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Multiwave methods via ultrasound

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We survey recent results by the authors on multiwave methods where the high-resolution method is ultrasound. We consider the inverse problem of determining a source inside a medium from ultrasound measurements made on the boundary of the medium. Some multiwave medical imaging methods where this is considered are photoacoustic tomography, thermoacoustic tomography, ultrasound modulated tomography, transient elastography and magnetoacoustic tomography. In the case of measurements on the whole boundary, we give an explicit solution in terms of a Neumann series expansion. We give almost necessary and sufficient conditions for uniqueness and stability when the measurements are taken on a part of the boundary. We study the case of a smooth speed and speeds having jump type of singularities. The latter models propagation of acoustic waves in the brain, where the skull has a much larger sound speed than the rest of the brain. In this paper we emphasize a microlocal viewpoint.

1. Introduction

Multiwave imaging methods, also called hybrid methods, attempt to combine the high resolution of one imaging method with the high contrast capabilities of another through a physical principle. One important medical imaging application is breast cancer detection. Ultrasound provides high (submillimeter) resolution, but it suffers from low contrast. On the other hand, many tumors absorb much more energy from electromagnetic waves (in some specific energy bands) than healthy cells. Photoacoustic tomography (PAT) [Wang 2009] consists of exposing tissues to relatively harmless optical radiation that causes temperature increases in the millikelvin range, resulting in the generation of propagating ultrasound waves (the photoacoustic effect). Such ultrasonic waves are readily measurable. The inverse problem then consists of reconstructing the optical properties of the tissue. In thermoacoustic tomography (TAT) — see, e.g., [Kruger et al. 1999] — low frequency microwaves, with wavelengths on the order of 1 m, are sent into the medium. The rationale for using the latter frequencies is that they are

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less absorbed than optical frequencies. In ultrasound modulated tomography (UMT), radiation is sent through the tissues at the same time as a modulating acoustic signal, which changes the local properties of the optical parameters (the acousto-optic effect) in a controlled manner. The objective is then the same as in PAT: to reconstruct the optical properties of the tissues. In both modalities, we seek to combine the large contrast in optical parameters between normal and cancerous tissues with the high (submillimeter) resolution of ultrasound imaging. Transient elastography (TE) [McLaughlin et al. 2010] images the propagation of shear waves using ultrasound. In magnetoacoustic tomography (MAT) [Xu and He 2005] the medium is located in a static magnetic field and a time-varying magnetic field. The time dependent magnetic field induces an eddy current and therefore induce an acoustic wave by the Lorentz force which are measured at the boundary of the medium. PAT, TAT, UMT, TE and MAT offer potential breakthroughs in the clinical application of multiwave methods to early detection of cancer, functional imaging, and molecular imaging among others.

We remark that we are only considering the first step in solving the inverse problem, namely recovering the source term from ultrasound measurements at the boundary. For a review of the results in recovering optical, elastic, electromagnetic and other properties of tissues see [Bal 2013] in this volume. This first step has been studied extensively in the mathematical literature; see, e.g., [Agranovsky et al. 2009; Finch et al. 2004; Finch and Rakesh 2009; Hristova 2009; Hristova et al. 2008; Kuchment and Kunyansky 2008; Patch 2004; Stefanov and Uhlmann 2009b; 2011] and the references there.

The purpose of this survey is to present an approach to the problem allowing us to treat variable and discontinuous sound speeds, and also consider partial data, based on [Stefanov and Uhlmann 2009b; 2011]. This approach is based on microlocal, PDE and functional analysis methods, rather than trying to find explicit closed form formulas for the partial case of a constant speed. We always assume a variable speed. We will actually formulate the problem in anisotropic media modeled by a Riemannian metric g in $\mathbb{R}^n$. Let $c > 0$, $q \geq 0$ be functions, all smooth and real-valued. Assume for convenience that g is Euclidean outside a large compact, and $c - 1 = q = 0$ there.

Let P be the differential operator

$$P = -c^2 \Delta_g + q, \qquad \Delta_g = \frac{1}{\sqrt{\det g}} \frac{\partial}{\partial x^i} g^{ij} \sqrt{\det g} \frac{\partial}{\partial x^j}. \tag{1-1}$$

Let u solve the problem

$$\begin{cases} (\partial_t^2 + P)u &= 0 \quad \text{in } (0,T) \times \mathbb{R}^n, \\ u|_{t=0} &= f, \\ \partial_t u|_{t=0} &= 0, \end{cases} \tag{1-2}$$

where $T > 0$ is fixed.

Assume that f is supported in $\overline{\Omega}$, where $\Omega \subset \mathbb{R}^n$ is some smooth bounded domain. The measurements are modeled by the operator

$$\Lambda f := u|_{[0,T]\times\partial\Omega}. \tag{1-3}$$

The problem is to reconstruct the unknown f, knowing c; and if possible, to reconstruct both. The same problem, but with data on a part of $\partial\Omega$ is of great practical interest, as well.

The accepted mathematical model is as described above with g Euclidean, and $q = 0$; see, e.g., [Xu and Wang 2006a; Wang and Wu 2007; Finch et al. 2004]. Including nontrivial g and q does not complicate the problem further, and one can even include a magnetic field [Stefanov and Uhlmann 2009b].

If $T = \infty$, then one can solve a problem with Cauchy data 0 at $t = \infty$ (as a limit), and boundary data $h = \Lambda f$. The zero Cauchy data are justified by local energy decay that holds for nontrapping geometry, for example (actually, it is always true but much weaker and not uniform in general). Then solving the resulting problem backwards recovers f. This is known as *time reversal* or *back-projection*. For a fixed T, one can still do the same thing with an error $\epsilon(T) \to 0$, as $T \to \infty$. In the nontrapping case, n odd, the error is uniform and $\epsilon(T) = O(e^{-T/C})$. There is no good control over C though. Error estimates based on local energy decay can be found in [Hristova 2009]; see also Corollary 4.2. Other reconstruction methods have been used as well (see, e.g., [Hristova et al. 2008] for a discussion) and they all use measurements for all t in the variable coefficients case, i.e., $T = \infty$; and they are only approximate for $T < \infty$ with an error depending on the local energy decay rate. Of course, if n is odd and $P = -\Delta$, any finite $T > \operatorname{diam}(\Omega)$ suffices by Huygens' principle. In the constant-speed case and for Ω of a specific type such as a ball or a box there are explicit closed-form inversion formulas; see [Finch et al. 2004; Xu and Wang 2005; Haltmeier et al. 2004; 2005; Finch et al. 2007] and references therein.

We describe now briefly the contents of this survey. We study what happens when $T < \infty$ is fixed. When the speed is smooth, Tataru's continuation principle [1995; 1999] provides a sharp time T_0 such that there is uniqueness for $T > T_0$ and no uniqueness for $T < T_0$. This time can be characterized as the least time T such that a signal from any point can reach $\partial\Omega$ before that time. For stable recovery, we need something more: from any point *and any direction*, we need the corresponding unit speed geodesic to hit $\partial\Omega$ for time t such that $|t| < T_1/2$. The optimal T_1 with that property is the length of the longest geodesic in $\overline{\Omega}$. Then when $T > T_1/2$, there is stability. In case of data on $[0, T] \times \partial\Omega$, $T > T_1/2$, we present an explicit Neumann series inversion formula. We also analyze the same questions for observations on a part of the boundary. In Section 3

we give an almost necessary and sufficient condition for uniqueness, and in Section 5 we give another almost necessary and sufficient condition for stability. In Proposition 5.1 we characterize Λ as a sum of two Fourier integral operators with canonical relations of graph type. Under the stability assumption, we do not have an explicit inversion anymore but we show that the problem reduces to a Fredholm equation with a trivial kernel.

In Section 6, we discuss a relation between the problems we consider and boundary control.

In Section 7 we give an estimate of the largest time interval for the geodesics to leave the medium which is important for the stability analysis.

In Section 8 we discuss briefly the connection with integral geometry.

In Section 9, we study the case where c is piecewise smooth, with jumps over smooth surfaces. This case is important for applications since in brain imaging, the acoustic speed jumps by a factor of two in the skull. Propagation of singularities is more complicated in this case: a single singularity can reflect and refract when hitting the boundary, then each branch can do the same. etc. Rays tangent to the boundary behave in an even more complicated manner. We present results similar to some of the ones above, under more restrictive assumptions which would allow us to avoid the analysis of the tangent rays. We review thoroughly the construction of geometrical optics solutions in this case.

In the Appendix we review briefly some basic concepts of microlocal analysis used in this survey. This is based mainly on [Stefanov 2012].

We also mention that a numerical method based on the theoretical developments considered here has been developed in [Qian et al. 2011].

We assume throughout the paper that the speed of sound is known. It has been suggested [Jin and Wang 2006] that one can use ultrasound transmission tomography, which measures travel times, to determine the speed of sound. For a numerical algorithm for UTT and also reflection tomography see [Chung et al. 2011]. This algorithm is based on the theoretical work [Stefanov and Uhlmann 1998a].

2. Preliminaries

2A. ***Energy spaces.*** Let g, $q \geq 0$ and c be in C^∞ first. The operator P is formally self-adjoint with respect to the measure $c^{-2}\mathrm{d\,Vol}$, where $\mathrm{d\,Vol}(x) = \sqrt{\det g}\,\mathrm{d}x$. Given a domain U, and a function $u(t,x)$, define the energy

$$E_U(t,u) = \int_U \left(|Du|^2 + c^{-2}q|u|^2 + c^{-2}|u_t|^2\right) \mathrm{d\,Vol},$$

where $D_j = -\mathrm{i}\partial/\partial x^j$, $D = (D_1, \ldots, D_n)$, $|Du|^2 = g^{ij}(D_i u)(\overline{D_j u})$. In particular, we define the space $H_D(U)$ to be the completion of $C_0^\infty(U)$ under the

Dirichlet norm

$$\|f\|_{H_D}^2 = \int_U \left(|Du|^2 + c^{-2}q|u|^2\right) \mathrm{d\,Vol}\,. \tag{2-1}$$

It is easy to see that $H_D(U) \subset H^1(U)$, if U is bounded with smooth boundary, therefore, $H_D(U)$ is topologically equivalent to $H_0^1(U)$. If $U = \mathbb{R}^n$, this is true for $n \geq 3$ only, if $q = 0$. By the finite speed of propagation, the solution with compactly supported Cauchy data always stays in H^1 even when $n = 2$. The energy norm for the Cauchy data (f, h), that we denote by $\|\cdot\|_{\mathcal{H}}$ is then defined by

$$\|(f,h)\|_{\mathcal{H}}^2 = \int_U \left(|Df|^2 + c^{-2}q|f|^2 + c^{-2}|h|^2\right) \mathrm{d\,Vol}\,.$$

This defines the energy space

$$\mathcal{H}(U) = H_D(U) \oplus L^2(U).$$

Here and below, $L^2(U) = L^2(U;\, c^{-2}\mathrm{d\,Vol})$. Note also that

$$\|f\|_{H_D}^2 = (Pf, f)_{L^2}. \tag{2-2}$$

The wave equation then can be written down as the system

$$\boldsymbol{u}_t = \boldsymbol{P}\boldsymbol{u}, \quad \boldsymbol{P} = \begin{pmatrix} 0 & I \\ -P & 0 \end{pmatrix}, \tag{2-3}$$

where $\boldsymbol{u} = (u, u_t)$ belongs to the energy space $\mathcal{H}$. The operator $\boldsymbol{P}$ then extends naturally to a skew-selfadjoint operator on $\mathcal{H}$. In this paper, we will deal with either $U = \mathbb{R}^n$ or $U = \Omega$. In the latter case, the definition of $H_D(U)$ reflects Dirichlet boundary conditions.

Assume now that c, $1/c$ and q are in L^∞. Then again, $\boldsymbol{P}$ is a skew-selfadjoint operator on $\mathcal{H}(U)$ (see [Stefanov and Uhlmann 2011]) and the statements above still hold. The important case for applications is $g = \{\delta_{ij}\}$ and $q = 0$.

By [Lasiecka et al. 1986; Katchalov et al. 2001], the operator

$$\Lambda : H_D(\Omega) \to H^1_{(0)}([0,T] \times \partial\Omega)$$

is bounded, where the subscript (0) indicates the subspace of functions vanishing for $t = 0$.

2B. ***Finite propagation speed and unique continuation for the wave equation.*** It is well known (see [Taylor 1996, Chapter 8], for example) that the wave equation (2-7) has the finite speed of propagation property: "signals" propagate with speed no greater that 1, in the metric $c^{-2}g$ (or with speed c, in the metric g).

More precisely, if u solves (2-7) and has Cauchy data (f, h) for $t = 0$, then

$$u(t, x) = 0 \quad \text{for} \quad t > \operatorname{dist}(x, \operatorname{supp}(f, h)), \tag{2-4}$$

where "dist" is the distance in the metric $c^{-2}g$. Another way to say this is that any solution of (2-7) at (t_0, x_0) has a domain of dependence given by the characteristic cone

$$\{(t, x);\ \operatorname{dist}(x, x_0) \le |t - t_0|\}. \tag{2-5}$$

The forward part of this cone is given by $t > t_0$, and the backward one by $t < t_0$.

Recall that given two subsets A and B of a metric space, the distance $\operatorname{dist}(A, B)$ is defined by

$$\operatorname{dist}(A, B) = \sup(\operatorname{dist}(a, B);\ a \in A). \tag{2-6}$$

This function is not symmetric in general; the Hausdorff distance is defined as

$$\operatorname{dist}_{\mathrm{H}}(A, B) = \max\big(\operatorname{dist}(A, B), \operatorname{dist}(B, A)\big).$$

The finite speed propagation property can then be formulated in the following form: if u has Cauchy data (f, h) at $t = 0$ supported in the set U, then $u(t, x) = 0$ when $\operatorname{dist}(x, U) > |t|$.

We recall next a Holmgren's type of unique continuation theorem for the wave equation $(\partial_t^2 + P)u = 0$ due mainly to Tataru [1995; 1999]. The local version of this theorem states that we have unique continuation across every surface that is not characteristic for P. One of its global versions, presented below, follows from its local version by Holmgren's type of arguments; see also [Katchalov et al. 2001].

Theorem 2.1. *Let P be the differential operator in $\mathbb{R}^n$ defined in* (1-1)*. Assume that $u \in H^1_{\mathrm{loc}}$ satisfies*

$$(\partial_t^2 + P)u = 0, \tag{2-7}$$

near the set in (2-8) *and vanishes in a neighborhood of $[-T, T] \times \{x_0\}$, with some $T > 0$, $x_0 \in \mathbb{R}^n$. Then*

$$u(t, x) = 0 \quad \textit{for } |t| + \operatorname{dist}(x_0, x) < T. \tag{2-8}$$

Proof. If P has analytic coefficients, this is Holmgren's theorem. In the non-analytic coefficients case, a version of this theorem was proved in [Robbiano 1991] with ρ replaced by $K\rho$ with an unspecified constant $K > 0$. It is derived there from a local unique continuation theorem across a surface that is "not too close to being characteristic". Hörmander [1992, Theorem 1 and Corollary 7] showed that one can choose $K = \sqrt{27/23}$, in both the local theorem and the global theorem. Moreover, he showed that K in the global one can be chosen to be

the same as the K in the local one. Finally, Tataru [1995; 1999] proved a unique continuation result that implies unique continuation across any noncharacteristic surface. This shows that actually $K = 1$ in Hörmander's work, and the theorem above then follows from [Hörmander 1992, Corollary 7]. □

For the partial data analysis we need a version of that theorem restricted to a bounded (connected) domain Ω. The inconvenience of the theorem above is that it requires u to solve the wave equation in a cone that may not fit in $\mathbb{R} \times \Omega$. The next theorem shows unique continuation of Cauchy data on $\mathbb{R} \times \partial\Omega$ to their domain of influence; see e.g., [Katchalov et al. 2001, Theorem 3.16].

Proposition 2.2. *Let $\Omega \subset \mathbb{R}^n$ be a domain, and let $u \in H^1$ solve the homogeneous wave equation $Pu = 0$ in $[-T, T] \times \Omega$. Assume that u has Cauchy data zero on $[-T, T] \times \Gamma$, where $\Gamma \subset \partial\Omega$ is open. Then $u = 0$ in the domain of influence $\{(t, x) \in [-T, T] \times \Omega;\ \operatorname{dist}(x, \Gamma) < T - |t|\}$.*

One way to derive Proposition 2.2 from the unique continuation theorem is to extend u as zero in a one sided neighborhood of Γ, in the exterior of Ω (by extending g and c there first), and this extension will still be a solution. Then we apply unique continuation along a curve connecting that exterior neighborhood with an arbitrary point x such that $\operatorname{dist}(x, \Gamma) < T$. To make sure that we always stay in some neighborhood of that curve in the x space, we need to apply the unique continuation Theorem 2.1 in small increments. We refer to the proof of [Stefanov and Uhlmann 2011, Theorem 6.1] for similar arguments.

3. Uniqueness for a smooth speed

Uniqueness and reconstruction results in the constant coefficients case based on spherical means have been known for a while; see e.g., the review paper [Kuchment and Kunyansky 2008]. If $P = -c^2(x)\Delta$, and Λf is known on $[0, T] \times \partial\Omega$, Finch and Rakesh [2009] have proved that Λf recovers f uniquely as long as $T > 2T_0$; see the definition below. A uniqueness result when Γ is a part of $\partial\Omega$ in the constant coefficients case is given in [Finch et al. 2004], and we follow the ideas of that proof below. Holmgren's uniqueness theorem for constant coefficients and its analogue for variable ones (see Theorem 2.1) play a central role in the proofs, which suggests possible instability without further assumptions; see also the remark following Theorem 5.2 below.

Stability of the reconstruction when $P = -\Delta$ and $T = \infty$ follows from known reconstruction formulas; see e.g., [Kuchment and Kunyansky 2008]. In the variable coefficients case, stability estimates as $T \to \infty$ based on local energy decay have been established recently in [Hristova 2009]. When T is fixed, there is the general feeling that if one can recover "stably" all singularities, and if there is uniqueness, there must be stability (although this has been viewed from the point

of view of integral geometry; see also Section 8). We prove this to be the case in Theorem 5.2, and we use the analysis in [Stefanov and Uhlmann 2009a] as well.

3A. ***Data on the whole boundary.*** We study first the uniqueness of recovery of f, given Λf. Since this is a linear problem, we just need to study conditions under which Λ has a trivial kernel.

We would like to use the unique continuation Theorem 2.1 but we only know that the solution u to (1-2) vanishes for $x \in \partial\Omega$ and $t \in [0, T]$. For the application of the uniqueness continuation theorem, we need to know that the normal derivative of u on $\partial\Omega$ vanishes, as well. Then we could apply Proposition 2.2. Here, we would use the simple fact that u extends as a solution to the wave equation for $t < 0$ in an even way, since $u_t = 0$ for $t = 0$.

