Local absorbing boundary conditions on fixed domains give order-one errors for high-frequency waves

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We consider approximating the solution of the Helmholtz exterior Dirichlet problem for a nontrapping obstacle, with boundary data coming from plane-wave incidence, by the solution of the corresponding boundary value problem where the exterior domain is truncated and a local absorbing boundary condition coming from a Padé approximation (of arbitrary order) of the Dirichlet-to-Neumann map is imposed on the artificial boundary (recall that the simplest such boundary condition is the impedance boundary condition). We prove upper- and lower-bounds on the relative error incurred by this approximation, both in the whole domain and in a fixed neighbourhood of the obstacle (i.e., away from the artificial boundary). Our bounds are valid for arbitrarily-high frequency, with the artificial boundary fixed, and show that the relative error is bounded away from zero, independent of the frequency, and regardless of the geometry of the artificial boundary.

Keywords: Helmholtz equation; absorbing boundary condition; high frequency.

1. Introduction and statement of the main results

1.1 *Informal discussion of the main results, their context, and their novelty*

Background on absorbing boundary conditions. Wave-scattering problems are usually posed in unbounded domains. However, when computing approximations to the solutions of such problems via discretization methods in the domain, such as finite-element methods (as opposed to discretization methods on the boundary such as boundary-element methods), an artificial boundary is introduced so that the computational domain is finite. The question then arises of what boundary condition to impose on this artificial boundary. If the exact Dirichlet-to-Neumann map for the domain exterior to the artificial boundary is used as the boundary condition, then the solution of the truncated problem is exactly the restriction to the truncated domain of the solution of the scattering problem. However, the Dirichlet-to-Neumann map is a nonlocal operator and is expensive to compute.

Since the late 1970s, starting with the papers Lindman (1975); Engquist & Majda (1977a,b, 1979); Bayliss & Turkel (1980); Bayliss *et al.* (1982), there has been much research on designing *local* boundary conditions to impose on the artificial boundary, with these boundary conditions approximating the (nonlocal) Dirichlet-to-Neumann map. Since the goal is for these boundary conditions to 'absorb' waves hitting this boundary, and not reflect them back into the computational domain, they are often called

'absorbing' or 'non-reflecting' boundary conditions. These boundary conditions are now standard tools in the numerical simulation of waves propagating in unbounded domains; see, e.g., Givoli (1991); Hagstrom (1997); (Ihlenburg, 1998, §3.3); Tsynkov (1998); Hagstrom (1999) and Givoli (2004).

The error incurred by absorbing boundary conditions. The following natural and important question then arises: what is the error between the solution of the truncated problem and the solution of the true scattering problem, and how does this error depend on the following factors?

(i) The shape of the artificial boundary.

(ii) The distance of the artificial boundary from the scatterer.

(iii) The position in the computational domain where the error is measured (e.g., is the error smaller away from the artificial boundary than near it?).

(iv) *Either* the time (for problems posed in the time domain) *or* the frequency of the waves (for problems posed in the frequency domain).

(v) The order of the artificial boundary condition.

Perhaps surprisingly, despite the decades-long interest in absorbing boundary conditions, there do not yet exist rigorous answers to many of these questions.

A summary of the existing answers to these questions is as follows: In the time domain, there exist error estimates describing how the error depends on the distance of the artificial boundary from the scatterer (Bayliss & Turkel, 1980, Theorem 3.2 and Diaz & Joly, 2005, Theorem 2.4), on the order of the boundary conditions (Hagstrom, 1997, §2.3) (for fixed boundary), and on the average frequency present in the solution (Halpern & Rauch, 1987, §5). In the frequency domain for fixed frequency, there exist error estimates describing how the error depends on the distance of the artificial boundary from the scatterer (Bayliss *et al.*, 1982, Theorems 4.1 and 4.2; Goldstein, 1982, Theorem 3.1).

The Helmholtz problem most studied by the numerical-analysis community: artificial boundary fixed and frequency arbitrarily high. One situation where, to our knowledge, there do not yet exist any estimates on the error incurred by absorbing boundary conditions is in the frequency domain when the artificial boundary is fixed and the frequency is arbitrarily high. This situation is a ubiquitous model problem for numerical methods applied to the Helmholtz equation.

Indeed, the following is a nonexhaustive list of papers analysing numerical methods applied to this set up, with the analyses valid in the high-frequency limit with the domain fixed. We highlight that this list includes some of the most influential work in the numerical analysis of the Helmholtz equation from the last ∼15 years.[1]

- Conforming FEMs (including continuous interior-penalty methods) (Shen & Wang, 2005; Han & Huang, 2008; Melenk & Sauter, 2011; Esterhazy & Melenk, 2012; Zhu & Wu, 2013; Esterhazy & Melenk, 2014; Wu, 2014; Du & Wu, 2015; Zhu & Du, 2015; Du & Zhu, 2016; Chaumont-Frelet & Nicaise, 2018; Burman *et al.*, 2019; Chaumont-Frelet, 2019; Diwan *et al.*, 2019; Chaumont-Frelet & Nicaise, 2020; Du *et al.*, 2020; Graham & Sauter, 2020; Melenk *et al.*, 2020).

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[1] More specifically, all of the following papers consider *either* the Helmholtz boundary-value problem (1.2) below with the impedance boundary condition (1.2c) on the truncation boundary, *or* the analogous boundary-value problem with variable coefficients in the PDE.

- Least-squares methods (Demkowicz *et al.*, 2012; Chen & Qiu, 2017; Bernkopf & Melenk, 2019; Hu & Song, 2020; Song & Lee, 2020).

- DG methods based on piece-wise polynomials (Feng & Wu, 2009, 2011; Demkowicz *et al.*, 2012; Chen *et al.*, 2013; Cui & Zhang, 2013; Feng & Xing, 2013; Hoppe & Sharma, 2013; Melenk *et al.*, 2013; Mu *et al.*, 2014; Sauter & Zech, 2015; Zhu & Du, 2015; Wang *et al.*, 2018; Cao & Wu, 2020; Zhao *et al.*, 2020; Zhu & Wu, 2021).

- Plane-wave/Trefftz-DG methods (Amara *et al.*, 2009; Hiptmair *et al.*, 2011; Amara *et al.*, 2014; Hiptmair *et al.*, 2014, 2016; Hu & Yuan, 2018; Mascotto *et al.*, 2019; Hu & Z., W., 2020; Yuan & Hu, 2020).

- Multiscale finite-element methods (Gallistl & Peterseim, 2015; Barucq *et al.*, 2017; Brown *et al.*, 2017; Peterseim, 2017; Ohlberger & Verfürth, 2018; Chaumont-Frelet & Valentin, 2020; Peterseim & Verfürth, 2020; Chen *et al.*, 2021; Freese *et al.*, 2021; Hauck & Peterseim, 2022; Ma *et al.*, 2023).

- Preconditioning methods (Gander *et al.*, 2015; Graham *et al.*, 2017, 2020; Liu *et al.*, 2020; Ramos & Nabben, 2020; Gong *et al.*, 2021, 2022, 2023).

- Uncertainty-quantification methods (Feng *et al.*, 2015; Li *et al.*, 2018; Ganesh *et al.*, 2021).

Informal summary of the results of this paper. The present paper proves error bounds on the accuracy of absorbing boundary conditions for the ubiquitous model problem discussed above. These bounds show how the error in this set up depends on each of the factors (i)–(v) described above, and all but one of our bounds are provably sharp.

More specifically, we consider the Helmholtz exterior Dirichlet problem with boundary data coming from plane-wave incidence when the artificial boundary is fixed and the frequency is arbitrarily high. We consider absorbing boundary conditions coming from a Padé approximation (of arbitrary order) of the Dirichlet-to-Neumann map; recall that this popular class of boundary conditions was introduced in Engquist & Majda (1977a,b, 1979) in the time-dependent setting.

These results are presented in §1.2 in the simplest-possible case of an impedance boundary condition, with these results illustrated in numerical experiments in §1.7. The results for the general Padé case are presented in §1.5 and §1.6. Our results about well-posedness of the truncated problem in §1.4 are also new and of independent interest. Of the results present in the existing literature, the results in this paper are closed to those of Halpern & Rauch (1987), and we compare and contrast these two sets of results in §1.8.

How the results are obtained, and their novelty from the point of view of analysis. The main results are obtained using techniques from semiclassical analysis; i.e., rigorous analysis of PDEs with a large/small parameter, with the analysis explicit in that parameter. In this case the parameter is the large frequency of the Helmholtz equation.

More specifically we use *semiclassical defect measures* (Zworski, 2012, Chapter 5; Dyatlov & Zworski, 2019, §E.3). These measures describe where the mass of Helmholtz solutions in phase space (i.e., the set of positions x and momenta ξ) is concentrated in the high-frequency limit; for an informal discussion of Helmholtz defect measures, see §9.1 in Lafontaine *et al.* (2022).

The main novelty of this paper is in applying these semiclassical techniques to this long-standing numerical-analysis question of the accuracy of absorbing boundary conditions. A large part of the analysis are delicate arguments (in §5) involving constructing geometric-optic rays and controlling their

properties with respect to the distance of the artificial boundary from the scatterer, and the geometry of both the artificial boundary and the scatterer. Indeed, controlling the properties of these rays is what allows us to determine how the error depends on the factors (i)–(iii) above. We highlight that the ideas behind the ray constructions are outlined in §5.6, and their use in the defect-measure arguments is described informally in §5.3.

In addition, the following two aspects of our paper are of independent interest in (non-numerical) analysis.

- The arguments in §4 that use defect measures to prove bounds on the solution operator over *families* of domains (as opposed to a single one), with the bounds explicit in both frequency and the characteristic length scale of the domains.

- The extension in §2.6 of the results in Miller (2000) about defect measures on the boundary to the case when the right-hand side of the Helmholtz equation is nonzero.

The wider context of absorbing boundary conditions in the numerical analysis of the Helmholtz equation. Another important use of local absorbing boundary conditions in the numerical analysis of the Helmholtz equation is in domain-decomposition (DD) methods. This large interest began with the use of impedance boundary conditions for nonoverlapping DD methods in Després (1991); Benamou & Després (1997) and the connection between absorbing boundary conditions and the optimal subdomain boundary conditions (involving appropriate Dirchlet-to-Neumann maps) was highlighted in Nataf *et al.* (1994); Engquist & Zhao (1998). Despite the large current interest in Helmholtz DD methods (see, e.g., the reviews in Gander & Zhang, 2019 and Graham *et al.*, 2020), there are no rigorous frequency-explicit convergence proofs for any practical DD method for the high-frequency Helmholtz equation, partly due to a lack of frequency-explicit bounds on the error when absorbing boundary conditions are used to approximate the appropriate Dirichlet-to-Neumann maps. We therefore expect the results and techniques in the present paper to be relevant for the frequency-explicit analysis of DD methods for the Helmholtz equation; preliminary results on this are given in Lafontaine & Spence (2022).

1.2 *Overview of the main results in the simplest-possible setting*

In this section, we present a selection of our bounds on the error in their simplest-possible setting when an impedance boundary condition is imposed on the truncation boundary. Our upper and lower bounds on the error when the absorbing boundary condition comes from a general Padé approximation of the Dirichlet-to-Neumann map are given in §1.5 and 1.6, with results on the well-posedness of this problem in §1.4.

Let $\Omega_- \subset \mathbb{R}^d$, $d \geq 2$, be a bounded open set such that the open complement $\Omega_+ := \mathbb{R}^d \setminus \overline{\Omega_-}$ is connected, and let $\Gamma_D := \partial \Omega_-$ be C^∞. Given $k > 0$ and $a \in \mathbb{R}^d$ with $|a| = 1$, let $u \in H^1_{\text{loc}}(\Omega_+)$ be the solution to the Helmholtz equation in Ω_+

$$(\Delta + k^2)u = 0 \quad \text{in } \Omega_+, \tag{1.1a}$$

with the Dirichlet boundary condition

$$u = \exp(ikx \cdot a) \quad \text{on } \Gamma_D \tag{1.1b}$$

and satisfying the Sommerfeld radiation condition

$$\frac{\partial u}{\partial r} - iku = o\left(\frac{1}{r^{(d-1)/2}}\right) \tag{1.1c}$$

as $r := |x| \to \infty$, uniformly in $\widehat{x} := x/r$. (The technical reason we only consider Dirichlet boundary conditions on Γ_D, and not also Neumann boundary conditions, is discussed in Remark 5.2 below.)

The physical interpretation of (1.1) is that u is minus the scattered wave for the plane-wave scattering problem with sound-soft boundary conditions; i.e., $\exp(ikx \cdot a) - u$ is the total field for the sound-soft scattering problem.

We assume throughout that the obstacle Ω_- is *nontrapping*, i.e., all billiard trajectories (in the sense of Hörmander, 1985, §24.3) starting in a neighbourhood of the convex hull of Ω_- escape that neighbourhood after some uniform time. Without loss of generality, we assume that Ω_- has characteristic length scale one (results explicit in the size of Ω_- can then be obtained by a scaling argument). In principle, our arguments could also cover the case when the Helmholtz equation (1.1) has variable coefficients, but the ray arguments would be more complicated, since the rays are no longer straight lines (at least in a neighbourhood of the scatterer).

Let v be the solution of the analogous exterior Dirichlet problem, but with the exterior domain Ω_+ truncated, and an impedance boundary condition prescribed on the truncation boundary. More precisely, let $\widetilde{\Omega}_R$ be such that $\widetilde{\Omega}_R \subset B(0, MR)$ for some $M > 0$, $\Gamma_{\mathrm{tr},R} := \partial\widetilde{\Omega}_R$ is C^∞ and $\Omega_- \Subset \widetilde{\Omega}_R$, where $\Subset$ denotes compact containment. The subscripts R on $\widetilde{\Omega}_R$ and $\Gamma_{\mathrm{tr},R}$ emphasize that both have characteristic length scale R, and the subscript tr on $\Gamma_{\mathrm{tr},R}$ emphasizes that this is the truncation boundary. We assume that the family $\{\Gamma_{\mathrm{tr},R}\}_{R\in[1,\infty)}$ is continuous in R and is such that the limit $\Gamma_{\mathrm{tr}}^\infty := \lim_{R\to\infty}(\Gamma_{\mathrm{tr},R}/R)$ exists. Let $\Omega_R := \widetilde{\Omega}_R \setminus \overline{\Omega_-}$, and let $v \in H^1(\Omega_R)$ be the solution of

$$(\Delta + k^2)v = 0 \quad \text{in } \Omega_R, \tag{1.2a}$$

$$v = \exp(ikx \cdot a) \quad \text{on } \Gamma_D, \quad \text{and} \tag{1.2b}$$

$$\partial_n v - ikv = 0 \quad \text{on } \Gamma_{\mathrm{tr},R}. \tag{1.2c}$$

THEOREM 1.1 (Lower and upper bounds when $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$). Suppose that Ω_- is nontrapping, $\Omega_- \subset B(0,1)$, and $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$ with $R \geq 1$. Then there exists $C_j = C_j(\Omega_-) > 0, j = 1, 2$, such that for any $R \geq 1$, there exists $k_0(R, \Omega_-) > 0$ such that, for any direction a, the solutions to (1.1) and (1.2), u and v, respectively, satisfy

$$\frac{C_1}{R^2} \leq \frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \leq \frac{C_2}{R^2}, \qquad \text{for all } k \geq k_0. \tag{1.3}$$

Furthermore, there exists $C_3 = C_3(\Omega_-) > 0$ such that for any $R \geq 2$, there exists $k_1 = k_1(R, \Omega_-) > 0$ such that, for any direction a,

$$\frac{\|u - v\|_{L^2(B(0,2)\setminus\Omega_-)}}{\|u\|_{L^2(B(0,2)\setminus\Omega_-)}} \geq \frac{C_3}{R^2} \qquad \text{for all } k \geq k_1. \tag{1.4}$$

Theorem 1.1 shows that, for sufficiently high frequency, the error is proportional to R^{-2} in *both* the whole domain Ω_R (1.3) *and* a neighbourhood of the obstacle (1.4).

We make two comments: (i) The reason that k_0 and k_1 depends on R is discussed below Theorem 1.7 (the more-general version of Theorem 1.1). (ii) When the impedance boundary condition is replaced by the more-general boundary condition corresponding to Padé approximation, the only changes in (1.3) and (1.4) are in the powers of R (see (1.14) and (1.19) below).

The following theorem shows that when $\Gamma_{\mathrm{tr}}^{\infty}$ is not a sphere centred at the origin, the relative error between u and v does not decrease with R.

THEOREM 1.2 (Lower bound for generic $\Gamma_{\mathrm{tr},R}$). Suppose that Ω_- is nontrapping, $\Omega_- \subset B(0,1)$, and there exists $M > 1$ such that

$$B(0, M^{-1}R) \subset \widetilde{\Omega}_R \subset B(0, MR).$$

Assume that $\Gamma_{\mathrm{tr},R}$ is smooth and strictly convex and (i) $\Gamma_{\mathrm{tr}}^{\infty}$ is *not* a sphere centred at the origin, and (ii) the convergence $\Gamma_{\mathrm{tr},R}/R \to \Gamma_{\mathrm{tr}}^{\infty}$ is in $C^{0,1}$ globally and in $C^{1,\varepsilon}$ (for some $\varepsilon > 0$) away from any corners of $\Gamma_{\mathrm{tr}}^{\infty}$.

Then there exists $C = C(\Omega_-, \{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}) > 0$ such that for all $R \geq 1$, there exists $k_0 = k_0(R, \Omega_-, \{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}) > 0$ such that, for any direction a, the solutions to (1.1) and (1.2), u and v, respectively, satisfy

$$\frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \geq C \qquad \text{for all } k \geq k_0. \tag{1.5}$$

REMARK 1.3 We highlight that the constant C in Theorem 1.2 depends on the family $\{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}$ (indexed by R), but is independent of the variable R itself. This also applies in Theorems 1.5, 1.8 and 1.9 below.

We make four comments: (i) Even under the more-general boundary condition corresponding to Padé approximation, the lower bound analogous to (1.5) is still independent of R; see Theorem 1.8 below. (ii) The numerical experiments in § 1.7 indicate that k_0 in Theorem 1.2 is independent of R, and in fact a lower bound holds uniformly in k and R; see Tables 3 and 4. (iii) Under further smoothness assumption on $\Gamma_{\mathrm{tr}}^{\infty}$, Theorem 1.9 proves an upper bound on the relative error. (iv) The reason why the error decreases with R when $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, but is independent of R for generic $\Gamma_{\mathrm{tr},R}$ is explained in the text immediately after the statement of Theorem 1.9.

1.3 *Definitions of the boundary conditions corresponding to Padé approximation of the Dirichlet-to-Neumann map*

We now consider a more-general truncated problem than (1.2). With $\Omega_-, \widetilde{\Omega}_R$ and Ω_R as in § 1.2, let $v \in H^1(\Omega_R)$ be the solution of

$$(\Delta + k^2)v = 0 \quad \text{in } \Omega_R, \tag{1.6a}$$

$$v = \exp(ikx \cdot a) \quad \text{on } \Gamma_D, \quad \text{and} \tag{1.6b}$$

$$\mathcal{N}\big(k^{-1}\partial_n v\big) - i\mathcal{D}(v) = 0 \quad \text{on } \Gamma_{\mathrm{tr},R}, \tag{1.6c}$$

where $\mathcal{N} \in \Psi^{2N}(\Gamma_{\text{tr},R})$, $\mathcal{D} \in \Psi^{2M}(\Gamma_{\text{tr},R})$ (i.e., $\mathcal{N}$ and $\mathcal{D}$ are semiclassical pseudodifferential operators on $\Gamma_{\text{tr},R}$ of order $2N$ and $2M$, respectively) and both have real-valued principal symbols (see § A for background material on semiclassical pseudodifferential operators).

While most of our analysis applies to much more general choices of $\mathcal{N}$ and $\mathcal{D}$, we focus on $\mathcal{N}$ and $\mathcal{D}$ corresponding to a Padé approximation (up to terms that are lower order both in k^{-1} and differentiation order) of the principal symbol of the Dirichlet-to-Neumann map; this class of $\mathcal{N}$ and $\mathcal{D}$ was introduced in Engquist & Majda (1977a,b, 1979) in the time-dependent setting. In the following assumption, Diff^m denotes the set of operators of the form

$$A(x, k^{-1}D) = \sum_{j=0}^{m} a_j(x) (k^{-1}D)^j,$$

with $a_j \in C^\infty$, $D = -i\partial$, Furthermore, we use Fermi normal coordinates $x = (x_1, x')$, $\xi = (\xi_1, \xi')$, with $\Gamma_{\text{tr},R} = \{x_1 = 0\}$, x_1 the signed distance to $\Gamma_{\text{tr},R}$, $\partial_{x'}$ and ∂_{x_1} orthogonal. We also let $r(x', \xi')$ denote the symbol of one plus the tangential Laplacian on $\Gamma_{\text{tr},R}$, i.e.,

$$r(x', \xi') := 1 - |\xi'|_g^2 \tag{1.7}$$

where $|\cdot|_g$ is the norm induced on the co-tangent space (i.e., the space of the Fourier variables ξ' corresponding to the tangential variables x') of $\Gamma_{\text{tr},R}$ from $\mathbb{R}^d$; see § 2.3 for more details.

Let the coefficients $(p_{M,N}^j)_{j=0}^M$ and $(q_{M,N}^j)_{j=1}^N$ be defined so that $p(t)/q(t)$ is the Padé approximant of of type $[M, N]$ at $t = 0$ to $\sqrt{1-t}$, where

$$p(t) = \sum_{j=0}^{M} p_{M,N}^j t^j \quad \text{and} \quad q(t) = \sum_{j=0}^{N} q_{M,N}^j t^j \tag{1.8}$$

with $q_{M,N}^0 = 1$ and $p_{M,N}^M, q_{M,N}^N \neq 0$. This definition implies that

$$\sqrt{1-t} - \left(\sum_{j=0}^{M} p_{M,N}^j t^j\right)\left(1 + \sum_{j=1}^{N} q_{M,N}^j t^j\right)^{-1} = O\left(t^{m_{\text{ord}}}\right) \quad \text{as } t \to 0, \tag{1.9}$$

where

$$m_{\text{ord}} \geq M + N + 1.$$

Assumption 1.4 (Boundary condition corresponding to Padé approximation). We assume that

$$\mathcal{D} - \mathcal{P}_{M,N}(x', k^{-1}D_{x'}) \in k^{-1}\,\text{Diff}^{2M-1}, \qquad \mathcal{N} - \mathcal{Q}_{M,N}(x', k^{-1}D_{x'}) \in k^{-1}\,\text{Diff}^{2N-1},$$

where

$$\mathcal{P}_{\mathsf{M},\mathsf{N}}(x',\xi') := \sum_{j=0}^{\mathsf{M}} p_{\mathsf{M},\mathsf{N}}^j \left(1 - r(x',\xi')\right)^j \text{ and } \mathcal{Q}_{\mathsf{M},\mathsf{N}}(x',\xi') := 1 + \sum_{j=1}^{\mathsf{N}} q_{\mathsf{M},\mathsf{N}}^j \left(1 - r(x',\xi')\right)^j.$$

By (1.7), $\mathcal{P}_{\mathsf{M},\mathsf{N}}$ and $\mathcal{Q}_{\mathsf{M},\mathsf{N}}$ involve powers of $|\xi'|_g^2$. Since $|\xi'|_g^2$ is a quadratic form in the variables ξ', the boundary condition (1.6c) involves differential operators, and is thus local.

Recall that the rationale behind these particular $\mathcal{D}$ and $\mathcal{N}$ consists of the following three points.

(i) The ideal condition to impose on $\Gamma_{\mathrm{tr},R}$ is that the Neumann trace, $\partial_n v$, equals the Dirichlet-to-Neumann map for the exterior of $\widetilde{\Omega}_R$ under the Sommerfeld radiation condition (1.1c) applied to the Dirichlet trace, v (see § 2.7 and the references therein).

(ii) When $\widetilde{\Omega}_R$ is strictly convex, the principal symbol of this Dirichlet-to-Neumann map (as a semiclassical pseudodifferential operator), away from glancing rays, i.e., rays that are tangent to the boundary, equals $\sqrt{r(x',\xi')} = \sqrt{1 - |\xi'|_g^2}$; see Remark 2.1 for more details.

(iii) The definitions of $p(t)$ and $q(t)$ (1.8) imply that if $\mathcal{D}$ and $\mathcal{N}$ satisfy Assumption 1.4, then the boundary condition (1.6c) corresponds to approximating $\sqrt{1 - |\xi'|_g^2}$ by the Padé approximant of type $[\mathsf{M},\mathsf{N}]$ at $|\xi'|_g^2 = 0$, i.e., at rays that are normal to the boundary.

The polynomials $p(t)$ and $q(t)$ are constructed based on their properties at $t = 0$. However, the quantity $q(t)\sqrt{1-t} - p(t)$ can have other zeros in $t \in (0,1]$, which corresponds to the boundary condition (1.6c) not reflecting certain non-normal rays. We record here notation used later in the paper for these other zeros. Given M,N, let $\{t_j\}_{j=1}^{m_{\mathrm{vanish}}}$ be the zeros of $q(t)\sqrt{1-t} - p(t)$ in $t \in (0,1]$ where $p(t)$ and $q(t)$ are defined by (1.8). Then $m_{\mathrm{vanish}} < \infty$ since $q(t)\sqrt{1-t} - p(t)$ is analytic on $(-1,1)$, continuous at 1, and $p(1) \neq 0$ (see Lemma 4.4 below). Let m_{mult} be the highest multiplicity of the zeros $\{t_j\}_{j=1}^{m_{\mathrm{vanish}}}$.

When $\mathcal{N} = \mathcal{D} = I$, (1.6c) is the impedance boundary condition

$$\partial_n v - ikv = 0, \tag{1.10}$$

and is covered by Assumption 1.4 with $\mathsf{M} = \mathsf{N} = 0$, i.e., $p(t) = q(t) = 1$. In this case, $m_{\mathrm{vanish}} = 0$, since $\sqrt{1-t} - 1$ has no zeros for $t \in (0,1]$.

1.4   *Well-posedness of the truncated problem and k-explicit bound on its solution*

THEOREM 1.5   Let $\Omega_- \Subset B(0,1)$ be a nontrapping obstacle, $M > 0$, $\widetilde{\Omega}_R \subset B(0,MR)$ be convex with smooth boundary $\Gamma_{\mathrm{tr},R}$ that is nowhere flat to infinite order and such that $\Gamma_{\mathrm{tr},R}/R \to \Gamma_{\mathrm{tr}}^\infty$ in C^∞. Let $\mathcal{N}$ and $\mathcal{D}$ satisfy Assumption 1.4 with *either* $\mathsf{M} = \mathsf{N}$ *or* $\mathsf{M} = \mathsf{N} + 1$.

There exists $C > 0$ such that given $R \geq 1$, there exists $k_0 = k_0(R) > 0$ such that, given $f \in L^2(\Omega_R)$, $g_D \in H^1(\Gamma_D)$ and $g_I \in L^2(\Gamma_{\mathrm{tr},R})$, if $k \geq k_0$, then the solution $v \in H^1(\Omega_R)$ of

$$(\Delta + k^2)v = f \quad \text{in } \Omega_R, \tag{1.11a}$$

$$v = g_D \quad \text{on } \Gamma_D, \quad \text{and} \tag{1.11b}$$

$$\mathcal{N}\left(k^{-1}\partial_n v\right) - i\mathcal{D}(v) = g_I \quad \text{on } \Gamma_{\mathrm{tr},R} \tag{1.11c}$$

exists, is unique, and satisfies

$$\|\nabla v\|_{L^2(\Omega_R)} + k \|v\|_{L^2(\Omega_R)}$$
$$\leq C \left(R \|f\|_{L^2(\Omega_R)} + R^{1/2} \big(\|\nabla_{\Gamma_D} g_D\|_{L^2(\Gamma_D)} + k\|g_D\|_{L^2(\Gamma_D)} \big) + R^{1/2} k \|g_I\|_{L^2(\Gamma_{\mathrm{tr},R})} \right). \qquad (1.12)$$

Note that results analogous to the well-posedness statement in Theorem 1.5 in the time domain are given in Theorem 4 of Trefethen & Halpern (1986) and Theorem 1 of Engquist & Majda (1979) for problems where the spatial domain is a half-plane.

Because of the importance of the truncated problem in numerical analysis, proving bounds analogous to (1.12) when v satisfies the impedance boundary condition

$$\partial_n v - ikv = g_I \quad \text{on } \Gamma_{\mathrm{tr},R} \qquad (1.13)$$

has been the subject of many investigations in the literature (Melenk, 1995, §8.1; Cummings & Feng, 2006; Hetmaniuk, 2007; Bao *et al.*, 2012; Li *et al.*, 2013; Moiola & Spence, 2014, Remark 4.7; Chaumont Frelet, 2015, §2.1; Bao & Yun, 2016; Baskin *et al.*, 2016; Chaumont-Frelet & Nicaise, 2018, Appendix B; Sauter & Torres, 2018; Graham *et al.*, 2019, Appendix A; Graham & Sauter, 2020). Indeed, the bound (1.12) under the boundary condition (1.13) and various assumptions on Ω_- and $\widetilde{\Omega}_R$ (often for star-shaped Ω_- and $\widetilde{\Omega}_R$ and sometimes with $\Omega_- = \emptyset$) in (Melenk, 1995, Proposition 8.1.4), (Cummings & Feng, 2006, Theorem 1), (Hetmaniuk, 2007, Proposition 3.3), (Chaumont Frelet, 2015, §2.1.5), (Baskin *et al.*, 2016, Theorem 1.8), (Sauter & Torres, 2018, Theorem 22), (Graham *et al.*, 2019, §A.2), (Graham & Sauter, 2020, Theorems 3.2 and 5.10) (with the last four references considering the variable-coefficient Helmholtz equation).

To our knowledge, the bound (1.12), however, is the first k-explicit bound for a truncated Helmholtz problem where a local absorbing boundary condition is posed other than the impedance boundary condition (1.13).

1.5 *Bounds on the relative error in Ω_R*

All the results in this section proved under the assumption that $\mathcal{N}$ and $\mathcal{D}$ satisfy Assumption 2.2 with *either* $\mathsf{M} = \mathsf{N}$ *or* $\mathsf{M} = \mathsf{N} + 1$, so the the truncated problem is well-posed by Theorem 1.5.

