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OPTIMAL CONSTANTS IN NONTRAPPING RESOLVENT ESTIMATES AND APPLICATIONS IN NUMERICAL ANALYSIS

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We study the resolvent for nontrapping obstacles on manifolds with Euclidean ends. It is well known that for such manifolds the outgoing resolvent satisfies $\|\chi R(k)\chi\|_{L^2 \to L^2} \leq Ck^{-1}$ for $k > 1$, but the constant C has been little studied. We show that, for high frequencies, the constant is bounded above by $\frac{2}{\pi}$ times the length of the longest generalized bicharacteristic of $|\xi|_g^2 - 1$ remaining in the support of χ. We show that this estimate is optimal in the case of manifolds without boundary. We then explore the implications of this result for the numerical analysis of the Helmholtz equation.

1. Introduction

Let (M, g) be a manifold with Euclidean ends and $\Omega \Subset M$ an obstacle with smooth boundary. Assume that all Melrose–Sjöstrand generalized bicharacteristics (i.e., geodesics) escape to infinity. Let $\Delta_{\Omega, g}$ be the Dirichlet realization of the Laplacian on $M \setminus \Omega$. It is well known that for any $\chi \in \mathcal{C}_c^\infty(M)$, there exists a constant $C > 0$ and $k_0 > 0$ so that

$$\|\chi(-\Delta_{\Omega, g} - k^2 - i0)^{-1}\chi\|_{L^2(M\setminus\Omega) \to L^2(M\setminus\Omega)} \leq C|k|^{-1}, \quad k > k_0.$$

In this paper we study how the constant $C > 0$ depends on the classical dynamics on $((M, g), \Omega)$.

Suppose that there are no geodesics tangent to $\partial\Omega$ to infinite order and let $\varphi_t : S^*M \to S^*M$ denote the Melrose–Sjöstrand generalized bicharacteristic flow [Hörmander 1994, Section 24.3]. Next, fix $R_1 > 0$ so that $\Omega \subset B(0, R_1)$ and (M, g) is Euclidean outside $B(0, R_1)$. Then define, for any $R \geq R_1$,

$$L(g, \Omega, R) := \inf\{t > 0 : \varphi_t(S^*_{B(0, R)}M) \cap S^*_{B(0, R)}M = \varnothing\}. \tag{1-1}$$

(We will omit the Ω from the notation when $\Omega = \varnothing$.)

In the statement of the following estimates, we will use a family of Sobolev spaces with appropriate semiclassical scaling, using the global definition, for $s \in \mathbb{R}$,

$$\|u\|_{H^s(M\setminus\Omega)}^2 = \langle(-\Delta_{\Omega, g} + k^2)^s u, u\rangle. \tag{1-2}$$

Theorem 1. *Let (M, g) be a manifold with Euclidean ends with $g \in \mathcal{C}^{1,1}$. Suppose that $\Omega \Subset M$ has smooth boundary, g is $\mathcal{C}^\infty$ near Ω, and Ω is nowhere tangent to the geodesic flow to infinite order. Assume the*

generalized geodesic flow on $M\setminus\Omega$ is nontrapping. Then for every $R > R_1$, $\chi \in \mathcal{C}_c^\infty(B(0, R); [0, 1])$ there exists $k_0 > 0$ so that, for $k > k_0$,

$$\|\chi(-\Delta_{\Omega,g} - k^2 - i0)^{-1}\chi\|_{L^2(M\setminus\Omega)\to L^2(M\setminus\Omega)} \le \frac{2L(g, \Omega, R)}{\pi k}. \tag{1-3}$$

More generally, for $0 \le s \le 2$,

$$\|\chi(-\Delta_{\Omega,g} - k^2 - i0)^{-1}\chi\|_{L^2(M\setminus\Omega)\to H^s(M\setminus\Omega)} \le \frac{2^{s/2+1}L(g, \Omega, R)}{\pi}k^{s-1}. \tag{1-4}$$

The constant k_0 may be chosen uniformly as g varies within a sufficiently small open neighborhood in $\mathcal{C}^{2,\alpha}$ ($\alpha > 0$) of a given nontrapping metric in $\mathcal{C}^{2,\alpha}$ (where all metrics are taken smooth near $\partial\Omega$).

Conversely, when $\Omega = \varnothing$ and $g \in \mathcal{C}^\infty$, for every $R' > R_1$ with $B(0, R') \subset \{\chi \equiv 1\}$, there is $k_0 > 0$ so that, for $k > k_0$,

$$\|\chi(-\Delta_g - k^2 - i0)^{-1}\chi\|_{L^2(M\setminus\Omega)\to L^2(M\setminus\Omega)} \ge \frac{2L(g, R')}{\pi k}. \tag{1-5}$$

Notice that in the interior of $M \setminus \Omega$, the Melrose–Sjöstrand flow is equal to the geodesic flow except that, on the unit cotangent bundle, the speed of the flow is 2 rather than 1. Thus, in the case where $\Omega = \varnothing$, the theorem states that the growth of the resolvent as a map on L^2 as $k \to \infty$ is controlled above and below by $\frac{1}{\pi}$ times the length of the longest geodesic contained entirely in $B(0, R_1)$.

1A. *More general operators.* In [Section 6B](#) below, we recall that several important physical applications of the Helmholtz equation involve an operator that differs slightly from $-\Delta_{\Omega,g}$, namely the divergence form operator $-\sum \partial_i g^{ij}\partial_j$, which is self-adjoint with respect to the Euclidean volume form on $\mathbb{R}^n$. In order to deal with this and similar operators, we will prove a slightly more general result.

Theorem 2. *Let (M, g) be a manifold with Euclidean ends, $g \in \mathcal{C}^{1,1}$. Suppose that $\Omega \subset M$ has smooth boundary, g is $\mathcal{C}^\infty$ in a neighborhood of Ω, and Ω is nowhere tangent to the geodesic flow to infinite order. Assume the generalized geodesic flow on $M\setminus\Omega$ is nontrapping. Suppose that $P(g) \in \mathrm{Diff}^2(M)$ so that*

$$P(g) + \Delta_g = \sum_j L_j\partial_{x_j} + L, \tag{1-6}$$

where $L_j, L \in \mathcal{C}_c^{0,\alpha}(B(0, R_1))$ for some $\alpha > 0$. Suppose further that ν is a density on M so that $P_\Omega(g)$ is self-adjoint with respect to $L^2(M \setminus \Omega; \nu)$, where $P_\Omega(g)$ is the Dirichlet realization of $P(g)$. Let

$$\|u\|_{H_\nu^s(M\setminus\Omega)}^2 := \langle(P_\Omega(g) + k^2)^s u, u\rangle_{L^2(M\setminus\Omega;\nu)}. \tag{1-7}$$

Then for every $R > R_1$, $\chi \in \mathcal{C}_c^\infty(B(0, R); [0, 1])$, there exists $k_0 > 0$ so that, for $k > k_0$ and $0 \le s \le 2$,

$$\|\chi(P_\Omega(g) - k^2 - i0)^{-1}\chi\|_{L_\nu^2(M\setminus\Omega)\to H_\nu^s(M\setminus\Omega)} \le \frac{2^{s/2+1}L(g, \Omega, R)}{\pi}k^{s-1}. \tag{1-8}$$

The constant k_0 may be chosen uniformly as g varies within sufficiently small open neighborhoods of in $\mathcal{C}^{2,\alpha}$ ($\alpha > 0$) of a given nontrapping metric in $\mathcal{C}^{2,\alpha}$ and L_j, L vary in small neighborhoods in $\mathcal{C}^{0,\alpha}$ (where all g, L_j, L are taken smooth near $\partial\Omega$ and the subset is assumed to be contained in a small open neighborhood in $\mathcal{C}^N$ for some sufficiently large N near $\partial\Omega$).

1B. *Motivation from, and applications to, numerical analysis.* In the last few years, there has been growing interest from the numerical-analysis community in proving bounds on solutions of the Helmholtz equation where the constants are explicit in the metric (i.e., the coefficients); see [Brown et al. 2017; Chaumont-Frelet 2016; Barucq et al. 2017; Ohlberger and Verfürth 2018; Sauter and Torres 2018; Moiola and Spence 2019; Graham et al. 2019; Graham and Sauter 2020]. Almost all of these previously obtained bounds used variants of the Morawetz commutator $x \cdot \nabla$, and thus are restricted to star-shaped domains and certain classes of coefficients (although this class includes discontinuous coefficients; see, e.g., [Graham et al. 2019]); the exception are the one-dimensional bounds in [Sauter and Torres 2018], which use the fact that the solution of the Helmholtz equation with piecewise-constant coefficients in one dimension can be expressed in terms of the solution of a linear system of algebraic equations.

This interest from the numerical-analysis community is because the analysis of *any* numerical method for solving the Helmholtz equation with variable coefficients requires a resolvent estimate, and if the constant in the resolvent estimate is not given explicitly in terms of the coefficients, then the numerical analysis will not be explicit in the coefficients. For example, having proved a bound explicit in the coefficients, [Chaumont-Frelet 2016; Graham and Sauter 2020] were then concerned with analyzing standard finite-element methods applied to Helmholtz problems with variable coefficients, and [Brown et al. 2017; Chaumont-Frelet 2016; Barucq et al. 2017; Ohlberger and Verfürth 2018] were concerned with designing and analyzing methods tailored to the coefficients.

The resolvent estimate (1-8) will therefore be a fundamental ingredient in the numerical analysis of variable-coefficient Helmholtz problems in nontrapping scenarios. In Section 6 we illustrate this fact by proving an error estimate for the finite-element method applied to the variable-coefficient Helmholtz equation posed in the exterior of a nontrapping Dirichlet obstacle, with this estimate explicit in k, the coefficients, and the parameters of the discretization; see Theorem 3 below. The key point is that Theorem 3 shows how the condition on the discretization for the error estimate to hold depends on the length of the longest ray, showing that this condition becomes more restrictive as the length of the longest ray grows.

In Section 6 we also briefly outline the implications of the estimate (1-8) for (i) preconditioning finite-element discretizations of the Helmholtz equation (see Remark 6.8), and (ii) "uncertainty quantification" of the Helmholtz equation (see Remark 6.9).

2. Manifolds with Euclidean ends

We now define the notion of a manifold with Euclidean ends. Note that the canonical example of a manifold with Euclidean ends is the space $\mathbb{R}^n$ with a metric g so that $I - g$ has compact support. In order to allow more general topologies, we define the general notion of a manifold with Euclidean ends.

Definition 2.1. (M, g) is an n-dimensional *manifold with Euclidean ends* if it is a noncompact, complete Riemannian manifold such that

- there exists a function $r \in \mathcal{C}^\infty(M; \mathbb{R})$ such that the sets $\{r \le c\}$ are compact for all c, and

- there exists $R_1 > 0$ such that $\{r \geq R_1\}$ is the disjoint union of finitely many components, each of which is isometric to $\mathbb{R}^n \setminus B(0, R_1)$ with the Euclidean metric, and the pullback of r under the isometry is the Euclidean norm.

The connected components of $\{r \geq R_1\}$ are called the *infinite ends* of M. The notation $B(0, R)$ is defined for $R \geq R_1$ and has the following meaning:

$$B(0, R) := \{r < R\}.$$

2A. *The outgoing resolvent on manifolds with Euclidean ends.* We now review (following the treatment in [Dyatlov and Zworski 2019, Section 4.2]) some properties of the outgoing resolvent on a manifold with Euclidean ends. Let E_i, $i = 1, \ldots, m$, be the infinite ends of M, and let $R_0(k)$ denote the free resolvent on $\mathbb{R}^n$. That is, $R_0(k) : L^2_{\mathrm{comp}}(\mathbb{R}^n) \to L^2_{\mathrm{loc}}(\mathbb{R}^n)$ is the meromorphic continuation of $(-\Delta - k^2)^{-1}$ from the half plane $\mathrm{Im}\, k > 0$. Define $\widetilde{R}_0(k) : L^2_{\mathrm{comp}}(M) \to L^2_{\mathrm{loc}}(M)$ by

$$\widetilde{R}_0(k)f := \sum_{i=1}^{m} 1_{E_i} R_0(k) 1_{E_i} f. \tag{2-1}$$

Next, let $\chi_i \in \mathcal{C}^\infty_c(M; [0, 1])$, $i = 0, \ldots, 3$, so that

$$\chi_i \equiv 1 \text{ on } \mathrm{supp}\, \chi_{i-1}, \quad \mathrm{supp}(1 - \chi_i) \subset M \setminus \overline{B(0, R_1)}, \quad \mathrm{supp}\, \chi_i \subset B(0, R) \tag{2-2}$$

for some $R > R_1$. Then for $k_0 \in \mathbb{C}$ with $\mathrm{Im}\, k_0 \gg 1$, let

$$Q(k, k_0) := Q_0(k) + Q_1(k_0),$$
$$Q_0(k) := (1 - \chi_0)\widetilde{R}_0(k)(1 - \chi_1), \quad Q_1(k) := \chi_2(-\Delta_g - k_0^2)^{-1}\chi_1.$$

Following the proof in [Dyatlov and Zworski 2019, Section 4.2], we can write

$$R(k) := (P_\Omega(g) - k^2)^{-1} = Q(k, k_0)(I + K(k, k_0)\chi_3)^{-1}(I - K(k, k_0)(1 - \chi_3)), \tag{2-3}$$

where $K(k, k_0) : L^2(M) \to L^2_{\mathrm{comp}}(M)$ and in particular, $(1 - \chi_3)K(k, k_0) = 0$. This implies $(1 - \chi_3)R(k)$ lies in the image of $\widetilde{R}_0(k)$.

3. The case of a manifold without boundary

To illustrate the methods we begin by proving (1-3) in the case of a manifold without boundary. The idea of the proof is identical when the boundary is nonempty, but the proofs of propagation statements are more involved. Thus we take $\partial M = \varnothing$ throughout this section.

3A. *Defect measures.* We will argue by contradiction. Let $h = k^{-1}$ and $P(h) := h^2 P_\Omega(g) - 1$. We also write L^2 for $L^2_\nu(M \setminus \Omega)$ and H^s for $H^s_\nu(M \setminus \Omega)$.

Remark 3.1. We will sometimes write $\|\cdot\|_{H^s_h}$ for $h^s\|\cdot\|_{H^s}$; since $\|\cdot\|_{H^s}$ has a semiclassical scaling built into it, this means that

$$\|u\|^2_{H^s_h} = \langle (h^2 \Delta_{\Omega,g} + 1)^s u, u \rangle.$$

Note that if χ_0, $\chi_1 \in C_c^\infty(M; [0, 1])$ and $\chi_1 \equiv 1$ on supp χ_0, then

$$\frac{\|\chi_0(P - i0)^{-1}\chi_0 f\|_{L^2}}{\|f\|_{L^2}} = \frac{\|\chi_0\chi_1(P - i0)^{-1}\chi_1\chi_0 f\|_{L^2}}{\|f\|_{L^2}} \leq \frac{\|\chi_0\chi_1(P - i0)^{-1}\chi_1\chi_0 f\|_{L^2}}{\|\chi_0 f\|_{L^2}}$$

$$\leq \frac{\|\chi_1(P - i0)^{-1}\chi_1\chi_0 f\|_{L^2}}{\|\chi_0 f\|_{L^2}} \leq \|\chi_1(P - i0)^{-1}\chi_1\|_{L^2 \to L^2}.$$

In particular,

$$\|\chi_0(P - i0)^{-1}\chi_0\|_{L^2 \to L^2} \leq \|\chi_1(P - i0)^{-1}\chi_1\|_{L^2 \to L^2},$$

and, since $R > R_1$, *we may assume without loss of generality that $\chi \equiv 1$ on $B(0, R_1)$.*

If (1-3) fails, there exists a sequence of discrete values of $h = h_j \downarrow 0$ and a sequence $0 \neq f(h) \in L^2$ such that

$$\|\chi(P - i0)^{-1}\chi h f(h)\|_{L^2} = 1$$

and

$$\lim_{h \to 0} \frac{\|\chi(P - i0)^{-1}\chi h f(h)\|_{L^2}}{\|f(h)\|_{L^2}} = M \geq 2L(g, R)$$

(note that we allow $M = \infty$). There exists $R' < R$ such that we still have supp $\chi \subset B(0, R')$; hence we have the strict inequality $M > L(g, R')$. Let

$$u(h) = (P - i0)^{-1}\chi h f \in L^2_{\text{loc}}$$

so that $\|\chi u\|_{L^2} = 1$.

Lemma 3.2. *For all $\tilde{\chi} \in C_c^\infty(M)$, there exists $C > 0$ so that $\|\tilde{\chi}u\|_{L^2} \leq C$.*

Proof. Let $\chi_i \in C_c^\infty(M; [0, 1])$, $i = 0, 1$, so that $\chi \equiv 1$ on supp χ_1, and $\chi_1 \equiv 1$ on supp χ_0, and $\chi_0 \equiv 1$ on $B(0, R_1)$. Then

$$(1 - \chi_0)P(1 - \chi_1) = \sum_i (1 - \chi_0)(-h^2\Delta_{\mathbb{R}^n} - 1)1_{E_i}(1 - \chi_1),$$

where E_i denotes the i-th Euclidean end of M.

Then,

$$P(1 - \chi_1)u = \sum_i (1 - \chi_0)1_{E_i}(-h^2\Delta_{\mathbb{R}^n} - 1)1_{E_i}(1 - \chi_1)u$$

$$= (1 - \chi_1)\chi h f - \sum_i (1 - \chi_0)[-h^2 1_{E_i}\Delta_{\mathbb{R}^n} 1_{E_i}, \chi_1]u$$

$$= (1 - \chi_1)\chi h f - \sum_i [-h^2 1_{E_i}\Delta_{\mathbb{R}^n} 1_{E_i}, \chi_1]u.$$

Next extend $u1_{E_i}$ by 0 to a function v_i on $\mathbb{R}^n$ so that $v_i \equiv u1_{E_i}$ on $\mathbb{R}^n \setminus B(0, R_1)$. Then

$$(-h^2\Delta_{\mathbb{R}^n} - 1)(1 - \chi_1)1_{E_i}v_i = 1_{E_i}(1 - \chi_1)\chi h f - [h^2\Delta_{\mathbb{R}^n}, 1_{E_i}\chi_1]v_i.$$

Since by (2-3) v_i is h^{-1} outgoing,

$$(1 - \chi_1)1_{E_i}v_i = h^{-2}R_0(h^{-1})(1_{E_i}(1 - \chi_1)\chi h f - [h^2\Delta_{\mathbb{R}^n}, 1_{E_i}\chi_1]v_i).$$

In particular, since $\chi \equiv 1$ on supp χ_1,

$$\|(1 - \chi_1)1_{E_i} v_i\|_{L^2} \le C(\|f\|_{L^2} + \|[\Delta_{\mathbb{R}^n}, 1_{E_i} \chi_1] v_i\|_{H^{-1}}) \le C(\|f\|_{L^2} + \|\chi u\|_{L^2}).$$

Now,

$$(1 - \chi_1)u = (1 - \chi_1) \sum_i 1_{E_i} v_i.$$

Therefore,

$$\|(1 - \chi_1)u\|_{L^2} \le C(\|f\|_{L^2} + \|\chi u\|_{L^2}).$$

Let $\tilde{\chi} \in C_c^\infty(M; [0, 1])$. Then using again that $\chi \equiv 1$ on supp χ_1,

$$\begin{aligned}
\limsup_{h \to 0} \|\tilde{\chi} u\|_{L^2} &\le \limsup_{h \to 0} (\|\tilde{\chi}(1 - \chi)u\|_{L^2} + \|\tilde{\chi}\chi u\|_{L^2}) \\
&\le \limsup_{h \to 0} (\|\tilde{\chi}(1 - \chi_1)u\|_{L^2} + \|\chi u\|_{L^2}) \\
&\le C \limsup_{h \to 0} (\|f\|_{L^2} + \|\chi u\|_{L^2}) \le C \left(\frac{1}{2L(g, R')} + 1 \right),
\end{aligned}$$

completing the proof of the lemma. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

By Lemma 3.2, u is uniformly bounded in L_{loc}^2 and, taking subsequences, we may assume that u has defect measure μ, χf has defect measure α, and u and χf have joint defect measure μ^j; in other words, for $h = h_j$ in this chosen subsequence, and for every $a \in C_c^\infty(T^*M)$,

$$\lim_{h \downarrow 0} \langle a(x, hD)u, u \rangle = \int a \, d\mu, \quad \lim_{h \downarrow 0} \langle a(x, hD)\chi f, \chi f \rangle = \int a \, d\alpha, \quad \lim_{h \downarrow 0} \langle a(x, hD)\chi f, u \rangle = \int a \, d\mu^j. \quad (3\text{-}1)$$

Note that we use a quantization procedure that sends symbols with compact support in x to operators with compactly supported kernel.

The Cauchy–Schwarz inequality gives us a simple inequality satisfied by these three measures. We use the notation

$$\mu(a) \equiv \int a \, d\mu$$

for the pairing of a function and a measure.