It turns out, that knowing $\Lambda \boldsymbol{f}$, one can recover the Neumann derivative of the solution at $[0, T] \times \partial\Omega$ as well. This is done by applying the nonlocal exterior Dirichlet-to-Neumann map to $\Lambda \boldsymbol{f}$; see Lemma 6.1. We will explain now briefly the uniqueness part of this recovery. Suppose that $\Lambda f = 0$ (on $[0, T] \times \Omega$). The function u also solves the wave equation in the exterior of Ω for $0 < t < T$, with vanishing Dirichlet data on $[0, T] \times \partial\Omega$ by assumption. The Cauchy data at $t = 0$ are zero as well, because supp $f \subset \overline{\Omega}$. Therefore, $u = 0$ on $[0, T] \times (\mathbb{R}^n \setminus \Omega)$. Take a normal derivative $\partial/\partial\nu$ on $\partial\Omega$ from the exterior, to get $\partial u/\partial\nu = 0$ on $[0, T] \times \partial\Omega$. We can extend those equalities for $t \in [-T, 0]$, as well, because u is an even function of t. By Proposition 2.2, $f(x) = 0$ for $\operatorname{dist}(x, \partial\Omega) < T$. Note that this is a sharp inequality by the finite speed of propagation. To get $f = 0$ for all $x \in \Omega$, we need to take T greater than the critical "uniqueness time"

$$T_0 = \operatorname{dist}(\Omega, \partial\Omega); \tag{3-1}$$

see (2-6).

We have therefore proved the following.

Theorem 3.1. *Let $\Lambda f = 0$ with $f \in H_D(\Omega)$. Then $f(x) = 0$ for $\operatorname{dist}(x, \partial\Omega) < T$. In particular*:

(a) *If $T < T_0$, then $f(x)$ can be arbitrary for $\operatorname{dist}(x, \partial\Omega) > T$.*

(b) *If $T > T_0$, then $f = 0$.*

If we restrict f to a subspace of functions supported in some compact set $K \subset \overline{\Omega}$, then the theorem above admits an obvious generalization with T_0 replaced by $T_0(K) := \operatorname{dist}(K, \partial\Omega)$. Also, f can be a distribution supported in $\overline{\Omega}$, and the theorem would still hold.

3B. ***Data on a part of $\partial\Omega$.*** The case of partial measurements has been discussed in the literature as well; see, e.g., [Kuchment and Kunyansky 2008; Xu et al.

2004; 2009]. One of the motivations is that in breast imaging, for example, measurements are possible only on part of the boundary. Remember that $P = -\Delta$ outside Ω. All geodesics below are related to the metric $c^{-2}g$.

Let $\Gamma \subset \partial\Omega$ be a relatively open subset of $\partial\Omega$. We are interested in what information about f can be obtained when making measurements on sets of the kind

$$\mathcal{G} := \{(t, x);\ x \in \Gamma,\ 0 < t < s(x)\}, \tag{3-2}$$

where s is a fixed continuous function on Γ. This corresponds to measurements taken at each $x \in \Gamma$ for the time interval $0 < t < s(x)$. The special case studied so far is $s(x) \equiv T$, for some $T > 0$; then $\mathcal{G} = [0, T] \times \Gamma$, and this is where our main interest is.

We assume now that the observations are made on $\mathcal{G}$ only, i.e., we assume we are given

$$\Lambda f|_{\mathcal{G}}, \tag{3-3}$$

where, with some abuse of notation, we denote by Λ the operator in (1-3), with $T = \infty$ that actually can be replaced by any upper bound of the function s.

We study below functions f with support in some fixed compact $\mathcal{K} \subset \overline{\Omega}$. By the finite speed of propagation, to be able to recover all f supported in $\mathcal{K}$, we want for any $x \in \mathcal{K}$, at least one signal from x to reach $\mathcal{G}$, i.e., we want to have a signal that reaches some $z \in \Gamma$ for $t \leq s(z)$. In other words, we should at least require that

$$\forall x \in \mathcal{K}, \exists z \in \Gamma \text{ such that } \operatorname{dist}(x, z) < s(z). \tag{3-4}$$

We strengthened slightly the condition by replacing the $\leq$ sign by $<$. In Theorem 3.2 below, we show that this is a sufficient condition, as well.

Another way to formulate this condition is to say that $f = 0$ in the domain of influence

$$\Omega_{\mathcal{G}} := \{x \in \Omega;\ \exists z \in \Gamma \text{ such that } \operatorname{dist}(x, z) < s(z)\}.$$

We have the following uniqueness result, which in particular generalizes the result in [Finch et al. 2004] to the case of variable coefficients.

Theorem 3.2. *Let $P = -\Delta$ outside Ω and let $\partial\Omega$ be strictly convex. Under the assumption* (3-4)*, if $\Lambda f = 0$ on $\mathcal{G}$ for $f \in H_D(\Omega)$ with* $\operatorname{supp} f \subset \mathcal{K}$*, then $f = 0$.*

As above, we can make this more precise.

Proposition 3.3. *Let $P = -\Delta$ outside Ω and let $\partial\Omega$ be strictly convex. Assume that $\Lambda f = 0$ on $\mathcal{G}$ for some $f \in H_D(\Omega)$ with* $\operatorname{supp} f \subset \Omega$ *that may not satisfy* (3-4)*. Then $f = 0$ in $\Omega_{\mathcal{G}}$. Moreover, no information about f in $\Omega \setminus \overline{\Omega}_{\mathcal{G}}$ is contained in $\Lambda f|_{\mathcal{G}}$.*

Sketch of the proof. We follow the proof in [Finch et al. 2004], where c is constant everywhere (and g is Euclidean).

The main difficulty in the partial data case is that we do not have the whole Cauchy data on $\mathcal{G}$, and unlike the case of the whole boundary, we cannot recover the Neumann data directly. If we assume for a moment that the Cauchy data on $\mathcal{G}$ vanishes, the unique continuation principle of Theorem 2.1 finishes the proof.

Note first that it is enough to prove the theorem if $\Gamma = U \times \partial\Omega$, where U is a small neighborhood of some $p \in \partial\Omega$, and $\Omega_{\mathcal{G}}$ given by $\operatorname{dist}(x, p) \le s(p)$. We fist recover the Neumann data on a part of $\mathbb{R}_+ \times \Gamma$ (smaller than we would want), using a finite domain of dependence result: Proposition 2 of [Finch et al. 2004], which shows, roughly speaking, that the corresponding solution u to the exterior problem with Dirichlet data equal to zero on $[0, T] \times \Gamma$ vanishes in an exterior neighborhood $[0, T_0] \times \{p\}$ (and therefore has zero normal derivative there) only for $T_0 > 0$ such that no signal traveling in the exterior of Ω can reach p for time not exceeding T_0. In other words, if we define a distance function $\operatorname{dist}_e(x, y)$ outside Ω as the infimum of the Euclidean distance of all curves *outside* Ω, connecting x and y, then any time T_1 with that property would not exceed $\operatorname{dist}_e(p, \partial\Omega \setminus \Gamma)$. A critical observation is that if we are not restricted to the exterior of Ω, the (geodesic) distance between p and $\partial\Omega \setminus \Gamma$ is strictly less. Moreover, if are restricted to a set on $\partial\Omega$ where either of those distances has a uniform positive lower bound, then so does the difference. Now, knowing that $u = 0$ near $[0, T_0] \times \{p\}$, we apply unique continuation to conclude that $f(x) = 0$ for $\operatorname{dist}(x, p) < T_0$, *and* to conclude that u has zero Dirichlet data on a larger part than Γ, by the reason explained above. Then we repeat the same argument using the fact that at each step, we improve the maximal distance at which we can get inside by at least a positive constant, independent of the step. □

4. Reconstruction with data on the whole boundary; the modified back-projection

One method to get an approximate solution of the thermoacoustic problem is the following time reversal (back-projection) method. Given h, which eventually will be replaced by Λf, let v_0 solve

$$\begin{cases} (\partial_t^2 + P)v_0 = 0 & \text{in } (0, T) \times \Omega, \\ v_0|_{[0,T]\times\partial\Omega} = h, \\ v_0|_{t=T} = 0, \\ \partial_t v_0|_{t=T} = 0. \end{cases} \tag{4-1}$$

Then we define the *back-projection*

$$A_0 h := v_0(0, \cdot) \quad \text{in } \overline{\Omega}.$$

The function $A_0\Lambda f$ is viewed as a candidate for a reconstructed f. Since h does not necessarily vanish at $t = T$, the compatibility condition of first order may not be satisfied because there might be a possible jump at $\{T\} \times \partial\Omega$. That singularity will propagate back to $t = 0$ and will affect v_0, and then v_0 may not be in the energy space. For this reason, h is usually cut off smoothly near $t = T$, i.e., h is replaced by $\chi(t)h(t, x)$, where $\chi \in C^\infty(\mathbb{R})$, $\chi = 0$ for $t = T$, and $\chi = 1$ in a neighborhood of $(-\infty, T(\Omega))$. See, e.g., [Hristova 2009, Section 2.2].

As we mentioned above, the back-projection v_0 converges to f, as $T \to \infty$; see [Hristova 2009] for rate of convergence estimates based on local energy decay results. In our analysis, T is fixed however.

We will modify this approach in a way that would make the problem Fredholm, and will make the error operator a contraction for certain explicit $T \gg 1$. Given h (that eventually will be replaced by Λf), solve

$$\begin{cases} (\partial_t^2 + P)v &= 0 \quad \text{in } (0, T) \times \Omega, \\ v|_{[0,T]\times\partial\Omega} &= h, \\ v|_{t=T} &= \phi, \\ \partial_t v|_{t=T} &= 0, \end{cases} \tag{4-2}$$

where ϕ solves the elliptic boundary value problem

$$P\phi = 0, \quad \phi|_{\partial\Omega} = h(T, \cdot). \tag{4-3}$$

Since P is a positive operator, 0 is not a Dirichlet eigenvalue of P in Ω, and therefore (4-3) is uniquely solvable. Now the initial data at $t = T$ satisfy compatibility conditions of first order (no jump at $\{T\} \times \partial\Omega$). Then we define the modified back-projection

$$Ah := v(0, \cdot) \quad \text{in } \overline{\Omega}. \tag{4-4}$$

The operator A maps continuously the closed subspace of $H^1([0, T] \times \partial\Omega)$ consisting of functions that vanish at $t = T$ (compatibility condition) to $H^1(\Omega)$; see [Lasiecka et al. 1986]. It also sends the range of Λ to $H_0^1(\Omega) \cong H_D(\Omega)$, as the proof below indicates.

To explain the idea behind this approach, let us assume for a moment that we knew the Cauchy data $[u, u_t]$ on $\{T\} \times \Omega$. Then one could simply solve the mixed problem in $[0, T] \times \Omega$ with that Cauchy data and boundary data Λf. Then that solution at $t = 0$ would recover f. We do not know the Cauchy data $[u, u_t]$ on $\{T\} \times \Omega$, of course, but we know the trace of u (a priori in H^1 for t fixed) on $\{T\} \times \partial\Omega$. The trace of u_t does not make sense because the latter is only in L^2 for $t = T$. The choice of the Cauchy data in (4-2) can then be explained by the following. Among all possible Cauchy data that belong to the "shifted linear

space"

$$\{\boldsymbol{g} = [g_1, g_2] \in H^1(\Omega) \oplus L^2(\Omega);\ g_1|_{\partial\Omega} = h(T, \cdot)\},$$

(the linear space $\mathcal{H}(\Omega)$ translated by a single element of the set above) we chose the one that minimizes the energy. The "error" will then be minimized. We refer to the proof of Theorem 4.1 for more details.

In the next theorem and everywhere below, $T_1 = T_1(\Omega)$ is the supremum of the lengths of all geodesics of the metric $c^{-2}g$ in $\overline{\Omega}$. Also, $\operatorname{dist}(x, y)$ denotes the distance function in that metric. We then call $(\Omega, c^{-2}g)$ nontrapping, if $T_1 < \infty$. It is easy to see that

$$T_0 \le T_1/2. \tag{4-5}$$

Theorem 4.1. *Let $(\Omega, c^{-2}g)$ be nontrapping, and let $T > T_1/2$. Then $A\Lambda = \mathrm{Id} - K$, where K is compact in $H_D(\Omega)$, and $\|K\|_{H_D(\Omega)} < 1$. In particular, $\mathrm{Id} - K$ is invertible on $H_D(\Omega)$, and the inverse thermoacoustic problem has an explicit solution of the form*

$$f = \sum_{m=0}^{\infty} K^m A h, \quad h := \Lambda f. \tag{4-6}$$

Sketch of the proof. Let u solve (1-2) with a given $f \in H_D$, and let v be the solution of (4-2) with $h = \Lambda f$. Then $w := u - v$ solves

$$\begin{cases} (\partial_t^2 + P)w = 0 & \text{in } (0, T) \times \Omega, \\ w|_{[0,T]\times\partial\Omega} = 0, \\ \quad w|_{t=T} = u|_{t=T} - \phi, \\ \quad w_t|_{t=T} = u_t|_{t=T}, \end{cases} \tag{4-7}$$

Restrict w to $t = 0$ to get

$$f = A\Lambda f + w(0, \cdot).$$

Therefore, the "error" is given by

$$Kf = w(0, \cdot).$$

First, we show that

$$\|Kf\|_{H_D(\Omega)} \le \|f\|_{H_D(\Omega)}, \quad \forall f \in H_D(\Omega), \tag{4-8}$$

for any fixed $T > 0$ (not necessarily greater than T_1). Since the Dirichlet boundary condition is energy preserving, it is enough to estimate th energy of $(u^T - \phi, u^T)$, where $u^T := u(T, \cdot)$.

In what follows, $(\cdot, \cdot)_{H_D(\Omega)}$ is the inner product in $H_D(\Omega)$ — see (2-1) — applied to functions that belong to $H^1(\Omega)$ but maybe not to $H_D(\Omega)$ (because

they may not vanish on $\partial\Omega$). By (2-2) and the fact that $u^T = \phi$ on $\partial\Omega$, we get

$$(u^T - \phi, \phi)_{H_D(\Omega)} = 0.$$

Then

$$\|u^T - \phi\|^2_{H_D(\Omega)} = \|u^T\|^2_{H_D(\Omega)} - \|\phi\|^2_{H_D(\Omega)} \le \|u^T\|^2_{H_D(\Omega)}.$$

Therefore, the energy of the initial conditions in (4-7) satisfies the inequality

$$E_\Omega(w, T) = \|u^T - \phi\|^2_{H_D(\Omega)} + \|u_t^T\|^2_{L^2(\Omega)} \le E_\Omega(u, T). \tag{4-9}$$

As mentioned above, the Dirichlet boundary condition is energy preserving, therefore

$$E_\Omega(w, 0) = E_\Omega(w, T) \le E_\Omega(u, T) \le E_{\mathbb{R}^n}(u, T) = E_\Omega(u, 0) = \|f\|^2_{H_D(\Omega)}.$$

This proves (4-8). Note that no condition on $T > 0$ was needed. If supp $f \subset K$, and $T < \operatorname{dist}(K, \partial\Omega)$, for example, then $K = \mathrm{Id}$, and $A\Lambda f = 0$. Then the "error" is 100%, and we have no information about f but (4-8) is still true.

We show next that the inequality above is strict when $T > T_0(\Omega)$:

$$\|Kf\|_{H_D(\Omega)} < \|f\|_{H_D(\Omega)}, \quad f \ne 0. \tag{4-10}$$

Assuming the opposite, we would get for some $f \ne 0$ that all inequalities leading to (4-8) are equalities. In particular,

$$u(T, x) = u_t(T, x) = 0 \quad \text{for } x \notin \Omega.$$

By the finite domain of dependence then

$$u(t, x) = 0 \quad \text{when } \operatorname{dist}(x, \Omega) > |T - t|. \tag{4-11}$$

One the other hand, we also have

$$u(t, x) = 0 \quad \text{when } \operatorname{dist}(x, \Omega) > |t|. \tag{4-12}$$

Therefore,

$$u(t, x) = 0 \quad \text{when } \operatorname{dist}(x, \partial\Omega) > T/2,\ -T/2 \le t \le 3T/2. \tag{4-13}$$

Since u extends to an even function of t that is still a solution of the wave equation, we get that (4-13) actually holds for $|t| < 3T/2$.

We will conclude next by the unique continuation Theorem 2.1 that $u = 0$ on $[0, T] \times \Omega$, and therefore $f = 0$ (see Figure 1). To this end, notice fist that by John's theorem (equivalent to Tataru's unique continuation result [Stefanov and Uhlmann 2009b, Theorem 2] in the Euclidean setting), we get $u = 0$ on $[-T, T] \times \mathbb{R}^n \setminus \Omega$. Fix $x_0 \in \Omega$. Then there is a piecewise smooth curve starting at x_0 in direction either ξ^0 or $-\xi^0$, where ξ^0 is arbitrary and fixed, of length less

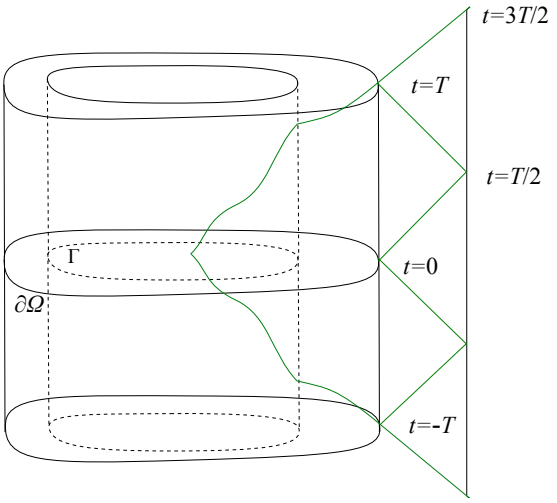

Figure 1

than T that reaches $\partial\Omega$ because $T > T_0$. This means that $\operatorname{dist}(x_0, \mathbb{R}^n \setminus \Omega) < T$. Then by Theorem 2.1, $u(0,\cdot) = 0$ near x_0. Since x_0 was arbitrary, we get $f = 0$. This completes the proof of (4-10).

Finally, we show that $\|K\| < 1$ if $T > T_1/2$ as claimed in the theorem. Indeed, for such T, and $(x,\xi) \in S^*\Omega$, at least one of the rays originating from $(x, \pm\xi)$ leaves $\overline{\Omega}$. Then for any $\varepsilon > 0$, K can be represented as a sum of an operator K_1 with norm not exceeding $1/2 + \varepsilon$, plus a compact one, K_2. The spectrum of K^*K on the interval $((1/2+\varepsilon)^2, 1]$ then is discrete and consists of eigenvalues only; and 1 cannot be among them, by (4-10). Then

$$\|Kf\|_{H_D(\Omega)} \le \sqrt{\lambda_1}\,\|f\|_{H_D(\Omega)}, \quad f \ne 0, \tag{4-14}$$

where $\lambda_1 < 1$ is the maximum of $1/2$ and the largest eigenvalue of K^*K greater than $1/2$, if any.

It is worth mentioning that for $T > T_1$, K is compact. □

The proof of Theorem 4.1 provides an estimate of the error in the reconstruction if we use the first term in (4-6) only that is Ah. It is in the spirit of [Hristova 2009] and relates the error to the local energy decay, as can be expected.