THEOREM 1.6 (Lower bound for general strictly-convex $\Gamma_{\mathrm{tr},R}$). If Ω_- is nontrapping and $\Gamma_{\mathrm{tr},R}$ is strictly convex, then there exists $C = C(\Omega_R, \mathsf{M}, \mathsf{N}) > 0$ that depends continuously on R and $k_0 = k_0(R, \Omega_R, \mathsf{M}, \mathsf{N}) > 0$, such that, for any direction a,

$$\frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \geq C \qquad \text{for all } k \geq k_0.$$

The following three results prove bounds on the relative error that are explicit in R. Theorem 1.7 considers the case $\Gamma_{\mathrm{tr},R} = \partial B(0, R)$, and Theorems 1.8 and 1.9 consider the case when $\Gamma_{\mathrm{tr},R}/R$ tends to a limiting object that is not a sphere.

THEOREM 1.7 (Quantitative lower and upper bounds when $\Gamma_{\mathrm{tr},R} = \partial B(0, R)$). Suppose that Ω_- is non-trapping, $\Omega_- \subset B(0, 1)$, and $\Gamma_{\mathrm{tr},R} = \partial B(0, R)$ with $R \geq 1$. Then, there exists $C_j = C_j(\Omega_-, \mathsf{M}, \mathsf{N}) > 0$,

$j = 1, 2$, such that for any $R \geq 1$, there exists $k_0(R, \Omega_-, \mathsf{M}, \mathsf{N}) > 0$ such that, for any direction a,

$$\frac{C_1}{R^{2m_{\mathrm{ord}}}} \leq \frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \leq \frac{C_2}{R^{2m_{\mathrm{ord}}}}, \qquad \text{for all } k \geq k_0. \tag{1.14}$$

The reason that k_0 in Theorem 1.7 depends on R is because of the difference between the limits $k \to \infty$ with R fixed and $R \to \infty$ with k fixed. To illustrate this difference, consider the boundary conditions

$$(\partial_n - ik)v = 0 \quad \text{and} \quad \left(\partial_n - ik + \frac{d-1}{2r}\right)v = 0. \tag{1.15}$$

Both satisfy Assumption 1.4 with $\mathsf{M} = \mathsf{N} = 0$, with, respectively $\mathcal{N} = 1$, $\mathcal{D} = 1$ and $\mathcal{N} = 1$, $\mathcal{D} = 1 - k^{-1}i(d-1)(2r)^{-1}$. Therefore, in both cases the error $\|u - v\|_{L^2(\Omega_R)}/\|u\|_{L^2(\Omega_R)} \sim R^{-2}$ for fixed R as $k \to \infty$ by Theorem 1.7. However, for fixed k as $r := |x| \to \infty$,

$$(\partial_n - ik)(u - v)(x) = (\partial_n - ik)u(x) = O(r^{-(d+1)/2})_{L^\infty} = O(r^{-1})_{L^2(\partial B(0,r))} \tag{1.16}$$

and

$$\left(\partial_n - ik + \frac{d-1}{2r}\right)(u - v)(x) = \left(\partial_n - ik + \frac{d-1}{2r}\right)u(x) = O(r^{-(d+3)/2})_{L^\infty} = O(r^{-2})_{L^2(\partial B(0,r))}. \tag{1.17}$$

The fact that the right-hand sides of (1.16) and (1.17) are different shows that, while the behaviour of $u - v$ for the two boundary conditions in (1.15) is the same as $k \to \infty$ with R fixed by Theorem 1.7, the behaviour as $R \to \infty$ with k fixed is different. We expect that the bounds in this paper – for the limit $k \to \infty$ with R fixed – in fact hold uniformly when $R \ll k^\gamma$ for some $\gamma < 1$ (i.e., when the large parameter R is smaller than the large parameter k).

When the limiting object $\Gamma_{\mathrm{tr}}^\infty$ is not a sphere, the lower and upper bounds are given separately in Theorems 1.8 and 1.9, respectively. This is because the lower bound allows the limiting object to, e.g., have corners, whereas the upper bound requires the limiting object to be smooth.

THEOREM 1.8 (Quantitative lower bound for generic $\Gamma_{\mathrm{tr},R}$). Suppose that Ω_- is nontrapping, $\Omega_- \subset B(0, 1)$, and there exists $M > 0$ such that

$$B(0, M^{-1}R) \subset \widetilde{\Omega}_R \subset B(0, MR). \tag{1.18}$$

Assume that $\Gamma_{\mathrm{tr},R}$ is smooth and strictly convex and such that (i) $\Gamma_{\mathrm{tr}}^\infty$ is *not* a sphere centred at the origin, and (ii) the convergence $\Gamma_{\mathrm{tr},R}/R \to \Gamma_{\mathrm{tr}}^\infty$ is in $C^{0,1}$ globally and in $C^{1,\varepsilon}$ (for some $\varepsilon > 0$) away from any corners of $\Gamma_{\mathrm{tr}}^\infty$.

Then there exists $C = C(\Omega_-, \mathsf{M}, \mathsf{N}, \{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}) > 0$ such that for all $R \geq 1$, there exists $k_0 = k_0(R, \Omega_-, \mathsf{M}, \mathsf{N}, \{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}) > 0$ such that, for any direction a,

$$\frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \geq C \qquad \text{for all } k \geq k_0.$$

THEOREM 1.9 (Quantitative upper bound for generic $\Gamma_{\mathrm{tr},R}$). Suppose that Ω_- is nontrapping with $\Omega_- \subset B(0,1)$. Suppose that, for every $R \geq 1$, $\widetilde{\Omega}_R \subset B(0,MR)$, $\Gamma_{\mathrm{tr},R}$ is smooth, convex, and nowhere flat to infinite order, and $(\Gamma_{\mathrm{tr},R}/R) \to \Gamma_{\mathrm{tr}}^\infty$ in C^∞ as $R \to \infty$. Then there exists $C = C(\Omega_-, \mathsf{M}, \mathsf{N}, \{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}) > 0$ such that for any $R \geq 1$, there exists $k_0 = k_0(R, \Omega_-, \mathsf{M}, \mathsf{N}, \{\Gamma_{\mathrm{tr},R}\}_{R \in [1,\infty)}) > 0$ such that for any $a \in \mathbb{R}^d$,

$$\frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \leq C \qquad \text{for all } k \geq k_0.$$

We now explain why the constants in the upper and lower bounds in Theorems 1.6–1.9 decrease with R when $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, but are independent of R for generic $\Gamma_{\mathrm{tr},R}$. Recall from §1.3 that the boundary condition (1.6c) corresponds to approximating $\sqrt{r(x', \xi')}$ by a Padé approximant in $|\xi'|_g^2$, with this approximation valid to order m_{ord} in $|\xi'|_g^2$ at $\xi' = 0$ (i.e., rays hitting $\Gamma_{\mathrm{tr},R}$ in the normal direction) by (1.9); recall also that there exists finitely-many other values of $|\xi'|_g^2$ such that $\mathcal{Q}_{\mathsf{M},\mathsf{N}}(x', \xi')\sqrt{r(x', \xi')} - \mathcal{P}_{\mathsf{M},\mathsf{N}}(x', \xi') = 0$, which corresponds to there being finitely-many non-normal angles such that rays hitting $\Gamma_{\mathrm{tr},R}$ at these angles are not reflected by $\Gamma_{\mathrm{tr},R}$. When $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$ and R is large, the rays originating from Ω_- hit $\Gamma_{\mathrm{tr},R}$ in a direction whose angle with the normal decreases with increasing R (in fact the angle $< R^{-1}$; see Lemma 5.14 below). Thus, if R is sufficiently large, the finitely-many special non-normal angles are avoided, and the error for large k decreases with R, with the accuracy, depending on m_{ord}; see Theorem 1.7. When $\Gamma_{\mathrm{tr}}^\infty$ is not a sphere centred at the origin, for every incident direction there exist rays hitting $\Gamma_{\mathrm{tr}}^\infty$ at a fixed, non-normal angle that is also not one of the finitely-many special non-normal angles (see Lemma 5.12 below). Since the Dirichlet-to-Neumann map is not approximated by the boundary condition (1.6c) at such an angle, the error is therefore independent of R and m_{ord}; see Theorems 1.8 and 1.9.

1.6 *Bounds on the relative error in subsets of Ω_R*

Given the upper and lower bounds on the error in Theorems 1.6–1.9, a natural question is: is the error any smaller in a neighbourhood of the obstacle (i.e., away from the artificial boundary)?

We focus on the case when *either* $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$ *or* $\Gamma_{\mathrm{tr},R}$ is the boundary of a hypercube with smoothed corners. We do this because the artificial boundaries most commonly used in applications are $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$ and $\Gamma_{\mathrm{tr},R}$ is a hypercube, but in the latter case we need to smooth the corners for technical reasons.

THEOREM 1.10 (Quantitative lower bound on subset of Ω_R when $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$). Suppose that Ω_- is nontrapping, $\Omega_- \subset B(0,1)$ and $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$ with $R \geq 1$. Then, there exists $C = C(\Omega_-, \mathsf{M}, \mathsf{N}) > 0$ and $R_0 = R_0(\mathsf{M}, \mathsf{N}) \geq 2$ such that for any $R \geq R_0$, there exists $k_0 = k_0(R, \Omega_-, \mathsf{M}, \mathsf{N}) > 0$ such that, for any direction a,

$$\frac{\|u - v\|_{L^2(B(0,2) \setminus \Omega_-)}}{\|u\|_{L^2(B(0,2) \setminus \Omega_-)}} \geq \frac{C}{R^{2m_{\mathrm{ord}}}} \qquad \text{for all } k \geq k_0. \tag{1.19}$$

Furthermore, if $\mathsf{M} = \mathsf{N} = 0$, then $R_0 = 2$.

That is, when $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, the error in $B(0,2)$ is bounded below, independently of k, and the lower bound has the same dependence on R as for the error in Ω_R (see Theorem 1.7). The fact that we

have explicit information about R_0 when $\mathsf{M} = \mathsf{N} = 0$ is because in this case $m_{\text{vanish}} = 0$, i.e., there are no non-normal angles for which the reflection coefficient vanishes, and the proof is simpler.

THEOREM 1.11 (Quantitative lower bound on subset of Ω_R when $\Gamma_{\text{tr},R}$ is the boundary of a smoothed hypercube), Suppose that Ω_- is nontrapping and $\Omega_- \subset B(0, 1)$. Let $\mathfrak{C}$ be the set of corners of $[-R/2, R/2]^d$ and, given $\epsilon > 0$, let

$$\mathfrak{C}_\epsilon := \bigcup_{x \in \mathfrak{C}} B(x, \epsilon);$$

i.e., $\mathfrak{C}_\epsilon$ is a neighbourhood of the corners. Then, there exists $C = C(\Omega_-, \mathsf{M}, \mathsf{N}) > 0$, and $\epsilon_0 = \epsilon_0(\Omega_-)$ such that, for any $R \geq 4$, if $\Gamma_{\text{tr},R}$ is smooth and

$$\Gamma_{\text{tr},R} \setminus \mathfrak{C}_\epsilon = \left[-\frac{R}{2}, \frac{R}{2} \right]^d \setminus \mathfrak{C}_\epsilon \quad \text{for } 0 < \epsilon \leq \epsilon_0,$$

then there exists $k_0 = k_0(\Gamma_{\text{tr},R}, \Omega_-, \mathsf{M}, \mathsf{N}) > 0$ such that, for any direction a,

$$\frac{\|u - v\|_{L^2(B(0,2) \setminus \Omega_-)}}{\|u\|_{L^2(B(0,2) \setminus \Omega_-)}} \geq \frac{C}{R^{(d-1)/2}}, \qquad \text{for all } k \geq k_0.$$

That is, when $\Gamma_{\text{tr},R}$ is a smoothed hypercube, the error in $B(0, 2)$ is bounded below independently of k, in a similar way to the error in Ω_R (see Theorem 1.8). However, whereas the lower bound in Theorem 1.8 is independent of R, Theorem 1.11 allows for the possibility that the large-k-limit of the error in $B(0, 2) \setminus \Omega_-$ decreases with R.

REMARK 1.12 (Smoothness of boundaries). Theorems 1.6, 1.7, 1.8, 1.9 and 1.5 are proved under the assumptions that Γ_D and $\Gamma_{\text{tr},R}$ are C^∞, with Theorem 1.5 also assuming that $\Gamma_{\text{tr}}^\infty$ is C^∞. In all these proofs one actually requires that these boundaries are C^m for some unspecified m. One could in principle go through the arguments in the present paper, and those in Miller (2000) about defect measures on the boundary (which we adapt in § 2), to determine the smallest m such that the results hold, but we have not done this.

1.7 *Numerical experiments in 2-d illustrating some of the main results*

These numerical experiments all consider the simplest boundary condition satisfying Assumption 1.4, i.e., the impedance boundary condition $\partial_n v - ikv = 0$, which is covered by Assumption 1.4 with $\mathcal{N} = \mathcal{D} = 1$.

We first describe the set up common to Experiments 1.13, 1.14 and 1.15. The set up for Experiments 1.16 and 1.17 is slightly different, and is described at the beginning of Experiment 1.16.
The absorbing boundary condition. We let $\Gamma_{\text{tr},R} = \partial B(0, R)$, for some specified $R > 0$, $d = 2$, $\mathcal{N} = \mathcal{D} = 1$ in (1.6c); therefore, $\mathsf{M} = \mathsf{N} = 0$, $m_{\text{ord}} = 1$ and $m_{\text{vanish}} = 0$.
The PML solution used as a proxy for the exact solution. As a proxy for the solution u to (1.1), we use u_{pml} defined to be the solution of the boundary value problem analogous to (1.1), but truncated with a radial PML in an annular region $B(0, R_{\text{pml}}) \setminus B(0, R)$, with $R_{\text{pml}} > R$, using the particular PML described

in (Collino & Monk, 1998, §3). The one change from (Collino & Monk, 1998, §3) is that we take the scaled variable to be independent of k, i.e.,

$$\widetilde{\rho} = \rho + i \int_R^\rho \sigma(s) \, ds, \quad \rho > R$$

(compare to Collino & Monk, 1998, Second displayed equation on page 2067 where R in our notation is a in their notation). We choose

$$\sigma(s) = (r-R)^2/(R_{\text{pml}} - R)^2. \tag{1.20}$$

With this set up, the error between the PML solution and the solution to (1.1) decreases exponentially with k by (Galkowski *et al.*, 2023, Theorem 1.2). (Note, in particular, that $\sigma = f'_\theta$ in the notation of Galkowski *et al.* (2023), and thus the choice of σ (1.20) satisfies the regularity assumptions in Galkowski *et al.* (2023) – indeed, this particular σ is given as an example in (Galkowski *et al.*, 2023, Equation 1.7).) The width of the PML, $R_{\text{pml}} - R$ is chosen as a constant independent of k (specified in each experiment), which is always larger than the largest wavelength considered.

The FEM approximation space. The boundary value problems for u_{pml} and v are discretized using the finite element method with P4 elements (i.e., conforming piecewise polynomials of degree 4) and implemented in FreeFEM++ (Hecht, 2012). The finite-element approximations to u_{pml} and v are denoted by $u_{\text{pml},h_{\text{FEM}}}$ and $v_{h_{\text{FEM}}}$, respectively, and the same mesh is used inside Ω_R when computing both. We then compute the *relative error*

$$\frac{\left\| u_{\text{pml},h_{\text{FEM}}} - v_{h_{\text{FEM}}} \right\|_{L^2(\Omega_R)}}{\left\| u_{\text{pml},h_{\text{FEM}}} \right\|_{L^2(\Omega_R)}}, \tag{1.21}$$

using an element-wise quadrature rule. In the figures we plot the total fields corresponding to $u_{\text{pml},h_{\text{FEM}}}$ and $v_{h_{\text{FEM}}}$, i.e., $\exp(ikx \cdot a) - u_{\text{pml},h_{\text{FEM}}}$ and $\exp(ikx \cdot a) - v_{h_{\text{FEM}}}$, respectively; this is because the total field is easier to interpret than the scattered fields.

Ensuring accuracy of the FEM solutions. The relative H^1 errors in the FEM approximations of u_{pml} and v are both controllably small, uniformly in k, if

$$kR(h_{\text{FEM}}k)^{2p} = C \tag{1.22}$$

for some $C > 0$, independent of all parameters, where p is the polynomial degree and h_{FEM} is the meshwidth. This is proved in (Galkowski & Spence, 2023, Theorems 4.9 and 5.3), following earlier results in (Du & Wu, 2015, Theorem 5.1 and Corollary 5.2) for the impedance problem with no scatterer and (Li & Wu, 2019, Theorem 4.4) for the PML problem with no scatterer and $p = 1$ (see also Chaumont-Frelet *et al.* (2022) for related results). Although $p = 4$, we choose h_{FEM} to satisfy (1.22) with $p = 3$. This choice ensures that the FEM error *decreases* as $k \to \infty$, and thus the difference between $u_{\text{pml},h_{\text{FEM}}} - v_{h_{\text{FEM}}}$ and $u_{\text{pml}} - v$ decreases as $k \to \infty$. We choose $C > 0$ (depending on R and p) such that when $k = 20$, $hk = 1$ (i.e., there are 2π points per wavelength at $k = 20$). We use triangular elements, and thus there is a variational crime caused by approximating the curved boundaries $\Gamma_{\text{tr},R}$ and $\partial\Omega_-$; empirically this error is controlled if hk is sufficiently small, and thus decreases as $k \to \infty$ under the

(a) Real part of total field corresponding to $u_{\mathrm{pml},h_{\mathrm{FEM}}}$ (b) Real part of total field corresponding to $v_{h_{\mathrm{FEM}}}$

(c) Real part of error $u_{\mathrm{pml},h_{\mathrm{FEM}}} - v_{h_{\mathrm{FEM}}}$
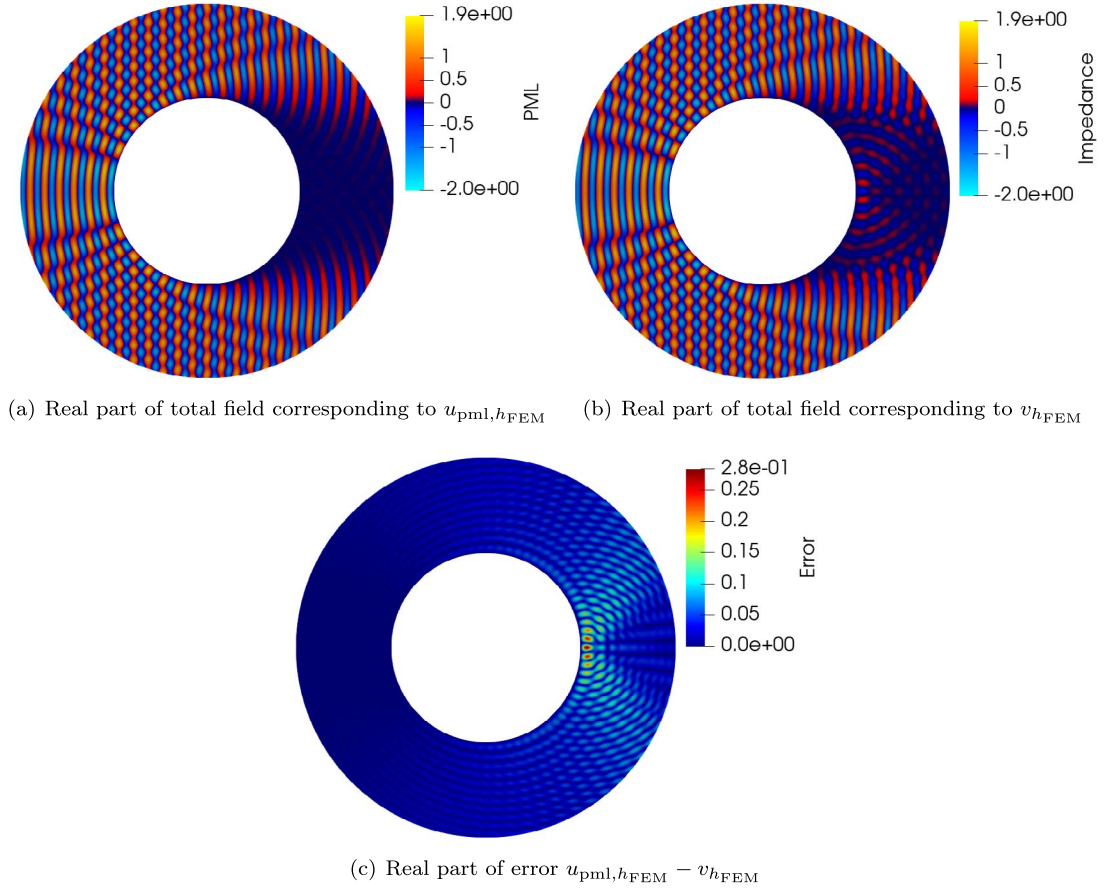
FIG. 1. Scattering by a unit ball for $k = 40$ (as described in Experiment 1.13).

meshthreshold (1.22). The linear systems are solved using preconditioned GMRES, using the package 'ffddm' with tolerance 10^{-6} and the preconditioner ORAS (Optimized Restricted Additive Schwarz), as described in FreeFEM++ (2020).

EXPERIMENT 1.13 (Scattering by ball, verifying Theorems 1.1/ 1.7).We choose $\Gamma_D = \partial B(0,1)$, $R = 2$, $R_{\mathrm{pml}} = 2 + 0.5$, and $a = (1,0)$ (i.e., the plane wave is incident from the left). Figure 1 shows the real parts of the total fields

$$\Re\big(\exp(ikx \cdot a) - u_{\mathrm{pml},h_{\mathrm{FEM}}}\big), \quad \Re\big(\exp(ikx \cdot a) - v_{\mathrm{pml},h_{\mathrm{FEM}}}\big) \quad \text{and} \quad \Re\big(u_{\mathrm{pml},h_{\mathrm{FEM}}} - v_{\mathrm{pml},h_{\mathrm{FEM}}}\big) \quad (1.23)$$

at $k = 40$. We see the error is largest in the shadow of the scatterer near Γ_D.

Table 1 then shows the relative error (defined by (1.21)) for increasing k for $R = 2, 4, 8$. The errors in Table 1 are constant for R fixed as k increases, in agreement with Theorems 1.1/1.7. The errors for $R = 4$ are roughly 4 to 4.5 times smaller than the errors for $R = 2$, and the errors for $R = 8$ are roughly 4 times smaller than the errors for $R = 4$. Since $m_{\mathrm{ord}} = 1$, the factor $R^{-2m_{\mathrm{ord}}} = R^{-2}$ in the bound (1.14)

TABLE 1 *The relative error* (1.21) *against k for scattering by a ball (described in Experiment* 1.13) *for two different values of R*

k	Relative error for ball $R = 2$	Relative error for ball $R = 4$	Relative error for ball $R = 8$
20	0.052557755	0.012321440	0.0035458354
40	0.050360302	0.011438903	0.0029200006
80	0.050034175	0.011050890	
160	0.049001901		

means that we expect the error for $R = 4$ to be 4 times smaller than that for $R = 2$, and the error for $R = 8$ to be 4 times smaller than that for $R = 4$, at least when $k \geq k_0(R)$ (with $k_0(R)$ the unspecified constant in Theorems 1.1/ 1.7).

EXPERIMENT 1.14 (Scattering by a butterfly-shaped obstacle, verifying Theorems 1.1/1.7).We choose Γ_D to be the curve defined in polar coordinates by

$$\Gamma_D := \left\{ (r, \theta) \,:\, r = (0.3 + \sin^2(\theta))(1.4\cos(2\theta) + 1.5), \theta \in [0, 2\pi) \right\}$$

$R = 2$ and $R_{\text{pml}} = 2 + 0.5$. We consider the two different incident plane waves corresponding to $a = (\cos(7\pi/16), \sin(7\pi/16))$ and $a = (\cos(\pi/16), \sin(\pi/16))$.

Figure 2 shows the real parts of the total fields (1.23) at $k = 40$ with $a = (\cos(7\pi/16), \sin(7\pi/16))$, computed with $p = 2$ and $h_{\text{FEM}} = (2\pi/5)k^{-1-1/4}$. In this case, the error is large in the shadow of the scatterer not only near Γ_D, but also away from the obstacle. The choice $a = (\cos(\pi/16), \sin(\pi/16))$ gives a qualitatively similar picture.

Table 2 shows the relative error (defined by (1.21)) for this set up for increasing k and the two different incident plane waves. For each a, the error is constant as k increases, again in agreement with Theorems 1.1/ 1.7. While the errors depend on a, the results are consistent with the statement in Theorems 1.1/1.7 that the error can be bounded, from above and below, uniformly in a.

EXPERIMENT 1.15 (Trapping created by the impedance boundary). We choose $R = 2$, $R_{\text{pml}} = 2 + 0.5$, $k = 50$, $a = (10/\sqrt{104}, 2/\sqrt{104})$, and Ω_- the polygon connecting the points $(0.5, 0.125)$, $(0.5, 0.5)$, $(-0.5, 0.5)$, $(-0.5, -0.5)$, $(0.8, -0.5)$, $(0.8, -0.125)$, $(0.55, -0.125)$, $(0.55, -0.375)$, $(-0.375, -0.375)$, $(-0.375, 0.375)$, $(0.25, 0.375)$, $(0.25, 0.125)$. The total fields are plotted in Fig. 3.

This set up is not included in Theorems 1.1/1.7, since Ω_- is trapping. However, we include this experiment to show that artificial reflections from the impedance boundary Γ_I can excite trapped waves not present in the PML solution (as long as the incident angle is chosen in a careful way, depending on Ω_-, k, and the position of Γ_I).

EXPERIMENT 1.16 (Square Γ_I, investigating accuracy for increasing k with Γ_I fixed). Both this experiment and Experiment 1.17 investigate the effect of a noncircular impedance boundary. Γ_I is the square of side length $2R_{\text{square}}$ centred at the origin. We still compute our proxy for u using a radial PML, posing the boundary-value problem for u_{pml} on $B(0, 3R_{\text{square}}/2)$, with the PML region being $B(0, 3R_{\text{square}}/2+1/2)\backslash B(0, 3R_{\text{square}}/2)$. Observe that $\Gamma_I \subset B(0, 3R_{\text{square}}/2)$, and so Γ_I is a fixed distance away from the PML region. We choose $\Omega_- = B(0, 1)$, $R_{\text{square}} = 2, 4, 8$ (observe that Γ_D is then inside Γ_I – as required), and incident direction $a = (\cos \pi/8, \sin \pi/8)$. Table 3 then shows the relative error for increasing k.

(a) Real part of total field corresponding to $u_{\mathrm{pml},h_{\mathrm{FEM}}}$ (b) Real part of total field corresponding to $v_{h_{\mathrm{FEM}}}$

(c) Real part of error $u_{\mathrm{pml},h_{\mathrm{FEM}}} - v_{h_{\mathrm{FEM}}}$
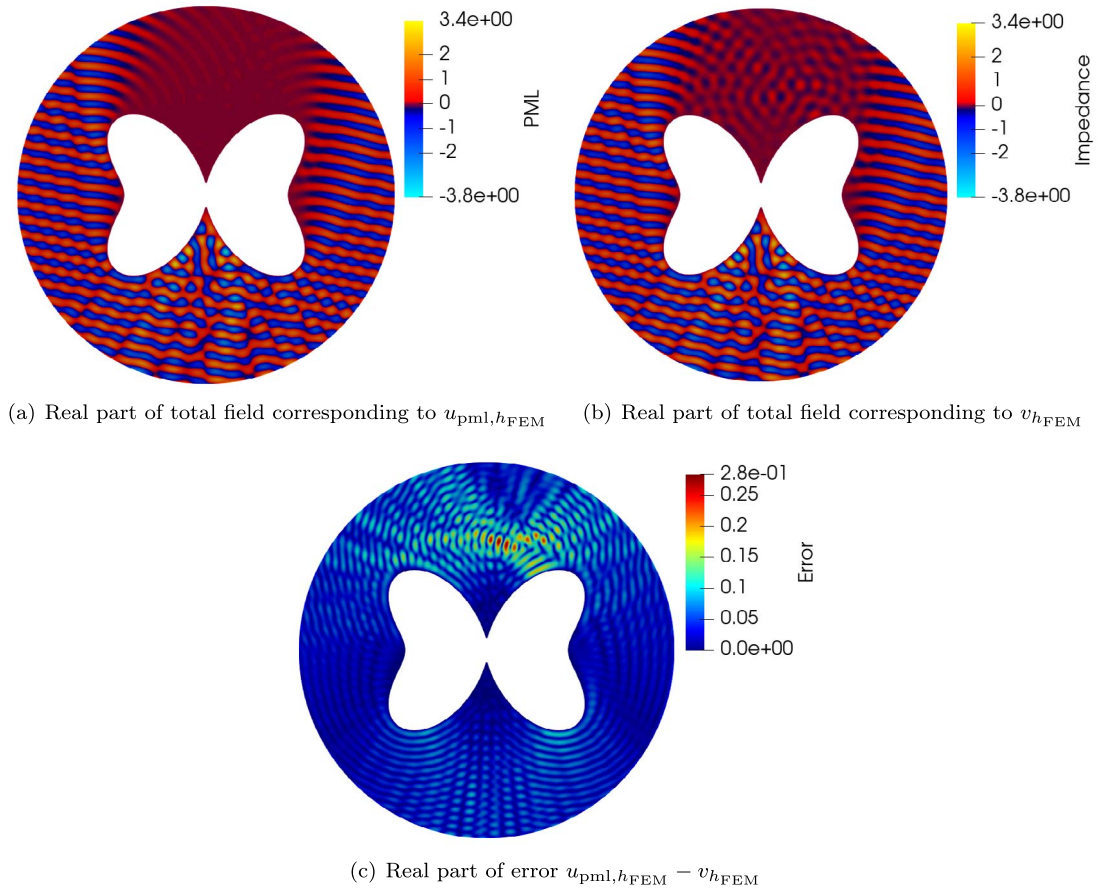
FIG. 2. Scattering by a butterfly-shaped obstacle for $k = 40$ (as described in Experiment 1.14).