Lemma 3.3. *For any* $a \in C_c^0(T^*M; \mathbb{R})$,

$$|\mu^j(a)| \le \sqrt{\mu(|a|)} \sqrt{\alpha(|a|)}.$$

Proof. If $b = \sqrt{a}$ is in $C_c^\infty(T^*M)$,

$$\begin{aligned}
\langle a(x, hD)\chi f, u \rangle = \langle b^2(x, hD)\chi f, u \rangle &= \langle b(x, hD)\chi f, b(x, hD)u \rangle + O(h) \\
&\le \sqrt{\langle b(x, hD)\chi f, b(x, hD)\chi f \rangle} \sqrt{\langle b(x, hD)u, b(x, hD)u \rangle} + O(h) \\
&\le \left(\int b^2 \, d\alpha \right)^{1/2} \left(\int b^2 \, d\mu \right)^{1/2} + o(1),
\end{aligned}$$

which proves the desired inequality by letting $h \to 0$.

Next, let $a \in C_c^\infty(T^*M)$ with $a \geq 0$, $\psi_i \in C_c^\infty(T^*M; [0, 1])$, $i = 0, 1$, have $\psi_i \equiv 1$ in a neighborhood of supp a and $\psi_1 \equiv 1$ in a neighborhood of supp ψ_0. Then we apply the previous result to $a_\epsilon = \psi_0^2(a + \epsilon \psi_1)$ and let $\epsilon \downarrow 0$ to see that $|\mu^j(a)| \leq \sqrt{\mu(a)}\sqrt{\alpha(a)}$.

Now, letting $0 \leq a \in C_c^0(T^*M)$, we have $0 \leq a_n \in C_c^\infty(T^*M)$ with $a_n \to a$ uniformly. Then we have

$$\mu^j(a_n) \to \mu^j(a), \quad \mu(a_n) \to \mu(a), \quad \alpha(a_n) \to \alpha(a).$$

In particular,

$$|\mu^j(a)| \leq \sqrt{\mu(a)}\sqrt{\alpha(a)}, \quad 0 \leq a \in C_c^0(T^*M).$$

Next, for $a \in C_c^0(T^*M; \mathbb{R})$, write $a = a_+ - a_-$ with $0 \leq a_\pm \in C_c^0(T^*M)$. Then,

$$|\mu^j(a)| \leq |\mu^j(a_+)| + |\mu^j(a_-)| \leq \sqrt{\mu(a_+)}\sqrt{\alpha(a_+)} + \sqrt{\mu(a_-)}\sqrt{\alpha(a_-)} \leq \sqrt{\mu(|a|)}\sqrt{\alpha(|a|)}. \qquad \square$$

Since $Pu = h\chi f$, for $a \in C_c^\infty(T^*M; \mathbb{R})$,

$$ih^{-1}\langle [P, a(x, hD)]u, u\rangle = ih^{-1}(\langle a(x, hD)u, Pu\rangle - \langle a(x, hD)Pu, u\rangle$$
$$= 2\operatorname{Im}\langle a(x, hD)\chi f, u\rangle. \tag{3-2}$$

Sending $h \to 0$ yields

$$\mu(H_p a) = 2\operatorname{Im}\mu^j(a). \tag{3-3}$$

For the proof of the following standard result, we use the formula (2-3) relating

$$R(k) := (P_\Omega(g) - k^2 - i0)^{-1}$$

to the free outgoing resolvent on $\mathbb{R}^n$ and refer the reader to, e.g., [Burq 2002, Proposition 3.5].

Lemma 3.4. *Let*

$$\mathcal{I} := \left\{\rho \in S^*M : \bigcup_{t \geq 0} \varphi_{-t}(\rho) \cap \operatorname{supp}\chi = \varnothing\right\}$$

be the directly incoming set. Then $\mu(\mathcal{I}) = 0$.

Next, we show that μ is supported on the characteristic variety and that u is oscillating at frequency roughly h^{-1}.

Lemma 3.5. *The measure μ is supported on S^*M. In addition, for $b \in S^1$,*

$$\lim_{h \to 0} \|b(x, hD)\chi u\|_{L^2}^2 = \mu(|b|^2\chi^2).$$

Proof. Suppose that $a \in C_c^\infty(T^*M)$ with $a \equiv 0$ in a neighborhood of $|\xi|_g = 1$. Then there exists $E \in \Psi^{-2}$ compactly supported so that

$$a(x, hD) = EP + O_{L^2_{\text{loc}} \to L^2_{\text{comp}}}(h^\infty).$$

Therefore,

$$\langle a(x, hD)u, u\rangle = \langle Eh\chi f, u\rangle + O(h^\infty) \to 0.$$

Hence, $\mu(a) = 0$. In particular, supp $\mu \subset S^*M$.

Fix $\psi \in \mathcal{C}_c^\infty(T^*M)$ with $\psi \equiv 1$ on supp $\chi \cap \{|\xi|_g^2 \leq 2\}$. Then, there exists $E \in \Psi^0$ compactly supported so that

$$\chi(x)b(x, hD)^*b(x, hD)\chi(x)(1 - \psi(x, hD)) = EP + O_{L_{\text{loc}}^2 \to L_{\text{comp}}^2}(h^\infty).$$

In particular,

$$\|b(x, hD)\chi u\|_{L^2}^2$$
$$= \langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)u, u \rangle$$
$$= \langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)\psi(x, hD)u, u \rangle + \langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)(1-\psi(x, hD))u, u \rangle$$
$$= \langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)\psi(x, hD)u, u \rangle + \langle hE\chi f, u \rangle + O(h^\infty)$$
$$\to \mu(|b|^2\chi^2\psi) = \mu(|b|^2\chi^2). \qquad \square$$

3B. *Hölder continuous metrics.* We now make the necessary adjustments to allow the metric g to be Hölder continuous. We refer the reader to [Taylor 2000, Chapter 3, Section 11] for an analogous account of propagation of singularities for the wave equation as well as a review of the history of propagation of singularities theorems for operators with rough coefficients. Stronger results (i.e., with weaker regularity hypotheses) are probably possible in line with [Burq and Zuily 2015, Remark 3.3], but low regularity is not our main focus here.

Lemma 3.6. *Let g_0, L_0, $L_{j,0}$ satisfy the hypotheses of Theorem 2. Suppose that $g(h) \in \mathcal{C}^{1,\alpha}$ and $L(h), L_j(h) \in \mathcal{C}^{0,\alpha}$ for some $\alpha > 0$ satisfy*

$$\lim_{h \to 0} \|g(h) - g_0\|_{C^{1,\alpha}} = 0,$$
$$\lim_{h \to 0} \|L(h) - L_0\|_{C^{0,\alpha}} = 0,$$
$$\lim_{h \to 0} \|L_j(h) - L_{j,0}\|_{C^{0,\alpha}} = 0, \quad j = 1, \ldots, n.$$

Then the measure μ is supported in S^*M, for $b \in S^1$,

$$\mu(|b|^2\chi^2) = \lim_{h \to 0} \|\operatorname{Op}_h(b)\chi u\|_{L^2}^2 \tag{3-4}$$

and, for $a \in \mathcal{C}_c^\infty(T^*M)$,

$$\mu(H_p a) = 2\operatorname{Im}\mu^j(a), \tag{3-5}$$

where $p = |\xi|_{g_0}^2 - 1$.

This lemma (together with the results of Section 3C below) suffices to prove our estimate *provided the bicharacteristic flow is unique*. Note that the lemma only requires the hypothesis that $g \in \mathcal{C}^{1,\alpha}$ for $\alpha > 0$ and that this regularity suffices to prove existence of solutions to Hamilton's equations. However, it is not adequate for proving uniqueness. Hence Theorem 1 is only stated for $\alpha = 1$, which is sufficient to guarantee the existence of a well-defined single-valued bicharacteristic flow. (A quantitative result using the dynamics of the multivalued flow for $\alpha < 1$ would be an interesting direction for further research.)

To prove Lemma 3.6, we will need a more general set of symbol classes. Let $r \in \mathbb{N}$, $0 < \alpha < 1$, $0 \leq \rho < 1$. We say that $p(x, \xi) \in \mathcal{C}^{r,\alpha} S_\rho^m$ if

$$\|D_\xi^\beta p(\,\cdot\,, \xi)\|_{C^{r,\alpha}} \leq C_\beta h^{-r\rho} \langle \xi \rangle^{m-|\beta|}.$$

We say $p \in S_\rho^m$ if $p \in \bigcap_r \mathcal{C}^{r,\alpha} S_\rho^m$. We need the following boundedness property for operators with symbol in $\mathcal{C}^{r,\alpha} S^m$.

Lemma 3.7. *For $r \geq 0$ and $\alpha > 0$, the map $\mathrm{Op}_h : \mathcal{C}^{r,\alpha} S^m \to \mathcal{L}(H_h^m, L^2)$ with $p \mapsto p(x, hD)$ is continuous with norm bounded independently of h.*

Proof. It is enough to show that $\mathrm{Op}_h : \mathcal{C}^{r,\alpha} S^0 \to \mathcal{L}(L^2, L^2)$ is continuous with norm bounded independently of h. For this, we rescale to $h = 1$. That is, let $T_h : L^2(\mathbb{R}^n) \to L^2(\mathbb{R}^n)$ be given by $(T_h u)(x) = h^{n/4} u(h^{1/2} x)$. Then T_h is unitary and

$$\mathrm{Op}_h(a)u = T_h^* \mathrm{Op}_1(a_h) T_h u,$$

where

$$a_h(x, \xi) = a(h^{1/2} x, h^{1/2} \xi).$$

Now, for $a \in \mathcal{C}^{r,\alpha} S^m$,

$$\|D_\xi^\beta a_h(\,\cdot\,, \xi)\|_{C^{r,\alpha}} \leq C_\beta h^{|\beta|/2} \langle h^{1/2} \xi \rangle^{-|\beta|}.$$

In particular, a_h is uniformly bounded in $\mathcal{C}^{r,\alpha} S^m$. Therefore, by [Taylor 2011, Chapter 13, Theorem 9.1] $\mathrm{Op}_1(a_h) : L^2 \to L^2$ uniformly in h with norm bounded by a finite sum of $\mathcal{C}^{r,\alpha} S^0$ seminorms. Since T_h is unitary, this completes the proof. □

Lemma 3.8. *Let $a \in \mathcal{C}_c^\infty(T^*M)$, $m \in \mathbb{R}$, and $0 < \alpha < 1$. Then*

$$\mathcal{C}^{1,\alpha} S^m \to \mathcal{L}(L^2, L^2), \quad p \mapsto h^{-1}[p(x, hD), a(x, hD)],$$

is continuous with norm bounded independently of h.

Proof. Let $p \in \mathcal{C}^{1,\alpha} S^m$ and choose $\rho \in (2/(2+\alpha), 1)$ so that $(1 + \alpha/2)\rho > 1$. Let $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ with $\psi \equiv 1$ on $[-2, 2]$. Define $p_h(x, \xi) = (\psi(h^\rho |D_x|)p)(x, \xi)$. Then, $p_h \in S_\rho^m$. Moreover,

$$|D_x D_\xi^\beta p_h(x, \xi)| \leq C_\beta \langle \xi \rangle^{m-|\beta|},$$
$$|D_x^\gamma D_\xi^\beta p_h(x, \xi)| \leq C_\beta h^{-\rho(|\gamma|-1)} \langle \xi \rangle^{m-|\beta|}, \quad |\gamma| > 1.$$

Note that the symbol classes S_ρ^m have a symbol calculus and, in particular,

$$h^{-1}[\mathrm{Op}_h(p_h), a(x, hD)] = \frac{1}{i} \mathrm{Op}_h(\{p_h, a\}) + O(h^{1-\rho})_{L^2 \to L^2}. \tag{3-6}$$

Next, note that by the characterization of Hölder spaces by Littlewood–Paley decomposition [Taylor 2011, Chapter 13, Theorems 8.1, 8.2],

$$\|(p - p_h)(\,\cdot\,, \xi)\|_{\mathcal{C}^{0,\alpha/2}} \leq h^{\rho(1+\alpha/2)} \|p(\,\cdot\,, \xi)\|_{\mathcal{C}^{1,\alpha}} = o(h)\|p(\,\cdot\,, \xi)\|_{\mathcal{C}^{1,\alpha}}.$$

In particular, $p - p_h \in o(h)\mathcal{C}^{0,\alpha/2}S^2$ and hence

$$h^{-1}[\mathrm{Op}_h(p - p_h), a(x, hD)] = o(1)_{L^2 \to L^2}.$$

Combining this with (3-6) completes the proof. $\qquad\square$

Proof of Lemma 3.6. We start with the proof of (3-4). Note that $P = \mathrm{Op}_h(p_0) + h\,\mathrm{Op}_h(p_1)$, where $p_0(h) = |\xi|^2_{g(h)} - 1 \in \mathcal{C}^{1,\alpha}S^2$ and $p_1(h) \in \mathcal{C}^{0,\alpha}S^1$ uniformly as $h \to 0$.

Fix $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ with $\psi \equiv 1$ on $[-2, 2]$ and let $\epsilon > 0$. Let $p_{i,\epsilon}(x, \xi) = (\psi(\epsilon|D_x|)p_i)(x, \xi)$. Then, $p_{i,\epsilon} \in S^{2-i}$ and again by Littlewood–Paley,

$$\|D_\xi^\beta(p_0 - p_{0,\epsilon})(\,\cdot\,, \xi)\|_{\mathcal{C}^{0,\alpha}} \leq C_\beta \epsilon \langle \xi \rangle^{2-|\beta|}.$$

In particular, for $\epsilon > 0$ small and $h < h_0$ small, p_ϵ is elliptic on $||\xi|_g - 1| \geq C\epsilon$. Therefore, for $a \in S^0(T^*M)$ supported away from $p = 0$, there is $\epsilon > 0$, h_0 small enough so that $p_{0,\epsilon}$ is elliptic on supp a. Hence there is $E_\epsilon \in \Psi^{-\infty}$ (uniformly for $\epsilon > 0$ small) so that

$$a(x, hD) = E_\epsilon \mathrm{Op}_h(p_{0,\epsilon}) + O(h^\infty)_{\Psi^{-\infty}}.$$

In particular,

$$a(x, hD) = E_\epsilon(P - \mathrm{Op}_h(p_0 - p_{0,\epsilon}) - h\,\mathrm{Op}_h(p_1)) + O(h^\infty)_{\Psi^{-\infty}}.$$

Therefore,

$$\mu(a) = \lim_{h \to 0}\langle E_\epsilon P u, u\rangle - \langle E_\epsilon[\mathrm{Op}_h(p_0 - p_{0,\epsilon}) + h\,\mathrm{Op}_h(p_1)]u, u\rangle$$

$$= \lim_{h \to 0}\langle E_\epsilon h\chi f, u\rangle + O(\epsilon) = O(\epsilon).$$

Since the left-hand side does not depend on ϵ, sending $\epsilon \to 0$, we have $\mu(a) = 0$ and hence supp $\mu \subset S^*M$.

Next, fix $K > 0$ large enough so that, for $h < h_0$, $\{|\xi|_{g(h)} \leq 2\} \subset \{|\xi| \leq K\}$. We apply the previous argument with $a(x, hD) = \chi(x)b(x, hD)^*b(x, hD)\chi(x)(1 - \psi(K^{-1}|hD|))$. In particular, there exists $E_\epsilon \in \Psi^0$ compactly supported so that

$$\chi(x)b(x, hD)^*b(x, hD)\chi(x)(1 - \psi(|hD|_g)) = E_\epsilon P + O_{L^2_{\mathrm{loc}} \to L^2_{\mathrm{comp}}}(\epsilon).$$

Therefore,

$$\lim_{h \to 0}\|b(x, hD)\chi u\|_{L^2}^2 = \lim_{h \to 0}\langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)u, u\rangle$$

$$= \lim_{h \to 0}\langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)\psi(K^{-1}|hD|)u, u\rangle$$

$$+ \lim_{h \to 0}\langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)(1 - \psi(K^{-1}|hD|))u, u\rangle$$

$$= \lim_{h \to 0}\langle \chi(x)b(x, hD)^*b(x, hD)\chi(x)\psi(K^{-1}|hD|)u, u\rangle + \lim_{h \to 0}\langle hE_\epsilon f, u\rangle + O(\epsilon)$$

$$= \mu(|b|^2\chi^2\psi(|\xi|_g)) + O(\epsilon) = \mu(|b|^2\chi^2) + O(\epsilon).$$

Again, since the left hand side is independent of ϵ, this proves (3-4).

We now prove (3-5). Let $a \in \mathcal{C}_c^\infty(T^*M; \mathbb{R})$. Then,

$$\frac{i}{h}\langle[P, a(x, hD)]u, u\rangle = i[(a(x, hD)u, h\chi f) - (ha(x, hD)\chi f, u)] \to 2\,\mathrm{Im}\,\mu^j(a).$$

Therefore, it remains to show that

$$\frac{i}{h}\langle[P, A]u, u\rangle \to \mu(H_p a). \tag{3-7}$$

First, observe that by Lemma 3.7 and the fact that

$$\|D_\xi^\beta(p_1 - p_{1,\epsilon})(\,\cdot\,, \xi)\|_{\mathcal{C}^{0,\alpha/2}} \le C_\beta \epsilon^{\alpha/2} \langle\xi\rangle^{1-|\beta|},$$

we obtain

$$\|ha(x, hD)\operatorname{Op}_h(p_1 - p_{1,\epsilon})\| + \|h\operatorname{Op}_h(p_1 - p_{1,\epsilon})a(x, hD)u\|_{L^2} \le Ch\epsilon^{\alpha/2}.$$

Therefore,

$$\|[h\operatorname{Op}_h(p_1), a(x, hD)u]\|_{L^2} \le Ch\epsilon^{\alpha/2}\|u\|_{L^2} + O_\epsilon(h^2). \tag{3-8}$$

Next, observe that by Lemma 3.8,

$$\|[\operatorname{Op}_h(p_0 - p_{0,\epsilon}), a(x, hD)]u\|_{L^2} \le C\epsilon h\|u\|_{L^2}. \tag{3-9}$$

Finally, with $q_\epsilon := \lim_{h\to 0} p_{0,\epsilon}$,

$$\lim_{h\to 0}\left\langle\frac{i}{h}[\operatorname{Op}_h(p_{0,\epsilon}), a(x, hD)]u, u\right\rangle = \mu(H_{q_\epsilon} a). \tag{3-10}$$

Combining (3-8), (3-9), and (3-10) gives

$$\left|\lim_{h\to 0}\frac{i}{h}\langle[P, A]u, u\rangle - \mu(H_{q_\epsilon} a)\right| \le C\epsilon^{\alpha/2}.$$

Since $p_0 \in \mathcal{C}^{1,\alpha}S^2$ uniformly in h, we have $H_{q_\epsilon} \to H_p$. In particular, sending $\epsilon \to 0$ and applying the dominated convergence theorem gives (3-7). □

3C. *Appearance of the Volterra operator.* To complete the proof of (1-3) in the boundaryless case, we prove the following measure-theoretic proposition. This lemma will be modified slightly in the case of a manifold with boundary to account for the fact that the generalized bicharacteristic flow is not generated by a vector field.

Proposition 3.9. *Suppose that μ, μ^j, and α are Radon measures on T^*M with α finite and μ finite on compact subsets of T^*M. Let X be a continuous vector field on T^*M and $\varphi_t : T^*M \to T^*M$ be given by $\varphi_t(q) = \exp(tX)(q)$. Let $\Sigma \subset T^*M$ be a hypersurface transverse to X so that the map $F : \mathbb{R} \times \Sigma \to T^*M$, $(t, q) \mapsto \varphi_t(q)$, is a homeomorphism onto its image. Suppose that $\mu(F((-\infty, 0) \times \Sigma)) = 0$ and, for $a \in \mathcal{C}_c^0(T^*M; \mathbb{R})$,*

$$|\mu^j(a)| \le \sqrt{\mu(|a|)\alpha(|a|)}. \tag{3-11}$$

Furthermore, for $\psi \in \mathcal{C}_c^1(\mathbb{R})$, $a \in \mathcal{C}_c^0(\Sigma)$, let $f_{\psi,a}(F(t, q)) = \psi(t)a(q)$ and assume that

$$\mu(f_{\partial_t\psi,a}) = 2\operatorname{Im}\mu^j(f_{\psi,a}). \tag{3-12}$$

Then,

$$\mu(F([0, L] \times \Sigma)) \le \frac{4L^2}{\pi^2}\alpha(F([0, L] \times \Sigma))).$$

Proof. For $0 \le a \in \mathcal{C}_c^0(T^*M)$, define the Radon measures $\mu_a^\sharp$, $\operatorname{Im} \mu^{j,\sharp}$, and $\alpha_a^\sharp$ on $\mathbb{R}$ by

$$\mu_a^\sharp(\psi) = \mu(f_{\psi,a}), \quad \mu_a^{j,\sharp}(\psi) = \mu^j(f_{\psi,a}), \quad \alpha_a^\sharp(\psi) = \mu(f_{\psi,a}).$$

Lemma 3.10. *The measure $\mu^\sharp$ is absolutely continuous with respect to Lebesgue measure and*

$$\mu_a^\sharp = \dot\mu_a^\sharp \, dt,$$

with $|\dot\mu_a^\sharp| \le C \sup |a|$.