Corollary 4.2.

$$\|f - A\Lambda f\|_{H_D(\Omega)} \le \left(\frac{E_\Omega(u,T)}{E_\Omega(u,0)}\right)^{\frac{1}{2}} \|f\|_{H_D(\Omega)}, \quad \forall f \in H_{D(\Omega)},\ f \ne 0,$$

where u is the solution of (1-2).

Note that the $f - A\Lambda f = Kf$, and the corollary actually provides an upper bound for $\|Kf\|$. The estimate above also can be used to estimate the rate of convergence of the Neumann series (4-6) when we have a good control over the uniform local energy decay from time $t = 0$ to time $t = T$.

5. Stability and a microlocal characterization of Λ and the back-projection

Note first that in case of observations on $[0, T]\times\partial\Omega$ with $T > T_1/2$, Theorem 4.1 already implies a Lipschitz stability estimate of the type below. We consider below the partial boundary data case, where Λf is known on $\mathcal{G}$; see (3-2).

If we want that recovery to be stable, we need to be able to recover all singularities of f "in a stable way." By the zero initial velocity condition, each singularity (x, ξ) splits into two parts (see Proposition 5.1 below and the Appendix): one that starts propagating in the direction ξ; and another one propagates in the direction $-\xi$. Moreover, neither one of those singularities vanishes at $t = 0$ (and therefore never vanishes), they actually start with equal amplitudes. For a stable recovery, we need to be able to detect at least one of them, in the spirit of [Stefanov and Uhlmann 2009a], i.e., at least one of them should reach $\mathcal{G}$.

Define $\tau_\pm(x, \xi)$ by the condition

$$\tau_\pm(x, \xi) = \max\big(\tau \geq 0;\ \gamma_{x,\xi}(\pm\tau) \in \overline{\Omega}\big).$$

Based on the arguments above, for a stable recovery we should assume that $\mathcal{G}$ satisfies the condition

$$\forall (x, \xi) \in S^*\mathcal{H},\ \big(\tau_\sigma(x, \xi), \gamma_{x,\xi}(\tau_\sigma(x, \xi)\big) \in \mathcal{G} \quad \text{for either } \sigma = + \text{ or } \sigma = - \text{ (or both).} \tag{5-1}$$

Compared to condition (3-4), this means that for each $x \in \mathcal{H}$ *and each unit direction* ξ, at least one of the signals from (x, ξ) and $(x, -\xi)$ reaches $\mathcal{G}$. This condition becomes necessary if we replace $\mathcal{G}$ by its closure above; see Remark 5.3. In Theorem 5.2 below, we show that it is also sufficient.

We start with a description of the operator Λ that is of independent interest as well. In the next proposition, we formally choose $T = \infty$. We restrict the result below to functions supported in Ω (the support cannot touch $\partial\Omega$) to avoid the analysis at the boundary, where Λ is of more general class.

Proposition 5.1. $\Lambda = \Lambda_+ + \Lambda_-$, *where* $\Lambda_\pm : C_0^\infty(\Omega) \to C^\infty((0, \infty)\times\partial\Omega)$ *are elliptic Fourier integral operators of zeroth order with canonical relations given by the graphs of the maps*

$$(y, \xi) \mapsto \big(\tau_\pm(y, \xi),\ \gamma_{y,\xi}(\pm\tau_\pm(y, \xi)),\ \mp|\xi|,\ \dot\gamma'_{y,\xi}(\pm\tau_\pm(y, \xi))\big), \tag{5-2}$$

where $|\xi|$ is the norm in the metric $c^{-2}g$, and $\dot\gamma'$ stands for the tangential projection of $\dot\gamma$ on $T\partial\Omega$.

Proof. This statement is well known and follows directly from [Duistermaat 1996], for example. See also the Appendix where microlocal analysis and geometric optics is briefly reviewed. We will give more details that are needed just for the proof of this proposition in order to be able to compute the principal symbol in Theorem 5.2.

We start with a standard geometric optics construction. See Section A.4 in the Appendix.

Fix $x_0 \in \Omega$. In a neighborhood of $(0, x_0)$, the solution to (4-2) is given by

$$u(t,x) = (2\pi)^{-n} \sum_{\sigma=\pm} \int e^{i\phi_\sigma(t,x,\xi)} a_\sigma(x,\xi,t)\, \hat f(\xi)\, d\xi, \tag{5-3}$$

modulo smooth terms, where the phase functions $\phi_\pm$ are positively homogeneous of order 1 in ξ and solve the eikonal equations (A-16), (A-17), while $a_\pm$ are classical amplitudes of order 0 solving the corresponding transport equations (A-18). Singularities starting from $(x,\xi) \in \mathrm{WF}(f)$ propagate along geodesics in the phase space issued from (x,ξ), i.e., they stay on the curve $(\gamma_{x,\xi}(t), \dot\gamma_{x,\xi}(\sigma t))$ for $\sigma = \pm$. This is consistent with the general propagation of singularities theory for the wave equation because the principal symbol of the wave operator $\tau^2 - c^2|\xi|_g$ has two roots $\tau = \pm c|\xi|_g$.

The construction is valid as long as the eikonal equations are solvable, i.e., along geodesics issued from $(x, \pm\xi)$ that do not have conjugate points. Assume that $\mathrm{WF}(f)$ is supported in a small neighborhood of (x_0, ξ_0) with some $\xi_0 \neq 0$. Assume first that the geodesic from (x_0, ξ_0) with endpoint on $\partial\Omega$ has no conjugate points. We will study the $\sigma = +$ term in (5-3) first. Let ϕ_b, a_b be the restrictions of ϕ_+, a_+, respectively, on $\mathbb{R}\times\partial\Omega$. Then, modulo smooth terms,

$$\Lambda_+ f := u_+(t,x)|_{\mathbb{R}\times\partial\Omega} = (2\pi)^{-n} \int e^{i\phi_b(t,x,\xi)} a_b(x,\xi,t)\, \hat f(\xi)\, d\xi, \tag{5-4}$$

where u_+ is the $\sigma = +$ term in (5-3). Set $t_0 = \tau_+(x_0,\xi_0)$, $y_0 = \gamma_{x_0,\xi_0}(t_0)$, $\eta_0 = \dot\gamma_{x_0,\xi_0}(t_0)$; in other words, (y_0,η_0) is the exit point and direction of the geodesic issued from (x_0,ξ_0) when it reaches $\partial\Omega$. Let $x = (x', x^n)$ be boundary normal coordinates near y_0. Writing $\hat f$ in (5-4) as an integral, we see that (5-4) is an oscillating integral with phase function $\Phi = \phi_+(t,x',0,\xi) - y\cdot\xi$. Then (see [Trèves 1980], for example), the set $\Sigma := \{\Phi_\xi = 0\}$ is given by the equation

$$y = \partial_\xi \phi_+(t,x',0,\xi)$$

It is well known (see Example 2.1 in [Trèves 1980, VI.2], for example) that this equation implies that $(x',0)$ is the endpoint of the geodesic issued from

(y,ξ) until it reaches the boundary, and $t=\tau_+(y,\xi)$, i.e., t is the time it takes to reach $\partial\Omega$. In particular, Σ is a manifold of dimension $2n$, parametrized by (y,ξ). Next, the map

$$\Sigma \ni (y,t,x',\xi) \mapsto (y,t,x',-\xi,\partial_t\phi_+,\partial_{x'}\phi_+) \tag{5-5}$$

is smooth of rank $2n$ at any point. This shows that Φ is a nondegenerate phase; see [Trèves 1980, VIII.1], and that $f\mapsto \Lambda_+ f$ is an FIO associated with the Lagrangian given by the right side of (5-5). The canonical relation is then given by

$$C := (y,\xi,t,x',\partial_t\phi_+,\partial_{x'}\phi_+), \quad (y,t,x',\xi)\in\Sigma.$$

Then (5-2) follows from the way ϕ_+ is constructed by the Hamilton-Jacobi theory. The proof in the $\sigma=-$ case is the same.

The proof above was done under the assumption that there are no conjugate points on $\gamma_{y_0,\xi_0}(t)$, $0\le t\le \tau_+(y_0,\xi_0)$. To prove the theorem in the general case, let $t_1\in(0,\tau_+(y_0,\xi_0))$ be such that there are no conjugate points on that geodesic for $t_1\le t\le\tau_+(y_0,\xi_0)$. Then each of the terms in (5-3) extends to a global elliptic FIO mapping initial data at $t=0$ to a solution at $t=t_1$; see, e.g., [Duistermaat 1996]. Its canonical relation is the graph of the geodesic flow between those two moments of time (for $\sigma=+$, and with obvious sign changes when $\sigma=-$). We can compose this with the local FIO constructed above, and the result is a well defined elliptic FIO of order 0 with canonical relation (5-2). □

We now consider the situation where Λf is given on a set $\mathcal{G}$ satisfying (5-1). Since $\mathcal{K}$ is compact and $\mathcal{G}$ is closed, one can always choose $\mathcal{G}'\Subset\mathcal{G}$ that still satisfies (5-1). Fix $\chi\in C_0^\infty([0,T]\times\partial\Omega)$ such that $\operatorname{supp}\chi\subset\mathcal{G}$ and $\chi=1$ on $\mathcal{G}'$. The measurements are then modeled by $\chi\Lambda f$, which depends on Λf on $\mathcal{G}$ only.

Choose and fix $T>\sup_\Gamma s$; see (3-2). Let A be the back-projection operator defined in (4-2) and (4-4). Note that A is always applied to $\chi\Lambda$ below, therefore $\phi=0$ in this case.

Theorem 5.2. *$A\chi\Lambda$ is a zero-order classical pseudodifferential operator* (ΨDO) *in some neighborhood of $\mathcal{K}$ with principal symbol*

$$\tfrac12\chi\big(\tau_+(x,\xi),\gamma_{x,\xi}(\tau_+(x,\xi))\big)+\tfrac12\chi\big(\tau_+(x,\xi),\gamma_{x,\xi}(\tau_-(x,\xi))\big).$$

If $\mathcal{G}$ satisfies (5-1), *then*

(a) *$A\chi\Lambda$ is elliptic,*

(b) *$A\chi\Lambda$ is a Fredholm operator on $H_D(\mathcal{K})$, and*

(c) *there exists a constant $C>0$ such that*

$$\|f\|_{H_D(\mathcal{K})}\le C\|\Lambda f\|_{H^1(\mathcal{G})}. \tag{5-6}$$

Remark 5.3. By [Stefanov and Uhlmann 2009a, Proposition 3], condition (5-1), with $\mathcal{G}$ replaced by its closure, is a necessary condition for stability in any pair of Sobolev spaces. In particular, $c^{-2}g$ has to be nontrapping for stability. Indeed, then the proof below shows that $A\chi\Lambda$ will be a smoothing operator on some nonempty open conic subset of $T^*\mathcal{H} \setminus 0$.

Remark 5.4. Note that $\Lambda : H_D(\mathcal{H}) \to H^1([0,T]\times\partial\Omega)$ is bounded. This follows for example from Proposition 5.1.

Sketch of the proof. To construct a parametrix for $A\chi\Lambda f$, we apply again a geometric optic construction, using the two characteristic roots $\pm c|\xi|_g$. It is enough to assume that $A\chi\Lambda f$ has a wave front set in a conic neighborhood of some point $(t_0, y_0, \tau_0, \xi_0') \in [0,T]\times\partial\Omega$, using the notation above. For simplicity, assume that the eikonal equation is solvable for t in some neighborhood of $[0,T]$. Let $\tau_0 < 0$, for example. We look for a parametrix of the solution of the wave equation (4-2) with zero Cauchy data at $t = T$ and boundary data $\chi\Lambda_+ f$ in the form

$$v(t,x) = (2\pi)^{-n} \int e^{i\phi_+(t,x,\xi)} b(x,\xi,t)\, \hat{f}(\xi)\, d\xi.$$

Let (x_0, ξ_0) be the intersection of the bicharacteristic issued from $(t_0, y_0, \tau_0, \xi_0')$ with $t = 0$. The choice of that parametrix is justified by the fact that all singularities of that solution must propagate along the geodesics close to γ_{x_0,ξ_0} in the opposite direction, as t decreases because there are no singularities for $t = T$. The critical observation is that the first transport equation for the principal term b_0 of b is a linear ODE along bicharacteristics, and starting from initial data $b_0 = \chi a_0$, where $a_0 = 1/2$, at time $t = 0$, we will get that $b_0(x,\xi)|_{t=0}$ is given by the value of $\chi/2$ at the exit point of $\gamma_{x,\xi}$ on $\partial\Omega$.

This proves the first statement of the theorem.

Parts (a), (b) follows immediately from the ellipticity of $A\chi\Lambda$ that is guaranteed by (5-1).

To prove part (c), note first that the ellipticity of $A\chi\Lambda$ and the mapping property of A (see [Lasiecka et al. 1986]) imply the estimate

$$\|f\|_{H_D(\mathcal{H})} \le C\left(\|\chi\Lambda f\|_{H^1} + \|f\|_{L^2}\right).$$

By Theorem 3.2, and (5-1), $\chi\Lambda$ is injective on $H_D(\mathcal{H})$. By [Taylor 1981, Proposition V.3.1], one gets estimate (5-6) with a constant $C > 0$ possibly different than the one above. □

6. Relations to boundary control and observability

This problem is closely related but not equivalent to the *observability problem* in boundary control. The observability problem asks the following. Let u solve

$$\begin{cases} (\partial_t^2 + P)u &= 0 \quad \text{in } (0,T)\times\Omega, \\ u|_{(0,T)\times\partial\Omega} &= 0, \\ u|_{t=0} &= f, \\ \partial_t u|_{t=0} &= h, \end{cases} \tag{6-1}$$

where Ω is a bounded domain with a smooth boundary as above and $T > 0$ is fixed. Comparing this with (1-2), we see that the Cauchy data at $t = 0$ given by (f, h) with h not necessarily zero (which is not essential for the discussion here) but the equation is satisfied for $x \in \Omega$ only and there is a Dirichlet boundary condition for $x \in \partial\Omega$. Then the question is: given $\partial u/\partial\nu$ on $(0,T)\times\Gamma$, with some $\Gamma \subset \Omega$, can we determine (f, h), and therefore, u? One can have Neumann or Robin boundary conditions in (6-1) and measure Dirichlet ones on $(0,T)\times\Gamma$. The essential assumption on a possibly different boundary condition is that the latter defines a well posed problem and the measurement determines the Cauchy data on $(0,T)\times\Gamma$. Physically, and microlocally, the presence of a boundary condition leads to waves that reflect off $\partial\Omega$. In the thermoacoustic case, they do not; actually then there is no boundary for the direct problem. The measurements consist of "half" of the Cauchy data only — the Dirichlet part.

6A. ***Measurements on the whole boundary.*** If $\Gamma = \partial\Omega$, then the two problems are actually equivalent *in a stable way*. Indeed, we will show here that knowing $\Lambda \boldsymbol{f}$, one can recover the normal derivative of the solution of (1-2) on $[0,T]\times\partial\Omega$ as well. This is done by applying a nonlocal ΨDO to $\Lambda \boldsymbol{f}$.

We will define first the outgoing DN map. Given $h \in C_0^\infty([0,\infty)\times\partial\Omega)$, let w solve the exterior mixed problem related to the Euclidean Laplacian:

$$\begin{cases} (\partial_t^2 - \Delta)w &= 0 \quad \text{in } (0,T)\times\mathbb{R}^n \setminus \overline{\Omega}, \\ w|_{[0,T]\times\partial\Omega} &= h, \\ w|_{t=0} &= 0, \\ \partial_t w|_{t=0} &= 0. \end{cases} \tag{6-2}$$

Then we set

$$Ng = \frac{\partial w}{\partial \nu}\Big|_{[0,T]\times\partial\Omega}.$$

By [Lasiecka et al. 1986], for $h \in H^1_{(0)}([0,T]\times\partial\Omega)$, we have

$$[w, w_t] \in C([0,T);\ \mathcal{H});$$

therefore,

$$N : H^1_{(0)}([0,T]\times\partial\Omega) \to C([0,T]\times H^{\frac{1}{2}}(\partial\Omega))$$

is continuous. Note that the results in [Lasiecka et al. 1986] require the domain to be bounded but by finite domain of dependence we can remove that restriction

in our case. We also refer to [Finch et al. 2004, Proposition 2] for a sharp domain of dependence result for exterior problems.

Lemma 6.1. *Let u solve* (1-2) *with $f \in H_D(\Omega)$ compactly supported in Ω. Assume that $P = -\Delta$ outside Ω. Then for any $T > 0$, $\Lambda \boldsymbol{f}$ determines uniquely u in $[0, T] \times \mathbb{R}^n \setminus \Omega$ and the normal derivative of u on $[0, T] \times \partial\Omega$ as follows*:

(a) *The solution u in $[0, T] \times \mathbb{R}^n \setminus \Omega$ coincides with the solution of* (6-2) *with $h = \Lambda \boldsymbol{f}$.*

(b) *We have*

$$\frac{\partial w}{\partial \nu}\Big|_{[0,T]\times\partial\Omega} = N\Lambda f. \tag{6-3}$$

Proof. Let w be the solution of (6-2) with $g = \Lambda \boldsymbol{f} \in H^1_{(0)}([0, T] \times \partial\Omega)$. Let u be the solution of (1-2). Then $u - w$ solves the unit speed wave equation in $[0, T] \times \mathbb{R}^n \setminus \Omega$ with zero Dirichlet data and zero initial data. Therefore, $u = w$ in $[0, T] \times \mathbb{R}^n \setminus \Omega$. □

The operator N is well known in scattering theory as the outgoing DN map, also called the Neumann operator sometimes. If $\partial\Omega$ is strictly convex, it is a classical ΨDO of order 1 restricted to noncharacteristic codirections (corresponding to either reflecting rays or evanescent waves) and has a more complicated structure near characteristic vectors (corresponding to glancing rays). The range of Λ acting in f with supp $f \subset \Omega$ can have a wave front set in the hyperbolic region only, corresponding to reflected rays.

Now, knowing Λf, we can recover the whole Cauchy data $(f, N\Lambda f)$ on $(0, T) \times \partial\Omega$. In this case, the observability problem is to recover f from the Cauchy data there as well. One can therefore use all results known in the literature about the observability problem (see [Bardos et al. 1992], for example) to obtain results for the thermoacoustic one. On the other hand, this may not be the best way to do, numerically, at least. Also, the special and in fact the simpler structure of the thermoacoustic solution of (1-2) (no reflected waves) would be ignored if we did so. An essential part of [Bardos et al. 1992] is devoted to the analysis of such reflected waves which do not exist in our case.