TABLE 2   *The relative error* (1.21) *against k for scattering by a butterfly-shaped obstacle* *(described in Experiment* 1.14*) and two different incident plane waves*

k	Relative error, incident angle $7\pi/16$	Relative error, incident angle $\pi/16$
20	0.066501411	0.060746128
40	0.063926342	0.061104428
80	0.063212656	0.058719452

When $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, Table 1 showed the error decreasing by roughly a factor of 4 as R doubled. In Table 3 we see very different behaviour: going from $R_{\mathrm{square}} = 2$ to $R_{\mathrm{square}} = 4$ the error decreases by less than a factor of 2, and going from $R_{\mathrm{square}} = 4$ to $R_{\mathrm{square}} = 8$ the error does not decrease. Although this experiment is not covered by Theorems 1.2/1.8, since the theorem requires $\Gamma_{\mathrm{tr},R}$ to be smooth, the behaviour of the error is consistent with the main result of Theorems 1.2/1.8, namely that

(a) Real part of total field corresponding to $u_{\mathrm{pml},h_{\mathrm{FEM}}}$

(b) Real part of total field corresponding to $v_{h_{\mathrm{FEM}}}$

(c) Real part of error $u_{\mathrm{pml},h_{\mathrm{FEM}}} - v_{h_{\mathrm{FEM}}}$
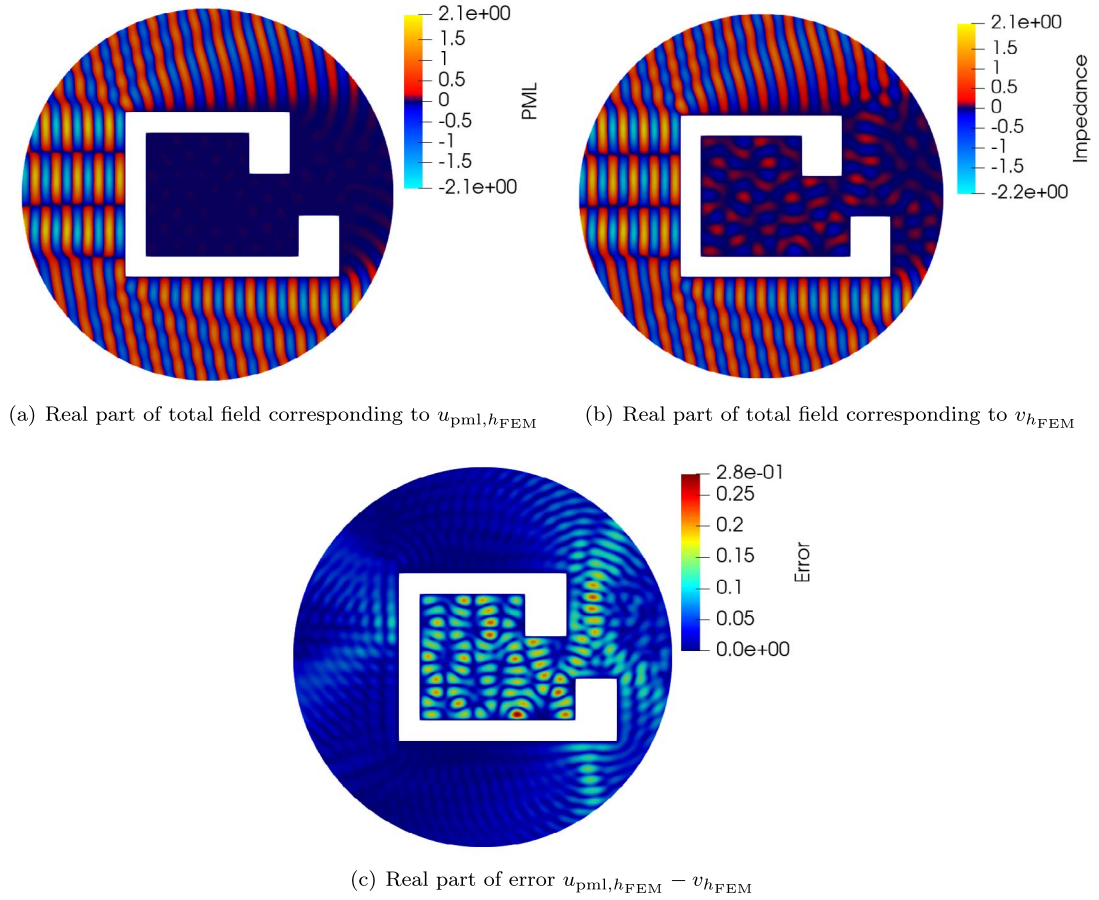
Fig. 3. Scattering by a trapping obstacle for $k = 50$ (as described in Experiment 1.15).

TABLE 3   *The relative error (1.21) against k for scattering by the ball of radius 1 with Γ_I a square of side length $2R_{square}$ centred at the origin and incident angle $\pi/8$ (described in Experiment 1.16)*

k	Relative error for $R_{\mathrm{square}} = 2$	Relative error for $R_{\mathrm{square}} = 4$	Relative error for $R_{\mathrm{square}} = 8$
20	0.0832432	0.0582767	0.0529081
40	0.0802578	0.0578435	0.0528049
80	0.0772090		

when $\Gamma_{\mathrm{tr}}^{\infty} := \lim_{R \to \infty}(\Gamma_{\mathrm{tr},R}/R)$ is not a ball centred at the origin, the relative error is bounded above and below, *independent of R*, as k increases.

EXPERIMENT 1.17 (Square $\Gamma_{\mathrm{tr},R}$, investigating accuracy for increasing $\mathrm{dist}(\Gamma_I, 0)$ with k fixed). We now investigate the error when $\Gamma_{\mathrm{tr},R}$ is a square as R_{square} increases with k fixed. This situation is not covered
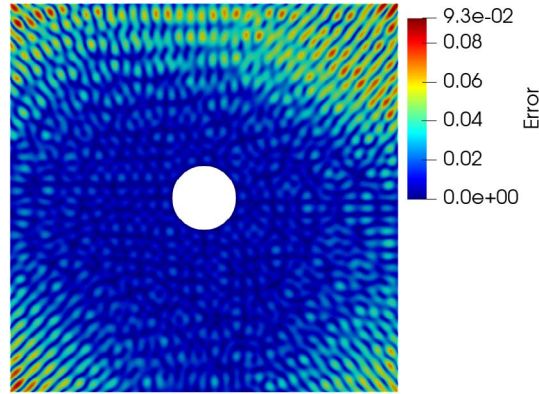
FIG. 4. Real part of error $u_{\mathrm{pml},h_{\mathrm{FEM}}} - v_{h_{\mathrm{FEM}}}$ for scattering by a circle radius one with $k = 10$, Γ_I the square of side length 12 centred at the origin, and incident direction $a = (\cos(\pi/8), \sin(\pi/8))$ (as described in Experiment 1.17).

TABLE 4 *The relative error* (1.21) *against* R_{square} *for scattering by the ball of radius* 1 *with* Γ_I *a square of side length* $2R_{square}$ *centred at the origin,* $k = 10$, *and incident direction* $a = (\cos(\pi/8), \sin(\pi/8))$ *(described in Experiment* 1.17*)*

R_{square}	Relative error
4	0.0593483
8	0.0532721
16	0.0515247

by any of Theorems 1.6–1.9. However, we include this experiment since its results, along with those in Experiment 1.16, indicate that the lower bound in Theorems 1.2/ 1.8 holds uniformly in R and k.

To investigate the case when R_{square} increases with k fixed, we consider an equivalent problem when R_{square} is fixed, k increases, and the obstacle diameter decreases like $1/k$. The set up is as in Experiment 1.16 with $R_{\mathrm{square}} = 2$ (so the PML region is $B(0, 3.5) \setminus B(0, 3)$), $\Omega_- = B(0, 10/k)$ (so that we need $k > 5$ for Γ_D to be inside Γ_I), and the incident direction $a = \pi/8$. Figure 4 plots the relative error for this set up with $k = 30$, and Table 4 displays the relative error (1.21) for $k = 20, 40, 80$. This set up is equivalent to $\Omega_- = B(0, 1)$, $k = 10$, and $R_{\mathrm{square}} = 4, 8, 16$ and Table 4 is labelled with these parameters.

The fact that the last three entries of Table 4 and the last entries in the second and third columns of Table 3 are all around 0.05 suggests that some value near 0.05 is a lower bound on the relative error in *both* the limit $k \to \infty$ with R_{square} fixed *and* the limit $R_{\mathrm{square}} \to \infty$ with k fixed.

1.8 *Comparison to the results of Halpern & Rauch (1987)*

Out of the existing results on absorbing boundary conditions in the literature, the closest to those in the present paper are in Halpern & Rauch (1987). Indeed, Halpern & Rauch (1987) used microlocal methods to study the time-domain analogue of the problems (1.1)/(1.6) when $\Omega_- = \emptyset$ (i.e., no obstacle), and proved a bound on the error between the solutions of the analogues of (1.1)/(1.6) at an arbitrary time.

While the results of the present paper also use microlocal methods (using defect measures instead of propagation of singularities used in Halpern & Rauch (1987)), differences between the results of the present paper and the results of Halpern & Rauch (1987) are the following.

- The constants in the main error bound in Halpern & Rauch (1987) (Halpern & Rauch, 1987, Equation 5.1) depend in an unspecified way on time. The results of the present paper hold uniformly for high-frequency in the frequency domain, which is analogous to proving results for arbitrarily-long times in the time domain.

- The constants in the main error bound in Halpern & Rauch (1987) are not explicit in the distance of the artificial boundary from the origin. In contrast, the error bounds in Theorems 1.8–1.11 are explicit in R.

- Halpern & Rauch (1987) does not have to deal with glancings rays because it assumes that (i) $\Omega_- = \emptyset$, and (ii) the data is supported away from the artificial boundary. In contrast, (i) we allow the obstacle Ω_- to be nonempty and have tangent points, and so have to deal with glancing here, and (ii) we allow f in (1.11a) to have support up to the boundary $\Gamma_{\mathrm{tr},R}$ (as is needed to use the bound (1.12) in, e.g., the analysis of finite-element methods); therefore a large part of the analysis in §4 takes place at glancing.

1.9 *Outline of paper*

§2 contains results about semiclassical defect measures of Helmholtz solutions, with these results used in proofs of both the upper and lower bounds in Theorems 1.6–1.11.

§3 proves three results about outgoing solutions of the Helmholtz equation (i.e., solutions satisfying the Sommerfeld radiation condition (1.1c)), Lemmas 3.1, 3.2 and 3.3, with the first used in the proof of the lower bounds, and the last two used in the proof of the upper bounds.

§4 proves Theorem 1.5 (the well-posedness result). Important ingredients for this proof are the trace bounds of Theorem 4.1; since the proofs of these are long and technical, they are postponed to §6.

§5 proves Theorems 1.6–1.11. The upper bounds follow immediately from Theorem 1.5 and Lemma 3.2. However, the lower bounds require showing that there exist rays, created by the incident plane wave, that reflect off Γ_D and hit $\Gamma_{\mathrm{tr},R}$ at an angle for which the reflection coefficient is not zero. Furthermore, to prove the qualitative bounds Theorems 1.7–1.11 we need to control various properties of these rays explicitly in R. §5.3 outlines the ideas used to construct these rays.

2. Results about defect measures of solutions of the Helmholtz equation

2.1 *Restatement of the boundary-value problems in semiclassical notation*

While we anticipate the vast majority of 'end users' of Theorems 1.6, 1.7, 1.8 and 1.9 will use the Helmholtz equation in the form (1.1) with frequency k (and be interested in the limit $k \to \infty$), the tools and existing results from semiclassical-analysis that we use to prove these results are more convenient to write using the semiclassical parameter $h = k^{-1}$ (and the corresponding limit $h \to 0$).

The boundary-value problem (1.1) therefore becomes,

$$(-h^2 \Delta - 1)u = 0 \qquad \text{in } \Omega_+, \tag{2.1a}$$

$$u = \exp(ix \cdot a/h) \qquad \text{on } \Gamma_D, \quad \text{and} \tag{2.1b}$$

$$h\frac{\partial u}{\partial r} - iu = o\left(\frac{1}{r^{(d-1)/2}}\right) \qquad \text{as } r \to \infty, \tag{2.1c}$$

and the boundary-value problem (1.6) becomes,

$$(-h^2\Delta - 1)v = 0 \qquad \text{in } \Omega_R, \tag{2.2a}$$

$$v = \exp(ix \cdot a/h) \qquad \text{on } \Gamma_D, \tag{2.2b}$$

$$\mathcal{N}h\partial_n v - i\mathcal{D}v = 0 \quad \text{on } \Gamma_{\text{tr},R}. \tag{2.2c}$$

In the rest of the paper, we use the 'h-notation' instead of the 'k-notation'.

Appendix A recaps semiclassical pseudodifferential operators and associated notation.

2.2 *The Helmholtz equation posed a Riemannian manifold M*

While the main results of this paper concern the Helmholtz equation posed in $\Omega_R \subset \mathbb{R}^d$, in the rest of this section (§2), in § 4, and in §6, unless specifically indicated otherwise, we consider the Helmholtz equation posed on a Riemannian manifold M with smooth boundary ∂M and such that there exists a smooth extension $\widetilde{M}$ of M. The reason we do this is that we expect the intermediary results of Theorems 2.15 and 4.1 to be of interest in this manifold setting, independent of their application in proving the main results (Theorems 1.6–1.11). This manifold setting involves the operator $P := -h^2\Delta_g - 1$, where Δ_g is the metric Laplacian. Nevertheless, for the reader unfamiliar with this set up, we highlight that M can be replaced by Ω_R, $\widetilde{M}$ replaced by $\mathbb{R}^d$, and Δ replaced by Δ_g, and all the statements and proofs remain unchanged.

2.3 *The local geometry and the flow*

Near the boundary ∂M, we use Riemannian/Fermi normal coordinates (x_1, x'), in which Γ is given by $\{x_1 = 0\}$ and Ω_R is $\{x_1 > 0\}$. The conormal and cotangent variables are given by (ξ_1, ξ'). In these coordinates,

$$P := -h^2\Delta_g - 1 = (hD_{x_1})^2 - R\left(x_1, x', hD_{x'}\right) + h\left(a_1(x)hD_{x_1} + a_0(x, hD_{x'})\right), \tag{2.3}$$

where $a_1 \in C^\infty$, a_0 and R are tangential pseudodifferential operators (in sense of §A.3), with a_0 of order 1, and R of order 2 with h-symbol $r(x_1, x', \xi')$, with $r(0, x', \xi') = 1 - |\xi'|^2_{g_\Gamma}$ (where the metric g_Γ in the norm is that induced by the boundary). That is, $r(0, x', \xi')$ is the symbol of one plus the tangential Laplacian; in what follows, we often abbreviate $r(0, x', \xi')$ to $r(x', \xi')$.

The fact that P is self adjoint implies that R is self adjoint, $a_1 = \overline{a_1}$, and $[hD_{x_1}, a_1] = a_0 - (a_0)^*$ (with the latter two conditions obtained by integration by parts in the x_1 variable near Γ). Let p denote the semiclassical principal symbol of $P := -h^2\Delta_g - 1$, i.e., $p = |\xi|^2_g - 1$. In a classical way (see, e.g., (Hörmander, 1985, §24.2 page 423)), the cotangent bundle to the boundary $T^*\partial M$ is divided in three regions, corresponding to the number of solutions of the second-order polynomial equation $p(\xi_1) = 0$:

- the *elliptic region* $\mathcal{E} := \left\{(x', \xi') \in T^*\partial M, \ r(x', \xi') < 0\right\}$, where this equation has no solution,

- the *hyperbolic region* $\mathcal{H} := \left\{(x', \xi') \in T^*\partial M, \ r(x', \xi') > 0\right\}$, where it has two distinct solutions

$$\xi_1^{\text{in}} = -\sqrt{r(x', \xi')} \quad \text{and} \quad \xi_1^{\text{out}} = \sqrt{r(x', \xi')}, \tag{2.4}$$

- the *glancing region* $\mathcal{G} := \left\{(x', \xi') \in T^*\partial M, \ r(x', \xi') = 0\right\}$, where it has exactly one solution, $\xi_1 = 0$.

The hyperbolic region plays a crucial role in obtaining the lower bounds in the main results, while we perform analysis near glancing to obtain the upper bounds.

With $p = |\xi|_g^2 - 1$ (i.e., the semiclassical principal symbol of $P := -h^2\Delta_g - 1$), the Hamiltonian vector field of p is defined for compactly supported a by

$$H_p a := \{p, a\},$$

where $\{\cdot, \cdot\}$ denotes the Poisson bracket. Let H_p^* denote the formal adjoint of $H_p a$, and let $\varphi_t(\rho)$ denote the *generalized bicharacteristic flow* in M (see (Hörmander, 1985, §24.3)), defined such that

$$(t, \rho) \in \mathbb{R} \times S_M^* \widetilde{M} \to \varphi_t(\rho) \in S_M^* \widetilde{M}. \tag{2.5}$$

In particular, when $M = \Omega_R$ and $\widetilde{M} = \mathbb{R}^d$, $\varphi_t(\rho) \in S_{\Omega_R}^* \mathbb{R}^d := \{(x, \xi) \in S^*\mathbb{R}^d, x \in \overline{\Omega_R}\} = \{x \in \overline{\Omega_R}, \xi \in \mathbb{R}^d$ with $|\xi| = 1\}$. By Hamilton's equations, away from the boundary of M, this flow satisfies $\dot{x}_i = 2\xi_i$ and $\dot{\xi}_i = 0$, so that it has speed 2 (since $|\xi| = 1$). Recall that the projection of the flow in the spatial variables are the *rays*.

We now defined some projection maps. Let $\pi_M : T^*\widetilde{M} \to \widetilde{M}$ be defined by $\pi_{\mathbb{R}^d}(x, \xi) = x$. Let $\pi_{\partial M} : T_{\partial M}^* \widetilde{M} \cap \{p = 0\} \to T^*\partial M$ be defined by

$$\pi_{\partial M}(0, x', \xi_1, \xi') = (x', \xi'). \tag{2.6}$$

Let $\pi_{\partial M, \text{in}} := \pi_{\partial M}|_{\xi_1 < 0}$ and let $\pi_{\partial M, \text{out}} := \pi_{\partial M}|_{\xi_1 > 0}$.

REMARK 2.1 (The Dirichlet-to-Neumann map away from glancing in local coordinates). In the notation above, locally on $\Gamma_{\text{tr},R}$, the map $u \mapsto hD_{x_1}u = -h\partial_n u/i$ has semiclassical principal symbol $-\sqrt{r(x', \xi')}$. The minus sign in front of the square root is chosen since, when $\xi' = 0$ (i.e., u corresponds to a normally-incident wave), the outgoing condition is that $hD_{x_1}u = -u$ (i.e., $\partial_n u = iku$), as opposed to $hD_{x_1}u = u$ (i.e., $\partial_n u = -iku$).

2.4 *Existence and basic properties of defect measures*

We first assume that $u \in L^2_{\text{loc}}(\mathbb{R}^d)$ is a solution to

$$Pu := \left(-h^2\Delta_g - 1\right)u = hf \quad \text{on } U, \qquad u|_{\mathbb{R}^d \setminus \overline{U}} = 0, \tag{2.7}$$

where $U \subset \mathbb{R}^d$ is open with smooth boundary Γ and $f \in L^2_{\text{comp}}(\mathbb{R}^d)$. When taking traces of u, we always do so from U rather than from $\mathbb{R}^d \setminus \overline{U}$. To define the defect measures associated with u we need the following boundedness assumption.

ASSUMPTION 2.2 Given $\chi \in C_c^\infty(\mathbb{R}^d)$, there exists $C > 0$, and $h_0 > 0$ such that for any $0 < h \le h_0$

$$\|\chi u\|_{L^2(U)} + \|u\|_{L^2(\Gamma)} + \|h\partial_n u\|_{L^2(\Gamma)} \le C.$$

We highlight that Assumption 2.2 is satisfied when the problem is nontrapping; see Lemma 5.1 below.

THEOREM 2.3 (Existence of defect measures). Suppose that u_{h_k} solves (2.7) and satisfies Assumption 2.2. Then there exists a subsequence $h_{k_\ell} \to 0$ and non-negative Radon measures μ and μ^j on $T^*\widetilde{M}$, ν_d, ν_n, ν_j on $T^*\partial M$ such that for any symbol $b \in C_c^\infty(T^*\widetilde{M})$ and tangential symbol $a \in C_c^\infty(T^*\partial M)$, as $\ell \to \infty$

$$\langle b\left(x, h_{k_\ell} D_x\right) u, u \rangle \to \int b(x, \xi)\, \mathrm{d}\mu, \qquad \langle b\left(x, h_{k_\ell} D_x\right) u, f \rangle \to \int b(x, \xi)\, \mathrm{d}\mu^j,$$

$$\langle a\left(x', h_{k_\ell} D_{x'}\right) u, u \rangle_\Gamma \to \int a(x', \xi')\, \mathrm{d}\nu_d, \qquad \langle a\left(x', h_{k_\ell} D_{x'}\right) h_{k_\ell} D_{x_1} u, u \rangle_\Gamma \to \int a(x', \xi')\, \mathrm{d}\nu_j,$$

$$\langle a\left(x', h_{k_\ell} D_{x'}\right) h_{k_\ell} D_{x_1} u, h_{k_\ell} D_{x_1} u \rangle_\Gamma \to \int a(x', \xi')\, \mathrm{d}\nu_n. \tag{2.8}$$

Reference for the proof. See (Zworski, 2012, Theorem 5.2).   □

REMARK 2.4 (The measure ν_j). The joint measure ν_j also describes pairings with the Neumann and Dirichlet traces swapped, since, by (A.2),

$$\langle a\left(x', h_{k_\ell} D_{x'}\right) u, h_{k_\ell} D_{x_1} u \rangle_\Gamma = \overline{\langle a\left(x', h_{k_\ell} D_{x'}\right)^* h_{k_\ell} D_{x_1} u, u \rangle_\Gamma} \to \overline{\int \bar{a}\, \mathrm{d}\nu_j} = \int a\, \mathrm{d}\nu_j.$$

We use the notation that $\mu(a) := \int a\, \mathrm{d}\mu$ for the pairing of a function and a measure. We also use the notation that $b\mu(f) := \int f\, b\, \mathrm{d}\mu$, where $b \in L^\infty(\mathrm{d}\mu)$ and $f \in L^1(\mathrm{d}\mu)$.

We now recall the following two fundamental results.

LEMMA 2.5 (Invariance and support of defect measures). Let u satisfy (2.7) and let μ be a defect measure of u.

(i) In the interior of U,

$$\mu(H_p a) = -2\Im\mu^j(a) \tag{2.9}$$

for all $a \in C_c^\infty(T^*U)$; in particular, if $f = o(1)$ as $h \to 0$, then μ is invariant under the flow.

(ii) μ is supported in the characteristic set:

$$\mathrm{supp}\,\mu \cap T^*U \subset \Sigma_p := \{p = 0\}. \tag{2.10}$$

References for the proof. (2.9) was originally proved in Gérard (1991); see also (Zworski, 2012, Theorem 5.4), (Dyatlov & Zworski, 2019, Theorem E.44). (2.10) was proved in the framework with boundary by (Miller, 2000, Lemma 1.3); see also (Galkowski *et al.*, 2020, Lemma 4.2).   □

Part (ii) of Lemma 2.5 implies that μ is only supported on $|\xi| = 1$; this is the reason why we only consider the flow (2.5) defined on $S_{\overline{M}}^* \widetilde{M}$.

2.5 *Evolution of defect measures under the flow*

LEMMA 2.6 (Integration by parts). Let $B_i \in C_c^\infty((-2\delta, 2\delta)_{x_1}; \Psi^{\ell_i}(\mathbb{R}^{d-1}))$, $i = 1, 2$, and let $B = B_0 + B_1 h D_{x_1}$. If

$$B_1^* = B_1, \qquad B_0^* + [h D_{x_1}, B_1] = B_0, \tag{2.11}$$

then, for all $u \in C^\infty(\overline{M})$,

$$
\begin{aligned}
\frac{i}{h} \left\langle [P, B]u, u \right\rangle_{L^2(M)} = &-\frac{2}{h} \Im \left\langle Bu, Pu \right\rangle_{L^2(M)} \\
&- \left\langle B_1 hD_{x_1} u, hD_{x_1} u \right\rangle_{L^2(\partial M)} - \left\langle \left(B_0 + h(D_{x_1} B_1) - h(B_1 a_1 - \overline{a_1} B_1)\right) hD_{x_1} u, u \right\rangle_{L^2(\partial M)} \\
&- \left\langle B_0 u, hD_{x_1} u \right\rangle_{L^2(\partial M)} - \left\langle \left(h(D_{x_1} B_0) + B_1(R - ha_0) + h\overline{a_1} B_0\right) u, u \right\rangle_{L^2(\partial M)}.
\end{aligned}
\tag{2.12}
$$

COROLLARY 2.7 Let u satisfy Assumption 2.2, and thus have defect measures as in Theorem 2.3. Given $a \in C_c^\infty(T^*\widetilde{M})$, let

$$
a_{\text{even}}(x, \xi_1, \xi') := \frac{a(x, \xi_1, \xi') + a(x, -\xi_1, \xi')}{2}, \quad a_{\text{odd}}(x, \xi_1, \xi') := \frac{a(x, \xi_1, \xi') - a(x, -\xi_1, \xi')}{2\xi_1},
$$

so that $a(x, \xi_1, \xi') = a_{\text{even}}(x, \xi_1, \xi') + \xi_1 a_{\text{odd}}(x, \xi_1, \xi')$. Then

$$
\mu(H_p a) = -2\Im \mu^j(a) - \nu_n(a_{\text{odd}}) - 2\Re \nu_j(a_{\text{even}}) - \nu_d(r(x', \xi') a_{\text{odd}}).
\tag{2.13}
$$

Proof of Lemma 2.6. First recall that R is self adjoint, $a_1 = \overline{a_1}$, and $[hD_{x_1}, a_1] = a_0 - (a_0)^*$; see §2.3. By integration by parts,

$$
\left\langle \left(hD_{x_1}\right)^2 Bu, u \right\rangle_{L^2(M)} = \left\langle Bu, \left(hD_{x_1}\right)^2 u \right\rangle_{L^2(M)} - \frac{h}{i} \left[\left\langle hD_{x_1} Bu, u \right\rangle_{L^2(\partial M)} + \left\langle Bu, hD_{x_1} u \right\rangle_{L^2(\partial M)} \right],
$$

and

$$
\left\langle a_1 hD_{x_1} Bu, u \right\rangle_{L^2(M)} = \left\langle Bu, \left(a_1 hD_{x_1} + [hD_{x_1}, a_1]\right) u \right\rangle_{L^2(M)} - \frac{h}{i} \left\langle Bu, a_1 u \right\rangle_{L^2(\partial M)}.
$$

Using theses two identities, the expression for P (2.3), the self-adjointness of R, and the fact that $[hD_{x_1}, a_1] = a_0 - (a_0)^*$, we obtain that

$$
\langle PBu, u \rangle_{L^2(M)} = \langle Bu, Pu \rangle_{L^2(M)} - \frac{h}{i} \left[\left\langle hD_{x_1} Bu, u \right\rangle_{L^2(\partial M)} + \left\langle Bu, hD_{x_1} u \right\rangle_{L^2(\partial M)} + h \left\langle Bu, a_1 u \right\rangle_{L^2(\partial M)} \right].
\tag{2.14}
$$

The definition of B and the form of P in (2.3) imply that

$$
\begin{aligned}
hD_{x_1} Bu &= B_1 \left(hD_{x_1}\right)^2 u + \left(hD_{x_1} B_1 + B_0\right) \left(hD_{x_1} u\right) + \left(hD_{x_1} B_0\right) u, \\
&= B_1 \left(R - ha_0 - ha_1 hD_{x_1}\right) u + B_1 Pu + \left(hD_{x_1} B_1 + B_0\right) \left(hD_{x_1} u\right) + \left(hD_{x_1} B_0\right) u.
\end{aligned}
\tag{2.15}
$$

Therefore, using (2.14) and (2.15), we have

$$
\begin{aligned}
\frac{i}{h} \langle [P,B]u, u \rangle_{L^2(M)} &= \frac{i}{h} \langle PBu, u \rangle_{L^2(M)} - \frac{i}{h} \langle B(Pu), u \rangle_{L^2(M)} \\
&= \frac{i}{h} \langle Bu, Pu \rangle_{L^2(M)} - \frac{i}{h} \langle B(Pu), u \rangle_{L^2(M)} \\
&\quad - \langle B_1 h D_{x_1} u, h D_{x_1} u \rangle_{L^2(\partial M)} - \langle \left(B_0 + h \left(D_{x_1} B_1 \right) - h(B_1 a_1 - \overline{a_1} B_1) \right) h D_{x_1} u, u \rangle_{L^2(\partial M)} \\
&\quad - \langle B_0 u, h D_{x_1} u \rangle_{L^2(\partial M)} - \langle \left[h(D_{x_1} B_0) + B_1 (R - h a_0) + h \overline{a_1} B_0 \right] u, u \rangle_{L^2(\partial M)} - \langle B_1 (Pu), u \rangle_{L^2(\partial M)}.
\end{aligned}
$$
(2.16)

Next, using the definition of B, integration by parts, and (2.11), we find that, for any v, u,

$$
\begin{aligned}
\langle Bv, u \rangle_{L^2(M)} &= -\frac{h}{i} \langle v, B_1^* u \rangle_{L^2(\partial M)} + \langle v, B_0^* u + h D_{x_1} \left(B_1^* u \right) \rangle_{L^2(M)} \\
&= -\frac{h}{i} \langle v, B_1 u \rangle_{L^2(\partial M)} + \langle v, Bu \rangle_{L^2(M)}.
\end{aligned}
$$
(2.17)

Letting $v = Pu$, combining (2.16) and (2.17), and using the fact that $B_1 = B_1^*$, we obtain

$$
\begin{aligned}
\frac{i}{h} \langle [P,B]u, u \rangle_{L^2(M)} &= \frac{i}{h} \langle Bu, Pu \rangle_{L^2(M)} - \frac{i}{h} \langle Pu, Bu \rangle_{L^2(M)} \\
&\quad - \langle B_1 h D_{x_1} u, h D_{x_1} u \rangle_{L^2(\partial M)} - \langle \left(B_0 + h \left(D_{x_1} B_1 \right) - h(B_1 a_1 - \overline{a_1} B_1) \right) h D_{x_1} u, u \rangle_{L^2(\partial M)} \\
&\quad - \langle B_0 u, h D_{x_1} u \rangle_{L^2(\partial M)} - \langle \left[h \left(D_{x_1} B_0 \right) + B_1 (R - h a_0) + h \overline{a_1} B_0 \right] u, u \rangle_{L^2(\partial M)},
\end{aligned}
$$

which is (2.12). $\qquad\square$

Proof of Corollary 2.7. Letting $h \to 0$ in (2.12), using the third equation in (A.2) and the definitions of the measures in Theorem 2.3, we have

$$
\mu(H_p b) = -2 \Im \mu^j(b) - \nu_n(b_1) - 2 \Re \nu_j(b_0) - \nu_d(r b_1),
$$
(2.18)

where $b = \sigma(B)$, $b_i = \sigma(B_i)$. The idea of the proof is to construct a B satisfying the assumptions of Lemma 2.6 with $\sigma(B_0) = a_{\mathrm{odd}}$ and $\sigma(B_1) = a_{\mathrm{even}}$ (and thus $\sigma(B) = a$). Since (2.13) is linear in a, without loss of generality, we assume that a is real. Since a_{even} and a_{odd} are both smooth, even functions of ξ_1, abusing notation slightly, we can write

$$
a_{\mathrm{even/odd}}(x, \xi_1, \xi') = a_{\mathrm{even/odd}}(x, \xi_1^2, \xi').
$$
(2.19)

Let

$$
\widetilde{a}_{\mathrm{even}}(x, \xi') = a_{\mathrm{even}} \left(x, r(x_1, x', \xi'), \xi' \right), \qquad \widetilde{a}_{\mathrm{odd}}(x, \xi') = a_{\mathrm{odd}} \left(x, r(x_1, x', \xi'), \xi' \right),
$$
(2.20)

and

$$\widetilde{a}(x,\xi') = \widetilde{a}_{\mathrm{even}}(x,\xi') + \xi_1 \widetilde{a}_{\mathrm{odd}}(x,\xi').$$

Since $S^*\widetilde{M} = \{\xi_1^2 - r(x_1,x',\xi') = 0\}$ and $H_p\left(\xi_1^2 - r(x_1,x',\xi')\right) = 0$ (by (2.3)),

$$\widetilde{a}|_{S^*\widetilde{M}} = a|_{S^*\widetilde{M}} \quad \text{and} \quad H_p a|_{S^*\widetilde{M}} = H_p\left(a|_{S^*\widetilde{M}}\right);$$

therefore

$$H_p a|_{S^*\widetilde{M}} = H_p\left(\widetilde{a}|_{S^*\widetilde{M}}\right).$$

Since μ is supported on $\{p = 0\}$ by (2.10),

$$\mu(H_p a) = \mu(H_p \widetilde{a}). \tag{2.21}$$

Let

$$B_0(x, hD_{x'}) := \frac{\widetilde{a}_{\mathrm{even}}(x, hD_{x'}) + (\widetilde{a}_{\mathrm{even}}(x, hD_{x'}))^*}{2} + \frac{1}{2}\left[hD_{x_1}, \frac{\widetilde{a}_{\mathrm{odd}}(x, hD_{x'}) + (\widetilde{a}_{\mathrm{odd}}(x, hD_{x'}))^*}{2}\right]$$

and

$$B_1(x, hD_{x'}) := \frac{\widetilde{a}_{\mathrm{odd}}(x, hD_{x'}) + (\widetilde{a}_{\mathrm{odd}}(x, hD_{x'}))^*}{2}.$$

Then (2.11) is satisfied and by (A.2), (2.20), and (2.19),

$$\sigma(B_0)(x,\xi') = \widetilde{a}_{\mathrm{even}}(x,\xi') = a_{\mathrm{even}}\left(x,\xi_1^2,\xi'\right) \quad \text{on } S^*\widetilde{M}.$$

Similarly, $\sigma(B_0)(x,\xi') = a_{\mathrm{odd}}(x,\xi_1^2,\xi')$, and thus $\sigma(B) = a(x,\xi_1,\xi')$ on $S^*\widetilde{M}$. The result (2.13) then follows from (2.18) and (2.21). $\qquad\square$

2.6 *Properties of defect measures on the boundary*

In this subsection we review the calculations from Miller (2000), adapting them to the case when the right-hand side of the PDE is nonzero.