Proof. First, observe that for $\psi \in \mathcal{C}_c^1(\mathbb{R})$, (3-12) implies

$$\mu_a^\sharp(\partial_t \psi) = 2 \operatorname{Im} \mu^j(f_{\psi,a}).$$

Let $[b, c] \subset \mathbb{R}$, $0 \le \chi_\epsilon \in \mathcal{C}_c^\infty(\mathbb{R}; [0, 1])$, with $\chi \equiv 1$ on $[b, c]$ and $\operatorname{supp} \chi_\epsilon \subset (b - \epsilon, c + \epsilon)$. Define

$$\psi_\epsilon(t) = -\int \chi_\epsilon(s) \, ds + \int_{-\infty}^t \chi_\epsilon(s) \, ds.$$

Then, since $\mu((-\infty, 0) \times \Sigma) = 0$, we have $\mu^j(F((-\infty, 0) \times \Sigma)) = 0$ and hence

$$|\mu_a^\sharp(\chi_\epsilon)| = 2|\operatorname{Im} \mu^j(1_{F([0,\infty) \times \Sigma)} f_{\psi_\epsilon,a})|$$

$$\le C \sup |a| \sup |\psi_\epsilon|$$

$$\le C \sup |a| \left| \int \chi_\epsilon \, ds \right| \le C \sup |a|(c - b + 2\epsilon).$$

Since $\chi_\epsilon \to 1_{[b,c]}$, we have by the dominated convergence theorem,

$$|\mu_a^\sharp([a, b])| \le C \sup |a|(c - b).$$

In particular, $\mu_a^\sharp$ is absolutely continuous with respect to Lebesgue measure since the intervals generate the Borel sets on $\mathbb{R}$. Moreover, its Radon–Nikodym derivative is linear in a and bounded by $C \sup |a|$. $\square$

By (3-11), since $\mu_a^\sharp$ is absolutely continuous with respect to Lebesgue measure, $\mu_a^{j,\sharp}$ is also. Let $\dot\mu_a^\sharp$, $\dot\mu_a^{j,\sharp}$, and $\dot\alpha_a^\sharp$ be the Radon–Nikodym derivatives of $\mu_a^\sharp$, $\mu_a^{j,\sharp}$, and $\alpha_a^\sharp$ respectively with respect to Lebesgue measure. In particular,

$$\mu_a^\sharp = \dot\mu_a^\sharp \, dt, \quad \operatorname{Im} \mu_a^{j,\sharp} = \operatorname{Im} \dot\mu_a^{j,\sharp} \, dt, \quad \alpha_a^\sharp = \dot\alpha_a^\sharp \, dt + \lambda,$$

where $\lambda \perp dt$. Now, by (3-11),

$$\frac{1}{2r}|\mu_a^{j,\sharp}([t - r, t + r])| \le \frac{1}{2r} \sqrt{\mu_a^\sharp([t - r, t + r])} \sqrt{\alpha_a^\sharp([t - r, t + r])}.$$

So, by the Lebesgue differentiation theorem [Folland 1999, Theorem 3.22], for Lebesgue a.e. t,

$$|\dot\mu_a^{j,\sharp}(t)| \le \sqrt{\dot\mu_a^\sharp(t)} \sqrt{\dot\alpha_a^\sharp(t)}. \tag{3-13}$$

Lemma 3.11. *With $\dot\mu_a^\sharp(t)$ as above, $\dot\mu_a^\sharp(t)$ is continuous and*

$$\dot\mu_a^\sharp(t) \le 2 \int_0^{\max(t,0)} |\operatorname{Im} \dot\mu_a^{j,\sharp}(s)| \, ds \le 2 \int_0^t \sqrt{\dot\mu_a^\sharp(s)} \sqrt{\dot\alpha_a^\sharp(s)} \, ds. \tag{3-14}$$

Proof. By (3-12), for $\psi \in \mathcal{C}_c^1(\mathbb{R})$,

$$\int \psi'(t) \dot{\mu}_a^\sharp(t) \, dt = 2 \int \psi(t) \operatorname{Im} \dot{\mu}_a^{j,\sharp}(t) \, dt. \tag{3-15}$$

Let $\chi \in \mathcal{C}_c^\infty(\mathbb{R}; [0,1])$ with $\int \chi(s) \, ds \equiv 1$ and define $\chi_{\epsilon,t'}(s) = \epsilon^{-1} \chi(\epsilon^{-1}(s - t'))$ and

$$\psi_{\epsilon,t'}(s) = -1 + \int_{-\infty}^{t} \chi_{\epsilon,t'}(s) \, ds.$$

Then by (3-15), together with the fact that $\mu_a^{j,\sharp}(t) = 0$ for $t < 0$,

$$\int \chi_{\epsilon,t'}(t) \dot{\mu}_a^\sharp(t) \, dt = 2 \int_0^\infty \psi_{\epsilon,t'}(t) \operatorname{Im} \dot{\mu}_a^{j,\sharp}(t) \, dt.$$

Applying the Lebesgue differentiation theorem on the left and dominated convergence on the right, we find for Lebesgue a.e. t'

$$\dot{\mu}_a^\sharp(t') = -2 \int_0^{\max(t',0)} \operatorname{Im} \dot{\mu}_a^{j,\sharp}(t) \, dt.$$

Note that this implies $\dot{\mu}_a^\sharp(t')$ is continuous. Applying (3-13) gives (3-14). □

Lemma 3.12. *Let* $0 \le b(t), c(t) \in L^2$ *with* $b(t)$ *continuous and*

$$b^2(t) \le 2 \int_0^t b(s) c(s) \, ds.$$

Then

$$b(t) \le \int_0^t c(s) \, ds. \tag{3-16}$$

Proof. Supposing (3-16) to be false, there exists $\epsilon > 0$ and $t > 0$ such that

$$b(t) \ge \int_0^t c(s) \, ds + \epsilon;$$

hence we may define

$$t_0 := \inf\left\{ t > 0 : \int_0^t c(s) \, ds + \epsilon \le b(t) \right\}.$$

Then,

$$\left[\int_0^{t_0} c(s) \, ds + \epsilon \right]^2 = b^2(t_0) \le 2 \int_0^{t_0} b(s) c(s) \, ds$$

$$\le 2 \int_0^{t_0} \int_0^s c(r) c(s) \, dr \, ds + 2\epsilon \int_0^{t_0} c(s) \, ds$$

$$= \left[\int_0^{t_0} \int_0^s c(r) c(s) \, dr \, ds + \int_0^{t_0} \int_s^{t_0} c(r) c(s) \, dr \, ds \right] + 2\epsilon \int_0^{t_0} c(s) \, ds$$

$$= \left[\int_0^{t_0} c(s) \, ds \right]^2 + 2\epsilon \int_0^{t_0} c(s) \, ds$$

$$= \left[\int_0^{t_0} c(s) \, ds + \epsilon \right]^2 - \epsilon^2,$$

which is a contradiction. □

Using the continuity of $\dot{\mu}_a^\sharp$ together with (3-14) to apply Lemma 3.12 with $b(t) = \sqrt{\dot{\mu}_a^\sharp(t)}$, $c(t) = \sqrt{\dot{\alpha}_a^\sharp(s)}$, we have

$$\sqrt{\dot{\mu}_a^\sharp(t)} \leq \int_0^t \sqrt{\dot{\alpha}_a^\sharp(s)} \, ds.$$

Now,

$$\mu(F([0, L] \times \Sigma) = \int_0^L \dot{\mu}_1^\sharp(t) \, dt \leq \int_0^L \left| \int_0^t \sqrt{\dot{\alpha}_1^\sharp(s)} \, ds \right|^2 dt$$

$$= \left\| V \sqrt{\dot{\alpha}_1^\sharp} \right\|_{L^2([0,L])}^2 \leq \| V \|_{L^2([0,L]) \to L^2([0,L])}^2 \int_0^L \dot{\alpha}_1^\sharp(t) \, dt,$$

where $V : L^2([0, L]) \to L^2([0, L])$ is the Volterra operator. Since the Volterra operator acting on $L^2([0, L])$ has norm $(2L)/\pi$ [Halmos 1967, Problem 188] and

$$\alpha(F([0, L] \times \Sigma)) = \int_0^L \dot{\alpha}_1^\sharp(t) \, dt,$$

we have

$$\mu(F([0, L] \times \Sigma)) \leq \frac{4L^2}{\pi^2} \alpha(F([0, L] \times \Sigma)). \qquad \square$$

3D. *Completion of the proof of (1-3) in the boundaryless case.* Let

$$\Sigma = \{ \rho \in T_{\partial B(0, R)}^* M : (H_p r)(\rho) < 0 \},$$

where r is the radial variable defined in the Euclidean end(s) as in Definition 2.1. Thus, these are the inward-pointing covectors over the boundary of the ball of radius R. By convexity of Euclidean balls,

$$\bigcup_{t>0} \exp(t H_p)(\Sigma) \supset \mathcal{I}^c, \quad \bigcup_{t \leq 0} \exp(t H_p)(\Sigma) \subset \mathcal{I},$$

and F as in Proposition 3.9 is a diffeomorphism onto its image.

Then, by (3-3) and Lemmas 3.3, 3.4, and 3.6, $(\mu, \mu^j, \alpha, \Sigma)$ satisfy the hypotheses of Proposition 3.9 with $\varphi_t = \exp(t H_p)$. Therefore,

$$\mu \left(\bigcup_{t=0}^L \varphi_t(\Sigma \cap S^* M) \right) \leq \frac{4L^2}{\pi^2} \alpha(T^* M),$$

where we may take $L = L(g, R')$. So, since $0 \leq \chi^2 \leq 1$ and

$$\text{supp} \, \chi \cap S^* M \subset \bigcup_{t=0}^{L(g,R')} \varphi_t(\Sigma \cap S^* M),$$

we conclude

$$\limsup_{h \to 0} \| \chi u \|_{L^2} = \sqrt{\mu(\chi^2)} \leq \frac{2L(g, R')}{\pi} \sqrt{\alpha(T^* M)} \leq \liminf \frac{2L(g, R')}{\pi} \| f(h) \|_{L^2}.$$

This completes the proof of (1-3) in the case of a manifold without boundary.

3E. *Uniformity of k_0 and Sobolev estimates.* In this section we prove the uniformity of k_0 statement from Theorem 1, as well as the more general Sobolev mapping property (1-4). We will omit the terms L, L_j from this discussion for brevity, but will on the other hand prove a slightly more general statement about metric perturbations as follows.

We begin with uniformity in the case $s = 0$, i.e., in the basic L^2 estimate. Fix $R_1 > 0$ and let $\mathcal{C}$ be a subset of $\mathcal{C}^{1,1}$ metrics so that, for $g \in \mathcal{C}$, g is nontrapping and $\mathrm{supp}(I - g) \subset B(0, R_1)$. Furthermore, suppose that for any $\{g_k\}_{k=1}^\infty \subset \mathcal{C}$, there exists a subsequence $\{g_{k_m}\}_{m=1}^\infty$, $\gamma > 0$, and $g \in \mathcal{C}$ so that $\|g_{k_m} - g\|_{\mathcal{C}^{1,\gamma}} \to 0$ and $\lim_{m \to \infty} L(g_{k_m}, R_1) \geq L(g, R_1)$. Let $\chi \in \mathcal{C}_c^\infty(B(0, R); [0, 1])$ and $R_1 < R' < R'' < R$ so that $\mathrm{supp}\,\chi \subset B(0, R')$.

We start by showing that there exists $k_0 > 0$ so that, for all $g \in \mathcal{C}$ and $k > k_0$,

$$\|\chi(P(g) - k^2 - i0)^{-1}\chi\|_{L^2 \to L^2} \leq \frac{2L(g, R'')}{\pi k}. \tag{3-17}$$

Suppose not. Then since $L(g, R') < L(g, R'')$, there exists $\{g_k\}_{k=1}^\infty \subset \mathcal{C}$, $h_k \to 0$, $f_k \in L^2(M)$, $u_k \in H_{\mathrm{loc}}^s(M)$, with $\|\chi u_k\|_{L^2} = 1$, and $\delta > 0$ so that

$$(h_k^2 P(g_k) - 1)u_k = h_k \chi f_k, \quad 1 = \|\chi u_k\|_{L^2} \geq \frac{2L(g_k, R')\|f_k\|_{L^2(M)}}{\pi} + \delta. \tag{3-18}$$

Extracting subsequences, we may assume that $g_k \to g$ in $\mathcal{C}^{1,\gamma}$ for some $\gamma > 0$ and $\lim L(g_k, R') \geq L(g, R')$. Note also that by Lemma 3.2, u_k is uniformly bounded in L_{loc}^2 and hence, by extracting further subsequences, we may assume that u_k has defect measure μ, χf_k has defect measure α, and u_k, χf_k have joint defect measure μ^j. Let Σ denote the set of directly incoming points on $T_{\partial B(0,R')}^* M$. By Lemmas 3.3, 3.4, and 3.6, $(\mu, \mu^j, \alpha, \Sigma)$ satisfy the hypotheses of Proposition 3.9 with $\varphi_t = \exp(t H_p)$ and $p = |\xi|_g^2 - 1$. Therefore,

$$\mu\left(\bigcup_{t=0}^L \varphi_t(\Sigma \cap S^*M)\right) \leq \frac{4L^2}{\pi^2}\alpha(T^*M),$$

and we arrive at a contradiction just as above.

Finally, to obtain the bound (1-4), we begin by considering the case $s = 2$. We compute

$$(P(g) + k^2)\chi(P(g) - k^2 - i0)^{-1}\chi f = \chi^2 f + ([-\Delta_{\mathbb{R}^n}, \chi] + 2k^2\chi)(P(g) - k^2 - i0)^{-1}\chi f.$$

We next consider $[-\Delta_{\mathbb{R}^n}, \chi]$ and show that there exists $k_1 > 0$ so that, for $k > k_1$ and $g \in \mathcal{C}$,

$$\|[-\Delta_{\mathbb{R}^n}, \chi](P - k^2 - i0)^{-1}\chi\|_{L^2 \to L^2} \leq \sup_{S^*M} |H_{|\xi|^2}\chi|\frac{2L(g_k, R'')}{\pi}. \tag{3-19}$$

Suppose that (3-19) does not hold. Then there is $\delta > 0$ and a sequence $h_k \to 0$, $f_k \in L^2(M)$, $u_k \in H^2(M)$ with $\|f_k\|_{L^2} = 1$, u_k so that

$$(h_k^2 P(g_k) - 1)u_k = \chi h_k f_k, \quad u_k|_{\partial M} = 0,$$

$$\|h_k^{-1}[-h_k^2\Delta_{\mathbb{R}^n}, \chi]u_k\|_{L^2} \geq \sup_{S^*M} |H_{|\xi|^2}\chi|\frac{2(L(g_k, R') + \delta)}{\pi}.$$

Let $\tilde{\chi} \in C_c^\infty(B(0, R'); [0, 1])$ with $\tilde{\chi} \equiv 1$ on supp χ. As before, we may assume that u_k has a defect measure and then, by Lemma 4.2 applied with χ replaced by $\tilde{\chi} \in C_c^\infty(B(0, R'))$,

$$\sup_{S^*M} |H_{|\xi|^2} \chi^2| \frac{4(L(g_k, R') + \delta)^2}{\pi^2} \le \|h^{-1}[-h^2\Delta_{\mathbb{R}^n}, \chi]\tilde{\chi}u_k\|_{L^2}^2 \to \mu(|H_{|\xi|^2}\chi|^2\tilde{\chi}^2)$$

$$\le \sup_{S^*M} |H_{|\xi|^2}\chi|^2 \mu(\tilde{\chi}^2) \le \sup_{S^*M} |H_{|\xi|^2}\chi|^2 \frac{4(L(g, R'))^2}{\pi^2},$$

a contradiction.

Thus, by (3-17), for $k > k_0$, and any $g \in \mathcal{C}$,

$$\|(P(g) + k^2)\chi(P(g) - k^2 - i0)^{-1}\chi f\|_{L^2}$$

$$\le 2k^2\|\chi(P(g) - k^2 - i0)^{-1}\chi f\|_{L^2} + \|\chi^2 f\| + \|[-\Delta_{\mathbb{R}^n}, \chi](P(g) - k^2 - i0)^{-1}\chi f\|$$

$$\le \frac{4L(g, R'')k}{\pi}\|\chi f\|_{L^2} + \|[-\Delta_{\mathbb{R}^n}, \chi](P(g) - k^2 - i0)^{-1}\chi f\|_{L^2} + \|\chi^2 f\|_{L^2}.$$

Using (3-19), we have for $k > k_1$, and any $g \in \mathcal{C}$,

$$\|[-\Delta_{\mathbb{R}^n}, \chi](P(g) - k^2 - i0)^{-1}\chi f\|_{L^2} \le \sup_{S^*M} |H_{|\xi|^2}\chi| \frac{2L(g_k, R'')}{\pi}\|f\|_{L^2}.$$

In particular, letting

$$k > \max\left(k_0, k_1, \frac{\sup_{S^*M} |H_{|\xi|^2}\chi|2L(g, R'') + \pi}{4(L(g, R) - L(g, R''))}\right),$$

we have for all $g \in \mathcal{C}$,

$$\|\chi(P(g) - k^2 - i0)^{-1}\chi f\|_{H^2} = \|(P(g) + k^2)\chi(P(g) - k^2 - i0)^{-1}\chi f\|_{L^2}$$

$$\le \frac{4L(g, R)k}{\pi}\|f\|_{L^2}. \tag{3-20}$$

Since $L(g, R'') \le L(g, R)$, the general case of $0 \le s \le 2$ then follows by interpolation between (3-17) and (3-20).

If we choose $\mathcal{C}$ to be a subset of an open neighborhood in the $\mathcal{C}^{2,\alpha}$ topology of a given $\mathcal{C}^{2,\alpha}$ nontrapping metric, then provided this neighborhood is chosen sufficiently small, all the metrics in $\mathcal{C}$ are nontrapping, and the subsequence condition is guaranteed by the compactness of the embedding $\mathcal{C}^{2,\alpha} \hookrightarrow \mathcal{C}^{1,\gamma}$; indeed we have subsequential convergence in $\mathcal{C}^{1,1}$, which ensures that $\lim L(g_{k_m}, R_1) = L(g, R_1)$. This choice of $\mathcal{C}$ then gives the uniformity assertion from Theorem 1. This completes the proof of (1-3) in the case of a manifold without boundary.

4. Manifolds with boundary

We now turn to the case of manifolds with boundary. Our treatment of the propagation of defect measures in this setting is motivated by [Miller 2000; Burq and Lebeau 2001]; see also [Burq 1997].

Let $\widetilde{M}$ be an open manifold extending M and extend P to an operator on $\widetilde{M}$. We then let $\underline{u}$ be the extension of u by 0. As in the boundaryless case, we will assume that we have a sequence $h = h_j \downarrow 0$ with

$$Pu(h) = h\chi f(h) \quad \text{in } M, \quad u|_{x_1=0} = 0,$$

and we take

$$\| f(h)\| = 1, \quad \lim_{h \to 0} \|\chi u\|_{L^2} = M > L(\Omega, g, R).$$

Since propagation of singularities is a local consideration, we may employ Riemannian normal coordinates (x_1, x') in which ∂M is given by $x_1 = 0$, $M = \{x_1 > 0\}$, and the operator P is given by

$$P = (hD_{x_1})^2 + R(x_1, x', hD_{x'}) + hE \tag{4-1}$$

for some self-adjoint $E \in \text{Diff}_h^1$ and for $R \in \text{Diff}_h^2$ with symbol $r(x_1, x', \xi')$.