6B. ***Measurements on a part of the boundary.*** When Λ is known restricted to $(0, T) \times \Gamma$, $\Gamma \subset \Omega$, the relation between the two problems is not so straightforward. First, the solution u to (1-2) and that to (6-1) are different as we explained already. In the observability problem, we know u on $[0, T] \times \partial\Omega$ (zero), and $\partial u/\partial \nu$ on the smaller set $(0, T) \times \Gamma$. In the thermoacoustic one, we know that the waves go through $\partial\Omega$, which is equivalent to the hidden boundary condition $\partial u/\partial \nu = Nu$ on $[0, T] \times \partial\Omega$, and we know u on $(0, T) \times \Gamma$. As Theorem 3.2 shows, we can, in a nontrivial way, recover $\partial u/\partial \nu$ on $(0, T) \times \Gamma$. The proof uses unique

continuation, which is unstable. Therefore, trying to reduce the thermoacoustic problem to an observability one this way (and no other is known to the authors) goes through a unstable step and will not lead to sharp results because we have showed in Theorem 5.2 that under certain conditions, the recovery is stable.

7. Estimating the uniqueness time T_0 and the stability time T_1

One practical question is how to estimate the times T_0 and T_1 from above, to be certain that the chosen T is large enough for uniqueness or stability.

The max-min Equation (3-1) of T_0 makes it easy to get an upper bound. First, to estimate $\operatorname{dist}(x, \partial\Omega)$ from above for x fixed, we can take any path $[a, b] \ni s \mapsto \gamma(s)$ from x to $\partial\Omega$ and compute the length of that path as $\int_a^b \frac{|\dot\gamma(s)|\mathrm{d}s}{c(\gamma(s))}$. Then we take an upper bound with respect to $x \in \Omega$. Let $R > 0$ be such that Ω is contained in the ball $B(0, R)$ and assume that $0 \in \Omega$. Then, for example,

$$T_0 < \max_{|\omega|=1} \int_0^R \frac{\mathrm{d}r}{c(r\omega)}.$$

In particular, if $c(x) \geq c_0 = \text{const.}$, we get

$$T_0 < \frac{R}{c_0}.$$

We estimate T_1 now, which (divided by 2) is critical for stability. A possible way to do this is to use a suitable *escape function*, a method well known and used in scattering theory. Consider the Hamiltonian

$$H(x, \xi) = \tfrac{1}{2} c^2(x) g^{ij}(x) \xi_i \xi_j$$

of P on the energy level $\Sigma := \{(x, \xi) \in T^*\overline{\Omega};\ H = 1/2\}$. Here, g^{ij} are the components of g^{-1}. Let $\psi(x, \xi)$ be a smooth function on $\Omega \times \mathbb{R}^n$ which we regard as $T^*\Omega$ in local coordinates. Assume that for some constant α,

$$X_H \psi \geq \alpha > 0 \quad \text{on } \Sigma, \tag{7-1}$$

where X_H is the Hamiltonian vector field related to H. Relation (7-1) tells us that ψ is strictly increasing along the Hamiltonian flow. Let

$$A = \max_{\Sigma} |\psi(x, \xi)|.$$

Then any Hamiltonian curve on Σ issued from $T^*\Omega$ will leave Ω for time t such that $\alpha t > 2A$. Thus $T_1 \leq 2A/\alpha$.

For example, assume that g is Euclidean. Then $H = \frac{1}{2} c^2 |\xi|^2$ and

$$X_H = \sum \left(c^2 \xi_j \frac{\partial}{\partial x^j} - c \frac{\partial c}{\partial x^j} |\xi|^2 \frac{\partial}{\partial \xi_j} \right).$$

Choose $\psi = x \cdot \xi$. Then

$$X_H \psi = c^2 |\xi|^2 - |\xi|^2 c x \cdot \partial_x c.$$

On the energy level Σ, we have

$$X_H \psi = 1 - c^{-1} x \cdot \partial_x c.$$

Condition (7-1) is then satisfied if

$$x \cdot \partial_x c(x) < c(x) \quad \text{in } \overline{\Omega}. \tag{7-2}$$

In particular, if $c = c(r)$ is radial, condition (7-2) reduces to $r \partial c / \partial r < c$ or $\partial_r (r/c(r)) > 0$. This is the condition imposed by Herglotz [1905] and Wiechert and Zoeppritz [1907] more than a century ago in their solution of the inverse kinematic problem for radial speeds arising in seismology.

We have therefore proved the following.

Proposition 7.1. *Let* $0 < c_0 \le c(x)$ *in* $\overline{\Omega} \subset \bar{B}(0, R)$. *Then*

$$T_0 < R/c_0.$$

Assume that

$$\alpha := \min_{\overline{\Omega}} (1 - c^{-1} x \cdot \partial_x c) > 0.$$

Then $T_1/2 \le R/(\alpha c_0)$.

To finish the proof it only remains to notice that $|\psi| \le |x||\xi| \le R/c(x)$ on the energy level Σ.

8. Multiwave tomography and integral geometry

If $P = -\Delta$, and if n is odd, the solution of the wave equation is given by Kirchhoff's formula and can be expressed in terms of integrals over spheres centered at $\partial\Omega$ with radius t, and their t-derivatives. Then the problem can be formulated as an integral geometry problem — recovering f from integrals over spheres centered at $\partial\Omega$, with radii in $[0, T]$. This point of view has been exploited a lot in the literature. Uniqueness theorems can be proved using analytic microlocal calculus, when the boundary is analytic (a ball, for example). Explicit formulas has been derived when $\partial\Omega$ is a ball. There are also works studying "uniqueness sets" — what configuration of the boundary, not necessarily smooth, provides unique recovery; see [Kuchment and Kunyansky 2008], for example.

One may attempt to apply the same approach in the variable coefficients case; then one has to integrate over geodesic spheres. This has two drawbacks. First, those integrals represent the leading order terms of the solution operator only, not the whole solution. That would still be enough for constructing a parametrix

however but not the Neumann series solution in Theorem 4.1. The second problem is that the geodesic spheres become degenerate in presence of caustics. The wave equation viewpoint that we use in this paper is not sensitive to caustics. We still have to require that the metric be nontrapping in some of our theorems. By the remark following Theorem 5.2 however, this is a necessary condition for stability. On the other hand, it is not needed for the uniqueness result as long as (3-4) is satisfied. Also, there is no clear integral geometry approach to uniqueness, except for analytic speeds, that would replace unique continuation. So in this sense, the integral geometry problem is "the wrong approach" when the speed is variable.

9. Brain imaging

In this section, we study the mathematical model of thermoacoustic and photoacoustic tomography when the sound speed has a jump across a smooth surface. This models the change in the sound speed in the skull when trying to image the human brain. This problem was proposed by Lihong Wang at the meeting in Banff on inverse transport and tomography in May, 2010 and it arises in brain imaging [Xu and Wang 2006b; Yang and Wang 2008]. We derive again an explicit inversion formula in the form of a convergent Neumann series under the assumptions that all singularities from the support of the source reach the boundary.

The main difference between the case of a smooth speed c and a discontinuous one with jump type of singularities is the propagation of singularities. In the present case, each ray may split into two parts when it hits the surface Γ where the speed jumps, then each branch may split again, etc. This is illustrated in Figure 2. Each such branch carries a positive fraction of the high frequency energy if there are segments tangent to Γ. The stability condition (9-5) then requires that we can detect at least one of those branches issued from supp f and any direction at time $|t| < T$. Then we also have an explicit inversion in the form of a convergent Neumann series as shown in Theorem 4.1. That reconstruction is based on applying a modified time reversal with a harmonic extension step, and then iterating it. While for a smooth speed, the classical time reversal already provides a parametrix but not necessarily an actual inversion, in the case under consideration the harmonic extension and the iteration are even more important because the first term or the classical time reversal are not parametrices. This has been also numerically observed in [Qian et al. 2011].

We describe the mathematical model now. Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary. Let $\Gamma \subset \Omega$ be a smooth closed, orientable, not necessarily connected surface. Let the sound speed $c(x) > 0$ be smooth up to Γ with a

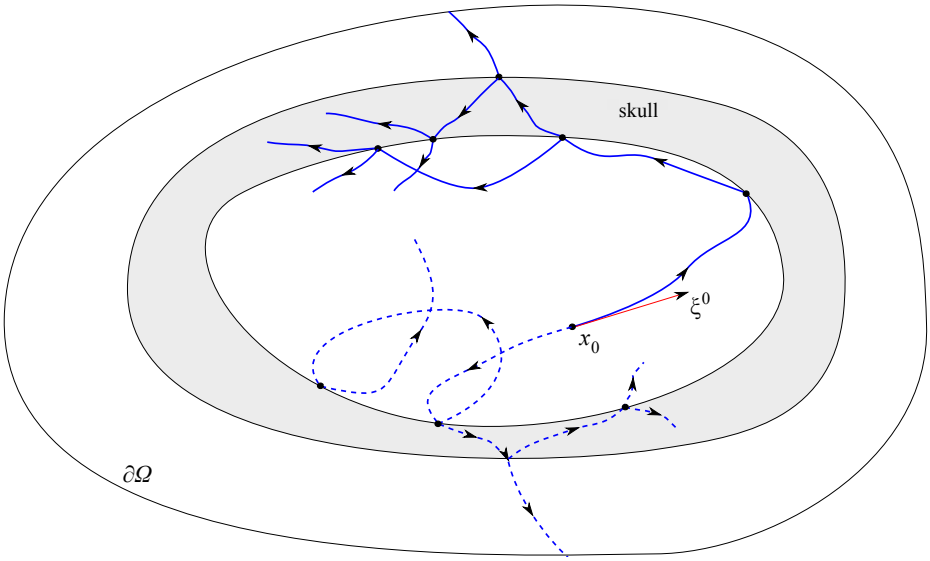

Figure 2. Propagation of singularities for the transmission problem in the skull example. The shaded region represents the skull, and the speed there is higher than in the nonshaded part. The dotted curves represent the propagation of the same singularity but moving with a negative wave speed.

nonzero jump across it. For $x \in \Gamma$, and a fixed orientation of Γ, we introduce the notation

$$c_{\text{int}}(x) = c|_{\Gamma_{\text{int}}}, \quad c_{\text{ext}}(x) = c|_{\Gamma_{\text{ext}}} \tag{9-1}$$

for the limits from the interior and from the exterior of $\Omega \setminus \Gamma$. Our assumption then is that those limits are positive as well, and

$$c_{\text{int}}(x) \neq c_{\text{ext}}(x) \quad \text{for all } x \in \Gamma. \tag{9-2}$$

In the case of brain imaging, the brain is represented by some domain $\Omega_0 \Subset \Omega$. Let Ω_1 be another domain representing the brain and the skull, so that $\Omega_0 \Subset \Omega_1 \Subset \Omega$, and $\overline{\Omega}_1 \setminus \Omega_0$ is the skull; see Figure 2. The measuring devices are then typically placed on a surface encompassing the skull, modeled by $\partial\Omega$ in our case. Then

$$c|_{\Omega_0} < c|_{\Omega_1 \setminus \Omega_0}, \quad c|_{\Omega_1 \setminus \Omega_0} > c|_{\Omega \setminus \Omega_1},$$

with the speed jumping by about a factor of two inside the skull $\overline{\Omega}_1 \setminus \Omega_0$. Another motivation to study this problem is to model the classical case of a smooth speed in the patient's body but account for a possible jump of the speed when the acoustic waves leave the body and enter the liquid surrounding it.

Let u solve the problem

$$\begin{cases} (\partial_t^2 - c^2\Delta)u &= 0 & \text{in } (0,T)\times\mathbb{R}^n, \\ u|_{\Gamma_{\text{int}}} &= u|_{\Gamma_{\text{ext}}}, \\ (\partial u/\partial\nu)|_{\Gamma_{\text{int}}} &= (\partial u/\partial\nu)|_{\Gamma_{\text{ext}}}, \\ u|_{t=0} &= f, \\ \partial_t u|_{t=0} &= 0, \end{cases} \tag{9-3}$$

where $T > 0$ is fixed, $u|_{\Gamma_{\text{int,ext}}}$ is the limit value (the trace) of u on Γ when taking the limit from the exterior and from the interior of Γ, respectively, and f is the source that we want to recover. We similarly define the interior/exterior normal derivatives, and ν is the exterior unit (in the Euclidean metric) normal to Γ.

Assume that f is supported in $\overline{\Omega}$, where $\Omega \subset \mathbb{R}^n$ is some smooth bounded domain. The measurements are modeled by the operator Λf as in (1-3). The problem is to reconstruct the unknown f.

We study the case where f is supported in some compact $\mathcal{K}$ in Ω. In applications, this corresponds to f, that is not necessarily zero outside $\mathcal{K}$ but are known there. By subtracting the known part, we arrive at the formulation that we described above. We also assume that $c = 1$ on $\mathbb{R}^n \setminus \Omega$.

The propagation of singularities for the transmission problem is well understood, at least away from possible gliding rays [Hansen 1984; Taylor 1976; Petkov 1982a; 1982b]. When a singularity traveling along a geodesic hits the interface Γ transversely, there is a reflected ray carrying a singularity, that reflects at Γ according to the usual reflection laws. If the speed on the other side is smaller, there is a transmitted (refracted) ray as well, at an angle satisfying Snell's law; see (9-41). In the opposite case, such a ray exists only if the angle with Γ is above some critical angle; see (9-42). If that angle is smaller than the critical one, there is no transmitted singularity on the other side of Γ. This is known as a full internal reflection. This is what happens in the case of the skull when a ray hits the skull boundary from inside at a small enough angle; see Figure 2. Therefore, the initial ray splits into two parts, or does not split; or it hits the boundary exactly at the critical angle. The latter case is more delicate, and we refer to Section 9B for some discussion on that.

Next, consider the propagation of each branch, if more than one. Each branch may split into two, etc. In the skull example, a ray coming from the interior of the skull hitting the boundary goes to a region with a smaller speed; and therefore there is always a transmitted ray, together with the reflected one. Then a single singularity starting at time $t = 0$ until time $t = T$ in general propagates along a few branches that look like a directed graph. This is true at least under the assumption than none of those branches, including possible transmitted ones, is tangent to the boundary.

Since $u_t|_{t=0} = 0$, singularities from (x_0, ξ^0) start to propagate in the direction ξ^0 and in the negative one $-\xi^0$. If none of the branches reaches $\partial\Omega$ at time T or less, a stable recovery is not possible [Stefanov and Uhlmann 1998b]. In the next subsection, we study the case where the initial data is supported in some compact $\mathcal{K} \subset \Omega \setminus \Gamma$ and for each $(x_0, \xi^0) \in T^*\mathcal{K} \setminus 0$, each ray through it, or through $(x_0, -\xi^0)$ has a branch that reaches $\partial\Omega$ transversely at time less than T. The main idea of the proof is to estimate the energy that each branch carries at high energies. If there is branching into rays not tangent to the boundary, we show that a positive portion of the energy is transmitted, and a positive one is reflected, at high energies. As long as one of these branches reaches the boundary transversely, at a time at which measurements are still done, we can detect that singularity. If we can do that for all singularities originating from $\mathcal{K}$, we have stability. This explains condition (9-5) below. Uniqueness follows from unique continuation results.

Similarly to the case of smooth speed studied above, assuming (9-5), we also get an explicit converging Neumann series formula for reconstructing f; see Theorem 4.1. As in the case of a smooth speed considered in [Stefanov and Uhlmann 2009b] the "error" operator K in (4-6) is a contraction. An essential difference in this case is that K is not necessarily compact. Roughly speaking, Kf corresponds to that part of the high frequency energy that is still held in Ω until time T due to reflected or transmitted signals that have not reached $\partial\Omega$ yet. While the first term only in (4-6) will still recover all singularities of f, it will not recover their strength, in contrast to the situation in [Stefanov and Uhlmann 2009b], where the speed is smooth. Thus one can expect somewhat slower convergence in this case.

9A. ***Main result.*** Let u solve the problem (9-3) where $T > 0$ is fixed. Let $\Lambda \boldsymbol{f} := u|_{[0,T]\times\partial\Omega}$ as in (1-3). The trace $\Lambda \boldsymbol{f}$ is well defined in $C_{(0)}\big([0, T];\ H^{1/2}(\partial\Omega)\big)$, where the subscript (0) indicates that we take the subspace of functions h such that $h = 0$ for $t = 0$. For a discussion of other mapping properties, we refer to [Isakov 2006], when c has no jumps. By finite speed of propagation, one can reduce the analysis of the mapping properties of Λ to that case.

As in the case of a smooth speed, one could use the standard back-projection that would serve as some kind of approximation of the actual solution. We cut off smoothly Λf near $t = T$ to satisfy the compatibility conditions in the next step; and then we solve a backward mixed problem with boundary data the so cut Λf; and Cauchy data $[0, 0]$ at $t = T$. As in the case of a smooth speed (see [Hristova 2009; Stefanov and Uhlmann 2009b]) one can show that such a back-projection would converge to f as $T \to \infty$ at a rate that depends on f and that is at least a slow logarithmic one if one knows a priori that $f \in H^2$; see [Bellassoued 2003].

If $\Gamma = \partial\Omega_0$, where $\Omega_0 \subset \Omega$ is strictly convex, then in the case that the speed outside Ω_0 is faster than the speed inside (then there is full internal reflection), the convergence would be no faster than logarithmic, as suggested by the result in [Popov and Vodev 1999]. In the opposite case, it is exponential if n is odd, and polynomial when n is even [Cardoso et al. 1999]. Our goal in this work is to fix T however.

Consider the modified back-projection described in (4-2)–(4-4). The function Ah with $h = \Lambda f$ can be thought of as the "first approximation" of f. On the other hand, the proof of Theorem 9.1 below shows that it is not even a parametrix, in contrast to the case where c is smooth; see Remark 9.2.

The discussion in the Introduction and in Section 9B indicates that the singularities that we are certain to detect at $\partial\Omega$ lie in the *nontrapped set*

$$\mathcal{U} = \big\{(x,\xi) \in S^*(\Omega \setminus \Gamma);\ \text{there is a geodesic path issued from either } (x,\xi) \text{ or } (x,-\xi) \text{ at } t=0, \text{ never tangent to } \Gamma, \text{ and outside } \overline{\Omega} \text{ at time } t = T\big\}. \quad (9\text{-}4)$$

Actually, $\mathcal{U}$ is the maximal open set with the property that a singularity in $\mathcal{U}$ is visible at $[0,T] \times \partial\Omega$; and what happens at the boundary of that set, that includes for example rays tangent to Γ, will not be important for our analysis. We emphasize here that "visible" means that some positive fraction of the energy and high frequencies can be detected as a singularity of the data; and of course there is a fraction that is reflected; then some trace of it may appear later on $\partial\Omega$, and so on.

One special case is the following. Take a compact set $\mathcal{K} \subset \Omega \setminus \Gamma$ with smooth boundary, and assume that

$$S^*\mathcal{K} \subset \mathcal{U}. \quad (9\text{-}5)$$

In other words, we require that for any $x \in \mathcal{K}$ and any unit $\xi \in S^*_x\mathcal{K}$, at least one of the multi-branched "geodesics" starting from (x,ξ), and from $(x,-\xi)$, at $t=0$ has a path that hits $\partial\Omega$ for time $t < T$ and satisfies the nontangency assumption of (9-4). Such a set may not even exist for some speeds c.