REMARK 2.8 (Notation in Miller (2000)). Since our results rely heavily on the results of Miller (2000), we record here the correspondence between the notation in Miller (2000) (on the left) and our notation (on the right):

$$\Delta_p = 4r, \quad k^{\mathrm{in/out}} = \xi_1^{\mathrm{in/out}}, \quad \sigma = \xi_1, \quad s = x_1, \quad \dot{v}^N = 4v_n, \quad v^{jN} = 2v_j.$$

Recall that u has defect measure μ, trace measures v_d, v_n and v_j, and f and u have joint defect measure μ^j. By (Galkowski *et al.*, 2020, Lemma 3.3), $\mu^j(a)$ is absolutely continuous with respect to μ,

and $\mu^j = \beta \, \mathrm{d}\mu$ for some $\beta \in L^1(\mathrm{d}\mu)$; hence (2.13) becomes

$$\mu(H_p a + 2\Im\beta a) = -\nu_n(a_{\mathrm{odd}}) - 2\Re\nu_j(a_{\mathrm{even}}) - \nu_d(r a_{\mathrm{odd}}). \tag{2.22}$$

For convenience, we define the differential operator

$$\mathcal{L} := H_p + 2\Im\beta.$$

LEMMA 2.9 There is a distribution μ^0 on $T^*_{\partial M}\widetilde{M}$ supported in $\overline{B^*\partial M}$ such that

$$\mathcal{L}^*\left(\mu 1_{x_1 > 0}\right) = \delta(x_1) \otimes \mu^0, \tag{2.23}$$

where $\otimes$ denotes tensor product of distributions. Furthermore, on $\pi_{\partial M}^{-1}(\mathcal{H})$,

$$\mu^0 := \delta\left(\xi_1 - \xi_1^{\mathrm{in}}\right) \otimes \mu^{\mathrm{in}} - \delta\left(\xi_1 - \xi_1^{\mathrm{out}}\right) \otimes \mu^{\mathrm{out}}, \tag{2.24}$$

where $\mu^{\mathrm{in/out}}$ are positive measures on $T^*\partial M$ supported in $\mathcal{H}$, and $\xi^{\mathrm{in/out}}$ are defined by (2.4).

Proof. The proof follows (Miller, 2000, Proposition 1.7), replacing H_p at every step by $\mathcal{L}$. In particular, by (2.22), $\mathcal{L}^*(\mu 1_{x_1 > 0})$ is supported in $\{x_1 = 0\}$, and hence is of the form $\sum_{k=0}^{\ell} \delta^{(k)}(x_1) \otimes \mu_k$ where each μ_k is a distribution on $T^*_{\partial M}\widetilde{M}$. But, letting $\chi \in C_c^\infty(\mathbb{R})$ with $\chi^{(k)}(0) = 1$, for $k \leq \ell$ and applying (2.22) to $a_\epsilon = \epsilon^\ell \chi(\epsilon^{-1}x_1)b(x', \xi)$, we have for $\ell \geq 1$,

$$\sum_{k=0}^{\ell} \epsilon^{\ell-k}\mu_k(b) = \mu\left(1_{x_1 > 0}\mathcal{L}a_\epsilon\right) = \mu\left(1_{x_1 > 0}\left(\epsilon^{\ell-1}H_p\chi + \epsilon^\ell \chi H_p b - 2\Im\beta a\right)\right) \to 0 \text{ as } \epsilon \to 0.$$

In particular, $\mu_k = 0$ for $k \geq 1$ and (2.23) follows.

The result (2.24) about the structure of μ^0 in the hyperbolic set follows by considering a small neighbourhood $\mathcal{V}$ in $T^*\partial M$ of a point $\rho \in \mathcal{H}$ and $\delta > 0$ such that each geodesic trajectory of length 2δ centered in $\pi_{\partial M}^{-1}(\mathcal{V})$ intersects the boundary exactly once. We may then use

$$(-\delta, \delta) \times \pi_{\partial M}^{-1}(\mathcal{V}) \ni (t, \rho) \to \varphi_t(\rho) \in \mathcal{V}_\delta \subset T^*\widetilde{M}$$

as coordinates on an open neighbourhood, $\mathcal{V}_\delta$ of $\pi_{\partial M}^{-1}(\mathcal{V})$. In these coordinates, writing $\widetilde{\mu}$ for the pull-back of $1_{x_1 > 0}\mu$ under φ_t, we obtain

$$(\partial_t + 2\Im\beta)\widetilde{\mu} = \delta(t) \otimes \mu^0.$$

In particular, $\widetilde{\mu}$ is null $\mathcal{V}_{t_0}$ for any $t_0 \in (-\delta, \delta)$, and testing by $\epsilon\chi(t\epsilon^{-1})b$ with $0 \leq b \in C_c^\infty(\pi_{\partial M}^{-1}(\mathcal{V}))$, and $\chi \in C_c^\infty(-\delta, \delta)$ with $t\chi'(t) < 0$ on $|t| > 0$, $\chi(0) = 1$, we have

$$\widetilde{\mu}(\chi'(\epsilon^{-1}t)b - 2\epsilon\Im\beta\chi(\epsilon^{-1}t)b) = \mu^0(b).$$

Now $\widetilde{\mu}$ is identically zero on $\pi_{\text{in}}^{-1}(\mathcal{V}) \times [0, \infty)$ and on $\pi_{\text{out}}^{-1}(\mathcal{V}) \times (-\infty, 0]$. Therefore, for b supported in $\pi_{\partial M \text{out}}^{-1}(\mathcal{V})$

$$\mu^0(b) \leq \liminf_{\epsilon \to 0} \widetilde{\mu} \left(\left[\chi'(\epsilon^{-1}t)b - 2\epsilon \Im \beta \chi(\epsilon^{-1}t)b \right] 1_{t>0} \right) \leq 0.$$

Similarly, for b supported in $\pi_{\text{in}}^{-1}(\mathcal{V})$, $\mu^0(b) \geq 0$. In particular, μ^0 is a positive distribution on $\pi_{\text{in}}^{-1}(\mathcal{H})$ and a negative distribution of $\pi_{\text{out}}^{-1}(\mathcal{H})$, and the result follows. $\qquad\square$

Next, we decompose μ into its interior and boundary components, with the following lemma the analogue of (Miller, 2000, Proposition 1.8).

LEMMA 2.10 There is a positive measure μ^∂ on $\mathcal{G} \subset T_{\partial M}^* \widetilde{M}$ such that

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

Proof. Let $\chi \in C_c^\infty(\mathbb{R})$ with $\chi(0) = \chi'(0) = 1$ and $b \in C_c^\infty(\mathbb{R} \times T^*\mathbb{R}^{n-1})$. Then, with $a_\epsilon = \epsilon \chi(x_1 \epsilon^{-1})b(x, \xi')$, (2.22) implies that

$$\mu(\mathcal{L}a_\epsilon) = -2\epsilon \Re \nu_j(b).$$

Now,

$$\mathcal{L}a_\epsilon = 2\chi'(x_1 \epsilon^{-1})H_p x_1 b + O(\epsilon).$$

Therefore, by the dominated convergence theorem,

$$\mu(\mathcal{L}a_\epsilon) \to \mu(1_{x_1=0}bH_p x_1)$$

and, since $|\nu_j(b)| < \infty$,

$$\mu(1_{x_1=0}bH_p x_1) = 0.$$

Since b was arbitrary, μ decomposes as claimed. $\qquad\square$

The following lemma is the analogue of (Miller, 2000, Lemma 1.9).

LEMMA 2.11 On $\mathcal{E}$ (i.e., $r < 0$), $\Re \nu_j = 0$ and $\nu_n = -r\nu_d$.

Proof. Let $\chi \in C^\infty(\mathbb{R})$ with $\chi \equiv 1$ on $(-\infty, -1]$ and $\text{supp } \chi \subset (-\infty, 0)$. Let $b = b(x, \xi') \in C_c^\infty$ and define $b_\epsilon = \chi(\epsilon^{-1}r)b$. Then, by (2.22) together with the fact that $\text{supp } \mu \subset S^*M$,

$$0 = \mu(H_p b_\epsilon + 2\Im \beta b_\epsilon) = -2\Re \nu_j(b_\epsilon).$$

Sending $\epsilon \to 0^+$, we obtain

$$0 = 2\Re \nu_j(b 1_{r<0}).$$

Since b was arbitrary, $v_j 1_{r<0} = 0$. Replacing b by $b(x, \xi')\xi_1$ and applying the same argument, we obtain

$$v_n 1_{r<0} = -r v_d 1_{r<0}.$$

$\square$

Next, we prove the analogue of (Miller, 2000, Proposition 1.10).

LEMMA 2.12 On the hyperbolic set $\mathcal{H}$,
(i)

$$2\mu^{\text{out}} = \sqrt{r(x', \xi')} v_d + 2\Re v_j + \frac{1}{\sqrt{r(x', \xi')}} v_n, \qquad 2\mu^{\text{in}} = \sqrt{r(x', \xi')} v_d - 2\Re v_j + \frac{1}{\sqrt{r(x', \xi')}} v_n. \tag{2.25}$$

(ii) If $\mu^{\text{in}} = 0$ on some Borel set $\mathcal{B} \subset \mathcal{H}$, then

$$\mu^{\text{out}} = 2\Re v_j = 2\sqrt{r(x', \xi')} v_d = \frac{2}{\sqrt{r(x', \xi')}} v_n. \tag{2.26}$$

(iii) If

$$-2\Re v_j = (\Re \alpha) v_d = 4(\Re \alpha) |\alpha|^{-2} v_n \tag{2.27}$$

on some Borel set $\mathcal{B} \subset \mathcal{H}$ for α a complex valued function such that $\alpha + 2\sqrt{r(x', \xi')}$ is never zero on $\mathcal{B}$, then

$$\mu^{\text{out}} = \alpha^{\text{ref}} \mu^{\text{in}}, \tag{2.28}$$

where

$$\alpha^{\text{ref}} := \left| \frac{2\sqrt{r(x', \xi')} - \alpha}{2\sqrt{r(x', \xi')} + \alpha} \right|^2 \text{ on } \mathcal{B}, \tag{2.29}$$

where the superscript 'ref' stands for 'reflected'. If instead, $\alpha - 2\sqrt{r}$ is never zero, then

$$(\alpha^{\text{ref}})^{-1} \mu^{\text{out}} = \mu^{\text{in}}.$$

Proof. (i) By combining Lemmas 2.9 and 2.10,

$$\mathcal{L}^* \mu = \delta(x_1) \otimes \mu^0 + \mathcal{L}^* \big(\delta(x_1) \otimes \delta(H_p x_1) \otimes \mu^{\partial} \big). \tag{2.30}$$

Let $\chi \in C^\infty(\mathbb{R})$ with $\chi \equiv 0$ on $(-\infty, 1]$ and $\chi \equiv 1$ on $[2, \infty)$. For $a \in C_c^\infty(\mathbb{R} \times T^*\partial M)$ (so $a = a(x_1, x', \xi')$), let $a_\epsilon = \chi(\epsilon^{-1}|H_p x_1|)a$. Since $H_p x_1 = 2\xi_1$, $a_\epsilon = a$ for $|\xi_1| \geq \epsilon$ and $a_\epsilon = 0$ for $|\xi_1| \leq \epsilon/2$. Combining (2.30) and (2.22), and using the facts that a_ϵ is even in ξ_1 and $a_\varepsilon = 0$ for $|H_p x_1| \leq \varepsilon/2$, we

find that

$$\mu^0\left(a_\epsilon|_{x_1=0}\right) = \mu(\mathcal{L}a_\epsilon) = -2\Re\nu_j\left(a_\epsilon|_{x_1=0}\right).$$

By (2.24),

$$\chi\left(2|\xi_1^{\text{in}}|/\epsilon\right)\mu^{\text{in}}\left(a|_{x_1=0}\right) - \chi\left(2|\xi_1^{\text{out}}|/\epsilon\right)\mu^{\text{out}}\left(a|_{x_1=0}\right) = 2\Re\nu_j\left(a_\epsilon|_{x_1=0}\right).$$

Therefore, by the dominated convergence theorem,

$$\mu^{\text{in}} - \mu^{\text{out}} = -2\Re\nu_j \quad \text{on } \mathcal{H}. \tag{2.31}$$

Similarly, since $a_\epsilon\xi_1$ is an odd function of ξ_1, (2.30) and (2.22) imply that

$$\mu^0(a_\epsilon\xi_1|_{x_1=0}) = \mu(\mathcal{L}a_\epsilon\xi_1) = -\nu_d(ra_\epsilon|_{x_1=0}) - \nu_n(a_\epsilon|_{x_1=0}).$$

By (2.24),

$$\xi_1^{\text{in}}\chi\left(2|\xi_1^{\text{in}}|/\epsilon\right)\mu^{\text{in}}\left(a|_{x_1=0}\right) - \xi_1^{\text{out}}\chi\left(2|\xi_1^{\text{out}}|/\epsilon\right)\mu^{\text{out}}\left(a|_{x_1=0}\right) = -\nu_d(ra_\epsilon|_{x_1=0}) - \nu_n(a_\epsilon|_{x_1=0}).$$

Therefore, by the dominated convergence theorem,

$$-\sqrt{r}(\mu^{\text{in}} + \mu^{\text{out}}) = -r\nu_d - \nu_n \quad \text{on } \mathcal{H}. \tag{2.32}$$

The result (2.25) now follows from solving (2.31) and (2.32) for μ^{in} and μ^{out}.

(ii) By the Cauchy–Schwarz inequality and similar reasoning used in the proof of (Galkowski *et al.*, 2020, Lemma 3.3),

$$|\nu_j| \le \sqrt{\sqrt{r}\nu_d}\sqrt{\nu_n/\sqrt{r}}. \tag{2.33}$$

By (2.25), when $\mu^{\text{in}} = 0$,

$$2\Re\nu_j = \sqrt{r}\nu_d + \nu_n/\sqrt{r}. \tag{2.34}$$

However, for both (2.33) and (2.34) to hold, we must have $\sqrt{r}\nu_d = \nu_n/\sqrt{r}$, and (2.28) follows.

(iii) The equation (2.28) follows from using (2.27) in (2.25). $\qquad\square$

LEMMA 2.13

$$-H_p^2 x_1\mu^\partial = 4\nu_n 1_{\mathcal{G}}.$$

In particular, μ^∂ is supported in $H_p^2 x_1 \le 0$ and $\nu_n 1_{\mathcal{G}}$ does not charge $H_p^2 x_1 \ge 0$.

Proof. We follow (Galkowski *et al.*, 2020, Lemma 4.7). Since $H_p x_1 = 2\xi_1$,

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

Now, put $a_\epsilon = \chi(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r(x,\xi'))2a\xi_1$ where $\chi \in C_c^\infty(\mathbb{R})$ has $\chi \equiv 1$ near 0. Then,

$$H_p a_\epsilon = a\chi(\epsilon^{-1}x_1)\chi(\epsilon^{-1}r)H_p^2 x_1 + O(1)\big(\big|\chi'(\epsilon^{-1}x_1)\big| + \big|\chi'(\epsilon^{-1}r)\big| + \epsilon^{1/2}\big),$$

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

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

Using (2.22), we have

$$\mu(H_p a_\epsilon) = -2\mu(\Im\beta a_\epsilon) - \nu_d(2\chi(\epsilon^{-1}r)ra) - \nu_n(2\chi(\epsilon^{-1}r)a).$$

Using the dominated convergence theorem again, using that $\xi_1 = O(\sqrt{r})$ on S^*M, we have

$$\mu(2\Im\beta a_\epsilon) \to 0,$$

and hence

$$\tfrac{1}{2}\mu^\partial\big([H_p^2 x_1]a\big) = -\nu_n(2a1_{\mathcal{G}}),$$

as claimed.   □

LEMMA 2.14 Let $q = q(x_1, x_1\xi_1, x', \xi) \in C_c^\infty(T^*\widetilde{M})$. Then,

$$\mu(H_p q) = -2\Im\beta\mu(q) + (\mu^{\mathrm{in}} - \mu^{\mathrm{out}})\,\big(q|_{x_1=0}\big) + \tfrac{1}{2}\mu^\partial\big(\Re(\dot{n}^j)H_p^2 x_1 q|_{x_1=0}\big),$$

where $\dot{n}^j\nu_n = \nu_j$.

Proof. By Lemma 2.12,

$$\mu(\mathcal{L}q) = -2\Re\nu_j(q|_{x_1=0}) = (\mu^{\mathrm{in}} - \mu^{\mathrm{out}})(q|_{x_1=0}) - 2\Re\nu_j(1_{\mathcal{G}}q|_{x_1=0}).$$

Now, since $\nu_j \ll \nu_n$ we may write $\nu_j = \dot{n}^j\nu_n$ and use Lemma 2.13 to obtain

$$-2\Re\nu_j(1_{\mathcal{G}}q|_{x_1=0}) = -2\Re\nu_n\big(\dot{n}^j 1_{\mathcal{G}}q|_{x_1=0}\big) = \frac{1}{2}\mu^\partial\big((\Re\dot{n}^j)H_p^2 x_1 q|_{x_1=0}\big),$$

and the claim follows.   □

THEOREM 2.15 Suppose that ∂M is nowhere tangent to H_p to infinite order. Then, for $q \in C_c^\infty(^bT^*M)$

$$\pi_*\mu(q \circ \varphi_t) - \pi_*\mu(q) = \int_0^t \left(-2\Im\pi_*\mu^j + \delta(x_1) \otimes (\mu^{\text{in}} - \mu^{\text{out}}) + \frac{1}{2}(\Re\dot{n}^j)H_p^2 x_1 \mu 1_{\mathcal{G}} 1_{x_1=0}\right)(q \circ \varphi^s)\,\mathrm{d}s, \tag{2.35}$$

where $^bT^*M$ denotes the b-cotangent bundle to M and $\pi : T^*M \rightarrow {}^bT^*M$ is defined by $\pi(x_1, x', \xi_1, \xi') := (x_1, x', x_1\xi_1, \xi')$ (see (Galkowski *et al.*, 2020, Section 4.2)).

Proof. This result is analogous to (Galkowski *et al.*, 2020, Lemma 4.8), except that (Galkowski *et al.*, 2020, Lemma 4.8) only considers zero Dirichlet boundary conditions, and thus only $-2\Im\pi_*\mu^j$ appears on the right-hand side of (Galkowski *et al.*, 2020, Equation 4.3) compared to (2.35) (note that Galkowski *et al.* (2020) defines the joint measure μ^j differently to (2.8), with the result that the signs of μ^j are changed here compared to in Galkowski *et al.* (2020) – compare the definitions (Galkowski *et al.*, 2020, Equation 3.1) and (2.8), and then the sign change in the propagation statements (Galkowski *et al.*, 2020, Lemma 4.4) and (2.13)).

Examination of the proof of (Galkowski *et al.*, 2020, Lemma 4.8) shows that the only time absolute continuity of the measure μ_1 in that proof is used is in the higher-order glancing set. Therefore, since Lemma 2.14 shows that $\mu(H_p q) = \mu_1(q)$ for some measure that is absolutely continuous with respect to μ on the glancing set, the result (2.35) follows in exactly the same way as in (Galkowski *et al.*, 2020, Equation 4.3 and Lemma 4.8). □

2.7 *Linking Lemma* 2.12 *to concepts in the applied literature*

The summary is that α^{ref} in (2.29) is the square of the reflection coefficient describing how plane waves interact with the boundary condition

$$hD_{x_1}v(0, x') = -\frac{\alpha(x', hD_{x'})}{2}v(0, x'), \tag{2.36}$$

where α is a semiclassical pseudodifferential operator. Indeed, when $\alpha = 2$, the boundary condition (2.36) corresponds to the first-order impedance boundary condition $(hD_{x_1} + 1)v = 0$ at $x_1 = 0$, i.e., $(-\partial_{x_1} - ik)v = 0$ (since $h = k^{-1}$). The Helmholtz solution

$$v(x) = \exp\left(ik\left(\xi' \cdot x' - \sqrt{1 - |\xi'|^2}\,x_1\right)\right) + R\exp ik\left(\xi' \cdot x' + \sqrt{1 - |\xi'|^2}\,x_1\right),$$

in the half-plane $x_1 > 0$, corresponds to an incoming plane wave with unit amplitude, and an outgoing plane wave with amplitude R. Imposing the boundary condition $(\partial_{x_1} - ik)v = 0$ at $x_1 = 0$, we obtain that

$$R = \frac{\sqrt{1 - |\xi'|^2} - 1}{\sqrt{1 - |\xi'|^2} + 1}$$

which equals $\sqrt{\alpha^{\text{ref}}}$ when $\alpha = 2$ (since $r(x', \xi') = \sqrt{1 - |\xi'|^2}$ when Γ is flat).

The interpretation of $\sqrt{\alpha^{\mathrm{ref}}}$ as the reflection coefficient is consistent with the relation $\mu^{\mathrm{out}} = \alpha^{\mathrm{ref}}\mu^{\mathrm{in}}$ in (2.28). Indeed, the defect measure of the solution v of (1.6) records where the mass of the solution is concentrated in phase space (x, ξ) in the high-frequency limit $h \to 0$ (see, e.g., the discussion and references in (Lafontaine *et al.*, 2022, §9.1)). The relation $\mu^{\mathrm{out}} = \alpha^{\mathrm{ref}}\mu^{\mathrm{in}}$ therefore describes how much mass of $|v|^2$ (since the defect measure is quadratic in v) is reflected from $\Gamma_{\mathrm{tr},R}$.

The expression for α^{ref} in (2.29) shows that, to minimize reflection from $\Gamma_{\mathrm{tr},R}$ (i.e., to make α^{ref} small), $\alpha/2$ must approximate the symbol of the Dirichlet-to-Neumann map $\sqrt{r(x', \xi')}$; recall the discussion in § 1.3 and see, e.g., (Ihlenburg, 1998, §3.3.2) for similar discussion in this frequency-domain setting, and, e.g., (Engquist & Majda, 1977b, pages 631–632), (Engquist & Majda, 1979, Equation 1.12), (Tsynkov, 1998, §2.2), and (Givoli, 2004, §3) for analogous discussion in the time domain.

2.8 *Relationship between boundary measures and the measure in the interior*

The goal of this subsection is to prove Lemma 2.16 relating the measures μ^{in} and μ^{out} to the measure $\mu|_{T^*U}$. We first introduce some notation.

Recall that $\pi_{\partial M}$ is defined by (2.6); let

$$p^{\mathrm{out/in}} : \mathcal{H} \to \pi_{\partial M}^{-1}\mathcal{H} \cap \{\xi_1 = \xi^{\mathrm{out/in}}\} \subset T_{\partial M}^*\widetilde{M}$$

be defined by

$$p^{\mathrm{out/in}}(x', \xi') := \big(0, x', \xi^{\mathrm{out/in}}(x', \xi'), \xi'\big) \tag{2.37}$$

(i.e., $p^{\mathrm{out/in}}$ takes a point in $\mathcal{H}$ and gives it outgoing/incoming normal momentum).

For $q \in \mathcal{H}$, let

$$t^{\mathrm{out}}(q) = \sup\big\{t > 0 \ : \ \pi_M\varphi_t(p^{\mathrm{out}}(q)) \cap \big(\Gamma \setminus \{\pi_M(q)\}\big) = \emptyset\big\}; \tag{2.38}$$

i.e., $t^{\mathrm{out}}(q)$ is the positive time at which the flow starting at $t = 0$ from $p^{\mathrm{out}}(q)$ hits Γ again. Similarly, let

$$t^{\mathrm{in}}(q) = \inf\big\{t < 0 \ : \ \pi_M\varphi_t(p^{\mathrm{in}}(q)) \cap \big(\Gamma \setminus \{\pi_M(q)\}\big) = \emptyset\big\};$$

i.e., $t^{\mathrm{in}}(q)$ is the negative time at which the flow starting at $t = 0$ from $p^{\mathrm{in}}(q)$ hits Γ again.

Given $\mathcal{V} \subset \mathcal{H}$, let $\mathcal{B}^{\mathrm{out}}(\mathcal{V}), \mathcal{B}^{\mathrm{in}}(\mathcal{V}) \subset T^*U$ be defined by

$$\mathcal{B}^{\mathrm{out}}(\mathcal{V}) := \bigcup_{q \in \mathcal{V}} \big\{\varphi_t\big(p^{\mathrm{out}}(q)\big), \ 0 < t < t^{\mathrm{out}}(q)\big\}, \quad \text{and}$$

$$\mathcal{B}^{\mathrm{in}}(\mathcal{V}) := \bigcup_{q \in \mathcal{V}} \big\{\varphi_t\big(p^{\mathrm{out}}(q)\big), \ t^{\mathrm{in}}(q) < t < 0\big\}.$$

i.e., $\mathcal{B}^{\mathrm{out}}(\mathcal{V})$ is the union of the outgoing flows from points in $\mathcal{V}$ up to their times t^{out} and i.e., $\mathcal{B}^{\mathrm{in}}(\mathcal{V})$ is the union of the incoming flows from points in $\mathcal{V}$ up to their (negative) times t_{in}.

The whole point of these definitions is that in $\mathcal{B}^{\text{out}}(\mathcal{V})$ we can work in geodesic coordinates

$$(\rho, t) \in \left(\pi_{\partial M}^{-1}\mathcal{V} \cap \left\{\xi_1 = \xi_1^{\text{out}}\right\}\right) \times \mathbb{R}_+ = p^{\text{out}}(\mathcal{V}) \times \mathbb{R}_+,$$

defined for $(x, \xi) \in \mathcal{B}$ by $(x, \xi) = \varphi_t(\rho)$ (in a similar way to in the proof of Lemma 2.9). Similarly, in $\mathcal{B}^{\text{in}}(\mathcal{V})$ we work in geodesic coordinates

$$(\rho, t) \in \left(\pi_{\partial M}^{-1}\mathcal{V} \cap \left\{\xi_1 = \xi_1^{\text{in}}\right\}\right) \times \mathbb{R}_- = p^{\text{in}}(\mathcal{V}) \times \mathbb{R}_-.$$

In the following lemma, recall that the pushforward measure $f_*\mu$ is defined by $(f_*\mu)(\mathcal{B}) = \mu(f^{-1}(\mathcal{B}))$.