We proceed as before, letting μ be a defect measure of $\underline{u}$, α be a defect measure of $\underline{\chi f}$, and μ^j a joint defect measure of $\underline{u}$ and $\underline{\chi f}$. Finally, let $\dot{\nu}$ be the defect measures of $hD_{x_1}u|_{x_1=0}$ on ∂M. Thus,

$$\lim_{h \downarrow 0} \langle a(x, hD)\underline{u}, \underline{u} \rangle = \int a \, d\mu, \qquad \lim_{h \downarrow 0} \langle a(x, hD)\underline{\chi f}, \underline{\chi f} \rangle = \int a \, d\alpha,$$

$$\lim_{h \downarrow 0} \langle a(x, hD)\underline{\chi f}, \underline{u} \rangle = \int a \, d\mu^j, \quad \lim_{h \downarrow 0} \langle b(x', hD')hD_x u, hD_x u \rangle_{\partial M} = \int_{\partial M} b \, d\dot{\nu}. \tag{4-2}$$

4A. *Local study of the measure μ.*

Lemma 4.1. *For $a = a_0(x, \xi') + a_1(x, \xi')\xi_1$ with $a_i \in C_c^\infty([0, \epsilon) \times T^*\partial M)$, we have*

$$\mu(H_p a) = 2 \operatorname{Im} \mu^j(a) - \dot{\nu}(a_1|_{x_1=0}).$$

Proof. Here we work in a small neighborhood of the boundary and write

$$A = a_0(x, hD') + a_1(x, hD')hD_{x_1}.$$

Equation (3-2) must now be modified owing to boundary terms arising in integration by parts. In particular,

$$\langle (hD_{x_1})^2 Au, u \rangle_M = ih(\langle hD_{x_1}Au, u \rangle_{L^2(\partial M)} + \langle Au, hD_{x_1}u \rangle_{L^2(\partial M)}) + \langle Au, (hD_{x_1})^2 u \rangle_{L^2(M)}.$$

There is also a term arising when we integrate by parts to change $\langle f, Au \rangle$ to $\langle Au, f \rangle$ but this term is $O(h)$. Now,

$$\langle hD_{x_1}Au, u \rangle_{L^2(\partial M)} = \langle a_0 hD_{x_1}u + a_1(hD_{x_1})^2 u, u \rangle_{L^2(\partial M)} + o(1)$$

$$= \langle a_0 hD_{x_1}u + a_1(1 + h^2\Delta_{\partial M})u, u \rangle_{L^2(\partial M)} + \langle a_1 h\chi f, u \rangle_{\partial M} + o(1).$$

With Dirichlet boundary conditions, this is actually just 0. Moreover,

$$\langle Au, hD_{x_1}u \rangle_{L^2(\partial M)} = \langle [a_0 + a_1 hD_{x_1}]u, hD_{x_1}u \rangle = \langle a_1 hD_{x_1}u, hD_{x_1}u \rangle.$$

So (3-2) now reads

$$ih^{-1}\langle [P, A]u, u \rangle_M = \operatorname{Im}\langle A\chi f, u \rangle_M - \langle a_1 hD_{x_1}u, hD_{x_1}u \rangle_{\partial M} + o(1). \qquad \square$$

We want to upgrade this to a statement for all functions in $C_c^\infty(T^*M)$. First, we need to show that μ is supported on S^*M.

Lemma 4.2. *Let μ be a defect measure associated to u as above. Then $\operatorname{supp}\mu \subset S^*M$ and $\mu(\chi^2) = 1$. Moreover, for $b \in S^1(T^*M)$, supported away from ∂M,*

$$\lim_{h \to 0} \| \operatorname{Op}_h(b)\chi u \|_{L^2}^2 = \mu(|b|^2\chi^2).$$

Proof. Note that

$$P\underline{u} = 1_{x_1 \geq 0}Pu + h(-\delta(x_1) \otimes h\partial_{x_1}u|_{x_1=0} + h\delta'(x_1) \otimes u|_{x_1=0}).$$

Now, suppose $a \in \mathcal{C}_c^\infty(T^*\widetilde{M})$ has $\operatorname{supp} a \cap \{p = 0\} = \varnothing$. Then, there exist $E \in \Psi^{-2}$ so that $a(x, hD) = EP + O_{\mathcal{D}' \to \mathcal{C}^\infty}(h^\infty)$. Therefore,

$$a(x, hD)\underline{u} = a(x, hD)1_{x_1 \geq 0}Pu + hE(-\delta(x_1) \otimes h\partial_{x_1}u|_{x_1=0}).$$

Since $E : H_h^s \to H_h^{s+2}$ is bounded and $\|h\partial_{x_1}u|_{x_1=0}\| \leq C$, we have

$$a(x, hD)\underline{u} = a(x, hD)1_{x_1 \geq 0}Pu + O_{L^2}(h^{1/2}).$$

In particular, this implies $\mu(a) = 0$ completing the proof.

To see that $\mu(\chi^2) = 1$, let $\psi \in \mathcal{C}_c^\infty(\mathbb{R})$ with $\psi \equiv 1$ on $|s| \leq 2$. Then, as above there exists $E \in S^{-2}$ so that

$$\chi(1 - \psi)(|hD|)\chi = EP + O_{\mathcal{D}' \to \mathcal{S}}(h^\infty)$$

and hence again

$$\chi(1 - \psi)(|hD|))\chi\underline{u} = O_{L^2}(h^{1/2}).$$

In particular,

$$1 = \langle \chi^2\underline{u}, \underline{u}\rangle = \langle \chi\psi(|hD|)\chi\underline{u}, \underline{u}\rangle + O(h^{1/2})$$
$$= \int \chi^2(x)\psi(|\xi|)\,d\mu = \int \chi^2\,d\mu,$$

where in the last line we use the fact that μ is supported on S^*M.

The last claim follows the same arguments as in the boundaryless case. $\square$

We now introduce notation for the even and odd parts of smooth functions on T^*M.

Definition 4.3. For $a \in \mathcal{C}^\infty(T^*M)$, let

$$a_o(x, \xi_1, \xi') = \frac{a(x, \xi_1, \xi') - a(x, -\xi_1, \xi')}{2\xi_1}, \quad a_e(x, \xi_1, \xi') = \frac{a(x, \xi_1, \xi') + a(x, -\xi_1, \xi')}{2}.$$

Thus, $a = a_e + \xi_1 a_o$ and a_e, a_o are both even functions of ξ_1.

Next we upgrade the test functions for which we can compute $\mu(H_p a)$.

Lemma 4.4. *For $a \in \mathcal{C}_c^\infty(T^*\widetilde{M})$,*

$$\mu(H_p a) = 2\operatorname{Im}\mu^j(a) - \dot{\nu}(a_o|_{x_1=0}).$$

In particular, for $a = a(x, x_1\xi_1, \xi') \in \mathcal{C}_c^\infty({}^bT^*\overline{\mathbb{R}_+^n})$,

$$\mu(H_p a) = 2\operatorname{Im}\mu^j(a).$$

Remark 4.5. Here, ${}^b T^* \overline{\mathbb{R}^n_+}$ denotes the b-cotangent bundle of this local model for a manifold with boundary, constructed so that smooth functions on this space are simply functions of $(x, x_1\xi_1, \xi')$. See Section 4B for a more precise description of this space and for additional references. We are regarding a here as extended to a smooth function on $T^* \widetilde{M}$; the choice of extension is immaterial, as μ is supported on M.

Proof. Since a_o and a_e are both even functions, we may write

$$a_{e/o}(x, \xi_1, \xi') = \tilde{a}_{e/o}(x, \xi_1^2, \xi')$$

for smooth functions $\tilde{a}_{e/o}$; thus,

$$a = \tilde{a}_e(x, \xi_1^2, \xi') + \tilde{a}_o(x, \xi_1^2, \xi')\xi_1.$$

Since H_p is tangent to $S^*\widetilde{M}$, we have $H_p 1_{S^*\widetilde{M}} a = 1_{S^*\widetilde{M}} H_p a$. In particular, since $\operatorname{supp}\mu \subset S^*\widetilde{M}$,

$$\mu(H_p a) = \mu(H_p 1_{S^*\widetilde{M}} a).$$

Now,

$$S^*\widetilde{M} := \{\xi_1^2 - r(x, \xi') = 0\}.$$

Therefore,

$$1_{S^*\widetilde{M}} a = 1_{S^*\widetilde{M}}[\tilde{a}_e(x, r(x, \xi'), \xi') + \tilde{a}_o(x, r(x, \xi'), \xi')\xi_1].$$

Let $b_{e/o} = a_{e/o}(x, r(x, \xi'), \xi')$. Then we have

$$\begin{aligned}
\mu(H_p a) &= \mu(H_p 1_{S^*\widetilde{M}}[b_e + b_o\xi_1]) \\
&= \mu(H_p(b_e + b_o\xi_1)) \\
&= 2\operatorname{Im}\mu^j(b_e + b_o\xi_1) - \dot{\nu}(b_o|_{x_1=0}).
\end{aligned}$$

Now, since $\operatorname{supp}\mu \subset S^*M$, we have $\operatorname{supp}\mu^j \subset S^*M$ (by Lemma 3.3) and hence

$$\mu^j(b_e + b_o\xi_1) = \mu^j(a).$$

Therefore, we have

$$\mu(H_p a) = 2\operatorname{Im}\mu^j(a) - \dot{\nu}(b_o|_{x_1=0}). \qquad \square$$

Before proceeding further, we recall the decomposition of $T^*_{\partial M} M$ into elliptic, hyperbolic, and glancing regions. In the notation of (4-1), with r the symbol of $R(x_1, x', hD_{x'})$, we write

$$\begin{aligned}
(y, \xi_1, \xi') &\in \mathcal{E} && \text{if } r(0, x', \xi') > 0, \\
(y, \xi_1, \xi') &\in \mathcal{H} && \text{if } r(0, x', \xi') < 0, \\
(y, \xi_1, \xi') &\in \mathcal{G} && \text{if } r(0, x', \xi') = 0
\end{aligned}$$

to denote the elliptic, hyperbolic, and glancing sets respectively.

We further split the glancing set into subsets as follows: we let

$$\begin{aligned}
\mathcal{G}_d &:= \mathcal{G} \cap \{H_p^2 x_1 > 0\}, \\
\mathcal{G}_g &:= \mathcal{G} \cap \{H_p^2 x_1 < 0\};
\end{aligned}$$

these are the *diffractive* and *gliding* sets respectively. We will also employ the filtration of the remainder of the glancing set given by the order of contact with the boundary as follows:

$$\mathcal{G}^k := \{\rho \in \mathcal{G} : (H_p^j x_1)(\rho) = 0 \text{ for } 0 \le j < k, \text{ and } (H_p^k x_1)(\rho) \ne 0\}.$$

(We remark that this definition differs from the G^k defined in [Hörmander 1994, Section 24.3] in that our $\mathcal{G}^k$ does not include higher-order glancing as well.)

With an open set $U \subset {}^b T^* M$ fixed, we will also use the notation

$$\widetilde{\mathcal{G}}^k := \{\rho \in U : \rho \text{ is connected to } \mathcal{G}^k \text{ by a generalized bicharacteristic}\}.$$

We further let

$$\widetilde{\mathcal{G}}^{\ge k} := \bigcup_{k' \ge k} \widetilde{\mathcal{G}}^{k'}.$$

Near glancing: We now commence the study of the measure μ near the glancing set $\mathcal{G}$. Here we follow an inductive strategy employed in [Burq and Lebeau 2001].

Lemma 4.6. *There exists a positive measure μ^∂ on the glancing set $\mathcal{G}$ so that*

$$\mu = \mu 1_{x_1 > 0} + \delta(x_1) \otimes \delta(H_p x_1) \otimes \mu^\partial.$$

In particular, $\mu(\mathcal{H}) = 0$.

Proof. Let $a_\epsilon = \varphi(x, \xi') \epsilon \chi(\epsilon^{-1} x_1)$, with $\chi \in \mathcal{C}_c^\infty(\mathbb{R})$, $\chi(0) = \chi'(0) = 1$.

By Lemma 4.4,

$$\mu(H_p a_\epsilon) = 2 \operatorname{Im} \mu^j(a_\epsilon).$$

By the dominated convergence theorem,

$$2 \operatorname{Im} \mu^j(a_\epsilon) \to 0.$$

On the other hand,

$$H_p a_\epsilon = \chi'(\epsilon^{-1} x_1) \varphi(x, \xi') H_p x_1 + O(\epsilon).$$

So, by dominated convergence,

$$\mu(H_p a_\epsilon) \to \mu(1_{x_1=0} H_p x_1 \varphi).$$

In particular,

$$\mu 1_{x_1=0}(H_p x_1 \varphi) = 0$$

for any φ and hence $\mu 1_{x_1=0}$ is supported on $\mathcal{G}$. Since it is a positive measure, $\mu 1_{x_1=0}$ takes the form specified. $\qquad\square$

Lemma 4.7. *We have*

$$-(H_p^2 x_1)\mu^\partial = 4\dot{v} 1_{\mathcal{G}}.$$

In particular, since μ^∂ and $\dot{v}$ are positive measures,

$$\operatorname{supp} \mu^\partial \cup \operatorname{supp} \dot{v} \subset \{H_p^2 x_1 \le 0\};$$

hence

$$\mu(\mathcal{G}_d) = 0,$$

and, for $E \subset \mathcal{G}$,

$$\dot{v}(E) = \dot{v}(E \cap \{H_p^2 x_1 < 0\}).$$

Proof. Since $H_p x_1 = 2\xi_1$,

$$H_p(2a(x,\xi)\xi_1) = aH_p^2 x_1 + 2\xi_1 H_p a.$$

Let $a_\epsilon = \chi(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r(x,\xi'))2a(x,\xi')\xi_1$, where $\chi \in \mathcal{C}_c^\infty(\mathbb{R})$ has $\chi(0) = 1$, $\chi'(0) = 0$. Then

$$\begin{aligned}
H_p a_\epsilon &= \epsilon^{-1}\chi'(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r(x,\xi'))2a\xi_1 H_p x_1 \\
&\quad + \epsilon^{-1}\chi(\epsilon^{-1}x_1)\chi'(\epsilon^{-1}r(x,\xi'))2a\xi_1 H_p r \\
&\quad + 2\xi_1\chi(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r(x,\xi'))H_p a + a\chi(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r(x,\xi'))H_p^2 x_1 \\
&= a\chi(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r(x,\xi'))H_p^2 x_1 + O(1)(|\chi'(\epsilon^{-1}x_1)| + |\chi'(\epsilon^{-1}r(x,\xi'))| + \epsilon^{1/2}).
\end{aligned}$$

Here we have used that on S^*M, we have $H_p r = -H_p \xi_1^2 = O(\xi_1)$. Then by dominated convergence,

$$\mu(H_p a_\epsilon) \to \tfrac{1}{2}\mu^\partial([H_p^2 x_1]a).$$

On the other hand, since $a_\epsilon = O(\sqrt{\epsilon})$ on S^*M,

$$\mu(H_p a_\epsilon) = 2\,\mathrm{Im}\,\mu^j(a_\epsilon) - \dot{v}(2a(0,x',\xi')\chi(\epsilon^{-1}r)) \to -\dot{v}(21_{\mathcal{G}}a).$$

So, $-H_p^2 x_1 \mu^\partial = 4\dot{v}1_{\mathcal{G}}$ as claimed. $\qquad\square$

4B. *Invariance of the measure* μ.

<u>The *b*-cotangent bundle, ${}^bT^*M$</u>: In our discussion of the invariance of μ, it will be convenient to have some facts about the *b*-cotangent bundle, ${}^bT^*M$. We refer the reader to [Hörmander 1994, Section 18.3] (where the notation $\widetilde{T}^*M$ is used) and [Vasy 2008] for more details on the ${}^bT^*M$. Recall that ${}^bT^*M$ is the dual to the vector bundle of vector fields tangent to ∂M. In local coordinates with $\partial M = \{x_1 = 0\}$, the bundle of vector fields tangent to M is generated over $\mathcal{C}^\infty(M)$ by the vector fields

$$\{x_1 \partial_{x_1}, \partial_{x_2}, \dots, \partial_{x_n}\}.$$

Over $x_1 > 0$, ${}^bT^*M$ is canonically diffeomorphic to T^*M with

$$(x, \zeta, \xi') \mapsto (x, \zeta/x_1, \xi').$$

In fact, we can identify T^*M as a subset of ${}^bT^*M$ using the canonical projection map $\pi : T^*M \to {}^bT^*M$ given in local coordinates by

$$\pi : (x, \xi_1, \xi') \mapsto (x, x_1\xi_1, \xi').$$

Using this map, we can push forward the measure μ to a measure on ${}^bT^*M$. It is actually this pushforward $\pi_*\mu$ for which we will show invariance under the generalized bicharacteristic flow.

Define

$$H_p^G = H_p + \frac{H_p^2 x_1}{H_{x_1}^2 p} H_{x_1}.$$

That is, H_p^G is the gliding vector field. Then H_p^G is tangent to $\mathcal{G}$; see [Hörmander 1994, Section 24.3]. Let also $\varphi_t : {}^b T^* M \to {}^b T^* M$ denote the generalized bicharacteristic flow on ${}^b T^* M$.

Invariance: The aim of the rest of this section is to show that

$$\pi_* \mu(q \circ \varphi_t) - \pi_* \mu(q) = \int_0^t 2 \operatorname{Im} \pi_* \mu^j (q \circ \varphi_s) \, ds, \quad q \in \mathcal{C}_c^\infty({}^b T^* M). \tag{4-3}$$

The main lemma is as follows.

Lemma 4.8. *Let μ and μ_1 be measures on $T^* M$ supported by $S^* M$ with $\mu_1 \ll \mu$. The following are equivalent*:

(1)
$$\pi_* \mu(q \circ \varphi_t) - \pi_* \mu(q) = \int_0^t \pi_* \mu_1 (q \circ \varphi_s) \, ds, \quad q \in \mathcal{C}_c^\infty({}^b T^* M). \tag{4-4}$$

(2) *For $a = a(x_1, x', x_1 \xi_1, \xi')$*
$$\mu(H_p a) = \mu_1(a) \tag{4-5}$$

   and $\mu(\mathcal{G}_d \cup \mathcal{H}) = 0$.

Once we prove this, Lemmas 4.4 and 4.7 imply that μ satisfies condition (ii) with $\mu_1 = 2 \operatorname{Im} \mu^j$ and hence satisfies (4-3).

Proof of Lemma 4.8. Here we follow [Burq and Lebeau 2001, Section 3.3].

(i) implies (ii): Let $a \in \mathcal{C}_c^\infty(T^* M)$ with $a = a(x, x_1 \xi_1, \xi')$. Then there exists $q \in \mathcal{C}_c^\infty({}^b T^* M)$ such that $a = \pi^* q$. Thus, $q \circ \varphi_s(\rho)$ is differentiable from the left and right for all s and

$$\partial_s^\mp (q \circ \varphi_s)(\rho) = H_p a(\pi_\pm^{-1}(\varphi_s(\rho))), \tag{4-6}$$

where $\pi_\pm^{-1}$ denotes the outward- and inward-pointing inverses of π. In particular, for s such that $\varphi_s(\rho) \notin \mathcal{H}$,

$$\partial_s (q \circ \varphi_s)(\rho) = H_p a(\varphi_s(\rho)).$$

Now, $\pi_* \mu(\mathcal{H}) = 0$ since $\pi_* \mu$ satisfies (4-4) and $\mathcal{H}$ is transverse to the flow φ_s. Therefore, since $\pi_* \mu$ satisfies (4-4), differentiating yields

$$\pi_* \mu(\partial_t q \circ \varphi_t|_{t=s}) = \pi_* \mu_1(q \circ \varphi_s)$$

and setting $s = 0$ gives

$$\mu(H_p a) = \mu_1(a).$$

Finally, since $\mathcal{G}_d$ is transverse to the flow, and $\pi_* \mu$ satisfies (i),

$$\pi_* \mu(1_{\mathcal{G}_d}) = \mu(1_{\mathcal{G}_d}) = 0.$$

This completes the proof of (ii).

<u>(ii) implies (i):</u>

Lemma 4.9. *For $b \in C_c^\infty(T^*M)$,*

$$\mu(H_p b) = \mu_1(b) + \mu(1_{x_1=0} \partial_{x_1} r b_o|_{\xi_1^2=r(x,\xi')}) + u^0(b_o|_{x_1=0, \xi_1^2=r(0,x',\xi')}),$$

where u^0 is a measure supported $\mathcal{H}$, $1_{x_1=0}\mu$ is supported by $\mathcal{G} \setminus \mathcal{G}_d$, and

$$b_o = \frac{b(x,\xi_1,\xi') - b(x,-\xi_1,\xi')}{2\xi_1}$$

is the ξ_1 odd part of b.