Example 1. Let $\Omega_0 \subset \Omega$ be two concentric balls, and let c be piecewise constant; more precisely, assume

$$\Omega = B(0,R), \quad \Omega_0 = B(0,R_0), \quad 0 < R_0 < R,$$

and let

$$c = \begin{cases} c_0 < 1 & \text{in } \Omega_0, \\ 1 & \text{in } \mathbb{R}^n \setminus \Omega_0. \end{cases}$$

Then such a set $\mathcal{K}$ always exist and can be taken to be a ball with the same center and small enough radius. Indeed, the requirement then is that all rays starting from $\mathcal{K}$ hit Γ at an angle greater than a critical one $\pi/2 - \alpha_0$; see (9-42).

This can be achieved by choosing $\mathcal{H} = B(0, \rho)$ with $\rho \ll R_0$. An elementary calculation shows that we need to satisfy the inequality $\rho/R_0 < \sin\alpha_0 = c_0$, i.e., it is enough to choose $\rho < c_0 < R_0$. Then there exists T_0 such that (9-5) holds for $T > T_0$, and T_0 is easy to compute. On can also add to $\mathcal{H}$ any compact included in $\{R_0 < |x| < R\}$. In other words, $\mathcal{H}$ can be any compact in Ω not intersecting $\{c_0 R_0 \le |x| \le R_0\}$, the zone where the trapped rays lie.

If $c = c_0 > 1$ in Ω_0, then any compact $\mathcal{H}$ in Ω satisfies (9-5). In that case, there is always a transmitted ray leaving Ω_0.

Example 2. This is a simplified version of the skull model. Let $\Omega_0 \subset \Omega_1 \subset \Omega$ be balls such that

$$\Omega = B(0, R), \quad \Omega_0 = B(0, R_0), \quad \Omega_1 = B(0, R_1) \quad 0 < R_0 < R_1 < R,$$

Assume that

$$c|_{\Omega_0} = c_0, \quad c|_{\Omega_1 \setminus \Omega_0} = c_1, \quad c|_{\mathbb{R}^n \setminus \Omega_1} = 1$$

with some constants c_0, c_1 such that $c_0 < c_1$, $c_1 > 1$. Here, c_0 models the acoustic speed in the brain, c_1 is the speed in the skull, and 1 is the acoustic speed in the liquid outside the head. If for a moment we consider Ω_0 and Ω_1 only, we have the configuration of the previous example. If $\mathcal{H} = B(0, \rho)$ with $\rho < (c_0/c_1)R_0$, then $\mathcal{H}$ satisfies (9-5) with an appropriate T. Now, since $c_1 > 1$, rays that hit $\partial\Omega_1$ always have a transmitted part outside Ω_1, and therefore (9-5) is still satisfied in Ω. Rays originating outside Ω_1 are not trapped, therefore, more generally, $\mathcal{H}$ can be any compact in $\Omega \setminus \{c_0 R_0/c_1 \le |x| \le R_0\}$.

Let $\Pi_{\mathcal{H}} : H_D(\Omega) \to H_D(\mathcal{H})$ be the orthogonal projection of elements of the former space to the latter (considered as a subspace of $H_D(\Omega)$). It is easy to check that $\Pi_{\mathcal{H}} f = f|_{\mathcal{H}} - P_{\partial\mathcal{H}}(f|_{\partial\mathcal{H}})$, where $P_{\partial\mathcal{H}}$ is the Poisson operator of harmonic extension in $\mathcal{H}$.

Our main result about discontinuous speeds is the following.

Theorem 9.1. *Let $\mathcal{H}$ satisfy* (9-5). *Then $\Pi_{\mathcal{H}} A_1 \Lambda = \mathrm{Id} - K$ in $H_D(\mathcal{H})$, with $\|K\|_{H_D(\mathcal{H})} < 1$. In particular, $\mathrm{Id} - K$ is invertible on $H_D(\mathcal{H})$, and Λ restricted to $H_D(\mathcal{H})$ has an explicit left inverse of the form*

$$f = \sum_{m=0}^{\infty} K^m \Pi_{\mathcal{H}} A h, \quad h = \Lambda f. \tag{9-6}$$

Remark 9.2. As discussed in the Introduction, K is not a compact operator as in the case of smooth sound speed. It follows from the proof of the theorem that the least upper bound of its essential spectrum (always less that 1) corresponds to the maximal portion of the high-frequency energy that is still held in Ω at time $t = T$.

Remark 9.3. Consider the case now where $\mathcal{K}$ does not satisfy (9-5). If there is an open set of singularities that does not reach $\partial\Omega$, a stable recovery is impossible [Stefanov and Uhlmann 1998b]. In either case however, a truncated version of the series (9-6) would provide an approximate parametrix that would recover the visible singularities, i.e., those in $\mathcal{U}$. By an approximate parametrix we mean a pseudodifferential operator elliptic in $\mathcal{U}$ with a principal symbol converging to 1 in any compact in that set as the number of the terms in (9-6) increases. This shows that roughly speaking, if a recovery of the singularities is the primary goal, then only those in $\mathcal{U}$ can be recovered in a "stable way", and (9-6) works in that case as well, without the assumption (9-5).

9B. ***Sketch of the proof; geometric optics.*** The proof of Theorem 9.1 is based on a detailed microlocal analysis of the solution of the forward equation (9-3). As we explained above, propagation of singularities is well understood, and we avoided the most delicate cases with our assumptions about $\mathcal{K}$. To prove that the "error operator" K is a contraction however, we show first that it is a contraction up to a compact operator by studying the parametrix first. Then we use a suitable adaptation of the unique continuation property to this setting, combined with arguments similar to those in the smooth case to show that the whole K is a contraction as well. The most essential part of the proof is to show that the parametrix is a contraction. This requires not only to trace the propagation of singularities but to show that each time a ray splits into a reflected and transmitted one (neither one tangent), both rays carry a positive fraction of the energy.

Analysis at the boundary. We will analyze what happens when the geodesic (x_0, ξ^0) issued from (x_0, ξ^0), $x_0 \notin \Gamma$, hits Γ for first time, under some assumptions. Let the open sets Ω_{int}, Ω_{ext}, be the interior and the exterior part of Ω near x_0, according to the orientation of Γ. They only need to be defined near the first contact with Γ. Let us assume that this geodesic hits Γ from Ω_{int}. We will construct here a microlocal representation of the reflected and the transmitted waves near the boundary. We refer to Section A.4 for the geometric optics construction.

Extend $c|_{\Omega_{\text{int}}}$ in a smooth way in a small neighborhood on the other side of Γ, and let u_+ be the solution described above, defined in some neighborhood of that geodesic segment. Since we are only going to use u_+ in the microlocal construction described below, and we will need only the trace of u_+ on $\mathbb{R}_+ \times \Gamma$ near the first contact of the bicharacteristic from (x_0, ξ^0) with Γ, the particular extension of c would not affect the microlocal expansion but may affect the smoothing part.

Set

$$h := u_+|_{\mathbb{R}\times\Gamma}. \tag{9-7}$$

Let $(t_1, x_1) \in \mathbb{R}_+ \times \Gamma$ be the point where the geodesic from γ_{x_0,ξ^0} hits Γ for the first time (see Figure 3). We assume that such a t_1 exists. Let ξ^1 be the tangent covector to that geodesic at (t_1, x_1). Assume that ξ^0 is unit covector in the metric $c^{-2}\mathrm{d}x^2$, then so is ξ^1 (in the metric $c_{\text{int}}^{-2}\mathrm{d}x^2$), i.e., $c_{\text{int}}|\xi| = 1$, where $|\xi|$ is the Euclidean norm. Assume that ξ^1 is transversal to Γ. In view of condition (9-5), this is the case that we need to study.

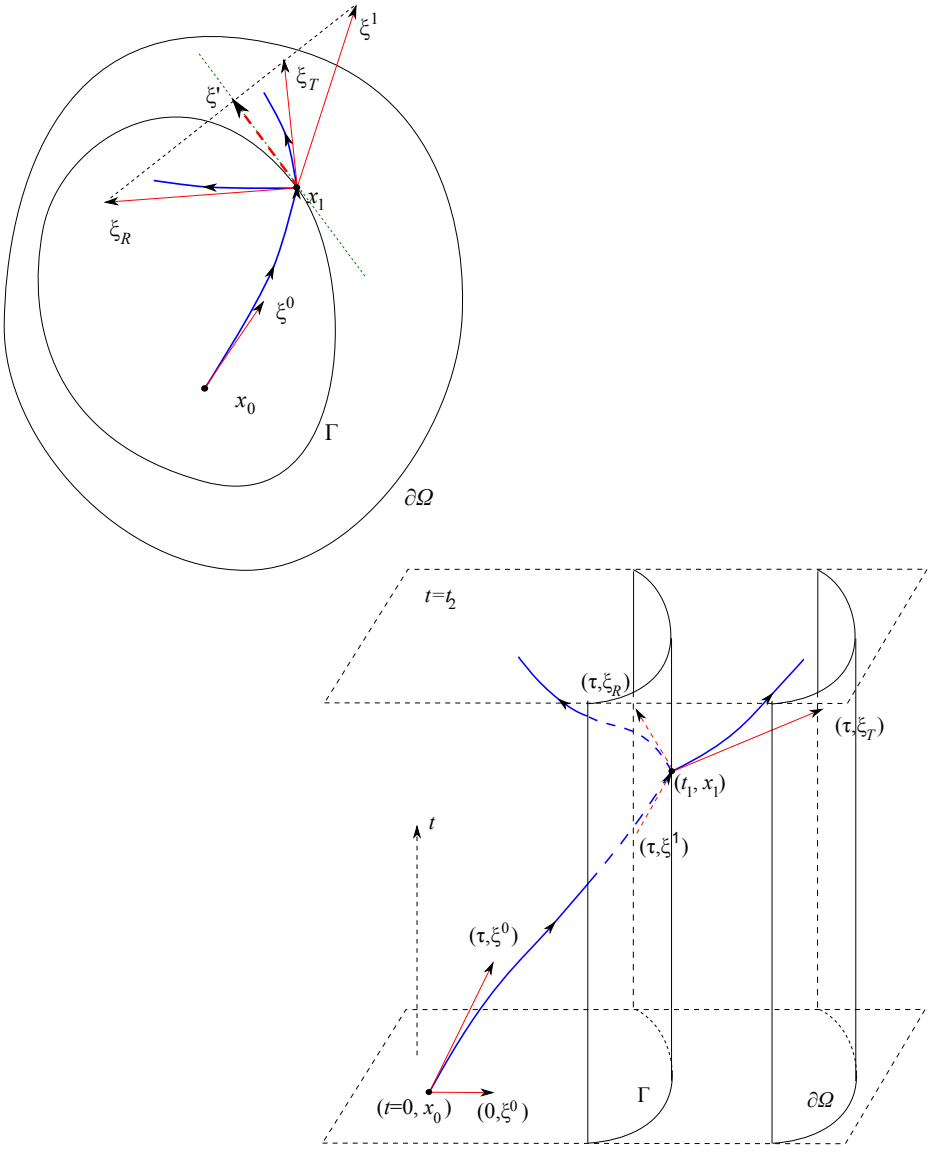

Figure 3. Reflected and the transmitted rays in x-space (top) and in (t, x)-space (bottom).

Standard microlocal arguments show that the map $[f_1, f_2] \mapsto h$ is an elliptic Fourier integral operator (FIO) with a canonical relation that is locally a canonical graph described in Proposition 3 of [Stefanov and Uhlmann 2009b]; see the proof of that proposition for details. That diffeomorphism maps (x_0, ξ^0) into $(t_1, x_1, 1, (\xi^1)')$, where the prime stands for the tangential projection onto $T^*\Gamma$; and that maps extends as a positively homogeneous one of order one with respect to the dual variable. In particular, the dual variable τ to t stays positive. In fact, $\mathrm{WF}(u)$ is in the characteristic set $\tau^2 - c^2(x)|\xi|^2 = 0$, and (x, ξ) belongs to some small neighborhood of (x_1, ξ^1). The wave front set $\mathrm{WF}(h)$ is given by $(x, \xi') \in T^*\Gamma$, $(x, \xi) \in \mathrm{WF}(u)$, where ξ' is the tangential projection of ξ to the boundary. Then (t, x, τ, ξ') is the image of some $(\tilde{x}, \tilde{\xi})$ close to (x_0, ξ^0) under the canonical map above. Here $(\tilde{x}, \tilde{\xi})$ is such that the x-projection $x(s)$ of the bicharacteristic from it hits Γ for the first time at time for the value of s given by $sc(\tilde{x}) = t$. Since $\tau^2 - c_{\mathrm{int}}^2(x)|\xi|^2 = 0$, for the projection ξ' we have $\tau^2 - c_{\mathrm{int}}^2(x)|\xi'|^2 > 0$, where $(x, \xi') \in T^*\Gamma$, and $|\xi'|$ is the norm of the covector ξ' in the metric on Γ induced by the Euclidean one.

The microlocal regions of $T^*(\mathbb{R} \times \Gamma) \ni (t, x, \tau, \xi')$ with respect to the sound speed c_{int}, i.e., in $\overline{\Omega}_{\mathrm{int}}$, are defined as follows:

hyperbolic region: $c_{\mathrm{int}}(x)|\xi'| < \tau$,

glancing manifold: $c_{\mathrm{int}}(x)|\xi'| = \tau$,

elliptic region: $c_{\mathrm{int}}(x)|\xi'| > \tau$.

One has a similar classification of $T^*\Gamma$ with respect to the sound speed c_{ext}. A ray that hits Γ transversely, coming from Ω_{int}, has a tangential projection on $T^*(\mathbb{R} \times \Gamma)$ in the hyperbolic region relative to c_{int}. If $c_{\mathrm{int}} < c_{\mathrm{ext}}$, that projection may belong to any of the three microlocal regions with respect to the speed c_{int}. If $c_{\mathrm{int}} > c_{\mathrm{ext}}$, then that projection is always in the hyperbolic region for c_{ext}. When we have a ray that hits Γ from Ω_{ext}, then those two cases are reversed.

Reflected and transmitted waves. We will analyze the case where $(\xi^1)'$ belongs to the hyperbolic region with respect to both c_{int} and c_{ext}, i.e., we will work with ξ' in a neighborhood of $(\xi^1)'$ satisfying

$$c_{\mathrm{int}}^{-2}\tau^2 - |\xi'|^2 > 0, \quad c_{\mathrm{ext}}^{-2}\tau^2 - |\xi'|^2 > 0. \tag{9-8}$$

The analysis also applies to the case of a ray coming from Ω_{ext}, under the same assumption. We will confirm below in this setting the well known fact that under that condition, such a ray splits into a reflected ray with the same tangential component of the velocity that returns to the interior Ω_{int}, and a transmitted one, again with the same tangential component of the velocity, that propagates in Ω_{ext}. We will also compute the amplitudes and the energy at high frequencies of the corresponding asymptotic solutions.

Choose local coordinates on Γ that we denote by x', and a normal coordinate x^n to Γ such that $x^n > 0$ in Ω_{ext}, and $|x^n|$ is the Euclidean distance to Γ; then $x = (x', x^n)$. We will express the solution u_+ in $\mathbb{R} \times \overline{\Omega}_{\text{int}}$ that we defined above, as well as a reflected solution u_R in the same set; and a transmitted one u_T in $\mathbb{R} \times \overline{\Omega}_{\text{ext}}$, up to smoothing terms in the form

$$u_\sigma = (2\pi)^{-n} \int e^{\mathrm{i}\varphi_\sigma(t,x,\tau,\xi')} b_\sigma(t, x, \tau, \xi') \hat{h}(\tau, \xi') \, \mathrm{d}\tau \, \mathrm{d}\xi', \quad \sigma = +, R, T, \tag{9-9}$$

where $\hat{h} := \int_{\mathbb{R}\times\mathbb{R}^{n-1}} e^{-\mathrm{i}(-t\tau + x'\cdot\xi')} h(t, x') \mathrm{d}t \, \mathrm{d}x'$. We chose to alter the sign of τ so that if $c = 1$, the phase function in (9-9) equals φ_+, i.e., then $\varphi_+ = -t\tau + x \cdot \xi$. The three phase functions φ_+, φ_R, φ_T solve the eikonal equation

$$\partial_t \varphi_\sigma + c(x) |\nabla_x \varphi_\sigma| = 0, \quad \varphi_\sigma|_{x^n=0} = -t\tau + x' \cdot \xi'. \tag{9-10}$$

The right choice of the sign in front of $\partial_t \varphi_+$ (see (A-16)) is the positive one because $\partial_t \varphi_+ = -\tau < 0$ for $x^n = 0$, and that derivative must remain negative near the boundary as well. We see below that $\varphi_{R,T}$ have the same boundary values on $x^n = 0$, therefore they satisfy the same eikonal equation, with the same choice of the sign.

Let now h be a compactly supported distribution on $\mathbb{R} \times \Gamma$ with $\mathrm{WF}(h)$ in a small conic neighborhood of $(t_1, x_1, 1, (\xi^1)')$. We will take h as in (9-7) eventually, with u_+ the solution corresponding to initial data $\boldsymbol{f}$ at $t = 0$ but in what follows, h is arbitrary as long as $\mathrm{WF}(h)$ has that property, and u_+ is determined through h. We now look for a parametrix

$$\tilde{u} = u_+ + u_R + u_T \tag{9-11}$$

near (t_1, x_1) with u_+, u_R, u_T of the type (9-9), satisfying the wave equation and (9-7). We use the notation for u_+ now for a parametrix in Ω_{int} having singularities that come from the past and hit Γ; i.e., for an outgoing solution. The subscript $+$ is there to remind us that this is related to the positive sound speed $c(x)|\xi|$. Next, u_R is a solution with singularities that are obtained form those of u_+ by reflection; they propagate back to Ω_{int}. It is an outgoing solution in Ω_{int}. And finally, u_T is a solution in Ω_{ext} with singularities that go away from Γ as time increases; hence it is outgoing there. To satisfy the first transmission condition in (9-3), we need to have

$$\varphi_T = \varphi_R = \varphi_+ = -t\tau + x \cdot \xi' \quad \text{for } x^n = 0, \tag{9-12}$$

that explains the same boundary condition in (9-10), and

$$1 + b_R = b_T \quad \text{for } x^n = 0. \tag{9-13}$$

In particular, for the leading terms of the amplitudes we get

$$b_T^{(0)} - b_R^{(0)} = 1 \quad \text{for } x^n = 0. \tag{9-14}$$

To satisfy the second transmission condition, we require

$$\mathrm{i}\frac{\partial \varphi_+}{\partial x^n} + \frac{\partial b_+}{\partial x^n} + \mathrm{i}\frac{\partial \varphi_R}{\partial x^n} b_R + \frac{\partial b_R}{\partial x^n} = \mathrm{i}\frac{\partial \varphi_T}{\partial x^n} b_T + \frac{\partial b_T}{\partial x^n} \quad \text{for } x^n = 0. \tag{9-15}$$

Expanding this in a series of homogeneous in (τ, ξ) terms, we get series of initial conditions for the transport equations that follow. Comparing the leading order terms only, we get

$$\frac{\partial \varphi_T}{\partial x^n} b_T^{(0)} - \frac{\partial \varphi_R}{\partial x^n} b_R^{(0)} = \frac{\partial \varphi_+}{\partial x^n} \quad \text{for } x^n = 0. \tag{9-16}$$

The linear system (9-14), (9-16) for $b_R^{(0)}|_{x^n=0}$, $b_T^{(0)}|_{x^n=0}$ has determinant

$$-\left(\frac{\partial \varphi_T}{\partial x^n} - \frac{\partial \varphi_R}{\partial x^n}\right)\Big|_{x^n=0}. \tag{9-17}$$

Provided that this determinant is nonzero near x_1, we can solve for $b_R^{(0)}|_{x^n=0}$ and $b_T^{(0)}|_{x^n=0}$. Moreover, the determination of each subsequent term $b_R^{(-j)}|_{x^n=0}$ or $b_T^{(-j)}|_{x^n=0}$ in the asymptotic expansion of $b_R|_{x^n=0}$ and $b_T|_{x^n=0}$ can be found from (9-15) by solving a linear system with the same (nonzero) determinant.

