\rangle\big|\, dX\, dY. \tag{A-11}$$

Proof. We may write $A = B_1 B_2$, where B_1 and B_2 are Hilbert–Schmidt. By using the fundamental property (2-16) of coherent states, one sees that for all X and Y in R^{2n},

$$\langle A\Psi_{Xh}, \Psi_{Yh}\rangle = \langle B_2\Psi_{Xh}, B_1^\star \Psi_{Yh}\rangle = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} u_{Zh}(X) v_{Zh}(Y)\, dZ,$$

where $u_{Zh}(X) = \langle B_2\Psi_{Xh}, \Psi_{Zh}\rangle$ and $v_{Zh}(X) = \langle \Psi_{Zh}, B_1^\star \Psi_{Xh}\rangle$. Let I_h be the left-hand side of (A-10). By Schur's lemma,

$$I_h \le (2\pi h)^{-3n} h^n \|G\|_{L^1(\mathbb{R}^{2n})} \int_{\mathbb{R}^{2n}} \|u_{Zh}\|_{L^2(\mathbb{R}^{2n})} \|v_{Zh}\|_{L^2(\mathbb{R}^{2n})}\, dZ.$$

By (2-16), we have $\|u_{Zh}\|_{L^2(\mathbb{R}^{2n})} = (2\pi h)^{n/2} \|B_2^\star \Psi_{Zh}\|$ and $\|v_{Zh}\|_{L^2(\mathbb{R}^{2n})} = (2\pi h)^{n/2} \|B_1\Psi_{Zh}\|$. Hence,

$$I_h \le (2\pi h)^{-2n} h^n \|G\|_{L^1(\mathbb{R}^{2n})} \int_{\mathbb{R}^{2n}} \|B_1\Psi_{Zh}\| \|B_2^\star \Psi_{Zh}\|\, dZ.$$

By the fundamental property (2-16) of coherent states,

$$(2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \|B_j\Psi_{Zh}\|^2\, dZ = (2\pi h)^{-n} \int_{\mathbb{R}^{2n}} \langle B_j^\star B_j \Psi_{Zh}, \Psi_{Zh}\rangle\, dZ = \operatorname{Tr}(B_j^\star B_j) = \|B_j\|^2_{\mathcal{L}^2(\mathcal{H})},$$

where $\|B_j\|_{\mathcal{L}^2(\mathcal{H})}$ is the Hilbert norm of B_j. Therefore,

$$I_h \leq (2\pi)^{-n} \|G\|_{L^1(\mathbb{R}^{2n})} \, \|B_1\|_{\mathcal{L}^2(\mathcal{H})} \, \|B_2\|_{\mathcal{L}^2(\mathcal{H})}.$$

By taking the infimum over all the decompositions $A = B_1 B_2$, one gets (A-10). The inequality (A-11) is deduced from the equality (A-8) since the operators P_{XYh} have a trace norm equal to 1. □

Proof of Proposition 2.1. For (a), we use the equality (A-4) and integrate by parts, as is done in [Rondeaux 1984]. Thus we see that

$$(2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-(1/4h)|X-Y|^2} |S_h(A)(X, Y)| \, dX \, dY \leq C h^{-n} \sum_{|\alpha|+|\beta|\leq 2n+2} h^{(|\alpha|+|\beta|)/2} \|\partial_x^\alpha \partial_\xi^\beta F\|_{L^1(\mathbb{R}^{2n})}.$$

One then deduces item (a) (the upper bound estimate of the trace norm of A), using Equation (A-11).

For parts (b) and (c), we are going to integrate by parts in the second equality (A-5) of Proposition A.1. One verifies that the function K_h defined in (A-6) is invariant by the differential operator

$$L(h) K_h = K_h, \quad L(h) = \left(1 + \frac{|X-Y|^2}{h}\right)^{-1} \left(1 + (\overline{Y} - \overline{X}) \partial_X\right).$$

Thus equality (A-5) implies, for every integer N,

$$\left|\sigma_h^{\mathrm{weyl}}(A)(Z)\right| \leq 2^n (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \left|K_h(X, Y, Z)\right| \left|({}^t L(h))^N S_h(A)(X, Y)\right| dX \, dY.$$

One verifies that

$$|K_h(X, Y, Z)| = e^{-(1/h)|Z-(X+Y/2)|^2 - (1/4h)|X-Y|^2}.$$

One chooses $N = 2n+2$. There exists $C > 0$ such that

$$\left|\sigma_h^{\mathrm{weyl}}(A)(Z)\right| \leq C \sum_{|\alpha|\leq 2n+2} h^{|\alpha|/2} (2\pi h)^{-2n} \int_{\mathbb{R}^{4n}} \left|K_h(X, Y, Z)\right| G\left(\frac{X-Y}{\sqrt{h}}\right) \left|\partial_X^\alpha S_h(A)(X, Y)\right| dX \, dY,$$

where

$$G(X) = (1 + |X|)^{-2n-2}.$$

By the classical formulas giving $S_h([P_j(h), A])$ and $S_h([Q_j(h), A])$ as an expression with the derivatives of $S_h(A)$, it follows that

$$\begin{aligned} &\left|\sigma_h^{\mathrm{weyl}}(A)(Z)\right| \\ &\leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{-2n-(|\alpha|+|\beta|)/2} \int_{\mathbb{R}^{4n}} e^{-(1/h)|Z-(X+Y/2)|^2 - (1/4h)|X-Y|^2} G\left(\frac{X-Y}{\sqrt{h}}\right) \left|S_h(A_{\alpha\beta h})(X, Y)\right| dX \, dY, \end{aligned}$$

where

$$A_{\alpha\beta h} = (\mathrm{ad}\, P(h))^\alpha (\mathrm{ad}\, Q(h))^\beta A.$$

The preceding equality can be also written as

$$\left|\sigma_h^{\mathrm{weyl}}(A)(Z)\right| \leq C \sum_{|\alpha|+|\beta|\leq 2n+2} h^{-2n-(|\alpha|+|\beta|)/2} \int_{\mathbb{R}^{4n}} e^{-\frac{1}{h}\left|Z - \frac{X+Y}{2}\right|^2} G\left(\frac{X-Y}{\sqrt{h}}\right) \left|\langle (A_{\alpha\beta h} \Psi_{Xh}, \Psi_{Yh}\rangle\right| dX \, dY.$$

Item (b) is a consequence of (A-11). Item (c) (an analogue of the Beals characterization) is then easily deduced. □

Appendix B: Proof of Theorems 3.1 and 3.2

First step, common to both theorems. We know that, for all suitable functions F and G, we can write $\mathrm{Op}_h^{\mathrm{weyl}}(F) \circ \mathrm{Op}_h^{\mathrm{weyl}}(G) = \mathrm{Op}_h^{\mathrm{weyl}}(C_h(F, G, \cdot))$, with

$$C_h(F, G, X) = (\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-(2i/h)\sigma(Y-X,Z-X)} F(Y)G(Z)\, dY\, dZ,$$

where σ is the symplectic form $\sigma((x, \xi), (y, \eta)) = y\xi - x\eta$. Consequently the Moyal bracket $M_h(F, G, \cdot)$ is defined by $M_h(F, G, X) = C_h(F, G, X) - C_h(G, F, X)$. Thus it suffices to write an asymptotic expansion $C_h(F, G, \cdot)$. We may write $C_h(F, G, X) = \Phi_h(X, 1)$ by setting, for every $\theta \in [0, 1]$,

$$\Phi_h(X, \theta) = (\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-(2i/h)\sigma(Y-X,Z-X)} F(Y)G\big(X + \theta(Z - X)\big)\, dY\, dZ.$$

Consequently, for every integer N,

$$C_h(F, G, X) = \sum_{k=0}^{N-1} \frac{1}{k!} \partial_t^k \Phi_h(X, 0) + \widetilde{R}_h^{(N)}(F, G, X),$$

with

$$\widetilde{R}_h^{(N)}(F, G, X) = \int_0^1 \frac{(1-\theta)^{N-1}}{(N-1)!}\, \partial_\theta^N \Phi_h(X, \theta)\, d\theta.$$

One sees, using integration by parts, that

$$\partial_\theta^k \Phi(X, \theta, h) = \left(\frac{h}{2i}\right)^k (\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-(2i/h)\sigma(Y-X,Z-X)} \big(\sigma(\nabla_1, \nabla_2)^k (F \otimes G)\big)\big(Y, X + \theta(Z - X)\big)\, dY\, dZ.$$

If a function Φ depends only on the Y variable, one has (in the sense of distributions)

$$(\pi h)^{-2n} \int_{\mathbb{R}^{4n}} e^{-(2i/h)\sigma(Y-X,Z-X)} \Phi(Y)\, dY\, dZ = \Phi(X),$$

and similarly if Φ depends only on the Z variable. For $\theta = 0$, one has, by the above two equalities,

$$\partial_\theta^k \Phi(X, 0, h) = \left(\frac{h}{2i}\right)^k \sigma(\nabla_1, \nabla_2)^k (F \otimes G)(X, X),$$

and therefore we do have indeed the equality (3-3) of Theorem 3.1, by setting

$$R_h^{(N)}(F, G, X) = \widetilde{R}_h^{(N)}(F, G, X) - \widetilde{R}_h^{(N)}(G, F, X). \tag{B-1}$$

It remains to obtain an upper bound for the norm of the two above terms. One also has

$$\widetilde{R}_h^{(N)}(F, G, X) = \left(\frac{h}{2i}\right)^N (\pi h)^{-2n} \int_{\mathbb{R}^{4n} \times [0,1]} \frac{(1-\theta)^{N-1}}{(N-1)!} K_h(X, Y, Z)\Psi(X, Y, Z, \theta)\, dY\, dZ\, d\theta,$$

where

$$K_h(X,Y,Z)=e^{-(2i/h)\sigma(Y-X,Z-X)},$$
$$\Psi(X,Y,Z,\theta)=\big(\sigma(\nabla_1,\nabla_2)^N(F\otimes G)\big)\big(Y,X+\theta(Z-X)\big).$$

The function K_h is invariant by the operator

$$L_h=\left(1+4\frac{|X-Y|^2}{h}+4\frac{|X-Z|^2}{h}\right)^{-1}(1-h\Delta_Y-h\Delta_Z).$$

Therefore, for all integers K and ℓ,

$$\big|\nabla^\ell\widetilde{R}_h^{(N)}(F,G,X)\big|\le\left(\frac{h}{2}\right)^N(\pi h)^{-2n}\int_{\mathbb{R}^{4n}\times[0,1]}\frac{(1-\theta)^{N-1}}{(N-1)!}\big|\nabla^\ell({}^tL)^K\Psi(X,Y,Z,\theta)\big|\,dY\,dZ\,d\theta.$$

Consequently,

$$h^{\ell/2}|\nabla^\ell\widetilde{R}_h^{(N)}(F,G,X)|\le C\sum_{\substack{\alpha+\beta\le\ell+2K+2N\\ \alpha\ge N,\,\beta\ge N}}h^{(\alpha+\beta)/2}I_{\alpha\beta}(X,h),\tag{B-2}$$

$$I_{\alpha\beta}(X,h)=h^{-2n}\int_{\mathbb{R}^{4n}\times[0,1]}(1-\theta)^{N-1}\left(1+\frac{|X-Y|+|X-Z|}{\sqrt{h}}\right)^{-2K}|\nabla^\alpha F(Y)|\big|\nabla^\beta G\big(X+\theta(Z-X)\big)\big|\,dY\,dZ\,d\theta.\tag{B-3}$$

End of the proof of Theorem 3.1. We integrate the equality (B-3) with respect to X by making the change of variables

$$X=(1-\theta)^{-1}(\widetilde{X}-\theta\widetilde{Z}),\quad Y=\widetilde{Y},\quad Z=\widetilde{Z}.$$

We obtain

$$\big\|I_{\alpha\beta}(\cdot,h)\big\|_{L^1(\mathbb{R}^{2n})}\le Ch^{-2n}\int_{\mathbb{R}^{6n}\times[0,1]}(1-\theta)^{N-2n-1}\left(1+\frac{|X-Y|+|X-Z|}{\sqrt{h}}\right)^{-2K}|\nabla^\alpha F(Y)||\nabla^\beta G(X)|\,dX\,dY\,dY\,dZ\,d\theta.$$

If one has $N\ge 2n+1$ and chooses $K=2n+1$, we deduce, by using Schur's lemma, that

$$\big\|I_{\alpha\beta}(\cdot,h)\big\|_{L^1(\mathbb{R}^{2n})}\le C\|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\,\|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}.$$

Adding these inequalities, we obtain

$$h^{\ell/2}\big|\nabla^\ell R_h^{(N,1)}(F,G,X)\big|\le C\sum_{\substack{\alpha+\beta\le\ell+2K+2N\\ \alpha\ge N,\,\beta\ge N}}h^{(\alpha+\beta)/2}\|\nabla^\alpha F\|_{L^p(\mathbb{R}^{2n})}\|\nabla^\beta G\|_{L^q(\mathbb{R}^{2n})}.$$

By proceeding similarly for $\widetilde{R}_h^{(N)}(G,F,\cdot)$, we arrive at the upper bound (3-5) of Theorem 3.1. Part (3-6) is then deduced by Proposition 2.1.

End of the proof of Theorem 3.2. If one chooses $K = 2n + 1$, it follows from (B-3) that

$$\left\| I_{\alpha\beta}(\cdot\,, h) \right\|_{L^\infty(\mathbb{R}^{2n})} \leq C \|\nabla^\alpha F\|_{L^\infty(\mathbb{R}^{2n})} \|\nabla^\beta G\|_{L^\infty(\mathbb{R}^{2n})}.$$

By substituting in (B-2), then in (B-1), we obtain the majorization (3-7) of Theorem 3.2.

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THE CLASSIFICATION OF FOUR-END SOLUTIONS TO THE ALLEN–CAHN EQUATION ON THE PLANE

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An entire solution of the Allen–Cahn equation $\Delta u = f(u)$, where f is an odd function and has exactly three zeros at ± 1 and 0, for example, $f(u) = u(u^2 - 1)$, is called a $2k$-end solution if its nodal set is asymptotic to $2k$ half lines, and if along each of these half lines the function u looks like the one-dimensional, heteroclinic solution. In this paper we consider the family of four-end solutions whose ends are almost parallel at ∞. We show that this family can be parametrized by the family of solutions of the Toda system. As a result we obtain the uniqueness of four-end solutions with almost parallel ends. Combining this result with the classification of connected components in the moduli space of the four-end solutions, we can classify all such solutions. Thus we show that four-end solutions form, up to rigid motions, a one parameter family. This family contains the saddle solution, for which the angle between the nodal lines is $\pi/2$, as well as solutions for which the angle between the asymptotic half lines of the nodal set is any $\theta \in (0, \pi/2)$.

1. Introduction

Some entire solutions to the Allen–Cahn equation in $\mathbb{R}^2$. This paper deals with the problem of classification of the family of four-end solutions (precise definition will follow) to the Allen–Cahn equation:

$$\Delta u = F'(u) \quad \text{in } \mathbb{R}^2. \tag{1-1}$$

The function F is a smooth double well potential, which means that we assume the following conditions for F: F is even, nonnegative, and has only two zeros at ± 1, $F'(t) \neq 0$, $t \in (0, 1)$. We also suppose $F''(1) \neq 0$, $F''(0) \neq 0$. For convenience, we assume that F is such that $F''(1) = 2$. A standard example is $F(u) = \frac{1}{4}(1 - u^2)^2$.

It is known that (1-1) has a solution whose nodal set is a straight line. This will be called a *planar solution*. It is obtained simply by taking the unique, odd, heteroclinic solution connecting -1 to 1

$$H'' = F'(H), \qquad H(\pm\infty) = \pm 1, \qquad H(0) = 0, \tag{1-2}$$

and letting $u(x, y) = H(ax + by + c)$ for some constants a, b, c such that $a^2 + b^2 = 1$. We note that if $a > 0$, then $\partial_x u = aH' > 0$. The De Giorgi conjecture says that if u with $|u| < 1$ is a smooth solution of (1-1)

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such that $\partial_{\boldsymbol{e}} u > 0$ for a certain fixed direction $\boldsymbol{e}$, then u must in fact be a planar solution. Indeed, this conjecture holds in $\mathbb{R}^N$, $N \le 8$ (see [Ghoussoub and Gui 1998] when $N = 2$, [Ambrosio and Cabré 2000] when $N = 3$, and [Savin 2009] for $4 \le N \le 8$ under an additional limit condition), while a counterexample can be given when $N \ge 9$ [del Pino et al. 2011]. It is worth mentioning that the De Giorgi conjecture is a direct analogue of the famous Bernstein conjecture in the theory of minimal surfaces.

In order to proceed with the statement of our results, we will define the family of four-end solutions of (1-1), which is a particular example of a more general family of $2k$-end solutions [del Pino et al. 2013]. Intuitively, a four-end solution u is characterized by the fact that its nodal set $N(u)$ is asymptotic at infinity to four half lines, and along each of these half lines it looks locally like the heteroclinic solution. To describe this precisely, we introduce the set Λ_4 of oriented and ordered four affine lines in $\mathbb{R}^2$. Thus Λ_4 consists of 4-tuples $(\lambda_1, \dots, \lambda_4)$ such that each λ_j can be uniquely written as

$$\lambda_j := r_j \boldsymbol{e}_j^{\perp} + \mathbb{R}\boldsymbol{e}_j$$

for some $r_j \in \mathbb{R}$ and some unit vector $\boldsymbol{e}_j = (\cos\theta_j, \sin\theta_j) \in S^1$, which defines the orientation of the line. Here, the symbol $\perp$ refers to the rotation of angle $\pi/2$ in $\mathbb{R}^2$. Observe that the affine lines are oriented, and hence we do not identify the line corresponding to (r_j, θ_j) and the line corresponding to $(-r_j, \theta_j + \pi)$. Additionally we require that these lines are ordered, which means

$$\theta_1 < \theta_2 < \theta_3 < \theta_4 < 2\pi + \theta_1.$$

For future purposes we denote by

$$\theta_\lambda := \tfrac{1}{2} \min\{\theta_2 - \theta_1, \theta_3 - \theta_2, \theta_4 - \theta_3, 2\pi + \theta_1 - \theta_4\} \tag{1-3}$$

the half of the minimum of the angles between any two consecutive oriented affine lines of $\lambda_1, \dots, \lambda_4$.

Assume that we are given a 4-tuple of oriented affine lines $\lambda = (\lambda_1, \dots, \lambda_4)$. It is easy to check that for all $R > 0$ large enough and for all $j = 1, \dots, 4$, there exists $s_j \in \mathbb{R}$ such that

(i) the point $\boldsymbol{x}_j := r_j \boldsymbol{e}_j^{\perp} + s_j \boldsymbol{e}_j$ belongs to the circle ∂B_R, with $R > 0$;

(ii) the half lines

$$\lambda_j^+ := \boldsymbol{x}_j + \mathbb{R}^+ \boldsymbol{e}_j \tag{1-4}$$

are disjoint and included in $\mathbb{R}^2 \setminus B_R$;

(iii) the minimum of the distance between two distinct half lines λ_i^+ and λ_j^+ is larger than 4.

The set of affine half lines $\lambda_1^+, \dots, \lambda_4^+$ together with the circle ∂B_R induces a decomposition of $\mathbb{R}^2$ into five slightly overlapping connected components

$$\mathbb{R}^2 = \Omega_0 \cup \Omega_1 \cup \cdots \cup \Omega_4,$$

where

$$\Omega_0 := B_{R+1},$$

and where, for $j = 1, \dots, 4$,

$$\Omega_j := \{ \boldsymbol{x} \in \mathbb{R}^2 : |\boldsymbol{x}| > R - 1 \text{ and } \operatorname{dist}(\boldsymbol{x}, \lambda_j^+) < \operatorname{dist}(\boldsymbol{x}, \lambda_i^+) + 2 \text{ for all } i \neq j \}, \tag{1-5}$$

where $\operatorname{dist}(\boldsymbol{x}, \lambda_j^+)$ denotes the distance of $\boldsymbol{x}$ to λ_j^+. Observe that, for all $j = 1, \dots, 4$, the set Ω_j contains the half line λ_j^+.

We consider a smooth partition of unity of $\mathbb{R}^2$ given by the functions $\mathbb{I}_0, \mathbb{I}_1, \dots, \mathbb{I}_4$, which is subordinate to the above decomposition of $\mathbb{R}^2$. Hence

$$\sum_{j=0}^{4} \mathbb{I}_j \equiv 1,$$

and the support of $\mathbb{I}_j$ is included in Ω_j for $j = 0, \dots, 4$. Without loss of generality, we can also assume that $\mathbb{I}_0 \equiv 1$ in

$$\Omega_0' := B_{R-1},$$

and $\mathbb{I}_j \equiv 1$ in

$$\Omega_j' := \{ \boldsymbol{x} \in \mathbb{R}^2 : |\boldsymbol{x}| > R + 1 \text{ and } \operatorname{dist}(\boldsymbol{x}, \lambda_j^+) < \operatorname{dist}(\boldsymbol{x}, \lambda_i^+) - 2 \text{ for all } i \neq j \}$$

for $j = 1, \dots, 4$. Finally, we assume that

$$\|\mathbb{I}_j\|_{\mathscr{C}^2(\mathbb{R}^2)} \leq C.$$

We now take $\lambda = (\lambda_1, \dots, \lambda_4) \in \Lambda_4$ with $\lambda_j^+ = \boldsymbol{x}_j + \mathbb{R}^+ \boldsymbol{e}_j$ and we define

$$u_\lambda(\boldsymbol{x}) := \sum_{j=1}^{4} (-1)^j \mathbb{I}_j(\boldsymbol{x}) H((\boldsymbol{x} - \boldsymbol{x}_j) \cdot \boldsymbol{e}_j^\perp). \tag{1-6}$$

Observe that, by construction, the function u_λ is, away from a compact set, asymptotic to copies of planar solutions whose nodal set is the affine half lines $\lambda_1^+, \dots, \lambda_4^+$. A simple computation shows that u_λ is not far from being a solution of (1-1) in the sense that $\Delta u_\lambda - F'(u_\lambda)$ is a function which decays exponentially to 0 at infinity (this uses the fact that $\theta_\lambda > 0$).

In this paper we are interested in four-end solutions of (1-1), which means that they are asymptotic to a function u_λ for some choice of $\lambda \in \Lambda_4$. More precisely, we have:

Definition 1.1. Let $\mathscr{S}_4$ denote the set of functions u which are defined in $\mathbb{R}^2$ and which satisfy

$$u - u_\lambda \in W^{2,2}(\mathbb{R}^2) \tag{1-7}$$

for some $\lambda \in \Lambda_4$. We also define the decomposition operator $\mathscr{J}$ by

$$\mathscr{J} : \mathscr{S}_4 \to W^{2,2}(\mathbb{R}^2) \times \Lambda_4, \quad u \mapsto (u - u_\lambda, \lambda).$$

The topology on $\mathscr{S}_4$ is the one for which the operator $\mathscr{J}$ is continuous (the target space being endowed with the product topology). We define the set $\mathscr{M}_4$ of four-end solutions of the Allen–Cahn equation to be the set of solutions u of (1-1) which belong to $\mathscr{S}_4$.

The set $\mathcal{M}_4$ is nonempty. Indeed, it is known [Dang et al. 1992] that (1-1) has a saddle solution U, which is bounded and symmetric:

$$U(x, y) = U(x, -y) = U(-x, y).$$

Moreover, the nodal set of U coincides with the lines $y = \pm x$. Along these two lines, U converges exponentially fast to the "heteroclinic" solution. In addition, in [del Pino et al. 2010] it is shown that there exists a small number ε_0 such that, for all $0 < \theta$ with $\tan\theta < \varepsilon_0$, there exists a four-end solution with corresponding angles of the half lines λ_j^+, $j = 1, \dots, 4$ given by

$$\theta_1 = \theta, \quad \theta_2 = \pi - \theta, \quad \theta_3 = \theta + \pi, \quad \theta_4 = 2\pi - \theta.$$

Observe that the fact that θ is small implies that the ends of this solution are almost parallel and their slopes, given by $\pm\varepsilon$, $\varepsilon = \tan\theta$, are small as well. Clearly, by symmetry, it is easy to see that there also exist solutions with almost parallel ends whose angles are given by

$$\theta_1 = \pi/2 - \theta, \quad \theta_2 = \pi/2 + \theta, \quad \theta_3 = -\theta + 3\pi/2, \quad \theta_4 = 3\pi/2 + \theta.$$

In this case we have $\tan\theta_1 > 1/\varepsilon_0$.

Clearly, any four-end solution can be translated and rotated and multiplied by -1, yielding another four-end solution. In fact, from [Gui 2012] we know that any $u \in \mathcal{M}_4$ is (modulo rigid motions and multiplication of a solution by -1) even in its variables, monotonic in x in the set $x > 0$, and monotonic in y in the set $y < 0$:

$$u(x, y) = u(-x, y) = u(x, -y), \quad u_x(x, y) > 0, \quad x > 0, \quad u_y(x, y) > 0, \quad y < 0. \tag{1-8}$$

Thus, when studying four-end solutions, it is natural to consider the set $\mathcal{M}_4^{\mathrm{even}} \subset \mathcal{M}_4$, consisting precisely of functions satisfying (1-8). With each such function u we may associate in a unique way the angle that the asymptotic line of its nodal set in the first quadrant makes with the x-axis. Thus we can define *the angle map*

$$\theta : \mathcal{M}_4^{\mathrm{even}} \to (0, \pi/2), \quad u \mapsto \theta(u). \tag{1-9}$$

In principle the value of the angle map is not enough to identify in a unique way a solution to (1-1) in $\mathcal{M}_4^{\mathrm{even}}$. However, for solutions with almost parallel ends, we have:

Theorem 1.2. *There exists a small number ε_0 such that, for any two solutions $u_1, u_2 \in \mathcal{M}_4^{even}$ satisfying $\tan\theta(u_1) = \tan\theta(u_2) < \varepsilon_0$, we necessarily have $u_1 \equiv u_2$.*

This result, in some sense, gives a classification of the subfamily of the family of four-end solutions which contains solutions with almost parallel ends. It says that this subfamily consists precisely of the solutions constructed in [del Pino et al. 2010]. Let us explain the importance of this statement from the point of view of classification of all four-end solutions. We will appeal to the following theorem.

Theorem 1.3 [Kowalczyk et al. 2012]. *Let M be any connected component of $\mathcal{M}_4^{even}$. Then the angle map $\theta : M \to (0, \pi/2)$ is surjective.*

Consider, for example, the connected component $M_0 \subset \mathcal{M}_4^{\text{even}}$ which contains the saddle solution U. Theorem 1.3 implies that U can be deformed along M_0 to a solution with the value of the angle map arbitrarily close to 0 or to $\pi/2$, thus yielding a solution in the subfamily of the solutions with almost parallel ends. But these solutions are uniquely determined by the value of the angle map, which follows from the uniqueness statement in Theorem 1.2. As a result we obtain the following classification theorem.

Theorem 1.4. *Any solution $u \in \mathcal{M}_4^{even}$ belongs to M_0 and is a continuous deformation of the saddle solution U.*

We observe that, according to the conjecture of De Giorgi, in two dimensions, any solution u with $|u| < 1$ which is monotone in one direction must be one-dimensional and equal to $u(\boldsymbol{x}) = H(\boldsymbol{a} \cdot \boldsymbol{x} + b)$, that is, it is a planar solution. In the language of multiple end solutions, this solution has *two* (heteroclinic, planar) ends. Theorem 1.4, on the other hand, gives the classification of the family of solutions with *four* planar ends. Since the number of ends of a solution to (1-1) must be even, the family of four-end solutions is the natural object to study. In this context, one may wonder if it is possible to classify solutions to (1-1) assuming, for instance, that the nodal sets of u_x and u_y have just one component. This question is beyond the scope of this paper, however, since partial derivatives of four-end solutions satisfy this assumption, it seems reasonable to conjecture that a result similar to Theorem 1.4 should hold in this more general setting. We should mention here that it is, in principle, possible to study the problem of classification of solutions assuming, for example, that their Morse index is 1. This is natural since the Morse index of u and the number of the nodal domains of u_x and u_y are related. We recall here that the heteroclinic is stable, and, from [Dancer 2005], we know that in dimension $N = 2$, stability of a solution implies that it is necessarily a one-dimensional solution (for the related minimality conjecture, see, for example, [Pacard and Wei 2013; Savin 2009]. We expect that in fact the family of four-end solutions should contain all multiple end solutions with Morse index 1. We recall here that the Morse index of the saddle solution is indeed 1 [Schatzman 1995].

Let us now explain the analogy of Theorem 1.4 with some aspects of the theory of minimal surfaces in $\mathbb{R}^3$. In 1834, Scherk discovered an example of a singly periodic, embedded, minimal surface in $\mathbb{R}^3$ which, in a complement of a vertical cylinder, is asymptotic to 4 half-planes with angle $\pi/2$ between them. This surface, after a rigid motion, has two planes of symmetry, say $\{x_2 = 0\}$ and $\{x_1 = 0\}$, and it is periodic, with period 1 in the x_3 direction. If θ is the angle between the asymptotic end of the Scherk surface contained in $\{x_1 > 0, x_2 > 0\}$ and the $\{x_2 = 0\}$ plane, then $\theta = \pi/4$. This is the so-called second Scherk surface and it will be denoted here by $S_{\pi/4}$. Karcher [1988] found Scherk surfaces other than the original example in the sense that the corresponding angle between their asymptotic planes and the $\{x_2 = 0\}$ plane can be any $\theta \in (0, \pi/2)$. The one parameter family $\{S_\theta\}_{\{0<\theta<\pi/2\}}$ of these surfaces is the family of Scherk singly periodic minimal surfaces. Thus, accepting that the saddle solution of the Allen–Cahn equation U corresponds to the Scherk surface $S_{\pi/4}$, Theorem 1.3 can be understood as an analogue of the result of Karcher. We note that, unlike in the case of the Allen–Cahn equation, the Scherk family is given explicitly. For example, it can be represented as the zero level set of the function

$$F_\theta(x_1, x_2, x_3) = \cos^2\theta \cosh\frac{x_1}{\cos\theta} - \sin^2\theta \cosh\frac{x_2}{\cos\theta} - \cos x_3.$$

From this, it follows immediately that the angle map in this context $S_\theta \mapsto \theta$ is a diffeomorphism. A corresponding result for the family $\mathcal{M}_4^{\text{even}}$ is of course more difficult, since no explicit formula is available in this case.

We will further explore the analogy of our result with the theory of minimal surfaces in $\mathbb{R}^3$, now in the context of the classification of the four-end solutions in Theorem 1.4. The corresponding problem can be stated as follows: if S is an embedded, singly periodic, minimal surface with 4 Scherk ends, what can be said about this surface? It is proven by Meeks and Wolf [2007] that S must be one of the Scherk surfaces S_θ described above (a similar result is proven in [Pérez and Traizet 2007] assuming additionally that the genus of S in the quotient $\mathbb{R}^3/\mathbb{Z}$ is 0). The key results to prove this general statement are in fact the counterparts of Theorem 1.2 and Theorem 1.3.

We now sketch the basic elements in the proof of Theorem 1.2. First of all, let us explain the existence result in [del Pino et al. 2010]. The starting point of the construction is the Toda system:

$$\begin{cases} q_1'' = -c_* e^{\sqrt{2}(q_1-q_2)}, \\ q_2'' = c_* e^{\sqrt{2}(q_1-q_2)}, \end{cases} \tag{1-10}$$

for which $q_1 < 0 < q_2$ and $q_1(x) = -q_2(x)$, as well as $q_j(x) = q_j(-x)$, $j = 1, 2$. Here c_* is a fixed constant depending only on F (when $F(u) = \frac{1}{4}(1-u^2)^2$, $c_* = 12\sqrt{2}$), and $\sqrt{2}$ appears because we have assumed $F''(1) = 2$. Any solution of this system is asymptotically linear, namely,

$$q_j(x) = (-1)^j(m|x| + b) + \mathcal{O}(e^{-2\sqrt{2}m|x|}), \quad x \to \infty,$$

where $m > 0$ is the slope of the asymptotic straight line in the first quadrant. On the other hand, given that we only consider solutions whose trajectories are symmetric with respect to the x-axis, the value of the slope m determines the unique solution of (1-10). When the asymptotic lines become parallel, $m \to 0$ or $m \to \infty$. By symmetry, it suffices to consider the case $m \to 0$, and in this paper we will denote small slopes by $m = \varepsilon$ and the corresponding solutions by $q_{\varepsilon,j}$. Note that if by $q_{1,j}$ we denote a solution with $m = 1$, then

$$q_{\varepsilon,j}(x) = q_{1,j}(\varepsilon x) + \frac{(-1)^j}{\sqrt{2}} \ln \frac{1}{\varepsilon}.$$

Then, the existence result in [del Pino et al. 2010] implies that given a small ε, there exists a four-end solution u to (1-1) whose nodal set $N(u)$ is close to the trajectories of the Toda system given by the graphs of $y = q_{\varepsilon,j}(x)$. It turns out that the idea of relating solutions of the Toda system and the four-end solutions of (1-1) [ibid.] is very important. In fact, what we want to achieve is to parametrize the manifold of four-end solutions with almost parallel ends using corresponding solutions of the Toda system as parameters. To do this, in Sections 3–5 we obtain a very precise control of the nodal sets of the four-end solutions. The key observation is that in every quadrant the nodal set $N(u)$ of any four-end solution is a bigraph, and if we assume that the slope of its asymptotic lines is small, it is a graph of a smooth function, both in the lower and in the upper half-plane. We then have

$$N(u) = \{(x, y) \in \mathbb{R}^2 : y = f_{\varepsilon,j}(x),\ j = 1, 2,\ f_{\varepsilon,1}(x) < 0,\ f_{\varepsilon,2}(x) = -f_{\varepsilon,1}(x)\}$$

for any $u \in \mathcal{M}_4^{\text{even}}$, with $\varepsilon = \tan\theta(u)$. Our main result in Section 4 says that, for each ε small,

$$f_{\varepsilon,1}(x) - q_{\varepsilon,1}(x) = C\varepsilon^\alpha + \mathbb{O}(\varepsilon^\alpha e^{-\varepsilon\beta|x|})$$

with some positive constants α, β. Next, we define (Section 6) a suitable approximate four-end solution based on the solution of the Toda system with slope ε. To explain this, by $\widetilde{\mathcal{N}}_{\varepsilon,1}$ we denote the graph of the function $y = q_{\varepsilon,1}(x)$, which is contained in the lower half-plane. In a suitable neighborhood of the curve $\widetilde{\mathcal{N}}_{\varepsilon,1}$, we introduce Fermi coordinates $\boldsymbol{x} = (x, y) \mapsto (x_1, y_1)$, where y_1 denotes the signed distance to $\widetilde{\mathcal{N}}_{\varepsilon,1}$, and x_1 is the x coordinate of the projection of the point $\boldsymbol{x}$ onto $\widetilde{\mathcal{N}}_{\varepsilon,1}$. With this notation, we write locally the solution u, with $\varepsilon = \tan\theta(u)$ in the form

$$u(\boldsymbol{x}) = H(y_1 - h_\varepsilon(x_1)) + \phi.$$

This definition is suitably adjusted to yield a globally defined function. Here the function h_ε is required to satisfy an orthogonality condition. Then it is proven in Section 6 that $h_\varepsilon : \mathbb{R} \to \mathbb{R}$ and $\phi : \mathbb{R}^2 \to \mathbb{R}$ are small functions of order $\mathbb{O}(\varepsilon^\alpha)$ in some weighted norms.

Finally, starting on page 1715 we prove the Lipschitz dependence of the solution u on the function h_ε and conclude the proof of Theorem 1.2 using the mapping property of the linearized operator of the Toda equation.

2. Preliminaries

In this section we collect some facts about the Allen–Cahn equation which will be used later on.

Refined asymptotics theorem for four-end solutions. Let $H(x)$ be the heteroclinic solution of the Allen–Cahn equation. Recall that $F''(1) = 2$. Then it is known that we have asymptotically

$$H(x) = 1 - a_F e^{-\sqrt{2}x} + \mathbb{O}(e^{-2\sqrt{2}x}), \quad H'(x) = a_F\sqrt{2}e^{-\sqrt{2}x} + \mathbb{O}(e^{-2\sqrt{2}x}), \quad x \to \infty, \tag{2-1}$$

with similar estimates when $x \to -\infty$, where a_F is a constant depending on F.

We consider the linearized operator

$$L_0\phi = -\phi'' + F''(H)\phi.$$

It is known that the principal eigenvalue of this operator is $\mu_0 = 0$ and the corresponding eigenfunction is H'. In general, the operator L_0 has possibly infinite, discrete spectrum $0 < \mu_1 < \cdots \le \alpha_0^2$, and essential spectrum which is $[\alpha_0^2, \infty)$, $\alpha_0 = \sqrt{F''(1)}$. It may also happen that L_0 has just one eigenvalue, $\mu_0 = 0$ and continuous spectrum, in which case we will set $\mu_1 = \alpha_0^2$.

Next, we recall some facts about the moduli space theory developed in [del Pino et al. 2013]. We will mostly use this theory in the case of four-end solutions. Thus we will restrict the presentation to this situation only. We keep the notations introduced above. Thus we let

$$\lambda = (\lambda_1, \ldots, \lambda_4) \in \Lambda_4,$$

and we write $\lambda_j^+ = \boldsymbol{x}_j + \mathbb{R}^+\boldsymbol{e}_j$ as in (1-4). We denote by $\Omega_0, \ldots, \Omega_4$ the decomposition of $\mathbb{R}^2$ associated to these four affine half lines and $\mathbb{I}_0, \dots, \mathbb{I}_4$ the partition of unity subordinate to this partition. Given $\gamma, \delta \in \mathbb{R}$, we define a *weight function* $\Gamma_{\gamma,\delta}$ by

$$\Gamma_{\gamma,\delta}(\boldsymbol{x}) := \mathbb{I}_0(\boldsymbol{x}) + \sum_{j=1}^{4} \mathbb{I}_j(\boldsymbol{x}) e^{\gamma(\boldsymbol{x}-\boldsymbol{x}_j)\cdot \boldsymbol{e}_j} (\cosh((\boldsymbol{x}-\boldsymbol{x}_j)\cdot \boldsymbol{e}_j^{\perp}))^{\delta}, \tag{2-2}$$

so that, by construction, γ is the rate of decay or blow up along the half lines λ_j^+, and δ is the rate of decay or blow up in the direction orthogonal to λ_j^+.

With this definition in mind, we define the weighted Lebesgue space

$$L^2_{\gamma,\delta}(\mathbb{R}^2) := \Gamma_{\gamma,\delta} L^2(\mathbb{R}^2), \tag{2-3}$$

and the weighted Sobolev space

$$W^{2,2}_{\gamma,\delta}(\mathbb{R}^2) := \Gamma_{\gamma,\delta} W^{2,2}(\mathbb{R}^2). \tag{2-4}$$

Observe that, even though this does not appear in the notation, the partition of unity, the weight function, and the induced weighted spaces all depend on the choice of $\lambda \in \Lambda_4$.

Our first result shows that, if u is a solution of (1-1) which is close to u_λ (in $W^{2,2}$ topology), then $u - u_\lambda$ tends to 0 exponentially fast at infinity.

Proposition 2.1 (refined asymptotics). *Assume that $u \in \mathcal{S}_4$ is a solution of (1-1) and define $\lambda \in \Lambda_4$, so that*

$$u - u_\lambda \in W^{2,2}(\mathbb{R}^2).$$

Then there exist $\delta \in (0, \alpha_0)$, $\alpha_0 = \sqrt{F''(1)}$ and $\gamma > 0$ such that

$$u - u_\lambda \in W^{2,2}_{-\gamma,-\delta}(\mathbb{R}^2). \tag{2-5}$$

More precisely, $\delta > 0$ and $\gamma > 0$ can be chosen so that

$$\gamma \in (0, \sqrt{\mu_1}), \quad \gamma^2 + \delta^2 < \alpha_0^2 \quad \textit{and} \quad \alpha_0 > \delta + \gamma \cot \theta_\lambda, \tag{2-6}$$

where θ_λ is equal to the half of the minimum of the angles between two consecutive oriented affine lines $\lambda_1, \dots, \lambda_4$ (see (1-3)), and μ_1 is the second eigenvalue of the operator L_0 (or $\mu_1 = \alpha_0^2$ if 0 is the only eigenvalue).

We recall here that in this paper for convenience we have assumed $\alpha_0 = \sqrt{F''(1)} = \sqrt{2}$.

It is well known that for any solution of (1-1) the following is true: if by $N(u)$ we denote the nodal set of u and by $\mathrm{d}(N(u), \boldsymbol{x})$ the distance of $\boldsymbol{x}$ to $N(u)$, then

$$|u(\boldsymbol{x})^2 - 1| + |\nabla u(\boldsymbol{x})| + |D^2 u(\boldsymbol{x})| \le C e^{-\beta \mathrm{d}(N(u),\boldsymbol{x})}, \tag{2-7}$$

where $\beta > 0$. This type of estimate is relatively easy to obtain using a comparison argument; see [Berestycki et al. 1997; Kowalczyk et al. 2012]. On the other hand, the estimate (2-5) is nontrivial.

The balancing formulas. We will now briefly describe the balancing formulas for four-end solutions in the form they were introduced in [del Pino et al. 2013]. Assume that u is a solution of (1-1) which is defined in $\mathbb{R}^2$. Assume that X and Y are two vector fields also defined in $\mathbb{R}^2$. In coordinates, we can write

$$X = \sum_j X^j \partial_{x_j}, \quad Y = \sum_j Y^j \partial_{x_j},$$

and, if f is a smooth function, we use the notations

$$X(f) := \sum_j X^j \partial_{x_j} f, \quad \nabla f := \sum_j \partial_{x_j} f \partial_{x_j}, \quad \operatorname{div} X := \sum_i \partial_{x_i} X^i,$$

and

$$\mathrm{d}^* X := \frac{1}{2} \sum_{i,j} (\partial_{x_i} X^j + \partial_{x_j} X^i)\, dx_i \otimes dx_j,$$

so that

$$\mathrm{d}^* X(Y, Y) = \sum_{i,j} \partial_{x_i} X^j Y^i Y^j.$$

We will need the following *balancing formula*, which is proved by direct computation:

$$\operatorname{div}\bigl(\bigl(\tfrac{1}{2}|\nabla u|^2 + F(u)\bigr)X - X(u)\nabla u\bigr) = \bigl(\tfrac{1}{2}|\nabla u|^2 + F(u)\bigr) \operatorname{div} X - \mathrm{d}^* X(\nabla u, \nabla u). \tag{2-8}$$

Translations of $\mathbb{R}^2$ correspond to the constant vector field

$$X := X_0,$$

where X_0 is a fixed vector, while rotations correspond to the vector field

$$X := x\partial_y - y\partial_x.$$

In either case, we have $\operatorname{div} X = 0$ and $\mathrm{d}^* X = 0$. Therefore, we conclude that

$$\operatorname{div}\bigl(\bigl(\tfrac{1}{2}|\nabla u|^2 + F(u)\bigr)X - X(u)\nabla u\bigr) = 0$$

for these two vector fields. The divergence theorem implies that

$$\int_{\partial\Omega} \bigl(\bigl(\tfrac{1}{2}|\nabla u|^2 + F(u)\bigr)X - X(u)\nabla u\bigr) \cdot \nu \, ds = 0, \tag{2-9}$$

where ν is the (outward pointing) unit normal vector field to $\partial\Omega$.

To see how this identity is applied let us fix a unit vector $\boldsymbol{e} \in \mathbb{R}^2$ and let $X = \boldsymbol{e}$. For any $s \in \mathbb{R}$ we consider a straight line $L_s = \{\boldsymbol{x} \in \mathbb{R}^2 : \boldsymbol{x} = s\boldsymbol{e} + t\boldsymbol{e}^\perp, t \in \mathbb{R}\}$. Then we get

$$\int_{L_s} \bigl[\tfrac{1}{2}|\nabla u|^2 - |\nabla u \cdot \boldsymbol{e}|^2 + F(u)\bigr]\, dS = \text{const}$$

for any 4 end solution u of (1-1), as long as the direction of L_s does not coincide with that of any end, that is, $\boldsymbol{e} \neq \boldsymbol{e}_j$, $j = 1, \dots, 4$. In a particular case $\boldsymbol{e} = (0, 1)$ we get a *Hamiltonian identity* [Gui 2008]:

$$\int_{y=s} \bigl[\tfrac{1}{2}(\partial_x u)^2 - \tfrac{1}{2}(\partial_y u)^2 + F(u)\bigr]\, dx = \text{const}. \tag{2-10}$$

Summary of the existence result for small angles in [del Pino et al. 2010]. To state the existence result precisely, we assume that we are given an even symmetric solution of the Toda system (1-10) represented by a pair of functions $q_1(t) < 0 < q_2(t)$, where $q_1(t) = -q_2(t)$ as well as $q_1(t) = q_1(-t)$. In addition let us assume that the slope of q_1 at ∞ is -1. Then, asymptotically we have

$$q_j(x) = (-1)^j(|x| + b) + \mathbb{O}(e^{-2\sqrt{2}|x|}), \quad x \to \infty.$$

Given $\varepsilon > 0$, we define the vector valued function $\boldsymbol{q}_\varepsilon$, whose components are given by

$$q_{j,\varepsilon}(x) := q_j(\varepsilon x) + \frac{(-1)^j}{\sqrt{2}} \ln \frac{1}{\varepsilon}. \tag{2-11}$$

It is easy to check that the $q_{j,\varepsilon}$ are again solutions of (1-10).

Observe that, according to the asymptotic description of the functions q_j, the graphs of the functions $q_{j,\varepsilon}$ are asymptotic to oriented half lines with slopes $\pm\varepsilon$ at infinity. In addition, for $\varepsilon > 0$ small enough, these graphs are disjoint and in fact their mutual distance is given by $\sqrt{2}\ln\frac{1}{\varepsilon} + \mathbb{O}(1)$ as ε tends to 0.

It will be convenient to agree that χ^+ (respectively χ^-) is a smooth cutoff function defined on $\mathbb{R}$ which is identically equal to 1 for $x > 1$ (respectively for $x < -1$) and identically equal to 0 for $x < -1$ (respectively for $x > 1$), and additionally $\chi^- + \chi^+ \equiv 1$. With these cutoff functions at hand, we define the four-dimensional space

$$D := \mathrm{Span}\{x \mapsto \chi^\pm(x),\ x \mapsto x\chi^\pm(x)\}, \tag{2-12}$$

and, for all $\mu \in (0, 1)$ and all $\tau \in \mathbb{R}$, we define the space $\mathscr{C}^{2,\mu}_\tau(\mathbb{R})$ of $\mathscr{C}^{2,\mu}$ functions r which satisfy

$$\|r\|_{\mathscr{C}^{\ell,\mu}_\tau(\mathbb{R})} := \|(\cosh x)^\tau r\|_{\mathscr{C}^{\ell,\mu}(\mathbb{R})} < \infty.$$

Theorem 2.2. *For all $\varepsilon > 0$ sufficiently small, there exists an entire solution u_ε of the Allen–Cahn equation (1-1) whose nodal set is the union of 2 disjoint curves $\widetilde{\Gamma}_{1,\varepsilon}$, $\widetilde{\Gamma}_{2,\varepsilon}$ which are the graphs of the functions*

$$x \mapsto q_{j,\varepsilon}(x) + r_{j,\varepsilon}(\varepsilon x)$$

for some functions $r_{j,\varepsilon} \in \mathscr{C}^{2,\mu}_\tau(\mathbb{R}) \oplus D$ satisfying

$$\|r_{j,\varepsilon}\|_{\mathscr{C}^{2,\mu}_\tau(\mathbb{R})\oplus D} \le C\varepsilon^\alpha$$

for some constants $C, \alpha, \tau, \mu > 0$ independent of $\varepsilon > 0$.

In other words, given a solution of the Toda system, we can find a one parameter family of four-end solutions of (1-1) which depend on a small parameter $\varepsilon > 0$. As ε tends to 0, the nodal sets of the solutions we construct become close to the graphs of the functions $q_{j,\varepsilon}$.

Going through the proof, one can be more precise about the description of the solution u_ε. If $\Gamma \subset \mathbb{R}^2$ is a curve in $\mathbb{R}^2$ which is the graph over the x-axis of some function, we denote by $\mathrm{Y}(\,\cdot\,, \Gamma)$ the signed distance to Γ which is positive in the upper half of $\mathbb{R}^2 \setminus \Gamma$ and is negative in the lower half of $\mathbb{R}^2 \setminus \Gamma$.

Proposition 2.3. *The solution of (1-1) provided by Theorem 2.2 satisfies*

$$\|e^{\varepsilon\hat{\alpha}|\boldsymbol{x}|}(u_\varepsilon - u_\varepsilon^*)\|_{L^\infty(\mathbb{R}^2)} \le C\varepsilon^{\bar{\alpha}}$$

for some constants $C, \bar{\alpha}, \hat{\alpha} > 0$ independent of ε, where $\boldsymbol{x} = (x, y)$ and

$$u_\varepsilon^* = \sum_{j=1}^{2}(-1)^{j+1} H(\Upsilon(\,\cdot\,, \widetilde{\Gamma}_{j,\varepsilon})) - 1, \tag{2-13}$$

in the set

$$V = \left\{(x, y) : |y| \le C\varepsilon^{-1}\sqrt{1+x^2}\right\},$$

with some positive constant C (depending on $\widetilde{\Gamma}_{j,\varepsilon}$), and outside of this set u^* is defined by smoothly interpolating with 1 in the upper half-plane and with -1 in the lower half-plane.

3. The nodal sets of solutions

After a rigid motion, any four-end solution is even symmetric [Gui 2012], and thus we will always consider solutions in $\mathcal{M}_4^{\text{even}}$ which in particular satisfy (1-8). Note that $\mathcal{M}_4^{\text{even}}$ is a one-dimensional manifold, possibly with more than one connected component. For any solution $u \in \mathcal{M}_4^{\text{even}}$, the angle map $\theta(u)$ is defined to be the asymptotic angle at ∞ between the nodal set of u in the first quadrant and the x-axis. By the results proven in [Kowalczyk et al. 2012], the angle map on any connected component of the moduli space $\mathcal{M}_4^{\text{even}}$ of four-end, even solutions is surjective, and in particular it contains solutions whose nodal lines are almost parallel ($\theta(u) \approx 0$ or $\pi/2 - \theta(u) \approx 0$).

By $N(u)$ we will denote in this paper the nodal set of $u \in \mathcal{M}_4^{\text{even}}$. We are interested in solutions whose nodal lines are almost parallel at ∞, and, by symmetry, we can restrict our considerations to the case $\theta(u) \approx 0$. In this case $N(u)$ will consist of two components, one of them is a graph of a smooth function in the lower half-plane and the other one is contained in the upper half-plane.

Basic properties of solutions with almost parallel ends. It is expected that as $\theta(u) \to 0$, the distance between the upper and the lower nodal line of u will tend to infinity. This is the content of Lemma 3.1 below. In the sequel we will denote the first quadrant in $\mathbb{R}^2$ by Q_1.

Lemma 3.1. *Suppose $\{u_n\}_{n=1}^\infty$ is a sequence of four-end solutions such that $\theta(u_n) \to 0$ and $p_n \in N(u_n) \cap \partial Q_1$. Then $|p_n| \to +\infty$, as $n \to +\infty$. Moreover, p_n is point on the y axis for n large.*

Proof. To show that $|p_n| \to \infty$, we suppose by contradiction that $p_n \to p^*$, $|p^*| < \infty$. We know that, up to a subsequence, u_n converges in $\mathscr{C}^2_{\text{loc}}(\mathbb{R}^2)$ to a solution u^* of the Allen–Cahn equation. By similar arguments as in [Kowalczyk et al. 2012, Lemma 5.1], we know that u^* cannot be identically zero. Since $|p^*| < \infty$, u^* cannot be the constant solution 1 or -1. Therefore, by the maximum principle, $u_x^* > 0$, $x > 0$, $u_y^* < 0$, $y > 0$. Then, by [Gui 2008, Theorem 4.4], u^* must be a solution to (1-1), whose nodal set in the first quadrant is asymptotically a straight line with positive slope equal to $\tan\theta^* \neq 0$. It can also be proven using the refined asymptotic theorem (Proposition 2.1), that $u^* \in \mathcal{M}_4^{\text{even}}$. By the Hamiltonian identity,

$$\int_{\mathbb{R}} \left(\frac{1}{2} \left| \frac{\partial u_n(x,0)}{\partial x} \right|^2 + F(u_n(x,0)) \right) dx = 2\boldsymbol{e}_F \sin\theta(u_n) \to 0, \tag{3-1}$$

where $\boldsymbol{e}_F = \int_{\mathbb{R}} (H')^2$. But on the other hand, for any fixed $r > 0$,

$$\int_{-r}^{r} \left(\frac{1}{2} \left| \frac{\partial u_n(x,0)}{\partial x} \right|^2 + F(u_n(x,0)) \right) dx \to \int_{-r}^{r} \left(\frac{1}{2} \left| \frac{\partial u^*(x,0)}{\partial x} \right|^2 + F(u^*(x,0)) \right) dx > \delta > 0.$$

This is a contradiction.

It remains to show that p_n is in the y axis when n is large enough. To this end, we argue by contradiction and assume that p_n is in the x axis for large n. Observe that as p_n goes to infinity, locally around the nodal line, u_n will resemble the heteroclinic solution. Therefore, for any $\varepsilon > 0$, if n is large enough,

$$\int_{\mathbb{R}} \left(\frac{1}{2} \left| \frac{\partial u_n(x,0)}{\partial x} \right|^2 + F(u_n(x,0)) \right) dx > 2\boldsymbol{e}_F - \varepsilon.$$

But on the other hand, by (3-1), the left side is equal to $2\boldsymbol{e}_F \sin\theta(u_n)$, which tends to zero. This is a contradiction. □

We know that when the angle of u_n is small, the nodal set $N(u_n)$ in the upper half-plane is a graph of a smooth function $y = f_n(x)$. For this function, we have the following.

Lemma 3.2. *Suppose $\{u_n\}$ is a sequence of solutions in $\mathcal{M}_4^{even}$ such that $\theta(u_n) \to 0$, as $n \to \infty$. We have*

$$\lim_{n\to+\infty} \|f_n'\|_{\mathscr{C}^0(\mathbb{R})} = 0.$$

Proof. Using the monotonicity of u_n in the upper half-plane and the validity of the De Giorgi conjecture in dimension 2, one can show that, for any $r > 0$,

$$\lim_{n\to+\infty} \|f_n'\|_{\mathscr{C}^0([-r,r])} = 0.$$

Now, we claim that for each $\delta > 0$, there exists $r(\delta) > 0$ such that

$$|f_n'(x) - \tan\theta(u_n))| < \delta \quad \text{for all } x > r(\delta) \text{ and } n \in \mathbb{N}.$$

Indeed, if this were not true, then, using the fact that

$$\lim_{x\to+\infty} f_n'(x) = \tan\theta(u_n) \to 0 \quad \text{as } n \to +\infty,$$

we could find sequences $\{n_k\}$, $\{x_k\}$, $\{y_k\}$, all tending to infinity and $x_k < y_k$, such that

$$\frac{\delta}{4} \le |f_{n_k}'(x)| \le C, \quad x \in [x_k, y_k],$$

and

$$|f_{n_k}'(x_k) - f_{n_k}'(y_k)| = \frac{\delta}{2}. \tag{3-2}$$

Now we consider two lines L_{1,n_k} and L_{2,n_k} with slopes -1 passing though the points $(x_k, f_{n_k}(x_k))$ and $(y_k, f_{n_k}(y_k))$, respectively. Note that since the nodal lines $N(u_{n_k})$ are bigraphs, the lines L_{i,n_k} must be transversal to $N(u_{n_k})$ at their points of intersection.

Next, consider the domain $\Omega_{n_k} \subset Q_1$ bounded by the two axes and the lines L_{i,n_k}, $i = 1, 2$. Let X be the vector field $(0, 1)$. The balancing formula (2-9) tells us

$$\int_{\partial\Omega_{n_k}} \big(\big(\tfrac{1}{2}|\nabla u_{n_k}|^2 + F(u_{n_k})\big)X - X(u_{n_k})\nabla u_{n_k}\big) \cdot \nu \, dS = 0.$$

Note that the integral over the segment $\partial\Omega_{n_k} \cap \{x = 0\}$ is automatically 0 by the choice of the vector field X and the evenness of u_{n_k}.