Proof. Write

$$b = b_e + \xi_1 b_o,$$

where

$$b_e = \frac{b(x,\xi_1,\xi') + b(x,-\xi_1,\xi')}{2}.$$

Then, $b_e = \tilde{b}_e(x,\xi_1^2,\xi')$, $b_0 = \tilde{b}_o(x,\xi_1^2,\xi')$, and so on S^*M,

$$b_e = \tilde{b}_e(x, r(x,\xi'), \xi') =: a_e(x,\xi'), \quad b_o = \tilde{b}_o(x, r(x,\xi'), \xi') =: a_o(x,\xi').$$

Since H_p is tangent to S^*M,

$$\mu(H_p b) = \mu(H_p(a_e + \xi_1 a_o)) = \mu(H_p \xi_1 a_o) + \mu_1(a_e).$$

Now, let

$$\chi \in C_c^\infty(\mathbb{R}), \quad \chi \equiv 1 \text{ near } 0, \quad \chi' \leq 0 \text{ on } x_1 \geq 0, \quad \chi_\epsilon(x_1) = \chi(\epsilon^{-1} x_1). \tag{4-7}$$

Then,

$$\mu(H_p(1-\chi_\epsilon)\xi_1 a_o)) = \mu_1((1-\chi_\epsilon)\xi_1 a_o) \to \mu_1(1_{x_1>0}\xi_1 a_o).$$

Now,

$$\mu(H_p(\chi_\epsilon \xi_1 a_o)) = \mu(\chi_\epsilon \xi_1 H_p a_o + \chi_\epsilon \partial_{x_1} r a_o + 2\epsilon^{-1}\chi_\epsilon' \xi_1^2 a_o) =: I_\epsilon + II_\epsilon + III_\epsilon.$$

By the dominated convergence theorem,

$$I_\epsilon \to \mu(1_{x_1=0}\xi_1 H_p a_o), \quad II_\epsilon \to \mu(1_{x_1=0}\partial_{x_1} r a_o).$$

Note that since $\mu(\mathcal{H}) = 0$ and $\xi_1 = 0$ on $\{x_1 = 0\} \setminus \mathcal{H}$, we have

$$I_\epsilon \to 0, \quad II_\epsilon \to \mu(1_{x_1=0}\partial_{x_1} r a_o). \tag{4-8}$$

Now, observe that

$$\mu_1((1-\chi_\epsilon)\xi_1 a_o) = \mu(H_p(1-\chi_\epsilon)\xi_1 a_o) = \mu((1-\chi_\epsilon)H_p\xi_1 a_o) - III_\epsilon.$$

So,

$$III_\epsilon = \mu((1-\chi_\epsilon)H_p\xi_1 a_o) - \mu_1((1-\chi_\epsilon)\xi_1 a_o)$$

and in particular

$$\lim_{\epsilon \to 0} III_\epsilon(a_o) = \mu(1_{x_1>0}H_p\xi_1 a_o) - \mu_1(1_{x_1>0}\xi_1 a_o). \tag{4-9}$$

On the other hand for $a_o \geq 0$,

$$III_\epsilon(a_o) \leq 0.$$

Therefore, III_ϵ is a family of measures with a weak limit. In particular, $III_\epsilon \to u^0$ for some measure u_0 supported in $x_1 = 0$. In fact, this also shows that

$$a_o \mapsto \mu(1_{x_1>0} H_p(\xi_1 a_o)) - \mu_1(\xi_1 a_o) =: u^0(a_o) \tag{4-10}$$

is a measure. We now check that u^0 is supported in $\mathcal{H}$. Note that once we show this the proof will be complete, since by (4-8) and (4-9) together with $\mu_1(\mathcal{H}) = 0$, we then have

$$\mu(H_p b) = \mu_1(a_e) + \mu_1(\xi_1 a_o) + \mu(1_{x_1=0}\partial_{x_1} r a_o) + u^0(a_o)$$
$$= \mu_1(b) + \mu(1_{x_1=0}\partial_{x_1} r a_o) + u^0(a_o)$$

as desired.

Let χ, χ_ϵ be as in (4-7). Note that for each $\epsilon > 0$, $a_o \chi_\epsilon(x_1)\chi_{\sqrt{\epsilon}}(\xi_1)$ can be written as a smooth function of $(x_1, x', x_1\xi_1, \xi')$. Using (4-10), we now have the decomposition

$$u^0(a_o \chi_\epsilon(x_1)\chi_{\sqrt{\epsilon}}(\xi_1)) = u_1^0(\epsilon) + u_2^0(\epsilon) + u_3^0(\epsilon) + u_4^0(\epsilon),$$

where

$$u_1^0(\epsilon) = \mu(1_{x_1>0}\chi_\epsilon(x_1)\chi_{\sqrt{\epsilon}}(\xi_1)\xi_1 H_p a_o),$$
$$u_2^0(\epsilon) = \mu(1_{x_1>0}\epsilon^{-1}\chi_\epsilon'(x_1)\chi_{\sqrt{\epsilon}}(\xi_1)2\xi_1^2 a_o),$$
$$u_3^0(\epsilon) = \mu(1_{x_1>0}\chi_\epsilon(x_1)(\xi_1\epsilon^{-1/2}\chi_{\sqrt{\epsilon}}'(\xi_1) + \chi_{\sqrt{\epsilon}}(\xi_1))\partial_{x_1} r a_o),$$
$$u_4^0(\epsilon) = -\mu_1(\xi_1 a_o \chi_\epsilon(x_1)\chi_{\sqrt{\epsilon}}(\xi_1)).$$

Clearly $u_1^0(\epsilon) \to 0$ by dominated convergence. The same is true of $u_2^0(\epsilon)$: the function $\chi_\epsilon'(x_1)\chi_{\sqrt{\epsilon}}(\xi_1)2\xi_1^2 a_o$ is uniformly bounded as $\epsilon \downarrow 0$ since $\xi_1^2 \leq C\epsilon$ on $\operatorname{supp}\chi_{\sqrt{\epsilon}}(\xi_1)$. Next,

$$u_3^0(\epsilon) \to 0$$

as $\xi_1\epsilon^{-1/2}\chi_{\sqrt{\epsilon}}'(\xi_1) + \chi_{\sqrt{\epsilon}}(\xi_1)$ likewise remains uniformly bounded. Finally,

$$u_4^0(\epsilon) \to -\mu_1(1_{x_1=0}1_{\xi_1=0}\xi_1 a_o) = 0.$$

In particular, this implies by the dominated convergence theorem that

$$u^0(a_o 1_{x_1=\xi_1=0}) = 0$$

and so u^0 is supported by $\mathcal{H}$. $\qquad\square$

<u>Invariance away from glancing</u>: We now prove the integral invariance statement (i) away from glancing.

Lemma 4.10. *Suppose $\tilde{a} = \tilde{a}(x, \sigma, \xi') \in \mathcal{C}_c^\infty$ and let $a = \tilde{a}(x, x_1\xi_1, \xi')$. Furthermore, assume that for $\rho \in \operatorname{supp} a$, on $[-T, 0]$ $\varphi_{-t}(\rho)$ intersects $x_1 = 0$ at most once and in a hyperbolic point. Then,*

$$\mu(a) - \mu(a \circ \varphi_{-T}) = \int_{-T}^0 \mu_1(a \circ \varphi_{-s})\, ds.$$

Proof. Let $-T(\rho)$ be the time that $\varphi_{-T(\rho)}(\rho) \in \mathcal{H}$. Then

$$\int_{-T}^{0} H_p(a \circ \varphi_s)(\rho)\, ds = \int_{-T}^{-T(\rho)-0} H_p(a \circ \varphi_s)\, ds + \int_{-T(\rho)+0}^{0} H_p(a \circ \varphi_s)\, ds$$

$$= a \circ \varphi_{-T(\rho)-0}(\rho) - a \circ \varphi_{-T}(\rho) + a - a \circ \varphi_{-T(\rho)+0}(\rho).$$

Now, since at $x_1 = 0$, $a(0, x', \xi_1, \xi') = a(0, x', -\xi_1, \xi')$, $a \circ \varphi_{-T(\rho)-0} = a \circ \varphi_{-T(\rho)+0}$, we have

$$\int_{-T}^{0} H_p(a \circ \varphi_s)(\rho)\, ds = a(\rho) - a \circ \varphi_{-T}(\rho).$$

Now, by Lemma 4.9

$$\iint_{-T}^{0} H_p(a \circ \varphi_s)(\rho)\, ds\, d\mu(\rho) = (H_p^*\mu)\left(\int_{-T}^{0} a \circ \varphi_s\, ds\right) = \mu_1\left(\int_{-T}^{0} a \circ \varphi_s\, ds\right) + u^0\left[\left(\int_{-T}^{0} a \circ \varphi_s\, ds|_{\mathcal{H}}\right)_o\right].$$

Note that

$$\rho \mapsto \int_{-T}^{0} a \circ \varphi_s\, ds|_{\mathcal{H}}(\rho)$$

is even under $\xi_1 \mapsto -\xi_1$, since points $(x = 0, y, \pm\xi, \eta)$ over the hyperbolic set are both mapped to the same point in T^*M° under the short-time flow; thus the u^0 term vanishes. Therefore,

$$\int_{-T}^{0} \int a \circ \varphi_{-s}(\rho)\, d\mu_1\, ds = \mu_1\left(\int_{-T}^{0} a \circ \varphi_s\, ds\right) = \int a - a \circ \varphi_{-T}\, d\mu. \qquad \square$$

<u>Invariance on the glancing set</u>: We now turn to analysis at the glancing set. Our strategy will be to prove (i) for all $t < t_0$ fixed and small. To do this, we may break up the support of q by a partition of unity and work locally, assuming that q is replaced by a function a supported in a neighborhood U of a point $\rho \in \mathcal{G}$; we will show that for each such U, if t_0 is taken to be small, (i) holds with q replaced by a.

We will do this using a "layer stripping" argument. First, we "strip away" the hyperbolic layer using the invariance established in Lemma 4.10. In particular, recall that $\widetilde{\mathcal{G}}$ denotes the set of generalized bicharacteristics in U which encounter $\mathcal{G}$. Then we have already seen that (i) holds on $\widetilde{\mathcal{G}}^c$. Since $\widetilde{\mathcal{G}}^c$ is open, $\pi_* 1_{\widetilde{\mathcal{G}}^c} \mu$ satisfies

$$\pi_* 1_{\widetilde{\mathcal{G}}^c} \mu(q \circ \varphi_t) - \pi_* 1_{\widetilde{\mathcal{G}}^c} \mu(q) = \int_0^t \pi_* 2\,\mathrm{Im}\, 1_{\widetilde{\mathcal{G}}^c} \mu_1(q \circ \varphi_s)\, ds, \quad q \in \mathcal{C}_c^\infty(^bT^*M). \tag{4-11}$$

In particular, since (i) implies (ii), $1_{\widetilde{\mathcal{G}}^c} \mu$ satisfies

$$1_{\widetilde{\mathcal{G}}^c} \mu(H_p a) = 1_{\widetilde{\mathcal{G}}^c} \mu_1(a). \tag{4-12}$$

Subtracting this from (4-5) for μ, $\mu 1_{\widetilde{\mathcal{G}}}$ satisfies

$$\mu 1_{\widetilde{\mathcal{G}}}(H_p a) = 1_{\widetilde{\mathcal{G}}} \mu_1(a). \tag{4-13}$$

Thus we may turn our attention to studying the new measures $\mu 1_{\widetilde{\mathcal{G}}}$, $1_{\widetilde{\mathcal{G}}} \mu_1$. By a slight abuse of notation, *we assume henceforth that μ and μ_1 are supported on $\widetilde{\mathcal{G}}$.*

As we proceed through the proof, we will "strip away" the higher-order tangent layers. We start by showing that at points where the bicharacteristics of H_p are tangent to exactly order 2, the measure is invariant in the sense of (i). Once we have shown this, we can argue as we did to remove the hyperbolic set and replace the measure μ by $\mu 1_{\widetilde{\mathcal{G}} \geq 3}$. We then prove invariance on $\widetilde{\mathcal{G}}^k$ by induction. As before, the fact that (i) implies (ii) allows us to assume that μ is supported on $\widetilde{\mathcal{G}}^{\geq k}$. Then, since the flow is transverse to $\mathcal{G}^k$ we may work with a measure supported on $\widetilde{\mathcal{G}}^k$ when showing invariance at order k. We will obtain this invariance by using the transversality of the flow to $\mathcal{G}^k$ to show that there is no jump in the measure across these points. In particular, this argument will show that μ accumulates no mass across $\mathcal{G}^k$ and thus that the invariance continues to hold.

The case of $\mathcal{G}_d$: We choose the neighborhood of U of $\rho \in \widetilde{\mathcal{G}}_d$ so small that $U \cap (\mathcal{H} \cup \mathcal{G} \setminus \mathcal{G}_d) = \varnothing$. Next, suppose that $a \in \mathcal{C}_c^\infty(U)$. Recall that

$$\mu(H_p a) = \mu_1(a) + \mu(1_{x_1=0} \partial_{x_1} r a_o|_{\xi_1^2 = r(x,\xi')}) + u^0(a_o),$$

with u^0 supported in $\mathcal{H} \cap \operatorname{supp} \mu$ and $\mu(\mathcal{G}_d) = 0$. Since $\operatorname{supp} \mu \subset \widetilde{\mathcal{G}}$ and $\operatorname{supp} a \subset U$, we have

$$\mu(H_p a) = \mu_1(a),$$

and hence (4-4) holds since the generalized bicharacteristics through $\mathcal{G}_d$ are bicharacteristics of H_p.

The case of $\mathcal{G}_g$: Let $\widetilde{\mathcal{G}}_g$ be the set of generalized bicharacteristics encountering $\mathcal{G}_g$ in U. Recall that we may assume μ and μ_1 are supported on $\widetilde{\mathcal{G}}_g$ and may further choose U small enough so that $U \cap \widetilde{\mathcal{G}}_g \subset \mathcal{G}_g$; hence we may in fact assume at this stage that μ and μ_1 are supported by $\mathcal{G}_g$.

Let $a \in \mathcal{C}_c^\infty(U)$. For $q = q(x_1, x', x_1\xi_1, \xi')$, we have $1_{\mathcal{G}} H_p^G q = 1_{\mathcal{G}} H_p q$. Moreover, since $H_p^G x_1 = H_p^G \xi_1 = 0$, letting $a_0 = a|_{\xi_1 = 0}$,

$$1_{\mathcal{G}} H_p^G a = 1_{\mathcal{G}} H_p^G a_0 = 1_{\mathcal{G}} H_p a_0. \tag{4-14}$$

Now, since on U, $\operatorname{supp} \mu \subset \mathcal{G}_g$,

$$\mu(H_p^G a) = \mu(1_{\mathcal{G}_g} H_p^G a) = \mu(1_{\mathcal{G}_g} H_p^G a_0) = \mu(H_p a_0) = \mu_1(a_0) = \mu_1(1_{\mathcal{G}_g} a_0) = \mu_1(a). \tag{4-15}$$

Since H_p^G generates the bicharacteristic flow in $\mathcal{G}_g$, this implies (4-4).

Remark 4.11. While it may seem at first that the argument used for $\mathcal{G}_g$ applies directly to higher-order tangencies, we observe that it does not. In fact, the equality $\mu(H_p q) = \mu_1(q)$ for $q = q(x, x_1\xi_1, \xi')$ a priori only implies that μ mass can either "stick" to the boundary as in $\mathcal{G}_g$ or instantly detach from the boundary as in $\mathcal{G}_d$. It does not rule out either case. The facts that, in $\mathcal{G}_g$, trajectories which detach from the boundary instantly leave $\overline{M}$, while in $\mathcal{G}_d$, $\mu(\mathcal{G}_d) = 0$, rule out detaching from and sticking to the boundary at $\mathcal{G}_g$ and $\mathcal{G}_d$ respectively. In order to determine whether mass at a point of higher-order tangency sticks or detaches, we will use the transversality of the flow to such points to show that mass can neither accumulate nor dissipate.

Higher-order tangencies: Recall that

$$\mathcal{G}^k := \{\rho \in \mathcal{G} : (H_p^j x_1)(\rho) = 0 \text{ for } 0 \leq j < k \text{ and } (H_p^k x_1)(\rho) \neq 0\}.$$

We have shown that (4-3) holds for $a \in C_c^\infty(T^*M)$ with $\mathrm{supp}\, a \cap \mathcal{G}^k = \varnothing$ for $k \geq 3$. We now proceed by induction on k.

Let $r_0(x', \xi') = r(0, x', \xi')$ and $r_1(x,', \xi') = \partial_{x_1} r(0, x', \xi')$. Then note that by [Hörmander 1994, Lemma 24.3.1],

$$\mathcal{G}^k = \{x_1 = 0 = 1 - r(0, x', \xi'),\ H_{r_0}^j r_1 = 0,\ 0 \leq j < k-2,\ H_{r_0}^{k-2} r_1 \neq 0\}.$$

For each k, let $\widetilde{\mathcal{G}}^k$ denote the set of generalized bicharacteristics encountering $\mathcal{G}^k$ in a small fixed neighborhood of $\mathcal{G}^k$.

Suppose (4-4) holds for $q \in C_c^\infty(T^*M)$ with $\mathrm{supp}\, q \cap \widetilde{\mathcal{G}}^k = \varnothing$ for $k \geq M-1$. We show that (4-4) holds for $a \in C_c^\infty(T^*M)$ with $a \cap \widetilde{\mathcal{G}}^k = \varnothing$ for $k \geq M$.

Let $\rho \in \mathcal{G}^M$ and U a neighborhood of ρ so that $U \cap \mathcal{G}^k = \varnothing$ for $k > M$. As before, we may assume μ and μ_1 are supported on $\widetilde{\mathcal{G}}^{\geq M}$; thus by our choice of U, we may in fact assume without loss of generality that μ, μ_1 are supported on $\widetilde{\mathcal{G}}^M$. Let (x_2, ρ) be coordinates on $T^*(\partial M)$ so that $\partial_{x_2} = H_{r_0}$. Shrinking U if necessary, by the implicit function theorem there exists $\Theta(\rho)$ such that on U

$$\widetilde{\mathcal{G}}^M \cap \mathcal{G}^M = \{(x, \xi) \in \widetilde{\mathcal{G}}^M : x_2 = \Theta(\rho)\}.$$

Let

$$\widetilde{\mathcal{G}}_0 := \widetilde{\mathcal{G}}^M \cap \mathcal{G}^M,$$
$$\widetilde{\mathcal{G}}^+ := \{(x, \xi) \in \widetilde{\mathcal{G}}^M : x_2 > \Theta(\rho)\}, \quad \widetilde{\mathcal{G}}^- : \{(x, \xi) \in \widetilde{\mathcal{G}}^M : x_2 < \Theta(\rho)\}.$$

We write

$$\mu 1_{\widetilde{\mathcal{G}}^M} = \mu_- + \mu_+ + \Upsilon, \quad \mu_- = 1_{\widetilde{\mathcal{G}}^-}\mu, \quad \mu_+ = 1_{\widetilde{\mathcal{G}}^+}\mu, \quad \Upsilon = 1_{\widetilde{\mathcal{G}}_0}\mu.$$

Then, for $q = q(x_1, x', x_1\xi_1, \xi')$ supported in U,

$$\Upsilon(H_p q) = -\mu_-(H_p q) - \mu_+(H_p q) + \mu_1(q). \tag{4-16}$$

Let

$$\widetilde{H}(\rho) = \begin{cases} H_p(\rho), & \rho \notin \mathcal{G}_g, \\ H_p^G(\rho), & \rho \in \mathcal{G}_g; \end{cases}$$

this vector field generates the bicharacteristic flow on $\widetilde{\mathcal{G}}^M$, so by our inductive hypothesis,

$$\widetilde{H}^*\mu = \mu_1 \tag{4-17}$$

on $\widetilde{\mathcal{G}}^M \setminus \mathcal{G}^M$. Moreover, since on $\widetilde{\mathcal{G}}^0$ we have $H_p^M x_1 \neq 0$, the flow within U (perhaps after further shrinking that set) for forward and backward time is either in $\{x_1 > 0\}$ or lies entirely in $\mathcal{G}_g$ (with separate cases for forward/backward flow depending on the parity of M and the sign of $H_p^M x_1$). In either case, the flow stays away from $\mathcal{H}$, and hence is generated by $\widetilde{H}$ on $\widetilde{\mathcal{G}}^M \cap U$.

Now as in Lemma 3.10 and the surrounding discussion, given any continuous a defined on $\mathcal{G}_0$ and $\psi \in C_c^\infty(\mathbb{R})$, we extend a to be constant on the flow, and set

$$\mu_a^\sharp(\psi) = \mu(\psi(s) a(\rho));$$

here we are using $\rho \in \mathcal{G}_0$ together with $s \in \mathbb{R}$ as local (nonsmooth) coordinates on $\widetilde{\mathcal{G}}^M$ defined by the flow, mapping $(-\delta, \delta) \times \mathcal{G}_0$ homeomorphically to $\widetilde{\mathcal{G}}^M$ via $(s, \rho) \mapsto \exp(t\widetilde{H})(\rho)$. Just as in Lemma 3.10, the flow invariance established on $\widetilde{\mathcal{G}}^M \backslash \mathcal{G}_0$ implies that $\mu_a^\sharp$ is AC with respect to Lebesgue measure on $\mathbb{R} \backslash 0$; moreover the Radon–Nikodym derivative is itself bounded by a multiple of $\sup|a|$, and hence is a function of s with values in measures on $\mathcal{G}_0$, denoted by $G(s)$. Finally, let $\operatorname{tr} \dot{\mu}_\pm = G(0^\pm)$ denote the restrictions of these functions to $\mathcal{G}_0$ from left and right; these are well-defined since the relation (4-17) together with the arguments in Lemma 3.11 show that G is continuous on $s \le 0$ and on $s \ge 0$ separately but that there may be a jump at $s = 0$.