Solving the eikonal equations. As is well known, the eikonal equation (9-10) in any fixed side of $\mathbb{R} \times \Gamma$, near (t_1, x_1), has two solutions. They are determined by a choice of the sign of the normal derivative on $\mathbb{R} \times \Gamma$ and the boundary condition. We will make the choice of the signs according to the desired properties for the singularities of u_+, u_R, u_T. Let $\nabla_{x'}$ denote the tangential gradient on Γ. By (9-12),

$$\nabla_{x'} \varphi_T = \nabla_{x'} \varphi_R = \nabla_{x'} \varphi_+ = \xi', \quad \partial_t \varphi_T = \partial_t \varphi_R = \partial_t \varphi_+ = -\tau \quad \text{for } x^n = 0. \tag{9-18}$$

Using the eikonal equation (9-10) and the boundary condition there, we get

$$\frac{\partial \varphi_+}{\partial t} = -\tau, \quad \frac{\partial \varphi_+}{\partial x^n} = \sqrt{c_{\text{int}}^{-2}\tau^2 - |\xi'|^2} \quad \text{for } x^n = 0. \tag{9-19}$$

We made a sign choice for the square root here based on the required property of u_+ described above. This shows in particular, that the map $h \mapsto \partial u_+ / \partial t$ (that is just $\mathrm{d}/\mathrm{d}t$), and the interior incoming Dirichlet-to-Neumann map

$$N_{\text{int,in}} : h \mapsto \frac{\partial u_+}{\partial \nu}\Big|_{\mathbb{R}\times\Gamma}$$

are locally ΨDOs of order 1 with principal symbols given by $-\mathrm{i}\tau$, and

$$\sigma_p(N_{\mathrm{int,in}}) = \mathrm{i}\frac{\partial\varphi_+}{\partial x^n} = \mathrm{i}\sqrt{c_{\mathrm{int}}^{-2}\tau^2 - |\xi'|^2}. \tag{9-20}$$

The notion "interior incoming" is related to the fact that locally, near (t_1, x_1), we are solving a mixed problem in $\mathbb{R}\times\Omega_{\mathrm{int}}$ with lateral boundary value h and zero Cauchy data for $t \gg 0$.

Consider φ_R next. The reflected phase φ_R solves the same eikonal equation, with the same boundary condition, as φ_+. By the eikonal equation (9-10), we must have

$$\frac{\partial\varphi_R}{\partial x^n} = \pm\frac{\partial\varphi_+}{\partial x^n} \quad \text{for } x^n = 0. \tag{9-21}$$

The "+" choice will give us the solution φ_+ for φ_R. We chose the negative sign, that uniquely determines a solution locally, that we call φ_R, i.e.,

$$\frac{\partial\varphi_R}{\partial x^n} = -\frac{\partial\varphi_+}{\partial x^n} \quad \text{for } x^n = 0. \tag{9-22}$$

Therefore, $\nabla\varphi_R$ on the boundary is obtained from $\nabla\varphi_+$ by inverting the sign of the normal derivative. This corresponds to the usual law of reflection. Therefore,

$$\frac{\partial\varphi_R}{\partial t} = -\tau, \quad \frac{\partial\varphi_R}{\partial x^n} = -\sqrt{c_{\mathrm{int}}^{-2}\tau^2 - |\xi'|^2} \quad \text{for } x^n = 0. \tag{9-23}$$

In particular, $\partial u_R/\partial x^n|_{\mathbb{R}\times\Gamma}$ can be obtained from $u_R|_{\mathbb{R}\times\Gamma}$, that we still need to determine, via the interior outgoing Dirichlet-to-Neumann map

$$N_{\mathrm{int,out}} : u_R\Big|_{\mathbb{R}\times\Gamma} \quad \longmapsto \quad \frac{\partial u_R}{\partial x^n}\Big|_{\mathbb{R}\times\Gamma}$$

that is locally a first order ΨDO with principal symbol

$$\sigma_p(N_{\mathrm{int,out}}) = \mathrm{i}\frac{\partial\varphi_R}{\partial t} = -\mathrm{i}\sqrt{c_{\mathrm{int}}^{-2}\tau^2 - |\xi'|^2}. \tag{9-24}$$

To construct φ_T, we work in $\overline{\Omega}_{\mathrm{ext}}$. We define φ_T as the solution of (9-10) with the following choice of a normal derivative. This time φ_T and φ_+ solve the eikonal equation at different sides of Γ, and c has a jump at Γ. By (9-18),

$$c_{\mathrm{ext}}^2\left(|\xi'|^2 + \Big|\frac{\partial\varphi_T}{\partial x^n}\Big|^2\right) = \tau^2 \quad \text{for } x^n = 0. \tag{9-25}$$

We solve this equation for $|\partial\varphi_T/\partial x^n|^2$. Under the assumption (9-8), this solution is positive, therefore we can solve for $\partial\varphi_T/\partial x^n$ to get

$$\frac{\partial\varphi_T}{\partial x^n} = \quad \sqrt{c_{\mathrm{ext}}^{-2}\tau^2 - |\xi'|^2} \quad \text{for } x^n = 0. \tag{9-26}$$

The positive sign of the square root is determined by the requirement the singularity to be outgoing. In particular, we get that the exterior outgoing Dirichlet-to-Neumann map

$$N_{\text{ext,out}} : u_T\big|_{\mathbb{R}\times\Gamma} \longmapsto \frac{\partial u_T}{\partial x^n}\Big|_{\mathbb{R}\times\Gamma}$$

has principal symbol

$$\sigma_p(N_{\text{ext,out}}) = \mathrm{i}\frac{\partial \varphi_T}{\partial x^n} = \mathrm{i}\sqrt{c_{\text{ext}}^{-2}\tau^2 - |\xi'|^2}. \tag{9-27}$$

For future reference, we note the inequality

$$0 \le \frac{\partial \varphi_T}{\partial x^n} \le \gamma \frac{\partial \varphi_+}{\partial x^n}, \quad \text{where } \gamma := \max_\Gamma \frac{c_{\text{int}}}{c_{\text{ext}}} < 1. \tag{9-28}$$

Amplitude and energy calculations. By (9-23), (9-26), the determinant (9-17) is negative. Solving (9-14) and (9-16) then yields

$$b_T^{(0)} = \frac{2\partial\varphi_+/\partial x^n}{\partial\varphi_+/\partial x^n + \partial\varphi_T/\partial x^n}, \quad b_R^{(0)} = \frac{\partial\varphi_+/\partial x^n - \partial\varphi_T/\partial x^n}{\partial\varphi_+/\partial x^n + \partial\varphi_T/\partial x^n} \quad \text{for } x^n = 0. \tag{9-29}$$

As explained below (9-17), we can get initial conditions for the subsequent transport equations, and then solve those transport equation. By (9-12), the maps

$$P_R : h \mapsto u_R|_{\mathbb{R}\times\Gamma}, \quad P_T : h \mapsto u_T|_{\mathbb{R}\times\Gamma} \tag{9-30}$$

are ΨDOs of order 0 with principal symbols equal to $b_R^{(0)}$, $b_T^{(0)}$ restricted to $\mathbb{R}\times\Gamma$; see (9-29). We recall (9-7) as well.

We estimate next the amount of energy that is transmitted in Ω_{ext}. We will do it only based on the principal term in our parametrix. That corresponds to an estimate of the solution operator corresponding to transmission, up to compact operators, as we show below.

A quick look at (9-29) (see also (9-14)) shows that $b_T^{(0)} > 1$. This may look strange because we should have only a fraction of the energy transmitted, and the rest is reflected. There is no contradiction however because the energy is not proportional to the amplitude.

Let u solve $(\partial_t^2 - c^2\Delta)u = 0$ in the bounded domain U with smooth boundary for $t' \le t \le t''$ with some $t' < t''$. A direct calculation yields

$$E_U(\boldsymbol{u}(t'')) = E_U(\boldsymbol{u}(t')) + 2\Re \int_{[t',t'']\times\partial U} u_t \frac{\partial \bar{u}}{\partial \nu}\, \mathrm{d}t\, \mathrm{d}S. \tag{9-31}$$

We will use this to estimate the energy of u_T in Ω_{ext}. Since the wave front set of u_T is contained in some small neighborhood of the transmitted bicharacteristic, we have smooth data for $t = 0$. Therefore, if $t_2 > t_1$ is fixed closed enough to

t_1, we can apply (9-31) to a large ball minus Ω_{int} to get that modulo a compact operator applied to h,

$$E_{\Omega_{\text{ext}}}(\boldsymbol{u}_T(t_2)) \cong 2\Re \int_{[0,t_2]\times\Gamma} \frac{\partial u_T}{\partial t}\frac{\partial \bar{u}_T}{\partial \nu}\,\mathrm{d}t\,\mathrm{d}S. \tag{9-32}$$

Therefore,

$$E_{\Omega_{ext}}(\boldsymbol{u}_T(t_2)) \cong 2\Re(P_t u_T, N_{\text{ext,out}} u_T) = \Re(2P_T^* N_{\text{ext,out}}^* P_t P_T h, h), \tag{9-33}$$

where $(\cdot,\cdot)$ is the inner product in $\mathbb{R}\times\mathbb{R}^{n-1}$, and $P_t = \mathrm{d}/\mathrm{d}t$.

Apply similar arguments to u_+ in Ω_{int}. Since the bicharacteristics leave Ω_{int}, we have modulo smoother terms

$$0 \cong E_{\Omega_{\text{int}}}(\boldsymbol{u}_+(0)) + 2\Re \int_{[0,t_2]\times\Gamma} \frac{\partial u_+}{\partial t}\frac{\partial \bar{u}_+}{\partial \nu}\,\mathrm{d}t\,\mathrm{d}S. \tag{9-34}$$

Similarly we get (see again (9-30))

$$E_{\Omega_{\text{int}}}(\boldsymbol{u}_+(0)) \cong -2\Re(P_t h, N_{\text{int,in}} h) = \Re(2N_{\text{int,in}}^* P_t h, h). \tag{9-35}$$

For the principal symbols of the operators in (9-33), (9-35) we have

$$\frac{\sigma_p(2P_T^* N_{\text{ext,out}}^* P_t P_T)}{\sigma_p(2N_{\text{int,in}}^* P_t)} = \frac{\partial\varphi_T/\partial\nu}{\partial\varphi_+/\partial\nu}(b_T^{(0)})^2 = \frac{4(\partial\varphi_+/\partial\nu)(\partial\varphi_T/\partial\nu)}{(\partial\varphi_+/\partial\nu + \partial\varphi_T/\partial\nu)^2}. \tag{9-36}$$

Denote for a moment $a := \partial\varphi_+/\partial\nu$, $b := \partial\varphi_T/\partial\nu$. Then the quotient above equals $4ab/(a+b)^2 \le 1$ that confirms that the reflected wave has less energy than the incident one. By (9-28), $0 \le b \le \gamma a$, $0 < \gamma < 1$. This easily implies

$$\frac{4ab}{(a+b)^2} \le \frac{4\gamma}{(1+\gamma)^2} < 1. \tag{9-37}$$

Therefore, the expression in the middle represents an upper bound of the portion of the total energy that gets transmitted in the asymptotic regime when the frequency tends to infinity. To get a lower bound, assume in addition that $b \ge b_0 > 0$ and $a \le a_0$ for some a_0, b_0, i.e.,

$$0 < b_0 < \frac{\partial\varphi_T}{\partial\nu}, \quad \frac{\partial\varphi_+}{\partial\nu} \le a_0. \tag{9-38}$$

Then

$$\frac{4ab}{(a+b)^2} \ge \frac{4b_0^2/\gamma}{(1+\gamma)^2 a_0^2} > 0. \tag{9-39}$$

This is a lower bound of the ratio of the high frequency energy that is transmitted. As we can see, if the transmitted ray gets very close to a tangent one, that ratio tends to 0.

So far this is still not a proof of such a statement but just a heuristic argument. For the a precise statement, see [Stefanov and Uhlmann 2011].

Snell's law. Now assume that $(\xi^1)'$ is in the hyperbolic region for c_{int} but not necessarily for c_{ext}. This corresponds to a ray hitting Γ from the interior Ω_{int}. There is no change in solving the eikonal equation for φ_R but a real phase φ_T does not exist if the expression under the square root in (9-26) is negative. This happens when $(\xi^1)'$ is in the elliptic region for c_{ext}. Then there is no transmitted singularity in the parametrix. We analyze this case below. If $c_{\text{int}} > c_{\text{ext}}$, then $(\xi^1)'$ that is in the hyperbolic region for c_{int} by assumption, also falls into the hyperbolic region for the speed c_{ext}, i.e., there is always a transmitted ray. If $c_{\text{int}} < c_{\text{ext}}$, then existence of a transmitted wave depends on where $(\xi^1)'$ belongs with respect to c_{ext}.

Let α be the angle that $\xi^1 = \partial\varphi_+/\partial x^n$ makes with the (co)-normal represented by $\mathrm{d}x^n$, and let β be the angle between the latter and $\xi_T := \partial\varphi_T/\partial x^n$. We have

$$|\xi'| = |\xi^1| \sin\alpha = c_{\text{int}}^{-1}\tau \sin\alpha, \quad |\xi'| = |\xi_T| \sin\beta = c_{\text{ext}}^{-1}\tau \sin\beta \tag{9-40}$$

By (9-40), we recover Snell's law

$$\frac{\sin\alpha}{\sin\beta} = \frac{c_{\text{int}}}{c_{\text{ext}}}, \tag{9-41}$$

Assume now that $c_{\text{int}} < c_{\text{ext}}$, which is the case where there might be no transmitted ray. Denote by

$$\alpha_0(x) = \arcsin(c_{\text{int}}(x)/c_{\text{ext}}(x)) \tag{9-42}$$

the critical angle at any $x \in \Gamma$ that places $(\xi^1)'$ in the glancing manifold with respect to c_{ext}. Then the transmitted wave does not exist when $\alpha > \alpha_0$; more precisely we do not have a real phase function φ_T in that case. It exists, when $\alpha < \alpha_0$. In the critical case $\alpha = \alpha_0$, this construction provides an outgoing ray tangent to Γ that we are not going to analyze.

The full internal reflection case. Assume now that $(\xi^1)'$ is in the elliptic region with respect to c_{ext}, then there is no transmitted singularity, but one can still construct a parametrix for the "evanescent" wave in Ω_{ext}; and there is a reflected ray. This is known as a full internal reflection. We give details below.

We proceed as above with one essential difference. There is no real-valued solution φ_T to the eikonal equation (9-10) outside Ω_0. Similarly to (9-26), we get formally,

$$\frac{\partial\varphi_T}{\partial\nu} = \quad \mathrm{i}\sqrt{|\xi'|^2 - c_{\text{ext}}^{-2}\tau^2} \quad \text{for } x^n = 0. \tag{9-43}$$

The choice of the sign of the square root is dictated by the requirement that the parametrix (9-9) with $\sigma = T$ be exponentially decreasing away from Γ instead of exponentially increasing.

In general, the eikonal equation may not be solvable but one can still construct solutions modulo $O((x^n)^\infty)$. The same applies to the transport equations. One can show that the $O((x^n)^\infty)$ error does not change the properties of u_T to be a parametrix. In particular, in (9-33) in this case one gets

$$E_{\Omega_{\text{ext}}}(\boldsymbol{u}_T(t_2)) \cong 0, \tag{9-44}$$

because the principal term of $\partial \bar{u}_T/\partial \nu$ in (9-32) now is pure imaginary instead of being real. Moreover, u_T is smooth in $\overline{\Omega}_{\text{ext}}$. Therefore, no energy, as far as the principal part only is considered, is transmitted to Ω_{ext}. That does not mean that the solution vanishes there, of course.

Glancing, gliding rays and other cases. We do not analyze the cases where $(\xi^1)'$ is in the glancing manifold with respect one of the speeds. We can do that because the analysis of those cases in not needed because of our assumptions guaranteeing no tangent rays. The analysis there is more delicate, and we refer to [Taylor 1976; Petkov 1982a; 1982b] for more details and examples. We do not analyze either the case where $(\xi^1)'$ is in the elliptic region with respect to either speed.

Justification of the parametrix. Denote by $\boldsymbol{u}_R = [u_R, \partial_t u_R]$, $\boldsymbol{u}_T = [u_T, \partial_t u_T]$ the approximate solutions constructed above, defined for t in some neighborhood of t_2. Then $\boldsymbol{u}_R = \boldsymbol{V}_R h$, $\boldsymbol{u}_T = \boldsymbol{V}_T h$, where $\boldsymbol{V}_{R,T}$ are the FIOs constructed above. Let $\boldsymbol{u}_+$ be the solution of (9-3) defined above, with initial data $\boldsymbol{\Pi}_+ \boldsymbol{f}$ at $t = 0$ having wave front set in a small neighborhood of (x_0, ξ^0). The map $\Lambda_+ : \boldsymbol{f} \mapsto u_+|_{\mathbb{R}\times\Gamma} = h$ is an FIO described in [Stefanov and Uhlmann 2009b]. Then near (t_1, x_1),

$$\boldsymbol{u}_R = \boldsymbol{V}_R \Lambda \boldsymbol{f}, \quad \boldsymbol{u}_T = \boldsymbol{V}_T \Lambda \boldsymbol{f},$$

the former supported in $\mathbb{R} \times \overline{\Omega}_{\text{int}}$, and the later in $\mathbb{R} \times \overline{\Omega}_{\text{ext}}$. So far we had two objects that we denoted by u_+: first, the parametrix of the solution of (9-3) corresponding to the positive sound speed $c(x)|\xi|$; and the parametrix in $\mathbb{R}\times\overline{\Omega}_{\text{int}}$ for the incoming solution corresponding to boundary value h. When $h = \Lambda_+ \boldsymbol{f}$, those two parametrices coincide up to a smooth term, as it is not hard to see (the second one is a back-projection and is discussed in [Stefanov and Uhlmann 2009b], in fact). This justifies the same notation for them that we will keep.