Following similar arguments as in [Kowalczyk et al. 2012, Lemma 5.2], one can show suitable exponential decay of $|u_n| - 1$ along the x axis, and it follows that, as $k \to +\infty$,

$$\int_{\partial\Omega_{n_k} \cap \{y=0\}} ((\tfrac{1}{2}|\nabla u_{n_k}|^2 + F(u_{n_k}))X - X(u_{n_k})\nabla u_{n_k}) \cdot \nu \, dS \to 0. \tag{3-3}$$

Now we estimate the integrals along the segments $\partial\Omega_{n_k} \cap L_{i,n_k}$. For this purpose it is convenient to denote

$$\alpha_{1,n_k} = \arctan f'_{n_k}(x_k), \quad \alpha_{2,n_k} = \arctan f'_{n_k}(y_k),$$

and

$$\boldsymbol{e}^{\perp}_{1,n_k} = (\sin\alpha_{1,n_k}, -\cos\alpha_{1,n_k}).$$

By the validity of the De Giorgi conjecture in dimension 2, we know that locally around $(x_k, f_{n_k}(x_k))$, as k goes to infinity, the function u_{n_k} converges to

$$H(\boldsymbol{e}^{\perp}_{1,n_k} \cdot (x - x_k, y - f_{n_k}(x_k)).$$

Moreover, by (2-7), on the segment $\partial\Omega_{n_k} \cap L_{1,n_k}$,

$$|u^2_{n_k}(\boldsymbol{x}) - 1| + |\nabla u_{n_k}(\boldsymbol{x})| \le Ce^{-\beta|x_k - x|}, \quad \boldsymbol{x} = (x, y).$$

Similar results hold around $(y_k, f_{n_k}(y_k))$. Using these facts, after some calculation, we get

$$\int_{\partial\Omega_{n_k} \cap L_{i,n_k}} \big(\big(\tfrac{1}{2}|\nabla u_{n_k}|^2 + F(u_{n_k})\big)X - X(u_{n_k})\nabla u_{n_k}\big) \cdot \nu \, dS = (-1)^{i+1} \sin\alpha_{i,n_k} \boldsymbol{e}_F + o(1),$$

where $o(1)$ is a term that goes to 0 as $k \to +\infty$. Combining all the above estimates, we infer

$$\sin\alpha_{1,n_k} - \sin\alpha_{2,n_k} = o(1),$$

which is a contradiction. $\square$

A refinement of the asymptotic behavior of the nodal set. Let u be a four-end solution with small angle $\theta(u)$. We set $\varepsilon = \tan\theta(u)$ and, for simplicity, use ε as a small parameter. To obtain more precise information about this solution, our first step is to define a good approximate solution and estimate the corresponding error term. As we will see later, this enables us to know more precisely the behavior of the nodal lines.

The nodal set $N(u)$ in the lower half-plane is the graph of a function $y = f(x)$. Strictly speaking the function f depends on u, but we will not indicate this dependence. We have shown that $\|f'\|_{\mathscr{C}^0(\mathbb{R})} \to 0$ as $\theta(u) \to 0$. Recall that by the validity of the De Giorgi conjecture in dimension 2, locally around the nodal line, u behaves like the heteroclinic solution. Using this fact and that $u(x, f(x)) = 0$, it is not difficult to show that $\|f'\|_{\mathscr{C}^1(\mathbb{R})} \to 0$ as $\theta(u) \to 0$. For future reference, we finally observe that, in general, $N(u) \cap Q_1$ is at least a $\mathscr{C}^3(\mathbb{R})$ function and, bootstrapping the above argument, it is not hard to show that $\|f'\|_{\mathscr{C}^2(\mathbb{R})} = o(1)$ as $\theta(u) \to 0$.

To fix attention, we will always work with the solution whose nodal lines have a small slope $\varepsilon = \tan\theta(u)$ at ∞. This means that these lines are asymptotically parallel, as $\varepsilon \to 0$, to the x axis, and one of them is contained in the lower half-plane and the other in the upper half-plane. We know that they are symmetric with respect to the x axis. In the sequel it will be convenient to denote the component of the nodal set $N(u)$ in the lower half-plane by $\mathscr{N}_{\varepsilon,1}$, and the one in the upper half-plane by $\mathscr{N}_{\varepsilon,2}$. Due to the evenness of u, the nodal lines are obviously graphs of some even functions: $\mathscr{N}_{\varepsilon,i} = \{(x, y) | y = f_{\varepsilon,i}(x)\}$.

To introduce the functional analytic tools used in this paper, we first define the weight functions

$$W_a(\boldsymbol{x}) := (\cosh x)^a, \quad \boldsymbol{x} = (x, y), \quad a \geq 0.$$

For $\ell = 0, 1, 2$, let $\mathscr{C}_a^{\ell,\mu}(\mathbb{R}^2) := W_a^{-1}\mathscr{C}^{\ell,\mu}(\mathbb{R}^2)$, endowed with the weighted norm

$$\|\phi\|_{\mathscr{C}_a^{\ell,\mu}(\mathbb{R}^2)} := \sup_{\boldsymbol{x}\in\mathbb{R}^2} W_a(\boldsymbol{x})\|\phi\|_{\mathscr{C}^{\ell,\mu}(B(\boldsymbol{x},1))}.$$

Likewise, we let $\overline{W}_a(x) = (\cosh x)^a$ and define the weighted space $\mathscr{C}_a^{\ell,\mu}(\mathbb{R})$ by

$$\|f\|_{\mathscr{C}_a^{\ell,\mu}(\mathbb{R})} := \sup_{x\in\mathbb{R}} \overline{W}_a(x)\|f\|_{\mathscr{C}^{\ell,\mu}((x-1,x+1))}.$$

In what follows we will measure the size of various functions involved in the $\mathscr{C}_a^{2,\mu}(\mathbb{R}^2)$, and in the $\mathscr{C}_a^{2,\mu}(\mathbb{R})$ norms. Mostly we will have $\mu \in (0, 1)$, $a \sim \varepsilon$, or $a = 0$.

Remark 3.3. In this paper, we will frequently estimate the usual $\mathscr{C}^{\ell,\mu}$ norm, as well as the $\mathscr{C}_a^{\ell,\mu}$ norm $(a \sim \varepsilon)$ of various functions. In many cases, the argument for the weighted norms and the usual $\mathscr{C}^{\ell,\mu}$ norm is almost identical. Therefore, for notational convenience, the symbol $\mathscr{C}_a^{\ell,\mu}$, with $a = 0$, will just denote the space $\mathscr{C}^{\ell,\mu}$, rather than the space of compactly supported functions.

Let us recall that a four-end solution u is asymptotic to a model solution u_λ defined in the introduction. Using Proposition 2.1, we know that $u - u_\lambda \in W^{2,2}_{-\varepsilon\tau_0,-\delta}(\mathbb{R}^2)$ with some small $\tau_0 > 0$ and $\delta > 0$, which can be chosen independent of the small parameter ε. It follows that

$$u - u_\lambda \in \mathscr{C}^{2,\mu}_{\varepsilon\tau_0}(\mathbb{R}^2). \tag{3-4}$$

To see this, we denote by $\boldsymbol{e}$ the asymptotic direction of the end of u in Q_1. Then, by definition of the weight function $\Gamma_{\varepsilon\tau_0,\delta}$ in (2-2), taking R large, we see that when $\delta \geq \varepsilon\tau_0$,

$$\Gamma_{\varepsilon\tau_0,\delta}(\boldsymbol{x}) \sim (\cosh((\boldsymbol{x}-\boldsymbol{x}_{\varepsilon,1})\cdot\boldsymbol{e}))^{\varepsilon\tau_0}(\cosh((\boldsymbol{x}-\boldsymbol{x}_{\varepsilon,1})\cdot\boldsymbol{e}^{\perp}))^{\delta} \geq C(\cosh x)^{\varepsilon\tau_0}, \quad \boldsymbol{x}\in Q_1\setminus B_R.$$

From this, $u-u_\lambda \in \mathscr{C}^{0,\mu}_{\varepsilon\tau_0}(\mathbb{R}^2)$ follows immediately. This estimate can be bootstrapped to yield the $\mathscr{C}^{2,\mu}_{\varepsilon\tau_0}(\mathbb{R}^2)$ estimate as claimed.

Additionally, using (3-4) and the fact that $u(x, f_{\varepsilon,2}(x))=0$, we get that, with some constant $\mathscr{A}_\varepsilon$,

$$H((f_{\varepsilon,2}(x)-\varepsilon x-\mathscr{A}_\varepsilon)\cos(\theta(u))) = \mathbb{O}_{\mathscr{C}^{2,\mu}_{\varepsilon\tau_0}(\mathbb{R})}(e^{-\varepsilon\tau_0|x|}), \quad x\to+\infty, \tag{3-5}$$

from which one can show

$$\|f_{\varepsilon,2}-\varepsilon|x|-\mathscr{A}_\varepsilon\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau_0}(\mathbb{R})} + \|f'_{\varepsilon,2}-\varepsilon\,\mathrm{sign}(x)\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau_0}(\mathbb{R})} + \|f''_{\varepsilon,2}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau_0}(\mathbb{R})} < \infty. \tag{3-6}$$

Fermi coordinates near the nodal lines. We will now describe some neighborhoods of the nodal lines $\mathscr{N}_{\varepsilon,i}$, $i=1,2$, where one can define the Fermi coordinates of $\boldsymbol{x}\in\mathbb{R}^2$ as the unique (x_i, y_i) such that

$$\boldsymbol{x} = (x_i, f_{\varepsilon,i}(x_i)) + y_i n_{\varepsilon,i}(x_i), \quad n_{\varepsilon,i}(x) := \frac{(-f'_{\varepsilon,i}(x), 1)}{\sqrt{1+(f'_{\varepsilon,i}(x))^2}}.$$

We will first find a large, expanding neighborhood of $\mathscr{N}_{\varepsilon,i}$ in which the map $\boldsymbol{x}\mapsto(x_i, y_i)$ is a diffeomorphism. Because of symmetry, it suffices to consider a neighborhood of $\mathscr{N}_{\varepsilon,1}$.

We define the (multivalued) projection of a point $\boldsymbol{x}\in\mathbb{R}^2$ onto $\mathscr{N}_{\varepsilon,1}$ to be the set of points that realize the distance between $\boldsymbol{x}$ and $\mathscr{N}_{\varepsilon,1}$:

$$\pi_{\varepsilon,1}(\boldsymbol{x}) := \{(x_1, f_{\varepsilon,1}(x_1)) : \mathrm{dist}(\boldsymbol{x}, (x_1, f_{\varepsilon,1}(x_1))) = \mathrm{dist}(\boldsymbol{x}, \mathscr{N}_{\varepsilon,1})\}.$$

Let $(-\bar{m}_\varepsilon(x_1), \bar{m}_\varepsilon(x_1))$ be the maximal interval where the projection function is single valued:

$$\bar{m}_\varepsilon(x_1) := \sup\{m : \pi_{\varepsilon,1}((x_1, f_{\varepsilon,1}(x_1)) + t n_{\varepsilon,1}(x_1)) = (x_1, f_{\varepsilon,1}(x_1)) \text{ for } |t|\leq m\}.$$

In a certain sense, we can regard the function $\bar{m}_\varepsilon$ as the measure of the size of the maximal neighborhood of $\mathscr{N}_{\varepsilon,1}$ where the Fermi coordinate could be defined. Finally, for technical reasons, for any $x_1\in\mathbb{R}$, let us define

$$m_\varepsilon(x_1) := \min\left\{\frac{1}{\sqrt{|f''_{\varepsilon,1}(x_1)|}}, \bar{m}_\varepsilon(x_1)\right\}.$$

Lemma 3.4. *Let τ be 0 or τ_0. Then there exists a constant C_0 such that*

$$e^{-m_\varepsilon(x)}(\cosh x)^{\varepsilon\tau} \leq C_0\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})}\|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}. \tag{3-7}$$

Proof. Given $x_1\in\mathbb{R}$, if $m_\varepsilon(x_1) = 1/\sqrt{|f''_{\varepsilon,1}(x_1)|}$, then

$$e^{-m_\varepsilon(x_1)}(\cosh x_1)^{\varepsilon\tau} \leq C|f''_{\varepsilon,1}(x_1)|^2(\cosh x_1)^{\varepsilon\tau} \leq C\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})}\|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}.$$

Therefore estimate (3-7) holds in this case.

If $m_\varepsilon(x_1) < 1/\sqrt{|f''_{\varepsilon,1}(x_1)|}$ by definition $m_\varepsilon(x_1) = \bar{m}_\varepsilon(x_1)$, and therefore one could find points $\boldsymbol{x}_1 = (x_1, f_{\varepsilon,1}(x_1))$, $\boldsymbol{x}_2 = (x_2, f_{\varepsilon,1}(x_2))$, and $\boldsymbol{x}_0$ with $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \pi_{\varepsilon,1}(\boldsymbol{x}_0)$ and

$$\|\boldsymbol{x}_0 - \boldsymbol{x}_1\| = \|\boldsymbol{x}_0 - \boldsymbol{x}_2\| = m_\varepsilon(x_1).$$

In particular, $\boldsymbol{x}_j$, $j = 1, 2$ lie on the circle S whose center is $\boldsymbol{x}_0$.

We observe that, by the choice of $\boldsymbol{x}_0$, the distance from $\boldsymbol{x}_0$ to $\mathcal{N}_{\varepsilon,1}$ is $m_\varepsilon(x_1)$, and therefore $\mathcal{N}_{\varepsilon,1}$ is tangent with S at $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$. Since $\mathcal{N}_{\varepsilon,1}$ is a graph, it is easy to see that the shorter arc of S between $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ is the graph of a function $y = g(x)$, $x \in [x_1, x_2]$.

Now an elementary calculation yields

$$\min_{x\in[x_1,x_2]} |g''(x)| \geq \frac{1}{m_\varepsilon(x_1)}.$$

On the other hand,

$$|g'(x_2) - g'(x_1)| = |f'_{\varepsilon,1}(x_2) - f'_{\varepsilon,1}(x_1)|.$$

Therefore, one can find a point $\boldsymbol{x}_3 = (x_3, f_{\varepsilon,1}(x_3)) \in \mathcal{N}_{\varepsilon,1}$, with $x_3 \in [x_1, x_2]$, which satisfies

$$|f''_{\varepsilon,1}(x_3)| \geq \min_{x\in[x_1,x_2]} |g''(x)| \geq \frac{1}{m_\varepsilon(x_1)}. \tag{3-8}$$

Observe that $x_3 \in (x_1 - 2m_\varepsilon(x_1), x_1 + 2m_\varepsilon(x_1))$. Therefore, as ε is small,

$$\begin{aligned} e^{-m_\varepsilon(x_1)}(\cosh x_1)^{\varepsilon\tau} &\leq C e^{-m_\varepsilon(x_1)} e^{2m_\varepsilon(x_1)\varepsilon\tau} (\cosh x_3)^{\varepsilon\tau} \\ &\leq e^{-(1/2)m_\varepsilon(x_1)} (\cosh x_3)^{\varepsilon\tau}. \end{aligned}$$

Then, using (3-8), we also get the desired estimate:

$$\begin{aligned} e^{-m_\varepsilon(x_1)}(\cosh x_1)^{\varepsilon\tau} &\leq e^{-1/(2|f''_{\varepsilon,1}(x_3)|)} (\cosh x_3)^{\varepsilon\tau} \\ &\leq C \|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})} \|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}. \end{aligned}$$

□

By the above lemma, we know that m_ε satisfies

$$m_\varepsilon(x) \geq \varepsilon\tau \ln\cosh x - \ln(C_0 \|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})} \|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}),$$

where τ is either 0 or τ_0, and, in particular, when $\tau = 0$,

$$m_\varepsilon(x) \geq -\ln(C_0 \|f''_{\varepsilon,1}\|^2_{\mathscr{C}^0(\mathbb{R})}).$$

Now we set

$$\hat{\mathrm{d}}_\varepsilon(x) = \max\{\varepsilon\tau_0 \ln\cosh x - \ln(C_0 \|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau_0}(\mathbb{R})} \|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}), -\ln(C_0 \|f''_{\varepsilon,1}\|^2_{\mathscr{C}^0(\mathbb{R})})\} - 1.$$

Recall that $\|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})} \to 0$ as $\varepsilon \to 0$. Therefore $\hat{\mathrm{d}}_\varepsilon(x)$ is positive. Modifying $\hat{\mathrm{d}}_\varepsilon(x)$ in a neighborhood of the point where it is not smooth, we get a smooth positive function $\mathrm{d}_\varepsilon(x)$ satisfying $\mathrm{d}_\varepsilon(x) \leq \hat{\mathrm{d}}_\varepsilon(x) + \frac{1}{2}$, $\|\mathrm{d}'_\varepsilon\|_{C^1(\mathbb{R})} \leq C$, and a similar estimate as (3-7):

$$e^{-\mathrm{d}_\varepsilon(x)}(\cosh x)^{\varepsilon\tau} \leq C \|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})} \|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}. \tag{3-9}$$

With this choice, the change of variables $\boldsymbol{x} = (x, y) = \boldsymbol{x}_{\varepsilon,1}(x_1, y_1)$ given by

$$(x_1, y_1) \mapsto (x_1, f_{\varepsilon,1}(x_1)) + y_1 n_{\varepsilon,1}(x_1) = (x, y)$$

is a diffeomorphism in the set $\{(x_1, y_1) : |y_1| < \mathrm{d}_\varepsilon(x_1)\}$. Denote the corresponding neighborhood of $\mathcal{N}_{\varepsilon,1}$ by $\mathcal{O}_1$. Note that the transformation $\boldsymbol{x}_{\varepsilon,1}$ is given explicitly by

$$x = x_1 - \frac{f'_{\varepsilon,1}(x_1)}{\sqrt{1+(f'_{\varepsilon,1}(x_1))^2}} y_1, \quad y = f_{\varepsilon,1}(x_1) + \frac{y_1}{\sqrt{1+(f'_{\varepsilon,1}(x_1))^2}}. \tag{3-10}$$

Similarly, for the graph of $y = f_{\varepsilon,2}(x) = -f_{\varepsilon,1}(x)$, which is the symmetric image $\mathcal{N}_{\varepsilon,2}$ of $\mathcal{N}_{\varepsilon,1}$ with respect to the x axis in the upper half-plane one can associate a Fermi coordinate $(x_2, y_2) \in \mathbb{R} \times (-\mathrm{d}_\varepsilon, \mathrm{d}_\varepsilon)$, in $\mathcal{O}_2$, which is the symmetric image of $\mathcal{O}_1$ defined above, and y_2 is the signed distance, positive in the upper part of $\mathcal{N}_{\varepsilon,2}$. Also, we use $\boldsymbol{x}_{\varepsilon,2}$ to denote the corresponding diffeomorphism

$$(x_2, y_2) \mapsto (x_2, f_{\varepsilon,2}(x_2)) + y_2 n_{\varepsilon,2}(x_2).$$

Furthermore, for any function $w : \mathcal{O}_i \to \mathbb{R}$, we will define its pullback by $\boldsymbol{x}_{\varepsilon,i}$ by setting $(\boldsymbol{x}^*_{\varepsilon,i} w)(x_i, y_i) = w \circ \boldsymbol{x}_{\varepsilon,i}(x_i, y_i)$.

4. Asymptotic profile of a solution near its nodal line

***An approximate solution of* (1-1).** We will now define an approximate solution to (1-1) which accounts accurately for the asymptotic behavior of the true solution as $\varepsilon \to 0$. We will use the nodal lines $\mathcal{N}_{\varepsilon,i}$ as the point of departure and will base our construction on the neighborhoods $\mathcal{O}_i$, which are expanding as $x \to \infty$.

To be precise, we let η_i be a smooth cutoff function satisfying $\eta_i(\boldsymbol{x}) = 0$, $\boldsymbol{x} \notin \mathcal{O}_i$, and $\eta_i(\boldsymbol{x}) = 1$ for any point $\boldsymbol{x} \in \mathcal{O}_i$ such that $\operatorname{dist}(\boldsymbol{x}, \partial\mathcal{O}_i) > 1$. Moreover, η_i could be chosen in such a way that $\|\eta_i\|_{\mathscr{C}^3(\mathbb{R}^2)} \le C$. We will use (x_i, y_i) to denote the Fermi coordinates associated to $\mathcal{N}_{\varepsilon,i}$, $i = 1, 2$. Finally, we introduce an unknown function $h_\varepsilon : \mathbb{R} \to \mathbb{R}$, which a priori is of class $\mathscr{C}^3$, and we let $H_{\varepsilon,1} : \mathbb{R}^2 \to \mathbb{R}$ be a $\mathscr{C}^3$ function that, outside of $\mathcal{O}_1$, is equal to 1 (above $\mathcal{N}_{\varepsilon,1}$) and -1 (below $\mathcal{N}_{\varepsilon,1}$), and otherwise is given by

$$(\boldsymbol{x}^*_{\varepsilon,1} H_{\varepsilon,1})(x_1, y_1) = (\boldsymbol{x}^*_{\varepsilon,1}\eta_1) H(y_1 - h_\varepsilon(x_1)) + (1 - \boldsymbol{x}^*_{\varepsilon,1}\eta_1) \frac{H(y_1 - h_\varepsilon(x_1))}{|H(y_1 - h_\varepsilon(x_1))|}. \tag{4-1}$$

Furthermore, we define

$$H_{\varepsilon,2}(x, y) = -H_{\varepsilon,1}(x, -y), \quad \bar{u}_\varepsilon = H_{\varepsilon,1} - H_{\varepsilon,2} - 1.$$

The function h_ε is called the modulation function and it will be defined (Lemma 5.1) through the orthogonality condition:

$$\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,i}[(u - \bar{u}_\varepsilon)\rho_{\varepsilon,i} H'_{\varepsilon,i}]\, dy_i = 0 \quad \text{for all } x_i \in \mathbb{R},$$

where

$$(\boldsymbol{x}^*_{\varepsilon,i} H'_{\varepsilon,i})(x_i, y_i) = (\boldsymbol{x}^*_{\varepsilon,i}\eta_i) H'(y_i - (-1)^{i+1} h_\varepsilon(x_i)), \quad i = 1, 2,$$

and the smooth cutoff functions $\rho_{\varepsilon,i}$ are defined by

$$(\boldsymbol{x}_{\varepsilon,i}^{*}\rho_{\varepsilon,i})(x_i, y_i) = \rho(y_i - (-1)^{i+1}h_\varepsilon(x_i)),$$

where ρ is an even function satisfying

$$\rho(t) = \begin{cases} 1, & |t| \le \min\{\mathrm{d}_\varepsilon(0), f_{\varepsilon,2}(0)\} - 2, \\ 0, & |t| \ge \min\{\mathrm{d}_\varepsilon(0), f_{\varepsilon,2}(0)\} - 1, \\ 0 < \rho < 1, & \text{otherwise.} \end{cases}$$

The proof of existence of the modulation function h_ε will be given later on, but, anticipating it, we observe that due to the exponential decay in x of the functions involved, we have $h_\varepsilon \in \mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})$, and in fact we will show

$$\|h_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})} \le C\varepsilon^2. \tag{4-2}$$

If we let $\phi = u - \bar{u}_\varepsilon$, we have

$$L_{\bar{u}_\varepsilon}\phi := -\Delta\phi + F''(\bar{u}_\varepsilon)\phi = E(\bar{u}_\varepsilon) - P(\phi),$$

where $E(\bar{u}_\varepsilon) = \Delta\bar{u}_\varepsilon - F'(\bar{u}_\varepsilon)$ and $P(\phi) = F'(\bar{u}_\varepsilon + \phi) - F'(\bar{u}_\varepsilon) - F''(\bar{u}_\varepsilon)\phi$. Our first result is the following.

Proposition 4.1. *Let τ be 0 or τ_0. For all $\mu \in (0, 1)$, the following estimate holds*:

$$\|h_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})} + \|\phi\|_{C^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} + \|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})} \le C\varepsilon^2.$$

The proof of this proposition, which is based on the a priori estimates for the linear operator $L_{\bar{u}_\varepsilon}$ and careful estimates of the error $E(\bar{u}_\varepsilon)$ of the approximation function is postponed for now and will be given in Section 5. However, it is not hard to show that, a priori, we have $\|\phi\|_{\mathscr{C}^0(\mathbb{R}^2)} = o(1)$ as $\varepsilon \to 0$. A proof of this fact is based on the validity of the De Giorgi conjecture in $\mathbb{R}^2$.

Precise asymptotics of the nodal lines. The point of this section is to describe precisely, and in particular uniformly as $\varepsilon \to 0$, estimates for the function $f_{\varepsilon,i}$. Our curve of reference will be given by a solution of the Toda system:

$$\begin{cases} q_1'' = -c_* e^{\sqrt{2}(q_1 - q_2)}, \\ q_2'' = c_* e^{\sqrt{2}(q_1 - q_2)}, \end{cases} \tag{4-3}$$

for which $q_1(x) = -q_2(x)$, as well as $q_j(x) = q_j(-x)$, $j = 1, 2$, and

$$c_* = \frac{a_F \int_{\mathbb{R}} [F''(1) - F''(H(y))] H'(y) e^{\sqrt{2}y}\, dy}{\int_{\mathbb{R}} (H'(y))^2\, dy}.$$

Here a_F is the constant appearing in the asymptotic expansion (2-1) of H. Keep in mind that we have assumed for convenience $F''(1) = 2$.

To find all solutions to (4-3) with the properties described above, we only need to solve

$$q_1'' = -c_* e^{2\sqrt{2}q_1} \tag{4-4}$$

in the class of even functions. It is easy to see that solutions of (4-4) form a one parameter family, and each solution of this family has asymptotically linear behavior. In fact this family can be parametrized by the slope of the asymptotic line. To describe this family precisely, let us consider the unique solution $U_0(x)$ of (4-4), whose slope at ∞ is -1. We have explicitly

$$U_0(x) = \frac{1}{2\sqrt{2}} \ln \frac{\sqrt{2}}{c_* \cosh^2(\sqrt{2}x)}. \tag{4-5}$$

Asymptotically, as $|x| \to \infty$, we have

$$U_0(x) = -|x| + b_0 + \mathcal{O}(e^{-2\sqrt{2}|x|}),$$

where b_0 is a fixed constant. Then the family of solutions can be written as

$$q_{\varepsilon,1}(x) = U_0(\varepsilon x) - \frac{1}{\sqrt{2}} \ln \frac{1}{\varepsilon}.$$

Thus, given the nodal line $\mathcal{N}_{\varepsilon,1}$ of a solution u, with $\varepsilon = \tan\theta(u)$, by $q_{\varepsilon,1}$ we will denote the solution of (4-4) whose slope at infinity is $-\varepsilon$. Respectively, we set

$$q_{\varepsilon,2} = -q_{\varepsilon,1}.$$

We will denote by $\widetilde{\mathcal{N}}_{\varepsilon,1}$ the curve $y = q_{\varepsilon,1}(x)$ in the lower half-plane and by $\widetilde{\mathcal{N}}_{\varepsilon,2}$ the graph of $y = q_{\varepsilon,2}(\,\cdot\,)$. The hope is that the nodal set in the lower half plane of a four-end solution u, with $\varepsilon = \tan\theta(u)$ small, and $\widetilde{\mathcal{N}}_{\varepsilon,1}$ should be close to each other. To quantify this, we state the next result.

Proposition 4.2. *Let u be a four-end solution of (1-1) such that $\varepsilon = \tan\theta(u)$ is small, let $\mathcal{N}_{\varepsilon,1}$ be the nodal line of this solution in the lower half-plane, given as the graph of the function $y = f_{\varepsilon,1}(x)$, and let $h_\varepsilon \in \mathscr{C}^{2,\mu}(\mathbb{R})$ be the modulation function described above. Then there exist $\alpha, \hat{\tau} > 0$ and a constant j_ε, with $|j_\varepsilon| \le C\varepsilon^\alpha$, such that the following estimates hold for the function $\omega_{\varepsilon,1} := f_{\varepsilon,1} + h_\varepsilon + j_\varepsilon - q_{\varepsilon,1}$:*

$$\begin{aligned}
\|\omega_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\hat{\tau}}(\mathbb{R})} &\le C\varepsilon^\alpha, \\
\|\omega'_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\hat{\tau}}(\mathbb{R})} &\le C\varepsilon^{1+\alpha}, \\
\|\omega''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\hat{\tau}}(\mathbb{R})} &\le C\varepsilon^{2+\alpha}.
\end{aligned} \tag{4-6}$$

This proposition is the main technical tool needed to prove the uniqueness and will be proven in the next section.

5. Proof of Propositions 4.1 and 4.2

We recall that by definition h_ε is required to be such that the following orthogonality condition is satisfied:

$$\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,i}[(u - \bar{u}_\varepsilon)\rho_{\varepsilon,i} H'_{\varepsilon,i}]\, dy_i = 0 \qquad \text{for all } x_i \in \mathbb{R},\ i = 1, 2. \tag{5-1}$$

We will refer to h_ε as the modulation function, and we keep in mind that h_ε is required to be small. Our first objective is to show that the modulation function h_ε indeed exists.

Lemma 5.1. *For each sufficiently small ε there exists a function $h_\varepsilon \in \mathscr{C}^3(\mathbb{R})$ such that (5-1) holds.*

Proof. To find h_ε such that the orthogonality condition (5-1) is satisfied, we first replace the function h_ε in the definition of the functions $H_{\varepsilon,1}$ and $H_{\varepsilon,2}$ by two undetermined, bounded functions $h_{\varepsilon,1}$ and $h_{\varepsilon,2}$. More precisely, given a function $h_{\varepsilon,2}$ in a suitable function space, we have a function $H_{\varepsilon,2}$ which, in the Fermi coordinate (x_2, y_2), is equal to $H(y_2+h_{\varepsilon,2}(x_2))$, at least near $\mathcal{N}_{\varepsilon,2}$. Given this, we want to find the function $h_{\varepsilon,1}$, corresponding to the modulation of the nodal line $\mathcal{N}_{\varepsilon,1}$ such that, for the resulting approximate function $H_{\varepsilon,1}$, the orthogonality condition (5-1) is satisfied for $i = 1$. So far the orthogonality condition for $i = 2$ still may not hold. However, if it happens that $h_{\varepsilon,2} = h_{\varepsilon,1}$, then, by symmetry, the orthogonality condition is also satisfied for $i = 2$ and this will yield the desired modulation function h_ε. To find an $h_{\varepsilon,2}$ such that $h_{\varepsilon,1} = h_{\varepsilon,2}$, we will use a fixed point argument. Now we give more details for this strategy.

Obviously,

$$\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[\bar{u}_\varepsilon \rho_{\varepsilon,1} H'_{\varepsilon,1}]\,dy_1 = -\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[(H_{\varepsilon,2}+1)\rho_{\varepsilon,1} H'_{\varepsilon,1}]\,dy_1.$$

This identity suggests that we should consider the function

$$k_\varepsilon(s, x_1) := \int_{\mathbb{R}} \rho(y_1 - s) H'(y_1 - s)\boldsymbol{x}^*_{\varepsilon,1}(u + H_{\varepsilon,2} + 1)(x_1, y_1)\,dy_1, \quad s, x_1 \in \mathbb{R}.$$

Note that the orthogonality condition (5-1) for $i = 1$ is equivalent to $k_\varepsilon(s, x_1) = 0$ with $s = h_{\varepsilon,1}(x_1)$. Let us calculate

$$\begin{aligned}
-\partial_s k_\varepsilon(s, x_1) &= \int_{\mathbb{R}} [\rho'(y_1 - s)H'(y_1 - s) + \rho(y_1 - s)H''(y_1 - s)]\boldsymbol{x}^*_{\varepsilon,1}(u + H_{\varepsilon,2} + 1)(x_1, y_1)\,dy_1\\
&= \underbrace{\int_{\mathbb{R}} [\rho'(y_1 - s)H'(y_1 - s) + \rho(y_1 - s)H''(y_1 - s)]H(y_1)\,dy_1}_{l_1}\\
&\quad + \underbrace{\int_{\mathbb{R}} [\rho'(y_1 - s)H'(y_1 - s) + \rho(y_1 - s)H''(y_1 - s)]\boldsymbol{x}^*_{\varepsilon,1}(H_{\varepsilon,2} + 1)(x_1, y_1)\,dy_1}_{l_2}\\
&\quad + \underbrace{\int_{\mathbb{R}} [\rho'(y_1 - s)H'(y_1 - s) + \rho(y_1 - s)H''(y_1 - s)][\boldsymbol{x}^*_{\varepsilon,1}u(x_1, y_1) - H(y_1)]\,dy_1}_{l_3}.
\end{aligned}$$

Fix a small constant a. It is easy to see that there exists constant $\delta > 0$, independent of ε, such that $l_1 > \delta$ for $s \in (-a, a)$. Obviously, the second term l_2 tends to 0 as $\varepsilon \to 0$. Moreover, since u converges locally as $\varepsilon \to 0$ to the heteroclinic solution, we have

$$l_3 \to 0 \quad \text{as } \varepsilon \to 0.$$

Therefore $\partial_s k_\varepsilon(s, x_1) > \delta/2$ for $s \in (-a, a)$, and $x_1 \in \mathbb{R}$, when ε is small enough.

Next let us write

$$k_\varepsilon(s,x_1)=\underbrace{\int_{\mathbb{R}}\rho(y_1-s)H'(y_1-s)H(y_1)\,dy_1}_{l_4}+\underbrace{\int_{\mathbb{R}}\rho(y_1-s)H'(y_1-s)\boldsymbol{x}^*_{\varepsilon,1}(H_{\varepsilon,2}+1)(x_1,y_1)\,dy_1}_{l_5}$$
$$+\underbrace{\int_{\mathbb{R}}\rho(y_1-s)H'(y_1-s)[\boldsymbol{x}^*_{\varepsilon,1}u(x_1,y_1)-H(y_1)]\,dy_1}_{l_6}.$$

We have

$$l_4(s)=s\int_{\mathbb{R}}\rho(y_1)(H'(y_1))^2\,dy_1+b(s),\quad b(s)\sim s^2, \tag{5-2}$$

while

$$l_5,l_6\to 0,\quad \varepsilon\to 0. \tag{5-3}$$

Hence, taking a smaller if necessary, we may assume $k_\varepsilon(a,x_1)>0$ and $k_\varepsilon(-a,x_1)<0$ for small ε. This together with the monotonicity of k_ε ensures the existence of $h_{\varepsilon,1}$, which fulfills the orthogonality condition (5-1) for $i=1$ and fixed $h_{\varepsilon,2}$.

The above argument implies that, for any $h_{\varepsilon,2}\in\mathscr{C}^0(\mathbb{R})$, $\|h_{\varepsilon,2}\|_{\mathscr{C}^0(\mathbb{R})}<a$, we have a nonlinear map T defined by $h_{\varepsilon,2}\mapsto h_{\varepsilon,1}$. The map T satisfies

$$T\,B(0,a)\subset B(0,a),\quad B(0,a)=\{h\in\mathscr{C}^0(\mathbb{R}):\|h\|_{\mathscr{C}^0(\mathbb{R})}<a\}.$$

The proof that T is a contraction map is standard and is omitted. At the end we obtain the existence of a fixed point $h_\varepsilon=h_{\varepsilon,1}=h_{\varepsilon,2}$.

One can verify that although $h_{\varepsilon,2}$ is only of class $\mathscr{C}^0$, the function k_ε is of class $\mathscr{C}^1$. Therefore, by the implicit function theorem, h_ε is also of class $\mathscr{C}^1$. It then follows that k_ε is $\mathscr{C}^2$. Therefore the regularity of h_ε can be bootstrapped. This ends the proof. □

Corollary 5.2. *The modulation function h_ε satisfies*

$$\|h_\varepsilon\|_{\mathscr{C}^{2,\mu}(\mathbb{R})}=o(1),\quad \varepsilon\to 0. \tag{5-4}$$

We also have $h_\varepsilon\in\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})$.

Proof. The fact that $\|h_\varepsilon\|_{\mathscr{C}^0(\mathbb{R})}$ tends to 0 as $\varepsilon\to 0$ essentially follows from (5-2) and (5-3). Then the same can be shown for the higher order derivatives. Once the existence of small h_ε is established, one can again use (5-2) and the fact that, a priori, $u\in\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)$ to show that $h_\varepsilon\in\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})$. □

Now let us recall that for a four-end solution with small angle, we have written $u=\bar{u}_\varepsilon+\phi$. The linearization of the Allen–Cahn equation around $\bar{u}_\varepsilon$ is $L_{\bar{u}_\varepsilon}=-\Delta+F''(\bar{u}_\varepsilon)$. The function ϕ satisfies

$$L_{\bar{u}_\varepsilon}\phi=\Delta\bar{u}_\varepsilon-F'(\bar{u}_\varepsilon)-P(\phi), \tag{5-5}$$

and

$$P(\phi)=F'(\bar{u}_\varepsilon+\phi)-F'(\bar{u}_\varepsilon)-F''(\bar{u}_\varepsilon)\phi\sim\phi^2$$

is a higher order term in ϕ. Note that our definition of $\bar{u}_\varepsilon$ and the construction of the function h_ε imply that $\phi=u-\bar{u}_\varepsilon$ satisfies the orthogonality condition (5-1). Our strategy to get suitable estimates for ϕ relies on the a priori estimates for the operator $L_{\bar{u}_\varepsilon}$, taking into account this orthogonality condition.

To carry out the analysis, we will study the error term $E(\bar{u}_\varepsilon) = \Delta\bar{u}_\varepsilon - F'(\bar{u}_\varepsilon)$. First we consider the projection of $E(\bar{u}_\varepsilon)$ onto the two-dimensional space $K = \operatorname{span}\{H'_{\varepsilon,i}\rho_{\varepsilon,i},\, i = 1, 2\}$, which we will denote by $E(\bar{u}_\varepsilon)^{\|}$. Explicitly, $E(\bar{u}_\varepsilon)^{\|} = E(\bar{u}_\varepsilon)^{\|}_1 + E(\bar{u}_\varepsilon)^{\|}_2$, where $E(\bar{u}_\varepsilon)^{\|}_i$ is equal to 0 outside $\mathbb{O}_i$ and

$$\boldsymbol{x}^*_{\varepsilon,i} E(\bar{u}_\varepsilon)^{\|}_i(x_i, y_i) := c_\varepsilon \boldsymbol{x}^*_{\varepsilon,i}(\rho_{\varepsilon,i} H'_{\varepsilon,i}) \int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,i}[E(\bar{u}_\varepsilon)\rho_{\varepsilon,i} H'_{\varepsilon,i}]\, dy_i \quad \text{in } \mathbb{O}_i,\ i = 1, 2.$$

Here

$$c_\varepsilon = \left(\int_{\mathbb{R}} [\boldsymbol{x}^*_{\varepsilon,1}(\rho_{\varepsilon,1} H_{\varepsilon,1})]^2\, dy\right)^{-1} = \left(\int_{\mathbb{R}} (\rho H)^2\, dy\right)^{-1}.$$

Furthermore we set $E(\bar{u}_\varepsilon)^{\perp} = E(\bar{u}_\varepsilon) - E(\bar{u}_\varepsilon)^{\|}$. The main idea in what follows is that the size of the function $f''_{\varepsilon,1}$ is related to $E(\bar{u}_\varepsilon)^{\|}$, while the size of $u - \bar{u}_\varepsilon = \phi$ is controlled by $E(\bar{u}_\varepsilon)^{\perp}$. Of course, both projections of the error $E(\bar{u}_\varepsilon)$ are coupled, in the sense that the dependence on $f_{\varepsilon,1}$ and ϕ appears in both of them, but, as we will see, this coupling is relatively easy to deal with.

As we said, we wish to analyze the error $E(\bar{u}_\varepsilon)$. Observe that

$$\begin{aligned} -F'(H_{\varepsilon,2}) - F'(H_{\varepsilon,1} - H_{\varepsilon,2} - 1) &= -F'(H_{\varepsilon,2}) - F'(H_{\varepsilon,1}) + F''(H_{\varepsilon,1})(H_{\varepsilon,2} + 1) + \mathbb{O}((H_{\varepsilon,2} + 1)^2) \\ &= -F'(H_{\varepsilon,1}) - [F''(1) - F''(H_{\varepsilon,1})](H_{\varepsilon,2} + 1) + \mathbb{O}((H_{\varepsilon,2} + 1)^2). \end{aligned}$$

It follows that

$$\begin{aligned} E(\bar{u}_\varepsilon) &= -\Delta(H_{\varepsilon,1} - H_{\varepsilon,2} - 1) + F'(H_{\varepsilon,1} - H_{\varepsilon,2} - 1) \\ &= -\Delta H_{\varepsilon,1} + F'(H_{\varepsilon,1}) + \Delta H_{\varepsilon,2} - F'(H_{\varepsilon,2}) + [F''(1) - F''(H_{\varepsilon,1})](H_{\varepsilon,2} + 1) + \mathbb{O}((H_{\varepsilon,2} + 1)^2). \end{aligned}$$

The expression of the Laplace operator in $\mathcal{N}_{\varepsilon,i}$ is

$$\Delta = \frac{1}{A_i}\partial^2_{x_i} + \partial^2_{y_i} + \frac{1}{2}\frac{\partial_{y_i} A_i}{A_i}\partial_{y_i} - \tfrac{1}{2}\frac{\partial_{x_i} A_i}{A_i^2}\partial_{x_i}, \tag{5-6}$$

where

$$A_i = 1 + (f'_{\varepsilon,i}(x_i))^2 - 2y_i \frac{f''_{\varepsilon,i}(x_i)}{\sqrt{1 + (f'_{\varepsilon,i}(x_i))^2}} + y_i^2 \frac{(f''_{\varepsilon,i}(x_i))^2}{(1 + (f'_{\varepsilon,i}(x_i))^2)^2}.$$

Using these formulas, we can write down the explicit expression of $E(\bar{u}_\varepsilon)$. Because of symmetry, it suffices to carry out the calculation in the lower half plane. The same calculation as that of [del Pino et al. 2010, (5.65)] shows that in the portion of the lower half-plane where both cutoff functions $\eta_{\varepsilon,i}$ equal 1, we have, for $i = 1, 2$,

$$\begin{aligned} E(\bar{u}_\varepsilon) = \left(\frac{1}{2}\frac{\partial_{y_1} A_1}{A_1} - \frac{h''_\varepsilon(x_1)}{A_1} + \frac{1}{2}\frac{\partial_{x_1} A_1}{A_1^2} h'_\varepsilon(x_1)\right) H'(y_1 - h_\varepsilon(x_1)) \\ - \left(\frac{1}{2}\frac{\partial_{y_2} A_2}{A_2} + \frac{h''_\varepsilon(x_2)}{A_2} - \frac{1}{2}\frac{\partial_{x_2} A_2}{A_2^2} h'_\varepsilon(x_2)\right) H'(y_2 - h_\varepsilon(x_2)) \\ + \left(\frac{(h'_\varepsilon(x_1))^2}{A_1} H''(y_1 - h_\varepsilon(x_1)) - \frac{(h'_\varepsilon(x_2))^2}{A_2} H''(y_2 + h_\varepsilon(x_2))\right) \\ - (F''(1) - F''(H_{\varepsilon,1}))(H_{\varepsilon,2} + 1) + \mathbb{O}((H_{\varepsilon,2} + 1)^2). \end{aligned} \tag{5-7}$$

Lemma 5.3. *Suppose τ is equal to* 0 *or* τ_0, *and define* $\mathfrak{D}(\boldsymbol{x}) := \operatorname{dist}(\boldsymbol{x}, \mathcal{N}_{\varepsilon,1}) + \operatorname{dist}(\boldsymbol{x}, \mathcal{N}_{\varepsilon,2})$. *Then, for any* $\mu \in (0, 1)$,

$$\|E(\bar{u}_\varepsilon)^\perp\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} = o(\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})} + \|h_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})}) + \mathbb{O}(\|\exp(-\sqrt{2}\mathfrak{D})\|_{C^0_{\varepsilon\tau}(\mathbb{R}^2)}), \tag{5-8}$$

Proof. First we note that, outside of the set $\mathbb{O}_1 \cup \mathbb{O}_2$, $\bar{u}_\varepsilon$ is equal to 1 or -1, hence the estimate is trivial in this region. Secondly, if $\boldsymbol{x} \in \mathbb{O}_i$ and $\operatorname{dist}(\boldsymbol{x}, \partial\mathbb{O}_i) < 1$, then, using the asymptotic behavior of the heteroclinic solution, it is not difficult to see that

$$\| - \Delta H_{\varepsilon,i} + F'(H_{\varepsilon,i})\|_{\mathscr{C}^{0,\mu}(B(\boldsymbol{x},1))} \le C e^{-\sqrt{2}\mathrm{d}_\varepsilon(x_i)},$$

where (x_i, y_i) is the Fermi coordinate of $\boldsymbol{x}$. Let (x, y) be the Euclidean coordinate of the point $\boldsymbol{x}$. Then elementary geometry tells us

$$|x_i - x| \le |f'_{\varepsilon,i}(x_i)|\mathrm{d}_\varepsilon(x_i).$$

Therefore, using (3-9), we get

$$\begin{aligned} e^{-\sqrt{2}\mathrm{d}_\varepsilon(x_i)} e^{\varepsilon\tau|x|} &\le e^{-\sqrt{2}\mathrm{d}_\varepsilon(x_i)} e^{\varepsilon\tau|x_i|+\varepsilon\tau|f'_{\varepsilon,i}(x_i)|\mathrm{d}_\varepsilon(x_i)} \\ &\le e^{-\mathrm{d}_\varepsilon(x_i)} e^{\varepsilon\tau|x_i|} \\ &\le C\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})}\|f''_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})}. \end{aligned}$$

Hence, to prove (5-8), it will suffice to consider the expression (5-7) for $E(\bar{u}_\varepsilon)$.

By (5-7), we get, for instance, the following term in $E(\bar{u}_\varepsilon)^\perp$:

$$T_1 := \frac{\partial_{y_1} A_1}{A_1} \boldsymbol{x}^*_{\varepsilon,1} H'_{\varepsilon,1} - c_\varepsilon \boldsymbol{x}^*_{\varepsilon,1}(\rho_{\varepsilon,1} H'_{\varepsilon,1}) \int_{\mathbb{R}} \frac{\partial_{y_1} A_1}{A_1} \rho_{\varepsilon,1}(H'_{\varepsilon,1})^2 \, dy_1.$$

Here we have used the fact that $\rho_{\varepsilon,1} H'_{\varepsilon,1}$ is supported in the lower half-plane and $\rho_{\varepsilon,2} H'_{\varepsilon,2}$ is supported in the upper half-plane. Recall that the main order term of A_1 is 1 and

$$\frac{\partial_{y_1} A_1}{A_1} = -2 \frac{f''_{\varepsilon,1}(x_1)}{A_1\sqrt{1 + (f'_{\varepsilon,1}(x_1))^2}} + 2 \frac{y_1 (f''_{\varepsilon,1}(x_1))^2}{A_1(1 + (f'_{\varepsilon,1}(x_1))^2)^2},$$

whose main order term is, roughly speaking, $-2f''_{\varepsilon,1}$. Substituting this into the expression of T_1 results in

$$T_1 = \frac{\partial_{y_1} A_1}{A_1} H'_{\varepsilon,1} + \frac{2c_\varepsilon \rho_{\varepsilon,1} H'_{\varepsilon,1} f''_{\varepsilon,1}(x_1)}{\sqrt{1 + (f'_{\varepsilon,1}(x_1))^2}} \int_{\mathbb{R}} \frac{\rho_{\varepsilon,1}(H'_{\varepsilon,1})^2}{A_1} \, dy_1 - \frac{2c_\varepsilon \rho_{\varepsilon,1} H'_{\varepsilon,1} (f''_{\varepsilon,1}(x_1))^2}{(1 + (f'_{\varepsilon,1}(x_1))^2)^2} \int_{\mathbb{R}} \frac{y_1 \rho_{\varepsilon,1}(H'_{\varepsilon,1})^2}{A_1} \, dy_1.$$

We notice that although it appears at first that T_1 carries a term of order $\mathbb{O}(\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})})$, there is a cancelation between the first and the second term in T_1. In estimating this term it is important to use the properties of the cut off function $\rho_{\varepsilon,1}$. Note also that although y_1 appears in $\partial_{y_1} A_1/A_1$, it is always multiplied by $f''_{\varepsilon,1}(x_1)$. Since in $\mathbb{O}_1$, $|y_1| \le \mathrm{d}_\varepsilon(x_1)$, we have $|y_1| \le 1/\sqrt{f''_{\varepsilon,1}(x_1)}$. Therefore $y_1 f''_{\varepsilon,1}(x_1)$ is always a small order term.

It is worth mentioning that when we estimate $\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})$ norms we need to take into account the relation between the Fermi coordinate (x_1, y_1) and the Euclidean coordinate (x, y) of a point $\boldsymbol{x} \in \mathbb{O}_1$. Typically, we have

$$|(\cosh x)^{\varepsilon\tau} f''_{\varepsilon,1}(x_1)| \le Ce^{\varepsilon\tau|x_1-x|}\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})} \le C\exp\{\varepsilon\tau|y_1|\mathbb{O}(\|f'_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})})\}\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})}.$$

Any term of this form is additionally multiplied by $o(1)H'_{\varepsilon,1}$ or $o(1)H''_{\varepsilon,1}$, thus yielding a term of order $o(\|f''_{\varepsilon,1}\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})})$.

Now, using the fact that $f'_{\varepsilon,1}$ and $f''_{\varepsilon,1}$ are of order $o(1)$ as $\varepsilon \to 0$ and the definition of the cutoff function $\rho_{\varepsilon,1}$, we conclude

$$\|T_1\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} = o(\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})}).$$

Similar estimates hold for the terms involving $h''_\varepsilon(x_1)$. Regarding terms involving $h'_\varepsilon(x_1)$, $h'_\varepsilon(x_2)$, $h''_\varepsilon(x_2)$, we note that they are all multiplied by small order terms. Finally, to estimate the norms of $(H_{\varepsilon,2}+1)H'_{\varepsilon,1}$, we use the fact that

$$(H_{\varepsilon,2}+1)H'_{\varepsilon,1} \sim e^{-\sqrt{2}(|y_1|+|y_2|)}.$$

It follows immediately that

$$\|(H_{\varepsilon,2}+1)H'_{\varepsilon,1}\|_{C^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} \le C\|\exp(-\sqrt{2}\mathfrak{D})\|_{C^0_{\varepsilon\tau}(\mathbb{R}^2)}.$$ □

Observe that there are terms involving h_ε which appear in the right hand side of (5-8). This complicates the situation somewhat. However, since the Fermi coordinates are defined using the nodal line, we have the following.

Lemma 5.4. *Let τ be 0 or τ_0. We have*

$$\|h_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})} \le C\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} + C\|\exp(-\sqrt{2}\mathfrak{D})\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R}^2)}. \tag{5-9}$$

Proof. We first recall that if $\boldsymbol{x} \in \mathbb{O}_1$ and $\operatorname{dist}(\boldsymbol{x}, \partial\mathbb{O}_1) > 1$, then

$$(\boldsymbol{x}^*_{\varepsilon,1}u)(x_1, y_1) = H(y_1 - h_\varepsilon(x_1)) - (\boldsymbol{x}^*_{\varepsilon,1}H_{\varepsilon,2})(x_1, y_1) - 1 + (\boldsymbol{x}^*_{\varepsilon,1}\phi)(x_1, y_1). \tag{5-10}$$

Now let us consider any point $\boldsymbol{x}$ on the curve $\mathcal{N}_{\varepsilon,1}$. That is, the Fermi coordinate of $\boldsymbol{x}$ is $(x_1, 0)$. Since the distance of $\boldsymbol{x}$ to $\mathcal{N}_{\varepsilon,2}$ is $\mathfrak{D}(\boldsymbol{x})$, we have

$$|(\boldsymbol{x}^*_{\varepsilon,1}H_{\varepsilon,2})(x_1, 0) + 1| \le C\exp(-\sqrt{2}\mathfrak{D}(\boldsymbol{x})).$$

Then, from $(\boldsymbol{x}^*_{\varepsilon,1}u)(x_1, 0) = 0$ and (5-10), one gets

$$\|h_\varepsilon\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R})} \le C\|\phi\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R}^2)} + C\|\exp(-\sqrt{2}\mathfrak{D})\|_{\mathscr{C}^0_{\varepsilon\tau}(\mathbb{R}^2)}.$$

This gives us the $\mathscr{C}^0$ estimate. To estimate the $\mathscr{C}^1$ norm of h_ε, we differentiate the relation (5-10) with respect to x_1 and let $y_1 = 0$ in the resulting equation. Then we find that

$$-H'(-h_\varepsilon(x_1))h'_\varepsilon(x_1) - \frac{\partial}{\partial x_1}(\boldsymbol{x}^*_{\varepsilon,1}H_{\varepsilon,2}) + \frac{\partial}{\partial x_1}(\boldsymbol{x}^*_{\varepsilon,1}\phi) = 0, \tag{5-11}$$

from which the $\mathscr{C}^1_{\varepsilon\tau}$ estimate follows. Similarly, we could differentiate (5-10) twice with respect to x_1 and let $y_1 = 0$ to estimate h''_ε.

Corresponding estimates for the Hölder norm are also straightforward. □

To proceed, we need the following a priori estimate.

Proposition 5.5. *Suppose φ is a solution of the equation*

$$-\Delta\varphi + F''(\bar{u}_\varepsilon)\varphi = f + \sum_{i=1,2} \kappa_{\varepsilon,i}\rho_{\varepsilon,i}H'_{\varepsilon,i} \quad \text{in } \mathbb{R}^2,$$

with some given functions $f \in \mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)$ and $\kappa_{\varepsilon,i} \in \mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})$. Assume furthermore that the function φ satisfies the orthogonality condition:

$$\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,i}(\varphi\rho_{\varepsilon,i}H'_{\varepsilon,i})\,dy_i = 0, \quad i = 1, 2. \tag{5-12}$$

Then we have

$$\|\varphi\|_{C^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} \le C\|f\|_{C^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)}, \quad \|\kappa_{\varepsilon,i}\|_{C^{0,\mu}_{\varepsilon\tau}(\mathbb{R})} \le C\|f\|_{C^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)},$$

provided ε is small enough.

Sketch of proof. The proof is by contradiction and is essentially the same as that of [del Pino et al. 2010, Proposition 5.1]. First an a priori estimate is proven for a solution of the problem

$$-\Delta\varphi + F''(\bar{u}_\varepsilon)\varphi = f_0 \quad \text{in } \mathbb{R}^2,$$

where φ satisfies the orthogonality condition (5-12). Indeed, using the fact that H', where H is the heteroclinic solution in $\mathbb{R}$, is the only element of the kernel of the corresponding one-dimensional linear operator $d^2/dt^2 + 1 - 3H^2$, one can prove that φ satisfies an estimate of the form claimed. This type of argument can be found, for example, in [del Pino et al. 2011].

Second, we project the equation on the functions of the form $\rho_{\varepsilon,i}H'_{\varepsilon,i}$, $i = 1, 2$, and get the identity

$$\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,i}\{\rho_{\varepsilon,i}H'_{\varepsilon,i}[-\Delta\varphi + F''(\bar{u}_\varepsilon)\varphi]\}\,dy_i - \int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,i}(\rho_{\varepsilon,i}H'_{\varepsilon,i}f)\,dy_i = \kappa_{\varepsilon,i}\int_R (\boldsymbol{x}^*_{\varepsilon,i}\rho_{\varepsilon,i}H'_{\varepsilon,i})^2\,dy_i.$$

After an integration by parts and some calculations, we can use the above identity to prove that the $\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})$ norm of the functions $\kappa_{\varepsilon,i}$ can be controlled by $o(1)\|\varphi\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} + C\|f\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)}$. From this and the first step the assertion follows. We omit the details. □

Lemma 5.6. *Let $\phi = u - \bar{u}_\varepsilon$ be the solution of (5-5). The following estimate is true*:

$$\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} \le o(\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})}) + C\|\exp(-\sqrt{2}\mathfrak{D})\|_{C^0_{\varepsilon\tau}(\mathbb{R}^2)}. \tag{5-13}$$

Proof. We will use Proposition 5.5. Thus we write

$$-\Delta\phi + F''(\bar{u}_\varepsilon)\phi = E(\bar{u}_\varepsilon)^{\perp} - P(\phi) + E(\bar{u}_\varepsilon)^{\parallel}.$$

Because of Proposition 5.5, to control the size of the function ϕ, it suffices to control the size of $E(\bar{u}_\varepsilon)^{\perp}$ (which we already do by Lemma 5.3) and the size of $P(\phi)$.