Moreover, denoting the function $\psi(s)a(\rho)$ by $\psi \otimes a$, for $0 \notin \operatorname{supp} \psi$, we have $\mu(\psi' \otimes a) = \mu_1(\psi \otimes a)$. So in particular,

$$\int [G(a)](s)\psi'(s)\,ds = \mu_1(\psi \otimes a).$$

Now, let $\chi \in \mathcal{C}_c^\infty(\mathbb{R})$ with $\chi \equiv 1$ on $[-1, 1]$ and $\operatorname{supp} \chi \subset (-2, 2)$ and $\chi_\epsilon(s) = \chi(\epsilon^{-1}s)$. Then,

$$\begin{aligned}
\mu((1 - \chi_\epsilon(s))\widetilde{H}(\psi \otimes a)) &= \mu(\widetilde{H}[(1 - \chi_\epsilon)\psi] \otimes a) + \mu([\psi \otimes a]\widetilde{H}\chi_\epsilon) \\
&= \mu(\widetilde{H}[(1 - \chi_\epsilon)\psi \otimes a]) + \mu(\epsilon^{-1}\psi\chi'(\epsilon^{-1}\cdot) \otimes a) \\
&= \mu_1((1 - \chi_\epsilon)\psi \otimes a) + \mu(\epsilon^{-1}\psi\chi'(\epsilon^{-1}\cdot) \otimes a).
\end{aligned}$$

Thus,

$$\begin{aligned}
\mu(\epsilon^{-1}\psi\chi'(\epsilon^{-1}\cdot) \otimes a) &= \epsilon^{-1}\int_{\mathbb{R}\backslash 0} [G(a)](s)\chi'(\epsilon^{-1}s)\psi(s)\,ds \\
&= \psi(0)(G_a(0^-) - G_a(0^+)) - \int_{\mathbb{R}\backslash 0} G_a(s)\chi_\epsilon(s)\psi'(s)\,ds + \mu_1(\chi_\epsilon\psi \otimes a) \\
&\to \psi(0)(G_a(0^-) - G_a(0^+)) + \mu_1((\psi \otimes a)1_{\widetilde{\mathcal{G}}^0}).
\end{aligned}$$

In particular,

$$\begin{aligned}
\mu_+(\widetilde{H}\psi \otimes a) + \mu_-(\widetilde{H}\psi \otimes a) &= \psi(0)([G(a)](0^-) - [G(a)](0^+)) + \mu_1(\psi \otimes a) \\
&= \operatorname{tr}\dot{\mu}_+(\psi \otimes a) - \operatorname{tr}\dot{\mu}_-(\psi \otimes a) + \mu_1(\psi \otimes a). \quad\quad (4\text{-}18)
\end{aligned}$$

Now we claim that we may also apply (4-16) to the function $q = \psi \otimes a$. We begin by approximating a with a smooth function on $\mathcal{G}_0$. Since $\widetilde{H}$ locally generates the flow and is at least Lipschitz across $\mathcal{G}_0$, we find that the flow on $\widetilde{\mathcal{G}}^M$ is at least $\mathcal{C}^1$. We note further that $\widetilde{\mathcal{G}}^M$ is without loss of generality disjoint from $\mathcal{H}$ (after appropriately shrinking U) since depending on the parity and sign of $H_p^M x_1$ along $\mathcal{G}_0$ the flow is either gliding or enters $x_1 > 0$ in each of $\widetilde{\mathcal{G}}^\pm$. In particular, $\pi(\widetilde{\mathcal{G}}^M) \subset {}^bT^*M$ is $\mathcal{C}^1$. Moreover,

$$(-\delta, \delta) \times \mathcal{G}_0 \to \pi(\widetilde{\mathcal{G}}^M), \quad (s, q) \mapsto \varphi_s(q),$$

are $\mathcal{C}^1$ coordinates on $\widetilde{\mathcal{G}}^M$. Hence $b = \pi^*\psi \otimes a$ is $\mathcal{C}^1$ on $\pi(\widetilde{\mathcal{G}}^M)$ and we may extend b to $\tilde{b}$, a $\mathcal{C}^1$ function on ${}^bT^*M$. Equivalently, setting $\tilde{q} = \pi^*\tilde{b}$, we have $\tilde{q} = \tilde{b}(x, x_1\xi_1, \xi')$ with $\tilde{b}$ a $\mathcal{C}^1$ function of its arguments and $\tilde{q}|_{\widetilde{\mathcal{G}}^M} = \psi \otimes a$.

Since $\tilde{b}$ is $\mathcal{C}^1$, we may approximate it in $\mathcal{C}^1$ by smooth functions $\tilde{b}_\epsilon$ and hence we obtain using the dominated convergence theorem that (4-16) holds for $\tilde{q}$. Finally, since $\tilde{q}|_{\widetilde{\mathcal{G}}^M} = \psi \otimes a$ and $\operatorname{supp}\mu \subset \widetilde{\mathcal{G}}^M$,

we obtain (4-16) for $q = \psi \otimes a$. Moreover, since $\mu_\pm$ are each supported in the interior or $\mathcal{G}_g$, we can replace $\widetilde{H}$ by H_p in (4-18).

Now (4-16) and (4-18) yield

$$\Upsilon(H_p\psi \otimes a) = -\operatorname{tr}(\dot{\mu}_+)(\psi \otimes a) + \operatorname{tr}(\dot{\mu}_-)(\psi \otimes a), \tag{4-19}$$

and hence

$$|\Upsilon(H_p\psi \otimes a)| \le C|\sup \psi \otimes a|.$$

Since Υ is supported at $\widetilde{\mathcal{G}}^0$, and the collection of functions $\psi \otimes a$ is dense, this implies that, for all q,

$$|\Upsilon(H_pq)| \le C|\sup q|.$$

Then, using that Υ is a measure supported at $\widetilde{\mathcal{G}}_0$ and H_p is transverse to $\widetilde{\mathcal{G}}_0$, this implies $\Upsilon = 0$. Finally, inserting $\Upsilon = 0$ into (4-19) yields

$$\operatorname{tr}(\dot{\mu}_-) = \operatorname{tr}(\dot{\mu}_+).$$

Moreover, since μ_1 is absolutely continuous with respect to μ, we have $\mu_1 1_{\widetilde{\mathcal{G}}^0} = 0$.

Let $\psi_{t_0}(s) = \psi(s + t_0)$. Then $(\psi \otimes a) \circ \varphi_t = \psi_t \otimes a$ and

$$\begin{aligned}
\mu(\psi_{t_0} \otimes a) - \mu(\psi \otimes a) &= \int_0^{t_0} \partial_t \int [G(a)](s)\psi(s + t) \, ds \, dt \\
&= \int_0^{t_0} \int_{-\infty}^0 [G(a)](s)\psi'(s + t) \, ds + \int_0^\infty [G(a)](s)\psi'(s + t) \, dt \\
&= \int_0^{t_0} \int_{-\infty}^\infty \mu_1(\psi_t \otimes a) \, ds + \operatorname{tr} \dot{\mu}_-(a)\psi(t) - \operatorname{tr} \dot{\mu}_+(a)\psi(t) dt \\
&= \int_0^{t_0} \mu_1(\psi_t \otimes a) \, dt.
\end{aligned}$$

In particular, we have

$$\mu((\psi \otimes a) \circ \varphi_{t_0}) - \mu(\psi \otimes a) = \int_0^{t_0} \mu_1([\psi \otimes a] \circ \varphi_t) \, dt.$$

Since the collection of functions of the form $\psi \otimes a$ is dense in $\mathcal{C}^0(^bT^*M)$, this completes the proof that μ is invariant on $\widetilde{\mathcal{G}}^M$.

As there are no infinite-order tangencies, $\mathcal{G} = \bigcup_M \mathcal{G}^M$ and this completes the proof of (4-4). □

Finally, to complete the proof of (1-3) we use Proposition 3.9 and the following lemma.

Lemma 4.12. *Suppose that μ satisfies (4-3). Let $\psi \in \mathcal{C}_c^1(\mathbb{R})$, Σ be a hypersurface transverse to the generalized bicharacteristic flow so that $\varphi_t : \mathbb{R} \times \Sigma \to {}^bT^*M$ is a homeomorphism onto its image, and $a \in \mathcal{C}_c^0(\Sigma)$. Define $f_{\psi,a}(\varphi_t(\rho)) = \psi(t)a(\rho)$. Then*

$$\pi_*\mu(f_{\partial_t\psi,a}) = 2\operatorname{Im}\mu^j(f_{\psi,a}).$$

Proof. We have, for $q \in \mathcal{C}_c^\infty(^bT^*M)$,

$$\partial_t \pi_*\mu(q \circ \varphi_t)|_{t=0} = 2\operatorname{Im}\mu^j(q).$$

Therefore, it is enough to show that we can move the derivative inside $\pi_* \mu$. This follows from the dominated convergence theorem since $\pi_* \mu(\mathcal{H}) = 0$. Now approximation of $f_{\psi, a}$ by smooth functions gives the result. $\qquad \square$

In order to obtain the required uniformity, we adjust the set $\mathcal{C}$ by fixing neighborhood U of Ω in which we assume that for $\{g_k\}_{k=1}^\infty \subset \mathcal{C}$ we not only have $\|g - g_{k_m}\|_{\mathcal{C}^{1,\gamma}} \to 0$ for some $\gamma > 0$ but also $\|g - g_{k_m}\|_{\mathcal{C}^\infty(U)} \to 0$. Arguing as in Section 3E then completes the proof of Theorem 2 when $\Omega \neq \varnothing$.

5. Lower bounds on manifolds without boundary

The idea behind our proof of the lower bounds in Theorem 1 is that near any segment of a geodesic γ, which is not trapped, P is *globally* microlocally equivalent to hD_{x_1} and hence it is enough to construct examples which saturate the $L^2_{\text{comp}} \to L^2_{\text{loc}}$ bounds for the solution operator for hD_{x_1} where we impose the condition that the solution be supported in $x_1 \geq 0$.

Let U be an open set. Assume there exists a null bicharacteristic curve γ such that

$$\{\pi(\gamma(s)) : s \in (0, L)\} \subset U, \quad \pi(\gamma(s)) \notin U \text{ for } s \notin (0, L). \tag{5-1}$$

For any interval I (open or closed), let

$$\Gamma_I \equiv \{\gamma(s) : s \in I\} \subset T^*M, \quad \Gamma_I^0 = \{x_1 \in I : \xi_1 = 0, x' = \xi' = 0\} \subset T^*\mathbb{R}^n.$$

Lemma 5.1. *There exist neighborhoods $V \subset T^*M$ of $\Gamma_{[0,L]}$, $U \subset T^*\mathbb{R}^n$ of $\Gamma_{[0,L]}^0$ and a symplectomorphism $\kappa : U \to V$ with*

$$\kappa : \Gamma_{[0,L]}^0 \to \Gamma_{[0,L]}, \quad \kappa^* p = \xi_1.$$

Proof. Let $\rho_0 = \gamma(0)$. Then by Darboux's theorem, there exist neighborhoods $V_1 \subset T^*M$ of ρ_0, $U_1 \subset T^*\mathbb{R}^n$ of 0 and a symplectomorphism $\kappa_1 : U_1 \to V_1$ so that

$$\kappa_1^* p = \xi_1, \quad \kappa_1 : \Gamma_{[0,L]}^0 \cap U_1 \to \Gamma_{[0,L]} \cap V_1.$$

We will extend κ_1 so that its image covers a neighborhood of $\Gamma_{[0,L]}$. For this, let $\Sigma := \kappa_1(\{x_1 = 0\} \cap U_1)$. Shrinking U_1 if necessary, we assume that there is $\epsilon > 0$ so that

$$(-\epsilon, L + \epsilon) \times \Sigma \to V \subset T^*M, \quad (t, q) \mapsto \varphi_t(q),$$

is a diffeomorphism onto its image, V. Then, let

$$x_i(\varphi_t(q)) = x_i(\kappa_1(q)), \quad 1 < i \leq n, \qquad \xi_i(\varphi_t(q)) = \xi_i(\kappa_i(q)), \quad 1 \leq i \leq n, \qquad x_1(\varphi_t(q)) = t.$$

In particular, we have

$$H_p x_i = 0, \quad 1 < i \leq n, \qquad H_p \xi_i = 0, \quad 1 \leq i \leq n, \qquad H_p x_1 = 1.$$

By Jacobi's identity, for $f, g \in \mathcal{C}^\infty(T^*M)$,

$$H_p\{g, f\} = \{g, H_p f\} - \{f, H_p g\}.$$

Therefore, since the corresponding identities hold at Σ,

$$\{x_i, x_j\} = 0, \quad \{\xi_i, \xi_j\} = 0, \quad \{\xi_i, x_j\} = \delta_{ij}.$$

In particular, this implies that $\kappa^{-1} : V \to T^*\mathbb{R}^n$

$$\kappa^{-1}(q) := (x(q), \xi(q))$$

is a symplectomorphism onto its image, U. Furthermore, since p is invariant under H_p, we have $\kappa^* p = \xi_1$, and hence also $\kappa(\Gamma^0_{[0,L]}) = \Gamma_{[0,L]}$. $\qquad\square$

Proposition 5.2. *Let γ be a geodesic and $U \subset M$ satisfy (5-1). Then for any $\epsilon > 0$ there exists $\chi \in \mathcal{C}_c^\infty(U)$ and $f \in L^2$ with $\operatorname{supp} f \subset \{\chi = 1\}$ and $u \in L^2_{\mathrm{loc}}$ with*

$$Pu = f$$

and

$$\mathrm{WF}_h\, u \subset \bigcup_{s \geq 0} [\exp(s H_p)\, \mathrm{WF}_h\, f],$$

and where

$$\|\chi u\|_{L^2} \geq \left(\frac{2L - \epsilon}{\pi h}\right) \|f\|_{L^2}.$$

Note that u is purely microlocally outgoing by the wavefront set statement, and hence is given by the outgoing resolvent applied to f (modulo $O(h^\infty)$).

Proof. We first let κ be a symplectomorphism from $T^*\mathbb{R}^n$ into T^*M with

$$\kappa : \Gamma^0_{[0,L]} \to \Gamma_{[0,L]}, \quad \kappa^* p = \xi_1,$$

where

$$\Gamma^0_I = \{x_1 \in I : \xi_1 = 0, x' = \xi' = 0\};$$

this exists by Lemma 5.1.

Now quantize κ to a microlocally unitary FIO $T : \mathcal{C}_c^\infty(\mathbb{R}^n) \to \mathcal{C}_c^\infty(M)$ with parametrix S such that $ST - I$, $TS - I$ have no microsupport near $\Gamma^0_{[0,L]}$ and $\Gamma^0_{[0,L]}$ respectively and such that

$$Th D_1 = PT + O(h^\infty) \text{ microlocally near } \Gamma^0_{[0,L]}.$$

(There are no obstructions to such a quantization as long as we work on a contractible neighborhood of Γ^0.) Assume without loss of generality that T is defined on a δ_0-neighborhood of $\Gamma^0_{[0,L]}$.

Now for any $\delta < \delta_0$ we define on $\mathbb{R}^n$

$$f_0 = \begin{cases} \varphi(x') \cos \pi (x_1 - \delta)/2(L - 2\delta), & x_1 \in [\delta, L - \delta], \\ 0, & \text{otherwise}, \end{cases}$$

where φ is smooth and compactly supported in $B(0, \delta)$, with

$$\int |\varphi(x')|^2 \, dx' = 1.$$

Let

$$v_0 = \begin{cases} 0, & x_1 < \delta, \\ ih^{-1}(2(L-2\delta)/\pi)\varphi(x')\sin\pi(x_1-\delta)/2(L-2\delta), & x_1 \in [\delta, L-\delta], \\ ih^{-1}(2(L-2\delta)/\pi)\varphi(x'), & x_1 > L-\delta. \end{cases}$$

Thus of course $hD_1v_0 = f_0$ as distributions. Let $\psi(x_1)$ be a smooth cutoff function supported in $(0, L-\delta/4)$ and equal to 1 on $[\delta, L-\delta/2]$. Set $u_0 = \psi(x_1)v_0$, $w = Tu_0$, and $f = Tf_0$ Then modulo $O(h^\infty)$,

$$Pw \equiv PTu_0 \equiv ThD_{x_1}u_0 \equiv Tf_0 + Tr_0 \equiv f + r,$$

where r_0 is the error term coming from the $hD_1(\psi)$ term. Note that

$$\mathrm{WF}\, r_0 \subset \{x_1 \in [L-\delta/2, L-\delta/4] : |x'| < \delta,\ \xi = 0\},$$

which is thus in an arbitrarily small neighborhood of the endpoint of $\Gamma^0_{[0,L]}$. Thus by the construction of T, $r \equiv Tr_0$ has wavefront set in an arbitrarily small neighborhood of $\gamma(L)$ (as $\delta \downarrow 0$).

Note also that we may construct a cutoff function $\chi \in \mathcal{C}^\infty_c(U)$ such that

$$\chi = \begin{cases} 1 & \text{on } \mathrm{WF}_h\, f, \\ 0 & \text{on } \pi\{\exp(sH_p)(\mathrm{WF}_h\, r) : s \geq 0\}. \end{cases}$$

This follows from our hypotheses since on $\mathbb{R}^n$ f is supported on $x_1 \in [\delta, L-\delta]$ in a small neighborhood of Γ^0, while

$$\mathrm{WF}_h\, r_0 \subset x_1 \in [L-\delta/2, L-\delta/4],$$

and the forward flowout is thus contained (in these local coordinates) in $\{x_1 \geq L-\delta/2\}$. Since the Hamilton flow is nonradial and x_1 maps to the flow parameter under κ, we know that $\mathrm{WF}_h\, r_0$ is separated from a neighborhood of $\Gamma_{[0,L-\delta]}$ in *base* variables, not just in the cotangent bundle, and shrinking δ if necessary we obtain the separation in the base variables. Note for use below that since $\chi = 1$ on $\mathrm{WF}_h\, f$, pulling back by T yields a fortiori $\kappa^*(\chi) = 1$ on $\mathrm{WF}_h\, f_0$ and hence

$$\kappa^*(\chi) = 1 \quad \text{on } \{x_1 \in [\delta, L-\delta] : |x'| < \delta,\ \xi = 0\}. \tag{5-2}$$

Finally we set

$$u = w - (P-i0)^{-1}r$$

so that

$$Pu = f.$$

Owing to the propagation of singularities for the outgoing resolvent, $\mathrm{WF}_h(u-w)$ lies in the *forward flowout* of $\mathrm{WF}_h\, r$; by construction this $\mathrm{WF}_h\, r$ is disjoint from the support of χ and by our geometric hypotheses, its forward flowout *remains* disjoint from U: here we use the fact that $\pi\gamma(L+s) \notin U$ for $s > 0$ and indeed this point escapes to infinity; hence $\pi\exp(sH_p)(\gamma(L)) \notin \mathrm{WF}_h\, f$ for all $s > 0$. By continuity, the same is true with $\gamma(L)$ replaced by any point in $\mathrm{WF}_h\, r$ for δ sufficiently small. Thus,

$$\chi u = \chi w + O(h^\infty).$$

By microlocal unitarity of T we compute by the Egorov theorem

$$\|\chi u\|^2 = \|\chi w\|^2 + O(h^\infty) = \|S\chi TSw\|^2 + O(h^\infty) = \|\mathrm{Op}(\kappa^*\chi)u_0\|^2 + O(h)$$

$$\geq \int_\delta^{1-\delta} \int_\delta^{L-\delta} |v_0|^2 \, dx' \, dx_1 + O(h)$$

$$\geq \int_\delta^{1-\delta} \int_\delta^{L-\delta} h^{-2} \frac{4(L-2\delta)^2}{\pi^2} |\varphi(x')|^2 \sin^2 \frac{\pi(x_1-\delta)}{2(L-2\delta)} \, dx' \, dx_1 + O(h)$$

$$= \frac{\pi}{4} \frac{1}{h^2\mu^3} + O(h),$$

where

$$\mu = \frac{\pi}{2(L-2\delta)};$$

here we have used the fact that $\kappa^*\chi$ equals 1 on the zero section over $[\delta, L-\delta] \times B(0, \delta)$, while the semiclassical wavefront set of u_0 lies within the zero section; hence the last inequality follows by existence of a microlocal parametrix for $\mathrm{Op}(\kappa^*\chi)$ on this set.