LEMMA 2.16 (Relationship between boundary measures and the measure in the interior). Let u satisfy (2.7) with $f = o(1)$ as $h \to 0$, and let μ be a defect measure of u. Let $\mu^{\text{out}}, \mu^{\text{in}}$ be defined by Lemma 2.9. Then, in the geodesic coordinates described above,

$$\mu = \left(p_*^{\text{out}}(2\sqrt{r}\mu^{\text{out}})\right) \otimes \mathrm{d}t \ \text{ on } \mathcal{B}^{\text{out}}(\mathcal{V}) \quad \text{and} \quad \mu = \left(p_*^{\text{in}}(2\sqrt{r}\mu^{\text{in}})\right) \otimes \mathrm{d}t \ \text{ on } \mathcal{B}^{\text{in}}(\mathcal{V}),$$

where $\mathrm{d}t$ denotes Lebesgue measure in t and $\otimes$ denotes product measure.

Proof. We prove the result for $\mathcal{B}^{\text{out}}(\mathcal{V})$; the proof for $\mathcal{B}^{\text{in}}(\mathcal{V})$ is similar. By Part (i) of Lemma 2.5, μ is invariant away from the boundary, therefore μ is invariant on $\pm t > 0$ (away from Γ). Since the flow is generated by ∂_t in geodesic coordinates, and, in these coordinates, $\mathcal{B}^{\text{out}} \subset \{t > 0\}$,

$$\mu = \mu(\rho, t) = \mu_1(\rho) \otimes \mathbf{1}_{t>0} \, \mathrm{d}t,$$

for some μ_1. Since $\mu|_{x_1<0} = 0$,

$$\mu_1 = \mu_1 \mathbf{1}_{\xi_1>0},$$

and thus, on $\mathcal{B}^{\text{out}}$

$$\mu = \mu_1(\rho)\mathbf{1}_{\xi_1>0} \otimes \mathbf{1}_{t>0} \, \mathrm{d}t, \tag{2.39}$$

from which

$$\partial_t\mu = \mu_1(\rho)\mathbf{1}_{\xi_1>0} \otimes \delta(t). \tag{2.40}$$

On the other hand, since $x_1 = 0$ is $t = 0$ in geodesic coordinates, Lemma 2.9 implies that

$$H_p^*\mu = \mathcal{L}^*\mu = (2\sqrt{r})\delta(t) \otimes \delta\left(\xi_1 - \xi_1^{\text{in}}\right) \otimes \mu^{\text{in}} - (2\sqrt{r})\delta(t) \otimes \delta\left(\xi_1 - \xi_1^{\text{out}}\right) \otimes \mu^{\text{out}}, \tag{2.41}$$

where the factors of $2\sqrt{r}$ arise because $|\partial x_1/\partial t| = 2|\xi_1| = 2\sqrt{r}$.

Therefore, since $\mathcal{B}^{\text{out}}(\mathcal{V}) \subset \pi_{\partial M}^{-1}\mathcal{V} \cap \{\xi_1 = \xi_1^{\text{out}}\}$ and $\partial_t\mu = -H_p^*\mu$, comparing (2.40) and (2.41), we find that $\mu_1 = p_*^{\text{out}}(2\sqrt{r}\mu^{\text{out}})$ in $\mathcal{B}^{\text{out}}$ (note that p_*^{out} appears because $\rho = p^{\text{out}}(q)$ for $q \in \mathcal{V}$ and μ^{out} acts on $\mathcal{V}$). The result then follows from (2.39). □

The following corollary of Lemma 2.16 is an essential ingredient of our proofs of the lower bounds in Theorems 1.6, 1.7, 1.8, 1.10 and 1.11.

COROLLARY 2.17 (Relationships between incoming boundary measures, outgoing boundary measures, and measures in the interior) Let u be a solution of (2.7), and let μ be any defect measure of u.

(i) (Between two pieces of the boundary.) Let $\mathcal{V}_1 \subset \mathcal{H}$. Assume that $\sup_{q \in \mathcal{V}_1} t^{\mathrm{out}}(q) < \infty$, and that $\pi_{\partial M}(\varphi_{t^{\mathrm{out}}(q)}(p^{\mathrm{out}}(q))) \in \mathcal{H}$ for all $q \in \mathcal{V}_1$. Let

$$\mathcal{V}_2 := \bigcup_{q \in \mathcal{V}_1} \pi_{\partial M}\Big(\varphi_{t^{\mathrm{out}}(q)}\big(p^{\mathrm{out}}(q)\big)\Big) \subset \mathcal{H}$$

(i.e., $\mathcal{V}_2$ is the union of the outgoing flows from points in $\mathcal{V}_1$, projected into $T^* \partial M$). Then

$$(2\sqrt{r}\mu^{\mathrm{in}})(\mathcal{V}_2) = (2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_1). \tag{2.42}$$

(ii) (Between the boundary and the interior.) Let $\mathcal{V} \subset \mathcal{H}$ and $A \subset T^*U$. Then

$$\mu(A) \geq \left(\inf_{q \in \mathcal{V}} \int_0^{t^{\mathrm{out}}(q)} \mathbf{1}_A\left(\varphi_t(p^{\mathrm{out}}(q))\right)\, \mathrm{d}t\right)(2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}) \tag{2.43}$$

and

$$\mu(A) \geq \left(\inf_{q \in \mathcal{V}} \int_{t^{\mathrm{in}}(q)}^0 \mathbf{1}_A\left(\varphi_t(p^{\mathrm{in}}(q))\right)\, \mathrm{d}t\right)(2\sqrt{r}\mu^{\mathrm{in}})(\mathcal{V}). \tag{2.44}$$

The integrals on the right-hand sides of (2.43) and (2.44) are the shortest times that elements of $\mathcal{V}$ spend in A under, respectively, the outgoing forward flow and the incoming backward flow, with the flows considered until they hit Γ again.

Proof of Corollary 2.17. (i) The definition of $\mathcal{V}_2$ implies that

$$\mathcal{B}_{\mathrm{out}}(\mathcal{V}_1) = \mathcal{B}_{\mathrm{in}}(\mathcal{V}_2);$$

let $\mathcal{B}$ denote this set. In $\mathcal{B}$, we work in both sets of geodesic coordinates:

$$(\rho_1, t_1) \in p^{\mathrm{out}}(\mathcal{V}_1) \times \mathbb{R}_+ \quad \text{and} \quad (\rho_2, t_2) \in p^{\mathrm{in}}(\mathcal{V}_2) \times \mathbb{R}_-$$

as defined above. The coordinates $(\rho_j(q), t_j(q)), j = 1, 2$, of $q \in \mathcal{B}$ satisfy

$$t_1 = t_+(p^{\mathrm{out}}(\rho_1)) + t_2 \quad \text{and} \quad \rho_2 = \varphi_{\tau(\rho_1)}(\rho_1) =: \Phi^{1 \to 2}(\rho_1). \tag{2.45}$$

The first equation in (2.45) implies that $\mathrm{d}t_1 = \mathrm{d}t_2$. By Lemma 2.16, in $\mathcal{B}$,

$$\mu = \left(p_*^{\mathrm{out}}(2\sqrt{r}\mu^{\mathrm{out}})\right)_{\mathcal{V}_1}(\rho_1) \otimes \mathrm{d}t_1 = \left(p_*^{\mathrm{in}}(2\sqrt{r}\mu^{\mathrm{in}})\right)_{\mathcal{V}_2}(\rho_2) \otimes \mathrm{d}t_2,$$

where the subscripts $\mathcal{V}_1$ and $\mathcal{V}_2$ show on which neighbourhood of $\mathcal{H}$ $p^{\mathrm{out}}, p^{\mathrm{in}}, \mu^{\mathrm{out}}$, and μ^{in} are considered. This last equality and the second equation in (2.45) imply that

$$\left(p^{\mathrm{in}}_*(2\sqrt{r}\mu^{\mathrm{in}})\right)_{\mathcal{V}_2} = \Phi^{1\to 2}_* \left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)_{\mathcal{V}_1}.$$

Then

$$\begin{aligned}
(2\sqrt{r}\mu^{\mathrm{in}})(\mathcal{V}_2) &= \left(p^{\mathrm{in}}_*(2\sqrt{r}\mu^{\mathrm{in}})\right)_{\mathcal{V}_2} \left(p^{\mathrm{in}}(\mathcal{V}_2)\right), \\
&= \left(p^{\mathrm{in}}_*(2\sqrt{r}\mu^{\mathrm{in}})\right)_{\mathcal{V}_2} \left(\pi^{-1}_{\partial M}\mathcal{V}_2 \cap \{\xi_1 = \xi^{\mathrm{in}}_1\}\right), \\
&= \Phi^{1\to 2}_* \left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)_{\mathcal{V}_1} \left(\pi^{-1}_{\partial M}\mathcal{V}_2 \cap \{\xi_1 = \xi^{\mathrm{in}}_1\}\right), \\
&= \left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)_{\mathcal{V}_1} \left((\Phi^{1\to 2})^{-1}\left(\pi^{-1}_{\partial M}\mathcal{V}_2 \cap \{\xi_1 = \xi^{\mathrm{in}}_1\}\right)\right), \\
&= \left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)_{\mathcal{V}_1} \left(\pi^{-1}_{\partial M}\mathcal{V}_1 \cap \{\xi_1 = \xi^{\mathrm{out}}_1\}\right), \\
&= \left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)_{\mathcal{V}_1} \left(p^{\mathrm{out}}(\mathcal{V}_1)\right), \\
&= (2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_1).
\end{aligned}$$

(ii) We prove (2.43); the proof of (2.44) is similar. Using Lemma 2.16 along with the definitions of $\mathcal{B}_{\mathrm{out}}$, t^{out}, and the geodesic coordinates, we have

$$\begin{aligned}
\mu\left(\mathcal{B}_{\mathrm{out}}(\mathcal{V}) \cap A\right) &= \left(\left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right) \otimes \mathrm{d}t\right)\left(\mathcal{B}_{\mathrm{out}}(\mathcal{V}) \cap A\right), \\
&= \int_{p^{\mathrm{out}}(\mathcal{V})} \int_0^{t^{\mathrm{out}}(\pi_{\partial M}(\rho))} \mathbf{1}_A(\rho, t)\ \mathrm{d}t\, \mathrm{d}\left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)(\rho), \\
&= \int_{p^{\mathrm{out}}(\mathcal{V})} \int_0^{t^{\mathrm{out}}(\pi_{\partial M}(\rho))} \mathbf{1}_A\left(\varphi_t(\rho)\right)\ \mathrm{d}t\, \mathrm{d}\left(p^{\mathrm{out}}_*(2\sqrt{r}\mu^{\mathrm{out}})\right)(\rho),
\end{aligned}$$

where we have used the fact that the point represented in geodesic coordinates by (ρ, t) is in A iff $\varphi_t(\rho) \in A$. Using the change of variables $\rho = p^{\mathrm{out}}(q)$, for $q \in \mathcal{V}$, and then Fubini's theorem, we then have that

$$\begin{aligned}
\mu(A) &\geq \int_{\mathcal{V}} \int_0^{t^{\mathrm{out}}(q)} \mathbf{1}_A\left(\varphi_t(p^{\mathrm{out}}(q))\right)\ \mathrm{d}t\, \mathrm{d}(2\sqrt{r}\mu^{\mathrm{out}})(q), \\
&\geq \left(\inf_{q \in \mathcal{V}} \int_0^{t^{\mathrm{out}}(q)} \mathbf{1}_A\left(\varphi_t(p^{\mathrm{out}}(q))\right)\ \mathrm{d}t\right)(2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}),
\end{aligned}$$

as required. $\qquad\square$

2.9   *The reflection coefficient on $\Gamma_{tr,R}$*

To understand how the defect measures of the solution v of the truncated problem (1.6) are affected by the artificial boundary $\Gamma_{tr,R}$, we now show that the hypotheses of Part (iii) of Lemma 2.12 are satisfied, and get expressions for the numerator and denominator in the reflection coefficient α^{ref} in (2.29).

LEMMA 2.18 If v is the solution to (1.6) and

$$\alpha(x',\xi') = 2\frac{\sigma(\mathcal{D})(x',\xi')}{\sigma(\mathcal{N})(x',\xi')}, \tag{2.46}$$

then, in the hyperbolic set $\mathcal{H}$ of $\Gamma_{tr,R}$

$$-2\Re v_j = (\Re\alpha)v_d = 4(\Re\alpha)|\alpha|^{-2}v_n. \tag{2.47}$$

Combining (2.46), (2.47), (2.28) and (2.29), we obtain the following corollary.

COROLLARY 2.19 Let v be the solution of (1.6), and let μ be a defect measure of v. Then, in the hyperbolic set $\mathcal{H}$ on $\Gamma_{tr,R}$, (2.28) holds with

$$\alpha^{\text{ref}} = \left|\frac{\sqrt{r} - \sigma(\mathcal{D})/\sigma(\mathcal{N})}{\sqrt{r} + \sigma(\mathcal{D})/\sigma(\mathcal{N})}\right|^2. \tag{2.48}$$

Proof of Lemma 2.18.   We prove that

$$\sigma(\mathcal{D})(x',\xi')\,\mathrm{d}v_d^{\text{tr}} = -\sigma(\mathcal{N})(x',\xi')\,\mathrm{d}v_j^{\text{tr}} \tag{2.49}$$

and

$$\left(\sigma(\mathcal{D})(x',\xi')\right)^2 \mathrm{d}v_d^{\text{tr}} = \left(\sigma(\mathcal{N})(x',\xi')\right)^2 \mathrm{d}v_n^{\text{tr}}. \tag{2.50}$$

The result then follows from Part (iii) of Lemma 2.12, since (2.49) and (2.50) imply that (2.27) is satisfied.

For $a \in C_c^\infty(T^*\Gamma_{tr,R})$, if the traces of v have associated defect measures, then, as $h \to 0$,

$$\langle a(x',hD_{x'})\mathcal{N}(hD_{x_1}v), v\rangle \to \int a(x',\xi')\sigma(\mathcal{N})(x',\xi')\,\mathrm{d}v_j^{\text{tr}}. \tag{2.51}$$

On the other hand, in local coordinates, the boundary condition (2.2c) is

$$\mathcal{N}hD_{x_1}v + \mathcal{D}v = 0, \tag{2.52}$$

so that

$$\langle a(x',hD_{x'})\mathcal{N}hD_{x_1}v, v\rangle = -\langle a(x',hD_{x'})\mathcal{D}v, v\rangle$$
$$\to -\int a(x',\xi')\sigma(\mathcal{D})(x',\xi')\,\mathrm{d}v_d^{\text{tr}}. \tag{2.53}$$

Comparing (2.51) and (2.53), we obtain (2.49).

We now use a similar, but slightly more involved, argument to obtain (2.50). First observe that if $\sigma(B)$ is real and the trace of w has an associated defect measure $d\mu$, then

$$
\begin{aligned}
\langle a(x', hD_{x'})Bw, Bw \rangle &= \langle B^* a(x', hD_{x'})Bw, w \rangle \\
&= \langle a(x', hD_{x'})B^2 + a(x', hD_{x'})(B^* - B)B + [B, a(x', hD_{x'})]Bw, w \rangle \\
&\to \int a(x', \xi') \left(\sigma(B)(x', \xi') \right)^2 d\mu
\end{aligned}
\tag{2.54}
$$

as $h \to 0$, since both $B^* - B$ and $[B, a(x', hD_{x'})]$ are $O(h)$(see (A.2) and (Dyatlov & Zworski, 2019, Proposition E.17)). Therefore, (2.54) with $B = \mathcal{N}$ and $w = hD_{x_1}v$ implies that

$$
\langle a(x', hD_{x'})\mathcal{N}hD_{x_1}v, \mathcal{N}hD_{x_1}v \rangle \to \int a(x', \xi') \left(\sigma(\mathcal{N})(x', \xi') \right)^2 dv_n^{\mathrm{tr}}.
\tag{2.55}
$$

On the other hand by (2.52) and (2.54) (with $B = \mathcal{D}$ and $w = v$),

$$
\begin{aligned}
\langle a(x', hD_{x'})\mathcal{N}hD_{x_1}v, \mathcal{N}hD_{x_1}v \rangle &= \langle a(x', hD_{x'})\mathcal{D}v, \mathcal{D}v \rangle \\
&\to \int a(x', \xi') \left(\sigma(\mathcal{D})(x', \xi') \right)^2 dv_d^{\mathrm{tr}}.
\end{aligned}
\tag{2.56}
$$

Comparing (2.55) and (2.56), we find (2.50). □

2.10   *The mass produced by the Dirichlet boundary data on Γ_D*

LEMMA 2.20   Suppose that $h_\ell \to 0$ and $a_\ell \to a$, then the defect measure of

$$
e^{ix \cdot a_\ell / h_\ell}|_{\Gamma_D}
$$

is given by

$$
d\mathrm{vol}_{\Gamma_D} \otimes \delta_{\xi' = (a_{T(x')})^\flat},
$$

where $d\mathrm{vol}_{\Gamma_D}$ denotes Lebesgue measure on Γ_D, $a_{T(x')} := a - (a \cdot n(x'))n(x')$ is the tangential component of the direction a at the point x', $(\cdot)^\flat$ denotes the lowering map $T\Gamma_D \to T^*\Gamma_D$ given by the metric, and δ denotes Dirac measure.

Proof. By using a partition of unity argument, it is sufficient to work locally in a neighbourhood of a point $x_0 \in \Gamma_D$. We work in Euclidean coordinates x such that in a neighbourhood of x_0,

$$
\Gamma_D = \{(\gamma(\mathrm{x}'), \mathrm{x}')\}.
$$

If $a_\ell = (a_{1,a'})$, then, since $n(x') = (1, -\nabla\gamma(x'))/\sqrt{1 + |\nabla\gamma(x')|^2}$,

$$a - (a \cdot n(x'))n(x') = \left(\frac{a_1|\nabla\gamma(x')|^2 + \langle a', \nabla\gamma(x')\rangle}{1 + |\nabla\gamma(x')|^2}, a' - \frac{\langle a', \nabla\gamma(x')\rangle - a_1}{1 + |\nabla\gamma(x')|^2}\nabla\gamma(x') \right),$$

and the metric on Γ_D in the x' coordinates is

$$g_{ij}(x') = \delta_{ij} + \partial_{x_i}\gamma(x')\partial_{x_j}\gamma(x'), \qquad i,j = 2,\ldots,n.$$

Therefore, since we identify the tangent space of Γ_D with ∂_{x_i} $i = 2,\ldots n$

$$
\begin{aligned}
(a^T)^\flat &= a' - \frac{\langle a', \nabla\gamma(x')\rangle - a_1}{1 + |\nabla\gamma(x')|^2}\nabla\gamma(x') + \left(\frac{a_1|\nabla\gamma(x')|^2 + \langle a', \nabla\gamma(x')\rangle}{1 + |\nabla\gamma(x')|^2} \right)\nabla\gamma(x') \\
&= a' + \frac{a_1 - \langle a', \nabla\gamma(x')\rangle}{1 + |\nabla\gamma(x')|^2}\nabla\gamma(x') + \left(\langle a', \nabla\gamma(x')\rangle + \frac{|\nabla\gamma(x')|^2}{1 + |\nabla\gamma(x')|^2}(a_1 - \langle a', \nabla\gamma(x')\rangle) \right)\nabla\gamma(x') \\
&= a' + a_1\nabla\gamma(x').
\end{aligned}
$$

Let $u_\ell = e^{ix\cdot a_\ell/h_\ell}|_{\Gamma_D}$; the previous calculation implies that $u_\ell(x') = \exp((i/h)(a'_\ell \cdot x' + a_{\ell,1}\gamma(x')))$. By change of variable for the semiclassical quantization (see, e.g., (Zworski, 2012, Theorem 9.3, p. 203)),

$$
\begin{aligned}
\langle b(x', h_\ell D_{x'})u_\ell, u_\ell \rangle_{\Gamma_D} &= \int_{\Gamma_D} \left(b(x', h_\ell D_{x'})u_\ell \right)(x')\overline{u_\ell(x')}\,\mathrm{d}x' \\
&= \int_{\Gamma_D} \left(b(x', h_\ell D_{x'})u_\ell \right)(x')\overline{u_\ell(x')}\sqrt{1 + |\nabla\gamma(x')|^2}\,\mathrm{d}x' + O(h_\ell) \\
&= (2\pi h_\ell)^{-n+1}\int_{\Gamma_D}\int_{\Gamma_D}\int_{\mathbb{R}^{n-1}} e^{\frac{i}{h}(x'-y')\cdot\xi'}b(x',\xi') \\
&\qquad \times e^{\frac{i}{h}(a'_\ell\cdot y' + a_{\ell,1}\gamma(y'))}e^{-\frac{i}{h}(a'_\ell\cdot x' + a_{\ell,1}\gamma(x'))}\sqrt{1 + |\nabla\gamma(x')|^2}\,\mathrm{d}\xi'\mathrm{d}y'\mathrm{d}x' + O(h_\ell).
\end{aligned}
$$

Observe that for x' fixed, the phase

$$
\begin{aligned}
\Phi(y', \xi') &= (x' - y')\cdot\xi' + a'_\ell\cdot y' + a_{\ell,1}\gamma(y') - a'_\ell\cdot x' - a_{\ell,1}\gamma(x'), \\
&= (x' - y')\cdot(\xi' - a'_\ell) + a_{\ell,1}(\gamma(y') - \gamma(x'))
\end{aligned}
$$

is stationary (i.e., $\partial_{y'}\Phi = \partial_{\xi'}\Phi = 0$) if and only if

$$(y', \xi') = (x', a'_\ell + \nabla\gamma(x')a_{\ell,1}),$$

where it is additionally nondegenerate. Consequently, by stationary phase (see, e.g., (Zworski, 2012, §3.5))

$$\langle b(x', h_\ell D_{x'})u_\ell, u_\ell\rangle_{\Gamma_D} = \int_{\Gamma_D} b(x', a'_\ell + \nabla\gamma(x')a_{\ell,1})\sqrt{1 + |\nabla\gamma(x')|^2}\, dx' + O(h_\ell)$$

$$= \int_{\Gamma_D} b(x', (a^T)^\flat(x'))\sqrt{1 + |\nabla\gamma(x')|^2}\, dx' + O(h_\ell).$$

The result follows by letting $\ell \to \infty$. □

3. Properties of outgoing solutions of the Helmholtz equation

The goal of this section is to prove three lemmas (Lemmas 3.1, 3.2 and 3.3), the first two of which concern the solution to the exterior Dirichlet problem:

$$\begin{cases} (-h^2\Delta - 1)u = 0 & \text{in } \Omega_+, \\ u = g & \text{on } \Gamma_D, \\ h\partial_r u - iu = o(r^{(1-d)/2}) & \text{as } r \to \infty; \end{cases} \tag{3.1}$$

observe that the problem (2.1) is a special case of (3.1) with $g = e^{ia\cdot x/h}$.

LEMMA 3.1 Suppose that $\Omega_- \Subset B(0,1)$ is nontrapping. Then there is $C_0 > 0$ such that for all $R \geq 1$ there is $h_0 > 0$ such that for u_h solving (3.1)

$$\|u_h\|_{H_h^1(B(0,R)\setminus\overline{\Omega_-})} \leq C_0 R^{1/2}\|g\|_{H_h^1(\Gamma_D)}, \qquad 0 < h < h_0.$$

LEMMA 3.2 Let $\mathcal{N}, \mathcal{D}$ be as in § 1.3 (i.e., $\mathcal{N} \in \Psi^{2N}(\Gamma_{\mathrm{tr},R})$, $\mathcal{D} \in \Psi^{2M}(\Gamma_{\mathrm{tr},R})$ and both have real-valued principal symbols). There exists $C > 0$ such that for any $R > 1$ there exists $h_0(R) > 0$ such that for $0 < h \leq h_0(R)$ the solution u of (3.1) satisfies

$$\left\|(\mathcal{N}hD_n - \mathcal{D})u\right\|_{L^2(\Gamma_{\mathrm{tr},R})} \leq C\frac{\Upsilon(R)}{R^{1/2}}\|u\|_{L^2(\Omega_R)},$$

where $n(x)$ is the normal vector field to $\Gamma_{\mathrm{tr},R}$, and

$$\Upsilon(R) := \sup\left\{\left|\sigma(\mathcal{N})(x',\xi')n(x)\cdot\xi - \sigma(\mathcal{D})(x',\xi')\right| + \left|H_p\left(\sigma(\mathcal{N})(x',\xi')n(x)\cdot\xi - \sigma(\mathcal{D})(x',\xi')\right)\right|\right.$$

$$\left. : x \in \Gamma_{\mathrm{tr},R}, \left|\xi\cdot\frac{x}{|x|} - 1\right| \leq \frac{C}{|x|^2}, |\xi| = 1\right\}. \tag{3.2}$$

The quantity $\Upsilon(R)$ controls, on all rays that are approximately radial, the reflection coefficient as well as the change of the reflection coefficient under the Hamiltonian flow.

LEMMA 3.3 (Bounds on $\Upsilon(R)$). If $\mathcal{N}$ and $\mathcal{D}$ satisfy Assumption 1.4, then the following hold.
(i) There exists $C_1 > 0$, independent of R, such that if $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, then $\Upsilon(R) \leq C_1 R^{-2m_{\mathrm{ord}}}$.

(ii) There exists $C_2 > 0$, independent of R, such that if $\Gamma_{\mathrm{tr},R}$ is C^2 uniformly in R, then $\Upsilon(R) \leq C_2$.

Regarding Lemma 3.1: this result gives us a lower bound on $1/\|u\|_{L^2(\Omega_R)}$, and we use this in proving the R-explicit lower bounds on the relative error in Theorems 1.7, 1.8, 1.9. The analogue of this result without the explicit dependence of the constant on R was proved in (Baskin *et al.*, 2016, Theorem 3.5).

Regarding Lemmas 3.2 and 3.3: the upper bounds in Theorem 1.7 and in Theorem 1.9 follow from applying Theorem 1.5 to $u - v$ and then using these two lemmas.

3.1   *Proof of Lemma* 3.1

We define the directly-incoming set $\mathcal{I}$ by

$$\mathcal{I} := \left\{ \rho \in S^* \Omega_R, \text{ s.t. } \pi_{\mathbb{R}^d}\left(\bigcup_{t \geq 0} \varphi_{-t}(\rho) \right) \cap \Omega_- = \emptyset \right\}, \tag{3.3}$$

where we recall that $\pi_{\mathbb{R}^d}$ denotes projection in the x variable. The following lemma reflects the fact that u is an outgoing solution.

LEMMA 3.4   If u solves (3.1) with $\|g\|_{H_h^1} \leq C$, then

$$\mathrm{WF}_h(u) \cap \mathcal{I} = \emptyset.$$

In particular, there exists $C > 0$, sufficiently large, such that

$$\mathrm{WF}_h(u) \cap \{|x| > C\} \subset \left\{ \left| \xi - \frac{x}{|x|} \right| < \frac{C}{|x|}, \quad \left| \xi \cdot \frac{x}{|x|} - 1 \right| \leq \frac{C}{|x|^2} \right\}.$$

Proof.   Let R_D be the outgoing resolvent for

$$(-h^2 \Delta - 1)w = f, \qquad w|_{\Gamma_D} = 0,$$

i.e., $w = R_D f$. Fix $0 < R_1 < R_2$ such that $\Omega_- \subset B(0, R_1)$, and let $\chi_i \in C_c^\infty(B(0, R_2))$, $i = 0, 1, 2$, with $\chi_i \equiv 1$ on $B(0, R_1)$, $\mathrm{supp}\, \chi_i \subset \{\chi_{i+1} \equiv 1\}$. We now extend the Dirichlet boundary data off Γ_D by letting $\widetilde{g}$ be the solution of

$$(-h^2 \Delta - 1)\widetilde{g} = 0 \quad \text{in } \Omega_+ \cap B(0, R_1),$$
$$\widetilde{g} = g \quad \text{on } \Gamma_D,$$
$$(hD_n - 1)\widetilde{g} = 0 \quad \text{on } \partial B(0, R_1).$$

We now show that u can be expressed as an outgoing resolvent plus a function with compact support. To this end, let

$$v := u - \chi_0 \widetilde{g} - R_D\big(\big[-h^2 \Delta, \chi_0 \big] \widetilde{g} \big),$$

and observe that $(-h^2\Delta - 1)v = 0$. Since the Dirichlet Laplacian is a black box Hamiltonian in the sense of (Dyatlov & Zworski, 2019, Chapter 4), by (Dyatlov & Zworski, 2019, Theorem 4.17), the radiation condition for u implies that $v = 0$, and hence $u = \chi_0\widetilde{g} + R_D([-h^2\Delta, \chi_0]\widetilde{g})$. Now, by, e.g., (Dyatlov & Zworski, 2019, Theorem 4.4), the range of $(1 - \chi_2)R_D$ lies in the range of $R_0\chi_1$ where R_0 denotes the free resolvent. In particular, by the outgoing property of R_0 (see e.g., (Dyatlov & Zworski, 2019, Theorem 3.37))

$$\mathrm{WF}_h(u) \cap \{|x| > R_2 + 1\} \subset \bigcup_{t \geq 0} \varphi_t\left(S^*_{B(0,R_2)}\mathbb{R}^d\right). \tag{3.4}$$

Now, suppose that $A \subset \mathcal{I}$, where $\mathcal{I}$ is as in (3.3). Then, for $t_0 \geq 0$ large enough,

$$\varphi_{-t_0}(A) \subset \{|x| > R_2 + 1\}$$

and, moreover,

$$\bigcup_{t \leq -t_0} \varphi_t(A) \cap S^*_{B(0,R_1)}\mathbb{R}^d = \emptyset.$$

Therefore, by (3.4), $\varphi_{-t_0}(A) \cap \mathrm{WF}_h(u) = \emptyset$. Now, since $(h^2\Delta + 1)u = 0$, and

$$\bigcup_{-t_0 \leq t \leq 0} \varphi_t(A) \cap S^*_{\Gamma_D}\mathbb{R}^d = \emptyset,$$

by propagation of singularities (see e.g., (Dyatlov & Zworski, 2019, Appendix E.4)), $A \cap \mathrm{WF}_h(u) = \emptyset$.