Next we observe that $P(\phi)$ is essentially quadratic in ϕ, and therefore it is not difficult to show

$$\|P(\phi)\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} = o(\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)}).$$

Collecting all these estimates, we conclude (5-13). □

The above result indicates that we can control ϕ by $\exp(-\sqrt{2}\mathfrak{D})$ and the second derivative of $f_{\varepsilon,1}$. However, this is not quite enough for our later purpose. Note that for the solution constructed in [del Pino et al. 2010], the corresponding error is, roughly speaking, controlled by $C\varepsilon^2$, and $\| f_{\varepsilon,1}-\varepsilon|x|\|_{\mathscr{C}^0(\mathbb{R})} \sim \ln \frac{1}{\varepsilon}$. For this purpose we first show the following:

Lemma 5.7. *The following estimate holds*:

$$\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} + \| f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})} \leq C\| \exp(-\sqrt{2}\mathfrak{D})\|_{C^0_{\varepsilon\tau}(\mathbb{R}^2)}.$$

Proof. Consider the integral $\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[E(\bar{u}_\varepsilon)\rho_{\varepsilon,1}H'_{\varepsilon,1}]\,dy_1$. We will show below (Step 1) that on the one hand its $\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})$ norm is controlled by $o(\|\phi\|_{C^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)})$. On the other hand (Step 2) we will show that this integral is related to $f''_{\varepsilon,1}$. The proof will follow by combining this with the previous estimates. (Step 1 can be avoided if we estimate the integral using Proposition 5.5. However, since the computations will be used in the last part of the proof of uniqueness (page 1715), we choose to present them here.)

Step 1. We claim that the relevant norm of the integral $\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[E(\bar{u}_\varepsilon)\rho_{\varepsilon,1}H'_{\varepsilon,1}]\,dy_1$ is controlled by $o(\|\phi\|_{C^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)})$.

In fact,

$$\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[E(\bar{u}_\varepsilon)\rho_{\varepsilon,1}H'_{\varepsilon,1}]\,dy_1 = \int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}\{[-\Delta\phi + F''(\bar{u}_\varepsilon)\phi]\rho_{\varepsilon,1}H'_{\varepsilon,1}\}\,dy_1 + \int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[P(\phi)\rho_{\varepsilon,1}H'_{\varepsilon,1}]\,dy_1.$$

To handle the first term appearing in the right side, we write $\Delta_{(x_1,y_1)} = \partial^2_{x_1} + \partial^2_{y_1}$ and

$$T_2 := \underbrace{\int_{\mathbb{R}} [-\Delta_{(x_1,y_1)}\boldsymbol{x}^*_{\varepsilon,1}\phi + F''(H)\boldsymbol{x}^*_{\varepsilon,1}\phi]\boldsymbol{x}^*_{\varepsilon,1}(\rho_{\varepsilon,1}H'_{\varepsilon,1})\,dy_1}_{T_{21}}$$
$$+ \underbrace{\int_{\mathbb{R}} [\Delta_{(x_1,y_1)}\boldsymbol{x}^*_{\varepsilon,1}\phi - \boldsymbol{x}^*_{\varepsilon,1}\Delta\phi + \boldsymbol{x}^*_{\varepsilon,1}(F''(\bar{u}_\varepsilon)\phi) - F''(H)\boldsymbol{x}^*_{\varepsilon,1}\phi]\boldsymbol{x}^*_{\varepsilon,1}(\rho_{\varepsilon,1}H'_{\varepsilon,1})\,dy_1}_{T_{22}}.$$

Since $\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}(\phi\rho_{\varepsilon,1}H'_{\varepsilon,1})\,dy_1 = 0$, we have $(d^2/dx_1^2)\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}(\phi\rho_{\varepsilon,1}H'_{\varepsilon,1})\,dy_1 = 0$. Using integration by parts and the fact that $-H'' + F'(H) = 0$, we find

$$\begin{aligned}
T_{21} &= 2\int_{\mathbb{R}} \frac{\partial(\boldsymbol{x}^*_{\varepsilon,1}\phi)}{\partial x_1}\frac{\partial(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'_{\varepsilon,1})}{\partial x_1}\,dy_1 + \int_{\mathbb{R}} (\boldsymbol{x}^*_{\varepsilon,1}\phi)\frac{\partial^2(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'_{\varepsilon,1})}{\partial x_1^2}\,dy_1 \\
&\qquad - \int_{\mathbb{R}} (\boldsymbol{x}^*_{\varepsilon,1}\phi)\left[\frac{\partial^2(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'_{\varepsilon,1})}{\partial y_1^2} - F''(H)(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'_{\varepsilon,1})\right]dy_1 \\
&= 2\int_{\mathbb{R}} \frac{\partial \boldsymbol{x}^*_{\varepsilon,1}\phi}{\partial x_1}\frac{\partial(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'_{\varepsilon,1})}{\partial x_1}\,dy_1 + \int_{\mathbb{R}} (\boldsymbol{x}^*_{\varepsilon,1}\phi)\frac{\partial^2(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'_{\varepsilon,1})}{\partial x_1^2}\,dy_1 \\
&\qquad - \int_{\mathbb{R}} (\boldsymbol{x}^*_{\varepsilon,1}\phi)\left[\frac{\partial^2(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1})}{\partial y_1^2}(\boldsymbol{x}^*_{\varepsilon,1}H'_{\varepsilon,1}) + 2\frac{\partial(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1})}{\partial y_1}\frac{\partial(\boldsymbol{x}^*_{\varepsilon,1}H'_{\varepsilon,1})}{\partial y_1}\right]dy_1.
\end{aligned}$$

Due to the presence of the derivatives of $\boldsymbol{x}_{\varepsilon,1}^{*}\rho_{\varepsilon,1}$ with respect to x_1, y_1, and also the presence of $H_{\varepsilon,1}'$ in each term, we now obtain that

$$\|T_{21}\|_{\mathscr{C}_{\varepsilon\tau}^{0,\mu}(\mathbb{R})} = o(\|\phi\|_{\mathscr{C}_{\varepsilon\tau}^{2,\mu}(\mathbb{R}^2)}). \tag{5-14}$$

On the other hand,

$$T_{22} = -\int_{\mathbb{R}} \left\{ \left(\frac{1}{A_1} - 1 \right) \partial_{x_1}^2 (\boldsymbol{x}_{\varepsilon,1}^{*}\phi) + \frac{1}{2} \frac{\partial_{y_1} A_1}{A_1} \partial_{y_1} (\boldsymbol{x}_{\varepsilon,1}^{*}\phi) - \frac{1}{2} \frac{\partial_{x_1} A_1}{A_1^2} \partial_{x_1} (\boldsymbol{x}_{\varepsilon,1}^{*}\phi) \right\} (\boldsymbol{x}_{\varepsilon,1}^{*}\rho_{\varepsilon,1} H_{\varepsilon,1}')\, dy_1 \\ + \int_{\mathbb{R}} [\boldsymbol{x}_{\varepsilon,1}^{*}(F''(\bar{u}_\varepsilon)) - F''(H)] \boldsymbol{x}_{\varepsilon,1}^{*}(\phi\rho_{\varepsilon,1} H_{\varepsilon,1}')\, dy_1.$$

The desired estimate for T_{22} essentially follows from the fact that $1 - 1/A_1$, $\partial_{y_1} A_1/A_1$, $\partial_{x_1} A_1/A_1^2$, $\boldsymbol{x}_{\varepsilon,1}^{*}(F''(\bar{u}_\varepsilon)) - F''(H)$ are small terms. Note that we should take into account the relation between the Fermi coordinates and the Euclidean coordinates. For example, let us estimate the Hölder norm of a typical term in T_{22}. First, observe that if $z_1 = (s_1, y_1)$, $z_2 = (s_2, y_1)$ in the Fermi coordinates with respect to $\mathcal{N}_{\varepsilon,1}$, then by the formula (3-10), it is easy to see that

$$|z_1 - z_2| \le C|s_1 - s_2|.$$

Therefore, denoting $(1/A_1 - 1)\partial_{x_1}^2 (\boldsymbol{x}_{\varepsilon,1}^{*}\phi)\boldsymbol{x}_{\varepsilon,1}^{*}(\rho_{\varepsilon,1} H_{\varepsilon,1}')$ by $\boldsymbol{x}_{\varepsilon,1}^{*}\mathfrak{G}$, we have

$$\sup_{|s_1 - s_2| \le 1} \left| \int_{\mathbb{R}} \frac{\boldsymbol{x}_{\varepsilon,1}^{*}\mathfrak{G}(s_1, y_1) - \boldsymbol{x}_{\varepsilon,1}^{*}\mathfrak{G}(s_2, y_1)}{|s_1 - s_2|^{\mu}}\, dy_1 \right| \le C \sup_{|s_1 - s_2| \le 1} \left| \int_{\mathbb{R}} \frac{\mathfrak{G}(z_1) - \mathfrak{G}(z_2)}{|z_1 - z_2|^{\mu}}\, dy_1 \right| \\ = o(\|\phi\|_{C^{2,\mu}(\mathbb{R})}).$$

Other terms appearing in the definition of T_{22} can be checked similarly. Hence we obtain

$$\|T_{22}\|_{\mathscr{C}_{\varepsilon\tau}^{0,\mu}(\mathbb{R})} = o(\|\phi\|_{\mathscr{C}_{\varepsilon\tau}^{2,\mu}(\mathbb{R}^2)}).$$

This together with (5-14) tells us

$$\|T_{2}\|_{\mathscr{C}_{\varepsilon\tau}^{0,\mu}(\mathbb{R})} = o(\|\phi\|_{\mathscr{C}_{\varepsilon\tau}^{2,\mu}(\mathbb{R}^2)}).$$

The desired estimate follows from this in a straightforward way.

Step 2. We want to relate the weighted norm of the integral $\int_{\mathbb{R}} \boldsymbol{x}_{\varepsilon,1}^{*}[E(\bar{u}_\varepsilon)\rho_{\varepsilon,1} H_{\varepsilon,1}']\, dy_1$ to $f_{\varepsilon,1}''$. To do this, we will now check more closely the above integral using the definition of $\bar{u}_\varepsilon$ and the expression of $E(\bar{u}_\varepsilon)$. We see that one term appearing in the integral is

$$\frac{1}{2} \int_{\mathbb{R}} \frac{\partial_{y_1} A_1}{A_1} \boldsymbol{x}_{\varepsilon,1}^{*}(\rho_{\varepsilon,1} H_{\varepsilon,1}'^{2})\, dy_1.$$

We will concentrate on this term since the $\mathscr{C}_{\varepsilon\tau}^{0,\mu}(\mathbb{R})$ norm of other terms can be estimated by

$$C\|h_\varepsilon\|_{C_{\varepsilon\tau}^{2,\mu}(\mathbb{R})} + C\|e^{-\sqrt{2}\mathfrak{D}}\|_{\mathscr{C}_{\varepsilon\tau}^{0}(\mathbb{R})},$$

as we have seen in the proof of Lemma 5.3. Plugging the formula for A_1 into the above integral, one gets

$$\begin{aligned}\frac{1}{2}\int_{\mathbb{R}}\frac{\partial_{y_1}A_1}{A_1}\boldsymbol{x}^*_{\varepsilon,1}(\rho_{\varepsilon,1}H'^2_{\varepsilon,1})\,dy_1 &= \int_{\mathbb{R}}\frac{1}{A_1}\biggl(y_1\frac{(f''_{\varepsilon,1}(x_1))^2}{(1+(f'_{\varepsilon,1}(x_1))^2)^2}-\frac{f''_{\varepsilon,1}(x_1)}{\sqrt{1+(f'_{\varepsilon,1}(x_1))^2}}\biggr)(\boldsymbol{x}^*_{\varepsilon,1}\rho_{\varepsilon,1}H'^2_{\varepsilon,1})\,dy_1\\ &= -\frac{1}{c_\varepsilon}f''_{\varepsilon,1}(x_1)+T_4,\end{aligned}$$

where T_4 is a function such that

$$\|T_4\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})}=o(\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})}).$$

Consequently,

$$\begin{aligned}\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})} &\le C\Bigl\|\int_{\mathbb{R}}\boldsymbol{x}^*_{\varepsilon,1}[E(\bar u_\varepsilon)\rho_{\varepsilon,1}H'_{\varepsilon,1}\,dy_1\Bigr\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})}\\ &\le C\|h_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})}+o(\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})})+C\|\exp(-\sqrt{2}\mathfrak{D})\|_{\mathscr{C}^{0}_{\varepsilon\tau}(\mathbb{R})}.\end{aligned}$$

This together with (5-9) and (5-13) implies that

$$\|f''_{\varepsilon,1}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})}\le C\|\exp(-\sqrt{2}\mathfrak{D})\|_{\mathscr{C}^{0}_{\varepsilon\tau}(\mathbb{R})}. \tag{5-15}$$

This combined with Lemma 5.6 yields

$$\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)}\le C\|\exp(-\sqrt{2}\mathfrak{D})\|_{\mathscr{C}^{0}_{\varepsilon\tau}(\mathbb{R})}.$$ □

To proceed, let us observe that $\|\exp(-\sqrt{2}\mathfrak{D})\|_{\mathscr{C}^0(\mathbb{R}^2)}\le e^{-2\sqrt{2}|f_{\varepsilon,1}(0)|}$. Our next goal is to estimate the quantity $f_{\varepsilon,1}(0)$. To this end, we first need to obtain some exponential decay estimate of ϕ along the y axis away from $\mathcal{N}_{\varepsilon,1}$. Note that, up to now, we have only analyzed the decay behavior of $E(\bar u_\varepsilon)$ along the x axis, but actually it also decays exponentially in the direction transversal to the nodal line $\mathcal{N}_{\varepsilon,1}$. The next lemma gives us the necessary information.

Lemma 5.8. *Fix a small constant $\iota_0>0$. We have*

$$|\phi(0,y)|\le Ce^{-(2\sqrt{2}-\iota_0)|f_{\varepsilon,1}(0)|}e^{-\iota_0|y-f_{\varepsilon,1}(0)|}\quad \textit{for } y\le 0.$$

Proof. This estimate follows from the maximum principle. We only sketch the proof for $f_{\varepsilon,1}(0)\le y\le 0$, since the case of $y\le f_{\varepsilon,1}(0)$ is similar.

We write the equation satisfied by ϕ as

$$-\Delta\phi+\biggl(F''(\bar u_\varepsilon)+\frac{P(\phi)}{\phi}\biggr)\phi=E(\bar u_\varepsilon). \tag{5-16}$$

Consider the region

$$\Omega:=\{(x,y)\in\mathbb{R}^2\,|\,f_{\varepsilon,1}(0)+r_0<y<-f_{\varepsilon,1}(0)-r_0\},$$

where r_0 is a fixed large constant satisfying

$$F''(\bar u_\varepsilon(\boldsymbol{x}))+\frac{P(\phi)(\boldsymbol{x})}{\phi(\boldsymbol{x})}\ge 1,\quad \boldsymbol{x}\in\Omega.$$

Let $B(x, y) := C_1 e^{2\sqrt{2} f_{\varepsilon,1}(0)} \cosh(\iota_0 y)$. Then

$$-\Delta B + \left(F''(\bar{u}_\varepsilon) + \frac{P(\phi)}{\phi} \right) B \geq (1 - \iota_0^2) B. \tag{5-17}$$

Using (5-16), (5-17), and $\|E(\bar{u}_\varepsilon)\|_{\mathscr{C}^0(\mathbb{R}^2)} + \|\phi\|_{\mathscr{C}^0(\mathbb{R}^2)} \leq C e^{-2\sqrt{2}|f_{\varepsilon,1}(0)|}$, we find that if the constant C_1 in the definition of B is large enough, $\phi - B < 0$ in $\partial\Omega$ and

$$-\Delta(\phi - B) + \left(F''(\bar{u}_\varepsilon) + \frac{P(\phi)}{\phi} \right)(\phi - B) \leq 0 \quad \text{in } \Omega.$$

By the maximum principle, for $f_{\varepsilon,1}(0) + r_0 < y < 0$, we have

$$\begin{aligned} |\phi(x, y)| &\leq C_1 e^{2\sqrt{2} f_{\varepsilon,1}(0)} \cosh(\iota_0 y) \\ &\leq C_1 e^{(2\sqrt{2} - \iota_0) f_{\varepsilon,1}(0)} e^{-\iota_0 |f_{\varepsilon,1}(0) - y|}. \end{aligned}$$

Therefore the lemma is true for $f_{\varepsilon,1}(0) + r_0 < y < 0$. For $f_{\varepsilon,1}(0) < y < f_{\varepsilon,1}(0) + r_0$, the lemma obviously holds since $\|\phi\|_{\mathscr{C}^0(\mathbb{R}^2)} \leq C e^{-2\sqrt{2}|f_{\varepsilon,1}(0)|}$. □

Now let us go back to the Toda system (4-3) and recall that by $q_{\varepsilon,1}(x) < 0 < q_{\varepsilon,2}(x)$ we have denoted the solution of this system whose slope at ∞ is ε (this means the tangent of the angle between the asymptotic line of $y = q_{\varepsilon,2}(x)$ in the first quadrant and the x axis). We note that the curve $\widetilde{\mathcal{N}}_{\varepsilon,1} := \{y = q_{\varepsilon,1}(x)\}$ is contained in the lower half-plane.

In the rest of the paper we will also use α, β to denote general positive constants, which may change from step to step, but are always independent of ε.

Our aim is to show that the curves $\mathcal{N}_{\varepsilon,1}$ and $\widetilde{\mathcal{N}}_{\varepsilon,1}$ are close to each other. First of all, we prove the following.

Lemma 5.9. *There exists $\alpha_1 > 0$ such that $|f_{\varepsilon,1}(0) - q_{\varepsilon,1}(0)| \leq C\varepsilon^{\alpha_1}$.*

Proof. The idea of the proof is to relate the asymptotic behavior of u along vertical straight lines, as $\varepsilon \to 0$, using the Hamiltonian identity,

$$\int_{\mathbb{R}} \left\{ \tfrac{1}{2} u_y^2(0, y) - \tfrac{1}{2} u_x^2(0, y) + F(u(0, y)) \right\} dy = \int_{\mathbb{R}} \left\{ \tfrac{1}{2} u_y^2(x, y) - \tfrac{1}{2} u_x^2(x, y) + F(u(x, y)) \right\} dy \quad \text{for all } x, \tag{5-18}$$

and in particular take $x \to \infty$ on the right side of (5-18). Indeed, using the asymptotic behavior of a four-end solution, it is not hard to show that

$$\lim_{x \to \infty} \int_{\mathbb{R}} \left\{ \tfrac{1}{2} u_y^2(x, y) - \tfrac{1}{2} u_x^2(x, y) + F(u(x, y)) \right\} dy = 2\boldsymbol{e}_F \cos\theta(u),$$

where $\boldsymbol{e}_F = \int_{\mathbb{R}} [\frac{1}{2}(H')^2 + F(H)]$. Since u is an even function of x, we also have $u_x(0, y) = 0$, and thus it follows from (5-18) that

$$\int_{\mathbb{R}} \left\{ \tfrac{1}{2} u_y^2(0, y) + F(u(0, y)) \right\} dy = 2\boldsymbol{e}_F \cos\theta(u).$$

We will now calculate the left side of the above identity using the estimate of the error ϕ.

Recall that the heteroclinic solution has the asymptotic behavior

$$H(s) = 1 - a_F e^{-\sqrt{2}s} + \mathcal{O}(e^{-2\sqrt{2}s}) \quad \text{as } s \to +\infty,$$

which can also be differentiated. Set $t = f_{\varepsilon,1}(0) + h_\varepsilon(0)$. Let η_1, η_2 be cut off functions appearing in the definition of the approximate solution (4-1). For the points on the y-axis we have $(x_1, y_1) = (0, y - f_{\varepsilon,1}(x))$, where (x_1, y_1) are their Fermi coordinates with respect to $\mathcal{N}_{\varepsilon,1}$. Then, abusing the notation slightly, we can write

$$\begin{aligned} u(0, y) = &\underbrace{H(y-t) - H(y+t) - 1 + \phi(0, y)}_{u_0(y)} \\ &+ \underbrace{(1 - \eta_1(0, y))\Big[\frac{H(y-t)}{|H(y-t)|} - H(y-t)\Big]}_{\psi_1(y)} - \underbrace{(1 - \eta_2(0, y))\Big[\frac{H(y+t)}{|H(y+t)|} - H(y+t)\Big]}_{\psi_2(y)}. \end{aligned}$$

We observe that $\psi_1(y) = 0$ for $|y_1| < \mathrm{d}_\varepsilon(0) - 1$ and

$$|\psi_1(y)| + |\psi_1'(y)| \le Ce^{-\sqrt{2}|y_1|} \quad \text{for } |y_1| \ge \mathrm{d}_\varepsilon(0) - 1.$$

Therefore

$$\int_{\mathbb{R}} [|\psi_1(y)| + |\psi_1'(y)|]\, dy \le Ce^{-\sqrt{2}\mathrm{d}_\varepsilon(0)} \le \|f_{\varepsilon,1}''\|^2_{C^0(\mathbb{R})} \le Ce^{-4\sqrt{2}|f_{\varepsilon,1}(0)|}.$$

Similarly,

$$\int_{\mathbb{R}} [|\psi_2(y)| + |\psi_2'(y)|]\, dy \le Ce^{-4\sqrt{2}|f_{\varepsilon,1}(0)|}.$$

This implies

$$\int_{\mathbb{R}} \big[\tfrac{1}{2} u_y^2(0, y) + F(u(0, y))\big]\, dy = \int_{\mathbb{R}} \big[\tfrac{1}{2}(u_0'(y))^2 + F(u_0(y))\big]\, dy + \mathcal{O}(e^{-4\sqrt{2}|f_{\varepsilon,1}(0)|}).$$

Now we calculate

$$\begin{aligned} \int_{-\infty}^0 \big[\tfrac{1}{2}(u_0'(y))^2 + F(u_0(y))\big]\, dy = &\underbrace{\int_{-\infty}^0 \big[\tfrac{1}{2}(H'(y-t))^2 + F(H(y-t))\big]\, dy}_{I_1} \\ &+ \underbrace{\int_{-\infty}^0 \big[H'(y-t)(\partial_y\phi - H'(y+t)) + F'(H(y-t))(\phi - H(y+t) - 1)\big]\, dy}_{I_2} \\ &+ \underbrace{\frac{1}{2}\int_{-\infty}^0 \big[(\partial_y\phi - H'(y+t))^2 + F''(H(y-t))(\phi - H(y+t) - 1)^2\big]\, dy}_{I_3} \\ &+ \mathcal{O}\Big(\int_{-\infty}^0 (\phi - H(y+t) - 1)^3\, dy\Big). \end{aligned} \tag{5-19}$$

The first term on the right side of (5-19) is equal to

$$\begin{aligned} I_1 &= \int_{-\infty}^{-t} \left[\tfrac{1}{2}(H'(y))^2 + F(H(y))\right] dy \\ &= \boldsymbol{e}_F - \int_{-t}^{+\infty} \left[\tfrac{1}{2}(H'(y))^2 + F(H(y))\right] dy \\ &= \boldsymbol{e}_F - \int_{-t}^{+\infty} 2a_F^2 e^{-2\sqrt{2}y}\, dy + \mathbb{O}(e^{-3\sqrt{2}|t|}) \\ &= \boldsymbol{e}_F - \frac{\sqrt{2}}{2} a_F^2 e^{-2\sqrt{2}|t|} + \mathbb{O}(e^{-3\sqrt{2}|t|}). \end{aligned}$$

Next we analyze the second term I_2. We observe that after an integration by parts,

$$I_2 = H'(-t)(\phi(0) - H(t) - 1) = -\sqrt{2}a_F^2 e^{-2\sqrt{2}|t|} + \mathbb{O}(e^{-3\sqrt{2}|t|}).$$

On the other hand, using Lemma 5.8, we can estimate

$$\begin{aligned} I_3 &= \frac{1}{2}\int_{-\infty}^{0} [(H'(y+t))^2 + F''(H(y-t))(H(y+t)-1)^2]\, dy + \mathbb{O}(e^{-(3\sqrt{2}-\iota_0)|t|}) \\ &= \frac{\sqrt{2}a_F^2}{4} e^{-2\sqrt{2}|t|} + \frac{a_F^2}{2}\int_{-\infty}^{0} [F''(H(y-t))e^{-2\sqrt{2}|y+t|}]\, dy + \mathbb{O}(e^{-(3\sqrt{2}-\iota_0)|t|}). \end{aligned}$$

But we have

$$\begin{aligned} \int_{-\infty}^{0} [F''(H(y-t))e^{-2\sqrt{2}|y+t|}]\, dy &= \int_{-\infty}^{0} 2e^{2\sqrt{2}(y+t)}\, dy + \int_{-\infty}^{0} \{[F''(H(y-t)) - F''(1)]e^{-2\sqrt{2}|y+t|}\}\, dy \\ &= \frac{\sqrt{2}}{2} e^{-2\sqrt{2}|t|} + \mathbb{O}\Big(\int_{-\infty}^{0} e^{-\sqrt{2}|y-t| - 2\sqrt{2}|y+t|}\, dy\Big) \\ &= \frac{\sqrt{2}}{2} e^{-2\sqrt{2}|t|} + \mathbb{O}(e^{-3\sqrt{2}|t|}). \end{aligned}$$

Hence

$$I_3 = \frac{\sqrt{2}a_F^2}{2} e^{-2\sqrt{2}|t|} + \mathbb{O}(e^{-(3\sqrt{2}-\iota_0)|t|}).$$

Consequently,

$$I_0 := \int_{\mathbb{R}} \left[\tfrac{1}{2}u_y^2(0,y) + F(u(0,y))\right] dy = 2\boldsymbol{e}_F - 2\sqrt{2}a_F^2 e^{-2\sqrt{2}|f_{\varepsilon,1}(0) + h_\varepsilon(0)|} + \mathbb{O}(e^{-3|f_{\varepsilon,1}(0)|}).$$

According to the Hamiltonian identity (5-18),

$$I_0 = 2\boldsymbol{e}_F \cos\theta(u).$$

Now, let u_ε with $\varepsilon = \tan\theta(u)$ be a solution constructed in [del Pino et al. 2010] whose nodal line in the lower half-plane is given by the curve $y = q_{\varepsilon,1}(x) + r_{\varepsilon,1}(\varepsilon x)$, where $q_{\varepsilon,1}$ is the solution of the Toda system whose asymptotic angle at ∞ is ε, and $r_{\varepsilon,1}(x)$ satisfies, as we stated in Theorem 2.2, with some $\alpha > 0$,

$$\|r_{\varepsilon,1}\|_{\mathscr{C}_\tau^{2,\mu}(\mathbb{R})\oplus D} \le C\varepsilon^\alpha.$$

We recall that since we are working in the class of even functions, $|r_{\varepsilon,1}(x)| \le C\varepsilon^{\alpha}$, which implies that $r_{\varepsilon,1}$ is a bounded, small function. Now, the Hamiltonian identity (5-18) can be used for u_ε as well, and, by a similar computation as for I_0, we get

$$2\boldsymbol{e}_F \cos\theta(u_\varepsilon) = 2\boldsymbol{e}_F - 2\sqrt{2}a_F^2 e^{-2\sqrt{2}|q_{\varepsilon,1}(0)+r_{\varepsilon,1}(0)|} + \mathbb{O}(e^{-3|q_{\varepsilon,1}(0)+r_{\varepsilon,1}(0)|}),$$

where $r_{\varepsilon,1}(0) = \mathbb{O}(\varepsilon^{\alpha})$. Therefore,

$$I_0 = 2\boldsymbol{e}_F - 2\sqrt{2}a_F^2 e^{-2\sqrt{2}|q_{\varepsilon,1}(0)+r_{\varepsilon,1}(0)|} + \mathbb{O}(e^{-3|q_{\varepsilon,1}(0)+r_{\varepsilon,1}(0)|}).$$

That is,

$$e^{-2\sqrt{2}|f_{\varepsilon,1}(0)+h_\varepsilon(0)|} + \mathbb{O}(e^{-3|f_{\varepsilon,1}(0)|}) = e^{-2\sqrt{2}|q_{\varepsilon,1}(0)+r_{\varepsilon,1}(0)|} + \mathbb{O}(e^{-3|q_{\varepsilon,1}(0)+r_{\varepsilon,1}(0)|}).$$

This yields

$$f_{\varepsilon,1}(0) + h_\varepsilon(0) + \mathbb{O}(e^{-(3-2\sqrt{2})|f_{\varepsilon,1}(0)+h_\varepsilon(0)|}) = q_{\varepsilon,1}(0) + \mathbb{O}(\varepsilon^{\alpha}).$$

Since $q_{\varepsilon,1}(0) - (\sqrt{2}/2)\ln\varepsilon = \mathbb{O}(1)$, we get

$$f_{\varepsilon,1}(0) + h_\varepsilon(0) = \frac{\sqrt{2}}{2}\ln\varepsilon + \mathbb{O}(1),$$

which leads to

$$f_{\varepsilon,1}(0) + h_\varepsilon(0) - q_{\varepsilon,1}(0) = \mathbb{O}(\varepsilon^{\alpha}),$$

as claimed. □

Now we are in a position to prove Proposition 4.2. As we will see, the proof of Proposition 4.1 is obtained as an intermediate step.

Proof of Propositions 4.1 and 4.2. Our first goal is to show the estimate (4-6), and this will be done in a few steps. For brevity let us denote $p_{\varepsilon,1} = f_{\varepsilon,1} + h_\varepsilon$ and $\chi_{\varepsilon,1} = p_{\varepsilon,1} - q_{\varepsilon,1}$.

Step 1. We want to show that, in the interval $I := [\ln\varepsilon/\varepsilon, -\ln\varepsilon/\varepsilon]$,

$$|\chi_{\varepsilon,1}(x)| \le C\varepsilon^{\alpha}, \quad |\chi'_{\varepsilon,1}(x)| \le C\varepsilon^{1+\alpha}, \quad \text{and } \|\chi''_{\varepsilon,1}\|_{C^{0,\mu}(I)} \le C\varepsilon^{2+\alpha}.$$

Claim 1. If $I_a := [-a, a] \subset I$ is an interval where

$$|p_{\varepsilon,1}(x)| < 2|\ln\varepsilon|, \quad |p'_{\varepsilon,1}(x)| < 2\varepsilon, \quad x \in I_a, \tag{5-20}$$

then $p_{\varepsilon,1}$ satisfies a perturbed Toda equation in I_a, that is,

$$p''_{\varepsilon,1}(x) = -c_* e^{2\sqrt{2}p_{\varepsilon,1}(x)} + \lambda_1(x), \quad x \in I_a, \tag{5-21}$$

where λ_1 is a function satisfying

$$\|\lambda_1\|_{C^{0,\mu}(I_a)} \le C\varepsilon^{2+\beta_1} \tag{5-22}$$

for some constant $\beta_1 > 0$.

To begin the proof of the claim, let us consider a point $\boldsymbol{x} = (x_1, y_1)$ in the Fermi coordinates of $\Gamma_{\varepsilon,1}$ with $|y_1| \le |f_{\varepsilon,1}(0)|$, and denote it's Fermi coordinates relative to $\Gamma_{\varepsilon,2}$ by (x_2, y_2). Then, using (5-20) and elementary geometry, one can show that if $|x_1| \le a$, we have

$$y_1 - y_2 = -2 f_{\varepsilon,1}(x_1)(1 + \mathbb{O}(\varepsilon^2)). \tag{5-23}$$

Using this and (5-7) and calculating $\int_{\mathbb{R}} \boldsymbol{x}^*_{\varepsilon,1}[E(\bar{u}_\varepsilon)\rho_{\varepsilon,1} H'_{\varepsilon,1}]\,dy_1$ as in Lemma 5.7, we get

$$(1 + \mathbb{O}_{\mathscr{C}^{0,\mu}}(\varepsilon^\alpha)) f''_{\varepsilon,1}(x) + (1 + \mathbb{O}_{\mathscr{C}^{0,\mu}}(\varepsilon^\alpha)) h''_\varepsilon(x) = -c_* e^{2\sqrt{2} p_{\varepsilon,1}(x)}(1 + \mathbb{O}_{\mathscr{C}^{0,\mu}}(\varepsilon^\alpha)) + \mathbb{O}_{\mathscr{C}^{0,\mu}}(\varepsilon^{2+\alpha}). \tag{5-24}$$

This relation gives the claim. (For details, we refer the reader to [del Pino et al. 2010], where similar calculations can be found.) We note here that the term $e^{2\sqrt{2}p_{\varepsilon,1}(x)}$ essentially comes from the integral

$$\int_{\mathbb{R}} \boldsymbol{x}^*_1[(F''(1) - F''(H_{\varepsilon,1}))(H_{\varepsilon,2} + 1)\rho_{\varepsilon,1} H'_{\varepsilon,1}]\,dy_1,$$

and to calculate this integral we have used (5-23).

Next we will use Claim 1 to show

$$|\chi_{\varepsilon,1}| \le C\varepsilon^\alpha \quad \text{in } I_a. \tag{5-25}$$

In fact, from (5-21) we deduce that in I_a, as long as $\chi_{\varepsilon,1}$ is small,

$$\chi''_{\varepsilon,1} = -2\sqrt{2} c_* e^{2\sqrt{2} q_{\varepsilon,1}} \chi + \underbrace{\mathbb{O}(\chi^2_{\varepsilon,1}) e^{-2\sqrt{2} q_{\varepsilon,1}} + \lambda_1(x)}_{\lambda_2(x)}. \tag{5-26}$$

Let ς_i, $i = 1, 2$, be two linearly independent solutions of the linearized Toda equation

$$\varsigma''_i(x) = -2\sqrt{2} c_* e^{2\sqrt{2} q_{\varepsilon,1}(x)} \varsigma_i(x).$$

We can assume that ς_1 is even, ς_2 is odd, $\varsigma_1(0) = 1$, $\varsigma'_2(0) = \varepsilon$, and $|\varsigma'_i| \le C\varepsilon$, $i = 1, 2$. Since $\chi_{\varepsilon,1}$ is an even function, the variation of parameters formula tells us

$$\chi_{\varepsilon,1}(x) = \frac{\varsigma_2(x)}{\varepsilon} \int_0^x \varsigma_1(s)\lambda_2(s)\,ds - \frac{\varsigma_1(x)}{\varepsilon} \int_0^x \varsigma_2(s)\lambda_2(s)\,ds + (p_{\varepsilon,1}(0) - q_{\varepsilon,1}(0))\varsigma_1(x),$$

and

$$\chi'_{\varepsilon,1}(x) = \frac{\varsigma'_2(x)}{\varepsilon} \int_0^x \varsigma_1(s)\lambda_2(s)\,ds - \frac{\varsigma'_1(x)}{\varepsilon} \int_0^x \varsigma_2(s)\lambda_2(s)\,ds + (p_{\varepsilon,1}(0) - q_{\varepsilon,1}(0))\varsigma'_1(x).$$

Let β_2 be a fixed constant satisfying $0 < \beta_2 < \min(\beta_1, \alpha_1)$, where α_1 is the constant appearing in the assertion of Lemma 5.9. If $I_{a_1} := [-a_1, a_1] \subset I_a$ is an interval where $|\chi_{\varepsilon,1}| \le \varepsilon^{\beta_2}$, then, by (5-26),

$$\|\lambda_2\|_{\mathscr{C}^0(I_{a_1})} \le C\varepsilon^{2+\beta_1} + C\varepsilon^{2+2\beta_2}.$$

Recall that $|p_{\varepsilon,1}(0) - q_{\varepsilon,1}(0)| \le C\varepsilon^{\alpha_1}$. Therefore

$$\|\chi_{\varepsilon,1}\|_{\mathscr{C}^0(I_a)} \le C\varepsilon(\varepsilon^{\beta_1} + \varepsilon^{2\beta_2})\left(|\varsigma_2(x)| \int_0^x |\varsigma_1(s)|\,ds + |\varsigma_1(x)| \int_0^x |\varsigma_2(s)|\,ds\right) + C\varepsilon^{\alpha_1}|\varsigma_1(x)|.$$

Since $|\varsigma_1(s)| \le C\varepsilon|s|$ and $|\varsigma_2(s)| \le C$, we find that, for $x \in [\ln\varepsilon/\varepsilon, -\ln\varepsilon/\varepsilon]$,

$$|\varsigma_2(x)| \int_0^x |\varsigma_1(s)|\, ds + |\varsigma_1(x)| \int_0^x |\varsigma_2(s)|\, ds \le C|\ln\varepsilon|^2/\varepsilon.$$

Therefore, in I_{a_1}, if ε is small enough,

$$\|\chi_{\varepsilon,1}\|_{\mathscr{C}^0(I_{a_1})} \le C(\varepsilon^{\beta_1} + \varepsilon^{2\beta_2})|\ln\varepsilon|^2 + C\varepsilon^{\alpha_1}|\ln\varepsilon| \le \frac{\varepsilon^{\beta_2}}{2}.$$

From this we deduce $\|\chi_{\varepsilon,1}\|_{\mathscr{C}^0(I_a)} \le \varepsilon^{\beta_2}$, which proves (5-25).

Since $|\varsigma_i'(x)| \le C\varepsilon$, it then follows that, for $x \in I_a$,

$$\begin{aligned} |\chi_{\varepsilon,1}'(x)| &= C\varepsilon(\varepsilon^{\beta_1} + \varepsilon^{2\beta_2})\left(|\varsigma_2'(x)| \int_0^x |\varsigma_1(s)|\, ds + |\varsigma_1'(x)| \int_0^x |\varsigma_2(s)|\, ds\right) + C\varepsilon^{\alpha_1}|\varsigma_1'(x)| \\ &\le C\varepsilon(\varepsilon^{\beta_1} + \varepsilon^{2\beta_2})|\ln\varepsilon|^2 + C\varepsilon^{1+\alpha_1} \le C\varepsilon^{1+\beta_2}. \end{aligned} \tag{5-27}$$

Now recall that in I, $|q_{\varepsilon,1}(x)| < \frac{9}{5}|\ln\varepsilon|$ and $|q_{\varepsilon,1}'(x)| < \frac{3}{2}\varepsilon$. It then follows from Claim 1, (5-25), and (5-27) that, for ε small enough, the interval I satisfies the assumption of Claim 1. Therefore

$$|\chi_{\varepsilon,1}(x)| \le C\varepsilon^{\alpha} \quad \text{and} \quad |\chi_{\varepsilon,1}'(x)| \le C\varepsilon^{1+\alpha} \quad \text{for } x \in I.$$

Moreover, using (5-26), we get $\|\chi_{\varepsilon,1}''\|_{\mathscr{C}^{0,\mu}(I)} \le C\varepsilon^{2+\alpha}$.

Step 2. Next we will prove that $\|\chi_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R})} \to 0$ as $\varepsilon \to 0$. By Step 1, it suffices to show that

$$\|\chi_{\varepsilon,1}\|_{\mathscr{C}^0(\mathbb{R}\setminus I)} \to 0 \quad \text{as } \varepsilon \to 0.$$

Let the asymptotic line of u in the fourth quadrant be $y = -\varepsilon x - \mathscr{A}_\varepsilon$. Define

$$a_\varepsilon := \inf\{t \ge |\ln\varepsilon|/\varepsilon : |f_{\varepsilon,1}(x) + (\varepsilon x + \mathscr{A}_\varepsilon)| \le 1 \text{ for } x \in [t, +\infty)\}.$$

We wish to show that in fact $a_\varepsilon = |\ln\varepsilon|/\varepsilon$. For this purpose, we consider the domain

$$\Omega_L := \left\{(x, y) : y < 0,\ x > a_\varepsilon,\ y > \frac{x}{\varepsilon} - L\right\}.$$

Here $L > \varepsilon a_\varepsilon$ is large and indeed we will finally let it go to $+\infty$. We use the balancing formula in this domain and with the vector field $X := (f_{\varepsilon,1}(a_\varepsilon) - y, x - a_\varepsilon)$. This formula tells us that

$$\int_{\partial\Omega_L} \left\{\left(\tfrac{1}{2}|\nabla u|^2 + F(u)\right)X - X(u)\nabla u\right\} \cdot \nu\, dS = 0.$$

Let us estimate the relevant boundary integrals. First,

$$\int_{\partial\Omega_L \cap \{y=0\}} \left\{\left(\tfrac{1}{2}|\nabla u|^2 + F(u)\right)X - X(u)\nabla u\right\} \cdot \nu\, dS = \int_{a_\varepsilon}^{\varepsilon L} \left(\tfrac{1}{2}u_x^2 + F(u)\right)(x - a_\varepsilon)\, dx$$

whose limit as $L \to \infty$ is

$$\int_{a_\varepsilon}^{\infty} \left(\tfrac{1}{2}u_x^2 + F(u)\right)(x - a_\varepsilon).$$

To estimate this integral, let us recall that, by symmetry and (2-7), we have, for $\boldsymbol{x} = (x, y)$, $y \le 0$, with some $\kappa > 0$,

$$|(u(\boldsymbol{x}))^2 - 1| + |\nabla u(\boldsymbol{x})| \le C e^{-\kappa \operatorname{dist}(\Gamma_{\varepsilon,1}, \boldsymbol{x})}.$$

Now, using this and the fact that

$$|\varepsilon a_\varepsilon + \mathcal{A}_\varepsilon| \ge |f_{\varepsilon,1}(a_\varepsilon)| - 1 \ge \left(1 + \frac{\sqrt{2}}{2}\right) |\ln \varepsilon| - C,$$

after some calculation, we deduce that, as $\varepsilon \to 0$,

$$\int_{\partial\Omega_L \cap \{y=0\}} \left\{\left(\tfrac{1}{2}|\nabla u|^2 + F(u)\right) X - X(u)\nabla u\right\} \cdot \nu \, dS \to 0.$$

On the other hand, using the asymptotic behavior of u in the lower half plane, we get

$$u = \bar{H} + o(1) e^{-\kappa \operatorname{dist}(\Gamma_{\varepsilon,1}, \boldsymbol{x})}, \quad (\boldsymbol{x}^*_{\varepsilon,1} \bar{H})(x_1, y_1) = H(y_1),$$

where (x_1, y_1) are the Fermi coordinates of the point $\boldsymbol{x}$. Since on the line $\{x = a_\varepsilon\}$ we have $X = (f_{\varepsilon,1}(a_\varepsilon) - y, 0)$, we get

$$\int_{\partial\Omega_L \cap \{x=a_\varepsilon\}} \left\{\left(\tfrac{1}{2}|\nabla u|^2 + F(u)\right) X - X(u)\nabla u\right\} \cdot \nu \, dS = o(1).$$

Finally, we compute:

$$\left| \int_{\partial\Omega_L \cap \{y=x/\varepsilon - L\}} \left\{\left(\tfrac{1}{2}|\nabla u|^2 + F(u)\right) X - X(u)\nabla u\right\} \cdot \nu \, dS \right| = \frac{|f_{\varepsilon,1}(a_\varepsilon) + \varepsilon a_\varepsilon + \mathcal{A}_\varepsilon|}{\sqrt{1+\varepsilon^2}} + o(1).$$

Collecting all these estimates, we conclude

$$|f_{\varepsilon,1}(a_\varepsilon) + \varepsilon a_\varepsilon + \mathcal{A}_\varepsilon| = o(1).$$

Appealing to the definition of a_ε, this implies that $a_\varepsilon = |\ln \varepsilon|/\varepsilon$, and consequently,

$$|f_{\varepsilon,1}(x) + \varepsilon x + \mathcal{A}_\varepsilon| = o(1) \quad \text{for } x \in [|\ln \varepsilon|/\varepsilon, +\infty).$$

This implies that outside this interval, $\mathcal{N}_{\varepsilon,1}$ is close to a straight line, which combined with the estimates (4-6) yields the desired result. Indeed, now we have

$$\begin{aligned} q_{\varepsilon,1}(a_\varepsilon) &= f_{\varepsilon,1}(a_\varepsilon) + o(1) \\ &= -\varepsilon a_\varepsilon - \mathcal{A}_\varepsilon + o(1). \end{aligned}$$

On the other hand, since $q_{\varepsilon,1}$ is the solution of the Toda equation, we have

$$q_{\varepsilon,1}(x) = -\varepsilon x - \widetilde{\mathcal{A}}_\varepsilon + o(1) \quad \text{for } x \ge a_\varepsilon.$$

It follows that $\mathcal{A}_\varepsilon = \widetilde{\mathcal{A}}_\varepsilon + o(1)$. This ends the proof of Step 2.

Step 3. At this point we can use what we have just proven in Step 2 to get

$$f_{\varepsilon,1}(x) = \frac{\sqrt{2}}{2}\ln\varepsilon - \varepsilon|x| + \mathcal{O}(1), \quad |x| \gg 1.$$

As a consequence,

$$\|\exp(-\sqrt{2}\mathcal{D})\|_{\mathcal{C}^0_{\varepsilon\tau}(\mathbb{R})} \leq C\varepsilon^2, \tag{5-28}$$

which, together with Lemma 5.7, yields

$$\|\phi\|_{\mathcal{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R}^2)} + \|f''_{\varepsilon,1}\|_{\mathcal{C}^{0,\mu}_{\varepsilon\tau}(\mathbb{R})} + \|h_\varepsilon\|_{\mathcal{C}^{2,\mu}_{\varepsilon\tau}(\mathbb{R})} \leq C\varepsilon^2. \tag{5-29}$$

Then, by a similar calculation to that of (5-20), we find that, in the half line $\mathbb{R}\backslash I = (|\ln\varepsilon|/\varepsilon, +\infty)$, the function $p_{\varepsilon,1}$ satisfies

$$\|p''_{\varepsilon,1}\|_{\mathcal{C}^{0,\mu}_{\varepsilon\hat{\tau}}(\mathbb{R}\backslash I)} = \mathcal{O}(\varepsilon^{2+\alpha}) \tag{5-30}$$

for some $\hat{\tau} > 0$ independent of ε. This implies that, in $\mathbb{R}\backslash I$,

$$\begin{aligned}|p'_{\varepsilon,1}(x) + \varepsilon| &\leq C\int_x^{+\infty} \varepsilon^{2+\alpha} e^{-\varepsilon\hat{\tau}|s|}\,ds\\ &= C\varepsilon^{1+\alpha}e^{-\varepsilon\hat{\tau}|x|}.\end{aligned}$$

Therefore,

$$|p_{\varepsilon,1}(x) + \varepsilon x + \mathcal{A}_\varepsilon| \leq C\varepsilon^\alpha e^{-\varepsilon\hat{\tau}|x|}, \quad x \in \mathbb{R}\setminus I. \tag{5-31}$$

On the other hand, by Step 1 and the fact that

$$|q_{\varepsilon,1}(x) + \varepsilon x + \widetilde{\mathcal{A}}_\varepsilon| \leq C\varepsilon^\alpha e^{-\varepsilon\beta|x|}, \quad x \in \mathbb{R}\setminus I, \tag{5-32}$$

we get

$$|p_{\varepsilon,1}(|\ln\varepsilon|/\varepsilon) + |\ln\varepsilon| + \widetilde{\mathcal{A}}_\varepsilon| \leq C\varepsilon^\alpha.$$

This together with (5-31) then yields $|\mathcal{A}_\varepsilon - \widetilde{\mathcal{A}}_\varepsilon| < C\varepsilon^\alpha$. Now, letting $j_\varepsilon = \mathcal{A}_\varepsilon - \widetilde{\mathcal{A}}_\varepsilon$, taking into account Step 1, (5-31), (5-32), and reducing $\hat{\tau}$ if necessary, the assertion of Proposition 4.2 follows. The conclusion of the proof of Proposition 4.1 is contained in (5-29). □

6. Uniqueness of solutions with almost parallel nodal lines

Parametrization of the family of solutions of (1-1) by the trajectories of the Toda system. Let us consider the curve $\widetilde{\mathcal{N}}_{\varepsilon,i}$ which is the graph of the function $y = q_{\varepsilon,i}(x)$. When $i = 1$, it is contained in the lower half-plane, and when $i = 2$, it is contained in the upper half-plane. We have $q_{\varepsilon,1}(x) = -q_{\varepsilon,2}(x)$. With these curves we will associate the Fermi coordinates $(\tilde{x}_i, \tilde{y}_i)$:

$$\boldsymbol{x} = (\tilde{x}_i, q_{\varepsilon,i}(\tilde{x}_i)) + \tilde{y}_i\tilde{n}_{\varepsilon,i}(\tilde{x}_i), \quad \tilde{n}_{\varepsilon,i}(x) = \frac{(-q'_{\varepsilon,i}(x), 1)}{\sqrt{1+q'_{\varepsilon,i}(x)^2}}, \quad i = 1, 2.$$

The change of variables $(\tilde{x}_i, \tilde{y}_i) \mapsto \boldsymbol{x} = (x, y)$ is a diffeomorphism in a neighborhood $\widetilde{\mathcal{O}}_i$ of $\widetilde{\mathcal{N}}_{\varepsilon,i}$. We denote this diffeomorphism by $\tilde{\boldsymbol{x}}_{\varepsilon,i}$ so that

$$\tilde{\boldsymbol{x}}_{\varepsilon,i}(\tilde{x}_i, \tilde{y}_i) = \boldsymbol{x} \in \widetilde{\mathcal{O}}_i.$$

For any function $w \colon \widetilde{\mathcal{O}}_i \to \mathbb{R}$ by $\tilde{\boldsymbol{x}}^*_{\varepsilon,i} w$ we denote its pullback by $\tilde{\boldsymbol{x}}_{\varepsilon,i}$:

$$(\tilde{\boldsymbol{x}}^*_{\varepsilon,i} w)(\tilde{x}_i, \tilde{y}_i) = (w \circ \tilde{\boldsymbol{x}}_{\varepsilon,i})(\tilde{x}_i, \tilde{y}_i).$$

Using basic properties (linear growth, scaling) of the trajectories of the solutions of the Toda system, one can check [del Pino et al. 2010] that there exists a constant C_1 such that we can choose $\widetilde{\mathcal{O}}_i$, i=1,2, to be the set

$$\{(x, y) \in \mathbb{R}^2 : |y| \le C_1 \varepsilon^{-1} \sqrt{1 + x^2}\}.$$

With these preparations, we would like to write locally any solution u, with $\tan\theta(u) = \varepsilon$ small, in the Fermi coordinates with respect to $\widetilde{\mathcal{N}}_{\varepsilon,i}$. To this end, we will construct a suitable approximation of u in $\widetilde{\mathcal{O}}_i$ based on the fact that the true solution is locally close to the heteroclinic one. By symmetry we may focus on the case $i = 1$, namely, consider the lower half plane. The nodal line $\mathcal{N}_{\varepsilon,1}$ of u in the lower half plane is the graph of $y = f_{\varepsilon,1}(x)$. Recall that $q_{\varepsilon,1}(x)$ is the solution of the Toda equation such that the assertions of Proposition 4.2 are satisfied. We let $\tilde{\eta}$ to be a smooth cut off function equal to 1 in $\widetilde{\mathcal{O}}_1 \cap \{\operatorname{dist}(\boldsymbol{x}, \partial\widetilde{\mathcal{O}}_1) > 1\}$ and equal to 0 in $\mathbb{R}^2 \setminus \widetilde{\mathcal{O}}_1$. A reasonable ansatz for an approximate solution is built defining the function $\widetilde{H}_{\varepsilon,1}$ by

$$\tilde{\boldsymbol{x}}^*_{\varepsilon,1} \widetilde{H}_{\varepsilon,1}(\tilde{x}_1, \tilde{y}_1) := \tilde{\boldsymbol{x}}^*_{\varepsilon,1} \tilde{\eta}(\tilde{x}_1, \tilde{y}_1) H(\tilde{y}_1 - \tilde{g}_\varepsilon(\tilde{x}_1)) + (1 - \tilde{\boldsymbol{x}}^*_{\varepsilon,1} \tilde{\eta}(\tilde{x}_1, \tilde{y}_1)) \frac{H(\tilde{y}_1 - \tilde{g}_\varepsilon(\tilde{x}_1))}{|H(\tilde{y}_1 - \tilde{g}_\varepsilon(\tilde{x}_1))|},$$

which is extended to the whole $\mathbb{R}^2$ by ± 1, setting $\widetilde{H}_{\varepsilon,2}(x, y) = -\widetilde{H}_{\varepsilon,1}(x, -y)$, and finally defining

$$\tilde{u}_\varepsilon := \widetilde{H}_{\varepsilon,1} - \widetilde{H}_{\varepsilon,2} - 1. \tag{6-1}$$

Note that the function $\tilde{g}_\varepsilon$ has not been specified so far. It turns out that, in order to have a good approximation of u by $\tilde{u}_\varepsilon$, we should impose the orthogonality condition

$$\int_{\mathbb{R}} \tilde{\boldsymbol{x}}^*_{\varepsilon,i} [(u - \tilde{u}_\varepsilon) \tilde{\rho}_{\varepsilon,i} \widetilde{H}'_{\varepsilon,i}](\tilde{x}_i, \tilde{y}_i)\, d\tilde{y}_i = 0 \quad \text{for all } \tilde{x}_i,\ i = 1, 2, \tag{6-2}$$

where smooth cutoff functions $\tilde{\rho}_{\varepsilon,i}$ are defined through

$$(\tilde{\boldsymbol{x}}^*_{\varepsilon,i} \tilde{\rho}_{\varepsilon,i})(\tilde{x}_i, \tilde{y}_i) = \tilde{\rho}(\tilde{y}_i - (-1)^{i+1} \tilde{g}_\varepsilon(\tilde{x}_i)),$$

and $\tilde{\rho}$ is an even cutoff function equal to 1 in the interval $(\sqrt{2}\ln\varepsilon/8, -\sqrt{2}\ln\varepsilon/8)$ and equal to 0 outside $(\sqrt{2}\ln\varepsilon/4, -\sqrt{2}\ln\varepsilon/4)$, while $\widetilde{H}'_{\varepsilon,i}$ is defined by

$$\tilde{\boldsymbol{x}}^*_{\varepsilon,i} \widetilde{H}'_{\varepsilon,i}(\tilde{x}_i, \tilde{y}_i) = H'(\tilde{y}_i - (-1)^{i+1} \tilde{g}_\varepsilon(\tilde{x}_i)).$$

To show the existence of the function $\tilde{g}_\varepsilon$, one can use an argument similar to the one in Lemma 5.1. However, since the graph of the function $y = q_{\varepsilon,i}(x)$ does not converge to the nodal set of the solution at infinity, the function $\tilde{g}_\varepsilon$ does not decay exponentially. To determine the behavior of the function $\tilde{g}_\varepsilon$ more precisely, we need the following.

Lemma 6.1. *There exist constants $\tilde{\tau} > 0$ and v_ε such that $|v_\varepsilon| \leq C\varepsilon^\alpha$, and the function $\tilde{h}_\varepsilon(x) := \tilde{g}_\varepsilon(x) + v_\varepsilon$ satisfies*

$$\begin{aligned} \|\tilde{h}_\varepsilon\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} &\leq C\varepsilon^\alpha, \\ \|\tilde{h}'_\varepsilon\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} &\leq C\varepsilon^{1+\alpha}, \\ \|\tilde{h}''_\varepsilon\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R})} &\leq C\varepsilon^{2+\alpha}. \end{aligned} \tag{6-3}$$

Proof. The function $\tilde{g}_\varepsilon$ is determined by

$$\int_{\mathbb{R}} \tilde{\boldsymbol{x}}^*_{\varepsilon,1}[(u - \tilde{u}_\varepsilon)\tilde{\rho}_{\varepsilon,1}\widetilde{H}'_{\varepsilon,1}]\, d\tilde{y}_1 = 0.$$

Changing variables, this relation can also be written as

$$\int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1)H'(\tilde{y}_1)\tilde{\boldsymbol{x}}^*_{\varepsilon,1}(u - \tilde{u}_\varepsilon)(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1))\, d\tilde{y}_1 = 0. \tag{6-4}$$

For this integral, it suffices to consider the points in the support of $\tilde{\rho}_{\varepsilon,1}$.