Meanwhile,

$$\|f\|^2 = \int_\delta^{1-\delta} \int_\delta^{L-\delta} |\varphi(x')|^2 \cos^2 \frac{\pi(x_1-\delta)}{2(L-2\delta)} \, dx' \, dx_1 = \frac{\pi}{4} \frac{1}{\mu}.$$

Thus

$$\frac{\|\chi u\|}{\|f\|} \geq \frac{1}{h\mu} = \frac{2(L-2\delta)}{\pi h}. \qquad \square$$

Finally, we apply [Proposition 5.2](#) in the case of a nontrapping manifold with Euclidean ends and $P = -h^2\Delta_g - 1$. Let $R_1 < R' < R''$ so that $B(0, R'') \subset \{\chi \equiv 1\}$. By the definition of $L(g, R'')$, there is a null-bicharacteristic (a speed-2 geodesic lifted to S^*M) γ with $\pi\gamma(0) \in \partial B(0, R'')$, $\pi\gamma(s) \in B(0, R'')$ for $s \in (0, L(g, R''))$ and $\gamma(s) \notin B(0, R'')$ for $s > L(g, R'')$. In particular, since $L(g, R') < L(g, R'')$, [Proposition 5.2](#) applies to γ with $U = B(0, R'')$ and $\epsilon < 2L(g, R'') - 2L(g, R')$. In particular, there exist $f \in L^2(M)$ with supp $f \subset B(0, R'')$ so that

$$Pu = hf, \quad \mathrm{WF}_h u \subset \bigcup_{s \geq 0} [\exp(sH_p) \, \mathrm{WF}_h \, f] \tag{5-3}$$

and

$$\|u\|_{L^2(B(0,R''))} \geq \frac{2L(g, R'') - 2L(g, R'') + 2L(g, R')}{\pi} \|f\|_{L^2} = \frac{2L(g, R')}{\pi} \|f\|_{L^2}.$$

Next, observe that [(5-3)](#) implies

$$u = (-h^2\Delta_g - 1 - i0)^{-1}hf + O(h^\infty\|f\|_{L^2})_{L^2_{\mathrm{loc}}}.$$

In particular, letting $k = h^{-1}$,

$$\|\chi(-\Delta_g - k^2 - i0)^{-1}f\|_{L^2} \geq \left(\frac{2L(g, R')}{\pi k} - C_N k^{-N} \right) \|f\|_{L^2}$$

completing the proof of the lower bound in [Theorem 1](#).

6. Application to numerical analysis of the finite-element method

6A. *Summary.* In this section, we focus on the implications the bound (1-8) has on the numerical analysis of solving the Helmholtz exterior Dirichlet problem by the finite-element method (FEM). We mention two other numerical-analysis applications of (1-8) in Remarks 6.8 and 6.9 at the end.

We consider the *h-version* of the FEM; i.e., the solution is approximated in spaces of piecewise polynomials of fixed degree on a mesh with mesh width h_{FEM} (we use this notation to avoid a notational clash with the semiclassical parameter $h := k^{-1}$ in the rest of the paper). The question of how fast h_{FEM} must decrease with k to maintain accuracy as $k \to \infty$ was thoroughly investigated in the case of the *constant-coefficient* Helmholtz equation (i.e., (6-2) below with $A = I$ and $\nu = 1$) by [Ihlenburg and Babuška 1995; 1997] when $d = 1$ and by [Melenk 1995; Melenk and Sauter 2010; 2011; Esterhazy and Melenk 2012] when $d = 2, 3$. For example, in the case of piecewise-linear polynomials, and when the solution of the boundary value problem is nontrapping, the FEM satisfies a *quasioptimal* error estimate (of the form (6-22) and (6-29) below) when

$$h_{\mathrm{FEM}} k^2 \leq c \tag{6-1}$$

for a sufficiently small constant c (the case when the boundary value problem is trapping is more complicated; see [Chandler-Wilde et al. 2017, Section 1.4] for some initial results).

In this section, we use the bound (1-8) to prove the analogue of the result above in the case of the *variable-coefficient* Helmholtz equation ((6-2) below) posed in the exterior of a nontrapping Dirichlet obstacle (see Theorem 3 below). In particular, we show how the constant c in (6-1) depends on the constant in (1-8). The key point is that our bound on h_{FEM} shows explicitly how the constant c in (6-1) *decreases* (i.e., the requirement on h_{FEM} for quasioptimality becomes more stringent) as the length of the longest ray *increases*.

6B. *The Helmholtz exterior Dirichlet problem and FEM set-up.*

Motivation from applications. Several important physical applications involve the PDE

$$\nabla \cdot (A \nabla u) + k^2 \nu u = -f \tag{6-2}$$

posed in $\mathbb{R}^n \setminus \Omega$, where A is a symmetric positive-definite matrix-valued function of position and ν is a strictly positive scalar-valued function of position. One example is via reductions of the time-harmonic Maxwell equations

$$\operatorname{curl} H + ik\epsilon E = (ik)^{-1} J, \quad \operatorname{curl} E - ik\mu H = 0 \quad \text{in } \mathbb{R}^3, \tag{6-3}$$

when all the fields involved depend only on two Cartesian space variables, say x and y. In the transverse-magnetic (TM) mode, J and E are given by $J = (0, 0, J_z(x, y))$ and $E = (0, 0, E_z(x, y))$ so, when additionally the permittivity ϵ is a scalar and the permeability μ satisfies

$$\mu = \begin{pmatrix} \tilde{\mu} & 0 \\ 0 & 1 \end{pmatrix} \tag{6-4}$$

for $\tilde{\mu}$ a 2×2 symmetric positive-definite matrix, E_z satisfies (6-2) with $\nu = \epsilon$,

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}^T (\tilde{\mu})^{-1} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \tag{6-5}$$

and $f = J_z$. Similarly, in the case of the transverse-electric (TE) mode, J and H are given by $J = (J_x(x, y), J_y(x, y), 0)$ and $H = (0, 0, H_z(x, y))$, so that when μ is a scalar and ϵ satisfies an equation analogous to (6-4), H_z satisfies (6-2) with A given by (6-5) with $\tilde{\mu}$ replaced by $\tilde{\epsilon}$, $\nu = \mu$, and

$$f = -\frac{1}{ik} \nabla \cdot \left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} (\tilde{\epsilon})^{-1} \begin{pmatrix} J_x \\ J_y \end{pmatrix} \right].$$

Additionally, the so-called acoustic-approximation of the elastodynamic wave equation is (6-2) with A the inverse of the (scalar) density and ν the inverse of the (scalar) bulk modulus; see, e.g., the derivation in [Chaumont-Frelet 2015, Section 1.2.6].

Placing the PDE (6-2) *in the framework of Section 1A.* We let $M := \mathbb{R}^n \setminus \Omega$, where Ω is a compact set such that its complement is connected,

$$g^{ij} := \frac{A_{ij}}{\nu}, \quad L_j := \sum_{i=1}^n \frac{g^{ij}}{\sqrt{\det g}} \partial_i (\sqrt{\det g}) + \sum_{i=1}^n \partial_i (g^{ij}) - \sum_{i=1}^n \frac{1}{\nu} \partial_i (A_{ij}), \quad L := 0,$$

and

$$P(g)\varphi := -\frac{1}{\nu} \sum_{i,j=1}^n \partial_i (A_{ij} \partial_j \varphi),$$

and then observe that (1-6) is satisfied, since

$$\Delta_g \varphi := \sum_{i,j=1}^n \frac{1}{\sqrt{\det g}} \partial_i (\sqrt{\det g} \, g^{ij} \, \partial_j \varphi).$$

With these definitions, the PDE (6-2) is $(P(g) - k^2)u = f/\nu$. The operator P_Ω is then self-adjoint with respect to $L^2(\mathbb{R}^n \setminus \Omega; \nu)$ and the H^1 norm defined by (1-7) becomes

$$\|\varphi\|_{H^1_\nu(\mathbb{R}^n \setminus \Omega)}^2 := \int_{\mathbb{R}^n \setminus \Omega} ((A\nabla\varphi) \cdot \overline{\nabla\varphi} + k^2 \nu |\varphi|^2) \, dx. \tag{6-6}$$

In this section (*Section 6*) *only*, to make contact with the standard numerical-analysis literature, *we use nonsemiclassically scaled Sobolev spaces*; i.e., the norms on the spaces H^s do *not* include powers of k unless otherwise indicated. Indeed, in this section we write (6-6) as the weighted H^1 norm

$$\|\varphi\|_{H^1_{k,A,\nu}(\mathbb{R}^n \setminus \Omega)}^2 := \|A^{1/2} \nabla\varphi\|_{L^2(\mathbb{R}^n \setminus \Omega)}^2 + k^2 \|\nu^{1/2}\varphi\|_{L^2(\mathbb{R}^n \setminus \Omega)}^2, \tag{6-7}$$

and we use analogous notation for norms over subsets of $\mathbb{R}^n \setminus \Omega$. We also define the norms

$$\|\varphi\|_{H^m(\mathbb{R}^n \setminus \Omega)}^2 := \sum_{|\alpha| \le m} \int_{\mathbb{R}^n \setminus \Omega} |\partial^\alpha \varphi|^2 \, dx;$$

i.e., if there are no A, ν in the subscript, the H^m norm is the "standard" H^m norm on $\mathbb{R}^n$.

By (1-1), $L(\nu A^{-1}, \Omega, R)$ is the length of the longest generalized bicharacteristic (informally, ray) in $B(0, R) \setminus \Omega$. Recall that, in the case $\Omega = \varnothing$, the (generalized) bicharacteristics are the projections in x of

the solutions $(x(s), \xi(s)) \in \mathbb{R}^n \times \mathbb{R}^n$ of the Hamiltonian system

$$\frac{dx_i}{ds}(s) = \frac{\partial}{\partial \xi_i} H(x(s), \xi(s)), \quad \frac{d\xi_i}{ds}(s) = -\frac{\partial}{\partial x_i} H(x(s), \xi(s)), \tag{6-8}$$

where the Hamiltonian $H(x, \xi)$ is given by

$$H(x, \xi) := \frac{1}{\nu(x)} \sum_{i=1}^n \sum_{j=1}^n A_{ij}(x)\xi_i \xi_j - 1. \tag{6-9}$$

Exterior Dirichlet problem and its variational formulation. With Ω a compact set such that its complement is connected, we define $\Omega_+ := \mathbb{R}^n \setminus \Omega$. Since the vast majority of numerical-analysis applications of the Helmholtz equation are in two and three dimensions, we restrict attention to $d = 2, 3$. Let $\gamma : H^1_{\text{loc}}(\Omega) \to H^{1/2}(\partial\Omega)$ be the trace operator. Let A be a symmetric positive-definite matrix-valued function of position such that $\text{supp}(I - A)$ is a compact subset of $\mathbb{R}^n$. Let ν be a strictly positive scalar-valued function of position such that $\text{supp}(1 - \nu)$ is a compact subset of $\mathbb{R}^n$. Let $A_{\min}$ and $A_{\max}$ be such that

$$A_{\min} \le A(x) \le A_{\max} \quad \text{for all } x \in \Omega_+, \text{ in the sense of quadratic forms,} \tag{6-10}$$

and $\nu_{\min}$ and $\nu_{\max}$ be such that

$$\nu_{\min} \le \nu(x) \le \nu_{\max} \quad \text{for all } x \in \Omega_+. \tag{6-11}$$

We consider solving *both* the exterior Dirichlet problem

$$\nabla \cdot (A\nabla u) + k^2 \nu u = -f \quad \text{in } \Omega_+, \tag{6-12a}$$

$$\gamma u = 0 \quad \text{on } \partial\Omega, \tag{6-12b}$$

$$\frac{\partial u}{\partial r}(x) - iku(x) = o\left(\frac{1}{r^{(d-1)/2}}\right) \quad \text{as } r := |x| \to \infty, \text{ uniformly in } \hat{x} := x/r, \tag{6-12c}$$

and the sound-soft scattering problem

$$\nabla \cdot (A\nabla u) + k^2 \nu u = 0 \quad \text{in } \Omega_+, \tag{6-13a}$$

$$\gamma u = 0 \quad \text{on } \partial\Omega, \tag{6-13b}$$

$$(u - u^I) \text{ satisfies the radiation condition (6-12c)}, \tag{6-13c}$$

where u^I is solution of $\Delta u^I + k^2 u^I = 0$ (such as a plane wave or point source) that is smooth in a neighborhood of $\text{supp}(I - A) \cup \text{supp}(1 - \nu) \cup \Omega$.

The standard variational formulations of these problems are posed on $\Omega_R := \Omega_+ \cap B(0, R) = B(0, R) \setminus \Omega$, where R is chosen large enough such that $\text{supp}(I - A)$, $\text{supp}(1 - \nu)$, and $\text{supp } f$ are all compactly contained in $B(0, R)$, and also such that u^I is smooth in $B(0, R)$. Let

$$H^1_{0,D}(\Omega_R) := \{v \in H^1(\Omega_R) : \gamma v = 0 \text{ on } \partial\Omega\}, \tag{6-14}$$

let $\Gamma_R := \partial B(0, R)$, and let $T_R : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$ be the Dirichlet-to-Neumann (DtN) map for the equation $\Delta u + k^2 u = 0$ posed in the exterior of $B(0, R)$ with the Sommerfeld radiation condition

(6-12c); the definition of T_R in terms of Hankel functions and polar coordinates (when $d = 2$) and spherical polar coordinates (when $d = 3$) is given in, e.g., [Chandler-Wilde and Monk 2008, Equations 3.5 and 3.6; Nédélec 2001, Section 2.6.3; Melenk and Sauter 2010, Equations 3.7 and 3.10]. The variational formulation of (6-12) is

$$\text{find } u \in H^1_{0,D}(\Omega_R) \text{ such that } a(u,v) = F(v) \text{ for all } v \in H^1_{0,D}(\Omega_R), \tag{6-15}$$

where

$$a(u,v) := \int_{\Omega_R} ((A\nabla u) \cdot \overline{\nabla v} - k^2 \nu u \bar{v}) \, dx - \langle T_R(\gamma u), \gamma v \rangle_{\Gamma_R} \quad \text{and} \quad F(v) := \int_{\Omega_R} f \bar{v} \, dx, \tag{6-16}$$

and where $\langle \cdot, \cdot \rangle_{\Gamma_R}$ denotes the duality pairing on Γ_R that is linear in the first argument and antilinear in the second. The variational formulation of (6-13) is (6-15) but with $F(v)$ instead given by

$$F(v) := \int_{\Gamma_R} \left(\frac{\partial u^I}{\partial r} - T_R u^I \right) \gamma \bar{v} \, ds.$$

Finite-element method. Let $\mathcal{T}_{h_{\text{FEM}}}$ be a family of triangulations of Ω_R (in the sense of, e.g., [Ciarlet 1991, page 67]) that is shape regular (see, e.g., [Brenner and Scott 2008, Definition 4.4.13; Ciarlet 1991, page 128]). Let

$$\mathcal{H}_{h_{\text{FEM}}} := \{ v \in \mathcal{C}(\overline{\Omega}_R) : v|_K \text{ is a polynomial of degree 1 for each } K \in \mathcal{T}_{h_{\text{FEM}}} \},$$

and observe that the dimension of $\mathcal{H}_{h_{\text{FEM}}}$ is proportional to h_{FEM}^{-n}. Our main result, Theorem 3 below, is valid when Ω is $\mathcal{C}^\infty$ (or, more precisely, $\mathcal{C}^m$ for some large m not given explicitly). For such Ω it is not possible to fit $\partial\Omega$ exactly with simplicial elements (i.e., when each element of $\mathcal{T}_{h_{\text{FEM}}}$ is a simplex), and fitting $\partial\Omega$ with isoparametric elements (see, e.g, [Ciarlet 1991, Chapter VI]) or curved elements (see, e.g., [Bernardi 1989]) is impractical, and therefore some analysis of nonconforming error is necessary; since this is very standard (see, e.g., [Brenner and Scott 2008, Chapter 10]), we ignore this issue here.

The finite-element method for the variational problem (6-15) is the Galerkin method applied to the variational problem (6-15), i.e.,

$$\text{find } u_{h_{\text{FEM}}} \in \mathcal{H}_{h_{\text{FEM}}} \text{ such that } a(u_{h_{\text{FEM}}}, v_{h_{\text{FEM}}}) = F(v_{h_{\text{FEM}}}) \text{ for all } v_{h_{\text{FEM}}} \in \mathcal{H}_{h_{\text{FEM}}}. \tag{6-17}$$

6C. *Main result.* Before stating the main result (Theorem 3 below) we define the following constants — all independent of k but dependent on one or more of A, ν, Ω, R, and k_0 — upon which the main result depends.

C_{int}: Recall that the *nodal interpolant* $I_{h_{\text{FEM}}} : \mathcal{C}(\overline{\Omega}_R) \to \mathcal{H}_{h_{\text{FEM}}}$ is well-defined for functions in $H^2(\Omega_R)$ (for $d = 2, 3$) and satisfies

$$\|\nu^{1/2}(v - I_{h_{\text{FEM}}}v)\|_{L^2(\Omega_R)} + h_{\text{FEM}} \|A^{1/2}\nabla(v - I_{h_{\text{FEM}}}v)\|_{L^2(\Omega_R)} \le C_{\text{int}}(h_{\text{FEM}})^2 \|v\|_{H^2(\Omega_R)} \tag{6-18}$$

for all $v \in H^2(\Omega_R)$, for some constant $C_{\text{int}} = C_{\text{int}}(A, \nu)$. The only reason C_{int} depends on A and ν is because of the weights A and ν in the norms on the left-hand side of (6-18). Indeed, by, e.g., [Brenner

and Scott 2008, Equation 4.4.28],

$$\|v - I_{h_{\text{FEM}}} v\|_{L^2(\Omega_R)} + h_{\text{FEM}} \|\nabla(v - I_{h_{\text{FEM}}} v)\|_{L^2(\Omega_R)} \leq \widetilde{C}_{\text{int}} (h_{\text{FEM}})^2 \|v\|_{H^2(\Omega_R)}$$

for all $v \in H^2(\Omega_R)$, for some $\widetilde{C}_{\text{int}}$ that depends only on the shape-regularity constant of the mesh, and thus (6-18) holds with

$$C_{\text{int}}(A, \nu) := \widetilde{C}_{\text{int}} \max\{(A_{\max})^{1/2}, (\nu_{\max})^{1/2}\}.$$

C_{DtN}: There exists $C_{\text{DtN}} = C_{\text{DtN}}(A, \nu, R, k_0)$ such that

$$|\langle T_R(\gamma u), \gamma v \rangle_{\Gamma_R}| \leq C_{\text{DtN}} \|u\|_{H^1_{k,A,\nu}(\Omega_R)} \|v\|_{H^1_{k,A,\nu}(\Omega_R)} \quad \text{for all } u, v \in H^1(\Omega_R) \text{ and for all } k \geq k_0; \quad (6\text{-}19)$$

see [Melenk and Sauter 2010, Lemma 3.3]. As above, the only reason C_{DtN} depends on A and ν is because of the weights A and ν in (6-7). Indeed, [Melenk and Sauter 2010, Lemma 3.3] bounds the left-hand side of (6-19) by $H^{1/2}(\Gamma_R)$ and $L^2(\Gamma_R)$ norms of γu and γv, and then uses trace theorems to prove that

$$|\langle T_R(\gamma u), \gamma v \rangle_{\Gamma_R}| \leq \widetilde{C}_{\text{DtN}}(R, k_0) \|u\|_{H^1_{k,I,1}(\Omega_R)} \|v\|_{H^1_{k,I,1}(\Omega_R)},$$

for some $\widetilde{C}_{\text{DtN}}(R, k_0)$ given explicitly in the proof of [Melenk and Sauter 2010, Lemma 3.3]. Therefore, (6-19) holds with

$$C_{\text{DtN}}(A, \nu, R, k_0) := \widetilde{C}_{\text{DtN}}(R, k_0) \max\left\{ \frac{1}{(A_{\min})^{1/2}}, \frac{1}{(\nu_{\min})^{1/2}} \right\}.$$

C_{H^2}: There exists $C_{H^2} = C_{H^2}(A, \Omega, R)$ such that, if $\tilde{f} \in L^2(\Omega_{R+1})$ and $v \in H^1(\Omega_{R+1})$ satisfy

$$\nabla \cdot (A \nabla v) = \tilde{f} \quad \text{in } \Omega_{R+1} \text{ and } \gamma v = 0 \text{ on } \partial \Omega,$$

then

$$\|v\|_{H^2(\Omega_R)} \leq C_{H^2}(\|A^{1/2} \nabla v\|_{L^2(\Omega_{R+1})} + \|v\|_{L^2(\Omega_{R+1})} + \|\tilde{f}\|_{L^2(\Omega_{R+1})}); \quad (6\text{-}20)$$

since $A \in \mathcal{C}^{0,1}$ and $\Omega \in \mathcal{C}^{1,1}$, such a C_{H^2} exists by, e.g., [McLean 2000, Theorem 4.18], and C_{H^2} depends on $A_{\min}$ in (6-10), the $\mathcal{C}^{0,1}$ norm of A, and the $\mathcal{C}^{1,1}$ norm of the parametrization of $\partial \Omega$. Note that the $R + 1$ in the norms on the right-hand side of (6-20) can be replaced by $R + b$ for any $b > 0$, but the constant C_{H^2} blows up as $b \to 0$.