Consider the parametrix $v_p := u_+ + u_R + u_T$. We can always assume that its support is in some small neighborhood of the geodesic that hits $\mathbb{R} \times \Gamma$ at (t_1, x_1) and is tangent to ξ^1 there; and then reflects, and another branch refracts (see Figure 3 on page 300). In particular, then h has t-support near $t = t_1$,

let us say that this included in the interval $[t_1-\varepsilon, t_1+\varepsilon]$ with some $\varepsilon > 0$. At $t = t_2 := t_1 + 2\varepsilon$, let x_2 be the position of the reflected ray, and let ξ^2 be its unit co-direction. Then $\mathrm{WF}(u_R(t_2, \cdot))$ is in a small conic neighborhood of (x_2, ξ^2).

Let $\boldsymbol{v}(t, \cdot) = e^{t\boldsymbol{P}}\boldsymbol{\Pi}_+\boldsymbol{f}$ be the exact solution — see (A-22) — with some fixed choice of the parametrix Q^{-1} in the definition of $\boldsymbol{\Pi}_+$, properly supported. Consider $w = v - v_p$ in $[0, t_2] \times \mathbb{R}^n$. It satisfies

$$\begin{gathered}(\partial_t^2 - c^2\Delta)w|_{[0,t_2]\times\overline{\Omega}_{\mathrm{int}}} \in C^\infty, \qquad (\partial_t^2 - c^2\Delta)w|_{[0,t_2]\times\overline{\Omega}_{\mathrm{ext}}} \in C^\infty, \\ w|_{[0,t_2]\times\Gamma_{\mathrm{ext}}} - w|_{[0,t_2]\times\Gamma_{\mathrm{int}}} \in C^\infty, \ \frac{\partial w}{\partial \nu}\Big|_{[0,t_2]\times\Gamma_{\mathrm{ext}}} - \frac{\partial w}{\partial \nu}\Big|_{[0,t_2]\times\Gamma_{\mathrm{int}}} \in C^\infty.\end{gathered} \tag{9-45}$$

On the other hand, for $0 \le t \ll 1$, v is smooth. Let $\chi \in C^\infty(\mathbb{R})$ be a function that vanishes in $(-\infty, \delta]$ and equals 1 on $[2\delta, \infty)$, $0 < \delta \ll 1$. Then $\tilde{w} := \chi(t)w(t, x)$ still satisfies (9-45) and also vanishes for $t \le 0$. By [Williams 1992, Theorem 1.36], $\tilde{w}$ is smooth in $[0, t_2] \times \overline{\Omega}_{\mathrm{int}}$, up to the boundary, and is also smooth in $[0, t_2] \times \overline{\Omega}_{\mathrm{ext}}$, up to the boundary. Therefore,

$$\boldsymbol{v}(t, \cdot) = \boldsymbol{v}_p(t, \cdot) + \boldsymbol{K}_t\boldsymbol{f}, \tag{9-46}$$

for any $t \in [0, t_2]$, where $\boldsymbol{K}_t$ is a compact operator in $\mathcal{H}$, depending smoothly on t. The operator $\boldsymbol{K}_t$ depends on $\boldsymbol{Q}$ as well. Therefore, the parametrix coincides with the exact solution up to a compact operator that is also smoothing in the sense described above.

This concludes the description of the microlocal part of the proof. The rest of the proof of Theorem 9.1 is as indicated above. Write $A\Lambda = \mathrm{Id} - K$, as in the smooth case. This time K is not compact any more, regardless of how large T is. Based on our assumptions and on what we proved, its essential spectrum is supported in a disk $|z| < C_0 < 1$ in the complex plane; and by unique continuation, we still have (4-10). This situation is similar to the proof of Theorem 4.1; see (4-14). The difference is that in the smooth case, $C_0 = 1/2$, if $T_1/2 < T < T_1$, and $C_0 = 0$, if $T > T_1$, while in the "skull" case, $0 < C_1 < 1$ and we can only make C_1 as small as we want but not zero, as $T \to \infty$, under our assumptions.

Numerical experiments done in [Qian et al. 2011] based on this approach show that one gets very good reconstruction even without restricting the support of f to sets $\mathcal{K}$ satisfying (9-5), i.e., if we allow for invisible singularities. The reconstruction is worse in the trapping region, and trapped conormal singularities are not recovered.

The partial data case for a discontinuous speed, i.e, when we have data on a part of $\partial\Omega$ has not been studied yet. It seems plausible that the methods in [Stefanov and Uhlmann 2009b] for a smooth speed described above can be extended but there are new technical difficulties. Even for a smooth speed however, a convergent series solution is not known. On the other hand, such

reconstruction has been tried numerically in [Qian et al. 2011] with success. Under the condition that all singularities issued from supp f are visible, for a smooth speed, the inverse problem reduces to a Fredholm equation with a trivial kernel. For a discontinuous speed of the type we study in this paper, it follows from our analysis that we still get a Fredholm equation but the triviality of the kernel is a more delicate question.

Appendix: Microlocal analysis and geometric optics

One of the fundamental ideas of classical analysis is a thorough study of functions near a point, i.e., locally. Microlocal analysis, loosely speaking, is analysis near points and directions, i.e., in the "phase space".

A.1. ***Wave front sets.*** The phase space in $\mathbb{R}^n$ is the cotangent bundle $T^*\mathbb{R}^n$ that can be identified with $\mathbb{R}^n \times \mathbb{R}^n$. Given a distribution $f \in \mathcal{D}'(\mathbb{R}^n)$, a fundamental object to study is the wave front set $\mathrm{WF}(f) \subset T^*\mathbb{R}^n \setminus 0$ that we define below.

The basic idea goes back to the properties of the Fourier transform. If f is an integrable compactly supported function, one can tell whether f is smooth by looking at the behavior of $\hat{f}(\xi)$ (that is smooth, even analytic) when $|\xi| \to \infty$. It is known that f is smooth if and only if for any N, $|\hat{f}(\xi)| \le C_N|\xi|^{-N}$ for some C_N. If we localize this requirement to a conic neighborhood V of some $\xi_0 \neq 0$ (V is conic if $\xi \in V \Rightarrow t\xi \in V, \forall t > 0$), then we can think of this as a smoothness in the cone V. To localize in the base x variable however, we first have to cut smoothly near a fixed x_0.

We say that $(x_0, \xi_0) \in \mathbb{R}^n \times (\mathbb{R}^n \setminus 0)$ is *not* in the wave front set $\mathrm{WF}(f)$ of $f \in \mathcal{D}'(\mathbb{R}^n)$ if there exists $\phi \in C_0^\infty(\mathbb{R}^n)$ with $\phi(x_0) \neq 0$ such that for any N, there exists C_N so that

$$|\widehat{\phi f}(\xi)| \le C_N|\xi|^{-N}$$

for ξ in some conic neighborhood of ξ_0. This definition is independent of the choice of ϕ. If $f \in \mathcal{D}'(\Omega)$ with some open $\Omega \subset \mathbb{R}^n$, to define $\mathrm{WF}(f) \subset \Omega \times (\mathbb{R}^n \setminus 0)$, we need to choose $\phi \in C_0^\infty(\Omega)$. Clearly, the wave front set is a closed conic subset of $\mathbb{R}^n \times (\mathbb{R}^n \setminus 0)$. Next, multiplication by a smooth function cannot enlarge the wave front set. The transformation law under coordinate changes is that of covectors making it natural to think of $\mathrm{WF}(f)$ as a subset of $T^*\mathbb{R}^n \setminus 0$, or $T^*\Omega \setminus 0$, respectively.

The wave front set $\mathrm{WF}(f)$ generalizes the notion $\mathrm{singsupp}(f)$ — the complement of the largest open set where f is smooth. The points (x, ξ) in $\mathrm{WF}(f)$ are referred too as *singularities* of f. Its projection onto the base is

$$\mathrm{singsupp}(f) = \{x;\ \exists \xi, (x, \xi) \in \mathrm{WF}(f)\}.$$

Examples. (a) $\mathrm{WF}(\delta) = \{(0,\xi);\ \xi \neq 0\}$. In other words, the Dirac delta function is singular at $x = 0$ in all directions.

(b) Let $x = (x', x'')$, where $x' = (x_1, \ldots, x_k)$, $x'' = (x_{k+1}, \ldots, x_n)$ with some k. Then $\mathrm{WF}(\delta(x')) = \{(0, x'', \xi', 0), \xi' \neq 0\}$, where $\delta(x')$ is the Dirac delta function on the plane $x' = 0$, defined by $\langle \delta(x'), \phi \rangle = \int \phi(0, x'')\, \mathrm{d}x''$. In other words, $\mathrm{WF}(\delta(x'))$ consists of all (co)vectors with a base point on that plane, perpendicular to it.

(c) Let f be a piecewise smooth function that has a nonzero jump across some smooth surface S. Then $\mathrm{WF}(f)$ consists of all (co)vectors at points of S, normal to it. This follows from (a) and a change of variables that flatten S locally.

(d) Let $f = \mathrm{pv}\frac{1}{x} - \pi \mathrm{i}\delta(x)$ in $\mathbb{R}$. Then $\mathrm{WF}(f) = \{(0,\xi);\ \xi > 0\}$.

In example (d) we see a distribution with a wave front set that is not symmetric under the change $\xi \mapsto -\xi$. In fact, wave front sets do not have a special structure except for the requirement to be closed conic sets; given any such set, there is a distribution with a wave front set exactly that set.

Two distributions cannot be multiplied in general. However, if their wave front sets do not intersect, there is a "natural way" to define a product.

A.2. *Pseudodifferential operators.*

Definitions. We first define the symbol class $S^m(\Omega)$, $m \in \mathbb{R}$, as the set of all smooth functions $p(x,\xi)$, $(x,\xi) \in \Omega \times \mathbb{R}^n$, called symbols, satisfying the following symbol estimates: for any compact $K \subset \Omega$, and any multi-indices α, β, there is a constant $C_{K,\alpha,\beta} > 0$ such that

$$|\partial_\xi^\alpha \partial_x^\beta p(x,\xi)| \leq C_{K,\alpha,\beta}(1 + |\xi|)^{m-|\alpha|} \quad \text{for all } (x,\xi) \in K \times \mathbb{R}^n. \tag{A-1}$$

More generally, one can define the class $S^m_{\rho,\delta}(\Omega)$ with $0 \leq \rho, \delta \leq 1$ by replacing $m - |\alpha|$ there by $m - \rho|\alpha| + \delta|\beta|$. Then $S^m(\Omega) = S^m_{1,0}(\Omega)$. Often, we omit Ω and simply write S^m. There are other classes in the literature, for example $\Omega = \mathbb{R}^n$, and (A-1) is required to hold for all $x \in \mathbb{R}^n$.

The estimates (A-1) do not provide any control of p when x approaches boundary points of Ω, or ∞.

Given $p \in S^m(\Omega)$, we define the ΨDO with symbol p, denoted by $p(x, D)$, by

$$p(x, D) f = (2\pi)^{-n} \int e^{\mathrm{i}x\cdot\xi} p(x,\xi) \hat{f}(\xi)\, \mathrm{d}\xi, \quad f \in C_0^\infty(\Omega). \tag{A-2}$$

The definition is inspired by the following. If $P = \sum_{|\alpha|\leq m} a_\alpha(x) D^\alpha$ is a differential operator, where $D = -\mathrm{i}\partial$, then using the Fourier inversion formula we can write P as in (A-2) with a symbol $p = \sum_{|\alpha|\leq m} a_\alpha(x)\xi^\alpha$ that is a polynomial in ξ with x-dependent coefficients. The symbol class S^m allows

for more general functions. The class of the pseudodifferential operators with symbols in S^m is denoted usually by Ψ^m. The operator P is called a ΨDO if it belongs to Ψ^m for some m. By definition, $S^{-\infty} = \cap_m S^m$, and $\Psi^{-\infty} = \cap_m \Psi^m$.

An important subclass is the set of the *classical symbols* that have an asymptotic expansion of the form

$$p(x,\xi) \sim \sum_{j=0}^{\infty} p_{m-j}(x,\xi), \tag{A-3}$$

where $m \in \mathbb{R}$, and p_{m-j} are smooth and positively homogeneous in ξ of order $m-j$ for $|\xi| > 1$, i.e., $p_{m-j}(x,\lambda\xi) = \lambda^{m-j} p_{m-j}(x,\xi)$ for $|\xi| > 1$, $\lambda > 1$; and the sign $\sim$ means that

$$p(x,\xi) - \sum_{j=0}^{N} p_{m-j}(x,\xi) \in S^{m-N-1} \quad \text{for all } N \geq 0. \tag{A-4}$$

Any ΨDO $p(x,D)$ is continuous from $C_0^\infty(\Omega)$ to $C^\infty(\Omega)$, and can be extended by duality as a continuous map from $\mathscr{E}'(\Omega)$ to $\mathscr{D}'(\Omega)$.

Principal symbol. The principal symbol of a ΨDO given by (A-2) is the equivalence class $S^m(\Omega)/S^{m-1}(\Omega)$, and any its representative is called a principal symbol as well. In case of classical ΨDOs, the convention is to choose the principal symbol to be the first term p_m, that in particular is positively homogeneous in ξ.

Smoothing operators. Those are operators than map continuously $\mathscr{E}'(\Omega)$ into $C^\infty(\Omega)$. They coincide with operators with smooth Schwartz kernels in $\Omega \times \Omega$. They can always be written as ΨDOs with symbols in $S^{-\infty}$, and vice versa — all operators in $\Psi^{-\infty}$ are smoothing. Smoothing operators are viewed in this calculus as negligible and ΨDOs are typically defined modulo smoothing operators, i.e., $A = B$ if and only if $A - B$ is smoothing. Smoothing operators are not "small".

The pseudolocal property. For any ΨDO P and any $f \in \mathscr{E}'(\Omega)$,

$$\operatorname{singsupp}(Pf) \subset \operatorname{singsupp} f. \tag{A-5}$$

In other words, a ΨDO cannot increase the singular support. This property is preserved if we replace singsupp by WF; see (A-11).

Symbols defined by an asymptotic expansion. In many applications, a symbol is defined by consecutively constructing symbols $p_j \in S^{m_j}$, $j = 0, 1, \ldots$, where $m_j \searrow -\infty$, and setting

$$p(x,\xi) \sim \sum_j p_j(x,\xi). \tag{A-6}$$

The series on the right may not converge but we can make it convergent by using our freedom to modify each p_j for ξ in expanding compact sets without changing the large ξ behavior of each term. This extends the Borel idea of constructing a smooth function with prescribed derivatives at a fixed point. The asymptotic (A-6) then is understood in a sense similar to (A-4). This shows that there exists a symbol $p \in S^{m_0}$ satisfying (A-6). That symbol is not unique but the difference of two such symbols is always in $S^{-\infty}$.

Amplitudes. A seemingly larger class of ΨDOs is defined by

$$Af = (2\pi)^{-n} \int e^{i(x-y)\cdot\xi} a(x, y, \xi) f(y)\, dy\, d\xi, \quad f \in C_0^\infty(\Omega), \tag{A-7}$$

where the amplitude a satisfies

$$|\partial_\xi^\alpha \partial_x^\beta \partial_y^\gamma a(x, y, \xi)| \le C_{K,\alpha,\beta,\gamma}(1+|\xi|)^{m-|\alpha|} \quad \text{for all } (x, y, \xi) \in K \times \mathbb{R}^n \tag{A-8}$$

for any compact $K \subset \Omega \times \Omega$, and any α, β, γ. In fact, any such ΨDO A is a ΨDO with a symbol $p(x, \xi)$ (independent of y) with the formal asymptotic expansion

$$p(x, \xi) \sim \sum_{\alpha \ge 0} D_\xi^\alpha \partial_y^\alpha a(x, x, \xi).$$

In particular, the principal symbol of that operator can be taken to be $a(x, x, \xi)$.

Transpose and adjoint operators to a ΨDO. The mapping properties of any ΨDO A indicate that it has a well defined transpose A', and a complex adjoint A^* with the same mapping properties. They satisfy

$$\langle Au, v\rangle = \langle u, A'v\rangle, \quad \langle Au, \bar{v}\rangle = \langle u, \overline{A^*v}\rangle \quad \text{for all } u, v \in C_0^\infty$$

where $\langle \cdot, \cdot \rangle$ is the pairing in distribution sense; and in this particular case just an integral of uv. In particular, $A^*u = \overline{A'\bar{u}}$, and if A maps L^2 to L^2 in a bounded way, then A^* is the adjoint of A in L^2 sense.

The transpose and the adjoint are ΨDOs in the same class with amplitudes $a(y, x, -\xi)$ and $\bar{a}(y, x, \xi)$, respectively; and symbols

$$\sum_{\alpha \ge 0} (-1)^{|\alpha|} \frac{1}{\alpha!} (\partial_\xi^\alpha D_x^\alpha p)(x, -\xi), \quad \sum_{\alpha \ge 0} \frac{1}{\alpha!} \partial_\xi^\alpha D_x^\alpha \bar{p}(x, \xi),$$

if $a(x, y, \xi)$ and $p(x, \xi)$ are the amplitude and/or the symbol of that ΨDO. In particular, the principal symbols are $p_0(x, -\xi)$ and $\bar{p}_0(x, \xi)$, respectively, where p_0 is (any representative of) the principal symbol.

Composition of ΨDO*s and* ΨDO*s with properly supported kernels.* Given two ΨDOs A and B, their composition may not be defined even if they are smoothing ones because each one maps C_0^∞ to C^∞ but may not preserve the compactness

of the support. For example, if $A(x, y)$, and $B(x, y)$ are their Schwartz kernels, the candidate for the kernel of AB given by $\int A(x, z)B(z, y)$ may be a divergent integral. On the other hand, for any ΨDO A, one can find a smoothing correction R such that $A + R$ has properly supported kernel, i.e., the kernel of $A + R$, has a compact intersection with $K \times \Omega$ and $\Omega \times K$ for any compact $K \subset \Omega$. The proof of this uses the fact that the Schwartz kernel of a ΨDO is smooth away from the diagonal $\{x = y\}$ and one can always cut there in a smooth way to make the kernel properly supported at the price of a smoothing error. ΨDOs with properly supported kernels preserve $C_0^\infty(\Omega)$, and also $\mathscr{E}'(\Omega)$, and therefore can be composed in either of those spaces. Moreover, they map $C^\infty(\Omega)$ to itself, and can be extended from $\mathscr{D}'(\Omega)$ to itself. The property of the kernel to be properly supported is often assumed, and it is justified by considering each ΨDO as an equivalence class.

If $A \in \Psi^m(\Omega)$ and $B \in \Psi^k(\Omega)$ are properly supported ΨDOs with symbols a and b, respectively, then AB is again a ΨDO in $\Psi^{m+k}(\Omega)$ and its symbol is given by

$$\sum_{\alpha \geq 0} (-1)^{|\alpha|} \frac{1}{\alpha!} \partial_\xi^\alpha a(x, \xi) D_x^\alpha b(x, \xi).$$

In particular, the principal symbol can be taken to be ab.