Recall that, by the definition of $\tilde{u}_\varepsilon$,

$$\tilde{\boldsymbol{x}}^*_{\varepsilon,1}\tilde{u}_\varepsilon(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1)) = H(\tilde{y}_1) - \tilde{\boldsymbol{x}}^*_{\varepsilon,1}(\widetilde{H}_{\varepsilon,2} + 1)(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1)).$$

It is not difficult to see that

$$\left\| \int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1)H'(\tilde{y}_1)\tilde{\boldsymbol{x}}^*_{\varepsilon,1}(\widetilde{H}_{\varepsilon,2} + 1)(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1))\, d\tilde{y}_1 \right\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \leq C\varepsilon^2$$

for some $\tilde{\tau} > 0$. This combined with (6-4) leads to

$$\left\| \int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1)H'(\tilde{y}_1)\tilde{\boldsymbol{x}}^*_{\varepsilon,1}u(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1))\, d\tilde{y}_1 \right\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \leq C\varepsilon^2. \tag{6-5}$$

On the other hand, $u = \bar{u}_\varepsilon + \phi$ with $\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau_0}(\mathbb{R}^2)} \leq C\varepsilon^2$. Hence, reducing $\tilde{\tau}$ if necessary, we get

$$\begin{aligned} &\left\| \int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1)H'(\tilde{y}_1)\tilde{\boldsymbol{x}}^*_{\varepsilon,1}\bar{u}_\varepsilon(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1))\, d\tilde{y}_1 \right\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \\ &\qquad \leq \left\| \int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1)H'(\tilde{y}_1)\tilde{\boldsymbol{x}}^*_{\varepsilon,1}\phi(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1))\, d\tilde{y}_1 \right\|_{\mathscr{C}^0_{\varepsilon\tau_0}(\mathbb{R})} + C\varepsilon^2 \leq C\varepsilon^2. \end{aligned} \tag{6-6}$$

Now, in the support of $\tilde{\rho}_{\varepsilon,1}$, $\bar{u}_\varepsilon = H(y_1 - h_\varepsilon(x_1)) - H(y_2 + h_\varepsilon(x_2)) - 1$. Denoting the function $(x, y) = \boldsymbol{x}_{\varepsilon,1}(x_1, y_1) \mapsto H(y_1 - h_\varepsilon(x_1))$ by $\mathfrak{R}$, it follows from (6-6) that (reducing $\tilde{\tau}$ if necessary)

$$\left\| \int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1)H'(\tilde{y}_1)\tilde{\boldsymbol{x}}^*_{\varepsilon,1}\mathfrak{R}(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1))\, d\tilde{y}_1 \right\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \leq C\varepsilon^2. \tag{6-7}$$

To proceed, let us investigate the relation between the Fermi coordinates (x_1, y_1) and $(\tilde{x}_1, \tilde{y}_1)$. Using $|f'_{\varepsilon,1}| \le C\varepsilon$, $|f_{\varepsilon,1} - q_{\varepsilon,1}| \le C\varepsilon^\alpha$, $|y_1| \le C|\ln\varepsilon|$, and elementary geometry, one can verify that

$$|\tilde{x}_1 - x_1| \le C||y_1| + C\varepsilon^\alpha|\varepsilon \le C\varepsilon^\alpha. \tag{6-8}$$

Additionally, recall that by Proposition 4.2, $\| f_{\varepsilon,1} - q_{\varepsilon,1} + j_\varepsilon\|_{C^0_{\varepsilon\hat{\tau}}(\mathbb{R})} \le C\varepsilon^\alpha$. Using (6-8) , one can show

$$y_1 = \tilde{y}_1 + \left(\sqrt{1 + (q'_{\varepsilon,1}(\tilde{x}_1))^2}\,\right)^{-1} j_\varepsilon + \mathbb{O}(\varepsilon^\alpha e^{-\varepsilon\beta|\tilde{x}_1|}). \tag{6-9}$$

Inserting this into (6-7), we find (again reducing $\tilde{\tau}$ if necessary)

$$\left\| \int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1) H'(\tilde{y}_1) H(\tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1) + \left(\sqrt{1 + (q'_{\varepsilon,1}(\tilde{x}_1))^2}\,\right)^{-1} j_\varepsilon)\, d\tilde{y}_1 \right\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \le C\varepsilon^\alpha. \tag{6-10}$$

As a consequence,

$$\|\tilde{g}_\varepsilon + \left(\sqrt{1 + (q'_{\varepsilon,1})^2}\,\right)^{-1} j_\varepsilon\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \le C\varepsilon^\alpha, \tag{6-11}$$

which together with the behavior of $q'_{\varepsilon,1}$ implies that

$$\|\tilde{h}_\varepsilon\|_{\mathscr{C}^0_{\varepsilon\tilde{\tau}}(\mathbb{R})} \le C\varepsilon^\alpha, \quad |v_\varepsilon| \le C\varepsilon^\alpha, \tag{6-12}$$

where $v_\varepsilon := j_\varepsilon/\sqrt{1+\varepsilon^2}$ and

$$\tilde{h}_\varepsilon(x) := \tilde{g}_\varepsilon(x) + v_\varepsilon. \tag{6-13}$$

Next we need to estimate the weighted norm of the first derivative of $\tilde{h}_\varepsilon$.

Let us denote the diffeomorphism $\boldsymbol{x}^{-1}_{\varepsilon,1} \circ \tilde{\boldsymbol{x}}_{\varepsilon,1}$ by $\Phi_{\varepsilon,1}$ and denote $\boldsymbol{x}^{-1}_{\varepsilon,2} \circ \tilde{\boldsymbol{x}}_{\varepsilon,1}$ by $\Phi_{\varepsilon,2}$. Then, using (6-8), (6-9), and formulas (3-10), after direct calculations, we find that

$$|D\Phi_{\varepsilon,1} - \mathrm{Id}_{2\times 2}| = \mathbb{O}(\varepsilon^{1+\alpha} e^{-\varepsilon\beta|\tilde{x}_1|}), \quad |D^2\Phi_{\varepsilon,1}| = \mathbb{O}(\varepsilon^{2+\alpha} e^{-\varepsilon\beta|\tilde{x}_1|}), \tag{6-14}$$

$$|D\Phi_{\varepsilon,2} - \mathrm{Id}_{2\times 2}| = \mathbb{O}(\varepsilon e^{-\varepsilon\beta|\tilde{x}_2|}), \qquad |D^2\Phi_{\varepsilon,2}| = \mathbb{O}(\varepsilon^2 e^{-\varepsilon\beta|\tilde{x}_2|}). \tag{6-15}$$

We now differentiate (6-4) with respect to $\tilde{x}_1$. Set

$$\mathfrak{R}_1 := \partial_{\tilde{x}_1} \tilde{\boldsymbol{x}}^*_{\varepsilon,1} u(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1)),$$
$$\mathfrak{R}_2 := \partial_{\tilde{y}_1} \tilde{\boldsymbol{x}}^*_{\varepsilon,1} u(\tilde{x}_1, \tilde{y}_1 + \tilde{g}_\varepsilon(\tilde{x}_1)).$$

By estimate (6-15), one has

$$\int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1) H'(\tilde{y}_1) \{\mathfrak{R}_1 + \mathfrak{R}_2 \tilde{g}'_\varepsilon(\tilde{x}_1)\}\, d\tilde{y}_1 = O(\varepsilon^2 e^{-\varepsilon\beta|\tilde{x}_1|}).$$

Therefore, using (6-13),

$$\tilde{h}'_\varepsilon(\tilde{x}_1) = -\frac{\int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1) H'(\tilde{y}_1) \mathfrak{R}_1\, d\tilde{y}_1}{\int_{\mathbb{R}} \tilde{\rho}(\tilde{y}_1) H'(\tilde{y}_1) \mathfrak{R}_2\, d\tilde{y}_1} + \mathbb{O}(\varepsilon^2 e^{-\varepsilon\beta|\tilde{x}_1|}). \tag{6-16}$$

Keep in mind that

$$\int_{\mathbb{R}} \tilde\rho(\tilde y_1)H'(\tilde y_1)\mathfrak{R}_1\,d\tilde y_1 = \int_{\mathbb{R}} \tilde\rho(\tilde y_1)H'(\tilde y_1)\partial_{\tilde x_1}\tilde{\boldsymbol{x}}^*_{\varepsilon,1}\bar u_\varepsilon(\tilde x_1,\tilde y_1+\tilde g_\varepsilon(\tilde x_1))\,d\tilde y_1+\int_{\mathbb{R}} \tilde\rho(\tilde y_1)H'(\tilde y_1)\partial_{\tilde x_1}\tilde{\boldsymbol{x}}^*_{\varepsilon,1}\phi(\tilde x_1,\tilde y_1+\tilde g_\varepsilon(\tilde x_1))\,d\tilde y_1. \tag{6-17}$$

Equations (6-14), (6-15) and (6-17), together with $\|\phi\|_{\mathscr{C}^2_{\varepsilon\tau_0}(\mathbb{R}^2)} \le C\varepsilon^2$, yield

$$\int_{\mathbb{R}} \tilde\rho(\tilde y_1)H'(\tilde y_1)\mathfrak{R}_1\,d\tilde y_1 = \mathbb{O}(\varepsilon^{1+\alpha}e^{-\varepsilon\beta|\tilde x_1|}).$$

It then follows from (6-16) that (reducing $\tilde\tau$ if necessary)

$$\|\tilde h'_\varepsilon\|_{\mathscr{C}^0_{\varepsilon\tilde\tau}(\mathbb{R})} \le C\varepsilon^{1+\alpha}.$$

It remains to estimate $\tilde h''_\varepsilon$. Setting

$$\mathfrak{R}_3 = \partial^2_{\tilde x_1}\tilde{\boldsymbol{x}}^*_{\varepsilon,1}(u-\tilde u_\varepsilon)(\tilde x_1,\tilde y_1+\tilde g_\varepsilon(\tilde x_1)), \qquad \mathfrak{R}_5 = \partial^2_{\tilde y_1}\tilde{\boldsymbol{x}}^*_{\varepsilon,1}(u-\tilde u_\varepsilon)(\tilde x_1,\tilde y_1+\tilde g_\varepsilon(\tilde x_1)),$$
$$\mathfrak{R}_4 = \partial^2_{\tilde x_1\tilde y_1}\tilde{\boldsymbol{x}}^*_{\varepsilon,1}(u-\tilde u_\varepsilon)(\tilde x_1,\tilde y_1+\tilde g_\varepsilon(\tilde x_1)), \qquad \mathfrak{R}_6 = \partial_{\tilde y_1}\tilde{\boldsymbol{x}}^*_{\varepsilon,1}(u-\tilde u_\varepsilon)(\tilde x_1,\tilde y_1+\tilde g_\varepsilon(\tilde x_1)),$$

from (6-4), one gets

$$\tilde h''_\varepsilon(\tilde x_1) = -\frac{\int_{\mathbb{R}} \tilde\rho(\tilde y_1)H'(\tilde y_1)[\mathfrak{R}_3+2\mathfrak{R}_4\tilde g'_\varepsilon(\tilde x_1)+\mathfrak{R}_5(\tilde g'_\varepsilon(\tilde x_1))^2]\,d\tilde y_1}{\int_{\mathbb{R}} \tilde\rho(\tilde y_1)H'(\tilde y_1)\mathfrak{R}_6\,d\tilde y_1}. \tag{6-18}$$

Recall that

$$\|\phi\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau_0}(\mathbb{R})} + \|h_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tau_0}(\mathbb{R})} \le C\varepsilon^2.$$

A refined argument which involves closer analysis of the main order of ϕ shows that in reality $\partial_x^2\phi$ and h''_ε have better estimates:

$$\|\partial_x^2\phi\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau_0}(\mathbb{R})} + \|h''_\varepsilon\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tau_0}(\mathbb{R})} \le C\varepsilon^{2+\alpha}.$$

This estimate follows by observing first that the orthogonality relation for ϕ can be differentiated in x twice. Then we note that, furthermore, differentiating the equation satisfied by ϕ twice, we gain powers of ε in the main order term, namely, the right side will be of order at least $\mathbb{O}(\varepsilon^{2+\alpha})$. Then $\partial_x^2\phi$ and h''_ε can be estimated using the same orthogonal decomposition as in Section 5. Combining this with (6-14), (6-15), and (6-18), after some calculations, we get, reducing $\tilde\tau$ if necessary,

$$\|\tilde h''_\varepsilon\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})} \le C\varepsilon^{2+\alpha}. \qquad \square$$

Given a solution u of (1-1) such that $\tan\theta(u)=\varepsilon$, we can define an approximate solution $\tilde u_\varepsilon$ by (6-1) using the solution of the Toda system with the asymptotic slope ε. Then we can write

$$u = \tilde u_\varepsilon + \tilde\phi.$$

By the definition of $\tilde g_\varepsilon$, we know that $\tilde\phi = u-\tilde u_\varepsilon$ satisfies the orthogonality condition (6-2). This allows us to control the size of $\tilde\phi$ in the weighted norm in terms of the error of the approximation

$$E(\tilde u_\varepsilon) = \Delta\tilde u_\varepsilon - F'(\tilde u_\varepsilon),$$

following essentially the same approach as in Section 5, and, in particular, relying on a version of Proposition 5.5. In fact, one can prove that

$$\|\tilde{\phi}\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \le C\varepsilon^2. \tag{6-19}$$

Conclusion of the proof: the Lipschitz property of solutions. Based on the results of the previous section, we know that any solution with a small angle can be written in the following way:

$$u(\,\cdot\,;\tilde{g}_\varepsilon,\tilde{\phi}) = \tilde{u}_\varepsilon(\,\cdot\,;\tilde{g}_\varepsilon)+\tilde{\phi},$$

where $\tilde{u}_\varepsilon$ is the approximate solution defined in (6-1). Here and below we will indicate the dependence of this solution on the modulation function $\tilde{g}_\varepsilon$ as well as on $\tilde{\phi}$. Now let us consider two solutions $u^{(j)}$, $j=1,2$, with the same asymptotic angle $\theta(u^{(j)}) = \arctan\varepsilon$. Since the asymptotic angle is the same for both solutions, there is just one solution of the Toda system represented by the functions $q_{\varepsilon,1}=-q_{\varepsilon,2}$. On the other hand, it may happen that $\tilde{g}^{(1)}_\varepsilon \ne \tilde{g}^{(2)}_\varepsilon$ and $\tilde{\phi}^{(1)} \ne \tilde{\phi}^{(2)}$. In the notation of [del Pino et al. 2010], we have that $\tilde{g}^{(j)}_\varepsilon \in \mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R})\oplus D$ (see also the summary on pages 1684–1685). In the previous section we have shown that $\|\tilde{g}^{(j)}_\varepsilon\|_{\mathscr{C}^{0}_{\varepsilon\tilde{\tau}}(\mathbb{R})\oplus D} \le C\varepsilon^\alpha$, with corresponding estimates for the higher-order derivatives. In addition, for the functions $\tilde{\phi}^{(j)}$, we have (6-19). Without loss of generality, we can assume that $\tilde{\tau}$ is small but independent of ε.

To prove the uniqueness of solutions with small angles, it is enough to prove "local uniqueness" in the following sense. Given two four-end solutions associated to the same solution of the Toda system, we have $\tilde{\phi}^{(1)}=\tilde{\phi}^{(2)}$ and $\tilde{g}^{(1)}_\varepsilon=\tilde{g}^{(2)}_\varepsilon$. Our strategy to prove this fact follows in some sense the strategy used to prove the existence of solutions with small angles employed in [del Pino et al. 2010]. To explain this, let us introduce the scaled functions $\hat{g}^{(j)}_\varepsilon(x) := \tilde{g}^{(j)}_\varepsilon(x/\varepsilon)$, $j=1,2$. We show the Lipschitz property of the map $\hat{g}_\varepsilon \mapsto E(\tilde{u}_\varepsilon(\,\cdot\,;\tilde{g}_\varepsilon))$, and then we use the linearized equation to show that $\tilde{\phi}^{(1)}-\tilde{\phi}^{(2)}$ can be controlled by a small constant times $\hat{g}^{(1)}_\varepsilon-\hat{g}^{(2)}_\varepsilon$. As a final step we show that the function $\hat{g}^{(1)}_\varepsilon-\hat{g}^{(2)}_\varepsilon$ satisfies the linearized Toda system with the right side again controlled by a small constant times $\hat{g}^{(1)}_\varepsilon-\hat{g}^{(2)}_\varepsilon$. This leads us to conclude that $\hat{g}^{(1)}_\varepsilon-\hat{g}^{(2)}_\varepsilon=0$, and as a result we infer the uniqueness.

Now we will present some details of the argument outlined above. Many of the calculations are quite similar to the ones in [del Pino et al. 2010].

Lemma 6.2. *The following estimates hold*:

$$\|E(\tilde{u}^{(1)}(\,\cdot\,;\tilde{g}^{(1)}_\varepsilon)) - E(\tilde{u}^{(2)}(\,\cdot\,;\tilde{g}^{(2)}_\varepsilon))\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \le C\varepsilon^2\|\hat{g}^{(1)}_\varepsilon-\hat{g}^{(2)}_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\tilde{\tau}}(\mathbb{R})\oplus D}, \tag{6-20}$$

$$\|\tilde{\phi}^{(1)}-\tilde{\phi}^{(2)}\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \le C\varepsilon^2\|\hat{g}^{(1)}_\varepsilon-\hat{g}^{(2)}_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\tilde{\tau}}(\mathbb{R})\oplus D}. \tag{6-21}$$

Remark 6.3. Essentially, up to some minor difference, this Lipschitz property has already been proven in [del Pino et al. 2010]. Here we give a sketch of the proof for completeness.

Proof. To begin with, let us mention that, for a function $g:\mathbb{R}\to\mathbb{R}$, we have the obvious estimates:

$$\|g(\varepsilon\cdot)\|_{C^{l,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R})} \le C\|g(\,\cdot\,)\|_{C^{l,\mu}_{\tilde{\tau}}(\mathbb{R})},$$
$$\|g(\,\cdot\,)\|_{C^{l,\mu}_{\tilde{\tau}}(\mathbb{R})} \le C\varepsilon^{-l-\mu}\|g(\varepsilon\cdot)\|_{C^{l,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R})}.$$

To prove (6-20) we use essentially the formula (5-7) for the error, replacing $\bar{u}_\varepsilon$ by $\tilde{u}_\varepsilon^{(j)}$, $j = 1, 2$, and then take the difference of the resulting terms $E(\tilde{u}^{(j)}(\,\cdot\,; \tilde{g}_\varepsilon^{(j)}))$.

To show (6-21), we should consider the equation satisfied by the difference $\tilde{\psi} = \tilde{\phi}^{(1)} - \tilde{\phi}^{(2)}$ and use Proposition 5.5. The slight technical problem is that $\tilde{\psi}$ does not satisfy the orthogonality condition as in (6-2). To overcome this, we further define a function $\tilde{\psi}^\perp$ by

$$\tilde{\psi}^\perp := \tilde{\psi} - \sum_{i=1,2} \tilde{\psi}_i^\parallel,$$

where $\tilde{\psi}_i^\parallel : \mathbb{R}^2 \to \mathbb{R}$ is equal to 0 outside $\widetilde{\mathcal{O}}_i$ and

$$\tilde{\boldsymbol{x}}_{\varepsilon,i}^* \tilde{\psi}_i^\parallel(\tilde{x}_i, \tilde{y}_i) := \tilde{c}_\varepsilon \tilde{\boldsymbol{x}}_{\varepsilon,i}^* (\tilde{\rho}_{\varepsilon,i}^{(1)} \widetilde{H}_{\varepsilon,i}^{(1)\prime}) \int_{\mathbb{R}} \tilde{\boldsymbol{x}}_{\varepsilon,i}^* [\tilde{\psi} \tilde{\rho}_{\varepsilon,i}^{(1)} \widetilde{H}_{\varepsilon,i}^{(1)\prime}]\, d\tilde{y}_i \quad \text{in } \widetilde{\mathcal{O}}_i,$$

where $\tilde{c}_\varepsilon = \{\int_{\mathbb{R}} [\tilde{\rho}(y) H'(y)]^2\, dy\}^{-1}$.

Using the fact that $\|\tilde{\phi}^{(2)}\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \le C\varepsilon^2$ and

$$\int_{\mathbb{R}} \tilde{\boldsymbol{x}}_{\varepsilon,i}^* [\tilde{\phi}^{(2)} \tilde{\rho}_{\varepsilon,i}^{(2)} \widetilde{H}_{\varepsilon,i}^{(2)\prime}]\, d\tilde{y}_i = 0, \quad i = 1, 2,$$

it is not hard to show that

$$\|\tilde{\psi}_i^\parallel\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \le C\varepsilon^2 \|\hat{g}_\varepsilon^{(1)} - \hat{g}_\varepsilon^{(2)}\|_{\mathscr{C}^{2,\mu}_{\tilde{\tau}}(\mathbb{R}) \oplus D}.$$

Hence

$$\|\tilde{\psi}^\perp\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \ge \|\tilde{\psi}\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} - C\varepsilon^2 \|\hat{g}_\varepsilon^{(1)} - \hat{g}_\varepsilon^{(2)}\|_{\mathscr{C}^{2,\mu}_{\tilde{\tau}}(\mathbb{R}) \oplus D}. \tag{6-22}$$

On the other hand, setting

$$L^{(i)} = -\Delta + F''(\tilde{u}_\varepsilon^{(i)}), \quad P^{(i)}(\tilde{\phi}^{(i)}) = F'(\tilde{u}_\varepsilon^{(i)} + \tilde{\phi}^{(i)}) - F'(\tilde{u}_\varepsilon^{(i)}) - F''(\tilde{u}_\varepsilon^{(i)})\tilde{\phi}^{(i)}, \quad i = 1, 2,$$

we get

$$L^{(1)}\tilde{\psi}^\perp = \underbrace{E(\tilde{u}_\varepsilon^{(1)}) - E(\tilde{u}_\varepsilon^{(2)}) - P^{(1)}(\tilde{\phi}^{(1)}) + P^{(2)}(\tilde{\phi}^{(2)}) - (L^{(1)} - L^{(2)})\tilde{\phi}^{(2)} - L^{(1)}(\tilde{\psi}_1^\parallel + \tilde{\psi}_2^\parallel)}_{\tilde{f}}. \tag{6-23}$$

Applying Lemma 6.2, one can see that

$$\|\tilde{f}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} \le o(1)\|\tilde{\psi}\|_{\mathscr{C}^{2,\mu}_{\varepsilon\tilde{\tau}}(\mathbb{R}^2)} + C\varepsilon^2 \|\hat{g}_\varepsilon^{(1)} - \hat{g}_\varepsilon^{(2)}\|_{\mathscr{C}^{2,\mu}_{\tilde{\tau}}(\mathbb{R}) \oplus D}.$$

From this and (6-22), the required estimate follows. □

As we have already seen, the Toda system appears in the projected equation. It turns out that we also need to analyze the linearized Toda system. Recall that we are always working in the space of even functions. Suppose q is an even solution of the Toda system

$$q''(t) = -c_* e^{2\sqrt{2}q(t)},$$

and the linearized operator is

$$\mathscr{P} : \varphi \to \varphi'' + 2\sqrt{2} c_* e^{2\sqrt{2}q} \varphi.$$

We want to know the mapping property of this operator. Let $\mathscr{C}^{l,\mu}_{\tilde\tau}(\mathbb{R})_e$ be the space of even functions in $\mathscr{C}^{l,\mu}_{\tilde\tau}(\mathbb{R})$, and let D_0 be the one-dimensional deficiency space spanned by the constant function.

Lemma 6.4. *For small $\tilde\tau > 0$, the map $\mathscr{P} : C^{2,\mu}_{\tilde\tau}(\mathbb{R})_e \oplus D_0 \to C^{0,\mu}_{\tilde\tau}(\mathbb{R})_e$ is an isomorphism and therefore has a bounded inverse.*

This result has already been proven in [del Pino et al. 2010] and we omit the proof. With all these properties understood, we are ready to prove the uniqueness of solutions with given small angles.

Proof of Theorem 1.2. Let us consider the quantity (cf. the proof of Lemma 5.7)

$$\mathscr{T} = \int_{\mathbb{R}} \tilde{\boldsymbol{x}}^*_{\varepsilon,1}[E(\tilde u^{(1)}_\varepsilon)\tilde\rho^{(1)}_{\varepsilon,1}\tilde H^{(1)\prime}_{\varepsilon,1}]\,d\tilde y_1 - \int_{\mathbb{R}} \tilde{\boldsymbol{x}}^*_{\varepsilon,1}[E(\tilde u^{(2)}_\varepsilon)\tilde\rho^{(2)}_{\varepsilon,1}\tilde H^{(2)\prime}_{\varepsilon,1}]\,d\tilde y_1.$$

Recall that

$$E(\tilde u^{(i)}_\varepsilon) = -\Delta\tilde\phi^{(i)} + F''(\tilde u^{(i)}_\varepsilon)\tilde\phi^{(i)} + P^{(i)}(\tilde\phi^{(i)}).$$

Inserting this into the expression of $\mathscr{T}$, calculating as in Step 1 in the proof of Lemma 5.7, using the estimates in Lemma 6.2, we get

$$\|\mathscr{T}\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})} \le C\varepsilon^{2+\alpha}\|\hat g^{(1)}_\varepsilon - \hat g^{(2)}_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\tilde\tau}(\mathbb{R})\oplus D_0}. \tag{6-24}$$

For brevity set

$$\tilde{\boldsymbol{g}}_\varepsilon := \tilde g^{(1)}_\varepsilon - \tilde g^{(2)}_\varepsilon \quad\text{and}\quad \hat{\boldsymbol{g}}_\varepsilon := \hat g^{(1)}_\varepsilon - \hat g^{(2)}_\varepsilon.$$

Now we calculate $\mathscr{T}$ using the explicit expressions for $\tilde u^{(i)}_\varepsilon$ in a manner similar to Step 2 of Lemma 5.7, and, as a result, we get a formula similar to (5-24), which reads

$$\mathscr{T} = (1+\mathbb{O}_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})}(\varepsilon^\alpha))\tilde{\boldsymbol{g}}''_\varepsilon + 2\sqrt{2}c_*(1+\mathbb{O}_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})}(\varepsilon^\alpha))e^{2\sqrt{2}q_{\varepsilon,1}}\tilde{\boldsymbol{g}}_\varepsilon + \mathbb{O}_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})}(\varepsilon^{1+\alpha})\tilde{\boldsymbol{g}}'_\varepsilon + \mathbb{O}_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})}(\varepsilon^{2+\alpha})\tilde{\boldsymbol{g}}_\varepsilon.$$

Thus, calculating $\mathscr{T}$ in two ways, we get at the end that

$$\tilde{\boldsymbol{g}}''_\varepsilon + 2\sqrt{2}c_*e^{2\sqrt{2}q_{\varepsilon,1}}\tilde{\boldsymbol{g}}_\varepsilon = \mathbb{G}_\varepsilon, \tag{6-25}$$

where the term $\mathbb{G}_\varepsilon$ on the right satisfies

$$\|\mathbb{G}_\varepsilon\|_{\mathscr{C}^{0,\mu}_{\varepsilon\tilde\tau}(\mathbb{R})} \le C\varepsilon^{2+\alpha}\|\hat{\boldsymbol{g}}_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\tilde\tau}(\mathbb{R})\oplus D_0}. \tag{6-26}$$

(6-25) could be written as

$$\hat{\boldsymbol{g}}''_\varepsilon + 2\sqrt{2}c_*e^{2\sqrt{2}q_1}\hat{\boldsymbol{g}}_\varepsilon = \varepsilon^{-2}\mathbb{G}_\varepsilon(\varepsilon^{-1}\cdot),$$

where $q = (q_1, q_2)$ is the even solution of the Toda system whose asymptotic lines have slopes ∓ 1 (cf. the function U_0 in (4-5)). Now we adapt Lemma 6.4 to the present context and use (6-26) to get

$$\|\hat{\boldsymbol{g}}_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\tilde\tau}(\mathbb{R})\oplus D_0} \le C\varepsilon^{-2}\|\mathbb{G}_\varepsilon(\varepsilon^{-1}\cdot)\|_{\mathscr{C}^{0,\mu}_{\tilde\tau}(\mathbb{R})} \le C\varepsilon^{\alpha-\mu}\|\hat{\boldsymbol{g}}_\varepsilon\|_{\mathscr{C}^{2,\mu}_{\tilde\tau}(\mathbb{R})\oplus D_0}, \tag{6-27}$$

from which it follows that $\hat{\boldsymbol{g}}_\varepsilon = 0$, provided that we choose $\mu < \alpha$ and ε is taken small. This in turn implies $\tilde g^{(1)}_\varepsilon = \tilde g^{(2)}_\varepsilon$ and $\tilde\phi^{(1)} = \tilde\phi^{(2)}$, hence we get uniqueness. This ends the proof of Theorem 1.2. □

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PSEUDOPARABOLIC REGULARIZATION OF FORWARD-BACKWARD PARABOLIC EQUATIONS: A LOGARITHMIC NONLINEARITY

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We study the initial-boundary value problem

$$\begin{cases} u_t = \Delta\varphi(u) + \varepsilon\Delta[\psi(u)]_t & \text{in } Q := \Omega \times (0, T], \\ \varphi(u) + \varepsilon[\psi(u)]_t = 0 & \text{in } \partial\Omega \times (0, T], \\ u = u_0 \geq 0 & \text{in } \Omega \times \{0\}, \end{cases}$$

with *measure-valued initial data*, assuming that the regularizing term ψ has logarithmic growth (the case of power-type ψ was dealt with in an earlier work). We prove that this case is intermediate between the case of power-type ψ and that of bounded ψ, to be addressed in a forthcoming paper. Specifically, the support of the singular part of the solution with respect to the Lebesgue measure remains constant in time (as in the case of power-type ψ), although the singular part itself need not be constant (as in the case of bounded ψ, where the support of the singular part can also increase). However, it turns out that the concentrated part of the solution with respect to the Newtonian capacity remains constant.

1. Introduction

In this paper we study the initial-boundary value problem

$$\begin{cases} u_t = \Delta\varphi(u) + \varepsilon\Delta[\psi(u)]_t & \text{in } Q := \Omega \times (0, T], \\ \varphi(u) + \varepsilon[\psi(u)]_t = 0 & \text{in } \partial\Omega \times (0, T], \\ u = u_0 \geq 0 & \text{in } \Omega \times \{0\}, \end{cases} \tag{1-1}$$

where ε and T are positive constants,

$$\psi(u) = \log(1+u) \quad \text{for } u \geq 0, \tag{1-2}$$

$\varphi : [0, \infty) \to [0, \infty)$ is nonmonotone, u_0 is a nonnegative Radon measure on Ω, and $\Omega \subset \mathbb{R}^N$ $(N \geq 1)$ is a bounded and connected domain, with smooth boundary $\partial\Omega$ if $N \geq 2$. More precisely, $\varphi \in C^\infty([0, \infty))$ is a Perona–Malik type nonlinearity which satisfies, for some $\alpha > 0$ and $q \in (1, \infty)$,

$$\varphi(0) = \varphi(\infty) = 0, \quad \varphi' > 0 \text{ in } [0, \alpha), \quad \varphi' < 0 \text{ in } (\alpha, \infty), \quad \varphi''(\alpha) \neq 0, \tag{1-3}$$

$$\varphi \in L^q((0, \infty)), \quad \varphi^{(j)} \in L^\infty((0, \infty)) \text{ for any } j \in \mathbb{N}, \tag{1-4}$$

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and, for some $C > 0$,

$$|\varphi'(u)| \leq C\psi'(u) = \frac{C}{1+u} \quad \text{for } u \geq 0. \tag{1-5}$$

In particular, $0 < \varphi(u) \leq \varphi(\alpha)$ holds for $u > 0$. A typical example is

$$\varphi(u) = \frac{u}{1+u^2}.$$

The partial differential equation in problem (1-1) can be regarded as the regularization of the forward-backward parabolic equation

$$u_t = \Delta\varphi(u),$$

which leads to ill-posed problems. The latter equation and its regularizations arise in several applications, such as edge detection in image processing [Perona and Malik 1990], aggregation models in population dynamics [Padrón 1998], and stratified turbulent shear flow [Barenblatt et al. 1993a].

This paper is the second of a series where we address problem (1-1) with *measure-valued initial data*; see [Bertsch et al. ≥ 2013]. It is natural to consider flows which allow measure-valued solutions, since it is known that initially smooth solutions may develop a singular part in finite time, if $N = 1$ and ψ is uniformly bounded [Barenblatt et al. 1993b]. On the other hand we have shown [Bertsch et al. ≥ 2013] that in the case of power-type nonlinearities,

$$\psi(u) = (1+u)^\theta - 1 \qquad (u \geq 0, \theta \in (0, 1]), \tag{1-6}$$

the singular part of the solutions does not evolve in time, and initially smooth functions remain smooth for each later time. Therefore, the qualitative behavior of measure-valued solutions turns out to depend critically on the behavior of the nonlinearity $\psi(u)$ as $u \to \infty$.

Our purpose is to make a detailed analysis of this dependence. Therefore we distinguish three cases in this series of papers: mild degeneracies (power-type ψ), strong degeneracies (bounded ψ), and the intermediate case of logarithmic ψ. Observe that if ψ' vanishes at infinity, the partial differential equation in problem (1-1) is of *degenerate pseudoparabolic type*. In the present paper we focus on the intermediate case of functions ψ with logarithmic growth, and we take (1-2) as a model case.

It turns out that the logarithmic ψ can be considered as a truly intermediate case, in the sense that

(i) as in the case of power-type ψ, singularities cannot appear spontaneously;

(ii) as in the case of bounded ψ, the singular part of u need not be constant with respect to t.

Specifically, in all three cases the singular part of the solution is nondecreasing in time: it is constant for a power-type ψ (see [Bertsch et al. ≥ 2013, Theorem 2.1]), whereas its support can expand (that is, new singularities can appear) in the case of bounded ψ. Instead, in the logarithmic case the support of the singular part is constant, yet the singular part can increase; see Theorem 3.5 and equalities (3-13)–(3-14).

To explain the above claims, let us discuss heuristically the behavior of solutions to problem (1-1) for a logarithmic ψ as in (1-2) or a power-type ψ as in (1-6); see [Bertsch et al. ≥ 2013]. By a suitable approximation procedure, which plays a key role in our approach (see Section 6), we prove in both cases that the *entropy solution* $u(\cdot\,,t)$ at time t of problem (1-1) and the corresponding value $v(\cdot\,,t)$ of the *chemical potential*

$$v := \varphi(u_r) + \varepsilon[\psi(u_r)]_t \tag{1-7}$$

satisfy a suitable elliptic problem. Here $u_r(\cdot\,,t)$ denotes the density of the absolutely continuous part of $u(\cdot\,,t)$; see after (2-5). When ψ is of power-type, (1-7) becomes

$$\begin{cases} -\varepsilon\Delta v(\cdot\,,t) + \dfrac{v(\cdot\,,t)}{\psi'(u_r(\cdot\,,t))} = \dfrac{\varphi(u_r(\cdot\,,t))}{\psi'(u_r(\cdot\,,t))} & \text{in } \Omega, \\ v = 0 & \text{on } \partial\Omega \end{cases} \tag{1-8}$$

for a.e. $t \in (0,T)$. Instead, for a logarithmic ψ the elliptic problem is

$$\begin{cases} -\varepsilon\Delta v(\cdot\,,t) + \dfrac{1}{\psi'([u(\cdot\,,t)]_{d,2})} v(\cdot\,,t) = \dfrac{\varphi(u_r(\cdot\,,t))}{\psi'(u_r(\cdot\,,t))} & \text{in } \Omega, \\ v(\cdot\,,t) = 0 & \text{on } \partial\Omega, \end{cases} \tag{1-9}$$

where $[u(\cdot\,,t)]_{d,2}$ denotes the diffuse part of $u(\cdot\,,t)$ with respect to the Newtonian C_2-capacity. Recalling that $1/\psi'(u) = 1+u$, the first equation of problem (1-9) is meant in the sense that

$$-\varepsilon\langle \Delta[v(\cdot\,,t)], \rho\rangle_\Omega + \big\langle \{1+u_r(\cdot\,,t) + [u_s(\cdot\,,t)]_{d,2}\}, v(\cdot\,,t)\rho\big\rangle_\Omega = \int_\Omega [1+u_r(x,t)]\varphi(u_r(x,t))\rho(x)\,dx \tag{1-10}$$

for any $\rho \in C_c(\Omega)$; here $u_s(\cdot\,,t)$ denotes the singular part of $u(\cdot\,,t)$ and, as we shall make precise in Section 2 (see (2-2) and Remark 2.1), $\langle \cdot\,,\,\cdot\rangle_\Omega$ denotes an extension of the duality map between the space $\mathcal{M}(\Omega)$ of finite Radon measures on Ω and the space $C_c(\Omega)$ of continuous functions with compact support. Notice that

$$0 \le (1+u_r)\varphi(u_r) \le \varphi(\alpha)(1+u_r) \in L^1(Q).$$

The presence of the singular term $\langle [u_s(\cdot\,,t)]_{d,2}, v(\cdot\,,t)\rho\rangle_\Omega$ in the left-hand side of (1-10), which does not appear in the power-type case (see (1-8)), depends on the weaker regularization properties of a logarithmic ψ with respect to a power-type ψ.

By the above definition of the chemical potential, the partial differential equation in (1-1) reads

$$u_t = \Delta v. \tag{1-11}$$

The coupling of the above evolutionary equation with the corresponding elliptic problem (either (1-8) or (1-9), depending on the choice of ψ) suggests that we could study the time evolution of $u_r(\cdot\,,t)$ and that of $u_s(\cdot\,,t)$ separately. For both choices of ψ our definition of the solution of problem (1-1) implies that $v \in L^1(Q)$; see Definition 3.1 and [Bertsch et al. $\ge$ 2013, Definition 2.1]. Then for a power-type ψ we obtain from (1-8) that $\Delta v \in L^1(Q)$, which, by (1-11), implies

$$u_s(\cdot\,,t) = u_{0s}, \quad [u_r]_t(\cdot\,,t) = u_t(\cdot\,,t) = \Delta v(\cdot\,,t), \tag{1-12}$$

namely, the singular part u_s does not evolve with time; see [Bertsch et al. $\ge$ 2013, Theorem 2.1].

Now consider a logarithmic ψ as in (1-2). By (1-11) and the arbitrariness of ρ, (1-10) gives

$$-\epsilon u_t(\cdot\,,t)+\{1+u_r(\cdot\,,t)+[u_s(\cdot\,,t)]_{d,2}\}v(\cdot\,,t)=[1+u_r(\cdot\,,t)]\varphi(u_r(\cdot\,,t)). \tag{1-13}$$

On the other hand, by definition of the chemical potential, we have

$$\epsilon[u_r]_t(\cdot\,,t)=[1+u_r(\cdot\,,t)][v(\cdot\,,t)-\varphi(u_r)(\cdot\,,t)], \tag{1-14}$$

which can be regarded as the equation governing the evolution of the regular part u_r, since $v\in L^1(Q)$. From (1-13)–(1-14) we obtain the following equation for the evolution of the singular part u_s:

$$\epsilon[u_s]_t(\cdot\,,t)=[u_s]_{d,2}(\cdot\,,t)v(\cdot\,,t), \tag{1-15}$$

namely,

$$\epsilon\langle[u_s]_t(\cdot\,,t),\rho\rangle_\Omega=\langle[u_s(\cdot\,,t)]_{d,2},v(\cdot\,,t)\rho\rangle_\Omega$$

for any $\rho\in C_c(\Omega)$. Since

$$u_s=u_{c,2}+[u_s]_{d,2} \tag{1-16}$$

(see (2-7)–(2-8)), from Equation (1-15) we obtain

$$u_{c,2}(\cdot\,,t)=[u_0]_{c,2}$$

(see Theorem 3.1 below) and

$$\langle[u_s]_{d,2}(\cdot\,,t),\rho\rangle_\Omega=\left\langle[u_{0s}]_{d,2},\exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot\,,s)\,ds\right\}\rho\right\rangle_\Omega, \tag{1-17}$$

which imply (see (3-1))

$$\langle u_s(\cdot\,,t),\rho\rangle_\Omega\le\exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\langle u_{0s},\rho\rangle_\Omega$$

for any $t\ge 0$ and $\rho\in C_c(\Omega)$.

If $N=1$, since every Radon measure is C_2-diffuse (see page 1725), problem (1-9) becomes

$$\begin{cases}-\varepsilon[v(\cdot\,,t)]_{xx}+\dfrac{1}{\psi'(u(\cdot\,,t))}v(\cdot\,,t)=\dfrac{\varphi(u_r(\cdot\,,t))}{\psi'(u_r(\cdot\,,t))} & \text{in } \Omega,\\ v(\cdot\,,t)=0 & \text{on } \partial\Omega.\end{cases} \tag{1-18}$$

Now the evolution of the singular part u_s is described by the equation

$$\epsilon[u_s]_t(\cdot\,,t)=u_s(\cdot\,,t)v(\cdot\,,t), \tag{1-19}$$

whence we obtain

$$\langle u_s(\cdot\,,t),\rho\rangle_\Omega=\left\langle u_{0s},\exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot\,,s)\,ds\right\}\rho\right\rangle_\Omega \tag{1-20}$$

for any $\rho\in C_c(\Omega)$.

In view of the above considerations, whether or not $u_s(\cdot, t)$ evolves in time clearly depends on the positivity of the chemical potential; see (1-17), (1-20). This point will be addressed by a generalized strong maximum principle (see Proposition 3.15). We shall also construct a solution of the form

$$u(\cdot, t) = u_r(\cdot, t) + A(t)\delta_{x_0}, \quad A(0) = 1,$$

δ_{x_0} denoting the Dirac mass centered at $x_0 \in \Omega$ (see Remark 3.20), to point out the importance of the elliptic problem (1-9) for ensuring uniqueness of the solutions of problem (1-1); see Theorem 3.11; a similar example was given in [Porzio et al. 2013, Remark 2.4]. Finally, in Theorem 3.17 we prove the existence of an *entropy solution* of (1-1) (see Definition 3.4), whereas in Theorem 3.18 we show that under suitable conditions this solution and the associated chemical potential satisfy problem (1-9).

2. Preliminaries

Nonnegative finite Radon measures. We denote by $\mathcal{M}(\Omega)$ the space of finite Radon measures on Ω, and by $\mathcal{M}^+(\Omega)$ the cone of positive (finite) Radon measures on Ω. By $\mathcal{M}^+_{ac}(\Omega)$ and $\mathcal{M}^+_s(\Omega)$ we denote the subsets of $\mathcal{M}^+(\Omega)$ whose elements are, respectively, absolutely continuous and singular with respect to the Lebesgue measure on Ω. We have $\mathcal{M}^+_{ac}(\Omega) \cap \mathcal{M}^+_s(\Omega) = \{0\}$, and for every $\mu \in \mathcal{M}^+(\Omega)$ there is a unique pair $(\mu_{ac} \in \mathcal{M}^+_{ac}(\Omega), \mu_s \in \mathcal{M}^+_s(\Omega))$ such that

$$\mu = \mu_{ac} + \mu_s. \tag{2-1}$$

For every $\mu \in \mathcal{M}^+(\Omega)$, we shall denote by μ_r the density of the absolutely continuous part μ_{ac} of μ; namely, according to the Radon–Nikodym Theorem, μ_r is the unique function in $L^1(\Omega)$ such that

$$\mu_{ac}(E) = \int_E \mu_r \, dx$$

for every Borel set $E \subseteq \Omega$.

Given $\mu \in \mathcal{M}(\Omega)$ and a Borel set $E \subseteq \Omega$, the restriction $\mu \llcorner E$ of μ to E is defined by

$$(\mu \llcorner E)(A) := \mu(E \cap A)$$

for every Borel set $A \subseteq \Omega$. We denote by $\langle \cdot, \cdot \rangle_\Omega$ the duality map between $\mathcal{M}(\Omega)$ and the space $C_c(\Omega)$ of continuous functions with compact support. For $\mu \in \mathcal{M}(\Omega)$ and $\rho \in L^1(\Omega, \mu)$ we set, by abuse of notation,

$$\langle \mu, \rho \rangle_\Omega := \int_\Omega \rho(x) \, d\mu(x) \quad \text{and} \quad \|\mu\|_{\mathcal{M}(\Omega)} := |\mu|(\bar{\Omega}). \tag{2-2}$$

Similar notations will be used for the space of Radon measures on $Q := \Omega \times (0, T)$. The Lebesgue measure of any Borel set $E \subseteq \Omega$ or $E \subseteq Q$, will be denoted by $|E|$. A Borel set E such that $|E| = 0$ is called a null set. By the expression "almost everywhere", henceforth abbreviated a.e., we always mean "up to null sets".

We denote by $L^\infty((0, T); \mathcal{M}^+(\Omega))$ the set of positive Radon measures $u \in \mathcal{M}^+(Q)$ such that for a.e. $t \in (0, T)$ there exists a measure $u(\cdot, t) \in \mathcal{M}^+(\Omega)$ satisfying the following conditions:

(i) For every $\zeta \in C(\bar{Q})$ the map $t \to \langle u(\cdot\,,t), \zeta(\cdot\,,t)\rangle_\Omega$ is Lebesgue measurable, and

$$\langle u, \zeta\rangle_Q = \int_0^T \langle u(\cdot\,,t), \zeta(\cdot\,,t)\rangle_\Omega \, dt. \tag{2-3}$$

(ii) $\operatorname{ess\,sup}_{t\in(0,T)} \|u(\cdot\,,t)\|_{\mathcal{M}(\Omega)} < \infty$.

If $u \in L^\infty((0,T); \mathcal{M}^+(\Omega))$, both u_{ac} and u_s belong to $L^\infty((0,T); \mathcal{M}^+(\Omega))$. By (2-3), for all $\zeta \in C(\bar{Q})$,

$$\langle u_{ac}, \zeta\rangle_Q = \iint_Q u_r \zeta \, dx\, dt \quad \text{and} \quad \langle u_s, \zeta\rangle_Q = \int_0^T \langle u_s(\cdot\,,t), \zeta(\cdot\,,t)\rangle_\Omega \, dt.$$

It is easily checked that for a.e. $t \in (0,T)$ the measures $[u(\cdot\,,t)]_{ac}, [u(\cdot\,,t)]_s \in \mathcal{M}^+(\Omega)$ satisfy the equalities

$$u_{ac}(\cdot\,,t) = [u(\cdot\,,t)]_{ac}, \quad u_s(\cdot\,,t) = [u(\cdot\,,t)]_s. \tag{2-4}$$

Observe that the first equality above implies

$$u_r(\cdot\,,t) = [u(\cdot\,,t)]_r, \tag{2-5}$$

where $[u(\cdot\,,t)]_r$ denotes the density of the measure $[u(\cdot\,,t)]_{ac}$:

$$\langle [u(\cdot\,,t)]_{ac}, \zeta\rangle_\Omega = \int_\Omega u_r(\cdot\,,t)\zeta \, dx \quad \text{for } \zeta \in C(\bar{\Omega}) \text{ and a.e. t.}$$

C_p-capacity. Let $p \in [1,\infty)$. The C_p-capacity in Ω of a Borel set $E \subseteq \Omega$ is defined as

$$C_p(E) := \inf_{v \in \mathcal{U}_\Omega^E} \int_\Omega |\nabla v|^p \, dx,$$

where $\mathcal{U}_\Omega^E$ is the set of all functions $v \in H_0^{1,p}(\Omega)$ such that $0 \le v \le 1$ a.e. in Ω and $v = 1$ a.e. in a neighborhood of E (analogous definitions can be given in $\mathbb{R}^N$). If $\mathcal{U}_\Omega^E = \varnothing$ we adopt the usual convention that $\inf \varnothing = \infty$. We use the notation $C_p(E,\Omega)$ when we want to stress the dependence on Ω. If $K \subseteq \Omega$ is compact, then

$$C_p(K) := \inf_{v \in \mathcal{F}_\Omega^K} \int_\Omega |\nabla v|^p \, dx,$$

where $\mathcal{F}_\Omega^K$ is the set of all functions $v \in C_0^\infty(\Omega)$ such that $0 \le v \le 1$ in Ω and $v = 1$ in K. Moreover, if $p \in [1,\infty)$, for every Borel set $E \subseteq \Omega$,

$$C_p(E) = \inf\{C_p(U) \mid U \subseteq \Omega \text{ open}, \ E \subseteq U\},$$

and, if $1 < p < \infty$, for every open set $U \subseteq \Omega$,

$$C_p(U) = \sup\{C_p(K) \mid K \text{ compact}, \ K \subseteq U\}.$$

For any $p \in [1,\infty)$ define

$$\mathcal{M}_{d,p}^+(\Omega) := \{\mu \in \mathcal{M}^+(\Omega) \mid \mu(E) = 0 \text{ for every Borel set } E \subseteq \Omega, \ C_p(E) = 0\},$$

the set of finite (positive) Radon measures on Ω which are absolutely continuous with respect to the C_p-capacity. Analogously,

$$\mathcal{M}^+_{c,p}(\Omega) := \{\mu \in \mathcal{M}^+(\Omega) \mid \exists \text{ a Borel set } E \subseteq \Omega \text{ s.t. } C_p(E) = 0 \text{ and } \mu = \mu \llcorner E\}$$

is the set of finite (positive) Radon measures on Ω which are singular with respect to the C_p-capacity. Clearly, $\mathcal{M}^+_{c,p}(\Omega) \cap \mathcal{M}^+_{d,p}(\Omega) = \{0\}$. Observe that $\mathcal{M}^+_{d,p_1}(\Omega) \subseteq \mathcal{M}^+_{d,p_2}(\Omega)$ and $\mathcal{M}^+_{c,p_2}(\Omega) \subset \mathcal{M}^+_{c,p_1}(\Omega)$ if $p_1 < p_2$.

Recall that every subset $E \subseteq \Omega$ such that $C_p(E) = 0$ for $p \in [1, \infty)$ is Lebesgue measurable and satisfies $|E| = 0$. This plainly implies

$$\mathcal{M}^+_{c,p}(\Omega) \subseteq \mathcal{M}^+_{s}(\Omega), \quad \mathcal{M}^+_{ac}(\Omega) \subseteq \mathcal{M}^+_{d,p}(\Omega) \quad \text{for every } p \in [1, \infty). \tag{2-6}$$

In connection with the first inclusion in (2-6), observe that if $N = 1$, then $\mathcal{M}^+_{c,p}(\Omega) = \varnothing$ for any $p \in [1, \infty)$. In fact, for *singletons* $E = \{x\}$ ($x \in \Omega$), we have

$$C_p(\{x\}, \Omega) > 0 \quad \text{if either } p > N \text{ or } p = N = 1.$$

Therefore, if $N = 1$, by monotonicity, we have $C_p(E) > 0$ ($p \in [1, \infty)$) for every nonempty Borel set $E \subseteq \Omega$. The claim follows.

For any $p \in (1, \infty)$ it is known that a measure $\mu \in \mathcal{M}^+(\Omega)$ belongs to $\mathcal{M}^+_{d,p}(\Omega)$ if and only if

$$\mu \in L^1(\Omega) + W^{-1,p'}(\Omega)$$

(where $W^{-1,p'}(\Omega)$ denotes the dual space of the Sobolev space $W^{1,p}_0(\Omega)$). Then the duality symbol $\langle \mu, \varphi \rangle_\Omega$ makes sense for any $\mu \in \mathcal{M}^+_{d,p}(\Omega)$ and $\varphi \in W^{1,p}_0(\Omega) \cap L^\infty(\Omega)$. Moreover, if $\mu \in \mathcal{M}^+_{d,p}(\Omega)$, every function $v \in W^{1,p}_0(\Omega) \cap L^\infty(\Omega)$ also belongs to $L^\infty(\Omega, \mu)$; for example, see [Evans and Gariepy 1992].

For every $\mu \in \mathcal{M}^+(\Omega)$, $p \in [1, \infty)$, we define the *concentrated* and *diffuse* parts of μ with respect to C_p-capacity as the (unique, mutually singular) measures $\mu_{c,p} \in \mathcal{M}^+_{c,p}(\Omega)$ and $\mu_{d,p} \in \mathcal{M}^+_{d,p}(\Omega)$ such that

$$\mu = \mu_{c,p} + \mu_{d,p}. \tag{2-7}$$

Combining the decompositions in (2-1) and (2-7) and using (2-6) gives

$$\mu_{c,p} = [\mu_s]_{c,p}, \tag{2-8}$$

$$\mu_{d,p} = \mu_{ac} + [\mu_s]_{d,p}, \tag{2-9}$$

for every $\mu \in \mathcal{M}^+(\Omega)$. From (2-7)–(2-9) we obtain

$$\mu = \mu_{ac} + [\mu_s]_{d,p} + \mu_{c,p}, \tag{2-10}$$

which in the case $N = 1$ reduces to (2-1).

Finally, recall that a function $f : \Omega \to \mathbb{R}$ is C_p-*quasicontinuous in* Ω if for any $\epsilon > 0$ there exists a set $E \subseteq \Omega$, with $C_p(E) < \epsilon$, such that the restriction $f\big|_{\Omega \setminus E}$ is continuous in $\Omega \setminus E$ (it is not restrictive to assume that the set E is open). It can be proven (for example, see [Evans and Gariepy 1992]) that every function $u \in W^{1,p}(\Omega)$ has a C_p-quasicontinuous representative $\tilde{u}$; moreover, if $\bar{u}$ is another C_p-quasicontinuous representative of u, then the equality $\bar{u} = \tilde{u}$ holds C_p-almost everywhere in Ω. In the following, every function $u \in W^{1,p}(\Omega)$ will be identified with its unique C_p-quasicontinuous representative.

Remark 2.1. Recalling that $v(\cdot, t) \in H_0^1(\Omega) \cap L^\infty(\Omega)$ for a.e. $t \in (0, T)$ (see Definition 3.1) and $[u_s(\cdot, t)]_{d,2} \in L^1(\Omega) + H^{-1}(\Omega)$ by the characterization of the diffuse measures, it is apparent that the singular term $\langle [u_s(\cdot, t)]_{d,2}, v(\cdot, t)\rho\rangle_\Omega$ in the left-hand side of (1-10) is well defined for any $\rho \in C_c^1(\Omega)$. Let us show that the same quantity is well defined for any $\rho \in C_c(\Omega)$.

In fact, let $\mu \in \mathcal{M}_{d,2}^+(\Omega)$, $v \in H_0^1(\Omega) \cap L^\infty(\Omega)$, and let $\tilde{v}$ be its C_2-quasicontinuous representative. Let us show that $\tilde{v}\rho$ belongs to $L^1(\Omega, \mu)$, so that the quantity

$$\langle \mu, v\rho\rangle_\Omega = \int_\Omega \tilde{v}(x)\rho(x)\, d\mu(x)$$

is well defined.

Let $\{\rho_n\} \subseteq C_c^\infty(\Omega)$ be any sequence such that

$$\rho_n \to \rho \quad \text{in } C(\overline{\Omega}). \tag{2-11}$$

Since $\tilde{v}$ is defined C_2-almost everywhere in Ω and $\mu \in \mathcal{M}_{d,2}^+(\Omega)$,

$$\tilde{v}(x)\rho_n(x) \to \tilde{v}(x)\rho(x) \qquad \text{for } \mu\text{-a.e. } x \in \Omega. \tag{2-12}$$

Moreover, by (2-11) there exists $C > 0$ such that for every $n \in \mathbb{N}$ we have

$$|\tilde{v}\rho_n| \le C|\tilde{v}| \in L^1(\Omega, \mu).$$

Then by the dominated convergence theorem the claim follows.

3. Main results

Definitions.

Definition 3.1. Given $u_0 \in \mathcal{M}^+(\Omega)$, a measure $u \in L^\infty((0, T); \mathcal{M}^+(\Omega))$ is called a *solution* of problem (1-1) if the following holds:

(i) $[\psi(u_r)]_t \in L^\infty(Q)$, the chemical potential v defined by (1-7) belongs to $L^\infty((0, T); H_0^1(\Omega))$,

$$\Delta v \in L^\infty((0, T); \mathcal{M}(\Omega)),$$

and

$$0 \le v \le \varphi(\alpha) \quad \text{a.e. in } Q. \tag{3-1}$$

(ii) for every $\zeta \in C^1([0, T]; C_c(\Omega))$ with $\zeta(\cdot, T) = 0$ in Ω,

$$\int_0^T \langle u(\cdot, t), \zeta_t(\cdot, t)\rangle_\Omega\, dt + \int_0^T \langle \Delta v(\cdot, t), \zeta(\cdot, t)\rangle_\Omega\, dt = -\langle u_0, \zeta(\cdot, 0)\rangle_\Omega. \tag{3-2}$$

Observe that the assumption $\Delta v \in L^\infty((0, T); \mathcal{M}(\Omega))$ implies $u \in C([0, T]; \mathcal{M}^+(\Omega))$.