Now, suppose $(x, \xi) \in \mathrm{WF}_h(u) \cap \{|x| \geq R\}$. Then, $(x, \xi) \notin \mathcal{I}$ and, in particular, there is $t \geq 0$ such that $\varphi_{-t}(x, \xi) \in S^*_{\Omega_-}\mathbb{R}^d$. Let

$$t_0 = \inf\left\{t \geq 0 \,:\, \varphi_{-t}(x, \xi) \in S^*_{\Omega_-}\mathbb{R}^d\right\}$$

and $(x_0, \xi_0) = \varphi_{-t_0}(x, \xi)$. Then, $|x_0| \leq R_1$, $t_0 \geq \frac{R - R_0}{2}$, $\xi = \xi_0$, and

$$x = x_0 + 2t_0\xi_0.$$

Observe that

$$|x_0 + 2t\xi_0| = \sqrt{|x_0|^2 + 4t\langle x_0, \xi_0\rangle + 4t^2} = 2t\sqrt{1 + |x_0|^2 t^{-2} + 2t^{-1}\langle x_0, \xi_0\rangle} = 2t + O(t^{-1}|x_0|^2).$$

Then consider

$$\left|\frac{x}{|x|} - \xi\right| = \left|\frac{x_0 + 2t\xi_0}{|x_0 + 2t\xi|_0} - \xi_0\right| = \left|\frac{x_0 + \xi_0 O\left(t^{-1}|x_0|^2\right)}{|x_0 + 2t\xi_0|}\right| = O(t^{-1}|x_0|) = O\left(\frac{R_1}{|x| - R_1}\right).$$

In particular, if $R \geq 2R_1$, $|x| - R_1 \geq \frac{1}{2}|x|$.

Next, observe that

$$\xi \cdot \frac{x}{|x|} = \frac{x_0 \cdot \xi_0 + 2t}{|x_0 + 2t\xi_0|}, \qquad |x_0 + 2t\xi_0|^2 = |x_0|^2 + 4t^2 + 4tx_0 \cdot \xi_0$$

so that

$$\frac{1}{|x_0 + 2t\xi_0|} = \frac{1}{2t}\left(1 - \frac{x_0 \cdot \xi_0}{2t} + O(R_1^2 t^{-2})\right).$$

In particular,

$$\frac{x_0 \cdot \xi_0 + 2t}{|x_0 + 2t\xi_0|} = 1 + \frac{x_0 \cdot \xi_0}{2t} - \frac{x_0 \cdot \xi_0}{2t} + O(R_1^2 t^{-2}) = 1 + O(R_1^2 t^{-2}) = 1 + O\left(\frac{R_1^2}{(|x| - R_1)^2}\right).$$

Taking $|x| \geq 2R_1$ completes the proof. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\square$

COROLLARY 3.5 There exists $t_0 > 0, r_0 > 0$ such that, if u solves (3.1) and has defect measure μ, then for any $r \geq r_0$, if $(x, \xi) \in \text{supp}\,\mu$ with $|x| = r$, then, for $0 \leq t \leq r - t_0$,

$$|x(\varphi_{-t}(x, \xi))|^2 = |x - 2t\xi|^2 = (r - 2t)^2 + O(tr^{-1}).$$

Proof. This follows from Lemma 3.4 by observing that, by the definition of defect measures, $\text{supp}\,\mu \subset \text{WF}_h(u)$; then, if $|x| = r$ and $|\xi| = 1$ with $|\xi \cdot \frac{x}{|x|} - 1| < \frac{C}{r^2}$, then $x \cdot \xi \geq r - \frac{1}{r}$. $\qquad\square$

By the definitions of $\text{WF}_h(u)$ and $\mathcal{I}$, another corollary of Lemma 3.4 is the following lemma, originally proved in (Burq, 2002, Proposition 3.5) (see also (Galkowski *et al.*, 2020, Lemma 3.4)).

LEMMA 3.6 Suppose that u solves (3.1) and has defect measure μ. Then $\mu(\mathcal{I}) = 0$.

We now prove Lemma 3.1.

Proof of Lemma 3.1. Suppose that the lemma fails. Then there exist $R \geq 1, \epsilon > 0, (h_\ell, g_\ell)$ such that $h_\ell \to 0$ as $\ell \to \infty$ and such that

$$\|u_{h_\ell}\|_{H^1_{h_\ell}(B(0,R)\setminus\overline{\Omega_-})} = 1 \quad \text{and} \quad \|g_\ell\|_{H^1_{h_\ell}(\Gamma_D)} \leq \frac{1}{R^{1/2}(C_0 + \epsilon)}. \qquad (3.5)$$

Let w_ℓ solve

$$(-h_\ell^2 \Delta - 1)w_\ell = 0, \qquad w_\ell|_{\Gamma_D} = g_\ell, \qquad (hD_n - 1)w_\ell|_{\partial B(0,1)} = 0.$$

Since Lemma 3.1 is not used in the proof of Theorem 1.5, the upper bound in this latter result implies that there exists a $C_1 > 0$ such that

$$\|w_\ell\|_{H^1_{h_\ell}(B(0,1)\setminus\overline{\Omega_-})} \leq C_1 \|g_\ell\|_{H^1_{h_\ell}(\Gamma_D)}.$$

Let $\chi \in C_c^\infty(B(0,1))$ with $\chi \equiv 1$ near Γ_D and put $v_\ell = u_\ell - \chi w_\ell$ so that

$$\begin{cases} \left(-h_\ell^2 \Delta - 1\right) v_\ell = -\left(-h_\ell^2 \Delta_\ell - 1\right) \chi w_\ell =: h_\ell f_\ell \\ v_\ell|_{\Gamma_D} = 0 \\ (h_\ell D_n - 1)v_\ell = o(r^{(1-d)/2}), \end{cases}$$

and $\|f_\ell\|_{L^2} \leq C_2 \|w_\ell\|_{H_h^1} \leq C_2 C_1 \|g_\ell\|_{H_h^1(\Gamma_D)}$, $\mathrm{supp} f_\ell \subset B(0,1)$. In particular, by e.g., (Galkowski *et al.*, 2020, Theorem 1) there is $C_3 > 0$ such that for any $\psi \in C_c^\infty$ with $\psi \equiv 1$ on $B(0,1)$ and $\mathrm{supp}\, \psi \subset B(0, R_0)$, and any h_ℓ small enough,

$$\|\psi v_\ell\|_{H_h^1} \leq C_3 R_0 \|f_\ell\|_{L^2} \leq R_0 C_1 C_2 C_3 \|g_\ell\|_{H_h^1(\Gamma_D)}. \tag{3.6}$$

Now, taking $C_0 \geq C_1(3C_2 C_3 + 1)$ the proof is complete for $1 \leq R \leq 2$. To see this, observe that using (3.6) with $R_0 = 3$ and $\psi \equiv 1$ on $B(0,2)$

$$\|u_{h_\ell}\|_{H_{h_\ell}^1(B(0,2) \setminus \overline{\Omega_-})} \leq \|\psi(v_\ell + \chi w_\ell)\|_{H_{h_\ell}^1} \leq \|\psi v_\ell\|_{H_{h_\ell}^1} + \|\chi w_\ell\|_{H_{h_\ell}^1} \leq C_1(3C_2 C_3 + 1)R^{1/2}\|g\|_{H_h^1} < 1$$

which contradicts (3.5).

Now, for $R \geq 2$, we can pass to a subsequence in ℓ, and assume that v_ℓ has defect measure μ. By Lemma 3.6, $\mu(\mathcal{I} \cap T^*\widetilde{M} \setminus \mathrm{supp} f) = 0$ and

$$\mu(H_p a) = 0, \qquad a \in C_c^\infty(T^*\widetilde{M} \setminus \mathrm{supp} f).$$

Therefore, since $\mathrm{supp} f \subset B(0,1)$

$$\mathrm{supp}\, \mu \cap T^*\widetilde{M} \setminus B(0,2) \subset \bigcup_{t \geq 0} \varphi_t \left(\left\{ (x, \xi) \,:\, |x| = 2,\, \exists s > 0 \text{ s.t. } \varphi_{-s}(x, \xi) \in T^*B(0,1) \right\} \right).$$

In particular, since μ is invariant under φ_t on $T^*(\mathbb{R}^d \setminus B(0,1))$,

$$\begin{aligned} \mu(T^*B(0,R) \setminus B(0,2)) &\leq \mu\left(\bigcup_{0 \leq t \leq \sqrt{R^2-4}} \varphi_t \left(\left\{ (x,\xi) \,:\, |x| = 2,\, \exists s > 0 \text{ s.t. } \varphi_{-s}(x,\xi) \in T^*B(0,1) \right\} \right) \right) \\ &= \sqrt{R^2 - 4}\, \mu\left(\bigcup_{-1 \leq t \leq 0} \varphi_t \left(\left\{ (x,\xi) \,:\, |x| = 2,\, \exists s > 0 \text{ s.t. } \varphi_{-s}(x,\xi) \in T^*B(0,1) \right\} \right) \right) \\ &\leq \sqrt{R^2 - 4} \lim_{\ell \to \infty} \|v_\ell\|_{L^2(B(0,2) - B(0,1))}^2 \\ &\leq 9 C_1^2 C_2^2 C_3^2 \sqrt{R^2 - 4} \lim_{\ell \to \infty} \|g_\ell\|_{H_h^1(\Gamma_D)}^2 \\ &\leq \frac{3 C_1 C_2 C_3 \sqrt{R^2 - 4}}{R(C_0 + \epsilon)^2}. \end{aligned}$$

By (Galkowski *et al.*, 2020, Lemma 4.2)

$$\mu\big(|\xi|^2 1_{T^*B(0,R)\setminus B(0,2)}\big) \geq \limsup_{\ell\to\infty} \|v_\ell\|^2_{H^1_{h_\ell}(B(0,R)\setminus B(0,5/2))}.$$

Therefore, using (3.6) with $R_0 = 3$, $\psi \equiv 1$ on $B(0,5/2)$,

$$\limsup_{\ell\to\infty} \|v_\ell\|^2_{H^1_{h_\ell}(B(0,R))} \leq \frac{9C_3^2 C_2^2 C_1^2(1+\sqrt{R^2-4})}{R(C_0+\epsilon)^2}.$$

Hence, letting

$$C_0 = C_1 \max\left(3C_2 C_3 + 1, \sup_{R\geq 2} \frac{3C_3 C_2\sqrt{1+\sqrt{R^2-4}}+1}{R^{1/2}}\right),$$

we have

$$\limsup_{\ell\to\infty} \|u_{h_\ell}\|_{H^1_{h_\ell}(B(0,R))} \leq \frac{3C_3 C_2 C_1\sqrt{1+\sqrt{R^2-4}}+C_1}{R^{1/2}(C_0+\epsilon)} < 1,$$

which contradicts (3.5).   □

3.2 *Proof of Lemmas* 3.2 *and* 3.3

In the next lemma, we identify $S^*\Gamma_{\mathrm{tr},R}$ with a subset of $S^*\mathbb{R}^d$.

LEMMA 3.7 Suppose that $A \in \Psi^m(\mathbb{R}^d)$ and $\mathrm{WF}'_h(A) \cap S^*\Gamma_{\mathrm{tr},R} = \emptyset$. Then there is $C > 0$ such that

$$\|Au\|_{L^2(\Gamma_{\mathrm{tr},R})} \leq C\|Au\|_{L^2} + Ch^{-1}\|PAu\|_{L^2} + O(h^\infty)\|u\|_{L^2}.$$

Proof. First, note that for $B \in \Psi^0$ with $\mathrm{WF}'_h(B)$ supported away from $S^*\mathbb{R}^d$, we can write using the elliptic parametrix construction (Lemma A2) that there is $E \in \Psi^{-2}$ such that

$$BAu = EPAu + O(h^\infty)_{\Psi^{-\infty}}.$$

In particular, by the Sobolev embedding as in (Galkowski, 2019a, Lemma 5.1) see also (Zworski, 2012, Lemma 7.10),

$$\|BAu\|_{L^2(\Gamma_{\mathrm{tr},R})} \leq Ch^{-1/2}\|BAu\|_{H^1_h} \leq Ch^{-1/2}\|EPAu\|_{H^1_h} + O(h^\infty)\|u\|_{L^2}$$
$$\leq Ch^{-1/2}\|PAu\|_{L^2} + O(h^\infty)\|u\|_{L^2}.$$

Therefore, we can assume that

$$\mathrm{WF}'_h(A) \subset \big\{1-\delta \leq |\xi|^2 \leq 1+\delta\big\}$$

for any $\delta > 0$. Next, if $\mathrm{WF}'_h(A) \cap S^*_{\Gamma_{\mathrm{tr},R}} \mathbb{R}^d = \emptyset$, then there is $\chi \in C_c^\infty(\mathbb{R}^d)$ with $\chi \equiv 1$ in a neighbourhood of $\Gamma_{\mathrm{tr},R}$ such that

$$\chi A = O(h^\infty)_{\Psi^{-\infty}}.$$

In particular,

$$\|\chi A u|_{\Gamma_{\mathrm{tr},R}}\|_{L^2(\Gamma_{\mathrm{tr},R})} = O(h^\infty)\|u\|_{L^2}.$$

By using a partition of unity, we can work locally, assuming that $\Gamma_{\mathrm{tr},R} = \{x_1 = 0\}$ as in § 2.3. We can then assume that $\mathrm{WF}'_h(A) \subset \{|x_1| < \delta\}$. Write $A = a(x, hD)$ where $d(\mathrm{supp}\, a, \{r(x,\xi) = 0\}) > \epsilon > 0$ and $\mathrm{supp}\, a \subset \{|x_1| < \delta\}$ for some $\epsilon > 0$. Then, choosing $\delta > 0$ small enough, we have $|\xi_1| > 0$ on $\mathrm{supp}\, a$, and hence there is $e \in C_c^\infty(T^*\mathbb{R}^d)$ with $|e| > 0$ on $\mathrm{supp}\, a$ and such that

$$e(x,\xi)(\xi_1 - b(x,\xi'))a(x,\xi') = \left(-\xi_1^2 + r(x,\xi')\right)a(x,\xi).$$

Therefore,

$$\left\|\left(hD_{x_1} - b(x, hD_{x'})\right) Au\right\|_{L^2} \le C\|PAu\|_{L^2} + O(h)\|Au\|_{L^2};$$

the result then follows by applying (Zworski, 2012, Lemma 7.11). $\qquad \square$

LEMMA 3.8 Let u be the solution to (3.1). For any $\eta > 0$, there exists $R_0 > 0$ such that, for $R \ge R_0$ and h small enough (depending on R)

$$\|u\|_{L^2(B(0,R+1)\setminus B(0,R-1))} \le (\sqrt{2} + \eta)R^{-\frac{1}{2}}\|u\|_{L^2(B(0,R))}. \tag{3.7}$$

Proof. We define $A_{r_0,r_1} := \overline{B(0,r_0)} \setminus B(0,r_1)$. First, observe that it is sufficient to prove that there exists $R_1(\eta) > 0$ such that, for any $R \ge R_1$ and any u solving (3.1) having defect measure μ,

$$\mu\left(T^*A_{R+1,R-1}\right) < \frac{(\sqrt{2}+\eta)^2}{R}\mu(T^*B(0,R)). \tag{3.8}$$

Indeed, if (3.7) fails, then there exists $\eta > 0$ and $h_n \to 0$ and $g_n \in H_h^1(\Gamma_D)$ such that, for $u(h_n)$ solving (3.1) with $g = g_n$ and some $R \ge R_1(\eta)$,

$$\|u(h_n)\|_{L^2(A_{R+1,R-1})} > \frac{\sqrt{2}+\eta}{R^{1/2}}\|u(h_n)\|_{L^2(B(0,R))}, \qquad \|u(h_n)\|_{L^2(B(0,R))} = 1. \tag{3.9}$$

Then, passing to a subsequence, we can assume that $u(h_n)$ has defect measure μ. Let $\epsilon > 0$ be arbitrary. Take χ_0^ϵ equal to one in $A_{R+1,R-1}$ and supported in $A_{R+1+\epsilon,R-1-\epsilon}$ and χ_1^ϵ supported in $B(0,R)$ and equal to one in $B(0,R-\epsilon)$. The estimate (3.9) implies

$$\left\|\chi_0^\epsilon u(h_n)\right\|_{L^2} > \frac{\sqrt{2}+\eta}{R^{1/2}}\left\|\chi_1^\epsilon u(h_n)\right\|_{L^2},$$

passing to the limit $h_n \to 0$ and using e.g., (Galkowski *et al.*, 2020, Lemma 4.2), we obtain

$$\mu\big(\big(\chi_0^\epsilon\big)^2\big) \geq \frac{(\sqrt{2}+\eta)^2}{R}\mu\big(\big(\chi_1^\epsilon\big)^2\big),$$

which in turn implies, by the support properties of $\chi_{0,1}$,

$$\mu\left(T^*A_{R+1+\epsilon,R-1-\epsilon}\right) \geq \frac{(\sqrt{2}+\eta)^2}{R}\mu\left(T^*B_{R-\epsilon}\right).$$

In particular, sending $\epsilon \to 0^+$, and using monotonicity of measures

$$\mu\left(T^*A_{R+1,R-1}\right) \geq \frac{(\sqrt{2}+\eta)^2}{R}\mu\left(T^*B_R\right),$$

which contradicts (3.8).

We therefore only need to prove (3.8). The definition of defect measures implies supp $\mu \subset \mathrm{WF}_h(u)$, thus, by Lemma 3.4,

$$\mathrm{supp}\,\mu \cap \{|x| > C\} \subset \left\{\left|\xi \cdot \frac{x}{|x|} - 1\right| < \frac{C}{|x|^2}\right\}.$$

Now, invariance of defect measures away from the obstacle combined with the above implies that, for $r_0 > C + 2$, so that $\Omega_- \subset B(0, r_0 - 2)$, and $0 \leq t \leq 1$,

$$\mu\left(T^*A_{r_1,r_0}\right) = \mu\left(\varphi_{-t}\left(T^*A_{r_1,r_0} \cap \left\{|\xi| = 1, \left|\xi \cdot \frac{x}{|x|} - 1\right| < \frac{C}{|x|^2}\right\}\right)\right).$$

By Corollary 3.5, there exist $C_0, C_1, C_2 > 0$ such that

$$\varphi_{-\frac{1}{2}-C_0R^{-2}}\left(T^*A_{R+1,R-1} \cap \mathrm{supp}\,\mu\right) \cap T^*\{|x| \geq R\} = \emptyset,$$

$$\varphi_{-1-1C_0R^{-2}}\left(T^*A_{R+1,R-1} \cap \mathrm{supp}\,\mu\right) \subset T^*\{|x| < R-1\}.$$

Fix $r_0 > 0$ such that $\Omega_- \Subset B(0, r_0)$. Then, for $0 \leq 2t \leq R-1-r_0$, we have $\varphi_{-t}(S^*A_{R+1,R-1}) \cap B(0, r_0) = \emptyset$. Therefore, using the fact that $\langle x, \xi \rangle > 0$ on supp $\mu \cap T^*A_{R+1,R-1}$, we have

$$\varphi_{-t}\left(T^*A_{R+1,R-1} \cap \mathrm{supp}\,\mu\right) \cap T^*A_{R+1,R-1} \cap \mathrm{supp}\,\mu = \emptyset \text{ for } t \in \left[1 + C_0R^{-2}, \frac{R-1-r_0}{2}\right]. \quad (3.10)$$

Now, let $T_{1,R} := (R-1-r_0)/2$ and $T_{0,R} := 1 + C_0R^{-2}$ and consider

$$f_{T,R}(x,\xi) := \int_{T_{0,R}}^{T_{1,R}} 1_{T^*A_{R+1,R-1}\cap\mathrm{supp}\,\mu} \circ \varphi_t(x,\xi)\,\mathrm{d}t.$$

We claim that $0 \leq f_{T,R} \leq T_{0,R}$; to see this, suppose that $\varphi_t(x,\xi) \in T^*A_{R+1,R-1} \cap \operatorname{supp} \mu$ and $\varphi_s(x,\xi) \in T^*A_{R+1,R-1} \cap \operatorname{supp} \mu$ with $T_{0,R} \leq s \leq t - T_{0,R}$ and $t \leq T_{1,R}$. Then,

$$\varphi_{-(t-s)}(x,\xi) \in T^*A_{R+1,R-1} \cap \operatorname{supp} \mu, \qquad (x,\xi) \in T^*A_{R+1,R-1} \cap \operatorname{supp} \mu$$

and $T_{0,R} \leq t - s \leq T_{1,R}$, contradicting (3.10).

Now, since μ is φ_t invariant,

$$(T_{1,R} - T_{0,R})\,\mu\big(1_{T^*A_{R+1,R-1}}\big) = \mu(f_{T,R}(x,\xi)) \leq T_{0,R}\,\mu(B(0,R)).$$

In particular,

$$\mu\big(1_{T^*A_{R+1,R-1}}\big) \leq \frac{T_0,R}{T_{1,R} - T_{0,R}}\mu(B(0,R)) \leq \frac{2}{R}(1 + O(R^{-1}))\mu(B(0,R)).$$

Choosing $R > 0$ large enough yields (3.8), and the proof is complete. $\qquad\square$

We now prove Lemmas 3.2 and 3.3.

Proof of Lemma 3.2. Let $\tilde{n}$ be a smooth extension of the normal vector field to $\Gamma_{\mathrm{tr},R}$, $n_R(x)$ and $C_0 > 0$ so that the conclusions of Lemma 3.4 hold, and, $\widetilde{\mathcal{N}}$, $\widetilde{\mathcal{D}}$ smooth extensions of $\mathcal{N}$ and $\mathcal{D}$. Next, fix $\epsilon > 0$ such that

$$\sup\left\{\left|\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}}\right| + \left|H_p(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})\right| \,:\, \operatorname{dist}(x, \Gamma_{\mathrm{tr},R}) < \epsilon, \left|\xi \cdot \frac{x}{|x|} - 1\right| \leq \frac{C_0}{|x|^2}, \left||\xi| - 1\right| < \epsilon\right\} \leq 2\Upsilon(R)$$

and let χ be smooth, supported in

$$\Gamma_\epsilon := \big\{x \,:\, \operatorname{dist}(x, \Gamma_{\mathrm{tr},R}) < \epsilon\big\},$$

and equal to one near $\Gamma_{\mathrm{tr},R}$. By Lemma 3.4, we can find $Z \in \Psi(\mathbb{R}^d)$ with $\mathrm{WF}_h'(Z) \cap \mathcal{I} = \emptyset$ such that

$$\chi u = \chi Z u + O_{C^\infty}\big(h^\infty \|u\|_{L^2}\big).$$

Now, since $\widetilde{\Omega}_R$ is convex, and $\Omega_- \Subset \widetilde{\Omega}_R$, $S^*\Gamma_{\mathrm{tr},R} \subset \mathcal{I}$. In particular, by Lemma 3.7,

$$\begin{aligned}
\|(\mathcal{N}hD_n - \mathcal{D})u\|_{L^2(\Gamma_{\mathrm{tr},R})} &= \|(\mathcal{N}hD_n - \mathcal{D})\chi Z u\|_{L^2(\Gamma_{\mathrm{tr},R})} + O(h^\infty)\|u\|_{L^2} \\
&\leq C\|(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})\chi Z u\|_{L^2} + Ch^{-1}\|(-h^2\Delta - 1)(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})\chi Z u\|_{L^2} + O(h^\infty)\|u\|_{L^2} \\
&= C\|(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})\chi u\|_{L^2} + Ch^{-1}\|(-h^2\Delta - 1)(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})\chi u\|_{L^2} + O(h^\infty)\|u\|_{L^2} \\
&\leq C\|(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})\chi u\|_{L^2} + Ch^{-1}\|(\widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}})(-h^2\Delta - 1)\chi u\|_{L^2} \\
&\quad + Ch^{-1}\big\|\big[-h^2\Delta - 1, \widetilde{\mathcal{N}}hD_{\tilde{n}} - \widetilde{\mathcal{D}}\big]\chi u\big\|_{L^2} + O(h^\infty)\|u\|_{L^2},
\end{aligned}$$

and, using the fact that $(-h^2\Delta - 1)u = 0$,

$$\|(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}})u\|_{L^2(\Gamma_{\mathrm{tr},R})} \le \|(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}})\chi u\|_{L^2} + h^{-1}\|(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}})[h^2\Delta + 1, \chi]u\|_{L^2}$$
$$+ h^{-1}\|[-h^2\Delta - 1, \widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}}]\chi u\|_{L^2}. \tag{3.11}$$

Let

$$R_1 := \sup\{R : \Gamma_{\mathrm{tr},R} \cap B(0, C_0 + 1) \neq \emptyset\}.$$

Then, for $1 \le R \le R_1$, the proof is completed, since $\|Bu\|_{H_h^1} + h^{-1}\|[B, (-h^2\Delta - 1)]u\|_{L^2} \le C_B\|u\|_{L^2}$ for any $B \in \Psi^\infty$. We now consider the case $R \ge C_0$.

Observe that, by Lemma 3.4,

$$\mathrm{WF}_h(\chi u) \subset \mathrm{supp}\,\chi \cap \mathrm{WF}_h(u) \subset \left\{\left|\xi \cdot \frac{x}{|x|} - 1\right| < \frac{C}{|x|^2}, \, x \in \Gamma_\epsilon, \, |\xi| = 1\right\}. \tag{3.12}$$

Now, let $\widetilde{\chi} \in C_c^\infty(\mathbb{R}^d)$ with $\widetilde{\chi} \equiv 1$ on $\mathrm{supp}\,\chi$ with $\mathrm{supp}\,\widetilde{\chi} \subset \Gamma_\epsilon$, and $\psi \in C_c^\infty(T^*\mathbb{R}^d)$ with

$$\mathrm{supp}\,\psi \subset \left\{\left|\xi \cdot \frac{x}{|x|} - 1\right| \le \frac{2C}{|x|^2}, \quad \left||\xi| - 1\right| < \epsilon\right\},$$

with $\psi \equiv 1$ on

$$\left\{\left|\xi \cdot \frac{x}{|x|} - 1\right| < \frac{C}{|x|^2}, \, |\xi| = 1\right\}.$$

and $\Psi := \mathrm{Op}_h(\psi\widetilde{\chi})$. By (3.12)

$$\|(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}})\chi u\|_{L^2} = \|\Psi(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}})\chi u\|_{L^2} + O(h^\infty)\|\chi u\|_{L^2},$$

where $\Psi(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}})$ has principal h-symbol

$$\Lambda(x,\xi) := \psi\widetilde{\chi}(\widetilde{\mathcal{N}}(x,\xi)\xi \cdot \widetilde{n}(x) - \widetilde{\mathcal{D}}(x,\xi)), \tag{3.13}$$

and thus $\Psi(\widetilde{\mathcal{N}}hD_{\widetilde{n}} - \widetilde{\mathcal{D}}) = \mathrm{Op}_h(\Lambda) + O(h)_{L^2 \to L^2}$, and then, by (Zworski, 2012, Theorem 5.1),

$$\|\Psi\chi u\|_{L^2} \le \left(\sup|\Lambda(x,\xi)| + O(h^{1/2})\right)\|\chi u\|_{L^2}.$$

However, by the support properties of $\widetilde{\chi}$ and ψ and the definition (3.13) of Λ,

$$\sup|\Lambda(x,\xi)| \le \Upsilon(R),$$

and it follows that, given $R > 0$, there exists $h_0(R) > 0$ such that, for $0 < h \le h_0$,

$$\|(\widetilde{\mathcal{N}} h D_{\widetilde{n}} - \widetilde{\mathcal{D}}) \chi u\|_{L^2} \lesssim \Upsilon(R) \|\chi u\|_{L^2}. \tag{3.14}$$

On the other hand, by Lemma 3.4,

$$\mathrm{WF}_h([-h^2\Delta - 1, \chi]u) \subset \left\{ \left| \xi \cdot \frac{x}{|x|} - 1 \right| < \frac{C}{|x|^2}, \ x \in \Gamma_\epsilon, \ |\xi| = 1 \right\};$$

we obtain in the same way as before, reducing h_0 if necessary, that for $0 < h \le h_0$

$$\|(\widetilde{\mathcal{N}} h D_{\widetilde{n}} - \widetilde{\mathcal{D}})[-h^2\Delta - 1, \chi]u\|_{L^2} \lesssim \Upsilon(R) \|[-h^2\Delta - 1, \chi]u\|_{L^2} \lesssim \Upsilon(R) h \|\chi_0 u\|_{H_h^1}, \tag{3.15}$$

where χ_0 is supported in the support of $\widetilde{\chi}$ and equal to one on the support of χ. But, since $(-h^2\Delta - 1)u = 0$, u has h-wavefront set in $\{|\xi|^2 = 1\}$, thus so does $\widetilde{\chi} u$, and it follows that, taking η compactly supported near one

$$\|\chi_0 u\|_{H_h^1} = \|\mathrm{Op}_h(\eta(|\xi|^2)) \chi_0 \widetilde{\chi} u\|_{H_h^1} + O(h^\infty) \|\widetilde{\chi} u\|_{L^2}$$

$$= \|\mathrm{Op}_h(\eta(|\xi|^2)\xi \chi_0) \widetilde{\chi} u\|_{H_h^1} + O(h) \|\widetilde{\chi} u\|_{L^2}$$

$$\lesssim \|\widetilde{\chi} u\|_{L^2}. \tag{3.16}$$

Hence, by (3.15), for $0 < h \le h_0$,

$$h^{-1} \|(\widetilde{\mathcal{N}} h D_{\widetilde{n}} - \widetilde{\mathcal{D}})[-h^2\Delta - 1, \chi]u\|_{L^2} \lesssim \Upsilon(R) \|\widetilde{\chi} u\|_{L^2}. \tag{3.17}$$