Change of variables and ΨDO*s on manifolds.* Let Ω' be another domain, and let $\phi : \Omega \to \tilde{\Omega}$ be a diffeomorphism. For any $P \in \Psi^m(\Omega)$, $\tilde{P} f := (P(f \circ \phi)) \circ \phi^{-1}$ maps $C_0^\infty(\tilde{\Omega})$ into $C^\infty(\tilde{\Omega})$. It is a ΨDO in $\Psi^m(\tilde{\Omega})$ with principal symbol

$$p(\phi^{-1}(y), (\mathrm{d}\phi)'\eta) \tag{A-9}$$

where p is the symbol of P, $\mathrm{d}\phi$ is the Jacobi matrix $\{\partial\phi_i/\partial x_j\}$ evaluated at $x = \phi^{-1}(y)$, and $(\mathrm{d}\phi)'$ stands for the transpose of that matrix. We can also write $(\mathrm{d}\phi)' = ((\mathrm{d}\phi^{-1})^{-1})'$. An asymptotic expansion for the whole symbol can be written down as well.

Relation (A-9) shows that the transformation law under coordinate changes is that of a covector. Therefore, the principal symbol is a correctly defined function on the cotangent bundle $T^*\Omega$. The full symbol is not invariantly defined there in general.

Let M be a smooth manifold, and $A : C_0^\infty(M) \to C^\infty(M)$ be a linear operator. We say that $A \in \Psi^m(M)$, if its kernel is smooth away from the diagonal in $M \times M$, and if in any coordinate chart (A, χ), where $\chi : U \to \Omega \subset \mathbb{R}^n$, we have $(A(u \circ \chi)) \circ \chi^{-1} \in \Psi^m(\Omega)$. As before, the principal symbol of A, defined in any local chart, is an invariantly defined function on T^*M.

Mapping properties in Sobolev spaces. In $\mathbb{R}^n$, Sobolev spaces $H^s(\mathbb{R}^n)$, $s \in \mathbb{R}$, are defined as the completion of $\mathcal{S}'(\mathbb{R}^n)$ in the norm

$$\|f\|^2_{H^s(\mathbb{R}^n)} = \int (1+|\xi|^2)^s |\hat{f}(\xi)|^2 \, d\xi.$$

When s is a nonnegative integer, an equivalent norm is the square root of $\sum_{|\alpha|\le s} \int |\partial^\alpha f(x)|^2 \, dx$. For such s, and a bounded domain Ω, one defines $H^s(\Omega)$ as the completion of $C^\infty(\overline{\Omega})$ using the latter norm with the integral taken in Ω. Sobolev spaces in Ω for other real values of s are defined by different means, including duality or complex interpolation.

Sobolev spaces are also Hilbert spaces.

Any $P \in \Psi^m(\Omega)$ is a continuous map from $H^s_{\text{comp}}(\Omega)$ to $H^{s-m}_{\text{loc}}(\Omega)$. If the symbols estimates (A-1) are satisfied in the whole $\mathbb{R}^n \times \mathbb{R}^n$, then $P : H^s(\mathbb{R}^n) \to H^{s-m}(\mathbb{R}^n)$.

Elliptic ΨDO*s and their parametrices.* The operator $P \in \Psi^m(\Omega)$ with symbol p is called elliptic of order m, if for any compact $K \subset \Omega$, there exist constants $C > 0$ and $R > 0$ such that

$$C|\xi|^m \le |p(x,\xi)| \quad \text{for } x \in K, \text{ and } |\xi| > R. \tag{A-10}$$

Then the symbol p is called also elliptic of order m. It is enough to require the principal symbol only to be elliptic (of order m). For classical ΨDOs, as in (A-3), the requirement can be written as $p_m(x,\xi) \neq 0$ for $\xi \neq 0$. A fundamental property of elliptic operators is that they have parametrices. In other words, given an elliptic ΨDO P of order m, there exists $Q \in \Psi^{-m}(\Omega)$ such that

$$QP - \mathrm{Id} \in \Psi^{-\infty}, \quad PQ - \mathrm{Id} \in \Psi^{-\infty}.$$

The proof of this is to construct a left parametrix first by choosing a symbol $q_0 = 1/p$, cut off near the possible zeros of p, that form a compact any time when x is restricted to a compact as well. The corresponding ΨDO Q_0 will then satisfy $Q_0 P = \mathrm{Id} + R$, $R \in \Psi^{-1}$. Then we take a ΨDO E with asymptotic expansion $E \sim \mathrm{Id} - R + R^2 - R^3 + \cdots$, that would be the formal Neumann series expansion of $(\mathrm{Id}+R)^{-1}$, if the latter existed. Then EQ_0 is a left parametrix that is also a right parametrix.

An important consequence is the following elliptic regularity statement. If P is elliptic (and properly supported), then

$$\mathrm{singsupp}(PF) = \mathrm{singsupp}(f) \quad \text{for all } f \in \mathcal{D}'(\Omega).$$

In particular, $Pf \in C^\infty$ implies $f \in C^\infty$.

ΨDO*s and wave front sets.* The microlocal version of the pseudolocal property is given by the following:

$$\mathrm{WF}(Pf) \subset \mathrm{WF}(f) \tag{A-11}$$

for any (properly supported) ΨDO P and $f \in \mathscr{D}'(\Omega)$. In other words, a ΨDO cannot increase the wave front set. If P is elliptic for some m, it follows from the existence of a parametrix that there is equality above, i.e., $\mathrm{WF}(Pf) = \mathrm{WF}(f)$.

We say that the ΨDO P is of order $-\infty$ in the open conic set $U \subset T^*\Omega \setminus 0$, if for any closed conic set $K \subset U$ with a compact projection on the base "x-space", (A-1) is fulfilled for any m. The *essential support* $\mathrm{ES}(P)$, sometimes also called the *microsupport* of P, is defined as the smallest closed conic set on the complement of which the symbol p is of order $-\infty$. Then

$$\mathrm{WF}(Pf) \subset \mathrm{WF}(f) \cap \mathrm{ES}(P).$$

Let P have a homogeneous principal symbol p_m. The characteristic set Char P is defined by

$$\mathrm{Char}\, P = \{(x,\xi) \in T^*\Omega \setminus 0;\ p_m(x,\xi) = 0\}.$$

Char P can be defined also for general ΨDOs that may not have homogeneous principal symbols. For any ΨDO P, we have

$$\mathrm{WF}(f) \subset \mathrm{WF}(Pf) \cup \mathrm{Char}\, P \quad \text{for all } f \in \mathscr{E}'(\Omega). \tag{A-12}$$

P is called *microlocally elliptic* in the open conic set U, if (A-10) is satisfied in all compact subsets, similarly to the definition of $\mathrm{ES}(P)$ above. If it has a homogeneous principal symbol p_m, ellipticity is equivalent to $p_m \neq 0$ in U. If P is elliptic in U, then Pf and f have the same wave front set restricted to U, as follows from (A-12) and (A-11).

A.3. ***The Hamilton flow and propagation of singularities.*** Let $P \in \Psi^m(M)$ be properly supported, where M is a smooth manifold, and suppose that P has a real homogeneous principal symbol p_m. The Hamiltonian vector field of p_m on $T^*M \setminus 0$ is defined by

$$H_{p_m} = \sum_{j=1}^{n} \left(\frac{\partial p_m}{\partial x_j} \frac{\partial}{\partial \xi_j} - \frac{\partial p_m}{\partial \xi_j} \frac{\partial}{\partial x_j} \right).$$

The integral curves of H_{p_m} are called *bicharacteristics* of P. Clearly, $H_{p_m} p_m = 0$, thus p_m is constant along each bicharacteristics. The bicharacteristics along which $p_m = 0$ are called *zero bicharacteristics*.

The Hörmander's theorem about propagation of singularities is one of the fundamental results in the theory. It states that if P is an operator as above, and

$Pu = f$ with $u \in \mathscr{D}'(M)$, then

$$\mathrm{WF}(u) \setminus \mathrm{WF}(f) \subset \mathrm{Char}\, P,$$

and is invariant under the flow of H_{p_m}.

An important special case is the wave operator $P = \partial_t^2 - \Delta_g$, where Δ_g is the Laplace Beltrami operator associated with a Riemannian metric g. We may add lower order terms without changing the bicharacteristics. Let (τ, ξ) be the dual variables to (t, x). The principal symbol is $p_2 = -\tau^2 + |\xi|_g^2$, where $|\xi|_g^2 := \sum g^{ij}(x)\xi_i\xi_j$, and $(g^{ij}) = (g_{ij})^{-1}$. The bicharacteristics equations then are $\dot{\tau} = 0$, $\dot{t} = -2\tau$, $\dot{x}^j = 2\sum g^{ij}\xi_i$, $\dot{\xi}_j = -2\partial_{x^j}\sum g^{ij}(x)\xi_i\xi_j$, and they are null one if $\tau^2 = |\xi|_g^2$. Here, $\dot{x} = \mathrm{d}x/\mathrm{d}s$, etc. The latter two equations are the Hamiltonian curves of $\tilde{H} := \sum g^{ij}(x)\xi_i\xi_j$ and they are known to coincide with the geodesics $(\gamma, \dot{\gamma})$ on TM when identifying vectors and covectors by the metric. They lie on the energy surface $\tilde{H} = \text{const}$. The first two equations imply that τ is a constant, positive or negative, and up to rescaling, one can choose the parameter along the geodesics to be t. That rescaling forces the speed along the geodesic to be 1. The null condition $\tau^2 = |\xi|_g^2$ defines two smooth surfaces away from $(\tau, \xi) = (0, 0)$: $\tau = \pm|\xi|_g$. This corresponds to geodesics starting from x in direction either ξ or $-\xi$. To summarize, for the homogeneous equation $Pu = 0$, we get that each singularity (x, ξ) of the initial conditions at $t = 0$ starts to propagate from x in direction either ξ or $-\xi$ or both (depending on the initial conditions) along the unit speed geodesic. In fact, we get this first for the singularities in $T^*(\mathbb{R}_t \times \mathbb{R}_x^n)$ first, but since they lie in Char P, one can see that they project to $T^*\mathbb{R}_x^n$ as singularities again.

A.4. ***Geometric optics.*** Geometric optics describes asymptotically the solutions of hyperbolic equations at large frequencies. It also provides a parametrix (a solution up to smooth terms) of the initial value problem for hyperbolic equations. The resulting operators are not ΨDOs anymore; they are actually examples of Fourier integral operators. Geometric optics also studies the large frequency behavior of solutions that reflect from a smooth surface (obstacle scattering) including diffraction; reflect from an edge or a corner; reflect and refract from a surface where the speed jumps (transmission problems).

As an example, consider the acoustic equation

$$(\partial_t^2 - c^2(x)\Delta)u = 0, \quad (t, x) \in \mathbb{R}^n, \tag{A-13}$$

with initial conditions $u(0, x) = f_1(x)$, $u_t(0, x) = f_2$. It is enough to assume first that f_1 and f_2 are in C_0^∞, and extend the resulting solution operator to larger spaces later.

We are looking for a solution of the form

$$u(t,x) = (2\pi)^{-n} \times \sum_{\sigma=\pm} \int e^{i\phi_\sigma(t,x,\xi)} \big(a_{1,\sigma}(x,\xi,t)\hat{f}_1(\xi) + |\xi|^{-1} a_{2,\sigma}(x,\xi,t)\hat{f}_2(\xi)\big) d\xi, \quad \text{(A-14)}$$

modulo terms involving smoothing operators of f_1 and f_2. The reason to expect two terms is already clear by the propagation of singularities theorem, and is also justified by the eikonal equation below. Here the phase functions $\phi_\pm$ are positively homogeneous of order 1 in ξ. Next, we seek the amplitudes in the form

$$a_{j,\sigma} \sim \sum_{k=0}^{\infty} a_{j,\sigma}^{(k)}, \quad \sigma = \pm,\ j = 1,2, \quad \text{(A-15)}$$

where $a_{j,\sigma}^{(k)}$ is homogeneous in ξ of degree $-k$ for large $|\xi|$. To construct such a solution, we plug (A-14) into (A-13) and try to kill all terms in the expansion in homogeneous (in ξ) terms.

Equating the terms of order 2 yields the *eikonal equation*

$$(\partial_t \phi)^2 - c^2(x)|\nabla_x \phi|^2 = 0. \quad \text{(A-16)}$$

Write $f_j = (2\pi)^{-n} \int e^{ix\cdot\xi} \hat{f}_j(\xi)\, d\xi$, $j = 1,2$, to get the following initial conditions for $\phi_\pm$

$$\phi_\pm|_{t=0} = x \cdot \xi. \quad \text{(A-17)}$$

The eikonal equation can be solved by the method of characteristics. First, we determine $\partial_t \phi$ and $\nabla_x \phi$ for $t = 0$. We get $\partial_t \phi|_{t=0} = \mp c(x)|\xi|$, $\nabla_x \phi|_{t=0} = \xi$. This implies existence of two solutions $\phi_\pm$. If $c = 1$, we easily get $\phi_\pm = \mp|\xi|t + x\cdot\xi$. Let for any (z,ξ), $\gamma_{z,\xi}(s)$ be unit speed geodesic through (z,ξ). Then ϕ_+ is constant along the curve $(t, \gamma_{z,\xi}(t))$ that implies that $\phi_+ = z(x,\xi)\cdot\xi$ in any domain in which (t,z) can be chosen to be coordinates. Similarly, ϕ_- is constant along the curve $(t, \gamma_{z,-\xi}(t))$. In general, we cannot solve the eikonal equation globally, for all (t,x). Two geodesics $\gamma_{z,\xi}$ and $\gamma_{w,\xi}$ may intersect, for example, giving a value for $\phi_\pm$ that is not unique. However, we always have a solution in a neighborhood of $t = 0$.

Now equate the first-order terms in the expansion of $(\partial_t^2 - c^2\Delta)u$ to get that the principal terms of the amplitudes must solve the *transport equation*

$$\big((\partial_t \phi_\pm)\partial_t - c^{A2}\nabla_x \phi_\pm \cdot \nabla_x + C_\pm\big) a_{j,\pm}^{(0)} = 0, \quad \text{(A-18)}$$

with

$$2C_\pm = (\partial_t^2 - c^2\Delta)\phi_\pm.$$

This is an ODE along the vector field $(\partial_t\phi_\pm, c^2\nabla_x\phi)$, and the integral curves of it coincide with the curves $(t, \gamma_{z,\pm\xi})$. Given an initial condition at $t = 0$, it has a unique solution along the integral curves as long as ϕ is well defined.

Equating terms homogeneous in ξ of lower order we get transport equations for $a^{(k)}_{j,\sigma}$, $j = 1, 2, \dots$ with the same left-hand side as in (A-18) with a right-hand side determined by $a^{(k-1)}_{k,\sigma}$.

Taking into account the initial conditions, we get

$$a_{1,+} + a_{1,-} = 1, \quad a_{2,+} + a_{2,-} = 0 \qquad \text{for } t = 0.$$

This is true in particular for the leading terms $a^{(0)}_{1,\pm}$ and $a^{(0)}_{2,\pm}$. Since $\partial_t\phi_\pm = \mp c(x)|\xi|$ for $t = 0$, and $u_t = f_2$ for $t = 0$, from the leading order term in the expansion of u_t we get

$$a^{(0)}_{1,+} = a^{(0)}_{1,-}, \quad \mathrm{i}c(x)(a^{(0)}_{2,-} - a^{(0)}_{2,+}) = 1 \qquad \text{for } t = 0.$$

Therefore,

$$a^{(0)}_{1,+} = a^{(0)}_{1,-} = \frac{1}{2}, \quad a^{(0)}_{2,+} = -a^{(0)}_{2,-} = \frac{\mathrm{i}}{2c(x)} \qquad \text{for } t = 0. \tag{A-19}$$

Note that if $c = 1$, then $\phi_\pm = x \cdot \xi \mp t|\xi|$, and $a_{1,+} = a_{1,-} = 1/2$, $a_{2,+} = -a_{2,-} = \mathrm{i}/2$. Using those initial conditions, we solve the transport equations for $a^{(0)}_{1,\pm}$ and $a^{(0)}_{2,\pm}$. Similarly, we derive initial conditions for the lower order terms in (A-15) and solve the corresponding transport equations. Then we define $a_{j,\sigma}$ by (A-15) as a symbol.

The so constructed u in (A-14) is a solution only up to smoothing operators applied to (f_1, f_2). Using standard hyperbolic estimates, we show that adding such terms to u, we get an exact solution to (A-13). As mentions above, this construction may fail for t too large, depending on the speed. On the other hand, the solution operator $(f_1, f_2) \mapsto u$ makes sense as a global Fourier integral operator for which this construction is just one if its local representations.

Projections to the positive and the negative wave speeds. The zeros of the principal symbol of the wave operator, in regions where c is smooth, are given by $\tau = \pm c(x)|\xi|$, that we call wave speeds. We constructed above parametrices $u_\pm$ for the corresponding solutions. We will present here a functional analysis point of view that allows us to project the initial data $\boldsymbol{f}$ to data $\boldsymbol{\Pi}_\pm \boldsymbol{f}$ such that, up to smoothing operators, $u_\pm$ corresponds to initial data $\boldsymbol{\Pi}_\pm \boldsymbol{f}$.

Assume that $c(x)$ is extended from the maximal connected component of $\mathbb{R}^n \setminus \Gamma$ containing x_0 to the whole $\mathbb{R}^n$ in a smooth way so that $0 < 1/C \le c(x) \le C$. Let

$$Q = (-c^2\Delta)^{1/2}, \tag{A-20}$$

where the operator in the parentheses is the natural self-adjoint extension of $-c^2\Delta$ to $L^2(\mathbb{R}^n, c^{-2}\mathrm{d}x)$, and the square root exists by the functional calculus. Moreover, Q is an elliptic ΨDO of order 1 in any open set; and let Q^{-1} denote a fixed parametrix.

It is well known that the solution to (9-3) can be written as

$$u = \cos(tQ)\, f_1 + \frac{\sin(tQ)}{Q} f_2, \tag{A-21}$$

and the latter operator is defined by the functional calculus as $\phi(t, Q)$ with $\phi(t, \cdot) = \sin(t\,\cdot)/\cdot \in C^\infty$. Based on that, we can write

$$e^{t\boldsymbol{P}} = e^{\mathrm{i}t\boldsymbol{Q}}\boldsymbol{\Pi}_+ + e^{-\mathrm{i}t\boldsymbol{Q}}\boldsymbol{\Pi}_-, \tag{A-22}$$

where

$$\boldsymbol{\Pi}_+ = \frac{1}{2}\begin{pmatrix} 1 & -\mathrm{i}Q^{-1} \\ \mathrm{i}Q & 1 \end{pmatrix}, \quad \boldsymbol{\Pi}_- = \frac{1}{2}\begin{pmatrix} 1 & \mathrm{i}Q^{-1} \\ -\mathrm{i}Q & 1 \end{pmatrix}. \tag{A-23}$$

It is straightforward to see that $\boldsymbol{\Pi}\pm$ are orthogonal projections in $\mathscr{H}$, up to errors of smoothing type. Then given $\boldsymbol{f} \in \mathscr{H}$ supported on Ω, one has $\boldsymbol{u}_\pm = e^{t\boldsymbol{P}}\boldsymbol{f}_\pm$, with $\boldsymbol{f}_\pm := \boldsymbol{\Pi}_\pm \boldsymbol{f}$.

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