Remark 3.2. Since $0 \le \varphi(u) \le \varphi(\alpha)$ for $u \ge 0$ by (1-3), it follows from (1-7) and (3-1) that

$$|[\psi(u_r)]_t| \le \frac{\varphi(\alpha)}{\varepsilon} \quad \text{a.e. in } Q. \tag{3-3}$$

Remark 3.3. Since $v \in L^\infty((0,T); H_0^1(\Omega))$ and $\Delta v \in L^\infty((0,T); \mathcal{M}(\Omega))$, for a.e. $t \in (0,T)$ we have that $v(\cdot,t) \in H_0^1(\Omega)$ and $\Delta v(\cdot,t) := [\Delta v](\cdot,t) \in \mathcal{M}(\Omega)$. Observe that

$$\Delta v(\cdot,t) = \Delta[v(\cdot,t)] \in H^{-1}(\Omega) \tag{3-4}$$

for a.e. $t \in (0,T)$. In fact, let j_σ ($\sigma > 0$) be a standard mollifier. Then

$$\langle [\Delta v(\cdot,t)] * j_\sigma, \rho\rangle_\Omega = \langle \Delta[v(\cdot,t)] * j_\sigma], \rho\rangle_\Omega = \langle v(\cdot,t) * j_\sigma, \Delta\rho\rangle_\Omega$$

for any $\rho \in C_c^2(\Omega)$. Letting $\sigma \to 0$ we obtain

$$\langle \Delta v(\cdot,t), \rho\rangle_\Omega = \langle v(\cdot,t), \Delta\rho\rangle_\Omega,$$

which shows that $\Delta v(\cdot,t)$ is the distributional Laplacian of $v(\cdot,t) \in H_0^1(\Omega)$. Hence (3-4) follows.

Given $g \in C^1([0,\varphi(\alpha)])$, we set

$$G(z) := \int_0^z g(\varphi(u))\, du \quad \text{for } z \ge 0. \tag{3-5}$$

Definition 3.4. Let $u_0 \in \mathcal{M}^+(\Omega)$. A solution u of problem (1-1) is called an *entropy solution* if for all $g \in C^1([0,\varphi(\alpha)])$ such that $g' \ge 0$ and $g(0) = 0$, and for all $\zeta \in C^1([0,T]; C_c^1(\Omega))$ such that $\zeta \ge 0$, $\zeta(\cdot,T) = 0$ in Ω, the following *entropy inequality* holds:

$$\iint_Q \{G(u_r)\zeta_t - g(v)\nabla v \nabla\zeta - g'(v)|\nabla v|^2\zeta\}\, dx\, dt \ge -\int_\Omega G(u_{0r})\zeta(x,0)\, dx, \tag{3-6}$$

where G is defined by (3-5).

Inequality (3-6) is called the entropy inequality for problem (1-1) by analogy with the entropy inequality for viscous conservation laws; see [Evans 2004; Serre 1999]. Such an inequality is known to hold

(i) when $u_0 \in L^\infty(\Omega)$ and $\psi(u) = u$ (this is the so-called Sobolev regularization), both for a cubic-like φ and for a φ of Perona–Malik type (see [Novick-Cohen and Pego 1991; Smarrazzo 2008]);

(ii) for problem (1-1) if $N = 1$ and $\psi'(u) \to 0$ as $u \to \infty$ (see [Smarrazzo and Tesei 2012]).

In such cases, entropy inequalities play an important role both to describe the time evolution of solutions of (1-1) and to address the "vanishing viscosity limit" of the problem as $\epsilon \to 0$.

Persistence and monotonicity. Given any solution u of problem (1-1), we prove in Section 4 that the C_2-concentrated part $[u(\cdot,t)]_{c,2}$ does not evolve in time if $N \ge 2$ (recall that $\mathcal{M}^+_{c,2}(\Omega) = \varnothing$ if $N = 1$).

Theorem 3.5. *Let $N \ge 2$ and let u be a solution to problem (1-1). Then*

$$[u(\cdot,t)]_{c,2} = [u_0]_{c,2} \quad \textit{for a.e. } t \in (0,T). \tag{3-7}$$

Therefore, with respect to the case of a power-type ψ in which the first equality of (1-12) holds, in the present case it is only the concentrated part $[u(\cdot\,,t)]_{c,2} = [u_s(\cdot\,,t)]_{c,2}$ of the solution which remains constant.

Concerning the density of the absolutely continuous part of an entropy solution, the following holds. The proof is the same as that of [Bertsch et al. $\geq$ 2013, Proposition 2.5], thus we omit it.

Proposition 3.6. *Let u be an entropy solution of problem (1-1). Then there exists a null set $F^* \subset (0,T)$ such that, for any $t_0 \in (0,T)\setminus F^*$ and any Borel set $E \subseteq \Omega$,*

$$u_r(\cdot\,,t_0) \leq \alpha \text{ a.e. in } E \implies u_r(\cdot\,,t) \leq \alpha \text{ a.e. in } E \text{ for every } t \in (t_0,T)\setminus F^*.$$

The singular part of an entropy solution does not decrease if time evolves.

Proposition 3.7. *Let u be an entropy solution of problem (1-1), and let $\rho \in C_c(\Omega)$, $\rho \geq 0$. Then, for a.e. $0 \leq t_1 \leq t_2 \leq T$,*

$$\langle u_s(\cdot\,,t_1),\rho\rangle_\Omega \leq \langle u_s(\cdot\,,t_2),\rho\rangle_\Omega \tag{3-8}$$

and, for a.e. $t \in (0,T)$,

$$\langle u_{0s},\rho\rangle_\Omega \leq \langle u_s(\cdot\,,t),\rho\rangle_\Omega. \tag{3-9}$$

Remark 3.8. If u is a solution of problem (1-1) satisfying (1-9), inequalities (3-8)–(3-9) immediately follow from (3-7) and (3-13) below. The relationship between entropy solutions and solutions satisfying (1-9) is addressed in Theorem 3.18.

Proposition 3.7 implies that a solution (satisfying estimate (3-10) below) with trivial absolutely continuous part is a steady state.

Corollary 3.9. *Let $u_0 \in \mathcal{M}^+(\Omega)$, let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5), and let u be an entropy solution of problem (1-1) such that, for a.e. $t \in (0,T)$,*

$$\|u(\cdot\,,t)\|_{\mathcal{M}(\Omega)} \leq \|u_0\|_{\mathcal{M}(\Omega)}. \tag{3-10}$$

Then

$$u_{0r} = 0 \text{ a.e. in } \Omega \quad \implies \quad u_r(\cdot\,,t) = 0 \text{ a.e. in } \Omega,\; u_s(\cdot\,,t) = u_0 \text{ for a.e. } t \in (0,T).$$

Proposition 3.7 and Corollary 3.9 will be proved in Section 4.

Remark 3.10. By the considerations above,

$$u_r(\cdot\,,t) = 0 \text{ a.e. } t \in (0,T) \iff u_s(\cdot\,,t) = u_0 \text{ for a.e. } t \in (0,T).$$

In fact, if $u_r(\cdot\,,t) = 0$ for a.e. $t \in (0,T)$, by (1-7) we have $v = 0$ a.e. in Q, hence $u(\cdot\,,t) = u_s(\cdot\,,t) = u_0$ by equality (3-2). Conversely, if $u_s(\cdot\,,t) = u_0$ for a.e. $t \in (0,T)$, we have $u_0 = u_{0s}$, thus $u_{0r} = 0$ a.e. in Ω which implies $u_r(\cdot\,,t) = 0$ by (3-10).

Uniqueness. In this subsection we consider solutions u of problem (1-1) such that for a.e. $t \in (0, T)$ the trace $v(\cdot\,, t)$ of the chemical potential solves the elliptic problem (1-9). This means that for a.e. $t \in (0, T)$, $v(\cdot\,, t) \in H_0^1(\Omega)$, $\Delta[v(\cdot\,, t)] \in \mathcal{M}(\Omega)$, and equality (1-10) is satisfied for every $\rho \in C_c(\Omega)$. The results described in this subsection will be proved in Section 5.

Satisfying problem (1-9) guarantees uniqueness of solutions.

Theorem 3.11. *Let $\varphi \in C^\infty([0, \infty))$ satisfy (1-3)–(1-4). Let there exist $C > 0$ such that*

$$\left|\left(\frac{\varphi}{\psi'}\right)'(u)\right| \le C \quad \text{for } u \ge 0. \tag{3-11}$$

Then problem (1-1) has at most one solution satisfying (1-9).

Below we consider in more detail the qualitative properties of solutions of problem (1-1) which satisfy (1-9). In fact, it turns out that the logarithmic form of ψ makes it possible to give precise estimates of the time evolution both for u_r and for u_s.

Proposition 3.12. *Let $\varphi \in C^\infty([0, \infty))$ satisfy (1-3)–(1-4), and let u be a solution of problem (1-1) satisfying (1-9). Then, for a.e. $t \in (0, T)$ and for any $\rho \in C_c(\Omega)$, $\rho \ge 0$,*

$$\int_\Omega [1 + u_r(x, t)]\rho(x)\,dx \le \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\int_\Omega [1 + u_{0r}(x)]\rho(x)\,dx, \tag{3-12}$$

$$\langle [u_s]_{d,2}(\cdot\,, t), \rho\rangle_\Omega = \langle [u_{0s}]_{d,2}, \exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot\,, s)\,ds\right\}\rho\rangle_\Omega, \tag{3-13}$$

$$\langle u_s(\cdot\,, t), \rho\rangle_\Omega \le \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\langle u_{0s}, \rho\rangle_\Omega. \tag{3-14}$$

In particular, $u_s(\cdot\,, t)$ is absolutely continuous with respect to u_{0s}, for a.e. $t \in (0, T)$.

The last statement above entails a regularity result: no singularity can arise at some positive time. Going into detail, we have the following remark.

Remark 3.13. By inequality (3-14), for any solution of problem (1-1) satisfying (1-9), we have:

(i) $u_0 \in L^1(\Omega)$, $u_0 \ge 0 \Longrightarrow u \in L^1(Q)$, $u \ge 0$.

(ii) $u_{0s} \in \mathcal{M}^+_{c,p}(\Omega) \Longrightarrow u_s(\cdot\,, t) \in \mathcal{M}^+_{c,p}(\Omega)$ for a.e. $t \in (0, T)$.

(iii) $u_0 \in \mathcal{M}^+_{d,p}(\Omega) \Longrightarrow u(\cdot\,, t) \in \mathcal{M}^+_{d,p}(\Omega)$ for a.e. $t \in (0, T)$ $(p \in [1, \infty))$.

Remark 3.14. By the arbitrariness of ρ in (3-12)–(3-14), for every Borel set $E \subseteq \Omega$ and a.e. $t \in (0, T)$, we have

$$\int_E [1 + u_r(x, t)]\,dx \le \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\int_E [1 + u_{0r}(x)]\,dx,$$

$$u_s(\cdot\,, t)(E) \le \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}u_{0s}(E).$$

Also observe that (3-12) and (3-14) imply

$$\langle [1 + u(\cdot\,, t)], \rho\rangle_\Omega \le \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\langle [1 + u_0], \rho\rangle_\Omega \tag{3-15}$$

for every $\rho \in C_c(\Omega)$, $\rho \geq 0$, thus

$$u(\,\cdot\,,t)(E) \leq \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}u_0(E) + \left(\exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\} - 1\right)|E|$$

for every Borel set $E \subseteq \Omega$.

Observe that by equalities (2-8) and (2-10)

$$u_s(\,\cdot\,,t) = [u_s(\,\cdot\,,t)]_{d,2} + [u(\,\cdot\,,t)]_{c,2}$$

for a.e. $t \in (0,T)$. Then from (3-7), (3-13) it is apparent that to describe the time evolution of $u_s(\,\cdot\,,t)$ it is important to know whether $v(\,\cdot\,,t)$ vanishes in Ω. In this sense the following maximum principle, which generalizes in a certain sense [Brezis and Ponce 2003, Theorem 1], is expedient.

Proposition 3.15. *Let $\mu \in \mathcal{M}^+(\Omega)$ be C_2-diffuse. Let $v \in H_0^1(\Omega) \cap L^\infty(\Omega)$ satisfy*

$$-\Delta v + \mu v \geq 0 \quad \text{in } \Omega,$$

in the sense that

$$\int_\Omega \nabla v \cdot \nabla \rho \, dx + \langle \mu, v\rho \rangle_\Omega \geq 0 \quad \text{for any } \rho \in H_0^1(\Omega) \cap L^\infty(\Omega),\ \rho \geq 0. \tag{3-16}$$

Then $v \geq 0$ a.e. in Ω, and $v = 0$ a.e. in Ω if $v = 0$ a.e. on a subset $E \subseteq \Omega$ such that $C_2(E) > 0$.

If $N = 1$, we have the following.

Proposition 3.16. *Let $N = 1$, and let u be a solution of problem (1-1) satisfying (1-18). Then, for a.e. $t \in (0,T)$, either $v(\,\cdot\,,t) > 0$ in Ω or $v(\,\cdot\,,t) \equiv 0$ in Ω.*

Existence. Set

$$\psi_n(u) := \psi(u) + \frac{u}{n} = \log(1+u) + \frac{u}{n} \quad \text{for } u \geq 0. \tag{3-17}$$

Observe that $\psi_n \to \psi$ as $n \to \infty$ and $\psi_n' \geq 1/n > 0$, thus the nonlinearities ψ_n are nondegenerate. Consider the regularized problems

$$\begin{cases} u_{nt} = \Delta v_n & \text{in } Q, \\ v_n = 0 & \text{on } \partial\Omega \times (0,T), \\ u_n = u_{0n} \geq 0 & \text{in } \Omega \times \{0\}, \end{cases} \tag{P_n}$$

where

$$v_n := \varphi(u_n) + \varepsilon[\psi_n(u_n)]_t \tag{3-18}$$

and $\{u_{0n}\}$ is a sequence of smooth nonnegative functions with the properties stated in Lemma 6.1 (Section 6 is dedicated to the approximating problem P_n).

Theorem 3.17. *Let $u_0 \in \mathcal{M}^+(\Omega)$ and let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5). Then problem (1-1) has an entropy solution u, which is a limiting point as $n \to \infty$ of the family of solutions of the approximating problems (P_n). Moreover:*

(i) *For a.e. $t \in (0,T)$, inequality (3-10) holds.*

(ii) *For a.e.* $t \in (0, T)$ *and for every Borel set* $E \subseteq \Omega$, *inequalities* (3-12) *and* (3-14) *hold. In particular*, $u_s(\,\cdot\,, t)$ *is absolutely continuous with respect to* u_{0s}.

In Theorem 3.18 below we show that the entropy solution given in Theorem 3.17 satisfies the elliptic problem (1-9) if $N = 1$; the same holds if $N \geq 2$ for a suitable class of initial data $u_0 \in \mathcal{M}^+(\Omega)$. In these cases claim (ii) of Theorem 3.17 follows directly from Proposition 3.12.

Theorem 3.18. *Let* $u_0 \in \mathcal{M}^+(\Omega)$, *and let* $\varphi \in C^\infty([0, \infty))$ *satisfy* (1-3)–(1-5). *Let* u *be the entropy solution of problem* (1-1) *given in Theorem 3.17 and let* v *be the chemical potential defined in* (1-7).

(a) *If* $N = 1$, *the pair* (u, v) *satisfies problem* (1-18).

(b) *Let* $N \geq 2$, *and let* u_0 *satisfy the following assumptions*:

  (i) $[u_0]_{c,2}$ *is concentrated on some compact* $K_0 \subset \Omega$ *such that* $C_2(K_0) = 0$;

  (ii) $[u_0]_{d,2} \in \mathcal{M}^+_{d,p}(\Omega)$ *for some* $p \in [1, 2)$.

  Then the pair (u, v) *satisfies problem* (1-9).

Theorems 3.17 and 3.18 will be proved in Sections 7 and 8, respectively.

For $N = 1$, from the above theorem we deduce that an entropy solution of problem (1-1) satisfying problem (1-9) (or equivalently (1-18)) can be obtained as a limiting point as $n \to \infty$ of the family of solutions to the approximating problems (P_n).

If $N \geq 2$, the same result holds for a suitable class of initial data u_0, subject to technical conditions involving both $[u_0]_{d,2}$ and $[u_0]_{c,2}$ (see Theorem 3.18-(b)). Assumption (ii) on $[u_0]_{d,2}$ is rather mild, yet the problem of removing it is open. On the other hand, the existence of an entropy solution of (1-1) satisfying (1-9) can also be proven without assumption (i). In fact, for every $u_0 \in \mathcal{M}^+(\Omega)$,

$$u_0 = [u_0]_{d,2} + [u_0]_{c,2},$$

with $[u_0]_{d,2} \in \mathcal{M}^+_{d,p}(\Omega)$ for some $p \in [1, 2)$, it suffices to consider the measure $u \in L^\infty((0, T); \mathcal{M}^+(\Omega))$ defined by setting

$$u(\,\cdot\,, t) := \tilde{u}(\,\cdot\,, t) + [u_0]_{c,2} \quad \text{for a.e. } t \in (0, T);$$

here $\tilde{u}$ denotes a solution of (1-1) with initial data $[u_0]_{d,2}$ which satisfies the elliptic problem (1-9) (the existence of such a solution is ensured by Theorem 3.18 above). Clearly, the solution u (whose uniqueness is ensured by Theorem 3.11, if (3-11) holds) need not be obtained by letting $n \to \infty$ in the associated problems (P_n).

Corollary 3.19. *Let* $u_0 \in \mathcal{M}^+(\Omega)$, *and let* $\varphi \in C^\infty([0, \infty))$ *satisfy* (1-3)–(1-5) *and* (3-11). *If either* $N = 1$, *or* $N \geq 2$ *and* $[u_0]_{d,2} \in \mathcal{M}^+_{d,p}(\Omega)$ *for some* $p \in [1, 2)$, *there is exactly one entropy solution of problem* (1-1) *satisfying problem* (1-9).

Remark 3.20. Problem (1-9) is essential to introduce a class of well-posedness for problem (1-1). In fact, it is easy to exhibit a weak solution to problem (1-1) which does not satisfy (1-9) and which, therefore, is different from the solution given by Theorem 3.17.

For this purpose, let $N = 1$ and $\Omega = (0, 1)$. Let $\hat{u}_0 \in C^\infty([0, 1])$ satisfy $0 < \hat{u}_0 < \alpha$ in $(0, 1)$, $\hat{u}_0(0) = \hat{u}_0(1) = 0$. Let $\hat{u}$ be the solution of problem (1-1) with Cauchy data $u_0 = u_{0r} = \hat{u}_0$ given by

Theorem 3.17 . Then $\hat{u} = \hat{u}_r \in C^\infty([0,1]\times[0,\infty))$, $0 < \hat{u} < \alpha$ in $[0,1]\times[0,\infty)$, and $\hat{u}_s \equiv 0$. By Theorem 3.18(i) the pair $(\hat{u}, \hat{v})$, where $\hat{v} := \varphi(\hat{u}) + \varepsilon[\psi(\hat{u})]_t$, satisfies the problem

$$\begin{cases} -\varepsilon\hat{v}_{xx} + (1+\hat{u})\hat{v} = (1+\hat{u})\varphi(\hat{u}) & \text{in } [0,1]\times[0,\infty), \\ \hat{v} = 0 & \text{in } \{0,1\}\times[0,\infty), \end{cases}$$

hence $0 < \hat{v} < \varphi(\alpha)$ in $(0,1)\times[0,\infty)$ by the maximum principle.

Let δ_{x_0} denote the Dirac mass centered at some point $x_0 \in \Omega$, and set

$$u_1 := \hat{u} + \delta_{x_0}.$$

On the other hand, let u_2 be the solution of problem (1-1) given by Theorem 3.17, with initial data $u_0 := \hat{u}_0 + \delta_{x_0}$. We claim that

$$u_1 \text{ is a solution of problem (1-1) different from } u_2.$$

It is easily seen that u_1 is a solution of (1-1). Clearly, $u_{1r} = \hat{u}$, so the corresponding potential $v_1 := \varphi(u_{1r}) + \varepsilon[\psi(u_{1r})]_t$ coincides with $\hat{v}$. Recalling that $\hat{u}_t = \hat{v}_{xx}$, we have

$$\int_0^T \langle u(\cdot,t), \zeta_t(\cdot,t)\rangle_\Omega\,dt = \int_0^T\int_0^1 \hat{u}\zeta_t\,dx\,dt - \zeta(x_0,0) = -\int_0^T\int_0^1 \hat{v}_{xx}\zeta\,dx\,dt = -\int_0^1 \hat{u}_0(x)\zeta(x,0)\,dx - \zeta(x_0,0),$$

namely, equality (3-2) for every $\zeta \in C^1([0,T]; C_c(\Omega))$ with $\zeta(\cdot,T) = 0$ in Ω.

On the other hand, by Theorem 3.18(i) the solution u_2 and the corresponding chemical potential satisfy the elliptic problem (1-18), whereas the pair $(u_1, v_1) = (u_1, \hat{v})$ does not. In fact, if it did, by equality (3-13) we would have

$$\langle u_{1s}(\cdot,t), \rho\rangle_\Omega = \exp\left\{\frac{1}{\epsilon}\int_0^t \hat{v}(x_0,s)\,ds\right\}\rho(x_0)$$

(since every Radon measure is C_2-diffuse if $N = 1$), whereas the very definition of u_1 implies that

$$\langle u_{1s}(\cdot,t), \rho\rangle_\Omega = \langle \delta_{x_0}, \rho\rangle_\Omega = \rho(x_0)$$

for every $t > 0$. Since $\hat{v} > 0$ in $(0,1)\times[0,\infty)$, this gives a contradiction if $\rho(x_0) \neq 0$. The claim follows.

4. Proofs of persistence and monotonicity results

The proof of the following lemma is almost identical to that of [Bertsch et al. ≥ 2013, Lemma 3.1]; thus we omit it.

Lemma 4.1. *Let u be a solution of problem (1-1). Then there exists a null set $F^* \subseteq (0,T)$ such that, for every $t \in (0,T)\setminus F^*$ and $\rho \in C_c(\Omega)$,*

$$\langle u(\cdot,t), \rho\rangle_\Omega - \langle u_0, \rho\rangle_\Omega = \int_0^t \langle \Delta v(\cdot,s), \rho\rangle_\Omega\,ds, \tag{4-1}$$

$$\lim_{n\to\infty} \frac{n}{2}\int_{t-1/n}^{t+1/n} |\langle u_s(\cdot,s), \rho\rangle_\Omega - \langle u_s(\cdot,t), \rho\rangle_\Omega|\,ds = 0. \tag{4-2}$$

Proof of Theorem 3.5. Let $F^* \subseteq (0,T)$ be the null set given by Lemma 4.1. For every $t \in (0,T) \setminus F^*$ consider the map

$$F_t : C_c(\Omega) \to \mathbb{R}, \qquad \rho \to \int_0^t \langle \Delta v(\cdot\,,s), \rho\rangle_\Omega \, ds.$$

By (4-1) we have $F_t \in \mathcal{M}(\Omega)$. Moreover, $F_t \in H^{-1}(\Omega)$ by Remark 3.3; thus $F_t \in \mathcal{M}_{d,2}(\Omega)$. Then (4-1) becomes

$$\langle [u(\cdot\,,t)]_{c,2}, \rho\rangle_\Omega - \langle [u_0]_{c,2}, \rho\rangle_\Omega = \langle F_t, \rho\rangle_\Omega - \langle [u(\cdot\,,t)]_{d,2} - [u_0]_{d,2}, \rho\rangle_\Omega. \tag{4-3}$$

By equality (4-3) the difference $[u(\cdot\,,t)]_{c,2} - [u_0]_{c,2}$ is both C_2-diffuse and C_2-concentrated; thus

$$[u(\cdot\,,t)]_{c,2} - [u_0]_{c,2} = 0. \qquad \square$$

Proof of Proposition 3.7. Let $\{g_n\} \subseteq \mathrm{Lip}([0,\varphi(\alpha)])$ be defined by

$$g_n(s) := \begin{cases} ns & \text{if } 0 \le s \le \dfrac{1}{n}, \\ 1 & \text{if } \dfrac{1}{n} < s \le \varphi(\alpha), \end{cases}$$

and let G_n be the function (3-5) with $g = g_n$. By standard approximation arguments, inequality (3-6) is still valid with $G = G_n$. Therefore,

$$\iint_Q \{G_n(u_r)\zeta_t - g_n(v)\nabla v \nabla \zeta\}\, dx\, dt \ge -\int_\Omega G_n(u_{0r}(x))\zeta(x,0)\, dx \tag{4-4}$$

for $\zeta \in C^1([0,T]; C_c^1(\Omega))$, $\zeta \ge 0$, $\zeta(\cdot\,,T) = 0$ in Ω.

Since $0 \le G_n(u_r) \le u_r$ a.e. in Q, $0 \le G_n(u_{0r}) \le u_{0r}$ a.e. in Ω, and $g_n(s) \to 1$ for any $s \in (0,\varphi(\alpha)]$, as $n \to \infty$, by the dominated convergence theorem, we have

$$G_n(u_r) \to u_r \text{ in } L^1(Q), \qquad G_n(u_{0r}) \to u_{0r} \text{ in } L^1(\Omega). \tag{4-5}$$

Moreover,

$$g_n(v)\nabla v = \nabla\biggl(\int_0^v g_n(s)\, ds\biggr) \quad \text{a.e. in } Q, \tag{4-6}$$

and

$$\|g_n(v)|\nabla v|\|_{L^2(Q)} \le \||\nabla v|\|_{L^2(Q)}.$$

Therefore the sequence $\{g_n(v)\nabla v\}$ is weakly relatively compact in $[L^2(Q)]^N$. By (4-6), since

$$\int_0^{v(x,t)} g_n(s)\, ds \to v(x,t) \quad \text{as } n \to \infty \quad \text{for a.e. } (x,t) \in Q,$$

we obtain

$$g_n(v)\nabla v \rightharpoonup \nabla v \quad \text{in } [L^2(Q)]^N. \tag{4-7}$$

By (4-5) and (4-7), letting $n \to \infty$ in inequality (4-4), we have

$$\iint_\Omega \{u_r\zeta_t - \nabla v \nabla \zeta\}\, dx\, dt \ge -\int_\Omega u_{0r}(x)\zeta(x,0)\, dx, \tag{4-8}$$

whence, by (3-2),

$$-\int_0^T \langle u_s(\cdot\,,t), \zeta_t(\cdot\,,t)\rangle_\Omega\,dt \ge \langle u_{0s}, \zeta(\cdot\,,0)\rangle_\Omega \tag{4-9}$$

for any ζ as above.

To prove inequality (3-8), let $t_1, t_2 \in (0,T)\setminus F^*$, where $F^* \subseteq (0,T)$ is the null set defined by Lemma 4.1, and set

$$h_1(t) := \begin{cases} 0 & \text{if } t < t_1 - \dfrac{1}{n}, \\ n\Big(t - t_1 + \dfrac{1}{n}\Big) & \text{if } t_1 - \dfrac{1}{n} \le t \le t_1, \\ 1 & \text{if } t_1 < t < t_2, \\ -n\Big(t - t_2 - \dfrac{1}{n}\Big) & \text{if } t_2 \le t \le t_2 + \dfrac{1}{n}, \\ 0 & \text{if } t \ge t_2 + \dfrac{1}{n}. \end{cases}$$

Choosing $\zeta(x,t) = \rho(x)h_1(t)$ in (4-9), with any $\rho \in C_c^1(\Omega)$, $\rho \ge 0$, we obtain

$$n\int_{t_2}^{t_2+1/n} \langle u_s(\cdot\,,t), \rho\rangle_\Omega\,dt \ge n\int_{t_1-1/n}^{t_1} \langle u_s(\cdot\,,t), \rho\rangle_\Omega\,dt.$$

Letting $n \to \infty$ in the above inequality and using (4-2), we obtain (3-8).

The proof of inequality (3-9) is similar. For any $\tau \in (0,T)\setminus F^*$ define

$$h_2(t) := \begin{cases} 1 & \text{if } t \le \tau, \\ -n\Big(t - \tau - \dfrac{1}{n}\Big) & \text{if } \tau < t < \tau + \dfrac{1}{n}, \\ 0 & \text{if } t \ge \tau + \dfrac{1}{n}. \end{cases}$$

Substitution of $\zeta(x,t) = \rho(x)h_2(t)$ in (4-9) gives

$$n\int_\tau^{\tau+1/n} \langle u_s(\cdot\,,t), \rho\rangle_\Omega\,dt \ge \langle u_{0s}, \rho\rangle_\Omega,$$

whence we obtain (3-9) as $n \to \infty$. This completes the proof. □

Proof of Corollary 3.9. Since by assumption $u_0 = u_{0s}$, by inequality (3-10) we have

$$\|u_s(\cdot\,,t)\|_{\mathcal{M}(\Omega)} \le \|u(\cdot\,,t)\|_{\mathcal{M}(\Omega)} \le \|u_{0s}\|_{\mathcal{M}(\Omega)}$$

for a.e. $t \in (0,T)$. On the other hand, by inequality (3-9)

$$\|u_{0s}\|_{\mathcal{M}(\Omega)} = \sup_{\rho\in C_c(\Omega),|\rho|\le 1} \langle u_{0s}, \rho\rangle_\Omega \le \sup_{\rho\in C_c(\Omega),|\rho|\le 1} \langle u_s(\cdot\,,t), \rho\rangle_\Omega = \|u_s(\cdot\,,t)\|_{\mathcal{M}(\Omega)}.$$

The above inequalities imply

$$\|u_s(\cdot\,,t)\|_{\mathcal{M}(\Omega)} = \|u(\cdot\,,t)\|_{\mathcal{M}(\Omega)} = \|u_{0s}\|_{\mathcal{M}(\Omega)} = \|u_0\|_{\mathcal{M}(\Omega)}, \tag{4-10}$$

whence $\|u_r(\cdot\,,t)\|_{L^1(\Omega)} = 0$ for a.e. $t \in (0,T)$.

It remains to prove that $u_s(\,\cdot\,,t)=u_0$ for a.e. $t\in(0,T)$. By inequality (3-9) and the arbitrariness of ρ, for every Borel set $E\subseteq\Omega$ and for a.e. $t\in(0,T)$,

$$u_s(\,\cdot\,,t)(E)\geq u_{0s}(E)=u_0(E). \tag{4-11}$$

So, arguing by contradiction, we suppose that there exists a Borel set $\widetilde{E}\subseteq\Omega$ such that

$$u_s(\,\cdot\,,t)(\widetilde{E})>u_0(\widetilde{E}). \tag{4-12}$$

By (4-10)–(4-12) and the identities

$$\|u_0\|_{\mathcal{M}(\Omega)}=u_0(\Omega),\qquad \|u_s(\,\cdot\,,t)\|_{\mathcal{M}(\Omega)}=u_s(\,\cdot\,,t)(\Omega),$$

we obtain

$$u_0(\Omega\setminus\widetilde{E})\leq u_s(\,\cdot\,,t)(\Omega\setminus\widetilde{E})=u_s(\,\cdot\,,t)(\Omega)-u_s(\,\cdot\,,t)(\widetilde{E})<u_0(\Omega)-u_0(\widetilde{E})=u_0(\Omega\setminus\widetilde{E}),$$

a contradiction. Hence the conclusion follows. □

5. Proof of uniqueness

Proof of Theorem 3.11. Let u_1,u_2 be two solutions of problem (1-1) satisfying (1-9), and let v_1,v_2 be the corresponding potentials defined by (1-7). By Theorem 3.5 it is sufficient to prove that

$$[u_1(\,\cdot\,,t)]_{d,2}=[u_2(\,\cdot\,,t)]_{d,2}\quad\text{for a.e. } t\in(0,T).$$

By (3-2), for each $\rho\in C_c(\Omega)$ and for a.e. $t\in(0,T)$,

$$\langle u_1(\cdot,t)-u_2(\cdot,t),\rho\rangle_\Omega=\int_0^t\langle\Delta[v_1(\cdot,s)-v(\cdot,s)],\rho\rangle_\Omega\,ds\leq\|\rho\|_{C(\bar{\Omega})}\int_0^t\|\Delta[v_1(\cdot,s)-v_2(\cdot,s)]\|_{\mathcal{M}(\Omega)}\,ds,$$

thus

$$\|u_1(\cdot,t)-u_2(\cdot,t)\|_{\mathcal{M}(\Omega)}=\sup_{\rho\in C_c(\Omega),|\rho|\leq 1}\langle u_1(\cdot,t)-u_2(\cdot,t),\rho\rangle_\Omega\leq\int_0^t\|\Delta[v_1(\cdot,s)-v_2(\cdot,s)]\|_{\mathcal{M}(\Omega)}\,ds. \tag{5-1}$$

Let

$$w(x,t):=v_1(x,t)-v_2(x,t)\qquad((x,t)\in Q).$$

By (1-9), $w\in L^\infty((0,T);H_0^1(\Omega)\cap L^\infty(\Omega))$, $\Delta w\in L^\infty((0,T);\mathcal{M}(\Omega))$, and w solves the elliptic equation

$$\begin{aligned}-\varepsilon\Delta w(\,\cdot\,,t)&+[u_1(\,\cdot\,,t)]_{d,2}w(\,\cdot\,,t)+w(\,\cdot\,,t)\\&=-([u_1(\,\cdot\,,t)]_{d,2}-[u_2(\,\cdot\,,t)]_{d,2})v_2(\,\cdot\,,t)+\left[\frac{\varphi(u_{1r})}{\psi'(u_{1r})}-\frac{\varphi(u_{2r})}{\psi'(u_{2r})}\right](\,\cdot\,,t)\quad\text{in }\mathcal{M}(\Omega)\end{aligned} \tag{5-2}$$

for a.e. $t\in(0,T)$.

Let $\{f_j\}\subseteq C^\infty(\mathbb{R})$ satisfy

$$\begin{cases} f_j(0)=0,\quad \|f_j\|_\infty\leq 1,\quad f_j'\geq 0\text{ in }\mathbb{R},\\ |f_j'(s)s|\leq 1\text{ for every }s\in\mathbb{R},\quad f_j(s)\to\dfrac{s}{|s|}\text{ for every }s\neq 0.\end{cases} \tag{5-3}$$

Since $f_j(w) \in L^\infty((0,T); H_0^1(\Omega)\cap L^\infty(\Omega))$ for every $j \in \mathbb{N}$, it makes sense to use $[f_j(w)](\cdot\,,t)$ as test function for equality (5-2). Using inequalities (3-1) and (3-11), this gives

$$\begin{aligned}
\varepsilon \int_\Omega f_j'(w)(x,t)|\nabla w|^2(x,t)\,dx + \langle [u_1(\cdot\,,t)]_{d,2}, [f_j(w)w](\cdot\,,t)\rangle_\Omega + \int_\Omega [f_j(w)w](x,t)\,dx \\
\le \varphi(\alpha)\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)} + \int_\Omega \left|\frac{\varphi(u_{1r})}{\psi'(u_{1r})} - \frac{\varphi(u_{2r})}{\psi'(u_{2r})}\right|(x,t) f_j(w)(x,t)\,dx \\
\le \varphi(\alpha)\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)} + C\|u_{1r}(\cdot\,,t) - u_{2r}(\cdot\,,t)\|_{L^1(\Omega)} \\
\le L\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)}
\end{aligned} \tag{5-4}$$

for a.e. $t \in (0,T)$ with some constant $L > 0$. By the properties of $\{f_j\}$ (see (5-3)) we have

$$\|\,|\nabla[f_j(w)w]|\,\|_{L^2(Q)} \le 2\|\,|\nabla w|\,\|_{L^2(Q)} \tag{5-5}$$

for every $j \in \mathbb{N}$; hence the sequence $\{\nabla[f_j(w)w]\}$ is weakly relatively compact in $[L^2(Q)]^N$. Since

$$[f_j(w)w](\cdot\,,t)) \to |w(\cdot\,,t)| \text{ a.e. in } \Omega$$

and $\|w\|_{L^\infty(Q)} \le \varphi(\alpha)$ by inequality (3-1), by the dominated convergence theorem we have

$$[f_j(w)w](\cdot\,,t)) \to |w(\cdot\,,t)| \text{ in } L^1(\Omega), \quad [f_j(w)w](\cdot\,,t)) \overset{*}{\rightharpoonup} |w(\cdot\,,t)| \text{ in } L^\infty(\Omega).$$

Moreover, by (5-5)

$$[f_j(w)w](\cdot\,,t)) \rightharpoonup |w(\cdot\,,t)| \quad \text{in } H_0^1(\Omega).$$

Then, letting $n \to \infty$ in (5-4) and recalling that $f_j' \ge 0$, we get

$$\langle [u_1(\cdot\,,t)]_{d,2}, |w(\cdot\,,t)|\rangle_\Omega + \int_\Omega |w(x,t)|\,dx \le L\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)}.$$

On the other hand, since $u_1(\cdot\,,t)$ is a nonnegative Radon measure, for any $\rho \in C_c(\Omega)$ we have

$$\begin{aligned}
\langle [u_1(\cdot\,,t)]_{d,2}, |w(\cdot\,,t)|\rho\rangle_\Omega + \int_\Omega |w(x,t)|\rho(x)\,dx \le \|\rho\|_{C(\bar\Omega)}\left\{\langle [u_1(\cdot\,,t)]_{d,2}, |w(\cdot\,,t)|\rangle_\Omega + \int_\Omega |w(x,t)|\,dx\right\} \\
\le L\|\rho\|_{C(\bar\Omega)}\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)}.
\end{aligned}$$

Then from (5-2), arguing as in the proof of (5-4), we obtain plainly

$$\varepsilon\langle \Delta w(\cdot\,,t), \rho\rangle_\Omega \le \widetilde{L}\|\rho\|_{C(\bar\Omega)}\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)}$$

for some constant $\widetilde{L} > 0$ and any $\rho \in C_c(\Omega)$, whence

$$\varepsilon\|\Delta[v_1(\cdot\,,t) - v_2(\cdot\,,t)]\|_{\mathcal{M}(\Omega)} = \varepsilon\|\Delta w(\cdot\,,t)\|_{\mathcal{M}(\Omega)} \le \widetilde{L}\|[u_1(\cdot\,,t)]_{d,2} - [u_2(\cdot\,,t)]_{d,2}\|_{\mathcal{M}(\Omega)}$$

for a.e. $t \in (0,T)$. Combined with equality (5-1) this yields

$$\varepsilon\|u_1(\cdot\,,t) - u_2(\cdot\,,t)\|_{\mathcal{M}(\Omega)} \le \widetilde{L}\int_0^t \|u_1(\cdot\,,s) - u_2(\cdot\,,s)\|_{\mathcal{M}(\Omega)}\,ds,$$

and since $u_1(\cdot,0) = u_2(\cdot,0) = u_0$, it follows from Gronwall's inequality that

$$\|u_1(\cdot,t) - u_2(\cdot,t)\|_{\mathcal{M}(\Omega)} = 0 \quad \text{for a.e. } t \in (0,T). \qquad \square$$

Proof of Proposition 3.12. (i) Since $[\psi(u_r)]_t \in L^\infty(Q)$ (see Remark 3.2), the map $t \to \psi(u_r)(x,t)$ is Lipschitz continuous, and hence differentiable a.e. in $(0,T)$ for a.e. $x \in \Omega$. Differentiating the identity $u_r(\cdot,t) = \psi^{-1}[\psi(u_r)](\cdot,t)$, we obtain that the derivative u_{rt} exists a.e. in $(0,T)$ and the equality $[\psi(u_r)]_t = \psi'(u_r)u_{rt}$ holds, whence, by (1-7),

$$\varepsilon u_{rt} = (1+u_r)[v - \varphi(u_r)] \in L^1(Q). \tag{5-6}$$

Integrating the above equality in $(0,t)$, we obtain

$$\varepsilon u_r(x,t) - \varepsilon u_{0r}(x) = \int_0^t \{(1+u_r)[v-\varphi(u_r)]\}(x,s)\,ds \tag{5-7}$$

for a.e. $x \in \Omega$, whence, by inequality (3-1),

$$\varepsilon u_r(x,t) - \varepsilon u_{0r}(x) \le \varphi(\alpha) \int_0^t (1+u_r)(x,s)\,ds.$$

Then by Gronwall's inequality

$$1 + u_r(x,t) \le [1+u_{0r}(x)] \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\} \qquad (t \in (0,T))$$

for a.e. $x \in \Omega$, which implies (3-12).

(ii) By (4-1) and (1-10) we have

$$\begin{aligned}\varepsilon \int_\Omega [u_r(x,t) - u_{0r}(x)]\rho(x)\,dx + \varepsilon\langle [u_s(\cdot,t) - u_{0s}], \rho\rangle_\Omega \\ = \int_0^t \int_\Omega \rho(x)\{(1+u_r)[v-\varphi(u_r)]\}(x,s)\,dx\,ds + \int_0^t \langle [u_s(\cdot,s)]_{d,2}, v(\cdot,s)\rho\rangle_\Omega\,ds\end{aligned} \tag{5-8}$$

for any $\rho \in C_c(\Omega)$. Then by (5-7)–(5-8) we get

$$\varepsilon\langle [u_s(\cdot,t) - u_{0s}], \rho\rangle_\Omega = \int_0^t \langle [u_s(\cdot,s)]_{d,2}, v(\cdot,s)\rho\rangle_\Omega\,ds.$$

It follows that the map

$$g : (0,T) \to \mathcal{M}^+_{d,2}(\Omega), \quad g(t) := [u_s(\cdot,t)]_{d,2} \qquad (t \in (0,T))$$

satisfies the problem

$$\begin{cases} \varepsilon \dfrac{d}{dt}\langle f(t), \rho\rangle_\Omega = \langle f(t), v(\cdot,t)\rho\rangle_\Omega & \text{in } (0,T), \\ \langle f(0), \rho\rangle_\Omega = \langle [u_{0s}]_{d,2}, \rho\rangle_\Omega \end{cases} \tag{5-9}$$

for any $\rho \in C_c(\Omega)$.

Claim. *The unique solution of problem (5-9) is*

$$f : (0,T) \to \mathcal{M}^+_{d,2}(\Omega), \quad f(t) := [u_{0s}]_{d,2} \exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot,s)\,ds\right\} \qquad (t \in (0,T)).$$

This implies that

$$[u_s(\cdot\,,t)]_{d,2}=[u_{0s}]_{d,2}\exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot\,,s)\,ds\right\}\ \text{in } \mathcal{M}^+_{d,2}(\Omega) \text{ for any } t\in(0,T), \tag{5-10}$$

whence equality (3-13) follows. Then inequality (3-14) follows by (3-7) and (3-13), which completes the proof.

To prove the claim, observe preliminarily that

$$\exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot\,,s)\,ds\right\}\in H^1(\Omega)\cap L^\infty(\Omega),$$

thus

$$\langle f(t),\rho\rangle_\Omega:=\left\langle [u_{0s}]_{d,2},\exp\left\{\frac{1}{\epsilon}\int_0^t v(\cdot\,,s)\,ds\right\}\rho\right\rangle_\Omega$$

is well defined for any $\rho\in C_c(\Omega)$. Then for any $t_0,t_0+h\in(0,T)$ we have

$$\left\langle f(t_0+h)-f(t_0)-\frac{h}{\varepsilon}[u_{0s}]_{d,2}\exp\left\{\frac{1}{\epsilon}\int_0^{t_0} v(\cdot\,,s)\,ds\right\}v(\cdot\,,t_0),\rho\right\rangle_\Omega \\ =\frac{|h|^2}{\epsilon^2}\left\langle [u_{0s}]_{d,2},\exp\left\{\frac{1}{\epsilon}\int_0^{t_0+\theta h} v(\cdot\,,s)\,ds\right\}v^2(\cdot\,,t_0),\rho\right\rangle_\Omega$$

for some $\theta\in(0,1)$ and any $\rho\in C_c(\Omega)$. Hence there exists $C>0$, only depending on the norm of v in $L^\infty((0,T);H_0^1(\Omega)\cap L^\infty(\Omega))$, such that

$$\left\| f(t_0+h)-f(t_0)-\frac{h}{\varepsilon}[u_{0s}]_{d,2}\exp\left\{\frac{1}{\epsilon}\int_0^{t_0} v(\cdot\,,s)\,ds\right\}v(\cdot\,,t_0)\right\|_{\mathcal{M}(\Omega)}\le\frac{C}{\epsilon^2}\|u_0\|_{\mathcal{M}(\Omega)}|h|^2.$$

This proves that f is differentiable and satisfies the first equation of problem (5-9). Since $f(0)=[u_{0s}]_{d,2}$, f is a solution of the problem.

Let us show that no other solutions exist, so that equality (5-10) holds. In fact, if f_1 and f_2 both solve problem (5-9), plainly we obtain

$$\|f_1(t)-f_2(t)\|_{\mathcal{M}(\Omega)}\le\frac{\varphi(\alpha)}{\epsilon}\int_0^t\|f_1(s)-f_2(s)\|_{\mathcal{M}(\Omega)}\,ds\qquad\text{for any } t\in(0,T),$$

whence $f_1=f_2$ in $(0,T)$ by Gronwall's inequality. This proves the claim, and Proposition 3.12 follows. □

Proof of Proposition 3.15. Writing $v=v_+-v_-$ and choosing $\rho=v_-$ in (3-16), we get

$$-\int_\Omega|\nabla v_-|^2\,dx-\langle\mu,v_-^2\rangle_\Omega\ge 0,$$

whence $v=v_+\ge 0$ a.e. in Ω. Therefore the function $1/(v+\delta)$ belongs to $H^1(\Omega)\cap L^\infty(\Omega)$ and we can choose in (3-16) $\rho=\chi^2/(v+\delta)$ for any $\chi\in C_c^\infty(\Omega)$ and $\delta>0$, thus obtaining

$$-\int_\Omega\nabla v\cdot\nabla\left(\frac{\chi^2}{v+\delta}\right)dx\le\left\langle\mu,\frac{v}{v+\delta}\chi^2\right\rangle_\Omega. \tag{5-11}$$

Integrating by parts, we plainly get

$$\begin{aligned}\int_\Omega \nabla v\cdot\nabla\left(\frac{\chi^2}{v+\delta}\right)dx &= -\int_\Omega \frac{|\nabla v|^2}{(v+\delta)^2}\chi^2\,dx + 2\int_\Omega \frac{\chi\nabla\chi\cdot\nabla v}{v+\delta}\,dx \\ &\le -\frac{1}{2}\int_\Omega \frac{|\nabla v|^2}{(v+\delta)^2}\chi^2\,dx + 2\int_\Omega |\nabla\chi|^2\,dx.\end{aligned}\tag{5-12}$$

Since

$$\frac{\nabla v}{v+\delta} = \nabla\Big[\log\Big(1+\frac{v}{\delta}\Big)\Big],$$

by (5-11)–(5-12) we have

$$\frac{1}{2}\int_\Omega \Big|\nabla\Big[\log\Big(1+\frac{v}{\delta}\Big)\Big]\Big|^2\chi^2\,dx \le \langle\mu,\chi^2\rangle_\Omega + 2\int_\Omega|\nabla\chi|^2\,dx.$$

Then, arguing as in the proof of [Brezis and Ponce 2003, Theorem 1], the conclusion follows. □

Proof of Proposition 3.16. Since $N=1$, for a.e. $t\in(0,T)$ $v(\cdot,t)\in C(\overline{\Omega})$ and every singleton $E=\{x_0\}$ ($x_0\in\Omega$) has positive C_2-capacity. The conclusion follows by Proposition 3.15. □

6. The approximating problems

Lemma 6.1. *Let* $u_0\in\mathcal{M}^+(\Omega)$,

$$u_0 = u_{0ac} + [u_{0s}]_{d,2} + [u_0]_{c,2} = u_{0ac} + u_{0s},$$

and let u_{0r} *denote the density of the absolutely continuous part* u_{0ac}. *Then there exist sequences* $\{u_{0rn}\}$, $\{([u_{0s}]_{d,2})_n\}$ $\{([u_0]_{c,2})_n\}\subseteq C_c^\infty(\Omega)$ *of nonnegative functions such that*

$$\|u_{0rn}\|_{L^1(\Omega)} \le \|u_{0r}\|_{L^1(\Omega)};\tag{6-1}$$

$$\|([u_{0s}]_{d,2})_n\|_{L^1(\Omega)} \le \|[u_{0s}]_{d,2}\|_{\mathcal{M}(\Omega)},\quad \|([u_0]_{c,2})_n\|_{L^1(\Omega)} \le \|[u_0]_{c,2}\|_{\mathcal{M}(\Omega)};\tag{6-2}$$

$$u_{0rn}\to u_{0r}\ \text{in } L^1(\Omega);\tag{6-3}$$

$$([u_{0s}]_{d,2})_n \overset{*}{\rightharpoonup} [u_{0s}]_{d,2},\quad ([u_0]_{c,2})_n \overset{*}{\rightharpoonup} [u_0]_{c,2},\quad u_{0sn}\overset{*}{\rightharpoonup} u_{0s}\ \text{in } \mathcal{M}(\Omega),\tag{6-4}$$

$$u_{0n}\to u_{0r}\ \text{a.e. in } \Omega,\quad u_{0n}\overset{*}{\rightharpoonup} u_0\ \text{in } \mathcal{M}(\Omega),\tag{6-5}$$

where $u_{0sn} := ([u_{0s}]_{d,2})_n + ([u_0]_{c,2})_n$, $u_{0n} := u_{0rn} + u_{0sn}$. *In addition, there exists* $C>0$ *such that*

$$\|u_{0n}\|_{L^\infty(\Omega)} \le C\sqrt{n}\quad \text{for all } n.\tag{6-6}$$

Proof. Define $\tilde{u}_0\in\mathcal{M}^+(\mathbb{R}^N)$ by setting $\tilde{u}_0 := \tilde{u}_{0r} + \tilde{u}_{0s}$, where

$$\tilde{u}_{0r}(x) := \begin{cases} u_{0r}(x) & \text{if } x\in\Omega,\\ 0 & \text{otherwise}\end{cases}$$

and

$$[\tilde{u}_{0s}]_{d,2}(E) := [u_{0s}]_{d,2}(\Omega\cap E),\quad [\tilde{u}_0]_{c,2}(E) := [u_0]_{c,2}(\Omega\cap E),\quad \tilde{u}_{0s}(E) := [\tilde{u}_{0s}]_{d,2}(E) + [\tilde{u}_0]_{c,2}(E)$$

for every Borel set $E \subseteq \mathbb{R}^N$. Observe that by definition

$$\tilde{u}_0 = \tilde{u}_0 \llcorner \Omega, \quad \tilde{u}_0(E) = u_0(E) \quad \text{for every Borel set } E \subseteq \Omega.$$

Hence, if $\rho \in C_c(\Omega)$ and $\tilde{\rho} \in C_c(\mathbb{R}^N)$ denotes its trivial extension to $\mathbb{R}^N$, we get

$$\langle \tilde{u}_0, \tilde{\rho} \rangle_{\mathbb{R}^N} = \langle u_0, \rho \rangle_{\Omega}.$$

Consider the sequence $\{\tilde{u}_{0n}\} \subset C_c^\infty(\mathbb{R}^N)$ where

$$\tilde{u}_{0n} := \tilde{u}_0 * j_n,$$

$\{j_n\} \subseteq C_c^\infty(\mathbb{R}^N)$ being a regularizing sequence. We also define

$$\tilde{u}_{0rn} := \tilde{u}_{0r} * j_n, \quad ([\tilde{u}_{0s}]_{d,2})_n := ([\tilde{u}_{0s}]_{d,2}) * j_n, \quad ([\tilde{u}_0]_{c,2})_n := ([\tilde{u}_0]_{c,2}) * j_n, \quad \tilde{u}_{0sn} := \tilde{u}_{0s} * j_n$$

with j_n as above. To be specific, we choose

$$j_n(x) = \frac{n^N}{\int_{\mathbb{R}^N} j(x)\,dx} \zeta(nx) \qquad (x \in \mathbb{R}^N),$$

where $j \in C_c^\infty(\mathbb{R}^N)$, $j(x) = j(|x|)$ is a standard mollifier.

Next, choose any sequence $\{\eta_n\} \subseteq C_c^\infty(\mathbb{R}^N)$ such that $\eta_n \in C_c^\infty(\Omega_{n+1})$, $0 \le \eta_n \le 1$, $\eta_n = 1$ in $\overline{\Omega}_n$; here Ω_n is open, $\overline{\Omega}_n \subset \Omega_{n+1} \subset \Omega$ for every $n \in \mathbb{N}$ and $\bigcup_{n=1}^\infty \Omega_n = \Omega$. Finally, set

$$u_{0rn} := \tilde{u}_{0rn}\eta_n, \quad ([u_{0s}]_{d,2})_n := ([\tilde{u}_{0s}]_{d,2})_n\eta_n, \quad ([u_0]_{c,2})_n := ([\tilde{u}_0]_{c,2})_n\eta_n, \quad u_{0sn} := \tilde{u}_{0sn}\eta_n.$$

It is easily checked that the sequences $\{u_{0rn}\}$, $\{([u_{0s}]_{d,2})_n\}$ $\{([u_0]_{c,2})_n\}$, $\{u_{0sn}\}$, and $\{u_{0n}\}$ have the asserted properties. □

Definition 6.2. A nonnegative function $u_n \in C^1([0,T]; C(\overline{\Omega}))$ is called a *solution* of problem (P_n) if the function v_n defined by (3-17) belongs to $C([0,T]; C_0(\overline{\Omega}) \cap H^{2,p}(\Omega))$ for all $p \in [1,\infty)$, $\Delta v_n \in C(\overline{Q})$, and the pair (u_n, v_n) satisfies (P_n) in the strong sense.

Remark 6.3. If u is a solution of problem (P_n), then $v \in C(\overline{Q})$ and $v_{x_i} \in C(\overline{Q})$ for $i \in \{1,\dots,N\}$. Moreover, v admits second order weak derivatives $v_{x_i x_j} \in L^p(Q)$ for all $p \in [1,\infty)$, and for every $t \in [0,T]$

$$v_{x_i x_j}(\cdot\,,t) = [v(\cdot\,,t)]_{x_i x_j} \quad \text{a.e. in } \Omega.$$

We omit the proof of the following result, as it is almost identical to those of [Bertsch et al. ≥ 2013, Theorems 4.1–4.2].

Theorem 6.4. *Let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-4). Then, for any $n \in \mathbb{N}$, problem (P_n) has a unique solution $u_n \ge 0$, and*

$$u_n = [\psi_n(u_n)]_t = 0 \quad \text{on } \partial\Omega \times [0,T].$$

The function $v_n(\cdot, t)$ *defined by* (3-18) *satisfies, for a.e.* $t \in (0, T)$,

$$\begin{cases} --\epsilon\Delta[v_n(\cdot,t)] + \dfrac{v_n(\cdot,t)}{\psi_n'(u_n(\cdot,t))} = \dfrac{\varphi(u_n(\cdot,t))}{\psi_n'(u_n(\cdot,t))} & \text{in } \Omega, \\ v_n(\cdot,t) = 0 & \text{on } \partial\Omega, \end{cases} \tag{6-7}$$

$$0 \le v_n(\cdot,t) \le \varphi(\alpha) \quad \text{in } \Omega, \tag{6-8}$$

$$\frac{\partial v_n}{\partial \nu}(\cdot,t) \le 0 \quad \text{on } \partial\Omega, \tag{6-9}$$

where $\partial/(\partial\nu)$ *denotes the outer derivative at* $\partial\Omega$.