Finally, observe that $h^{-1}[-h^2\Delta - 1, \widetilde{\mathcal{N}} h D_{\widetilde{n}} - \widetilde{\mathcal{D}}]$ has principal h-symbol

$$\sigma\left(h^{-1}[-h^2\Delta - 1, (\widetilde{\mathcal{N}} h D_{\widetilde{n}} - \widetilde{\mathcal{D}})]\right) = \frac{1}{i}\left\{|\xi|^2 - 1, \widetilde{\mathcal{N}}(x,\xi)\xi \cdot \widetilde{n}(x) - \widetilde{\mathcal{D}}(x,\xi)\right\}$$

$$= \frac{1}{i} H_p\left(\widetilde{\mathcal{N}}(x,\xi)\xi \cdot \widetilde{n}(x) - \widetilde{\mathcal{D}}(x,\xi)\right),$$

therefore, using Lemma 3.4 in the same way as before, we obtain

$$h^{-1}\|[h^2\Delta + 1, \widetilde{\mathcal{N}} h D_{\widetilde{n}} - \widetilde{\mathcal{D}}]\chi u\|_{L^2} \lesssim \sup \left|\widetilde{\chi}\psi H_p\left(\widetilde{\mathcal{N}}(x,\xi)\xi \cdot \widetilde{n}(x) - \widetilde{\mathcal{D}}(x,\xi)\right)\right| \|\chi u\|_{L^2} + O(h^{1/2})\|\chi u\|_{L^2}.$$

By the support properties of ψ and $\widetilde{\chi}$

$$\sup \left|\widetilde{\chi}\psi H_p\left(\widetilde{\mathcal{N}}(x,\xi)\xi \cdot \widetilde{n}(x) - \widetilde{\mathcal{D}}(x,\xi)\right)\right| \lesssim \Upsilon(R).$$

Reducing $h_0 > 0$, depending on R if necessary, we obtain that for $0 < h \le h_0$

$$h^{-1}\|[-h^2\Delta - 1, \widetilde{\mathcal{N}}(x,\xi)\xi \cdot \widetilde{n}(x) - \widetilde{\mathcal{D}}(x,\xi)]\chi u\|_{L^2} \lesssim \Upsilon(R) \|\chi u\|_{L^2}. \tag{3.18}$$

Combining (3.11) with (3.14), (3.17) and (3.18), we have, for $0 < h \le h_0(R)$,

$$\|(\mathcal{N}hD_n - \mathcal{D})u\|_{L^2(\Gamma_{\mathrm{tr},R})} \lesssim \Upsilon(R)\|\widetilde{\chi}u\|_{L^2},$$

and then Lemma 3.8 implies that

$$\big\|(\mathcal{N}hD_n - \mathcal{D})u\big\|_{L^2(\Gamma_{\mathrm{tr},R})} \le C\frac{\Upsilon(R)}{R^{1/2}}\,\|u\|_{L^2(\Omega_R)}.$$

To obtain the bound on Au, we observe that, by Lemma 3.4, $S^*\Gamma_{\mathrm{tr},R} \subset \mathcal{I}$, and, by Lemma 3.7,

$$\|Au\|_{L^2(\Gamma_{\mathrm{tr},R})} \le \|A\chi u\|_{L^2} + h^{-1}\|(-h^2\Delta - 1)A\chi u\|_{L^2} + O(h^\infty)\|\chi u\|_{L^2}.$$

However, in the same way as we obtained (3.16), the fact that u has h-wavefront set in $\{|\xi|^2 = 1\}$ implies that

$$\|A\chi u\|_{L^2} + h^{-1}\|(-h^2\Delta - 1)A\chi u\|_{L^2} \lesssim \|\widetilde{\chi}u\|_{L^2},$$

and the bound on Au follows by reducing $h_0(R) > 0$ again if necessary. $\qquad\square$

Proof of Lemma 3.3.
Proof of (i). First observe that if $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, then for $x \in \Gamma_{\mathrm{tr},R}$, $n(x) = x/|x|$. Therefore, on

$$\mathcal{O} := \left\{ (x,\xi) \,:\, x \in \Gamma_{\mathrm{tr},R},\ \left|\xi \cdot \frac{x}{|x|} - 1\right| \le \frac{C}{R^2},\ |\xi| = 1 \right\}$$

since $n(x) \cdot \xi = \sqrt{1 - |\xi'|_g^2}$, we have

$$|\xi'|_g^2 = 1 - |n(x) \cdot \xi|^2 \le \frac{C}{R^2}.$$

We now claim that

$$\sigma(\mathcal{N})(x',\xi')n(x) \cdot \xi - \sigma(\mathcal{D})(x',\xi') = e(x',\xi')|\xi'|_g^{2m_{\mathrm{ord}}} \quad \text{on } \mathcal{O}, \tag{3.19}$$

where $e(x',\xi')$ is smooth on $\mathcal{O}$. Indeed, the existence of $e(x',\xi')$ follows from the definition of m_{ord} (1.8) and that $n(x) \cdot \xi = \sqrt{1 - |\xi'|_g^2}$ on $\mathcal{O}$.
    Therefore,

$$\sup_{\mathcal{O}} \left|\sigma(\mathcal{N})(x',\xi')n(x) \cdot \xi - \sigma(\mathcal{D})(x',\xi')\right| \le C|\xi'|_g^{2m_{\mathrm{ord}}} \le CR^{-2m_{\mathrm{ord}}}. \tag{3.20}$$

Next, we bound the terms in $\Upsilon(R)$ (3.2) involving the Hamiltonian vector field $H_p = 2\langle\xi, \partial_x\rangle$. First, using again that $\xi = (n(x) \cdot \xi)n(x) + \xi'$ (where we abuse notation slightly to identify vectors and

covectors), we have $H_p = 2n(x) \cdot \xi \, \partial_n + 2\langle \xi', \partial_{x'} \rangle$. Thus, on $\mathcal{O}$,

$$H_p \left(\sigma(\mathcal{N}) n(x) \cdot \xi - \sigma(\mathcal{D}) \right) = \sigma(\mathcal{N}) 2 \left(\frac{x}{|x|} \cdot \xi \right) \left\langle \frac{x}{|x|}, \partial_x \right\rangle \left(\frac{x}{|x|} \cdot \xi \right) + 2 \langle \xi', \partial_{x'} \rangle \left(\sigma(\mathcal{N}) n(x) \cdot \xi - \sigma(\mathcal{D}) \right)$$

$$= 2 \langle \xi', \partial_{x'} \rangle \left(\sigma(\mathcal{N}) \sqrt{1 - |\xi'|_g^2} - \sigma(\mathcal{D}) \right), \tag{3.21}$$

where we have used that $\partial_{x'}$ is tangent to $\Gamma_{\mathrm{tr},R} \cap \{|\xi| = 1\}$ to write $n(x) \cdot \xi = \sqrt{1 - |\xi'|_g^2}$ in the last line. Now, by (3.19),

$$\partial_{x'} \left(\sigma(\mathcal{N}) \sqrt{1 - |\xi'|_g^2} - \sigma(\mathcal{D}) \right) = O\big(|\xi'|_g^{2m_{\mathrm{ord}}}\big).$$

In particular,

$$2 \langle \xi', \partial_{x'} \rangle \left(\sigma(\mathcal{N}) \sqrt{1 - |\xi'|_g^2} - \sigma(\mathcal{D}) \right) = O\big(|\xi'|_g^{2m_{\mathrm{ord}}+1}\big) = O(R^{-2m_{\mathrm{ord}}-1}). \tag{3.22}$$

The required bound on $\Upsilon(R)$ follows by combining (3.20) (3.21), and (3.22).

Proof of (ii). This follows from the fact that $\sigma(\mathcal{N})$ and $\sigma(\mathcal{D})$ have uniformly bounded C^1 norms in R. □

4. Proof of well-posedness of the truncated problem (Theorem 1.5)

4.1 *Trace bounds for higher order boundary conditions*

In this section, we consider the solution to

$$\begin{cases} \left(-h^2 \Delta_g - 1 \right) u = hf & \text{in } M, \\ \mathcal{N}_i h D_n u - \mathcal{D}_i u = g_i & \text{on } \Gamma_i \subset \partial M, \end{cases} \tag{4.1}$$

where (M, g) is a Riemannian manifold with smooth boundary $\partial M = \cup_{i=1}^N \Gamma_i$ such that Γ_i are the connected components of ∂M, and $\mathcal{N}_i \in \Psi^{m_{1,i}}(\Gamma_i)$, and $\mathcal{D}_i \in \Psi^{m_{0,i}}(\Gamma_i)$ have real-valued principal symbols. We further assume that for all $i = 1, \ldots, N$,

$$|\sigma(\mathcal{N}_i)|^2 \langle \xi' \rangle^{-2m_{1,i}} + |\sigma(\mathcal{D}_i)|^2 \langle \xi' \rangle^{-2m_{0,i}} \geq c > 0 \quad \text{on } T^*\Gamma_i,$$

$$|\sigma(\mathcal{D}_i)| > 0 \quad \text{on } S^*\Gamma_i, \tag{4.2}$$

and for each i one of the following holds:

$$m_{0,i} = m_{1,i} + 1, \qquad \text{or} \tag{4.3}$$

$$|\sigma(\mathcal{N}_i)|^2 \langle \xi' \rangle^{-2m_{1,i}} \geq c > 0, \qquad |\xi'| \geq C, \qquad \text{and} \qquad m_{0,i} \leq m_{1,i} + 1, \qquad \text{or} \tag{4.4}$$

$$|\sigma(\mathcal{D}_i)|^2 \langle \xi' \rangle^{-2m_{0,i}} \geq c > 0, \qquad |\xi'| \geq C, \qquad \text{and} \qquad m_{1,i} + 1 \leq m_{0,i}. \tag{4.5}$$

The first condition in (4.2) ensures nondegeneracy at infinity in ξ (with (4.3), (4.4) and (4.5) the different options for which term in the boundary condition is dominant), and the second condition in (4.2) ensures that the Dirichlet trace is bounded.

THEOREM 4.1 Suppose that u solves (4.1) where $\mathcal{N}_i \in \Psi^{m_{1,i}}(\Gamma_i)$, $\mathcal{D}_i \in \Psi^{m_{0,i}}(\Gamma_i)$ have real-valued principal symbols and satisfy (4.2) and one of (4.3)–(4.5). Then, there exist $C > 0$ and $h_0 > 0$ such that for $0 < h < h_0$, and i and all ℓ_i, satisfying

$$-\frac{m_{0,i} + m_{1,i}}{2} \le \ell_i \le \frac{1}{2} - \frac{m_{0,i} + m_{1,i}}{2}, \tag{4.6}$$

$$\|u\|_{H_h^{\ell_i + m_{0,i}}(\Gamma_i)} + \|hD_\nu u\|_{H_h^{\ell_i + m_{1,i}}(\Gamma_i)} \le C\left(\|u\|_{L^2(M)} + \|f\|_{H_h^{\ell_i + \frac{m_{1,i} + m_{0,i} - 1}{2}}(M)} + \|g_i\|_{H_h^{\ell_i}(\Gamma_i)}\right), \tag{4.7}$$

$$\|u\|_{H_h^1(M)} \le C\left(\|u\|_{L^2(M)} + h\|f\|_{L^2(M)} + \sum_i \|g_i\|_{H_h^{\ell_i}(\Gamma_i)}\right), \tag{4.8}$$

and for $s \le 0$,

$$\|hD_\nu u\|_{H_h^s(\Gamma_i)} \le C\left(\|u\|_{H_h^{s+1}(\Gamma_i)} + \|u\|_{L^2(M)} + \|f\|_{L^2(M)} + \sum_i \|g_i\|_{H_h^{\ell_i}(\Gamma_i)}\right). \tag{4.9}$$

The proof of Theorem 4.1 is postponed until Section 6. Here we proceed directly to its application.

4.1.1   *Application of Theorem 4.1 with L^2 right hand sides.*

COROLLARY 4.2 Suppose that

$$m_0 \ge 0, \quad m_0 + m_1 \ge 0, \quad m_1 \le m_0 + 1, \tag{4.10}$$

and *either*

$$m_0 \le m_1 + \min\{1, m_0 + m_1\}, \tag{4.11}$$

or

$$m_0 \ge m_1 + 1 \quad \text{and} \quad m_0 \ge 1. \tag{4.12}$$

Then there exists $C > 0$ and $h_0 > 0$ such that, for $0 < h \le h_0$, the solution to

$$\begin{cases} (-h^2\Delta - 1)u = hf & \text{in } \Omega, \\ (\mathcal{N}hD_n - \mathcal{D})u = g & \text{on } \Gamma, \end{cases}$$

with $f \in L^2(\Omega)$ and $g \in L^2(\Gamma)$ satisfies

$$\|u\|_{L^2(\Gamma)} + \|hD_n u\|_{L^2(\Gamma)} + \|u\|_{H^1_h(\Omega_R)} \leq C \left(\|u\|_{L^2(\Omega_R)} + \|f\|_{L^2(\Omega_R)} + \|g\|_{L^2(\Gamma)} \right). \tag{4.13}$$

Proof. Let

$$\ell = r - \frac{m_0 + m_1}{2}.$$

If $0 \leq r \leq \frac{1}{2}$, then Theorem 4.1 holds and (4.7) and (4.8) become

$$\|u\|_{H^{r+\frac{m_0-m_1}{2}}_h(\Gamma)} + \|hD_\nu u\|_{H^{r+\frac{m_1-m_0}{2}}_h(\Gamma)} \leq C \left(\|u\|_{L^2(\Omega_R)} + \|f\|_{H^{r-\frac{1}{2}}_h(\Omega_R)} + \|g\|_{H^{r-\frac{m_1+m_0}{2}}_h(\Gamma)} \right) \tag{4.14}$$

and

$$\|u\|_{H^1_h(M)} \leq C \left(\|u\|_{L^2(M)} + h\|f\|_{L^2(M)} + \|g\|_{H^{r-\frac{m_1+m_0}{2}}_h(\Gamma)} \right), \tag{4.15}$$

respectively. Focusing on (4.14), we therefore impose the conditions that

$$r \geq \frac{m_1 - m_0}{2}, \qquad 0 \leq r \leq \frac{1}{2}, \qquad r \leq \frac{m_1 + m_0}{2},$$

i.e.,

$$\max \left(0, \frac{m_1 - m_0}{2} \right) \leq r \leq \min \left(\frac{1}{2}, \frac{m_1 + m_0}{2} \right)$$

(observe that this range of r is nonempty since $m_0 \geq 0$, $m_1 - m_0 \leq 1$, and $m_1 + m_0 \geq 0$). Choosing $r = \min\{1/2, (m_1 + m_0)/2\}$, we have

$$\|u\|_{L^2(\Gamma)} + \|hD_\nu u\|_{H^{s^*}_h(\Gamma)} \leq C \left(\|u\|_{L^2(\Omega_R)} + \|f\|_{L^2(\Omega_R)} + \|g\|_{L^2(\Gamma)} \right), \tag{4.16}$$

where

$$s^* := \min \left(\frac{1}{2}, \frac{m_1 + m_0}{2} \right) + \frac{m_1 - m_0}{2}.$$

If $s^* \geq 0$, i.e., if (4.11) holds, then the result (4.13) follows from combining (4.16) with (4.15).

If (4.11) doesn't hold, we seek control of $\|hD_n u\|_{L^2(\Gamma)}$ via the bound (4.9) with $s = 0$, i.e.,

$$\|hD_\nu u\|_{L^2(\Gamma)} \leq C \left(\|u\|_{H^1_h(\Gamma)} + \|u\|_{L^2(M)} + \|f\|_{L^2(M)} + \|g_i\|_{H^{r-\frac{m_1+m_0}{2}}_h(\Gamma)} \right).$$

To prove (4.13), therefore, we only need to bound $\|u\|_{H^1_h(\Gamma)}$ in terms of the right-hand side of (4.13). This follows from (4.14) if

$$\max\left(0, 1 + \frac{m_1 - m_0}{2}\right) \le r \le \min\left(\frac{1}{2}, \frac{m_1 + m_0}{2}\right),$$

which is ensured if (4.12) holds.   □

4.1.2 *Application of Theorem* 4.1 *to Dirichlet boundary conditions.*

COROLLARY 4.3 There exist $C > 0$ and $h_0 > 0$ such that if $0 \le h \le h_0$, then the solution of

$$\begin{cases} (-h^2 \Delta - 1)u = hf & \text{in } \Omega \\ u = g & \text{on } \Gamma, \end{cases}$$

with $f \in L^2(\Omega)$ and $g \in H^1_h(\Gamma)$ satisfies

$$\|u\|_{H^1_h(\Gamma)} + \|hD_\nu u\|_{L^2(\Gamma)} + \|u\|_{H^1_h(\Omega_R)} \le C\big(\|u\|_{L^2(\Omega_R)} + \|f\|_{L^2(\Omega_R)} + \|g\|_{H^1_h(\Gamma)}\big).$$

Proof of Lemma 3.3. The Dirichlet boundary condition corresponds to $\mathcal{D} = I, \mathcal{N} = 0$, and so satisfies the assumptions of Theorem 4.1 with $m_0 = 0$ and $m_1 = -1$, say. The result follows by choosing $\ell = 1$ and combining (4.7) and (4.8).   □

4.2 *Recap of results of Trefethen & Halpern (1986) about Padé approximants*

We now recall results of Trefethen & Halpern (1986) about Padé approximants. These results consider a larger class of approximants than covered in our Assumption 1.4; before stating these results, we explain this difference.

With $p(t)$ and $q(t)$ defined by (1.8), by Assumption 1.4,

$$\sigma(\mathcal{D})(x', \xi') = \mathcal{P}_{\mathsf{M,N}}(x', \xi') = p\big(|\xi'|_g^2\big) \quad \text{and} \quad \sigma(\mathcal{N})(x', \xi') = \mathcal{Q}_{\mathsf{M,N}}(x', \xi') = q\big(|\xi'|_g^2\big). \qquad (4.17)$$

As described in § 1.3, this choice of $\mathcal{D}$ and $\mathcal{N}$ is based on approximating $\sqrt{1 - |\xi'|_g^2}$ with a rational function in $|\xi'|_g^2$.

The boundary conditions in Trefethen & Halpern (1986) are based on approximating $\sqrt{1 - |\xi'|_g^2}$ with a rational function in $|\xi'|_g$, i.e., Trefethen & Halpern (1986) consider Padé approximants with polynomials $\widetilde{p}(s)$ and $\widetilde{q}(s)$, where the degrees $\widetilde{p}(s)$ and $\widetilde{q}(s)$ allowed to be either even or odd. Our polynomials p, q fit into the framework of Trefethen & Halpern (1986) with

$$\widetilde{p}(s) := p(s^2) \quad \text{and} \quad \widetilde{q}(s) := q(s^2), \qquad (4.18)$$

and then $\widetilde{p}$ has degree 2M and $\widetilde{q}$ has degree 2N. For $d - 1 \ge 2$ (i.e., when the boundary dimension is ≥ 2), polynomials with odd powers of $|\xi'|_g$ do not lead to $\mathcal{N}$ and $\mathcal{D}$ being local differential operators, but for $d - 1 = 1$ (i.e., $d = 2$) they do, since in this case $\sqrt{|\xi'|_g^2} = \sqrt{g(x')}\xi'$, i.e., a polynomial in ξ'.

Our arguments also apply to polynomials with odd powers of $|\xi'|_g$ in $d = 2$, but we do not analyze them specifically, instead leaving this to the interested reader.

To state the results of Trefethen & Halpern (1986), we let $\widetilde{p}(s)$ and $\widetilde{q}(s)$ be polynomials of degree m_0 and m_1, respectively; this notation is chosen so that, when we specialize the results to our case with (4.18), these m_0 and m_1 are the same as in Theorem 4.1/Corollary 4.2, i.e., $m_0 = 2\mathsf{M}$ and $m_1 = 2\mathsf{N}$. Finally, we let

$$\widetilde{r}(s) := \frac{\widetilde{p}(s)}{\widetilde{q}(s)}.$$

LEMMA 4.4 (Trefethen & Halpern, 1986, Theorems 2 and 4) If, and only if, $m_0 = m_1$ or $m_0 = m_1 + 2$, then

(a) $\widetilde{r}(s) > 0$ for $s \in [-1, 1]$, and
(b) the zeros and poles of $\widetilde{r}(s)/s$ are real and simple and interlace along the real axis.

COROLLARY 4.5 If $m_0 = m_1$ or $m_0 = m_1 + 2$, then neither $\widetilde{p}(s)$ nor $\widetilde{q}(s)$ has any zeros in $[-1, 1]$.

Proof. For $\widetilde{p}(s)$, this property follows directly from Part (a) of Lemma 4.4. For $\widetilde{q}(s)$, this property follows from Parts (a) and (b) of Lemma 4.4; indeed, if there were a zero of $\widetilde{q}(s)$ (i.e., a pole of $\widetilde{r}(s)$) in $[-1, 1]$, since the zeros of $\widetilde{q}(s)$ are simple and interlace with the zeros of $\widetilde{p}(s)$ (by Part (b)), $\widetilde{r}(s)$ would change sign in $[-1, 1]$, contradicting Part (a). □

4.3 *Proof of Theorem 1.5*

Throughout this section, we let $\widetilde{\Omega}_R$ be a smooth family of domains, depending on R and assume that there is $M > 0$ such that

$$B(0, 1) \subset \widetilde{\Omega}_R \subset B(0, MR),$$
(4.19)

$\widetilde{\Omega}_R$ is convex with smooth boundary, $\Gamma_{\mathrm{tr},R}$, that is nowhere flat to infinite order

Furthermore, we assume that

$$\widetilde{\Omega}_R/R \to \Omega_\infty$$

in the sense that $\partial\widetilde{\Omega}_R/R \to \partial\Omega_\infty$ in C^∞.

We prove below that Theorem 1.5 is a consequence of the following result, combined with the results from Trefethen & Halpern (1986) in § 4.2.

THEOREM 4.6 Let $\widetilde{\Omega}_R$ be as in (4.19) and $\Omega_- \Subset B(0, 1)$ with Ω_- nontrapping. Let $\mathcal{N} \in \Psi^{m_1}(\Gamma_{\mathrm{tr},R})$, $\mathcal{D} \in \Psi^{m_0}(\Gamma_{\mathrm{tr},R})$ have real-valued principal symbols and satisfy (4.2) and one of (4.3)–(4.5). Let m_0 and m_1 satisfy the assumptions of Corollary 4.2, and furthermore let $\mathcal{N}$ and $\mathcal{D}$ satisfy

$$\sigma(\mathcal{N})\sigma(\mathcal{D}) > 0 \text{ on } \overline{B^*\Gamma_{\mathrm{tr},R}}.$$
(4.20)

Let

$$G_h^R: L^2(\Gamma_{\mathrm{tr},R}) \oplus H_h^1(\Gamma_D) \oplus L^2(\widetilde{\Omega}_R \setminus \Omega_-) \to H_h^1(\widetilde{\Omega}_R \setminus \Omega_-)$$

satisfy

$$\begin{cases} (-h^2\Delta - 1)G_h^R(g_I, g_D, f) = hf & \text{on } \widetilde{\Omega}_R \setminus \Omega_- \\ (\mathcal{N}hD_n - \mathcal{D})\, G_h^R(g_I, g_D, f) = g_I & \text{on } \Gamma_{\text{tr},R} \\ G_h^R(g_I, g_D, f) = g_D & \text{on } \Gamma_D. \end{cases}$$

Then there exists $C > 0$ such that for $R \geq 1$, there is $h_0 = h_0(R) > 0$ such that for $0 < h < h_0$, G_h^R is well defined and satisfies

$$\left\| G_h^R(g_I, g_D, f) \right\|_{H_h^1(\widetilde{\Omega}_R \setminus \Omega_-)} \leq CR^{1/2} \big(\|g_I\|_{L^2(\Gamma_{\text{tr},R})} + \|g_D\|_{H_h^1(\Gamma_D)} \big) + CR \|f\|_{L^2(\widetilde{\Omega}_R \setminus \Omega_-)}. \tag{4.21}$$

Proof of Theorem 1.5 *using Theorem* 4.6. Theorem 1.5 will follow from Theorem 4.6 (translating between the *h*- and *k*-notations using § 2.1) if we can show that the boundary conditions in Assumption 1.4 with either $\mathsf{M} = \mathsf{N}$ or $\mathsf{M} = \mathsf{N} + 1$, with $\mathsf{M}, \mathsf{N} \geq 0$, satisfy

   (i)   (4.2),

  (ii)   one of (4.3)–(4.5),

 (iii)   the assumptions of Corollary 4.2, and

  (iv)   (4.20),

where $m_0 = 2\mathsf{M}$ and $m_1 = 2\mathsf{N}$.

Regarding (iii): the first two inequalities in (4.10) are satisfied since $m_0, m_1 \geq 0$, and the third inequality is satisfied both when $m_0 = m_1$ and when $m_0 = m_1 + 2$. If $m_0 = m_1$, then (4.11) is satisfied, and if $m_0 = m_1 + 2$ then (4.12) is satisfied (since $m_1 \geq 0$, and thus $m_0 \geq 2$).

Regarding (ii): if $m_0 = m_1$, then (4.4) holds since $q_{\mathsf{M},\mathsf{N}}^{\mathsf{N}} \neq 0$ by definition. If $m_0 = m_1 + 2$, then (4.5) holds since $p_{\mathsf{M},\mathsf{N}}^{\mathsf{M}} \neq 0$ by definition.

Regarding (i) and (iv): using (4.17), the conditions (4.2) and (4.20) become (with $t = |\xi'|_g^2$)

$$|q(t)|^2 t^{-2\mathsf{N}} + |p(t)|^2 t^{-2\mathsf{M}} > 0 \quad \text{for all } t \quad \text{and} \quad |p(\pm 1)| > 0, \tag{4.22}$$

and

$$|p(t)q(t)| > 0 \quad \text{on} -1 \leq t \leq 1, \tag{4.23}$$

respectively

If $\widetilde{p}(s)$ and $\widetilde{q}(s)$ are defined by (4.18), then (4.22) and (4.23) become

$$|\widetilde{q}(s)|^2 s^{-2m_1} + |\widetilde{p}(s)|^2 s^{-2m_0} > 0 \quad \text{for all } s \quad \text{and} \quad |\widetilde{p}(\pm 1)| > 0, \tag{4.24}$$

and

$$|\widetilde{p}(s)\widetilde{q}(s)| > 0 \quad \text{on} -1 \leq s \leq 1. \tag{4.25}$$

The first condition in (4.24) holds since, by Part (a) of Lemma 4.4, $\widetilde{p}(s)$ and $\widetilde{q}(s)$ have no common zeros. Both the second condition in (4.24) and the condition in (4.25) hold by Corollary 4.5. □

We now prove Theorem 4.6. We first show that, for each $z \in \mathbb{C}$ and $s \geq 0$ the operator

$$\widetilde{P}(z) : H^{2+s}(\widetilde{\Omega}_R \setminus \Omega_-) \ni u \mapsto \left(-h^2\Delta - z, \left(\mathcal{N}hD_n - \mathcal{D}\right)u|_{\Gamma_{\mathrm{tr},R}}, u|_{\Gamma_D}\right)$$
$$\in H^s(\widetilde{\Omega}_R \setminus \Omega_-) \oplus H^{3/2+s-m}(\Gamma_{\mathrm{tr},R}) \oplus H^{3/2+s}(\Gamma_D)$$

is Fredholm with $m = \max(m_0, m_1 + 1)$; we do this by checking the conditions of (Hörmander, 1985, Theorem 20.1.8, page 249). Observe that, for fixed $h > 0$, as a homogeneous pseudodifferential operator, $(-h^2\Delta - z^2)$ has symbol $p(x, \xi) = |\xi|^2$. Therefore, in Fermi normal coordinates at $\Gamma_{\mathrm{tr},R}$, we need to check that the map

$$M_{x,\xi'} \ni u \to \left(b\left(x, (D_t, \xi')\right)u\right)(0)$$

is bijective, where $M_{x,\xi'}$ denotes the solutions to $(D_t^2 + |\xi'|_g^2)u(t) = 0$ with u is bounded on $\mathbb{R}_+$, and

$$b(x, \xi) = \lim_{\lambda \to \infty} \left(-\sigma(\mathcal{N})(x, \lambda\xi')\lambda\xi_1 - \sigma(\mathcal{D})(x, \lambda\xi')\right)\lambda^{-m}.$$

Since $u = Ae^{-t|\xi'|_g}$,

$$\left(b\left(x, (D_t, \xi')\right)u\right)(0) = A\lim_{\lambda \to \infty}\left(-\sigma(\mathcal{N})(x, \lambda\xi')\lambda i|\xi'| - \sigma(\mathcal{D})(x, \lambda\xi')\right)\lambda^{-m},$$

and bijectivity follows if the limit on the right-hand side is nonzero. Since $\mathcal{N}$ and $\mathcal{D}$ are both real, this is ensured by (4.2) and any of (4.3)–(4.5).