Theorem 3 (quasioptimality of the Galerkin method). *Let Ω, A, and ν be as in Section 6B; i.e., Ω is a compact set such that its complement Ω_+ is connected, A is a symmetric positive-definite matrix-valued function of position such that $\text{supp}(I - A)$ is a compact subset of $B(0, R)$ and ν a strictly positive scalar-valued function of position such that $\text{supp}(1 - \nu)$ is a compact subset of $B(0, R)$. Furthermore, let Ω be $\mathcal{C}^\infty$, and let $A, \nu \in \mathcal{C}^{1,1}(\Omega_R)$ be such that A and ν are $\mathcal{C}^\infty$ in a neighborhood of $\partial \Omega$. Finally assume that Ω is nowhere tangent to infinite order to the geodesic flow generated by A and ν via the Hamiltonian (6-9), and that this flow on Ω_+ is nontrapping.*

There exists a $k_0 > 0$ such that if

$$1 \geq h_{\text{FEM}} k^2 \sqrt{1 + (h_{\text{FEM}} k)^2} \, L(\nu A^{-1}, \Omega, R+2) \, C_{\text{int}} C_{H^2} (1 + C_{\text{DtN}}) \left(\frac{\nu_{\max}}{\nu_{\min}} \right)^{1/2} \frac{4\sqrt{2}}{\pi}$$

$$\times \left((\nu_{\max})^{1/2} + \frac{1 + (\nu_{\min})^{1/2}}{k_0} + \frac{1}{k_0^2 (\nu_{\min})^{1/2}} \right), \quad (6\text{-}21)$$

then the Galerkin equations (6-17) *have a unique solution which satisfies*

$$\|u - u_{h_{\text{FEM}}}\|_{H^1_{k,A,\nu}(\Omega_R)} \leq 2(1 + C_{\text{DtN}}) \left(\min_{v_{h_{\text{FEM}}} \in \mathcal{H}_{h_{\text{FEM}}}} \|u - v_{h_{\text{FEM}}}\|_{H^1_{k,A,\nu}(\Omega_R)} \right). \quad (6\text{-}22)$$

(Note that k_0 depends on A, ν, and Ω but—as in Theorem 2—is uniform on small $\mathcal{C}^{2,\alpha}$ neighborhoods of A and ν; see Section 3E.)

Remark 6.1 (the mesh threshold (6-21)). If one assumes that $h_{\text{FEM}} k \leq C$, then the mesh threshold (6-21) can be written in the form (6-1), i.e., $h_{\text{FEM}} k^2 \leq c$. The key point is that if A, ν, and Ω are as in the statement of the theorem with the $\mathcal{C}^{0,1}$ norms of A and ν and the $\mathcal{C}^{1,1}$ norm of Ω all bounded by $\widetilde{C}$, say, then all the constants in c apart from $L(\nu A^{-1}, \Omega, R+2)$ (namely, $A_{\max}$, C_{int}, C_{H^2}, C_{DtN}) are bounded in terms of $\widetilde{C}$, $A_{\min}$ and $\nu_{\min}$, but $L(\nu A^{-1}, \Omega, R+2)$ can be arbitrarily large. Furthermore, *c decreases* as $L(\nu A^{-1}, \Omega, R+2)$ *increases*; i.e., the condition on the mesh threshold for quasioptimality becomes more restrictive as the length of the longest ray grows.

Remark 6.2 (quasioptimality for higher-order finite-element spaces). We have only considered the lowest-order conforming finite-element space of H^1, namely continuous piecewise-linear polynomials. In the case of the constant-coefficient Helmholtz equation, the mesh threshold for quasioptimality (analogous to (6-1)) has been determined by [Melenk and Sauter 2010; 2011; Esterhazy and Melenk 2012] for spaces of arbitrary order p (possibly depending on k), with the threshold then explicit in k, h, and p. These results are obtained by a careful splitting of the solution that does not immediately generalize to the case $A \neq I$. However, in the case of p fixed, the mesh thresholds for quasioptimality from [Melenk and Sauter 2010; 2011; Esterhazy and Melenk 2012] have recently been obtained in [Chaumont-Frelet and Nicaise 2019] using a simpler method (relying on well-known elliptic regularity results such as (6-20)), although the constants are not given explicitly in p. In the case when the DtN map is approximated by an impedance boundary condition, the results of [Chaumont-Frelet and Nicaise 2019] immediately apply to the case $A \neq I$, and they can in principle be extended to the full scattering problem considered here.

Remark 6.3 (comparison to existing results in the literature). The only existing results in the literature on quasioptimality (explicit in all parameters and coefficients) for the Galerkin method applied to the variable-coefficient Helmholtz equation are in [Chaumont-Frelet 2016; Graham and Sauter 2020]. The main similarity between these two works and the present paper is that they all use the "Schatz argument" described in Lemma 6.6 below (and pioneered for Helmholtz problems in [Sauter 2006; Banjai and Sauter 2007]). The main differences between [Chaumont-Frelet 2016; Graham and Sauter 2020] and the present paper are that (i) both [Chaumont-Frelet 2016] and [Graham and Sauter 2020] consider the Helmholtz equation in a bounded domain ([Chaumont-Frelet 2016] in one dimension, [Graham and Sauter

2020] in one, two, or three dimensions) with an impedance boundary condition (recall that this is the simplest-possible approximation to the DtN map operator T_R), and (ii) to get an a priori bound explicit in k and the coefficients, both [Chaumont-Frelet 2016] and [Graham and Sauter 2020] impose conditions on the coefficients and the domain that are *stronger* than the analogue of nontrapping for the interior impedance problem (i.e., the assumption that every ray reaches the boundary in a uniform time).

6D. *Proof of Theorem 3.* The heart of the proof is Lemma 6.6 below. This gives a condition for quasioptimality to hold in terms of how well the solution of the adjoint problem is approximated by the finite-element space, and relies on the fact that $a(\,\cdot\,,\,\cdot\,)$ satisfies a Gårding inequality. This argument essentially goes back to [Schatz 1974] (using the Aubin–Nitsche technique; see, e.g., the references in [Spence 2015, Remark 26]) and was extensively used in the analysis of the FEM for Helmholtz problems by [Sauter 2006; Melenk and Sauter 2010; 2011; Esterhazy and Melenk 2012].

Before stating Lemma 6.6 we need to introduce some notation. Let $C_{\text{cont}} = C_{\text{cont}}(A, \nu, R, k_0)$ be the *continuity constant* of the sesquilinear form $a(\,\cdot\,,\,\cdot\,)$ (defined in (6-16)) in the norm $\|\cdot\|_{H^1_{k,A,\nu}(\Omega_R)}$; i.e.,

$$a(u, v) \leq C_{\text{cont}} \|u\|_{H^1_{k,A,\nu}(\Omega_R)} \|v\|_{H^1_{k,A,\nu}(\Omega_R)} \quad \text{for all } u, v \in H^1_{0,D}(\Omega_R).$$

By the Cauchy–Schwarz inequality and (6-19) we have

$$C_{\text{cont}} \leq 1 + C_{\text{DtN}}. \tag{6-23}$$

Definition 6.4 (the adjoint sesquilinear form $a^*(\,\cdot\,,\,\cdot\,)$). The adjoint sesquilinear form, $a^*(u, v)$, to the sesquilinear form $a(\,\cdot\,,\,\cdot\,)$ defined in (6-16) is given by

$$a^*(u, v) := \overline{a(v, u)} = \int_{\Omega_R} ((A\nabla u) \cdot \overline{\nabla v} - k^2 \nu u \bar{v}) - \langle \gamma u, T_R(\gamma v)\rangle_{\Gamma_R}. \tag{6-24}$$

Lemma 6.5. *Given $F \in (H^1_{0,D}(\Omega_R))'$, if u is the solution to the variational problem*

$$a^*(u, v) = F(v) \quad \text{for all } v \in H^1_{0,D}(\Omega_R), \tag{6-25}$$

then $\bar{u}$ satisfies

$$a(\bar{u}, v) = \overline{F(\bar{v})} \quad \text{for all } v \in H^1_{0,D}(\Omega_R). \tag{6-26}$$

Proof of Lemma 6.5. By (6-25),

$$\overline{a^*(u, \bar{v})} = \overline{F(\bar{v})} \quad \text{for all } v \in H^1_{0,D}(\Omega_R).$$

The result then follows from the definition of $a^*(\,\cdot\,,\,\cdot\,)$ and the following property of the DtN map T_R:

$$\langle T_R \psi, \bar{\varphi}\rangle_\Gamma = \langle T_R \varphi, \bar{\psi}\rangle_\Gamma \quad \text{for all } \varphi, \psi \in H^{1/2}(\Gamma_R).$$

This property follows from the fact that, if u and v are solutions of the homogeneous Helmholtz equation $\Delta u + k^2 u = 0$ in $\mathbb{R}^n \setminus \overline{B(0, R)}$, both satisfying the Sommerfeld radiation condition (6-12c), then

$$\int_{\Gamma_R} (\gamma u) \frac{\partial v}{\partial n} = \int_{\Gamma_R} (\gamma v) \frac{\partial u}{\partial n}$$

by Green's second identity; see, e.g., [Spence 2015, Lemma 6.13]. $\qquad \square$

Lemma 6.6 (conditions for quasioptimality). *Given $f \in L^2(\Omega_R)$, let $S^* f$ be the solution of the adjoint problem* (6-25) *with $F(v)$ defined in* (6-16). *Let*

$$\eta(\mathcal{H}_{h_{\text{FEM}}}) := \sup_{0 \neq f \in L^2(\Omega_R)} \min_{v_{h_{\text{FEM}}} \in \mathcal{H}_{h_{\text{FEM}}}} \frac{\|S^* f - v_{h_{\text{FEM}}}\|_{H^1_{k,A,\nu}(\Omega_R)}}{\|f\|_{L^2(\Omega_R)}}. \tag{6-27}$$

If

$$\eta(\mathcal{H}_{h_{\text{FEM}}}) \leq \frac{1}{2C_{\text{cont}}(\nu_{\max})^{1/2}k} \tag{6-28}$$

then the Galerkin equations (6-17) *have a unique solution which satisfies*

$$\|u - u_{h_{\text{FEM}}}\|_{H^1_{k,A,\nu}(\Omega_R)} \leq 2C_{\text{cont}}\Big(\min_{v_{h_{\text{FEM}}} \in \mathcal{H}_{h_{\text{FEM}}}} \|u - v_{h_{\text{FEM}}}\|_{H^1_{k,A,\nu}(\Omega_R)} \Big). \tag{6-29}$$

Proof. Since

$$\text{Re}(-\langle T_R \varphi, \varphi \rangle_{\Gamma_R}) \geq 0 \quad \text{for all } \varphi \in H^{1/2}(\Gamma_R) \text{ and for all } k \geq k_0 \tag{6-30}$$

(see [Chandler-Wilde and Monk 2008, Corollary 3.1] or [Nédélec 2001, Theorem 2.6.4]), $a(\cdot, \cdot)$ satisfies the Gårding inequality

$$\text{Re}(a(v, v)) \geq \|v\|^2_{H^1_{k,A,\nu}(\Omega_R)} - 2k^2 \nu_{\max}\|v\|^2_{L^2(\Omega_R)}$$

and the result follows from the account of the Schatz argument in, e.g., [Spence 2015, Theorem 6.32]. □

The condition (6-28) on $\eta(\mathcal{H}_{h_{\text{FEM}}})$ is implicitly a condition on the mesh width h_{FEM}. To make this condition explicit, we observe that the polynomial-approximation bound (6-18) implies that a bound on $\eta(\mathcal{H}_{h_{\text{FEM}}})$ (defined by (6-27)) can be obtained from a bound on the H^2 norm of the (adjoint of the) exterior Dirichlet problem.

Lemma 6.7 (bound on H^2 norm). *If Ω, A, and ν are as in Theorem 3, then there exists a $k_0 > 0$ such that the solution of the exterior Dirichlet problem with f, $I - A$, and $1 - \nu$ supported in Ω_R satisfies*

$$\|u\|_{H^2(\Omega_R)}$$
$$\leq k\, C_{H^2} \frac{2\sqrt{2}}{\pi(\nu_{\min})^{1/2}} L(\nu A^{-1}, \Omega, R+2)\Big((\nu_{\max})^{1/2} + \frac{1 + (\nu_{\min})^{1/2}}{k_0} + \frac{1}{k_0^2(\nu_{\min})^{1/2}} \Big)\|f\|_{L^2(\Omega_R)}. \tag{6-31}$$

Proof. Choosing χ such that $\text{supp}\, \chi \subset B_{R+2}$ but $\chi = 1$ on B_{R+1}, Theorem 2 with $s = 1$ implies that there exists $k_0 > 0$ such that

$$\|A^{1/2}\nabla u\|^2_{L^2(\Omega_{R+1})} + k^2\|\nu^{1/2}v\|^2_{L^2(\Omega_{R+1})} \leq \Big(\frac{2\sqrt{2}}{\pi} L(\nu A^{-1}, \Omega, R+2) \Big)^2 \frac{1}{\nu_{\min}}\|f\|^2_{L^2(\Omega_+)} \tag{6-32}$$

for all $k \geq k_0$. Since the χ in our argument can be chosen independent of A and ν, the constant k_0 can be chosen uniformly as A and ν vary within a sufficiently small open neighborhood in $\mathcal{C}^{2,\alpha}$ ($\alpha > 0$), just as in Theorem 2.

We then apply (6-20) with $v = u$, $\tilde{f} = -k^2\nu u - f$, and recall that $\text{supp}\, f \subset \Omega_R$, to obtain

$$\|u\|_{H^2(\Omega_R)} \leq C_{H^2}\Big(\frac{2\sqrt{2}}{\pi(\nu_{\min})^{1/2}} L(\nu A^{-1}, \Omega, R+2)\Big(k(\nu_{\max})^{1/2} + 1 + \frac{1}{k(\nu_{\min})^{1/2}} \Big) + 1 \Big)\|f\|_{L^2(\Omega_R)}.$$

The result (6-31) then follows by noting that $L(\nu A^{-1}, \Omega, R+2) \geq 2$; this last inequality holds since the geodesic needs to at least travel from the boundary of the ball of radius $R+2$ into the ball of radius R and out again (a distance of at least 4), and in this annular region the metric is Euclidean and the flow has speed 2. □

We can now prove Theorem 3.

Proof of Theorem 3. Using the polynomial approximation result (6-18) and the definitions of $\eta(\mathcal{H}_{h_{\text{FEM}}})$ (6-27) and $\|\cdot\|_{H^1_{k,A,\nu}(\Omega_R)}$ (6-7), we have

$$\eta(\mathcal{H}_{h_{\text{FEM}}}) \leq C_{\text{int}} h_{\text{FEM}} \sqrt{1 + (h_{\text{FEM}} k)^2} \sup_{0 \neq f \in L^2(\Omega_R)} \frac{\|S^* f\|_{H^2(\Omega_R)}}{\|f\|_{L^2(\Omega_R)}}.$$

By Lemma 6.5, the solution of the adjoint exterior Dirichlet problem with data f is the complex conjugate of the solution of the exterior Dirichlet problem with data $\bar{f}$. Therefore, the bound (6-31) for the solution of the exterior Dirichlet problem also holds for the solution of the adjoint problem, and implies

$$\eta(\mathcal{H}_{h_{\text{FEM}}}) \leq C_{\text{int}} h_{\text{FEM}} \sqrt{1 + (h_{\text{FEM}} k)^2} \, k \, C_{H^2} \frac{2\sqrt{2}}{\pi (\nu_{\min})^{1/2}} L(\nu A^{-1}, \Omega, R+2)$$
$$\times \left((\nu_{\max})^{1/2} + \frac{1 + (\nu_{\min})^{1/2}}{k_0} + \frac{1}{k_0^2 (\nu_{\min})^{1/2}} \right);$$

the result then follows from using this bound on $\eta(\mathcal{H}_{h_{\text{FEM}}})$ in Lemma 6.6. □

Remark 6.8 (how the bound (1-8) can be used in the analysis of preconditioning strategies). The Galerkin method (6-17) is equivalent to a linear system of equations; denote the matrix of this linear system by A. Linear systems involving A are difficult to solve because (a) the dimension of A is proportional to h_{FEM}^{-n} and (by Theorem 3) h_{FEM} must decrease like k^{-2} for the Galerkin solution to be quasioptimal, therefore A is large, and (b) since A is large and sparse (when using standard piecewise-polynomial bases of $\mathcal{H}_{h_{\text{FEM}}}$), iterative methods are usually used to solve the linear system, but A is sign-indefinite when k is sufficiently large, and the efficient iterative solution of linear systems involving such matrices is difficult. One therefore seeks to *precondition* A; i.e., to find a B such that (i) B^{-1} approximates A^{-1} and (ii) the action of B^{-1} is cheap to compute, and one then applies the iterative solver to $B^{-1} A$.

A very popular and successful preconditioner for A is based on choosing B^{-1} to be a cheap approximation of $(A_\alpha)^{-1}$, where A_α is the Galerkin matrix arising from the exterior Dirichlet problem with $k^2 \mapsto k^2 + i\alpha$, i.e., with artificial absorption α added. The rationale behind this method (introduced in [Erlangga et al. 2006]) is that the larger α is, the less oscillatory the problem is, and hence the easier it is to find a cheap approximation to $(A_\alpha)^{-1}$. However, the larger α is, the further $(A_\alpha)^{-1}$ is from A^{-1}; hence the question of what is the optimal α is nontrivial.

Although one of the advantages of preconditioning with absorption, compared to other Helmholtz-preconditioning strategies, is its easy applicability to variable-coefficient problems (see, e.g., [Oosterlee et al. 2010]), the only existing analysis is for constant-coefficient Helmholtz problems (i.e., (6-2) with $A = I$ and $\nu = 1$). As a component of determining the optimal α, [Gander et al. 2015, Theorem 1.4] proved that, when $A = I$, $\nu = 1$, Ω is star-shaped, and a quasioptimal error estimate (similar to (6-22))

holds for Galerkin discretizations of the problem with absorption, there exists $C > 0$ (independent of k and h_{FEM}, but dependent on Ω and $\mathcal{T}_{h_{\text{FEM}}}$) such that

$$\|I - (A_\alpha)^{-1}A\| \leq C\alpha/k; \tag{6-33}$$

i.e., choosing α to be a sufficiently small multiple of k guarantees that $(A_\alpha)^{-1}$ is a good approximation to A^{-1}, uniformly as $k \to \infty$. Using the bound (1-8) in the arguments of [Gander et al. 2015] one can show that the bound (6-33) holds when A, ν, and Ω satisfy the conditions of Theorem 3 with C a constant multiple of $L(\nu A^{-1}, \Omega, R+1)$; i.e., as the length of the longest ray increases, less absorption is allowed for $(A_\alpha)^{-1}$ to be a good approximation to A^{-1}. This result is then consistent with the numerical experiments in [Gander et al. 2015, Tables 8 and 9]: the geometry corresponding to Table 9 supports longer rays than the geometry corresponding to Table 8, and the numerical results in the tables (the number of iterations required to solve $(A_\alpha)^{-1}A$ with GMRES) show that a lower amount of absorption is allowed in the former case than in the latter for $(A_\alpha)^{-1}$ to be a good preconditioner for A.

Remark 6.9 (how the bound (1-8) can be used in "uncertainty quantification"). In the last 10 years there has been a surge of interest in "uncertainty quantification (UQ)" of PDEs, understood as theory and algorithms for computing statistics of quantities of interest involving PDEs *either* posed on a random domain *or* having random coefficients.

There is a large literature on UQ for the Poisson equation

$$-\nabla \cdot (A(\omega)\nabla u(\omega)) = f(\omega) \tag{6-34}$$

(where ω is an element of the underlying probability space), due, in part, to its large number of applications (e.g., in modeling groundwater flow). The fact that a priori bounds on the solution of (6-34) that are explicit in the coefficient A can easily be obtained is the starting point for the rigorous analysis of UQ algorithms; see, e.g., [Babuška et al. 2004; 2007; Gittelson 2010; Mugler and Starkloff 2011; Charrier 2012; Charrier et al. 2013]. For example, for (6-34) posed in a bounded Lipschitz domain D with homogeneous Dirichlet boundary conditions and $A \in L^\infty(D)$ with $A_{\min} > 0$ (in the sense of quadratic forms as in (6-10)), the Lax–Milgram theorem implies

$$\|u\|_{H^1(D)} \leq \frac{C_D}{A_{\min}}\|f\|_{L^2(D)}, \tag{6-35}$$

where C_D is the constant appearing in the Poincaré inequality $\|v\|_{H^1(D)} \leq C_D^{1/2}\|\nabla v\|_{L^2(D)}$ for all $v \in H_0^1(D)$. In contrast, there has been essentially no rigorous theory of UQ for the Helmholtz equation with large k because a priori bounds on the solution that are explicit in both k and the coefficients have not been available.

The recent paper [Pembery and Spence 2018] presented general measure-theory arguments that convert a bound on the (deterministic) Helmholtz equation that is explicit in both k and the coefficients into a bound, and associated well-posedness result, on the Helmholtz equation with random coefficients (and random data). The paper [Pembery and Spence 2018] used as input to these general arguments the deterministic bounds from [Graham et al. 2019] for star-shaped Lipschitz Ω and coefficients satisfying

radial monotonicity-like conditions which are stronger than nontrapping. We highlight that the bound (1-8) can be used with the arguments of [Pembery and Spence 2018] to obtain well-posedness results and a priori bounds on the Helmholtz equation (6-2) where the coefficients and domain are such that the problem is almost surely nontrapping.

Acknowledgements

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