In addition, $v_n \in C^1(\bar{Q}_T)$, $v_{nt} \in C([0,T]; C_0(\bar{\Omega}) \cap H^{2,p}(\Omega))$ *for* $p \in [1,\infty)$ *and, for a.e* $t \in (0,T)$, $v_{nt}(\cdot,t)$ *satisfies*

$$\begin{cases} -\varepsilon\Delta[v_{nt}(\cdot,t)] + \dfrac{v_{nt}(\cdot,t)}{\psi_n'(u_n(\cdot,t))} = \left[\dfrac{\varphi'(u_n)u_{nt} + \varepsilon\psi_n''(u_n)u_{nt}^2}{\psi_n'(u_n)}\right](\cdot,t) & \text{in } \Omega, \\ v_{nt}(\cdot,t) = 0 & \text{on } \partial\Omega. \end{cases}$$

The following result is analogous to [Bertsch et al. $\ge$ 2013, Proposition 4.3]. The proof is omitted.

Proposition 6.5. *Let* u_n *be the solution of problem* (P_n), *let* $g \in C^1([0,\varphi(\alpha)])$ *with* $g' \ge 0$, *and let* G *be defined by* (3-5). *Then, for any* $\zeta \in C^1([0,T]; C_c^1(\Omega))$, $\zeta \ge 0$ *and for any* $0 \le t_1 \le t_2 \le T$,

$$\begin{aligned} \int_\Omega G(u_n(x,t_2))\zeta(x,t_2)\,dx &- \int_\Omega G(u_n(x,t_1))\zeta(x,t_1)\,dx \\ &\le \int_{t_1}^{t_2}\int_\Omega \{G(u_n)\zeta_t - g(v_n)\nabla v_n \nabla\zeta - g'(v_n)|\nabla v_n|^2\zeta\}\,dx\,dt. \end{aligned} \tag{6-10}$$

Next, the following a priori estimates hold.

Proposition 6.6. *Let* $\varphi \in C^\infty([0,\infty))$ *satisfy* (1-3)–(1-5). *Let* u_n *be the solution of problem* (P_n). *Then*

$$\|u_n\|_{L^\infty((0,T);L^1(\Omega))} \le \|u_0\|_{\mathcal{M}(\Omega)}, \tag{6-11}$$

$$\|[\psi_n(u_n)]_t\|_{L^\infty(Q)} \le \frac{\varphi(\alpha)}{\varepsilon}. \tag{6-12}$$

Moreover, there exists $C > 0$ *such that, for any* $n \in \mathbb{N}$,

$$\|v_n\|_{L^\infty((0,T);H_0^1(\Omega))} \le C, \tag{6-13}$$

$$\|v_{nt}\|_{L^\infty((0,T);L^1(\Omega))} \le C, \tag{6-14}$$

$$\|\Delta v_n\|_{L^\infty((0,T);L^1(\Omega))} \le C. \tag{6-15}$$

For the proofs of inequalities (6-11)–(6-14) we refer the reader to those of the analogous statements in [Bertsch et al. $\ge$ 2013, Proposition 5.1]. Let us only mention that in the proof of (6-13)–(6-14) we use the inequalities

$$\frac{\varphi(u_n)v_n}{\psi_n'(u_n)} \le [\varphi(\alpha)]^2(1+u_n)$$

and

$$\frac{|\psi_n''(u)|}{[\psi'(u)]^3} \le (1+u) \quad \text{for any } u \ge 0,$$

respectively.

Concerning inequality (6-15), observe that by, (6-7)–(6-8), we have

$$\varepsilon \int_\Omega |\Delta v_n|\, dx \le \int_\Omega \frac{|v_n - \varphi(u_n)|}{\psi_n'(u_n)}\, dx \le \varphi(\alpha) \int_\Omega [1+u_n]\, dx$$

for all $t \in (0,T)$. Then (6-15) follows from (6-11).

Finally, let us show that, for every $t \in (0,T)$, the sequence $\{1+u_n(\,\cdot\,,t)\}$ satisfies an inequality analogous to (3-12).

Proposition 6.7. *Let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-4). Let u_n be the solution of problem (P_n). Then, for any $t \in (0,T)$ and $\rho \in C_c(\Omega)$, $\rho \ge 0$,*

$$\int_\Omega [1+u_n(x,t)]\rho(x)\, dx \le \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\} \int_\Omega [1+u_{0n}(x)]\rho(x)\, dx. \tag{6-16}$$

Proof. From (3-18) we obtain

$$\varepsilon u_{nt} = \frac{v_n - \varphi(u_n)}{\psi_n'(u_n)}.$$

Integrating the above equality in $(0,t)$ and using inequality (6-8), we obtain, for every $x \in \Omega$,

$$\varepsilon[1+u_n(x,t)] - \varepsilon[1+u_{0n}(x)] \le \varphi(\alpha) \int_0^t [1+u_n(x,s)]\, ds.$$

Then, by Gronwall's inequality,

$$1+u_n(x,t) \le [1+u_{0n}(x)] \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\} \qquad (t \in (0,T)) \tag{6-17}$$

for every $x \in \Omega$, which implies (6-16). □

7. Proof of existence results

To prove Theorem 3.17 we need some preliminary results concerning convergence of solutions of the sequences $\{u_n\}$, $\{v_n\}$. From the estimates in Proposition 6.6 we obtain the following.

Proposition 7.1. *Let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5). Let u_n be the solution of problem (P_n) and let v_n be defined by (3-18). Then there exist $u \in L^\infty((0,T);\mathcal{M}^+(\Omega))$, $v \in L^\infty((0,T);H_0^1(\Omega)) \cap BV(Q)$*

with $\Delta v \in L^\infty((0,T);\mathcal{M}(\Omega))$, *and subsequences* $\{u_{n_k}\}$, $\{v_{n_k}\}$ *such that*

$$u_{n_k}(\cdot,t) \overset{*}{\rightharpoonup} u(\cdot,t) \quad \text{in } \mathcal{M}(\Omega), \tag{7-1}$$

$$v_{n_k} \to v \quad \text{a.e. in } Q, \tag{7-2}$$

$$\Delta v_{n_k} \overset{*}{\rightharpoonup} \Delta v \quad \text{in } \mathcal{M}(Q), \tag{7-3}$$

$$v_{n_k} \rightharpoonup v \quad \text{in } L^p((0,T);H_0^1(\Omega)) \qquad (p \in [1,\infty)), \tag{7-4}$$

$$v_n(\cdot,t) \rightharpoonup v(\cdot,t) \quad \text{in } H_0^1(\Omega) \tag{7-5}$$

for a.e. $t \in (0,T)$. *In addition*,

$$\|u\|_{L^\infty((0,T);\mathcal{M}(\Omega))} \le \|u_0\|_{\mathcal{M}(\Omega)} \tag{7-6}$$

and v *satisfies inequality* (3-1).

Proof. The convergence in (7-1) and inequality (7-6) are proven as in [Bertsch et al. ≥ 2013, Proposition 5.3]. The convergence in (7-2)–(7-4) and inequality (3-1) follow from (6-13)–(6-15) and (6-8).

To prove the convergence in (7-5), observe that, by (7-2),

$$v_{n_k}(\cdot,t) \to v(\cdot,t) \quad \text{a.e. in } \Omega$$

for a.e. $t \in (0,T)$. Hence, by inequality (6-8) and the dominated convergence theorem,

$$v_{n_k}(\cdot,t) \to v(\cdot,t) \quad \text{in } L^1(\Omega),$$

On the other hand, by inequality (6-13), the sequence $\{v_n(\cdot,t)\}$ is contained in a weakly compact subset of $H_0^1(\Omega)$ for a.e. $t \in (0,T)$; hence the conclusion follows. □

The sequence $\{u_{n_k}\}$ converges a.e. in Q to the density u_r of u_{ac}.

Proposition 7.2. *Let* $\varphi \in C^\infty([0,\infty))$ *satisfy* (1-3)–(1-5). *Let* $\{u_{n_k}\}$, u, *and* v *be as in Proposition 7.1, and let* $u_r \in L^1(Q)$ *be the density of the absolutely continuous part of* u. *Then*

$$u_{n_k} \to u_r \quad \text{a.e. in } Q, \tag{7-7}$$

$$[\psi(u_r)]_t \in L^\infty(Q), \quad u_{rt} \in L^1(Q), \tag{7-8}$$

$$[\psi_{n_k}(u_{n_k})]_t \overset{*}{\rightharpoonup} [\psi(u_r)]_t \quad \text{in } L^\infty(Q). \tag{7-9}$$

Moreover,

(i) *we have*

$$v = \varphi(u_r) + \varepsilon[\psi(u_r)]_t \quad \text{a.e. in } Q, \tag{7-10}$$

$$\|[\psi(u_r)]_t\|_{L^\infty(Q)} \le \frac{\varphi(\alpha)}{\varepsilon}; \tag{7-11}$$

(ii) $u_r(\cdot,t)$, $u_s(\cdot,t)$, $u(\cdot,t)$ *satisfy inequalities* (3-12), (3-14), (3-15), *respectively, for a.e.* $t \in (0,T)$ *and for any* $\rho \in C_c(\Omega)$, $\rho \ge 0$.

Proof. Arguing as in [Bertsch et al. ≥ 2013, Proposition 5.4], it can be proven that $u_{n_k} \to z$ a.e. in Q for some $z \in L^1(Q)$, $z \geq 0$. Let us show that

$$z = u_r \quad \text{a.e. in } Q. \tag{7-12}$$

For a.e. $t \in (0, T)$, we can assume without loss of generality that

$$u_{n_k}(\cdot\,, t) \to z(\cdot\,, t) \quad \text{a.e. in } \Omega \tag{7-13}$$

and the convergence in (7-1) holds. As in the proof of [Bertsch et al. ≥ 2013, Proposition 5.5], there exist a subsequence $\{u_{n_{k_j}}(\cdot\,, t)\}$ (possibly depending on t) and a sequence of subsets $\{A_j\}$, with $A_{j+1} \subseteq A_j \subseteq \Omega$ for any j and $|A_j| \to 0$, such that the family $\{u_{n_{k_j}}(\cdot\,, t)\chi_{\Omega\setminus A_j}\}$ is uniformly integrable in Ω and

$$u_{n_{k_j}}(\cdot\,, t)\chi_{\Omega\setminus A_j} \rightharpoonup z(\cdot\,, t) \quad \text{in } L^1(\Omega).$$

For example, see [Valadier 1994]. Then, by (7-1), we have

$$u_{n_{k_j}}(\cdot\,, t)\chi_{A_j} \overset{*}{\rightharpoonup} u(\cdot\,, t) - z(\cdot\,, t) =: \mu(\cdot\,, t) \quad \text{in } \mathcal{M}(\Omega). \tag{7-14}$$

Since $u_{n_{k_j}}(\cdot\,, t)\chi_{A_j} \geq 0$ in Ω for every j, the measure $\mu(\cdot\,, t)$ is nonnegative.

By (6-16), for every $\rho \in C_c(\Omega)$, $\rho \geq 0$, we get

$$\begin{aligned}\int_{A_j} u_{n_{k_j}}(x, t)\rho(x)\,dx &\leq \int_{A_j} [1 + u_{n_{k_j}}(x, t)]\rho(x)\,dx \leq \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\} \int_{A_j} [1 + u_{0n_{k_j}}(x)]\rho(x)\,dx \\ &\leq \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\left\{\int_{A_j} [1 + u_{0rn_{k_j}}(x)]\rho(x)\,dx + \int_\Omega u_{0sn_{k_j}}(x)\rho(x)\,dx\right\}.\end{aligned} \tag{7-15}$$

Since $u_{0rn_{k_j}} \to u_{0r}$ in $L^1(\Omega)$, $|A_j| \to 0$, and $u_{0sn_{k_j}} \overset{*}{\rightharpoonup} u_{0s}$ in $\mathcal{M}(\Omega)$ as $j \to \infty$,

$$\lim_{j\to\infty}\left\{\int_{A_j} [1 + u_{0rn_{k_j}}(x)]\rho(x)\,dx + \int_\Omega u_{0sn_{k_j}}(x)\rho(x)\,dx\right\} = \langle u_{0s}, \rho\rangle_\Omega.$$

Then, letting $j \to \infty$ in (7-15) and using (7-14), we have

$$\langle \mu(\cdot\,, t), \rho\rangle_\Omega \leq \exp\left\{\frac{\varphi(\alpha)t}{\varepsilon}\right\}\langle u_{0s}, \rho\rangle_\Omega \tag{7-16}$$

for every ρ, as above.

Since $\mu(\cdot\,, t)$ is nonnegative, by (7-16) it is absolutely continuous with respect to u_{0s}, thus singular with respect to the Lebesgue measure over Ω. Therefore, since $z(\cdot\,, t) \in L^1(\Omega)$ and $u(\cdot\,, t) = z(\cdot\,, t) + \mu(\cdot\,, t)$ by definition, the uniqueness of the Lebesgue decomposition of $u(\cdot\,, t)$ ensures that

$$z(\cdot\,, t) = [u(\cdot\,, t)]_r = [u_r(\cdot\,, t)], \qquad \mu(\cdot\,, t) = [u(\cdot\,, t)]_s = [u_s(\cdot\,, t)], \tag{7-17}$$

(see (2-4)–(2-5)). This proves (7-12), whence (7-7) follows. By the same token, inequality (7-16) and the second equality in (7-17) show that $u_s(\cdot\,, t)$ satisfies inequality (3-14).

Let us prove the remaining claims. By inequality (6-11) and the convergence in (7-7), we have

$$\psi_{n_k}(u_{n_k}) \to \psi(u_r) \quad \text{in } L^1(Q). \tag{7-18}$$

Then $[\psi(u_r)]_t \in L^\infty(Q)$, by (7-18) and inequality (6-12). The convergence in (7-9) follows. Inequality (7-11) follows by (6-12), (7-9), and the lower semicontinuity of the norm. By the continuity of φ, from (7-7) and the results in Proposition 7.1, we obtain equality (7-10). On the other hand, the fact that $u_{rt} \in L^1(Q)$ follows as in the proof of Proposition 3.12.

Finally, arguing as in the proof of Proposition 3.12, from equality (5-6), we obtain that $u_r(\cdot\,, t)$ satisfies inequality (3-12). As a consequence of (3-12) and (3-14), $u(\cdot\,, t)$ satisfies (3-15). This completes the proof. □

The proof of the following result is the same as that of [Bertsch et al. ≥ 2013, Proposition 5.6], hence we omit it.

Proposition 7.3. *Let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5). The pair (u, v) defined by Proposition 7.1 satisfies the entropy inequality (3-6).*

Proof of Theorem 3.17. Let u and v be defined by Proposition 7.1. Then $u \in L^\infty((0,T); \mathcal{M}^+(\Omega))$, $v \in L^\infty((0,T); H_0^1(\Omega))$, and $\Delta v \in L^\infty((0,T); \mathcal{M}(\Omega))$. Moreover, $[\psi(u_r)]_t \in L^\infty(Q)$ by (7-11), equality (7-10) holds, and inequality (3-1) is satisfied.

By (6-5), (6-11), (7-1), (7-3), and the dominated convergence theorem, letting $n \to \infty$ in the weak formulation of (P_n) shows that the limiting measure u satisfies equality (3-2) for any $\zeta \in C^1([0,T]; C_c(\Omega))$. The other claims follow by Propositions 7.1–7.2. This completes the proof. □

8. Proof of Theorem 3.18

Let us first prove Theorem 3.18 when $N = 1$. This is the content of the following proposition.

Proposition 8.1. *Let $N = 1$, $u_0 \in \mathcal{M}^+(\Omega)$, and let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5). Let u be the entropy solution of problem (1-1) given in Theorem 3.17 and v the chemical potential defined in (1-7). Then the pair (u, v) satisfies problem (1-18).*

Proof. Fix any $t \in (0,T)$ such that

$$\begin{aligned} u_{n_k}(\cdot\,,t) &\overset{*}{\rightharpoonup} u(\cdot\,,t) && \text{in } \mathcal{M}(\Omega),\\ u_{n_k}(\cdot\,,t) &\to u_r(\cdot\,,t) && \text{a.e. in } \Omega,\\ v_{n_k}(\cdot\,,t) &\rightharpoonup v(\cdot\,,t) && \text{in } H_0^1(\Omega) \end{aligned}$$

(see (7-1), (7-5), and (7-12)–(7-13)). By inequality (6-13) we can also assume

$$v_{n_k}(\cdot\,,t) \to v(\cdot\,,t) \quad \text{in } C(\overline{\Omega}).$$

Given $\rho \in C_c^1(\Omega)$, let us study the limit as $k \to \infty$ of the weak formulation of (6-7) with $n = n_k$, namely,

$$\varepsilon \int_\Omega v_{n_k x}(x,t)\rho_x(x)\,dx + \int_\Omega \frac{v_{n_k}(x,t)}{\psi'_{n_k}(u_{n_k}(x,t))}\rho(x)\,dx = \int_\Omega \frac{\varphi(u_{n_k}(x,t))}{\psi'_{n_k}(u_{n_k}(x,t))}\rho(x)\,dx. \tag{8-1}$$

(i) Since $\varphi \in L^q([\alpha,\infty))$ (see (1-4)) and

$$\{(1+u)[\varphi(u)]^q\}' = [\varphi(u)]^q + q[(1+u)[\varphi(u)]^{q-1}]\varphi'(u) \le [\varphi(u)]^q \quad \text{for any } u \ge \alpha,$$

we have

$$(1+u)[\varphi(u)]^q \le (1+\alpha)[\varphi(\alpha)]^q + \int_\alpha^u [\varphi(u)]^q\,ds = (1+\alpha)[\varphi(\alpha)]^q + \|\varphi\|^q_{L^q(\mathbb{R}^+)} \quad \text{for any } u \ge \alpha,$$

whence we get

$$[\varphi(u)] \le C(1+u)^{-1/q} \quad \text{for any } u \ge 0,$$

for some constant $C > 0$. It follows that

$$\frac{\varphi(u_{n_k})}{\psi'_{n_k}(u_{n_k})} \le (1+u_{n_k})\varphi(u_{n_k}) \le C(1+u_{n_k})^{1-1/q} \quad \text{a.e. in } Q. \tag{8-2}$$

Then, for every Borel set $E \subseteq \Omega$ and for a.e. $t \in (0,T)$,

$$\int_E \frac{\varphi(u_{n_k}(x,t))}{\psi'_{n_k}(u_{n_k}(x,t))}\,dx \le C\int_E [1+u_{n_k}(x,t)]^{1-1/q}\,dx \le |E|^{1/q}\left(\int_E [1+u_{n_k}(x,t)]\,dx\right)^{1-1/q}. \tag{8-3}$$

Inequalities (6-11) and (8-3) imply that the sequence

$$\left\{\frac{\varphi(u_{n_k}(\cdot,t))}{\psi'_{n_k}(u_{n_k}(\cdot,t))}\right\}$$

is bounded in $L^1(\Omega)$ and uniformly integrable in Ω. As a consequence, there exists a subsequence, for simplicity, denoted again by

$$\left\{\frac{\varphi(u_{n_k}(\cdot,t))}{\psi'_{n_k}(u_{n_k}(\cdot,t))}\right\},$$

such that

$$\frac{\varphi(u_{n_k}(\cdot,t))}{\psi'_{n_k}(u_{n_k}(\cdot,t))} \rightharpoonup \frac{\varphi(u_r(\cdot,t))}{\psi'(u_r(\cdot,t))} \quad \text{in } L^1(\Omega). \tag{8-4}$$

(ii) By inequalities (6-6) and (6-17),

$$1+u_{n_k} \le \exp\left\{\frac{\varphi(\alpha)T}{\varepsilon}\right\}(1+\sqrt{n_k}) \quad \text{a.e. in } Q. \tag{8-5}$$

Observe that

$$\left|\frac{1}{\psi'_{n_k}(u)} - \frac{1}{\psi'(u)}\right| = \frac{1}{n_k}\left(\frac{1+u}{1/(1+u)+1/n_k}\right) \le \frac{(1+u)^2}{n_k}. \tag{8-6}$$

Then, by (6-11) and (8-5)–(8-6),

$$\begin{aligned}\left\| \frac{1}{\psi'_{n_k}(u_{n_k}(\cdot,t))} - \frac{1}{\psi'(u_{n_k}(\cdot,t))} \right\|_{L^1(\Omega)} &\le \frac{2}{\sqrt{n_k}} \exp\left\{\frac{\varphi(\alpha)T}{\varepsilon}\right\} \int_\Omega [1+u_{n_k}(x,t)]dx \\ &\le \frac{2}{\sqrt{n_k}} \exp\left\{\frac{\varphi(\alpha)T}{\varepsilon}\right\} [|\Omega| + \|u_0\|_{\mathcal{M}(\Omega)}] \to 0 \quad \text{as } k\to\infty. \end{aligned} \tag{8-7}$$

Since $v_{n_k}(\cdot,t) \to v(\cdot,t)$ in $C(\overline{\Omega})$ and

$$\frac{1}{\psi'(u_{n_k}(\cdot,t))} = 1 + u_{n_k}(\cdot,t)) \overset{*}{\rightharpoonup} 1 + u(\cdot,t) \quad \text{in } \mathcal{M}(\Omega),$$

we have

$$\int_\Omega \frac{v_{n_k}(x,t)}{\psi'_{n_k}(u_{n_k}(x,t))} \rho(x)\,dx \to \langle [1+u(\cdot,t)],\, v(\cdot,t)\rho\rangle_\Omega. \tag{8-8}$$

Now let $k\to\infty$ in equality (8-1). By (7-5), (8-4), and (8-8), we obtain

$$\varepsilon \int_\Omega v_x(x,t)\rho_x(x)\,dx + \langle [1+u(\cdot,t)],\, \rho v(\cdot,t)\rangle_\Omega = \int_\Omega \frac{\varphi(u_r(x,t))}{\psi'(u_r(x,t))}\rho(x)\,dx.$$

Since by Definition 3.1, $v_{xx} \in L^\infty((0,T);\mathcal{M}(\Omega))$, this implies

$$-\varepsilon\langle v_{xx}(\cdot,t),\rho\rangle_\Omega + \langle [1+u(\cdot,t)],\, \rho v(\cdot,t)\rangle_\Omega = \int_\Omega \frac{\varphi(u_r(x,t))}{\psi'(u_r(x,t))}\rho(x)\,dx$$

for a.e. $t\in(0,T)$ and any $\rho \in C_c(\Omega)$. Hence the result follows. □

To complete the proof of Theorem 3.18, let us prove the following result.

Proposition 8.2. *Let $u_0 \in \mathcal{M}^+(\Omega)$, and let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5). Let u be the entropy solution of problem (1-1) given in Theorem 3.17 and v the chemical potential defined in (1-7). Let $N\ge 2$, and let u_0 satisfy the following assumptions*:

(i) *$[u_0]_{c,2}$ is concentrated on some compact $K_0 \subset \Omega$ such that $C_2(K_0)=0$;*

(ii) *$[u_0]_{d,2} \in \mathcal{M}^+_{d,p}(\Omega)$ for some $p\in[1,2)$.*

Then the pair (u,v) satisfies problem (1-9).

The main step in the proof of Proposition 8.2 is given by the following lemma.

Lemma 8.3. *Let $\varphi \in C^\infty([0,\infty))$ satisfy (1-3)–(1-5). Let $\{u_{n_k}\}$, $\{v_{n_k}\}$ be the subsequences given by Proposition 7.1. Then, for every $\rho \in C^1_c(\Omega)$,*

$$\lim_{k\to\infty} \int_\Omega [1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx = \langle [1+u(\cdot,t)]_{d,2},\, v(\cdot,t)\rho\rangle_\Omega. \tag{8-9}$$

Proof of Proposition 8.2. Fix any $t\in(0,T)$ such that the convergence in (7-1) and (7-5) hold, namely,

$$\begin{aligned} u_{n_k}(\cdot,t) &\overset{*}{\rightharpoonup} u(\cdot,t) && \text{in } \mathcal{M}(\Omega),\\ v_{n_k}(\cdot,t) &\rightharpoonup v(\cdot,t) && \text{in } H^1_0(\Omega),\\ u_{n_k}(\cdot,t) &\to u_r(\cdot,t) && \text{a.e. in } \Omega \end{aligned}$$

(see (7-12)–(7-13)). Consider the weak formulation of (6-7) with $n = n_k$, namely,

$$\varepsilon \int_\Omega \nabla v_{n_k}(x,t)\cdot\nabla\rho(x)\,dx + \int_\Omega \frac{v_{n_k}(x,t)}{\psi'_{n_k}(u_{n_k}(x,t))}\rho(x)\,dx = \int_\Omega \frac{\varphi(u_{n_k}(x,t))}{\psi'_{n_k}(u_{n_k}(x,t))}\rho(x)\,dx \tag{8-10}$$

where $\rho \in C^1_c(\Omega)$. Arguing as in the proof of Proposition 8.1, it is easily seen that

$$\lim_{k\to\infty}\int_\Omega \nabla v_{n_k}(x,t)\cdot\nabla\rho(x)\,dx = \int_\Omega \nabla v(x,t)\cdot\nabla\rho(x)\,dx;$$
$$\lim_{k\to\infty}\int_\Omega \frac{\varphi(u_{n_k}(x,t))}{\psi'_{n_k}(u_{n_k}(x,t))}\rho(x)\,dx = \int_\Omega \frac{\varphi(u_r(x,t))}{\psi'(u_r(x,t))}\rho(x)\,dx;$$
$$\lim_{k\to\infty}\left\| \frac{1}{\psi'_{n_k}(u_{n_k}(\cdot,t))} - \frac{1}{\psi'(u_{n_k}(\cdot,t))}\right\|_{L^1(\Omega)} = 0.$$

thus

$$\lim_{k\to\infty}\int_\Omega \frac{v_{n_k}(x,t)}{\psi'_{n_k}(u_{n_k}(x,t))}\rho(x)\,dx = \lim_{k\to\infty}\int_\Omega \frac{v_{n_k}(x,t)}{\psi'(u_{n_k}(x,t))}\rho(x)\,dx$$

(here we use (6-8)). Then, by Lemma 8.3, the conclusion follows. □

The proof of Lemma 8.3, which was used in the proof of Proposition 8.2, requires a few intermediate steps. Let $K_0 \subset \Omega$, $C_2(K_0) = 0$, be a compact set where $[u_0]_{c,2}$ is concentrated. Then for every $\delta > 0$ there exists an open set $\Omega^c_\delta \subseteq \Omega$ such that

$$K_0 \subset \Omega^c_\delta, \quad C_2(\Omega^c_\delta) < \delta. \tag{8-11}$$

Set

$$\Omega^d_\delta := \Omega \setminus \Omega^c_\delta. \tag{8-12}$$

Moreover, observe that the convergence in (7-5) guarantees the existence of a compact set $E_\delta \subseteq \Omega^d_\delta$ such that

$$C_p(E^c_\delta) < \delta, \qquad \text{where } E^c_\delta := \Omega^d_\delta \setminus E_\delta \tag{8-13}$$

and $p \in [1,2)$ is chosen so that $[u_0]_{d,2} \in \mathcal{M}^+_{d,p}(\Omega)$, and

$$v_{n_k}(\cdot,t) \to v(\cdot,t) \quad \text{uniformly in } E_\delta. \tag{8-14}$$

By (8-12) and the definition in (8-13), we have the disjoint union

$$\Omega = \Omega^c_\delta \cup E^c_\delta \cup E_\delta.$$

Therefore

$$\int_\Omega [1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx = \int_{\Omega^c_\delta}[1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx + \int_{E^c_\delta}[1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx + \int_{E_\delta}[1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx. \tag{8-15}$$

Concerning the first two integrals in the right-hand side of (8-15), we have the following two lemmata, whose proofs will be given at the end of this section.

Lemma 8.4. *Let $\Omega_\delta^c \subseteq \Omega$ be the set in (8-11), and $\rho \in C_c^1(\Omega)$. Then there exists a function*

$$f_1 = f_1(\delta) \geq 0$$

with $f_1(\delta) \to 0$ as $\delta \to 0$, such that

$$\limsup_{k\to\infty} \int_{\Omega_\delta^c} [1 + u_{n_k}(x,t)] v_{n_k}(x,t) |\rho(x)| \, dx \leq f_1(\delta). \tag{8-16}$$

Lemma 8.5. *Let E_δ^c be the set in (8-13), and $\rho \in C_c^1(\Omega)$. Then there exists a function $f_2 = f_2(\delta) \geq 0$, $f_2(\delta) \to 0$ as $\delta \to 0$, such that*

$$\limsup_{k\to\infty} \int_{E_\delta^c} [1 + u_{n_k}(x,t)] v_{n_k}(x,t) |\rho(x)| \, dx \leq f_2(\delta). \tag{8-17}$$

We also prove the following result.

Lemma 8.6. *Let $\rho \in C_c^1(\Omega)$ and let $\phi_\delta \in C_c^\infty(\Omega)$ such that*

$$\begin{cases} 0 \leq \phi_\delta \leq 1 & \text{a.e. in } \Omega, \\ \phi_\delta = 1 & \text{a.e. in } E_\delta, \\ \operatorname{dist}(K_0, \operatorname{supp} \phi_\delta) > 0. \end{cases} \tag{8-18}$$

Then there exists a function $f_3 = f_3(\delta) \geq 0$, $f_3(\delta) \to 0$ as $\delta \to 0$, such that

$$\limsup_{k\to\infty} \int_{\Omega_\delta^c \cup E_\delta^c} [1 + u_{n_k}(x,t)] v(x,t) \phi_\delta(x) |\rho(x)| \, dx \leq f_3(\delta), \tag{8-19}$$

Relying on the above results we can prove Lemma 8.3.

Proof of Lemma 8.3. For every $k \in \mathbb{N}$ we have

$$\begin{aligned}
&\left| \int_\Omega [1 + u_{n_k}(x,t)] v_{n_k}(x,t) \rho(x) \, dx - \langle [1 + u(\cdot,t)]_{d,2}, v(\cdot,t)\rho \rangle_\Omega \right| \\
&\qquad \leq \left| \int_{E_\delta} [1 + u_{n_k}(x,t)] v_{n_k}(x,t) \rho(x) \, dx - \langle [1 + u(\cdot,t)]_{d,2}, v(\cdot,t)\rho \rangle_\Omega \right| \\
&\qquad\qquad + \int_{\Omega_\delta^c \cup E_\delta^c} [1 + u_{n_k}(x,t)] v_{n_k}(x,t) |\rho(x)| \, dx \\
&\qquad \leq \int_{E_\delta} [1 + u_{n_k}(x,t)] |v_{n_k}(x,t) - v(x,t)| |\rho(x)| \, dx \\
&\qquad\qquad + \left| \int_\Omega [1 + u_{n_k}(x,t)] v(x,t) \phi_\delta(x) \rho(x) \, dx - \langle [1 + u(\cdot,t)]_{d,2}, v(\cdot,t)\phi_\delta \rho \rangle_\Omega \right| \\
&\qquad\qquad + \int_{\Omega_\delta^c \cup E_\delta^c} [1 + u_{n_k}(x,t)] [v_{n_k}(x,t) + v(x,t)\phi_\delta(x)] |\rho(x)| \, dx \\
&\qquad\qquad + |\langle [1 + u(\cdot,t)]_{d,2}, (1 - \phi_\delta) v(\cdot,t) |\rho| \rangle_\Omega|;
\end{aligned} \tag{8-20}$$

here we have used the equality (recall that $\phi_\delta = 1$ a.e. in E_δ)

$$\int_{E_\delta}[1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx=\int_{E_\delta}[1+u_{n_k}(x,t)]v_{n_k}(x,t)\phi_\delta(x)\rho(x)\,dx$$
$$=\int_\Omega[1+u_{n_k}(x,t)]v_{n_k}(x,t)\phi_\delta(x)\rho(x)\,dx-\int_{\Omega_\delta^c\cup E_\delta^c}[1+u_{n_k}(x,t)]v_{n_k}(x,t)\phi_\delta(x)\rho(x)\,dx.$$

By (6-11) and (8-14), we have

$$\lim_{k\to\infty}\int_{E_\delta}[1+u_{n_k}(x,t)]|v_{n_k}(x,t)-v(x,t)|\rho(x)\,dx=0;$$

while by (8-16)–(8-19),

$$\limsup_{k\to\infty}\int_{\Omega_\delta^c\cup E_\delta^c}[1+u_{n_k}(x,t)][v_{n_k}(x,t)+v(x,t)\phi_\delta(x)]|\rho(x)|\,dx\le f_1(\delta)+f_2(\delta)+f_3(\delta).$$

Moreover, observe that, by (8-11) and (8-13),

$$C_p(\Omega_c^\delta\cup E_\delta^c)\le C_p(\Omega_c^\delta)+C_p(E_\delta^c)\le AC_2(\Omega_\delta^c)+C_p(E_\delta^c)<(A+1)\delta \tag{8-21}$$

for some constant $A>0$ (here we used the condition $p<2$). Since the support of the function $(1-\phi_\delta)$ is contained in the set $\Omega_c^\delta\cup E_\delta^c$, by (8-21) and the assumption $[u_0]_{d,2}\in\mathcal{M}^+_{d,p}(\Omega)$, there exists a function $f_4=f_4(\delta)\ge 0$, $f_4(\delta)\to 0$ as $\delta\to 0$, such that

$$\left|\left\langle[1+u(\,\cdot\,,t)]_{d,2},(1-\phi_\delta)v(\,\cdot\,,t)|\rho|\right\rangle_\Omega\right|\le f_4(\delta). \tag{8-22}$$

In addition, we prove that

$$\lim_{k\to\infty}\int_\Omega[1+u_{n_k}(x,t)]v(x,t)\phi_\delta(x)\rho(x)\,dx=\langle[1+u(\,\cdot\,,t)]_{d,2},v(\,\cdot\,,t)\phi_\delta\rho\rangle_\Omega. \tag{8-23}$$

Then, from (8-20), we obtain

$$\limsup_{k\to\infty}\left|\int_\Omega[1+u_{n_k}(x,t)]v_{n_k}(x,t)\rho(x)\,dx-\langle[1+u(\,\cdot\,,t)]_{d,2},v(\,\cdot\,,t)\rho\rangle_\Omega\right|$$
$$\le f_1(\delta)+f_2(\delta)+f_3(\delta)+f_4(\delta)\qquad\text{for any }\delta>0. \tag{8-24}$$

By the arbitrariness of δ the conclusion follows.

It remains to prove equality (8-23). By the weak formulation of (P_n), we have

$$\int_\Omega u_{n_k}(x,t)v(x,t)\phi_\delta(x)\rho(x)\,dx$$
$$=-\int_0^t\int_\Omega\nabla v_{n_k}(x,s)\cdot\nabla[v(x,t)\phi_\delta(x)\rho(x)]\,dx\,ds+\int_\Omega u_{0n_k}(x)v(x,t)\phi_\delta(x)\rho(x)\,dx, \tag{8-25}$$

where

$$\int_\Omega u_{0n_k}v(x,t)\phi_\delta(x)\rho(x)\,dx=\int_\Omega([u_0]_{d,2})_{n_k}v(x,t)\phi_\delta(x)\rho(x)\,dx \tag{8-26}$$

for every k large enough, since $\operatorname{dist}(K_0,\operatorname{supp}\phi_\delta)>0$ and K_0 is the set where $[u_0]_{c,2}$ is concentrated. Therefore, by (7-4), letting $k\to\infty$ in equality (8-25), we have

$$\lim_{k\to\infty}\int_\Omega u_{n_k}(x,t)v(x,t)\phi_\delta(x)\rho(x)\,dx$$
$$= -\int_0^t\int_\Omega \nabla v(x,s)\cdot\nabla[v(x,t)\phi_\delta(x)\rho(x)]\,dx\,ds + \langle [u_0]_{d,2}, v(\,\cdot\,,t)\phi_\delta\rho\rangle_\Omega. \quad (8\text{-}27)$$

On the other hand, in view of (3-7), equality (4-1) gives

$$\langle [u(\,\cdot\,,t)]_{d,2},\rho\rangle_\Omega - \langle [u_0]_{d,2},\rho\rangle_\Omega = \int_0^t \langle \Delta v(\,\cdot\,,s),\rho\rangle_\Omega\,ds,$$

which makes sense for any $\rho\in H_0^1(\Omega)\cap L^\infty(\Omega)$. Therefore we can choose $v(\,\cdot\,,t)\phi_\delta\rho$ as a test function, obtaining

$$\langle [u(\,\cdot\,,t)]_{d,2}, v(\,\cdot\,,t)\phi_\delta\rho\rangle_\Omega - \langle [u_0]_{d,2}, v(\,\cdot\,,t)\phi_\delta\rho\rangle_\Omega = -\int_0^t\int_\Omega \nabla v(x,s)\cdot\nabla[v(x,t)\phi_\delta(x)\rho(x)]\,dx\,ds.$$

Comparing this equality with (8-27), we obtain (8-23). This completes the proof. □

Finally, let us prove Lemmata 8.4–8.6.

Proof of Lemma 8.4. Since $C_2(\Omega_c^\delta)<\delta$, there exists $\eta_\delta\in H_0^1(\Omega)$ such that

$$\begin{cases} \|\eta_\delta\|_{H_0^1(\Omega)} \le 2\delta, & \\ 0\le \eta_\delta\le 1 & \text{a.e. in } \Omega,\\ \eta_\delta = 1 & \text{a.e. in } \Omega_c^\delta. \end{cases}$$

By (8-5)–(8-6), we have

$$\int_{\Omega_\delta^c}[1+u_{n_k}(x,t)]v_{n_k}(x,t)|\rho(x)|\,dx$$
$$\le \int_\Omega\left|\frac{1}{\psi'(u_{n_k})}-\frac{1}{\psi'_{n_k}(u_{n_k})}\right|(x,t)v_{n_k}(x,t)|\rho(x)|\eta_\delta(x)\,dx + \int_\Omega \frac{v_{n_k}}{\psi'_{n_k}(u_{n_k})}(x,t)|\rho(x)|\eta_\delta(x)\,dx$$
$$\le C\int_\Omega \eta_\delta\,dx + \int_\Omega \frac{v_{n_k}}{\psi'_{n_k}(u_{n_k})}(x,t)|\rho(x)|\eta_\delta(x)\,dx.$$

Since $|\rho|\eta_\delta\in H_0^1(\Omega)$, by (6-7) we get

$$\int_{\Omega_\delta^c}[1+u_{n_k}(x,t)]v_{n_k}(x,t)|\rho(x)|\,dx$$
$$\le \epsilon\int_\Omega |\nabla v_{n_k}(x,t)|\,|\nabla(|\rho|\eta_\delta)|\,dx + \int_\Omega \frac{\varphi(u_{n_k})}{\psi'_{n_k}(u_{n_k})}(x,t)|\rho(x)|\eta_\delta(x)\,dx + C\int_\Omega \eta_\delta(x)\,dx,$$

whence we get

$$\int_{\Omega_\delta^c}[1+u_{n_k}(x,t)]v_{n_k}(x,t)|\rho(x)|\,dx \le C_1\|\,|\rho|\eta_\delta\|_{H_0^1(\Omega)} + C_2\int_\Omega u_{n_k}^{1-1/q}(x,t)\eta_\delta(x)\,dx + C\int_\Omega \eta_\delta(x)\,dx$$
$$\le \widetilde{C}\left[\|\,|\rho|\eta_\delta\|_{H_0^1(\Omega)} + \left(\int_\Omega \eta_\delta^q(x)\,dx\right)^{1/q} + \int_\Omega \eta_\delta(x)\,dx\right]$$

(here we used (6-11), (6-13), and (8-2)). Setting

$$f_1(\delta) := \widetilde{C}\left[\| |\rho| \eta_\delta \|_{H_0^1(\Omega)} + \left(\int_\Omega \eta_\delta^q(x)\,dx \right)^{1/q} + \int_\Omega \eta_\delta(x)\,dx \right],$$

the conclusion follows. □

Proof of Lemma 8.5. By (6-16) (see also Remark 3.14) we obtain

$$\begin{aligned} \int_{E_\delta^c} [1+u_{n_k}(x,t)] v_{n_k}(x,t) |\rho(x)|\,dx &\le C_1 \int_{E_\delta^c} [1+u_{0n_k}(x)] v_{n_k}(x,t) |\rho(x)|\,dx \\ &\le C_1 \int_{E_\delta^c} u_{0n_k}(x) v_{n_k}(x,t) |\rho(x)|\,dx + C_2 |E_\delta^c|. \end{aligned} \tag{8-28}$$

Moreover, by the definition of the sequence $\{u_{0n}\}$ in Lemma 6.1, we have

$$u_{0n_k} = ([u_0]_{c,2})_{n_k} + ([u_0]_{d,2})_{n_k},$$

where

$$([u_0]_{d,2})_{n_k} := u_{0rn_k} + ([u_{0s}]_{d,2})_{n_k},$$

and

$$\int_{E_\delta^c} ([u_0]_{c,2})_{n_k}(x)\,dx = 0 \tag{8-29}$$

holds for every k large enough. In fact, recall that the sequence $([u_0]_{c,2})_n$ is defined by convolution, $[u_0]_{c,2}$ is concentrated on the compact set $K_0 \subset \Omega_\delta^c$, the set Ω_δ^c is open, and $E_\delta^c \subseteq \Omega \setminus \Omega_\delta^c$. Combining (8-28) with (8-29) gives

$$\int_{E_\delta^c} [1+u_{n_k}(x,t)] v_{n_k}(x,t) |\rho(x)|\,dx \le C_1 \int_{E_\delta^c} ([u_0]_{d,2})_{n_k}(x) v_{n_k}(x,t) |\rho(x)|\,dx + C_2 |E_\delta^c| \tag{8-30}$$

for every k sufficiently large. Moreover, since $C_p(E_\delta^c) < \delta$ (see (8-13)) there exists $\rho_\delta \in H_0^{1,p}(\Omega)$ such that

$$\begin{cases} \|\rho_\delta\|_{H_0^{1,p}(\Omega)} \le 2\delta, \\ 0 \le \rho_\delta \le 1 & \text{a.e. in } \Omega, \\ \rho_\delta = 1 & \text{a.e. in } E_\delta^c. \end{cases}$$

By the above remarks, using inequality (6-8), we obtain

$$\int_{E_\delta^c} ([u_0]_{d,2})_{n_k}(x) v_{n_k}(x,t) |\rho(x)|\,dx \le C_3 \int_\Omega ([u_0]_{d,2})_{n_k}(x) \rho_\delta(x) |\rho(x)|\,dx. \tag{8-31}$$

Since, by assumption, $[u_0]_{d,2} \in \mathcal{M}_{d,p}^+(\Omega)$, by the first convergence in (6-4) we have

$$\lim_{k\to\infty} \int_\Omega ([u_0]_{d,2})_{n_k}(x) \rho_\delta(x) |\rho(x)|\,dx = \langle [u_0]_{d,2}, \rho_\delta |\rho| \rangle_\Omega.$$

Hence, by (8-30) and (8-31), we obtain

$$\limsup_{k\to\infty}\int_{E_\delta^c}[1+u_{n_k}(x,t)]v_{n_k}(x,t)|\rho(x)|\,dx \le C_2|E_\delta^c| + C_3\langle [u_0]_{d,2},\rho_\delta|\rho|\rangle_\Omega. \tag{8-32}$$

Then, setting

$$f_2(\delta) := C_2|E_\delta^c| + C_3\langle [u_0]_{d,2},\rho_\delta|\rho|\rangle_\Omega,$$

by (8-32) and the assumption $[u_0]_{d,2}\in\mathcal{M}^+_{d,p}(\Omega)$, the conclusion follows. □

Proof of Lemma 8.6. By (6-16) (see also Remark 3.14), for every k sufficiently large we have

$$\begin{aligned}\int_{\Omega_\delta^c\cup E_\delta^c}[1+u_{n_k}(x,t)]v(x,t)\phi_\delta(x)|\rho(x)|\,dx &\le C\int_{\Omega_\delta^c\cup E_\delta^c} u_{0n_k}(x)v(x,t)\phi_\delta(x)|\rho(x)|\,dx\\ &= C\int_{\Omega_\delta^c\cup E_\delta^c}([u_0]_{d,2})_{n_k}(x)v(x,t)\phi_\delta(x)|\rho(x)|\,dx.\end{aligned} \tag{8-33}$$

In fact, for k sufficiently large

$$\int_{\Omega_\delta^c\cup E_\delta^c}([u_0]_{c,2})_{n_k}(x)v(x,t)\phi_\delta(x)|\rho(x)|\,dx = 0,$$

since $\operatorname{dist}(K_0,\operatorname{supp}\phi_\delta)>0$ and $[u_0]_{c,2}$ is concentrated on K_0.

Let $g_\delta\in H_0^{1,p}(\Omega)$ be any function such that

$$\begin{cases}\|g_\delta\|_{H_0^{1,p}(\Omega)}\le 4\delta, & \\ 0\le g_\delta\le 1 & \text{a.e. in } \Omega,\\ g_\delta = 1 & \text{a.e. in } \Omega\setminus E_\delta.\end{cases}$$

In view of (8-21), since $[u_0]_{d,2}\in\mathcal{M}^+_{d,p}(\Omega)$, we have

$$\begin{aligned}\limsup_{k\to\infty}\int_{\Omega_\delta^c\cup E_\delta^c}([u_0]_{d,2})_{n_k}(x)v(x,t)\phi_\delta(x)|\rho(x)|\,dx &\le C\lim_{k\to\infty}\int_\Omega([u_0]_{d,2})_{n_k}(x)g_\delta(x)\,dx\\ &= C\langle [u_0]_{d,2},g_\delta\rangle_\Omega.\end{aligned} \tag{8-34}$$

Since

$$f_3(\delta) := C\langle [u_0]_{d,2},g_\delta\rangle_\Omega \to 0 \quad \text{as } \delta\to 0,$$

by (8-33)–(8-34), the conclusion follows. □

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THE HEAT KERNEL ON AN ASYMPTOTICALLY CONIC MANIFOLD

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We investigate the long-time structure of the heat kernel on a Riemannian manifold M that is asymptotically conic near infinity. Using geometric microlocal analysis and building on results of Guillarmou and Hassell, we give a complete description of the asymptotic structure of the heat kernel in all spatial and temporal regimes. We apply this structure to define and investigate a renormalized zeta function and determinant of the Laplacian on M.

1. Introduction

We study the heat kernel on asymptotically conic manifolds. Asymptotically conic manifolds should be thought of as those complete manifolds which are approximately conic near infinity. More specifically:

Definition [Guillarmou and Hassell 2008]. Let (M, g) be a complete Riemannian manifold without boundary of dimension n, and let $\overline{M}$ be the usual radial compactification of M. Let (N, h_0) be a closed Riemannian manifold of dimension $n-1$. We say that (M, g) is asymptotically conic with cross-section (N, h_0) if in a neighborhood of $\partial\overline{M}$, $\overline{M}$ is isometric to $[0, \delta)_x \times N_y$ with the metric

$$g = \frac{dx^2}{x^4} + \frac{h(x)}{x^2}. \tag{1}$$

Here x is a smooth function on $\overline{M}$ with $x = 0$ and $dx \neq 0$ on $\partial\overline{M}$ (we call this a *boundary defining function* for $\partial\overline{M}$) and a smooth family of metrics $h(x)$ on N with $h(0) = h_0$. Throughout, we let z be a global coordinate on M, writing $z = (x, y)$ in a neighborhood of the boundary of $\overline{M}$.

In particular, Euclidean space $\mathbb{R}^n$ is asymptotically conic with cross-section S^{n-1}; we may choose $x = r^{-1}$. Any complete manifold which is exactly Euclidean or conic near infinity is, of course, also asymptotically conic. The condition (1) may be weakened by replacing $h(x)$ with any symmetric 2-tensor $h'(x, y)$ which restricts to a metric $h_0(x)$ on the boundary at $x = 0$; an observation of Melrose and Wunsch [2004] shows that these conditions are in fact equivalent.

Asymptotically conic manifolds are a relatively well-behaved class of manifolds, and as such the theory of the heat equation is relatively advanced. In particular, it is easy to see from (1) that all sectional curvatures of (M, g) approach zero as x goes to zero, and thus that (M, g) has bounded sectional curvature. For complete manifolds of bounded sectional curvature, a classical theorem of Cheng, Li, and Yau gives the following Gaussian upper bound for the heat kernel:

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Theorem 1 [Cheng et al. 1981]. *There are nonzero constants C_1 and C_2 such that the heat kernel on M, denoted $H^M(t,z,z')$, satisfies*

$$H^M(t,z,z') \leq \frac{C_1}{t^{n/2}} e^{-|z-z'|^2/C_2 t}. \tag{2}$$

However, for many applications to spectral theory, one needs finer information about the structure of the heat kernel. The example we have in mind is the definition of the zeta function. Recall that if M is compact, the zeta function is defined for $\Re s > n/2$ by

$$\zeta_M(s) = \frac{1}{\Gamma(s)} \int_0^\infty (\operatorname{Tr} H^M(t) - 1)\, t^{s-1}\, dt. \tag{3}$$

The zeta function has a well-known meromorphic continuation to all of $\mathbb{C}$ with a regular value at $s=0$; the key is that the trace of the heat kernel has a short-time asymptotic expansion, which, along with the long-time exponential decay, enables us to write down an explicit meromorphic continuation [Rosenberg 1997]. The *determinant of the Laplacian* is then given by $\exp(-\zeta_M'(0))$; the determinant plays a key role in many problems in spectral theory, including the isospectral compactness results of Osgood, Phillips, and Sarnak [1988b; 1988a; 1989].

We would like to define such a zeta function and determinant when M is asymptotically conic, with an eye towards applying these concepts to the spectral and scattering theory of asymptotically conic manifolds. There are several obstacles. First, the heat kernel is no longer trace class, so $\operatorname{Tr} H^M(t)$ does not make sense. Instead, we define the *renormalized heat trace* ${}^R\operatorname{Tr} H^M(t)$ to be the finite part at $\delta = 0$ of the divergent asymptotic expansion in δ of

$$\int_{x \geq \delta} H^M(t,z,z)\, dz. \tag{4}$$

Details, including the existence of this divergent asymptotic expansion, may be found in Section 3. We then formally define the *renormalized zeta function*:

$${}^R\zeta_M(s) = \frac{1}{\Gamma(s)} \int_0^\infty {}^R\operatorname{Tr} H^M(t)\, t^{s-1}\, dt. \tag{5}$$

However, to make sense of this definition and obtain a meromorphic continuation, we still need to understand the behavior of the renormalized trace — and hence of the heat kernel itself — as $t \to 0$ and $t \to \infty$. In particular, we need asymptotics in both the short and long time regimes.

The short-time behavior of the heat kernel on an asymptotically conic manifold is relatively well-understood. Short-time heat kernels may be analyzed using techniques from semiclassical analysis. In this approach, the goal is to develop a "semiclassical functional calculus" containing the heat kernel, modeled on standard semiclassical techniques as developed, for example, in [Dimassi and Sjöstrand 1999]. The key functional calculus for this purpose, at least in the asymptotically Euclidean setting, is the Weyl calculus of Hörmander [1979].

An alternate approach, and one more suited to analysis of the renormalized trace and determinant, is to use geometric microlocal analysis to first construct the heat kernel and then analyze its fine structure. The techniques of geometric microlocal analysis were first developed by Melrose and Mendoza [1983] to study elliptic PDE on manifolds with asymptotically cylindrical ends. They have been extended by many other mathematicians and play a key role in the modern analysis of linear PDE on singular and non-compact spaces. In particular, Melrose [1994] discusses some aspects of spectral and scattering theory on asymptotically conic manifolds. Albin [2007] uses these methods to investigate the short-time heat kernel on a variety of complete spaces, including asymptotically conic manifolds. His work can be used to obtain the fine structure that we need for the short-time heat kernel.

The long-time problem is trickier: in the asymptotically conic setting, we no longer have exponential decay of the heat kernel as $t \to \infty$. Indeed, from the structure of the Euclidean heat kernel and (2), we expect that the leading-order behavior of $H^M(t, z, z')$ as $t \to \infty$ will be $Ct^{-n/2}$, and the leading-order behavior of the renormalized heat trace may be even worse. This lack of decay means that the zeta function may not be well-defined a priori for any s. We may split (5) into two integrals by breaking it up at $t = 1$, but there is no obvious reason for the integral from $t = 1$ to ∞ to have a meromorphic continuation to all of $\mathbb{C}$. In order to obtain such a meromorphic continuation, we need an asymptotic expansion for the heat kernel as $t \to \infty$. Moreover, we must understand how this expansion interacts with the heat trace renormalization.

1.1. ***Main results.*** We solve this problem by using the methods of geometric microlocal analysis to obtain a complete description of the asymptotic structure of the heat kernel on M in all spatial and temporal regimes. The key concepts, including blow-ups and polyhomogeneous conormal functions, were originally introduced by Melrose [1993; 1996], and a good introduction may be found in [Grieser 2001]. In Section 2, we discuss these concepts briefly and then use them to define a new blown-up manifold with corners which we call $M^2_{w,\mathrm{sc}}$. The space $M^2_{w,\mathrm{sc}}$ was originally defined by Guillarmou and Hassell [2008], and we use their labeling of the boundary hypersurfaces; see Section 2 for the definitions. Our main theorem is the following:

Theorem 2. *Let M be asymptotically conic. For any $n \geq 2$, and for any fixed time $T > 0$, the heat kernel on M is polyhomogeneous conormal on $M^2_{w,\mathrm{sc}}$ for $t > T$, where $w = t^{-1/2}$. The leading orders at the boundary hypersurfaces are at least* 0 *at* sc *and n at each of* bf_0, rb_0, lb_0, *and* zf, *with infinite-order decay at* lb, rb, *and* bf.

This theorem gives a complete description of the asymptotic structure of the heat kernel for long time; previously, only estimates such as Theorem 1 were known. The analogous structure for the short-time heat kernel is well-understood (see Section 2 for the definition of M^2_{sc}):

Theorem 3. *For $t < 1$, the heat kernel $H^M(t, z, z')$ is polyhomogeneous conormal on*

$$\left[M^2_{\mathrm{sc}}(z, z') \times [0, 1]_{\sqrt{t}}\,;\, \{\sqrt{t} = 0, z = z'\}\right].$$

Moreover, there is infinite-order decay at all faces except the scattering front face sc *and the face F obtained by the final blow-up.*

Theorem 3 follows immediately from the work of Albin [2007]; however, the precise statement above does not appear in the literature. Therefore, in the Appendix, we give a simple proof using the machinery

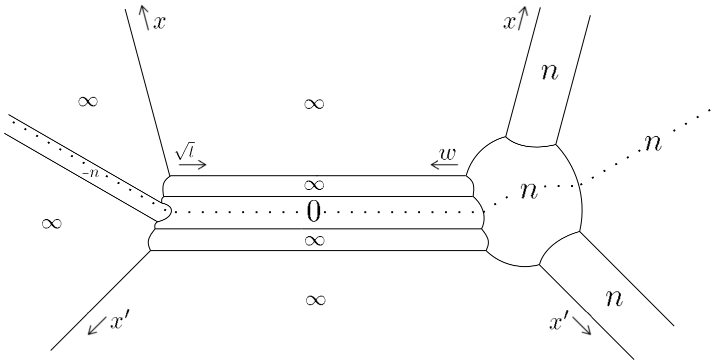

Figure 1. Asymptotic structure of the heat kernel on M.

developed in [Albin 2007]. Combining Theorem 2 with Theorem 3 gives a complete geometric-microlocal description of the structure of the heat kernel. This structure is illustrated in Figure 1; the short-time structure is the left-hand side of the diagram, and the long-time structure is the right-hand side. We also indicate the leading order of the heat kernel at each of the boundary hypersurfaces, in terms of $\sqrt{t}$ at $t=0$, $w=t^{-1/2}$ at $t=\infty$, and x or x' respectively at all the finite-time boundaries.

As an example of how polyhomogeneous structure may be used to read off the behavior in all asymptotic regimes, let a be a parameter, and fix (y, x', y'); consider the heat kernel $H^Z(a^2, a^{-1}, y, x', y')$ as a approaches infinity. In the compactified space in Figure 1, as a approaches infinity, the arguments approach a point in the center of the face lb_0, where the leading order of the heat kernel is n. Since $w=a^{-1}$, and w is a boundary defining function for lb_0, we conclude that $H^Z(a^2, a^{-1}, y, x', y')$ has a polyhomogeneous asymptotic expansion in a^{-1} as $a\to\infty$, with leading term $C_n a^{-n}$. A similar analysis may be performed in any asymptotic regime.

As an application, Theorems 2 and 3 give us precisely the polyhomogeneous structure we need to define and investigate the renormalized zeta function on M:

Theorem 4. *Let M be asymptotically conic. The renormalized zeta function, defined formally by (5), is well-defined and has a meromorphic continuation to all of $\mathbb{C}$.*

We may then define the *renormalized determinant* of the positive Laplacian Δ_M on M by

$$\log {}^R\det \Delta_M = -{}^R\zeta_M'(0),$$

where ${}^R\zeta_M'(0)$ is the coefficient of s in the Laurent series for ${}^R\zeta_M(s)$ around $s=0$.

In a companion paper [Sher 2012a], we use Theorems 2, 3, and 4 to analyze the behavior of the determinant of the Laplacian on a family of manifolds degenerating to a manifold with conical singularities. We expect that this work will have applications to spectral theory and to index theory on singular spaces, including the study of the Cheeger–Müller theorem on manifolds with conical singularities. The key theorem from [Sher 2012a] is as follows: let Ω_0 be a manifold with an exact conic singularity (with arbitrary base) and let Z be a manifold conic near infinity with the same base. For each $\epsilon>0$, we define a smooth manifold Ω_ϵ replacing the tip of Ω_0 with an ϵ-scaled copy of Z; as $\epsilon \to 0$, the manifolds Ω_ϵ converge to Ω_0 in the Gromov–Hausdorff sense. Then it is proven in [Sher 2012a] that

Theorem 5. *As* $\epsilon \to 0$,

$$\log\det\Delta_{\Omega_\epsilon} = -2\log\epsilon\,({}^R\zeta_Z(0)) + \log\det\Delta_{\Omega_0} + \log{}^R\!\det\Delta_Z + o(1).$$

1.2. ***Outline of the proofs.*** The usual geometric-microlocal approach to the fine structure of the heat kernel is a direct parametrix construction, which involves the construction of an initial approximation to the heat kernel and then the removal of the error via a Neumann series argument. This is the method adopted in [Albin 2007]. However, parametrix constructions are not well-suited for analysis of the long-time heat kernel; the problem is global rather than local. In order to obtain the asymptotic structure of the heat kernel at long time, we instead take an indirect approach. Recall that the functional calculus shows that the heat kernel and the resolvent are related by

$$H^M(t) = \frac{1}{2\pi i}\int_\Gamma e^{\lambda t}(\Delta_M + \lambda)^{-1}\,d\lambda, \tag{6}$$

where Γ is a contour around the spectrum. Guillarmou and Hassell [2008; 2009] have analyzed the asymptotic structure of the resolvent $(\Delta_M + \lambda)^{-1}$ at low energy, again giving a complete description in all regimes. They have shown:

Theorem 6 [Guillarmou and Hassell 2008]. *Suppose that M is an asymptotically conic manifold of dimension $n \geq 3$. Then the Schwartz kernel of $(\Delta_M + e^{i\theta}k^2)^{-1}$ is polyhomogeneous conormal on $M^2_{k,\mathrm{sc}}$ for each $\theta \in (-\pi, \pi)$, with a conormal singularity at the spatial diagonal and all coefficients smoothly depending on θ. It decays to infinite order at the faces* lb, rb, *and* bf, *with leading orders at* sc, bf_0, rb_0, lb_0 *and* zf *given by* 0, $n-2$, $n-2$, $n-2$, *and* 0 *respectively.*

Note that Guillarmou and Hassell require $n \geq 3$. In Section 4, we adapt their methods to extend Theorem 6 to the two-dimensional case:

Theorem 7. Theorem 6 *also holds when $n = 2$; all the leading orders are the same, except that we have logarithmic growth instead of order* 0 *at* zf.

In Section 2, we use geometric microlocal analysis, in particular Melrose's pushforward theorem, to prove Theorem 2. The key is to push the structure of Theorems 6 and 7 through the contour integral (6). To state the main technical theorem, we must first compactify $M^2_{k,\mathrm{sc}}$ to $\overline{M}^2_{k,\mathrm{sc}}$ by introducing a new boundary face at $k = \infty$, with boundary defining function k^{-1}. In a neighborhood of the new face, which we call tf, $\overline{M}^2_{k,\mathrm{sc}}$ is $M^2_{\mathrm{sc}} \times [0, 1)_{k^{-1}}$. The main technical theorem is this:

Theorem 8. *Let M be an asymptotically conic manifold, and let E be a vector bundle over M. Let $A : C^\infty(E) \to C^{-\infty}(E)$ be a pseudodifferential operator with the following properties*:

(a) $\sigma(A) \subset [0, \infty]$.

(b) (*Low-energy resolvent behavior*) *If k is bounded above, the Schwartz kernel of the resolvent $(A + e^{i\theta}k^2)^{-1}$ is polyhomogeneous conormal on $M^2_{k,\mathrm{sc}}$ for each $\theta \in (-\pi, \pi)$, with a conormal* *singularity at the spatial diagonal and all coefficients smoothly depending on* θ. *Moreover, it decays to infinite order at the faces* lb, rb, *and* bf, *with index sets at* sc, bf_0, rb_0, lb_0, *and* zf *given by* R_{sc}, R_{bf_0}, R_{rb_0}, R_{lb_0}, *and* R_{zf} *respectively.*

(c) (*High-energy resolvent behavior*) *For each* $\theta \in (-\pi, \pi)$ *and for* k *bounded below, the Schwarz kernel of* $(A + e^{i\theta}k^2)^{-1}$ *is phg conormal on* $\overline{M}^2_{k,\mathrm{sc}}$, *with infinite-order decay at* lb, rb, *and* bf, *index set* R_{sc} *at* sc, *and index set* R_{tf} *at tf.*

Then for t *greater than any fixed* $T > 0$, *the kernel of* e^{-tA} *is polyhomogeneous conormal on* $M^2_{w,\mathrm{sc}}$, *where* $w = t^{-1/2}$. *It decays to infinite order at* lb, rb, *and* bf, *and has index sets at* sc, bf_0, rb_0, lb_0, *and* zf *which are subsets of* R_{sc}, $R_{\mathrm{bf}_0} + 2$, $R_{\mathrm{rb}_0} + 2$, $R_{\mathrm{lb}_0} + 2$, *and* $R_{\mathrm{zf}} + 2$ *respectively.*

Once we have proven Theorem 8, Theorem 2 is an almost immediate consequence, though there is a slight twist involving the leading orders.

In Section 3, we use Theorem 2 and some additional geometric microlocal techniques to analyze the renormalized heat trace and prove Theorem 4. We also analyze the renormalized zeta function and determinant in the special case where M is exactly conic (or Euclidean) outside a compact set. In Section 4, we extend the methods of [Guillarmou and Hassell 2008] to prove Theorem 7. Finally, in the Appendix, we use the framework in [Albin 2007] to prove Theorem 3.

2. From resolvent to heat kernel

The goal of this section is to prove Theorems 8 and 2.

2.1. *Preliminaries.* We first give a brief summary of the key relevant concepts in geometric microlocal analysis; again, a self-contained introduction may be found in [Grieser 2001]. A *manifold with corners* of dimension n is a topological space which is locally modeled on $\mathbb{R}^k_+ \times \mathbb{R}^{n-k}$ for some k; a simple example is the n-dimensional unit cube. *Blow-up* is a way of creating new manifolds with corners from old ones, and is used to resolve certain geometric singularities. The idea is to formally introduce polar coordinates around a submanifold of a manifold with corners, in order to distinguish between directions of approach to that submanifold. For example, consider the origin as a submanifold of $\mathbb{R}^2_+$. To blow up the origin, we introduce polar coordinates (r, θ), which corresponds to replacing the point $(0, 0)$ with a quarter-circle, which corresponds to the inward-pointing spherical normal bundle of $(0, 0) \subset \mathbb{R}^2_+$. See [Melrose 1993; 1996; Grieser 2001], or the appendix of [Sher 2012b] for a more detailed explanation and more general examples of blow-ups.

By Taylor's theorem, smooth functions on a manifold with corners are precisely those functions which have Taylor expansions at each boundary hypersurface and joint Taylor expansions at every corner. *Polyhomogeneous conormal distributions*, which we abbreviate as phg or phg conormal, are a generalization of smooth functions. In particular, if we let x be a boundary defining function, we allow terms of the form $x^s(\log x)^p$ for any $x \in \mathbb{C}$ and any $p \in \mathbb{N}_0$ to appear in the asymptotic expansions at the boundary and in the joint expansions at the corners. The *index set* of a phg conormal distribution u at a particular boundary hypersurface H is simply the set of (s, p) which appear in the asymptotic expansion of u at H.

Polyhomogeneous conormal functions are well-behaved under addition and multiplication, but also under more complicated operations, namely pullback and pushforward. To discuss these, we first need to discuss properties of a map $f : W \to Z$ between manifolds with corners. Roughly, we say that f is a *b-map* if it is smooth up to the boundary and product-type near the boundary in terms of the local coordinate models (see [Grieser 2001] for a precise definition). If additionally f does not map any boundary hypersurface of W into a corner of Z, and f is also a fibration over the interior of every boundary hypersurface, we call f a *b-fibration*. Two results of Melrose will be critical in the analysis to follow:

Proposition 9 (Melrose's [1992] pullback and pushforward theorems). *Let $f : W \to Z$ be a smooth map of manifolds with corners.*

(a) *If f is a b-map and u is phg conormal on Z, then f^*u is phg conormal on W. Moreover, the index sets of f^*u may be computed explicitly from those of u and the geometry of the map f.*

(b) *If f is also a b-fibration, v is phg conormal on W, and f_*v is well-defined (the pushforward is integration along the fibers, which may not converge), then f_*v is phg conormal on Z, and again the index sets may be computed explicitly.*

Finally, we need to consider distributions which have pseudodifferential-type *conormal singularities* at submanifolds in the interior of a manifold with corners.

Definition [Grieser 2001]. Let $y = (x_1, \dots, x_k)$ and $z = (x_{k+1}, \dots, x_n)$, and let N be the set $\{z = 0\}$ in $\mathbb{R}^n_{y,z}$. A distribution u on $\mathbb{R}^n$ has a conormal singularity at N of order m if it can be written

$$u(y, z) = \int_{\mathbb{R}^{n-k}} e^{iz\cdot\xi} a(y, \xi)\, d\xi,$$

where a is a classical symbol; that is, a has asymptotics as $|\xi| \to \infty$

$$a(y, \xi) \sim \sum_{j=0}^{\infty} a_{m-j}\Big(y, \frac{\xi}{|\xi|}\Big)|\xi|^{m-j},$$

with each coefficient a_{m-j} smooth in y and $\xi/|\xi|$.

This definition may be extended, by using the local coordinate models, to define distributions with a conormal singularity at any *p-submanifold* of a manifold with corners; a p-submanifold is a subset which, in each local coordinate chart, may be identified with a coordinate submanifold. Variants of the pullback and pushforward theorems also hold for polyhomogeneous conormal distributions with interior conormal singularities [Melrose 1996; Epstein et al. 1991].

2.2. ***The space $M^2_{k,\mathrm{sc}}$.*** We now introduce the space $M^2_{k,\mathrm{sc}}$, which appears in [Guillarmou and Hassell 2008; 2009; Guillarmou et al. 2012] and was first proposed in an unpublished note of Melrose and Sá Barreto. To construct $M^2_{k,\mathrm{sc}}$, we begin with the space $M^2_k = [0, \infty)_k \times \overline{M} \times \overline{M}$; coordinates on this space near $[0, \infty)_k \times \partial\overline{M} \times \partial\overline{M}$ are (k, x, y, x', y'). There are three boundary hypersurfaces: $\{k = 0\}$, which we call zf, $\{x = 0\}$, which we call lb, and $\{x' = 0\}$, which we call rb.

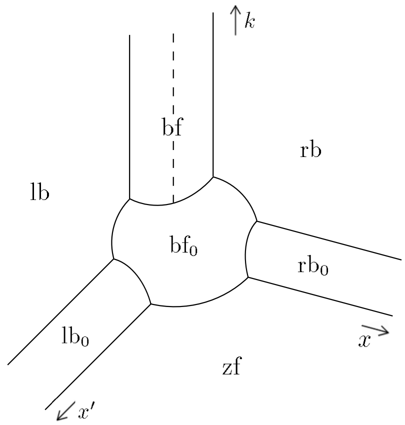

Figure 2. The space $M^2_{k,b}$.

First we blow up the corner $\{x = 0, x' = 0, k = 0\}$, which corresponds to the introduction of polar coordinates near that corner; we call the front face of this blow-up bf_0. We then blow up three codimension-2 submanifolds: we blow up $\{x = 0, x' = 0\}$ and call the new face bf, we blow up $\{x = 0, k = 0\}$ and call the resulting face lb_0, and we blow up $\{x' = 0, k = 0\}$ and call the resulting face rb_0. The resulting manifold with corners, which we call $M^2_{k,b}$ (as in [Guillarmou et al. 2012]), is shown in Figure 2, with y and y' suppressed. Using the definition of a "b-stretched product" from [Melrose and Singer 2008], we can identify this manifold near $x = 0, x' = 0$ with $X^3_b(x, x', k) \times N_y \times N_{y'}$. We use these b-stretched products X^n_b from [Melrose and Singer 2008] throughout the arguments.

Finally, consider the intersection of the closure of the interior spatial diagonal with the face bf. In coordinates near the boundary, this is $\{x/x' = 1, y = y', x/k = 0\}$, and it is marked with a dotted line in Figure 2. We blow this up to create a new boundary hypersurface, which we call sc (for "scattering"). The resulting space is $M^2_{k,\mathrm{sc}}$, and it has eight boundary hypersurfaces, illustrated in Figure 3. The spatial diagonal $D_{k,\mathrm{sc}}$ is defined to be the closure in $M^2_{k,\mathrm{sc}}$ of the interior spatial diagonal; its intersection with the boundary is marked with a dotted line in Figure 3.

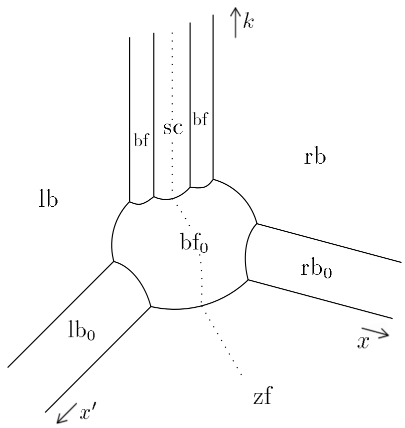

Figure 3. The space $M^2_{k,\mathrm{sc}}$.

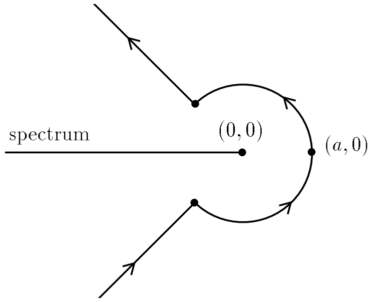

Figure 4. Contour of integration Γ_a.

We now describe some useful coordinate systems on $M^2_{k,\mathrm{sc}}$. Near the intersection of zf, rb_0, and bf_0, we use the coordinates

$$\left(x, \sigma = \frac{x'}{x}, y, y', \kappa' = \frac{k}{x}\right).$$

In these coordinates, x is a boundary defining function (bdf) for bf_0, σ is a bdf for rb_0, and κ' is a bdf for zf. Similarly, near the intersection of zf, lb_0, and bf_0, we use the coordinates

$$\left(x', \sigma' = \frac{x}{x'}, y, y', \kappa = \frac{k}{x}\right).$$

Coordinates near sc are slightly more complicated; before the final blow-up, good coordinates are $(x', \sigma', y, y', x/k)$. After the blow-up, we use the coordinates

$$\left(X = k\left(\frac{1}{x'} - \frac{1}{x}\right), Y = k\frac{y - y'}{x}, \lambda = \frac{x}{k}, y, k\right).$$

These are valid in a neighborhood of the intersection of $D_{k,\mathrm{sc}}$ with sc and bf_0; however, they are not good coordinates as we approach bf.

In addition to the b-stretched products of [Melrose and Singer 2008] and the space $M^2_{k,\mathrm{sc}}$, we also define the *scattering double space* $M^2_{\mathrm{sc}}(z, z')$, originally described in [Melrose 1994]. It is a blown-up version of $\overline{M} \times \overline{M}$; the first blow-up is of $\{x = x' = 0\}$, and the second blow-up is of the boundary fiber diagonal $\{x' = 0, x/x' = 1, y = y'\}$. Notice that each cross-section of $M^2_{k,\mathrm{sc}}$ corresponding to a fixed $k > 0$ is a copy of M^2_{sc}.

2.3. ***Proof of Theorem 8.*** Let A be an operator satisfying hypotheses (a)–(c) of Theorem 8, and let $R(\lambda, z, z')$ be the Schwartz kernel of $(A+\lambda)^{-1}$. The spectrum of A is $[0, \infty]$, so $R(\lambda, z, z')$ is holomorphic outside the non-positive real axis. Fix $\varphi \in (\pi/2, \pi)$. For any $a > 0$, let Γ_a be the path in $\mathbb{C}$ consisting of two half-rays along $\theta = -\varphi$ and $\theta = \varphi$, connected by the portion of the circle of radius a from $\theta = -\varphi$ to $\theta = \varphi$, and traversed counterclockwise. Moreover, let $\Gamma_{a,1}$ be the portion of Γ_a along the circle of radius a, and let $\Gamma_{a,2}$ be the remainder; that is, the two half-rays. These contours are illustrated in Figure 4.

Let $F(w, z, z')$ be the heat kernel at time $t = w^{-2}$. Then, by the functional calculus, we have

$$F(w, z, z') = \frac{1}{2\pi i}\int_\Gamma e^{\lambda/w^2} R(\lambda, z, z')\, d\lambda. \tag{7}$$

We let $a = w^2$ and $\Gamma = \Gamma_{w^2}$, and then consider the integral (7) over $\Gamma_{w^2,1}$ and $\Gamma_{w^2,2}$ separately.

On $\Gamma_{w^2,1}$, $\lambda = w^2 e^{i\theta}$, so $d\lambda = w^2 d\theta$, and we have

$$\frac{w^2}{2\pi i}\int_{-\varphi}^{\varphi} e^{e^{i\theta}} R(\theta, w, z, z')\, d\theta. \tag{8}$$

By condition (b), for each θ, the integrand in (8) is phg conormal on $M^2_{w,\mathrm{sc}}$ with a conormal singularity at $\Delta_{w,\mathrm{sc}}$, and the dependence of all coefficients on $\theta \in [-\varphi, \varphi]$ is smooth. Therefore, the integral (8) is phg conormal on $M^2_{w,\mathrm{sc}}$, with a possible conormal singularity at $D_{w,\mathrm{sc}}$. The index sets of (8) on $M^2_{w,\mathrm{sc}}$ are those of w^2 plus those of $R(w, z, z')$. The function w^2 is smooth and has order 2 as a function at zf, bf_0, rb_0, and lb_0 and order 0 everywhere else, so we add 2 to the index sets of the resolvent at those faces. This procedure gives precisely the index sets claimed in Theorem 8.

It remains to consider the integral over $\Gamma_{w^2,2}$. $\Gamma_{w^2,2}$ consists of two half-rays; we consider only the half-ray corresponding to $\theta = \varphi$, as the other is analogous. Since θ is fixed, we suppress θ in the notation; the integral runs from $r = w^2$ to $r = \infty$. After changing variables from r to $s = \sqrt{r}$, and dropping the overall factor of $(2\pi i)^{-1}$ (which does not affect polyhomogeneity), the $\Gamma_{w^2,2}$ portion of (7) becomes

$$\int_{w}^{\infty} 2s e^{(\cos\varphi)s^2/w^2} e^{i(\sin\varphi)s^2/w^2} R(s^2, z, z')\, ds. \tag{9}$$

First consider the behavior of the integrand as $s \to \infty$. Since $\cos\varphi < 0$ and w is bounded above, the term $\exp((\cos\varphi)s^2/w^2)$, and hence the entire integrand of (9), will decay to infinite order at $s = \infty$. There will still be a conormal singularity at the spatial diagonal, but the coefficients decay to infinite order at $s = \infty$.

In order to analyze (9), we break $R(s^2, z, z')$ into pieces. First we separate out the conormal singularity in a neighborhood of $D_{s,\mathrm{sc}}$ and analyze (9) using explicit local coordinates. Then we deal with the remainder, which is smooth on $M^2_{s,\mathrm{sc}}$, by breaking it into two pieces and applying the pushforward theorem.

2.4. ***The conormal singularity.*** Using a partition of unity, we let $R = R_s + R_c$, where R_c is supported in a neighborhood of $D_{s,\mathrm{sc}}$ and R_s is supported away from $D_{s,\mathrm{sc}}$, as in Figure 5. In a neighborhood of $\mathrm{sc} \cap \mathrm{bf}_0$, we use the coordinates

$$\left(X = s\left(\frac{1}{x} - \frac{1}{x'}\right), Y = s\frac{y-y'}{x}, y, \mu = \frac{x}{s}, s\right).$$

In these coordinates, R has a conormal singularity at $\{X = Y = 0\}$. On the other hand, in a neighborhood of $\mathrm{bf}_0 \cap \mathrm{zf} \cap D_{s,\mathrm{sc}}$, we use a slight modification of the coordinates in the previous subsection:

$$\left(\hat{X} = \left(1 - \frac{x}{x'}\right), \hat{Y} = y - y', y, \frac{s}{x}, x\right).$$

Since we use different coordinates in different regimes, write $R_c = R_1 + R_2 + R_3$ by using a smooth partition of unity near $x/s = 1$; R_1 is supported near the boundary but away from sc (say $s/x < 2$), R_2

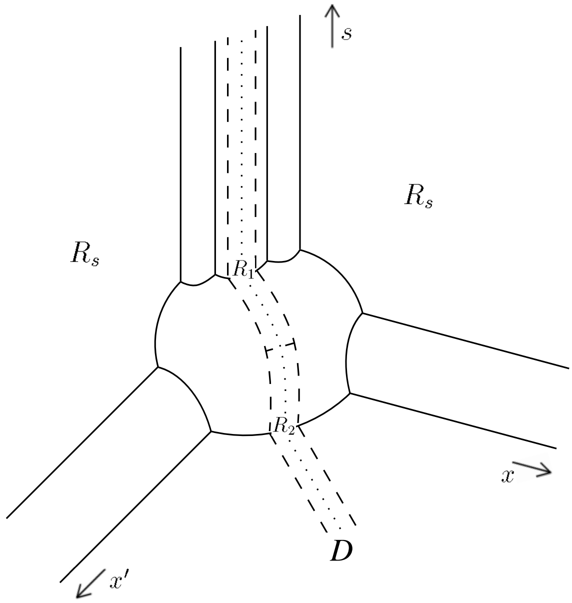

Figure 5. Decomposition of R.

near the boundary but away from zf (say $x/s < 2$), and R_3 in the interior. The decomposition at the boundary is illustrated in Figure 5.

First look at R_1. Using the explicit symbolic form of a conormal singularity, we may write

$$R_1 \sim \int_{\mathbb{R}^n} e^{i(\hat{X},\hat{Y})\cdot(\xi_1,\xi_2)} \sum_{j=0}^{\infty} a_j\left(\frac{s}{x}, x, y, \frac{\xi}{|\xi|}\right)|\xi|^{2-j}\, d\xi. \tag{10}$$

This is an asymptotic sum, modulo smooth functions on $M^2_{s,\mathrm{sc}}$; we pick a particular representative which is supported in a small neighborhood of $D_{s,\mathrm{sc}}$, and absorb the remainder into R_s. The coefficients a_j are phg conormal in x and s/x with index sets independent of j; they are also smooth in y and $\xi/|\xi|$. We plug (10) into (9) and then interchange the convergent s-integral with the asymptotic sum and the oscillatory integral over $\mathbb{R}^n$. The result is

$$\int_{\mathbb{R}^n} e^{i(\hat{X},\hat{Y})\cdot(\xi_1,\xi_2)} \sum_{j=0}^{\infty} \int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} a_j\left(\frac{s}{x}, x, y, \frac{\xi}{|\xi|}\right) ds\, |\xi|^{2-j}\, d\xi. \tag{11}$$

By Melrose's pullback theorem [1996], the pullback of each a_j to $X^3_b(s,x,w) \times N_y \times S^{n-1}_{\xi/|\xi|}$ via projection is also phg conormal with index sets independent of j. As a result, the integrand in

$$\int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} a_j\left(\frac{s}{x}, x, y, \frac{\xi}{|\xi|}\right) ds \tag{12}$$

is phg conormal on $X^3_b(s,w,x) \times N_y \times S^{n-1}_{\xi/|\xi|}$, with a cutoff singularity at $s/w = 1$. Moreover, it has infinite-order decay at $s = \infty$, independent of $w < 1$ and $x < 1$, and hence integration in s is well-defined. Integration in s is a b-fibration from $X^3_b(s,w,x)$ to $X^2_b(w,x)$, by [Melrose and Singer 2008, Proposition 4.4], and is hence also a b-fibration when we take the direct product with $N_y \times S^{n-1}_{\xi/|\xi|}$. Moreover, integration in s is transverse to the cutoff singularity at $s/w = 1$. Therefore, by the pushforward theorem with conormal singularities (from the appendix of [Epstein et al. 1991]), (12) is phg conormal on $X^2_b(w, x) \times N_y \times S^{n-1}_{\xi/|\xi|}$, with index sets independent of j.

Since $w < s < 2x$ on the support of R_1, (12) has a phg conormal expansion in $(w/x, x)$. Therefore, the integral (11), in the coordinates $(\hat{X}, \hat{Y}, y, w/x, x)$, corresponding to the R_1 piece of (9), is phg conormal in $(w/x, x)$ with index sets independent of j, and smoothly dependent on y, with an interior conormal singularity at $\hat{X} = \hat{Y} = 0$. Thus (11) is phg conormal on $M^2_{w,\mathrm{sc}}$ with a conormal singularity at the diagonal.

We now consider R_2; the analysis is similar. Write

$$R_2 \sim \int_{\mathbb{R}^n} e^{i(X,Y)\cdot(\xi_1,\xi_2)} \sum_{j=0}^{\infty} b_j\left(\frac{x}{s}, s, y, \frac{\xi}{|\xi|}\right)|\xi|^{2-j}\, d\xi, \tag{13}$$

where the b_j are phg conormal in x/s and s with index sets independent of j, and also smooth in y and $\xi/|\xi|$.

It is helpful to consider the regimes $w > x/2$ and $w < 2x$ separately. First assume that $w > x/2$, and let $\bar{X} = w(1/x - 1/x')$, $\bar{Y} = w(y - y')/x$, and $\bar{\lambda} = x/w$. We expect a conormal singularity at $\bar{X} = \bar{Y} = 0$ in this regime. Noting that $(X, Y) = (s/w)(\bar{X}, \bar{Y})$, we change variables in (13) and let $\zeta = (s/w)\xi$. The result is

$$R_2 \sim \int_{\mathbb{R}^n} e^{i(\bar{X},\bar{Y})\cdot(\zeta_1,\zeta_2)} \sum_{j=0}^{\infty} b_j\left(\frac{x}{s}, s, y, \frac{\zeta}{|\zeta|}\right)\left(\frac{s}{w}\right)^{j-2-n}|\zeta|^{2-j}\, d\zeta. \tag{14}$$

As before, plug (14) into (9) and interchange the sums and convergent integrals: the part of (9) coming from R_2 is

$$\int_{\mathbb{R}^n} e^{i(\bar{X},\bar{Y})\cdot(\zeta_1,\zeta_2)} \sum_{j=0}^{\infty} \int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} b_j\left(\frac{x}{s}, s, y, \frac{\zeta}{|\zeta|}\right)\left(\frac{s}{w}\right)^{j-2-n} ds\, |\zeta|^{2-j}\, d\zeta. \tag{15}$$

Consider the coefficients

$$\int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} b_j\left(\frac{x}{s}, s, y, \frac{\zeta}{|\zeta|}\right)\left(\frac{s}{w}\right)^{j-2-n} ds. \tag{16}$$

If we can show that the coefficients (16) are phg conormal in $(x/w, w)$ with respect to some index sets independent of j, with smooth dependence on y and $\zeta/|\zeta|$, then (15) is phg conormal on $M^2_{w,\mathrm{sc}}$ with a conormal singularity at the diagonal when $w > x/2$. To show this phg conormality, note that again the integrands in (16) are each phg conormal on $X^3_b(s, x, w) \times N_y \times S^{n-1}_{\zeta/|\zeta|}$. Moreover, the index sets are independent of j, as $s/w > 1$, and there is always infinite-order decay at $s = \infty$, independent of w. As before, we use the pushforward theorem to integrate in s, and we conclude that the coefficients (16) are phg conormal on $X^2_b(x, w) \times N_y \times S^{n-1}_{\zeta/|\zeta|}$ with respect to index sets independent of j. Since $w > x/2$, this yields expansions in x/w and w, which is precisely what we need.

On the other hand, suppose that $w < 2x$. Then we expect a conormal singularity at $\hat{X} = \hat{Y} = 0$. Since $(X, Y) = (s/x)(\hat{X}, \hat{Y})$, we change variables in (13), letting $\zeta' = (s/x)\xi$. Following the exact same procedure as in the $w > x/2$ case, we see that the part of (9) coming from R_2, when $w < 2x$, is

$$\int_{\mathbb{R}^n} e^{i(\hat{X},\hat{Y})\cdot(\zeta_1',\zeta_2')} \sum_{j=0}^{\infty} \int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} b_j\left(\frac{x}{s}, s, y, \frac{\zeta'}{|\zeta'|}\right)\left(\frac{s}{x}\right)^{j-2-n} ds\,|\zeta'|^{2-j}\,d\zeta'. \tag{17}$$

The coefficients can be rewritten as

$$\left(\frac{w}{x}\right)^{j-2-n} \int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} b_j\left(\frac{x}{s}, s, y, \frac{\zeta}{|\zeta|}\right)\left(\frac{s}{w}\right)^{j-2-n} ds. \tag{18}$$

These are just $(w/x)^{j-2-n}$ times (16), and $(w/x)^{j-2-n}$ is phg conormal on $X_b^2(w, x)$, so (18) is also phg conormal on $X_b^2(w, x)$ for each j. Since we are only considering $w < 2x$, the orders only improve as j increases. In particular, all the coefficients are phg conormal on $X_b^2(w, x)$ with respect to subsets of the index set of the $j = 0$ coefficient. This is again sufficient to prove that (17) is phg conormal on $M_{w,\mathrm{sc}}^2$ with a conormal singularity at the diagonal.

Finally, consider the interior term R_3; it is the simplest of the lot, since z and z' are in a compact subset of M. We let η be a dual variable to $z - z'$ and write

$$R_3 \sim \int_{\mathbb{R}^n} e^{i(z-z')\cdot\eta} \sum_{j=0}^{\infty} c_j\left(s, z, \frac{\eta}{|\eta|}\right)|\eta|^{2-j}\,d\eta. \tag{19}$$

Here the c_j are phg conormal at $s = 0$ and $s = \infty$, with index sets independent of j at $s = 0$ and $s = \infty$. Following the same procedure as in the previous two cases, simplified since $z - z'$ and η are independent of s, we conclude that the part of (9) coming from R_3 is

$$\int_{\mathbb{R}^n} e^{i(z-z')\cdot\eta} \sum_{j=0}^{\infty} \int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} c_j\left(s, z, \frac{\eta}{|\eta|}\right) ds\,|\eta|^{2-j}\,d\eta. \tag{20}$$

Analyzing the coefficients, we see that the integrand in each is phg conormal on $X_b^2(s, w)$, with index sets independent of j, z, and $\eta/|\eta|$, and with infinite-order decay at $s = \infty$. By the pushforward theorem, each coefficient is phg conormal at $w = 0$, with index sets independent of j, z, and $\eta/|\eta|$. Moreover, (20) has compact support in (z, z'). Therefore, (20), and hence the part of (9) corresponding to R_c, is phg conormal on $M_{w,\mathrm{sc}}^2$ with a conormal singularity at the diagonal.

Technically, we need to compute the index sets of the coefficients of the conormal singularity at each boundary face of $M_{w,\mathrm{sc}}^2$. This may be done directly via the pushforward theorem, but it is easier to apply the analysis we will develop in the next section. Note that a_j and b_j may be viewed as phg conormal functions on the diagonal $D_{s,\mathrm{sc}} \subset M_{s,\mathrm{sc}}^2$, with fixed index sets R_{sc}, R_{bf_0}, and R_{zf} at the boundary hypersurfaces sc, bf_0, and zf. Observe that they can be extended smoothly to functions defined in a neighborhood of $D_{s,\mathrm{sc}}$ which are themselves phg conormal on $M_{s,\mathrm{sc}}^2$ with the given index sets; call these extensions d_j. Then the coefficients of the conormal singularity of the integral (9) are the restrictions to the diagonal of

$$\int_w^{\infty} 2se^{-(s/w)^2 e^{i\varphi}} d_j(s, x, y, x', y')\,ds.$$

Applying Lemma 10 to each d_j, these coefficients are all phg conormal on $M^2_{w,\mathrm{sc}}$, with index sets obtained by adding 2 at the faces bf_0, rb_0, lb_0, and zf. Therefore the restrictions to the diagonal are all phg conormal on $D_{w,\mathrm{sc}}$, with leading orders matching those in Theorem 8, as expected. This completes the analysis of the conormal singularity.

2.5. ***Finishing the proof.*** It remains to consider the integral

$$\int_w^\infty 2se^{-(s/w)^2 e^{i\varphi}} R_s(s^2, z, z')\, ds, \tag{21}$$

where $R_s(s^2, z, z')$ is phg conormal on $\overline{M}^2_{s,\mathrm{sc}}$ and smooth across the diagonal. We claim:

Lemma 10. *Let $T(s, z, z')$ be any function which is phg conormal on $\overline{M}^2_{s,\mathrm{sc}}$, smooth in the interior, and decaying to infinite order at* lb, rb, *and* bf. *Then*

$$\int_w^\infty 2se^{-(s/w)^2 e^{i\varphi}} T(s, z, z')\, ds \tag{22}$$

is phg conormal on $M^2_{w,\mathrm{sc}}$ for w bounded above. Moreover, if the index sets of T at the various boundary hypersurfaces are T_{sc}, T_{bf_0}, T_{zf}, T_{rb_0}, T_{lb_0}, and T_{tf}, then the index sets of (22) are

$$T_{\mathrm{sc}}, \quad T_{\mathrm{bf}_0}+2, \quad T_{\mathrm{zf}}+2, \quad T_{\mathrm{rb}_0}+2, \quad T_{\mathrm{lb}_0}+2.$$

We defer the proof for the moment. Applying Lemma 10 to $T(s) = R_s(s^2)$, we conclude that (21) is phg conormal on $M^2_{w,\mathrm{sc}}$ with index sets precisely as in Theorem 8. Combining this with our analysis of R_c, we have now shown that $F(w, z, z')$ is phg conormal on $M^2_{w,\mathrm{sc}}$ possibly with a conormal singularity at the spatial diagonal, and with leading orders as specified in Theorem 8. However, $F(w, z, z')$ is a heat kernel, so it has no conormal singularity at the diagonal. This completes the proof of Theorem 8.

Finally, to prove Theorem 2, we apply Theorem 8. Condition (a) is true since the Laplacian is essentially self-adjoint and non-negative. Condition (b) follows from Theorems 6 and 7. Condition (c) is a well-known consequence of the semiclassical scattering calculus. The scattering calculus was first introduced by Melrose [1994] and the semiclassical version was developed by Vasy, Wunsch, and Zworski among others [Vasy and Zworski 2000; Wunsch and Zworski 2000]. The exact statement we need, along with a summary of the semiclassical scattering calculus, may be found in [Hassell and Wunsch 2008, Section 10]; $\hbar$ in the semiclassical calculus corresponds to k^{-1} in our context. Applying Theorem 8 gives us the polyhomogeneity we claim, and once we plug in the leading orders from [Guillarmou and Hassell 2008] and the Appendix, we see that the heat kernel has leading orders of 0 at sc and n at each of bf_0, rb_0, and lb_0.

Unfortunately, Theorem 8 does not by itself give us the claimed order-n behavior at zf; instead, we only see quadratic decay at zf when $n \geq 3$ and decay of the form $w^2 \log w$ when $n = 2$. However, by the estimate of Cheng–Li–Yau (Theorem 1), the heat kernel is uniformly bounded for large time by $Ct^{-n/2} = Cw^n$. Thus the leading order of the heat kernel at zf must actually be at least n, which completes the proof of Theorem 2.

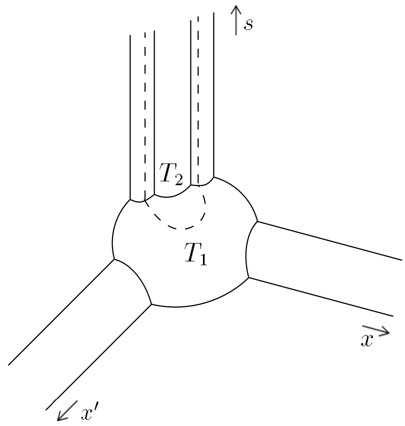

Figure 6. Decomposition of T.

Note that the lack of sharpness in the order calculation of Theorem 8 reflects the fact that our real-analytic approach does not take into account the complex-analytic structure of the resolvent; there is cancellation between the top and bottom parts of the integral that our approach cannot see. In particular, we could instead move the contour Γ towards the spectrum and represent the heat kernel as an integral with respect to the spectral measure. Guillarmou, Hassell, and Sikora demonstrate in [Guillarmou et al. 2012] that there is cancellation between the top and bottom parts of the contour in the spectral measure. In particular, the spectral measure at zf vanishes to order $n-1$ by Theorem 1.2 of their paper; integrating $e^{-\lambda t}$ against this spectral measure, we obtain an alternative proof of the fact that the heat kernel vanishes to order n at zf.

2.6. *Proof of Lemma 10.* We now prove Lemma 10; the proof involves extensive use of Melrose's pullback and pushforward theorems. First, write $T(s, z, z')$ as $T_1 + T_2$, where T_1 is supported away from sc and T_2 is supported in a neighborhood of sc. This partition is illustrated in Figure 6. Then decompose (22) into two integrals, corresponding to T_1 and T_2.

Consider the first integral:

$$\int_0^\infty \chi(\{s \geq w\})\, 2se^{-(s/w)^2 e^{i\varphi}} T_1(s, z, z')\, \frac{ds}{s}. \tag{23}$$

Notice that $T_1(s, z, z')$ is phg conormal on $M^2_{s,\mathrm{sc}}$ but supported away from sc, so it is in fact phg conormal on the blown-down space $M^2_{s,b}(z, z')$ (see Figure 2). The rest of the terms in the integrand are phg conormal on $X^2_b(s, w)$, with a cutoff singularity (which is an example of a conormal singularity) at $s = w$. We now define a space $M^2_{s,w,b}(z, z')$ as follows: start with $[0, T)_w \times [0, \infty]_s \times M_z \times M_{z'}$. Then blow up, in order,

- The submanifold where all four of (x, x', s, w) are zero;
- The four now-disjoint submanifolds where exactly three of (x, x', s, w) are zero;
- The six now-disjoint submanifolds where exactly two of (x, x', s, w) are zero.

This construction mimics the construction of the b-stretched product $X_b^4(x, x', s, w)$, and in fact $M^2_{s,w,b}(z, z')$ is precisely $X_b^4(x, x', s, w) \times N_y \times N_{y'}$ in a neighborhood of $\{x = x' = s = w = 0\}$. By the same arguments as for the b-stretched products in [Melrose and Singer 2008], the projection-induced maps from $M^2_{s,w,b}(z, z')$ to $M^2_{w,b}(z, z')$ (isomorphic to $X_b^3(x, x', w) \times N_y \times N_{y'}$ near $\{x = x' = w = 0\}$) and to $X_b^2(s, w)$ are well-defined b-fibrations. Therefore, by the pullback theorem, the integrand of (23) is phg conormal on $M^w_{s,w,b}(z, z')$, with a conormal singularity at $s = w$. Since the fibers of the projection map to $M^2_{w,b}(z, z')$ are transverse to the singularity at $s = w$, and the integrand has order ∞ at $s = \infty$, the pushforward theorem implies that (23) itself is phg conormal on $M^2_{w,b}(z, z')$. Since $M^2_{w,b}(z, z')$ is a blow-down of $M^2_{w,\mathrm{sc}}(z, z')$, we conclude that (23) is phg conormal on $M^2_{w,\mathrm{sc}}(z, z')$ as desired.

For T_2, we may use $(z, z') = (x, y, x', y')$ since T_2 is supported in a small neighborhood of sc. We have

$$\int_0^\infty \chi(\{s \geq w\})\, 2se^{-(s/w)^2 e^{i\varphi}}\, T_2(s, x, y, x', y')\, \frac{ds}{s}. \tag{24}$$

Let $\bar\sigma = (x/x' - 1, y - y')$; $\bar\sigma$ is an n-dimensional coordinate, and $M^2_{s,\mathrm{sc}}$ is created from $X_b^3(s, x, x') \times N_y \times N_{y'}$ by blowing up $\{\bar\sigma = x/s = 0\}$. In particular, $T_2(s, x, y, x', y')$, having compact support in x/x', is phg conormal on

$$\big[X_b^2(s, x) \times N_y\,;\, \{\bar\sigma = x/s = 0\}\big].$$

This space is the subset of $M^2_{w,\mathrm{sc}}$ with $1/2 < x/x' < 2$, so label its boundary hypersurfaces bf, sc, bf_0, and zf. In this labeling, T_2 is supported away from zf, decays to infinite order at bf, and has leading orders t_{sc} at sc and t_{bf_0} at bf_0.

We analyze the integrand in (24) as a function on the space

$$S = \big(X_b^3(s, w, x) \cap \{s \geq w\}\big) \times B(\bar\sigma) \times N_y.$$

Here B is the unit ball in $\mathbb{R}^n$. A diagram of S is given in Figure 7, with $\bar\sigma$ and y suppressed; we label the boundary hypersurfaces A–E.

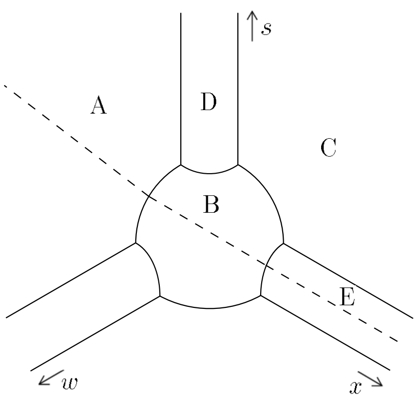

Figure 7. The space S.

We now define an iterated blow-up of S. Let P_1 be the p-submanifold of S given by $A \cap \{\bar{\sigma} = 0\}$. Blowing up P_1 creates a new space $S_1 = [S\,;\, P_1]$; call the front face of this blow-up F. Now let P_2 be the p-submanifold of S_1 given by the closure of the lift of $D^\circ \cap \{\bar{\sigma} = 0\}$. Then let

$$S_2 = [S_1\,;\, P_2] = [[S\,;\, P_1]\,;\, P_2],$$

and let G be the new front face. The following two propositions allow us to analyze (24); their proofs are deferred for the moment.

Proposition 11. *The map*

$$\pi_w : S_2 \cap \{s \geq x\} \to \left[\left(X_b^2(s, x) \cap \{s \geq x\}\right) \times B_1(\bar{\sigma}) \times N_y\,;\, \{\bar{\sigma} = x/s = 0\}\right],$$

given in the interior of S_2 by projection off the variable w and extending continuously to the boundary, is a b-map.

Proposition 12. *The map*

$$\pi_s : S_1 \to \left[X_b^2(w, x) \times B_1(\bar{\sigma}) \times N_y\,;\, \{\bar{\sigma} = x/w = 0\}\right],$$

given in the interior of S_1 by projection off the variable s and extending continuously to the boundary, is a b-fibration. Moreover, if we let ρ_H be a bdf for each hypersurface H, we have

$$(\pi_s)^*(\rho_{\mathrm{zf}}) = \rho_C \rho_E, \quad (\pi_s)^*(\rho_{\mathrm{bf}_0}) = \rho_B \rho_D, \quad (\pi_s)^*(\rho_{\mathrm{sc}}) = \rho_F, \quad (\pi_s)^*(\rho_{\mathrm{bf}}) = \rho_A. \tag{25}$$

Since T_2 is supported in $\{s \geq x\}$ and its support does not intersect the lift of $\{s = x\}$, Proposition 11 and the pullback theorem imply that the pullback of T_2 is phg conormal on S_2. Moreover, the remainder of the integrand in (24) is phg conormal on $X_b^2(s, w) \cap \{s > w\}$, so pulling back first to $X_b^3(s, w, x) \cap \{s > w\}$, and then to S_2, we see that it is phg conormal on S_2 as well. Therefore, the entire integrand in (24) is phg conormal on $S_2 = [S_1\,;\, P_2]$. However, the factor of e^{-s^2/w^2}, and hence the integrand, vanishes to infinite order at the front face G; consequently the integrand in (24) is actually phg conormal on S_1. By the pushforward theorem from [Epstein et al. 1991], since π_s is a b-fibration transverse to the conormal singularity at $s = w$, the pushforward (24) is phg conormal on the target space $[X_b^2(w, x) \times B_1(\bar{\sigma}) \times N_y\,;\, \{\bar{\sigma} = x/w = 0\}]$. From Figure 8, we see that this space is a subset of $M^2_{w,\mathrm{sc}}$; we have therefore shown that (24) is phg conormal on $M^2_{w,\mathrm{sc}}$. This completes the proof of the polyhomogeneity statement in Lemma 10, modulo the proofs of Propositions 11 and 12.

It remains to check the index sets claimed in Lemma 10. However, this calculation is a straightforward application of the pullback and pushforward theorems (explicit descriptions of the pullback and pushforward index sets may be found in [Grieser 2001]). A computation of the leading orders may be found in [Sher 2012b] and computing the index sets themselves is no harder.

2.7. *Propositions 11 and 12.* Finally, we prove Propositions 11 and 12. These propositions are proved in [Sher 2012b] using explicit local coordinates, but here we instead give a simpler proof based on the machinery developed by Hassell, Mazzeo, and Melrose [Hassell et al. 1995].

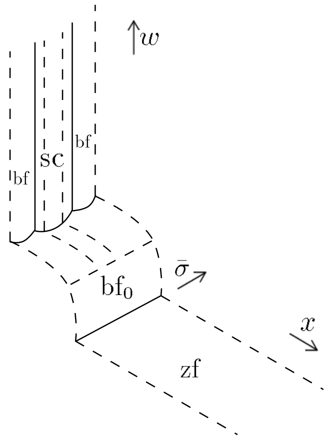

Figure 8. $[X_b^2(w,x)\,;\{\bar\sigma = x/w = 0\}]$.

Observe first that there are projection-induced maps from S to both $X_b^2(s,x) \times B(\bar\sigma) \times N_y$ and $X_b^2(w,x) \times B(\bar\sigma) \times N_y$. We call these maps $\tilde\pi_w$ and $\tilde\pi_s$ respectively. It is easy to see directly that both of these maps are in fact b-fibrations; see also the analysis of b-stretched products in [Melrose and Singer 2008]. Moreover, it may be checked by hand [ibid.] that each entry of the "exponent matrix" associated to each of these maps is either 0 or 1; see [Grieser 2001] or [Mazzeo 1991] for a discussion of exponent matrices.

To prove Proposition 11, consider the p-submanifold $\{\bar\sigma = x/s = 0\}$ of the target space of $\tilde\pi_w$. Its lift under $\tilde\pi_w$ is a union of two p-submanifolds of S: $A \cap \{\bar\sigma = 0\}$ and $D \cap \{\bar\sigma = 0\}$. S_2 is precisely the space we obtain from S by blowing up those two p-submanifolds (first A, then D). We may therefore apply Lemma 10 from [Hassell et al. 1995, Section 2] to conclude that the lift of $\tilde\pi_w$ to a map from S_2 to $[X_b^2(s,x) \times B(\bar\sigma) \times N_y\,;\{\bar\sigma = x/s = 0\}]$ is a b-fibration; but this lift is precisely π_w. Since a b-fibration is certainly a b-map, this completes the proof of Proposition 11.

Proposition 12 is proved in exactly the same way: the lift of $\{\bar\sigma = x/w = 0\}$ to S under $\tilde\pi_s$ is just $A \cap \{\bar\sigma = 0\}$, which is precisely P_1. An identical application of the lemma just cited allows us to conclude that π_s is a b-fibration. The computation of the pullbacks of boundary defining functions is not hard and may be done directly using local coordinates; the details may be found in [Sher 2012b].

3. Renormalized heat trace and zeta function

In this section, we define the renormalized heat trace, zeta function, and determinant on an asymptotically conic manifold M. These definitions ultimately allow us, in [Sher 2012a], to state and prove Theorem 5. The first step is to define the *renormalized trace*. This definition is inspired by Melrose's b-heat trace, which is a renormalized heat trace for manifolds with asymptotically cylindrical ends. Albin [2007] also defined renormalized heat traces in the asymptotically hyperbolic setting; later, Albin, Aldana, and Rochon [Albin et al. 2013] defined and investigated a renormalized determinant of the Laplacian on asymptotically hyperbolic surfaces.

3.1. *The renormalized heat trace.* Pick any cutoff function $\chi_1(r)$ on $\mathbb{R}_+$ which is supported on $\{r \le 2\}$ and equal to 1 on $\{r \le 1/2\}$. Assume that either

(a) $\chi_1(r)$ is a non-increasing smooth function of r (smooth cutoff), or

(b) $\chi_1(r)$ is precisely the characteristic function of [0, 1] (sharp cutoff).

Then for any $\delta < 1/2$, let $\chi_{1,\delta}$ be a function on M, equal to $\chi_1(r\delta)$ for $r \ge 1$ and equal to 1 inside $\{r = 1\}$. Consider the integral

$$\int_M \chi_{1,\delta}(z) H^M(t, z, z)\, dz. \tag{26}$$

Theorem 13. *Let χ_1 be either the smooth or the sharp cutoff. The integral (26) has a polyhomogeneous expansion in δ for each fixed t. Moreover, the finite part at $\delta = 0$, which we denote $P(t)$, has polyhomogeneous expansions in t at $t = 0$ and t^{-1} at $t = \infty$.*

This theorem allows us to define the renormalized heat trace on an asymptotically conic manifold. Roughly, this corresponds to integrating the heat kernel on the diagonal over regions where $r \le \delta^{-1}$, and renormalizing by subtracting the divergent parts at $\delta = 0$. Renormalization in this fashion is often called Hadamard renormalization (for details, see [Albin 2007; Albin et al. 2013]).

Definition. Let $\chi_1(r)$ be the sharp cutoff. The renormalized heat trace, denoted ${}^R\mathrm{Tr}\, H^M(t)$, is the finite part at $\delta = 0$ of (26).

Proof of Theorem 13. The key ingredient is the following observation on the structure of the heat kernel on the diagonal near the boundary, which is a consequence of the structure theorem we have proven for the heat kernel. The asymptotic structure of $H^M(t, x, y, x, y)$ reflected in this proposition is illustrated in Figure 9.

Proposition 14. (a) *For t bounded above, $H^M(t, x, y, x, y)$ is phg conormal in $(\sqrt{t}, x)$, with smooth dependence on y.*

(b) *For t bounded below, let $w = t^{-1/2}$; then $H^M(t, x, y, x, y)$ is phg conormal as a function of w and x on $X_b^2(w, x)$, again with smooth dependence on y.*

Proof. Proposition 14 is an immediate consequence of restricting to the spatial diagonal D in Theorem 2; since D is a p-submanifold of the space on which H^M is polyhomogeneous, the restriction of H^M to D

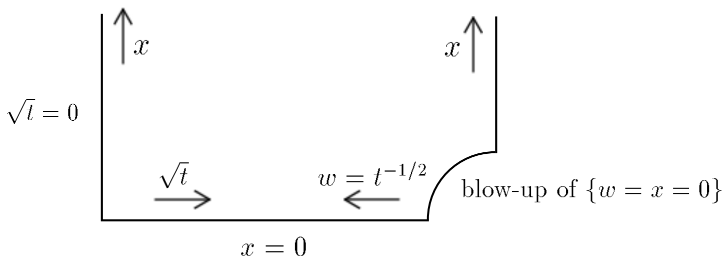

Figure 9. Asymptotic structure of $H^M(t, x, y, x, y)$.

is also polyhomogeneous. Comparing D with Figure 9, we see that D is precisely the space described in Proposition 14. $\square$

To prove Theorem 13, we analyze (26), which may be rewritten as

$$\int_N \int_0^1 \chi_1(\delta/x) H^M(t,x,y,x,y) x^{-n-1}\, dx\, dy + \int_{x\geq 1} H^M(t,z,z)\, dz. \tag{27}$$

First analyze the second term; the region $\{x \geq 1\}$ is bounded away from spatial infinity. Therefore, by Theorem 2, $H^M(t,z,z)$ has polyhomogeneous expansions in t at $t=0$ and $t^{-1/2}$, hence t^{-1}, at $t=\infty$, and these expansions are uniform in z with smooth coefficients. Integrating in z results in a function of t which is phg conormal at $t=0$ and $t=\infty$; this function contributes only to the finite part $P(t)$ at $\delta=0$ and satisfies the polyhomogeneity claimed in Theorem 13.

It remains to analyze the first term in (27). We consider the small-t and large-t regimes separately, analyzing the integrand

$$\chi_1(\delta/x) H^M(t,x,y,x,y) x^{-n-1} \tag{28}$$

in each regime as a function of (t,x,δ). In each case, $\chi_1(\delta/x)$ is phg conormal on $X_b^2(x,\delta)$; if χ_1 is the sharp cutoff, there is also a cutoff singularity, which is a type of conormal singularity, at $\delta/x=1$.

For small t, $H^M(t,x,y,x,y)$ is phg conormal in $(\sqrt{t},x)$, so (28) is phg conormal on $\mathbb{R}_+(\sqrt{t}) \times X_b^2(x,\delta)$, possibly with a conormal singularity at $\delta/x=1$. The projection map π_x is a b-fibration from this space onto the first quadrant in $(\sqrt{t},\delta)$ and is transverse to $\delta/x=1$; moreover, the integral in x is well-defined, as the integrand is supported away from the $x=0$, $\delta>0$ face. By the pushforward theorem from [Epstein et al. 1991], the first term of (27) is phg conormal in $(\sqrt{t},\delta)$ for bounded t.

On the other hand, for large t, H^M is phg conormal on $X_b^2(w,x)$ and χ_1 is phg conormal on $X_b^2(x,\delta)$. Since the maps from $X_b^3(w,x,\delta)$ to each of these spaces are b-maps (also b-fibrations), the integrand is phg conormal on $X_b^3(w,x,\delta)$ by the pullback theorem; there may again be a conormal singularity at $\delta/x=1$. Integration in x is pushforward by a b-fibration onto $X_b^2(w,\delta)$. Again, the integrand is supported in $\{x>\delta\}$, and the fibration is transverse to $\delta/x=1$, so we apply the pushforward theorem from [Epstein et al. 1991] to conclude that the first term in (27) is phg conormal on $X_b^2(w,\delta)$ for bounded w. Combining these results, we have shown that (27) is phg conormal on the space in Figure 10.

In particular, for any fixed t, (27) has a polyhomogeneous expansion as $\delta\to 0$. Moreover, $P(t)$ is simply the coefficient of the t^0 term at the $(0<t<\infty, \delta=0)$ face. By the definition of phg conormality

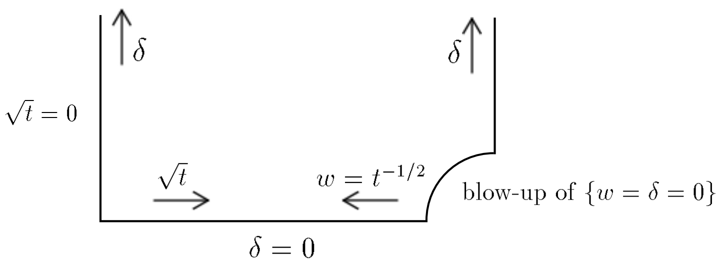

Figure 10. Asymptotic structure of (27).

(also see the discussion surrounding [Mazzeo 1991, Lemma A.4]), $P(t)$ therefore has polyhomogeneous conormal expansions at $t = 0$ and $t = \infty$. This completes the proof of Theorem 13. □

Using Theorem 13, we now define the meromorphic continuation of the renormalized zeta function:

$$ {}^R\zeta_M(s) = \frac{1}{\Gamma(s)} \int_0^\infty {}^R\mathrm{Tr}\, H^M(t)\, t^{s-1}\, dt. \tag{29} $$

We break up the integral (29) at $t = 1$, and consider first the short-time piece,

$$ \frac{1}{\Gamma(s)} \int_0^1 {}^R\mathrm{Tr}\, H^M(t)\, t^{s-1}\, dt. \tag{30} $$

By the phg conormality of ${}^R\mathrm{Tr}\, H^M(t)$, we can write, for any $N > 0$,

$$ {}^R\mathrm{Tr}\, H^M(t) = \sum_{i=0}^{k_N} a_i t^{z_i} (\log t)^{p_i} + \mathbb{O}(t^N). $$

Plug this expansion into (30). The $\mathbb{O}(t^N)$ contribution is well-defined and meromorphic whenever $\Re s > -N$, and the continuations of the other terms are integrals of the form

$$ \frac{a_i}{\Gamma(s)} \int_0^1 t^{z_i+s-1} (\log t)^{p_i}\, dt. $$

These integrals may be evaluated directly, and give explicit meromorphic functions of s, each with finitely many poles. Therefore, (30), though initially defined only when $\Re s > -z_0$, has a meromorphic extension to all of $\mathbb{C}$.

On the other hand, the long-time piece is

$$ \frac{1}{\Gamma(s)} \int_1^\infty {}^R\mathrm{Tr}\, H^M(t)\, t^{s-1}\, dt. \tag{31} $$

Writing $u = 1/t$ and substituting, this becomes

$$ \frac{1}{\Gamma(-(-s))} \int_0^1 {}^R\mathrm{Tr}\, H^M(1/u)\, u^{(-s)-1}\, du. $$

We have a phg conormal expansion for ${}^R\mathrm{Tr}\, H^M(1/u)$ as $u \to 0$; say the leading order term is of the form $u^{z_\infty}(\log u)^p$. Proceeding exactly as in the analysis of (30), we conclude that (31), though initially defined only when $\Re(-s) > -z_\infty$, has a meromorphic continuation to all of $\mathbb{C}$.

This allows us to define the renormalized zeta function and determinant on any asymptotically conic manifold M.

Definition. The renormalized zeta function on M, ${}^R\zeta_M(s)$, is given by the meromorphic continuation of (29).

Depending on the orders, there may be no s in $\mathbb{C}$ for which (29) is defined; however, once we split the integral at $t = 1$, both pieces are defined in half-planes and continue meromorphically to all of $\mathbb{C}$.

Definition. The *renormalized determinant* of the Laplacian on M is $e^{-{}^R\zeta_M'(0)}$, where ${}^R\zeta_M'(0)$ is the coefficient of s in the Laurent series for ${}^R\zeta_M(s)$ at $s=0$.

3.2. ***Manifolds conic near infinity.*** We now specialize to the case of manifolds which are precisely conic outside a compact set. In particular, let Z be any asymptotically conic manifold without boundary which is isometric to a cone outside a compact set. Without loss of generality, assume that Z is isometric to a cone when $r \geq 1/2$. We examine the asymptotic expansion of $\int_Z \chi_{1,\delta}(z) H^Z(t,z,z)\,dz$ as $\delta \to 0$; the finite part is precisely the renormalized heat trace. However, for applications, such as the study of conic degeneration in [Sher 2012a], we are also interested in identifying the divergent terms in the expansion. The fact that Z is conic near infinity allows us to identify those terms:

Theorem 15. *Let Z be conic near infinity as above, and let χ_1 be the sharp cutoff. We have the following asymptotic expansion for $\int_Z \chi_{1,\delta}(z) H^Z(t,z,z)\,dz$ as $\delta \to 0$:*

$$\int_Z \chi_{1,\delta}(z) H^Z(t,z,z)\,dz = \sum_{k=0}^{n-1} f_k(t)\delta^{k-n} + f_{\log}(t)\log\delta + {}^R\mathrm{Tr}\, H^Z(t) + R(\delta,t). \tag{32}$$

Here $R(\delta,t)$ goes to zero as δ goes to zero for each fixed t. Moreover, if we let $u_k(1,y)$ be the coefficient of $t^{(k-n)/2}$ in the short-time heat expansion on C_N at the point $(1,y)$, then

$$f_k(t) = \frac{t^{(k-n)/2}}{k-n}\int_N u_k(1,y)\,dy \quad \textit{and} \quad f_{\log}(t) = -\int_N u_n(1,y)\,dy.$$

Proof of Theorem 15. Note first that $\int_Z \chi_{1,\delta}(z) H^Z(t,z,z)$ does in fact have a polyhomogeneous expansion in δ, by Theorem 13, so it is just a matter of identifying the terms. The proof involves a comparison of the heat kernels on Z and on C_N; Z and C_N are identical near infinity, which allows us to formulate and prove the following lemma:

Lemma 16. *Let C_N be the infinite cone over N. Then $\left|H^{C_N}(t,z,z) - H^Z(t,z,z)\right|$, defined whenever $r \geq 1$, decays to infinite order in $|z|$ as $|z|$ goes to infinity.*

Proof. Let $\hat{Z} = Z \cap \{r \geq 1\}$. It is a complete manifold with boundary at $r=1$, and is a subset of both C_N and Z. On $\hat{Z}$, $H^{C_N}(t,z,z') - H^Z(t,z,z')$ is a solution of the heat equation for each z', with initial data equal to zero and boundary data at $r=1$ given by $H^{C_N}(t,1,y,z') - H^Z(t,1,y,z')$. Fix any $T>0$. We claim that for all $t<T$, $y \in N$, and z' with $|z'|>2$, there is a constant K so that the absolute value of the boundary data is less than K.

We show this for $H^{C_N}(t,1,y,z')$ and for $H^Z(t,1,y,z')$ separately. For C_N, by scaling and noting that $|z'|<2$,

$$H^{C_N}(t,1,y,z') = \frac{1}{|z'|^n} H^{C_N}\left(\frac{t}{|z'|^2}, \frac{1}{|z'|}, y, \frac{z'}{|z'|}\right) < H^{C_N}\left(\frac{t}{|z'|^2}, \frac{1}{|z'|}, y, 1, y'\right).$$

For each fixed y', the heat kernel with point source at $(1,y')$ is continuous for $r<1/2$ (i.e., the tip of the cone), and hence is bounded for $r<1/2$ and for $t/|z'|^2 < t < T$ by some universal constant K. Since y'

varies only over a compact set, the proof is complete. As for $H^Z(t,1,y,z')$, consider the region

$$W = \left\{(t,1,y,x',y') \;\middle|\; t<T,\, x'<\tfrac{1}{2},\, y\in N,\, y'\in N\right\}$$

as a subset of (t,x,y,x',y') space. The kernel H^Z has infinite-order decay at each boundary hypersurface of the space in Figure 1 with which W has nontrivial intersection. We conclude that H^Z is bounded on W, so there is a constant K so that $H^Z(t,1,y,z')<K$ for all $t<T$, all $y\in N$, and all z' with $|z'|>2$.

Since we have an upper bound for the boundary data, we can construct a supersolution and apply the parabolic maximum principle. Let $g(t,r)$ be the solution of the heat equation on $\hat{Z}$ with zero initial condition and boundary data at $r=1$ equal to K for all t. By the maximum principle, we see that $\left|H^{C_N}(t,z,z',t)-H^Z(t,z,z')\right|<g(t,|z'|)$ uniformly for $|z'|>2$ and $t<T$. We claim that $g(t,r)$ decays to infinite order in r, uniformly in t for $t<T$. This can be seen either from Bessel function expansions or by constructing a further supersolution $\hat{g}(t,r)$ modeled on the heat kernel on $\mathbb{R}^n$. In particular, we can use

$$\hat{g}(t,r)=\frac{K/\alpha}{(4\pi)^{n/2}}\sum_{k=-1}^{T_0}\frac{1}{(t-k)^{n/2}}\,e^{-r^2/4(t-k)}\chi_{\{t>k\}},$$

where $\alpha=(8\pi)^{n/2}e^{1/4}$ and T_0 is the greatest integer less than or equal to T. This supersolution has the uniform exponential decay property we want, so a final application of the parabolic maximum principle finishes the proof of the lemma. □

Corollary 17. *For any fixed t and any $\chi_{1,\delta}$ (either a sharp cutoff or a smooth cutoff),*

$$\left|\int_{C_N}\chi_{1,\delta}(z)H^{C_N}(t,z,z)\,dz-\int_Z\chi_{1,\delta}(z)H^Z(t,z,z)\,dz\right| \tag{33}$$

converges as $\delta\to 0$.

It now suffices to show that

$$\int_{C_N}\chi_{1,\delta}(z)H^{C_N}(t,z,z)\,dz$$

has a divergent asymptotic expansion of the form claimed in Theorem 15, as (33) converges as $\delta\to 0$ and hence contributes only to the finite part of the expansion. (Recall that χ is the sharp cutoff.)

Lemma 18. *Fix t. The divergent terms in the expansion of $\int_{|z|\le 1/\delta}H^{C_N}(t,z,z)$ as $\delta\to 0$ are given by*

$$\sum_{k=0}^{n-1}\frac{t^{(k-n)/2}}{k-n}\,\delta^{k-n}\int_N u_k(1,y)\,dy - C\log\delta,$$

where C is equal to $\int_N u_n(1,y)\,dy$.

Proof. The integral is, modulo a term independent of δ,

$$\int_1^{1/\delta}\int_N H^{C_N}(t,r,y,r,y)\,r^{n-1}\,dy\,dr.$$

By the conformal homogeneity of C_N, $H^{C_N}(t, r, y, r, y) = r^{-n} H^{C_N}(t/r^2, 1, y, 1, y)$. So the integral becomes

$$\int_1^{1/\delta} \int_N H^{C_N}\left(\frac{t}{r^2}, 1, y, 1, y\right) \frac{1}{r}\, dy\, dr.$$

Now let $s = t/r^2$ and switch to an integral in s; we get

$$\frac{1}{2} \int_{\delta^2 t}^{t} \int_N H^{C_N}(s, 1, y, 1, y) \frac{1}{s}\, dy\, ds. \tag{34}$$

From short-time heat asymptotics, we know that

$$\int_N H^{C_N}(s, 1, y, 1, y)\, dy = \sum_{k=0}^{n-1} s^{(k-n)/2} \int_N u_k(1, y)\, dy + \int_N u_n(1, y)\, dy + \mathbb{O}(s^{1/2}). \tag{35}$$

Here $u_k(1, y)$ are the heat coefficients on the cone C_N at the point $(1, y)$. We plug (35) into (34) and get

$$\sum_{k=0}^{n-1} \frac{t^{(k-n)/2}}{k-n} \delta^{k-n} \int_N u_k(1, y)\, dy - \log\delta \int_N u_n(1, y)\, dy + g(\delta, t),$$

where $g(\delta, t)$ is finite as $\delta \to 0$. This is what we wanted to prove. □

Combining this lemma with the preceding corollary and the definition of the renormalized heat trace completes the proof of Theorem 15. □

Finally, it is also useful to investigate the analogous divergent expansion when a smooth cutoff, rather than a sharp cutoff, is used.

Lemma 19. *Let $\chi_1(r)$ be as in condition (a) of Section 3.1: smooth and non-increasing, supported in $r \leq 2$ and* 1 *when $r \leq 1/2$. Then*

$$\int_Z \chi_{1,\delta}(z) H^Z(t, z, z)\, dz = \sum_{k=0}^{n-1} l_k f_k(t) \delta^{k-n} + f_{\log}(t) \log\delta + {}^R\mathrm{Tr}\, H^Z(t) + l_{\log} f_{\log}(t) + \tilde{R}(\delta, t), \tag{36}$$

where $l_k = -\int_{1/2}^{2} \chi_1'(r) r^{k-n}\, dr$ and $l_{\log} = -\int_{1/2}^{2} \chi_1'(r) \log r\, dr$, and $\tilde{R}(\delta, t)$ goes to zero as δ goes to zero for every fixed t.

Proof. Let $\xi(r)$ be any function which is equal to a constant a for $r \leq 1/2$ and supported in $\{r \leq 2\}$. For any $\delta < 1/2$, we may define a function $\xi_\delta(z)$ on Z by letting $\xi_\delta(z)$ be equal to $\xi\delta r$ for $r = |z| \geq 1$ and a for $\{r \leq 1\}$. Then consider the integral

$$\int_Z \xi_\delta(z) H^Z(t, z, z)\, dz, \tag{37}$$

and examine its behavior as $\delta \to 0$.

When $\xi(r)$ is the characteristic function of $[0, 1]$, we have the expansion (32). By replacing δ with δ/b for any $b \in [1/2, 2]$, we can compute the $\delta \to 0$ expansion of (37) for $\xi(r)$ equal to the characteristic function of $[0, b]$. By linearity, we see that the expansion of (37) for $\xi(r) = (\Delta h)\chi_{[a,b]}$ is

$$\sum_{k=0}^{n-1}(\Delta h) f_k(t)\big(b^{k-n} - a^{k-n}\big)\, \delta^{k-n} + (\Delta h) f_{\log}(t)\big(\log b - \log a\big) + (\Delta h)\big(R(\delta/b, t) - R(\delta/a, t)\big).$$

Now let $\xi(r) = \chi_1(r) - \chi_{\{r\leq 1\}}$; this is the difference between the sharp and smooth cutoffs. Since the expansions of (37) are linear in ξ, we can approximate by step functions and then integrate by summing over thin horizontal rectangles. Assume for simplicity that $\chi_1(r) = 1$ for all $r \leq 1$ (in the general case, there are some negative signs, but we get the same answer). The thickness of the rectangle at height h is Δh. The length of the rectangle is $\chi_1^{-1}(h) - 1$. Putting all of this together, the expansion of (37) with respect to $\xi(r)$ is

$$\sum_{k=0}^{n-1} f_k(t) \int_0^1 \big((\chi_1^{-1}(h))^{k-n} - 1\big)\, dh\, \delta^{k-n} + f_{\log}(t) \int_0^1 \log \chi_1^{-1}(h)\, dh + \tilde{R}(\delta, t),$$

where $\tilde{R}(\delta, t)$ is the contribution from the remainder terms.

Finally, perform the change of variables $u = \chi_1^{-1}(h)$, then add the expansion for $\chi_{\{r\leq 1\}}$; we obtain precisely the expansion claimed in the statement of the lemma. This finishes the proof, as long as we can control the remainder term $\tilde{R}(\delta, t)$. Indeed, for each fixed t, we claim that $\tilde{R}(\delta, t)$ goes to zero as δ goes to zero; define a new function $S(\delta, t)$ by letting

$$S(\delta, t) = \sup_{1/2\leq\gamma\leq 2} \big|R(\delta/\gamma, t)\big|.$$

When $\xi(r) = (\Delta h)\chi_{[a,b]}$, the remainder is bounded in absolute value by $(\Delta h)S(\delta, t)$. So the integral from $h = 0$ to 1 is bounded by $S(\delta, t)$, which goes to zero as $\delta \to 0$; this shows boundedness of the remainder term and finishes the proof of the lemma. □

It is worth examining the dependence on the zeta function on the choice of cutoff χ_1; we used a sharp cutoff to define it, but we could use a smooth cutoff instead. In this case, the finite part of the divergent δ-expansion changes from ${}^R\mathrm{Tr}\, H^Z(t)$ to ${}^R\mathrm{Tr}\, H^Z(t) + l_{\log} f_{\log}(t)$. But $f_{\log}$ and $l_{\log}$ are constants. So the renormalized heat trace only depends on the choice of cutoff function by the addition of a constant, independent of t. However, it can be easily shown by breaking up the integral at $t = 1$ that the meromorphic continuation of $\int_0^\infty Ct^k t^{s-1}\, dt$ is identically zero for any constant C. We have shown:

Proposition 20. *Let Z be conic near infinity. The renormalized zeta function and determinant of the Laplacian on Z are independent of the choice of cutoff function $\chi_{1,\delta}$.*

We have now shown the existence of a renormalized zeta function and determinant of the Laplacian on any asymptotically conic manifold M; moreover, when M is conic near infinity, we have computed the divergent terms in the expansion which leads to those renormalizations.

4. The low-energy resolvent in two dimensions

In this section, we extend the techniques used by Guillarmou and Hassell in [2008] to prove Theorem 7. In particular, we construct the low-energy resolvent on an asymptotically conic surface. The resolvent is

$$R(\theta, k, z, z') = (\Delta_M + e^{i\theta}k^2)^{-1}(z, z').$$

For simplicity, we set $\theta = 0$, so that R is a function of (k, z, z'). At the end of the section, we return to discuss allowing arbitrary $\theta \in [-\varphi, \varphi]$ and showing smoothness in θ; however, this is not difficult.

4.1. ***Strategy.*** Our goal is to construct the Schwartz kernel of the resolvent, $R(k, z, z')$, as a distribution on $M^2_{k,\mathrm{sc}}$. To do this, as in [Guillarmou and Hassell 2008], we will first construct a parametrix $G(k)$ so that $(\Delta_M + k^2)G(k) = \mathrm{Id} + E(k)$, where $E(k)$ is an error term. $G(k)$ will be a family (in k) of pseudodifferential operators on M whose Schwartz kernel is polyhomogeneous conormal on $M^2_{w,\mathrm{sc}}$ with an interior conormal singularity at the spatial diagonal. By examining the leading order behavior of the equation $(\Delta_M + k^2)G(k) = \mathrm{Id}$ at each boundary hypersurface of $M^2_{w,\mathrm{sc}}$, we obtain a model problem at each hypersurface. The leading order of the parametrix $G(k)$ at each hypersurface should solve the model problem. We first choose solutions of the model problem at each hypersurface, and then check that they are consistent; that is, that they may be glued together to obtain a parametrix $G(k)$. Finally, we analyze the error $E(k)$ and show that it can be removed via a Neumann series argument.

In order to define the appropriate space of pseudodifferential operators, we use certain density conventions, all the same as in [Guillarmou and Hassell 2008]. We consider $P = \Delta_M$ as an operator on *scattering half-densities* by writing

$$P\big(f(x, y)\,|x^{-n-1}\,dx\,dy|^{1/2}\big) = (\Delta_M f)(x, y)\,|x^{-n-1}\,dx\,dy|^{1/2}.$$

As in [Guillarmou and Hassell 2008], we expect a transition between scattering behavior for $k > 0$ and b-behavior at $k = 0$, which leads us to define the conformally related b-metric $g_b = x^2 g$. The space (M, g_b) is asymptotically cylindrical. We then define $P_b = x^{-n/2-1} P x^{n/2-1}$ with respect to scattering half-densities. However, we want to consider P_b acting with respect to *b-half densities* $|x^{-1}\,dx\,dy|^{1/2}$. After this shift, the relationship between P_b acting on b-half densities and P acting on scattering half-densities is $P = x P_b x$.

Let $\tilde{\Omega}_b^{1/2}$ be the bundle of half-densities on $M^2_{k,\mathrm{sc}}$ which is spanned by sections of the form

$$\left| f(k, x, y, x', y')\,\frac{dg_b\,dg_b'\,dk}{k} \right|^{1/2}.$$

Let ν be a smooth nonvanishing section of this bundle. Since it involves the b-metric g_b, $\tilde{\Omega}_b^{1/2}$ is not the natural bundle near sc. In particular, the kernel of the identity operator on M has leading order $-n/2$ at sc with respect to $\tilde{\Omega}_b^{1/2}$ [Guillarmou and Hassell 2008]. We can now define spaces of pseudodifferential operators, precisely as in [Guillarmou and Hassell 2008]:

Definition. Let ρ_{sc} be a boundary defining function for sc. The space $\Psi_k^{m,\mathcal{E}}(M\,;\tilde{\Omega}_b^{1/2})$ is the space of half-density kernels $K = K_1 + K_2$ on $M^2_{k,\mathrm{sc}}$ satisfying:

(1) $\rho_{\mathrm{sc}}^{n/2} K_1$ is supported near $\Delta_{k,\mathrm{sc}}$, and has an interior conormal singularity of order m at $\Delta_{k,\mathrm{sc}}$, with coefficients whose behavior at the boundary is specified by $\mathcal{E}$;

(2) $\rho_{\mathrm{sc}}^{n/2} K_2$ is polyhomogeneous conormal on $M^2_{k,\mathrm{sc}}$ with index family $\mathcal{E}$, and moreover decays to infinite order at bf, lb, and rb.

The factor of $\rho_{\mathrm{sc}}^{n/2}$ corrects for the use of b-half densities near sc. Using this definition, we can compute as in [Guillarmou and Hassell 2008] that

$$(P+k^2) \in \Psi_k^{2,\mathcal{E}}(M\,;\tilde{\Omega}_b^{1/2}),$$

with index sets 0 at sc, 2 at bf_0, 0 at zf, 2 at lb_0, and 2 at rb_0.

As proven in [Guillarmou and Hassell 2008], these spaces satisfy a composition rule:

Proposition 21. *Suppose that $A \in \Psi_k^{m,\mathcal{E}}$ and $B \in \Psi_k^{m',\mathcal{F}}$. Then $A \circ B$ is well defined and an element of $\Psi_k^{m+m',\mathcal{G}}$, where*

$$\mathcal{G}_{\mathrm{sc}} = \mathcal{E}_{\mathrm{sc}} + \mathcal{F}_{\mathrm{sc}}, \quad \mathcal{G}_{\mathrm{zf}} = (\mathcal{E}_{\mathrm{zf}} + \mathcal{F}_{\mathrm{zf}}) \,\overline{\cup}\, (\mathcal{E}_{\mathrm{rb}_0} + \mathcal{F}_{\mathrm{lb}_0}), \quad \mathcal{G}_{\mathrm{bf}_0} = (\mathcal{E}_{\mathrm{bf}_0} + \mathcal{F}_{\mathrm{bf}_0}) \,\overline{\cup}\, (\mathcal{E}_{\mathrm{lb}_0} + \mathcal{F}_{\mathrm{rb}_0}),$$
$$\mathcal{G}_{\mathrm{lb}_0} = (\mathcal{E}_{\mathrm{bf}_0} + \mathcal{F}_{\mathrm{lb}_0}) \,\overline{\cup}\, (\mathcal{E}_{\mathrm{lb}_0} + \mathcal{F}_{\mathrm{zf}}), \quad \mathcal{G}_{\mathrm{rb}_0} = (\mathcal{E}_{\mathrm{rb}_0} + \mathcal{F}_{\mathrm{bf}_0}) \,\overline{\cup}\, (\mathcal{E}_{\mathrm{zf}} + \mathcal{F}_{\mathrm{rb}_0}).$$

We therefore expect our parametrix G to be in $\Psi_k^{-2,\mathcal{G}}$ for some index family $\mathcal{G}$. To gain more information, we need to start analyzing the model problems.

4.2. ***The two-dimensional problem.*** We begin our analysis of the model problems at the face zf. In order to identify the leading-order part of the equation at a boundary hypersurface, we need to pick a coordinate to use as a boundary defining function in the interior of that face. For all the faces in the lift of $\{k=0\}$, we use k, which is the easiest choice, since it commutes with P. Since $P+k^2 = xP_b x + k^2$, the leading order part of the operator at zf, which we call the *normal operator*, is $xP_b x$, and the model problem is $(xP_b x)G^0_{\mathrm{zf}} = \mathrm{Id}$. We therefore expect that G^0_{zf} will be $(xx')^{-1}$ times some right inverse for P_b.

In order to invert P_b, we use the b-calculus of [Melrose 1993], identifying zf, near bf_0, with the b-double space $X_b^2(x,x') \times N_y \times N_{y'}$. The corner $\mathrm{zf} \cap \mathrm{bf}_0$ corresponds to the front face ff in the b-double space. An easy calculation, following [Guillarmou and Hassell 2008], shows that

$$P_b = -(x\partial_x)^2 + \left(\frac{n}{2}-1\right)^2 + \Delta_N + W,$$

where W is a lower-order term; that is, W vanishes as a b-differential operator at $x=0$. In fact, P_b is an elliptic b-differential operator, and hence may be inverted by following the procedure of Melrose, which is described in [Melrose 1993] and [Mazzeo 1991].

The first step in this procedure is to consider the indicial operator, which is the leading order part of P_b at the front face ff. Using the coordinates $(\sigma' = x/x', x', y, y')$, this is

$$I_{\mathrm{ff}}(P_b) = -(\sigma'\partial_{\sigma'})^2 + \left(\frac{n}{2}-1\right)^2 + \Delta_N.$$

With this terminology, the key theorem is as follows:

Theorem 22 [Melrose 1993]. *P_b is Fredholm as an operator between $x^\delta H_b^2$ and $x^\delta L_b^2$ if and only if δ is not an* indicial root *of $I_{\text{ff}}(P_b)$*. (See [Melrose 1993] or [Mazzeo 1991] for definitions of $x^\delta H_b^2$ and $x^\delta L_b^2$).

In our setting, as in [Guillarmou and Hassell 2008], the indicial roots are precisely

$$\pm\nu_i = \pm\sqrt{\left(\frac{n}{2}-1\right)^2 + \lambda_i}\,; \qquad \lambda_i \in \sigma(\Delta_N).$$

When $n > 2$, 0 is not an indicial root, and Guillarmou and Hassell show that P_b is not only Fredholm but invertible for $\delta = 0$, and then set G^0_{zf} to be $(xx')^{-1}$ times that inverse. However, in our case, $n = 2$, so $\nu_i = \sqrt{\lambda_i}$, and 0 is an indicial root. So P_b is not even Fredholm from H_b^2 to L_b^2. This is precisely why the $n = 2$ case is not considered by Guillarmou and Hassell.

4.3. ***An example: Euclidean space.*** In order to gain some intuition for the behavior of the resolvent near zf in the $n = 2$ setting, we examine the simplest case, which is $M = \mathbb{R}^2$. The resolvent on $\mathbb{R}^2$, acting on scattering half-densities $|dz| = |x^{-3}\,dx\,dy|$, is

$$-\frac{1}{2\pi}H_0\big(k|z-z'|\big) = -\frac{1}{2\pi}H_0\left(k\left|\frac{y}{x}-\frac{y'}{x'}\right|\right),$$

where H_0 is the Hankel function of order zero. From the asymptotics of the Hankel function, we know that $H_0(r)$ decays exponentially as $r \to \infty$, and for small r,

$$H_0(r) \sim -\log r + \log 2 - \gamma + \mathbb{O}(r).$$

Using these asymptotics, one can show that the resolvent on $\mathbb{R}^2$ is phg conormal on $M^2_{k,\text{sc}}$. We are most interested in the leading order behavior near zf. In a neighborhood of zf, we have $k|z-z'| < 1$, so this leading order behavior is controlled by the small-r asymptotics

$$H_0\big(k|z-z'|\big) \sim -\log\big(k|z-z'|\big) + \log 2 - \gamma = -\log k - \log|z-z'| + \log 2 - \gamma.$$

Some observations on these asymptotics:

- As we approach zf, the resolvent increases logarithmically. This is a major difference from the $n \geq 3$ case studied in [Guillarmou and Hassell 2008], in which the resolvent is continuous down to zf. On the other hand, the resolvent is continuous down to bf_0, lb_0, and rb_0.
- The function $-(1/2\pi)\log|z-z'|$ is the Green's function for the Laplacian on $\mathbb{R}^2$.

These observations suggest that in two dimensions, we will have a logarithmic term at zf in addition to a zero-order term. We write these terms as $G^{0,1}_{\text{zf}}\log k$ and G^0_{zf} respectively. From the Euclidean-space example, we expect that, on scattering half-densities,

$$G^{0,1}_{\text{zf}}\log k + G^0_{\text{zf}} = -C\log k + F(z,z'),$$

where $F(z,z')$ is a right inverse for the operator P. Moreover, since $-C\log k$ has logarithmic growth at bf_0, lb_0, and rb_0 but the resolvent on $\mathbb{R}^2$ does not, we expect that $F(z,z')$ will have logarithmic growth at those faces, with the right coefficient to cancel the logarithmic growth coming from $-C\log k$.

4.4. ***Construction of the initial parametrix.*** We now construct our parametrix $G(k)$ by specifying its leading order behavior at each boundary hypersurface and then checking that the models are consistent.

4.4.1. *The diagonal,* sc*, and* bf_0. The resolvent has an interior conormal singularity at the diagonal $\{z, z'\}$. The symbol of $P+k^2$ is $|\eta|^2+k^2$, where η is the dual variable of $z-z'$. One can compute that $|\eta|^2+k^2$ is elliptic on $M^2_{k,\mathrm{sc}}$, with leading orders 0 at sc, 2 at bf_0, and 0 at zf. As in [Guillarmou and Hassell 2008], we let the symbol of $G(k)$ be the inverse of $|\eta|^2+k^2$, in the sense of operator composition. This determines the diagonal symbol of $G(k)$ up to symbols of order $-\infty$, and hence determines $G(k)$ up to operators with smooth Schwartz kernels in the interior of $M^2_{w,\mathrm{sc}}$.

At sc, the analysis is identical to that of Guillarmou and Hassell, so we omit some of the details. The key point is that sc can be described as a fiber bundle with $\mathbb{R}^n$ fibers, parametrized by $y' \in N$ and k. The normal operator of $P+k^2$ is $\Delta_{\mathbb{R}^n}+k^2$, which has a well-defined inverse for $k>0$. In each fiber, we let

$$G^0_{\mathrm{sc}} = \left(\Delta_{\mathbb{R}^2}+k^2\right)^{-1}.$$

At bf_0, we again follow [Guillarmou and Hassell 2008] exactly. We use the coordinates $(\kappa = k/x, \kappa' = k/x', y, y')$, with k a bdf for bf_0. Note that these are only good coordinates on the interior of bf_0 — for example, they become degenerate near zf. We then view the interior of bf_0 as $\mathbb{R}_+(\kappa)\times\mathbb{R}_+(\kappa')\times N_y\times N'_y$. The normal operator at bf_0 is

$$I_{\mathrm{bf}_0}\left(k^{-2}(P+k^2)\right) = \kappa^{-1}\left(-(\kappa\partial_\kappa)^2+\Delta_N+\kappa^2\right)\kappa^{-1}.$$

Letting $P_{\mathrm{bf}_0} = -(\kappa\partial_\kappa)^2+\Delta_N+\kappa^2$, the model problem is $(\kappa P_{\mathrm{bf}_0}\kappa)G^{-2}_{\mathrm{bf}_0} = \delta\kappa-\kappa'\delta{-}y'$. To solve it, we separate variables and invert P_{bf_0}. For each eigenvalue λ_j of Δ_N, write $\nu_j = \sqrt{\lambda}_j$ (these are the indicial roots). Let $E_{\nu_j} \subset L^2(N)$ be the corresponding eigenspace of Δ_N, and let $\Pi_{E_{\nu_j}}$ be projection in $L^2(N)$ onto E_{ν_j}. Then the inverse of P_{bf_0} is

$$Q_{\mathrm{bf}_0} = \sum_{j=0}^{\infty}\Pi_{E_{\nu_j}}\left(I_{\nu_j}(\kappa)K_{\nu_j}(\kappa')\chi_{\{\kappa'>\kappa\}}+I_{\nu_j}(\kappa')K_{\nu_j}(\kappa)\chi_{\{\kappa'<\kappa\}}\right).$$

The only difference between our setting and Guillarmou and Hassell's is that we have $\nu_0=0$ as opposed to $\nu_0>0$. We then set

$$G^{-2}_{\mathrm{bf}_0} = (\kappa\kappa')Q_{\mathrm{bf}_0}.$$

We need to check consistency between G^0_{sc} and $G^{-2}_{\mathrm{bf}_0}$; that is, we need to show that they agree to leading order in a neighborhood of $\mathrm{sc}\cap\mathrm{bf}_0$. This proof is the same as in [Guillarmou and Hassell 2008]; the model problems and formal expressions for G^0_{sc} and $G^{-2}_{\mathrm{bf}_0}$ are identical. We do have $\nu_0=0$, and $K_0(r)$ has different small-r asymptotics from $K_{\nu_j}(r)$ for $\nu_j>0$; this will be reflected in the asymptotics of $G^{-2}_{\mathrm{bf}_0}$ near zf. However, since κ and κ' both approach infinity near sc, only the large-r asymptotics are relevant for this consistency check, and the large-r asymptotics of $I_\nu(r)$ and $K_\nu(r)$ are no different when $\nu=0$.

Technically, we also need to check consistency between the diagonal symbol and the models at bf_0 and sc. However, this is also the same as in [Guillarmou and Hassell 2008]; the models at bf_0 and sc themselves satisfy elliptic pseudodifferential equations given by the leading order part of $(P+k^2)G(k)=\mathrm{Id}$ at those faces. As a result, their symbols at the diagonal are determined up to symbols of order $-\infty$, and agree up to order $-\infty$ with the inverse of $|\xi|^2+k^2$.

4.4.2. *The leading order term at* zf. At zf, the model problem with respect to b-half-densities is

$$(x P_b x)\big(G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}\big) = \mathrm{Id},$$

which translates to

$$(x P_b x) G^0_{\mathrm{zf}} = \mathrm{Id}, \quad (x P_b x) G^{0,1}_{\mathrm{zf}} = 0.$$

Translating our observations in the $M=\mathbb{R}^2$ case to b-half-densities, we expect

$$G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}} = (xx')^{-1}(-C\log k + F(z,z')),$$

where $F(z,z')$ is a right inverse for P_b. We need to pick the correct right inverse; in particular, if we have one right inverse, we may add any function of z' to obtain another right inverse. The correct choice should have logarithmic singularities at all faces and should be consistent with our choice of $G^{-2}_{\mathrm{bf}_0}$. To check consistency, we need to show that $k^0\big(G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}\big)$ and $k^{-2}G^{-2}_{\mathrm{bf}_0}$ agree to leading order at $\mathrm{ff}=\mathrm{bf}_0\cap\mathrm{zf}$, which is the same as checking if $(xx')\big(G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}\big)$ and $Q_{\mathrm{bf}_0} = (\kappa\kappa')^{-1}G^{-2}_{\mathrm{bf}_0}$ agree to leading order there.

First examine the leading order part of Q_{bf_0} at zf. When $x<x'$, we use the coordinates (s,κ,x',y,y'), and we have, where $V=\mathrm{Vol}(N)$,

$$Q_{\mathrm{bf}_0} = V^{-1} I_0(\kappa\sigma')K_0(\kappa) + \sum_{j=1}^{\infty} \Pi_{E_j} I_{\nu_j}(\kappa\sigma')K_{\nu_j}(\kappa). \tag{38}$$

The boundary defining function for zf is κ, so we need to examine the small-κ asymptotics. For $\nu>0$ we know by standard asymptotics of Bessel functions in [Watson 1944] that

$$I_0(r)\sim 1, \quad K_0(r)\sim -\log r + \log 2 - \gamma, \quad I_\nu(r)\sim \frac{1}{\Gamma(\nu+1)}\left(\frac{r}{2}\right)^{\nu}, \quad K_\nu(r)\sim \frac{\Gamma(\nu)}{2}\left(\frac{r}{2}\right)^{-\nu}.$$

Here γ is the Euler–Mascheroni constant. Plugging these asymptotics into (38) shows that the leading order term in κ is

$$V^{-1}\big(-\log\kappa + \log 2 - \gamma\big) + \sum_{j=1}^{\infty} \Pi_{E_{\nu_j}} \frac{(\sigma')^{\nu_j}}{2\nu_j}.$$

On the other hand, when $x>x'$, we use the coordinates (σ,κ',x,y,y') and perform the same sort of calculations to obtain that the leading order term in κ is

$$V^{-1}\big(-\log\kappa' + \log 2 - \gamma\big) + \sum_{j=1}^{\infty} \Pi_{E_{\nu_j}} \frac{\sigma^{\nu_j}}{2\nu_j}.$$

The $x<x'$ and $x>x'$ cases may be combined; we see that the leading order term of Q_{bf_0} at zf is

$$V^{-1}\big(-\log k + \log 2 - \gamma + \log x' + \chi_{\sigma'<1}\log\sigma'\big) + \sum_{j=1}^{\infty} \Pi_{E_{\nu_j}} \frac{e^{-\nu_j|\log\sigma'|}}{2\nu_j}. \tag{39}$$

We see immediately that we must have $C=V^{-1}$, and hence we set

$$G_{\mathrm{zf}}^{0,1} = -V^{-1}(xx')^{-1}.$$

We then need to construct G_{zf}^0 so that $(xx')G_{\mathrm{zf}}^0$ has leading order at bf_0 given by

$$V^{-1}\big(\log 2 - \gamma + \log x' + \chi_{\sigma'<1}\log\sigma'\big) + \sum_{j=1}^{\infty} \Pi_{E_{\nu_j}} \frac{e^{-\nu_j|\log\sigma'|}}{2\nu_j}. \tag{40}$$

To construct G_{zf}^0, we must first find the correct right inverse for P_b. Fix δ with $0 < \delta < \nu_1$; then P_b is Fredholm from $x^{-\delta}H_b^2$ to $x^{-\delta}L_b^2$ by Theorem 22. Following the usual b-calculus construction in [Melrose 1993] and [Mazzeo 1991], we obtain a generalized inverse $Q_b^{-\delta}$. We claim:

Lemma 23. *P_b is surjective onto $x^{-\delta}L_b^2$.*

The lemma implies that $Q_b^{-\delta}$ is an exact right inverse for P_b.

Proof. By taking adjoints, the lemma is equivalent to the statement that P_b is injective on $x^{\delta}L_b^2$. Suppose that $u|dg_b|^{1/2}$ is in $x^{\delta}L_b^2$ and satisfies $P_b u = 0$. By regularity of solutions to b-elliptic equations, u is phg conormal on M near $x = 0$; since $u \in x^{\delta}L_b^2$, it decays to at least order δ at $x = 0$. On the other hand, since $P = xP_b x$ and $|dg_b|^{1/2} = x|dg|^{1/2}$, $u|dg|^{1/2}$ is in the kernel of $P = \Delta_M$, and hence $\Delta_M u = 0$. By the maximum principle, $u = 0$, which completes the proof of the lemma. $\square$

The correct right inverse will be a slight modification of $Q_b^{-\delta}$. In order to check consistency, we need to understand the structure of $Q_b^{-\delta}$ near the front face $\mathrm{ff} = \mathrm{bf}_0 \cap \mathrm{zf}$. This structure is described in detail in [Melrose 1993] and [Mazzeo 1991]. In particular, the leading order of $Q_b^{-\delta}$ at ff is precisely the indicial operator $I_{\mathrm{ff}}(Q_b^{-\delta})$, which satisfies the equation

$$\big(-(\sigma'\partial_{\sigma'})^2 + \Delta_N\big)I_{\mathrm{ff}}(Q_b) = \delta(\sigma' = 1, y = y'). \tag{41}$$

Moreover, from [Melrose 1993] and [Mazzeo 1991], $I_{\mathrm{ff}}(Q_b^{-\delta})$ has polyhomogeneous expansions at $\sigma' = 0$ and $\sigma' = \infty$, with leading order terms at worst $(\sigma')^{-\delta}$ at each end; that is, a small amount of growth is allowed at $\sigma' = 0$, and a small amount of decay is required at $\sigma' = \infty$.

We now separate variables and solve (41) directly. For each $j \geq 1$, $(\sigma')^{\pm\nu_j}$ span the kernel of $-(\sigma'\partial_{\sigma'})^2 + \nu_j^2$. Therefore, the solutions corresponding to E_{ν_j} are combinations of $(\sigma')^{\nu_j}$ and $(\sigma')^{-\nu_j}$ away from $\sigma' = 1$. By the requirements at $\sigma' = 0$ and $\sigma' = \infty$, our solution is a multiple of $(\sigma')^{-\nu_j}$ for $\sigma' > 1$ and of $(\sigma')^{\nu_j}$ for $\sigma' < 1$. Using the matching conditions at $\sigma' = 1$ arising from the delta function singularity, the solution on the eigenspace E_{ν_j} is

$$\Pi_{E_{\nu_j}} \frac{e^{-\nu_j|\log\sigma'|}}{2\nu_j}.$$

We have to consider $\nu_0 = 0$ separately; the kernel of $-(\sigma'\partial_{\sigma'})^2$ is spanned by 1 and $\log\sigma'$. Because we require decay at $\sigma' = \infty$, the solution for $\sigma' > 1$ must be zero. Then the matching conditions at $\sigma' = 1$ imply that the solution is $\log\sigma'$ for $\sigma' < 1$. Since projection onto E_0 is simply V^{-1}, the zero-eigenspace solution is $V\chi_{\{\sigma'<1\}}\log\sigma'$. Therefore the leading order part of $Q_b^{-\delta}$ at ff is

$$I_{\mathrm{ff}}(Q_b^{-\delta}) = V^{-1}\chi_{\{\sigma'<1\}}\log\sigma' + \sum_{j=1}^{\infty}\Pi_{E_{\nu_j}}\frac{e^{-\nu_j|\log\sigma'|}}{2\nu_j}. \tag{42}$$

Now compare (42) with (39). Let $\chi(z')$ be a smooth cutoff function on M, equal to 1 when $x'\in[0,1]$ and 0 whenever $x'\geq 2$. We see immediately that if we let

$$G^0_{\mathrm{zf}} = (xx')^{-1}\big(Q_b^{-\delta} + V^{-1}\chi(z')\log x' + V^{-1}(\log 2-\gamma)\big),$$

then $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$ and $G^{-2}_{\mathrm{bf}_0}$ are consistent. Additionally, G^0_{zf} solves the model problem $(xP_bx)G^0_{\mathrm{zf}}=\mathrm{Id}$ at zf; the key is that any function of z' is independent of (x,y) and hence is in the kernel of P_b. Similarly, $G^{0,1}_{\mathrm{zf}}\log k = -(Vxx')^{-1}\log k$ is in the kernel of xP_bx and hence solves the model problem. Moreover, the diagonal symbol is consistent with $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$ for the same reason that it is consistent with G^0_{sc} and $G^{-2}_{\mathrm{bf}_0}$.

4.4.3. *The model terms at* rb_0. Finally, we need to specify the leading-order behavior of the parametrix at rb_0; in fact, we need to specify some lower-order terms as well. We use the coordinates (x,y,κ',y'); the $\kappa'=0$ face is $\mathrm{rb}_0\cap\mathrm{zf}$ and the $x=0$ face is $\mathrm{rb}_0\cap\mathrm{bf}_0$. There will be a term $G^{\nu_j-1}_{\mathrm{rb}_0}$ for each ν_j in $[0,1)$. The model problem near this face, with k as a boundary defining function, is $(xP_bx)u=0$, so we need $P_b(xG^{-\nu_j}_{\mathrm{rb}_0})=0$ for each $\nu_j\in[0,1)$.

First we focus on the model of order -1. We let

$$G^{-1}_{\mathrm{rb}_0} = V^{-1}x^{-1}\kappa' K_0(\kappa'),$$

and claim that this is consistent with $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$ and $G^{-2}_{\mathrm{bf}_0}$.

To check consistency with $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$, we need to show that the leading order of $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$ agrees with the leading order of $k^{-1}G^{-1}_{\mathrm{rb}_0}$ at $\mathrm{zf}\cap\mathrm{rb}_0$. Recall that at rb_0, which corresponds to $s=\infty$, $Q_b^{-\delta}$ decays to a positive order. So $(xx')^{-1}Q_b^{-\delta}$ has leading order greater than -1 at rb_0; therefore, the leading order part of $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$ at rb_0 is precisely

$$(xx')^{-1}\big(V^{-1}(-\log\kappa' + \log 2-\gamma)\big).$$

But by Bessel function asymptotics,

$$k^{-1}G^{-1}_{\mathrm{rb}_0} = V^{-1}(xx')^{-1}K_0(\kappa') \sim (xx')^{-1}V^{-1}\big(-\log\kappa' + \log 2-\gamma\big).$$

Therefore $G^{0,1}_{\mathrm{zf}}\log k + G^0_{\mathrm{zf}}$ and $G^{-1}_{\mathrm{rb}_0}$ are consistent.

We must also check consistency of $G^{-1}_{\mathrm{rb}_0}$ with $G^{-2}_{\mathrm{bf}_0}$. Near rb_0,

$$k^{-2}G^{-2}_{\mathrm{bf}_0} = V^{-1}(xx')^{-1}I_0(\kappa)K_0(\kappa') + (xx')^{-1}\sum_{j=1}^{\infty}\Pi_{E_{\nu_j}}I_{\nu_j}(\kappa)K_{\nu_j}(\kappa').$$

We are only interested in the order -1 part of this term. Since x' and κ both vanish to first order at rb_0, all the $j>0$ terms have leading order $-1+\nu_j$ at rb_0. Since $I_0(0)=1$, the order -1 part of $k^{-2}G^{-2}_{\mathrm{bf}_0}$ at

rb_0 is precisely

$$(xx')^{-1}V^{-1}K_0(\kappa') = k^{-1}\big(V^{-1}x^{-1}\kappa' K_0(x')\big) = k^{-1}G^{-1}_{\mathrm{bf}_0}.$$

We conclude that $G^{-1}_{\mathrm{rb}_0}$ is consistent with the models at zf and bf_0.

We also need to specify some lower order terms at bf_0; for this we precisely follow [Guillarmou and Hassell 2008, Section 4]. At zf, they need to match with the asymptotics of $Q_b^{-\delta}$, and at bf_0, they need to match with the higher order Bessel functions. Both of these involve only the nonzero indicial roots, so the terms and arguments are identical to [Guillarmou and Hassell 2008]. In particular, for any $0 < \nu_j < 1$ in the indicial set, we let

$$G^{\nu_j-1}_{\mathrm{rb}_0} = x^{-1}\frac{\kappa' K_{\nu_j}(\kappa')}{\Gamma(\nu_j)2^{\nu_j-1}}\, v_{\nu_j}(z, y'),$$

where $v_{\nu_j}(z, y')$ is in the kernel of P_b with asymptotic

$$v_{\nu_j}(x, y, y') = (2\nu_j)^{-1}\Pi_{E_j}x^{-\nu_j} + \mathcal{O}(x^{-\nu_j-1}\log x).$$

The function v_{ν_j} is there to match with the asymptotics of Q_b at rb_0, as in [Guillarmou and Hassell 2008, Section 4]. In fact, these models are consistent with our models at bf_0 and at zf by precisely the same argument as in [Guillarmou and Hassell 2008]; we will not repeat it here.

4.5. ***The final parametrix and resolvent.*** We have now constructed models at sc, bf_0, zf, and rb_0 which are consistent with each other and also with the diagonal symbol. Moreover, all the models decay to infinite order as we approach lb, rb, or bf. Therefore, we specify our parametrix $G(k)$ to be any pseudodifferential operator in $\Psi_k^{-2,\mathscr{E}}$ with kernel having the specified diagonal symbol and specified leading-order terms at sc, bf_0, zf, and rb_0. The consistency we checked guarantees that such an operator exists. The behavior of the kernel of $G(k)$ at lb_0 may be freely chosen as long as the leading-order term is order -1 and it matches with our models at zf and bf_0; a term of order -1 will, however, be required.

Now let $E(k) = (P+k^2)G(k) - \mathrm{Id}$. Since $G(k)$ has diagonal symbol equal to the inverse of the symbol of $P+k^2$, the Schwartz kernel of $E(k)$ is smooth on the interior of $M^2_{w,\mathrm{sc}}$. Moreover, since $P+k^2$ is a differential operator, the Schwartz kernel of $E(k)$ is phg conormal on $M^2_{w,\mathrm{sc}}$.

- At lb, rb, and bf, the Schwartz kernel of $G(k)$ vanishes to infinite order along with all derivatives, so the same is true of $E(k)$.
- At sc, G^0_{sc} solves the model problem, so $E(k)$ has positive leading order at sc.
- At bf_0, $G(k)$ has order -2, but $G^{-2}_{\mathrm{bf}_0}$ solves the model problem, and moreover $P+k^2$ vanishes to second order. Therefore $E(k)$ has positive leading order at bf_0.
- At zf, G^0_{zf} and $G^{0,1}_{\mathrm{zf}}$ solve the model problem, so $E(k)$ has positive leading order.
- At lb_0, $G(k)$ has order -1. The variables k and x both vanish at lb_0, so $k^2G(k)$ has order 1 and $xG(k)$ has order 0. Since P_b is a b-differential operator, $P_b(xG(k))$ also has order 0, and hence $(P+k^2)G(k) = (xP_bx+k^2)G(k)$ has order 1. Since Id is supported away from lb_0, $E(k)$ decays to at least order 1 at lb_0.

- At rb_0, $G(k)$ has order -1, but all the terms G^{ν_j-1} for $\nu_j \in [0, 1)$ solve the model problem. Therefore, the error $E(k)$ has leading order at worst 0.

To summarize, if $\mathcal{E}$ is the index set for $E(k)$, we have shown:

$$\mathcal{E}_{\mathrm{sc}} > 0, \quad \mathcal{E}_{\mathrm{zf}} > 0, \quad \mathcal{E}_{\mathrm{bf}_0} > 0, \quad \mathcal{E}_{\mathrm{lb}_0} \geq 1, \quad \mathcal{E}_{\mathrm{rb}_0} \geq 0, \quad \mathcal{E}_{\mathrm{lb}} = \mathcal{E}_{\mathrm{rb}} = \mathcal{E}_{\mathrm{bf}} = \varnothing.$$

Now we iterate away the error. By Proposition 21, $E(k)^2$ vanishes to positive order at all faces of $M^2_{k,\mathrm{sc}}$; suppose that the order of vanishing at each face is greater than $\epsilon > 0$. Again applying Proposition 21, we see that for each $N \in \mathbb{N}$, the order of vanishing of $E(k)^{2N}$ and $E(k)^{2N+1}$ at each face of $M^2_{k,\mathrm{sc}}$ is greater than $N\delta$. Therefore the Neumann series

$$\big(\mathrm{Id} + E(k)\big)^{-1} = \sum_{i=0}^{\infty} E(k)^i$$

may be summed asymptotically, and the sum defines an element of $\Psi_k^{-\infty,\hat{\mathcal{E}}}$ for some index family $\hat{\mathcal{E}}$.

Finally, let $R(k) = G(k)(\mathrm{Id} + E(k))^{-1}$; we see that $(P + k^2)R(k) = \mathrm{Id}$. Since $P + k^2$ is invertible for all positive k, its only right inverse is the resolvent. We conclude that $R(k)$ is in fact the resolvent, and it is an element of $\Psi_k^{-\infty,\mathcal{R}}(M, \tilde{\Omega}_b^{1/2})$ for some index family $\mathcal{R}$.

In order to prove Theorem 7, we need to perform this construction for any angle $\theta \in (-\pi, \pi)$, not just for $\theta = 0$. However, as claimed in [Guillarmou and Hassell 2008], the construction is essentially unchanged. Indeed, we just use $e^{i\theta/2}k$ as our boundary defining function for the $k = 0$ faces instead of k, and correspondingly change the model at sc from $(\Delta_{\mathbb{R}^2} + k^2)^{-1}$ to $(\Delta_{\mathbb{R}^2} + e^{i\theta}k^2)^{-1}$. The construction is then precisely analogous to the $\theta = 0$ case; by construction, the index sets are independent of θ. Moreover, by the continuity of the resolvent outside the spectrum (also by construction), all the dependence on θ is smooth. This completes the proof.

4.6. ***Leading orders of the resolvent.*** Since $R(k) = G(k) - G(k)E(k) + G(k)E(k)^2 - \cdots$, we can obtain some information about the leading orders of $R(k)$ at each face. For $n \geq 3$, it is shown in [Guillarmou and Hassell 2008] that the leading orders of $R(k)$ are the same as those of $G(k)$; we claim that the same is true when $n = 2$.

When $n = 2$, $G(k)$ has leading orders -1 at lb_0 and rb_0, order 0 at sc, order -2 at bf_0, and logarithmic growth at zf. $E(k)$ has non-negative leading orders at all faces, and it is easy to use Proposition 21 to show that the leading orders of $G(k)E(k)$ are no worse than those of $G(k)$. Similarly, it may be shown that the leading orders of $G(k)E(k)^l$ are no worse than those of $G(k)$. Since $G(k)$ is fixed and $\mathrm{Id} - E(k) + E(k)^2 - \cdots$ is asymptotically summable, the series $G(k) - G(k)E(k) + \cdots$ is also asymptotically summable; therefore, the leading orders of $R(k)$ are no worse than those of $G(k)$. The leading order terms themselves may be affected by $G(k)E(k)$, but the orders are not.

To summarize, when $n = 2$, the leading orders of the exact resolvent $R(k)$ are no worse than 0 at sc, -2 at bf_0, logarithmic at zf, and -1 at lb_0 and rb_0. When $n \geq 3$, the orders are at worst 0 at sc, -2 at bf_0, 0 at zf, and $n/2 - 2$ at lb_0 and rb_0, as in [Guillarmou and Hassell 2008]. However, these orders are for the resolvent acting on b-half-densities, rather than the more natural scattering half-densities. Switching to scattering half-densities requires an order shift, adding $n/2$ at each of $\{x=0\}$ and $\{x'=0\}$. So we need to add $n/2$ to the orders at lb_0 and rb_0, and n at bf_0. The order at sc remains unchanged, because the extra factor of $\rho_{\mathrm{sc}}^{n/2}$ in the definition of the calculus already incorporates the shift. So: viewing the resolvent as a scattering half-density $|dg\,dg'|^{1/2}$ acting on scattering half-densities for each k, or equivalently as a function acting on functions on M by integration against dg, it has leading orders given by

- 0 at sc and $n-2$ at bf_0, rb_0, and lb_0;
- r_{zf} at zf, where $r_{\mathrm{zf}}=0$ if $n\geq 3$ and $r_{\mathrm{zf}}=(0,1)$ (that is, leading order behavior of $\log\rho_{\mathrm{zf}}$) if $n=2$.

Appendix: Construction of the short-time heat kernel

Albin has created a framework for the construction of the heat kernel on an asymptotically conic manifold; essentially all of the hard work involved in this construction has already been done [2007]. To complete the construction and prove Theorem 3, all we need to do is create an initial parametrix for the heat kernel. This construction is the content of this short appendix and is based on [Albin 2007, Section 5], in which the heat kernel on an edge manifold is constructed.

The space in Theorem 3, which we call S_{heat}, is obtained by taking the manifold $M_{\mathrm{sc}}^2\times[0,T)_t$ and then blowing up the $t=0$ diagonal. We call the scattering face of $M_{\mathrm{sc}}^2\times[0,T)_t$ sf and call the front face at $t=0$ ff. The heat operator is precisely $\partial_t+\Delta_M$. Our goal is to create a parametrix which, to first order, solves the normal equations at sf and ff.

First analyze the situation at sf. As first discussed in [Melrose 1994] and elaborated upon in [Guillarmou and Hassell 2008], sf has a Euclidean structure, parametrized by $y\in N$ and $t\in[0,T)$. By the same analysis as in the latter paper, the normal operator at sf is precisely $\partial_t+\Delta_{\mathbb{R}^n}$. We then simply let the model at sf be the Euclidean heat kernel, $H^{\mathbb{R}^n}$. This is analogous to the construction in [Albin 2007, Section 5] for the edge setting, in which the model is the heat kernel on hyperbolic space times the heat kernel on the fiber.

The analysis at ff is also standard, since ff corresponds to the short-time regime on the interior of the manifold, where the heat kernel asymptotics are local. We know that $d(z,z')/\sqrt{t}$ is a good coordinate along ff, zero at the spatial diagonal and increasing to infinity as we approach the original $t=0$ face. We therefore let the leading-order model at ff be

$$H_{\mathrm{ff}}=\frac{1}{(4\pi t)^{n/2}}\,e^{-d(z,z')^2/4t}.$$

The choice of model at ff is again based on the Euclidean heat kernel, and is precisely the same as the choice of model in the edge setting [Albin 2007].

Each model vanishes to infinite order as we approach all boundary hypersurfaces other than sf and ff. Moreover, the models are consistent, as the leading orders of each are precisely the Euclidean heat kernel at sf $\cap$ ff. We may therefore pick a pseudodifferential operator whose Schwartz kernel agrees with our models to leading order at sf and ff, and decays to infinite order at all other boundary faces. Albin [2007, Section 4] proves a composition rule for time-dependent pseudodifferential operators whose kernels are polyhomogeneous conormal on S_{heat} — our setting is the "scattering" setting, which is included in his analysis. We then use this composition rule and an iteration argument, precisely as in [Albin 2007, Section 5], to construct the heat kernel as a polyhomogeneous conormal distribution on S_{heat}. This completes the proof of Theorem 3.

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