Now, to see that $\widetilde{P}$ is invertible somewhere, consider $z = -1$. First, note that for $s \geq 0$ the map

$$P_D : \left(H^{2+s}(\widetilde{\Omega}_R \setminus \Omega_-) \ni u \mapsto \to (-h^2\Delta + 1)u, u|_{\Gamma_{\mathrm{tr},R}}, u|_{\Gamma_D}\right) \in H^s(\widetilde{\Omega}_R \setminus \Omega_-) \oplus H^{s-\frac{1}{2}}(\Gamma_I) \oplus H^{s-\frac{1}{2}}(\Gamma_D)$$

is invertible with inverse $G_D : H_h^s(\widetilde{\Omega}_R \setminus \Omega_-) \oplus H_h^{s-\frac{1}{2}}(\Gamma_{\mathrm{tr},R}) \oplus H_h^{s-\frac{1}{2}}(\Gamma_D) \to H_h^{2+s}(\widetilde{\Omega}_R \setminus \Omega_-)$ (see e.g., (Evans, 1998, Chapter 6)). In particular, the Dirichlet to Neumann map

$$\Lambda : g_1 \mapsto hD_nu|_{\Gamma_I}, \quad \text{where} \quad \begin{cases} (-h^2\Delta + 1)u = 0 & \text{on } \widetilde{\Omega}_R \setminus \Omega_-, \\ u = g_1 & \text{on } \Gamma_{\mathrm{tr},R}, \\ u = 0 & \text{on } \Gamma_D, \end{cases}$$

is well defined. Furthermore, $\Lambda \in \Psi^1(\Gamma_{\mathrm{tr},R})$ is a semiclassical pseudodifferential operator with symbol $\sigma(\Lambda) = -i\sqrt{|\xi'|_g + 1}$ (see, e.g., (Galkowski, 2019b, Proposition 4.1.1, Lemma 4.27)). In particular, by (4.2) and (4.3)–(4.5), $(-i\mathcal{N}\Lambda - \mathcal{D})^{-1}$ exists, and hence

$$[\widetilde{P}(-1)]^{-1}(f, g_I, g_D) = G_D\left(f, (-i\mathcal{N}\Lambda - \mathcal{D})^{-1}g_I, g_D\right).$$

Therefore, since for $z = -1$, the operator is invertible, by the analytic Fredholm Theorem (see e.g., (Dyatlov & Zworski, 2019, Theorem C.8)) the family $G_h^R(z)$ of operators solving

$$\begin{cases} (-h^2\Delta - z)G_h^R(z)(g_I, 0, f) = hf & \text{on } \widetilde{\Omega}_R \setminus \Omega_- \\ (\mathcal{N}hD_\nu - \mathcal{D})\, G_h^R(z)(g_I, 0, f) = g_I & \text{on } \Gamma_{\text{tr},R} \\ G_h^R(z)(g_I, 0, f) = 0 & \text{on } \Gamma_D \end{cases}$$

is a meromorphic family of operators with finite rank poles. To include the Dirichlet boundary values, we observe that by standard elliptic theory, the operator $\widetilde{G}_h(z) : H_h^1(\Gamma_D) \to H^{3/2}(B(0,1) \setminus \overline{\Omega_-})$ solving

$$\begin{cases} (-h^2\Delta - z)\widetilde{G}(z)g = 0 & \text{on } B(0,1) \setminus \overline{\Omega_-} \\ \widetilde{G}_h(z)g = g & \text{on } \Gamma_D \\ (hD_n - 1)\widetilde{G}_h(z)g = 0 & \text{on } \partial B(0,1) \end{cases}$$

is a meromorphic family of operators with finite rank poles. With $\chi \in C_c^\infty(B(0,1))$ with $\chi \equiv 1$ near Ω_-,

$$G_h^R(g_I, g_D, f) = G_h^R\big(g_I, 0, f - h^{-1}[-h^2\Delta, \chi]\widetilde{G}_h g_D\big) + \chi\widetilde{G}_h g_D,$$

and thus the operator G_h^R is well defined.

We start by studying $G_h^R(0, g, 0)$.

LEMMA 4.7 Let $R > 0$ and assume that $\mathcal{N}$ and $\mathcal{D}$ satisfy the assumptions of Theorem 4.1. Then there exist $C, h_0 > 0$ such that $u = G_h^R(0, g, 0)$, the solution to

$$\begin{cases} (-h^2\Delta - 1)u = 0 & \text{in } \Omega_R, \\ u = g & \text{on } \Gamma_D, \\ (\mathcal{N}hD_\nu - \mathcal{D})\, u = 0 & \text{on } \Gamma_{\text{tr},R}, \end{cases}$$

satisfies

$$\|u\|_{H_h^1(\widetilde{\Omega}_R\setminus\Omega_-)} \leq C\|g\|_{H_h^1(\Gamma_D)}.$$

Proof. Suppose the lemma fails. Then there exist (h_n, g_n) with $h_n \to 0$ such that $u_n = G_{h_n}^R(0, g_n, 0)$,

$$\|u_n\|_{H_{h_n}^1(\widetilde{\Omega}_R\setminus\Omega_-)} = 1, \qquad \|g_n\|_{H_{h_n}^1(\Gamma_D)} = n^{-1}.$$

Extracting subsequences, we can assume that u_n has defect measure μ. Moreover, by Corollaries 4.2 and 4.3, we can assume that the trace measures $\nu_d^{D/\text{tr}}$, $\nu_j^{D/\text{tr}}$ and $\nu_n^{D/\text{tr}}$ exist. In particular, since $g_n \to 0$ in H_h^1, $\nu_d^D = 0$. Let φ_t denote the billiard flow outside Ω_-. Then by Lemma 2.12 together with (Galkowski *et al.*, 2020, Section 4),

$$\mu(\varphi_t(A)) = \mu(A) \qquad \text{if} \qquad \bigcup_{0 \leq t \leq T} \varphi_t(A) \cap \Gamma_{\text{tr},R} = \emptyset. \tag{4.26}$$

Furthermore, using again Corollaries 4.2 and 4.3, we find that

$$1 = \limsup_n \|u_n\|^2_{H^1_{h_n}} \geq \mu(T^*\mathbb{R}^d) \geq \liminf_n \|v_n\|^2_{L^2} \geq c \liminf_n \|\widetilde{v}_n\|^2_{H^1_{h_n}} = c > 0.$$

Note also that $\mu^{\text{in/out,tr}}$, v^{tr}_d, v^{tr}_j and v^{tr}_n satisfy the relations in Lemma 2.12. Next, by Lemma 2.18,

$$\mu^{\text{out,tr}} = \alpha^{\text{ref}}\mu^{\text{in,tr}} \quad \text{where} \quad \alpha^{\text{ref}} = \left|\frac{\sqrt{r}\mathcal{N} - \mathcal{D}}{\sqrt{r}\mathcal{N} + \mathcal{D}}\right|^2 \in C^\infty(\{r > 0\}). \tag{4.27}$$

Here, we abuse notation slightly, since when $\sigma(\mathcal{N})\sigma(\mathcal{D}) < 0$, $\sqrt{r}\mathcal{N} + \mathcal{D}$ may take the value 0. In that case, the first equation in (4.27) is replaced by $(\alpha^{\text{ref}})^{-1}\mu^{\text{out,tr}} = \mu^{\text{in,tr}}$.

Finally, these measures satisfy Theorem 2.15 with $\dot{n}^j = \sigma(\mathcal{N})/\sigma(\mathcal{D})$ which is well defined and satisfies $\pm\dot{n}^j \geq m > 0$ since $\pm\sigma(\mathcal{N})\sigma(\mathcal{D}) > 0$ on $\overline{B^*\Gamma_{\text{tr},R}}$.

The proof of Lemma 4.7 is completed by the following lemma.

LEMMA 4.8 Suppose that Ω_- is nontrapping, and let $M > 0$. Then there exist $T_0, \delta_0 > 0$ such that the following holds for all $R \geq 1$. Suppose $\Omega_- \Subset B(0,1) \subset \widetilde{\Omega}_R \subset B(0, MR)$ has smooth boundary and is convex and that μ is a finite measure supported in $S^*_{\overline{\widetilde{\Omega}_R \setminus \Omega_-}} \mathbb{R}^d$ satisfying (4.26), (4.27) and Theorem 2.15 with $\Re\dot{n}^j = \frac{\sigma(\mathcal{N})}{\sigma(\mathcal{D})}$ with $0 < \pm\sigma(\mathcal{N})\sigma(\mathcal{D})$ on $\overline{B^*\Gamma_{\text{tr},R}}$ Then, for all $A \subset S^*_{\overline{\widetilde{\Omega}_R \setminus \Omega_-}} \mathbb{R}^d$,

$$\mu\left(\varphi_{\mp T_0 R}(A)\right) \geq (1 + \delta_0)\mu(A).$$

To see that Lemma 4.8 completes the proof of Lemma 4.7 observe that our defect measure μ has $\mu(T^*\mathbb{R}^d) \neq 0$, is finite, and is supported in $S^*_{\overline{\widetilde{\Omega}_R \setminus \Omega_-}} \mathbb{R}^d$. Therefore, there is $A \subset S^*_{\overline{\widetilde{\Omega}_R \setminus \Omega_-}} \mathbb{R}^d$ such that $\mu(A) > 0$. But then

$$\mu\left(\varphi_{\mp NRT_0}(A)\right) = (1 + \delta_0)^N \mu(A) \to \infty,$$

which is a contradiction. □

Proof of Lemma 4.8. We consider only the case where $\sigma(\mathcal{N})\sigma(\mathcal{D}) > 0$. The other case follows from an identical argument, but reversing the time direction.

By (4.26), μ is invariant under φ_t away from $\Gamma_{\text{tr},R}$. We first study the glancing set, $\mathcal{G} = T^*\Gamma_{\text{tr},R} \cap \{r = 0\}$. Note that since $\Gamma_{\text{tr},R}$ is convex, $\mathcal{G} \subset \{H^2_p x_1 \leq 0\}$ where x_1 is a boundary defining function for $\Gamma_{\text{tr},R}$. Note that for $\rho \in \mathcal{G}$, since $\widetilde{\Omega}_R(R)$ is convex and $\widetilde{\Omega}_R(R) \subset B(0, MR)$, there exist $c > 0$ and $T_0 > 0$ independent of R such that

$$\int_{-T_0 R}^0 -H^2_p x_1(\varphi_s(\rho)) \, \mathrm{d}s \geq c > 0.$$

In particular, since $\sigma(\mathcal{N})\sigma(\mathcal{D}) > m > 0$ on $S^*\Gamma_{\mathrm{tr},R}$ (by (4.20)), $\Re \dot{n}^j \geq m > 0$, and hence by Theorem 2.15, for $A \subset \mathcal{G}$,

$$\mu(\varphi_{-T_0 R}(A)) \geq e^{mc}\mu(A).$$

Next, we study the case where $A \subset S^*_{\widetilde{\Omega}_R \setminus \Omega_-}\mathbb{R}^d \setminus \mathcal{G}$. Let $\beta^{-1} : B^*\Gamma_{\mathrm{tr},R} \to B^*\Gamma_{\mathrm{tr},R}$ be the reversed billiard ball map induced by φ_t. That is, let $\pi : S^*_{\Gamma_{\mathrm{tr},R}}\mathbb{R}^d \to B^*\Gamma_{\mathrm{tr},R}$ be the natural projection map and $\pi_{\pm}^{-1} : B^*\Gamma_{\mathrm{tr},R} \to S^*_{\Gamma_{\mathrm{tr},R}}\mathbb{R}^d$ the inward- and outward-pointing inverse maps. Next, for $(x,\xi) \in S^*_{\Gamma_{\mathrm{tr},R}}\mathbb{R}^d$ define

$$T_-(x,\xi) = \inf\left\{t > 0 \,:\, \varphi_{-t}(x,\xi) \in S^*_{\Gamma_{\mathrm{tr},R}}\mathbb{R}^d\right\}.$$

Since Ω_- is nontrapping, there is $T_0 > 0$ such that for all $(x,\xi) \in S^*_{\widetilde{\Omega}_R \setminus \Omega_-}\mathbb{R}^d \cup \pi_-^{-1}(B^*\Gamma_{\mathrm{tr},R})$, $T_-(x,\xi) \leq T_0 R$. In particular, every trajectory intersects the boundary in time $T_0 R$.

The reversed billiard map is then given by

$$\beta^{-1}(q) : \pi\left(\varphi_{-T_-(\pi_-^{-1}(q))}(\pi_-^{-1}(q))\right).$$

Since $\Gamma_{\mathrm{tr},R}$ is convex $\beta : B^*\Gamma_{\mathrm{tr},R} \to B^*\Gamma_{\mathrm{tr},R}$ is well defined and, since μ is invariant under φ_t, $\beta_*\mu^{\mathrm{out,tr}} = \mu^{\mathrm{in,tr}}$. Then, using (4.27), we have

$$\mu^{\mathrm{out,tr}} = \alpha^{\mathrm{ref}}\mu^{\mathrm{in,tr}} = \alpha^{\mathrm{ref}}\beta_*\mu^{\mathrm{out,tr}}. \tag{4.28}$$

Fix $0 < c < 1$ and for $\rho \in B^*\Gamma_{\mathrm{tr},R}$, let

$$N(\rho,c) := \inf\left\{N \geq 0 \,:\, \sum_{j=0}^N \log(r(\beta^{-j}(\rho))) < -c\right\}.$$

We claim that there exist $c_0, T_0 > 0$ such that for all $\rho \in B^*\Gamma_{\mathrm{tr},R}$

$$\sum_{j=0}^{N(\rho,c_0)} T_-(\beta^{-j}(\rho)) < T_0 R. \tag{4.29}$$

Once we prove this claim, using (4.28) together with the definition of $\mu^{\mathrm{out,tr}}$ as the derivative along the flow of μ, we see that if $A \subset S^*_{\widetilde{\Omega}_R \setminus \Omega_-}\mathbb{R}^d \setminus \mathcal{G}$, then

$$\mu\left(\varphi_{-T_0 R}(A)\right) \geq e^{-c_0}\mu(A),$$

and hence the proof will be complete.

We now prove (4.29). If the claim fails then there is a sequence

$$(R_n, \rho_n, M_n) \in [1, \infty) \times B^* \Gamma_{\mathrm{tr},R}(R_n) \times \mathbb{Z}$$

such that

$$\sum_{j=0}^{M_n} T_-(\beta^{-j}(\rho_n)) \geq nR_n, \qquad \sum_{j=0}^{M_n} \log \alpha^{\mathrm{ref}}(r(\beta^{-j}\rho_n)) > -\frac{1}{n}. \tag{4.30}$$

Without loss of generality, we can assume that $R_n \to R_\infty \in [1, \infty]$. Note that

$$\log \alpha^{\mathrm{ref}}(\rho) = -\frac{4\sigma(\mathcal{N})}{\sigma(\mathcal{D})}\sqrt{r(\rho)} + O(r(\rho)).$$

By (4.20), since $\frac{\sigma(\mathcal{N})}{\sigma(\mathcal{D})} > m > 0$ on $S^* \Gamma_{\mathrm{tr},R}$,

$$\sum_{j=0}^{M_n} \sqrt{(r(\beta^{-j}\rho_n))} \leq \frac{1}{4mn} \tag{4.31}$$

and in particular,

$$\sup_{0 \leq j \leq M_n} r(\beta^{-j}(\rho_n)) \leq \frac{1}{16m^2n^2}. \tag{4.32}$$

Now, let $\pi_M : T^*M \to M$ and $\rho \in B^* \partial \widetilde{\Omega}_R$. We consider the angle between the two vectors

$$V_\pm(\rho) := \mathrm{d}\pi_M\big(\partial_t \varphi_t\big(\pi_\pm^{-1}(\rho)\big)\big) = 2\xi\big(\pi_\pm^{-1}(\rho)\big).$$

Note that $V_\pm$ are the tangent vectors to the billiard trajectory just before $(-)$ and after $(+)$ reflection. We define the angle accumulated at ρ, $\Delta(\rho) \in [0, \pi]$ by

$$\langle V_+(\rho), V_-(\rho)\rangle = 4\cos \Delta(\rho).$$

As can be seen, e.g., in Fig. 5,

$$\sin(\Delta(\rho)/2) = \sqrt{r(\rho)}, \qquad \cos(\Delta(\rho)/2) = \sqrt{1 - r(\rho)}.$$

In particular,

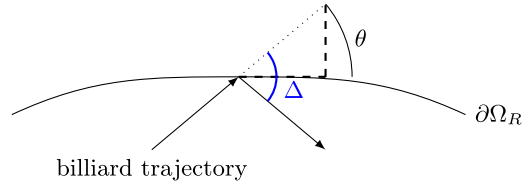$$\sin(\Delta(\rho)) = 2\sqrt{r(\rho)}\sqrt{1 - r(\rho)}.$$

FIG. 5. Ray construction showing the change, Δ, in the angle of a ray when hitting the boundary at angle θ. Note that $r = \sin^2 \theta$.

Therefore,

$$\Delta(\rho) = 2\sqrt{r(\rho)} + O(r(\rho)^{3/2}).$$

Now, note that if

$$\sum_{j=0}^{k} \Delta(\beta^{-j}(\rho)) < \frac{\pi}{4},$$

then

$$\left|\pi_M(\rho) - \pi_M(\beta^{-k}(\rho))\right| \geq \frac{1}{\sqrt{2}} \sum_{j=0}^{k} T_-(\beta^{-j}(\rho)). \tag{4.33}$$

By (4.31) and (4.32),

$$\sum_{j=0}^{M_n} \Delta\left(\beta^{-j}(\rho_n)\right) = \sum_{j=0}^{M_n} 2\sqrt{r\left(\beta^{-j}(\rho_n)\right)} + Or\left(\beta^{-j}(\rho_n)\right)^{3/2} \leq \frac{1}{2mn} + O(n^{-3}) < \frac{\pi}{4}$$

for n large enough. In particular, (4.30) and (4.33) imply that

$$\left|\pi_M(\rho_n) - \pi_M\left(\beta^{-k}(\rho_n)\right)\right| \geq \frac{1}{\sqrt{2}} \sum_{j=0}^{k} T_-\left(\beta^{-j}(\rho_n)\right) \geq \frac{1}{\sqrt{2}} n R_n$$

which, for n large enough, is impossible since $\widetilde{\Omega}_R \subset B(0, MR)$. $\square$

We now set up our contradiction argument to prove the bound (4.21). Suppose there is no constant $C > 0$ such that for all $R \geq 1$ the estimate fails. Then, there exists $\{R_\ell\}_{\ell=1}^{\infty} \subset [1, \infty)$, $\{h_{k,\ell}\}_{k,\ell=1}^{\infty}$, with $\lim_{k \to \infty} h_{k,\ell} = 0$, $u_{k,\ell}$, and $g_{k,\ell,\text{tr}/D}, f_{k,\ell}$ such that $\|u_{k,\ell}\|_{H_h^1(\widetilde{\Omega}_{R_\ell} \backslash \Omega_-)} = 1$,

$$\left(\|g_{k,\ell,I}\|_{L^2(\Gamma_{\text{tr},R}(R_\ell))} + \|g_{k,\ell,D}\|_{H_{h_{k,\ell}}^1(\Gamma_D)}\right) \leq R_\ell^{-1/2} \ell^{-1}, \qquad \|f_{k,\ell}\|_{L^2(\widetilde{\Omega}(R_\ell) \backslash \Omega_-)} \leq R_\ell^{-1} \ell^{-1},$$

and such that

$$\begin{cases} \left(-h_{k,\ell}^2 \Delta - 1\right) u_{k,\ell} = h_{k,\ell} f_{k,\ell} & \text{on } \widetilde{\Omega}_{R_\ell} \setminus \Omega_- \\ (\mathcal{N} h_{k,\ell} D_n - \mathcal{D}) u_{k,\ell} = g_{k,\ell,I} & \text{on } \Gamma_{\text{tr},R_\ell} \\ u_{k,\ell} = g_{k,\ell,D} & \text{on } \Gamma_D. \end{cases}$$

Rescaling, we define

$$\widetilde{u}_{k,\ell}(x) = R_\ell^{\frac{n}{2}} v_{k,\ell}(xR_\ell), \quad \widetilde{g}_{k,\ell,I}(x) = R_\ell^{\frac{n}{2}} g_{k,\ell,I}(xR_\ell),$$

$$\widetilde{f}_{k,\ell}(x) = R_\ell^{\frac{n+2}{2}} f_{k,\ell}(xR_\ell), \quad \widetilde{G}_{k,\ell,D} = R_\ell^{\frac{n}{2}} g_{l,\ell,D}(xR_\ell).$$

Then,

$$\|\widetilde{g}_{k,\ell,I}\|_{L^2(\Gamma_{\text{tr},R_\ell}/R_\ell)} + \|\widetilde{g}_{k,\ell,D}\|_{L^2(\Gamma_D/R_\ell)} \leq \frac{1}{\ell}, \qquad \|\widetilde{u}_{k,\ell}\|_{H^1_{h_{k,\ell}}(\widetilde{\Omega}_{R_\ell})} \geq 1 - \frac{C}{R_\ell^{1/2}\ell}, \qquad \|\widetilde{f}_{k,\ell}\|_{L^2} \leq \frac{1}{\ell},$$

and, with $U_\ell = (\widetilde{\Omega}_{R_\ell}/R_\ell) \setminus \overline{(\Omega_-/R_\ell)}$, $\widetilde{\Gamma}_{D,\ell} = \Gamma_D/R_\ell$, $\widetilde{\Gamma}_{I,\ell} = \Gamma_{\text{tr},R_\ell}/R_\ell$,

$$\begin{cases} \left(-\left(h_{k,\ell} R_\ell^{-1}\right)^2 \Delta - 1\right) \widetilde{u}_{k,\ell} = \left(h_{k,\ell} R_\ell^{-1}\right) \widetilde{f}_{k,\ell} & \text{on } U_\ell \\ (\widetilde{\mathcal{N}} h_{k,\ell} R_{k,\ell}^{-1} D_n - \widetilde{\mathcal{D}}) \widetilde{u}_{k,\ell} = \widetilde{g}_{k,\ell,I} & \text{on } \widetilde{\Gamma}_{I,\ell} \\ \widetilde{u}_{k,\ell}|_{\widetilde{\Gamma}_{D,\ell}} = \widetilde{G}_{k,\ell,D}, \end{cases}$$

where, if a pseudodifferential operator B on $\Gamma_{\text{tr},R}$ is given by

$$B = \text{Op}_h(b), \qquad b \sim \sum_j h^j b_j,$$

then

$$\widetilde{B} = \text{Op}_{hR^{-1}}(\widetilde{b}), \qquad \widetilde{b} \sim \sum_j (hR^{-1})^j R^j b_j.$$

Putting $\widetilde{h}_{k,\ell} = h_{k,\ell} R_\ell^{-1}$, we have $\widetilde{h}_{k,\ell} \underset{k\to\infty}{\to} 0$ hence, extracting subsequences if necessary, we can assume that $u_{k,\ell}$ ($k \to \infty$) has a defect measure μ_ℓ and by Corollaries 4.2 and 4.3 we can assume that the trace measures for $u_{k,\ell}$, $v_{d,\ell}^{I/D}$, $v_{n,\ell}^{I/D}$ and $v_{j,\ell}^{I/D}$ exist. Moreover, μ_ℓ satisfies the relations from Proposition 2.12 where $\mu^{\text{in/out}}$. Finally, extracting even further subsequences, we can assume $\widetilde{g}_{k,\ell,I/D}$ have defect measures

$\omega_{\ell,I/D}, \widetilde{f}_{k,\ell}$ has defect measure α_ℓ, and the joint measure of $\tilde{u}_{k,\ell}$ and $\tilde{f}_{k,\ell}$ is μ_ℓ^j with

$$\omega_{\ell,I}(T^*\widetilde{\Gamma}_{I,\ell}) \le \frac{1}{\ell^2}, \qquad \omega_{\ell,D}(T^*\widetilde{\Gamma}_{D,\ell}) \le \frac{1}{\ell^2}, \qquad \alpha_\ell(T^*U_\ell) \le \frac{1}{\ell^2},$$

$$|\mu_\ell^j(A)| \le \sqrt{\mu_\ell(A)\alpha_\ell(A)}$$

and $R_\ell \to R \in [1,\infty]$. Therefore, using e.g., (Galkowski *et al.*, 2020, Lemma 4.2) together with Corollaries 4.2 and 4.3 to estimate the $H^1_{h_\ell/R_\ell}$ norm of $\widetilde{v}$ by its L^2 norm,

$$1 = \limsup_k \|\widetilde{v}_{k,\ell}\|^2_{H^1_{h_{k,\ell}/R_\ell}} \ge \mu_\ell(T^*\mathbb{R}^d) \ge \liminf_k \|\widetilde{v}_{k,\ell}\|^2_{L^2} \ge c \liminf_k \|\widetilde{v}_{k,\ell}\|^2_{H^1_{h_{k,\ell}/R_\ell}} \ge \frac{c}{2} > 0.$$

Note that each μ_ℓ is a finite measure satisfying $\operatorname{supp}\mu_\ell \subset S^*_{B(0,M)}\mathbb{R}^d$. Therefore, the sequence μ_ℓ is tight and bounded, and hence by Prokhorov's theorem (see, e.g., (Billingsley, 1999, Theorem 5.1, page 59) we can assume that $\mu_\ell \rightharpoonup \mu$ for some measure μ. Moreover, $\operatorname{supp}\mu \subset S^*_{\overline{U_\infty}}\mathbb{R}^d$ and

$$1 \ge \mu(S^*\mathbb{R}^d) > c > 0. \tag{4.34}$$

Lemma 4.9 The sequences of boundary measures $\nu^{\mathrm{tr}}_{d,\ell}$, $\nu^{\mathrm{tr}}_{n,\ell}$ and $\nu^{\mathrm{tr}}_{j,\ell}$, and $\nu^D_{n,\ell}$ are tight.

Proof. Since $\{r \ge 0\} \subset T^*\partial M_{I,\ell}$ is a compact set, we need only consider $r < 0$. By Lemma 2.11,

$$\Re\nu^{I/D}_{j,\ell}1_{r<0} = 0, \qquad \nu^{I/D}_{n,\ell}1_{r<0} = -r\nu^{I/D}_{d,\ell}1_{r<0}. \tag{4.35}$$

On the other hand, the boundary condition on $\Gamma_{\mathrm{tr},R}$ gives for $a \in C^\infty_c(\{r < 0\})$,

$$\langle a(x,\tilde{h}D)\widetilde{\mathcal{N}}\tilde{h}D_n u, u\rangle = \langle a(x,\tilde{h}D)\widetilde{\mathcal{D}}u, u\rangle + O(\ell^{-1}) + o(1)_{\tilde{h}\to 0}.$$

Sending $\tilde{h} \to 0$, we obtain

$$\nu^{\mathrm{tr}}_{j,\ell}(\sigma(\mathcal{N})a) = \nu^{\mathrm{tr}}_{d,\ell}(\sigma(\mathcal{D})a) + O(\ell^{-1}).$$

In particular,

$$\left\|\nu^{\mathrm{tr}}_{j,\ell}(\sigma(\mathcal{N}))1_{r<0} - \nu^{\mathrm{tr}}_{d,\ell}(\sigma(\mathcal{D}))1_{r<0}\right\| = O(\ell^{-1}).$$

Now, since $\Re\nu^{\mathrm{tr}}_{j,\ell} = 0$ and $\nu^{\mathrm{tr}}_{d,\ell}$, $\sigma(\mathcal{D})$ are real,

$$\left\|\nu^{\mathrm{tr}}_{d,\ell}(\sigma(\mathcal{D}))1_{r<0}\right\| = O(\ell^{-1}).$$

Similarly, for $a \in C^\infty_c(\{r < 0\})$,

$$\langle a(x,\tilde{h}D)\tilde{h}D_n u, \mathcal{D}u\rangle = \langle a(x,\tilde{h}D)u, \widetilde{\mathcal{N}}hD_\nu u\rangle + O(\ell^{-1}) + o(1)_{\tilde{h}\to 0},$$

so that, since $\sigma(\mathcal{N})$ and $\sigma(\mathcal{D})$ are both real,

$$\left\| v_{j,\ell}^{\mathrm{tr}}(\sigma(\mathcal{D}))1_{r<0} - v_{n,\ell}^{\mathrm{tr}}(\sigma(\mathcal{N}))1_{r<0} \right\| = O(\ell^{-1}),$$

and hence

$$\left\| v_{j,\ell}^{\mathrm{tr}}(\sigma(\mathcal{D}))1_{r<0} + r v_{d,\ell}^{\mathrm{tr}}(\sigma(\mathcal{N}))1_{r<0} \right\| = O(\ell^{-1}),$$

which again implies

$$\left\| r v_{d,\ell}^{\mathrm{tr}}(\sigma(\mathcal{N}))1_{r<0} \right\| = O(\ell^{-1}).$$

We now claim that

$$\text{there exists } \epsilon > 0 \text{ such that } \{r|\sigma(\mathcal{N})| \le \epsilon\} \cap \{|\sigma(\mathcal{D})| \le \epsilon\} \text{ is compact,} \tag{4.36}$$

which then implies that $v_{d,\ell}^{\mathrm{tr}}$ is tight. We now show that (4.36) holds in each of the three cases: $m_0 > m_1 + 1$, $m_0 < m_1 + 1$ and $m_0 = m_1 + 1$. If $m_0 > m_1 + 1$, then $\{|\sigma(\mathcal{D})| \le c/2\}$ is compact by (4.5) since $m_0 \ge 0$ by (4.10). If $m_0 < m_1 + 1$ and $m_1 \ge -2$ then $\{r|\sigma(\mathcal{N})| \le c/2\}$ is compact by (4.4); observe that the inequality $m_1 \ge -2$ follows from $m_0 < m_1 + 1$ since $m_0 \ge 0$ by (4.10). We now show that if $m_0 = m_1 + 1$ then the first inequality in (4.2) implies that there exists $C > 0$ such that if $|\xi'| \ge C$ then the intersection (4.36) with $\epsilon = \sqrt{c/2}$ (with c the constant in (4.3) is empty (and hence compact)). Indeed, since $m_0 \ge 0$ and $\langle \xi \rangle \ge 1$,

$$\text{if } |\sigma(\mathcal{D})|^2 \le (c/2) \quad \text{then} \quad |\sigma(\mathcal{D})|^2 \le (c/2)\langle \xi \rangle^{2m_0}.$$

Now, by the first inequality in (4.2)

$$\text{if } |\sigma(\mathcal{D})|^2 \le (c/2)\langle \xi \rangle^{2m_0} \quad \text{then} \quad |\sigma(\mathcal{N})|^2 \le (c/2)\langle \xi \rangle^{2m_1}.$$

If $|\sigma(\mathcal{N})|^2 \le (c/2)\langle \xi \rangle^{2m_1}$ then, since $m_1 > -2$, $r^2|\sigma(\mathcal{N})|^2 \ge c/2$ for sufficiently large ξ, and thus (4.36) indeed holds with $\epsilon = \sqrt{c/2}$.

The tightness of $v_{d,\ell}^{\mathrm{tr}}$ and (4.35) then imply that $v_{n,\ell}^{\mathrm{tr}}$ is tight and $|v_{j,\ell}^{\mathrm{tr}}| \le \sqrt{v_{d,\ell}^{\mathrm{tr}} v_{n,\ell}^{\mathrm{tr}}}$ implies that $v_{j,\ell}^{\mathrm{tr}}$ is tight. Next, the boundary condition on Γ_D gives that

$$v_{d,\ell}^{D} = \omega_{\ell,D} \le \frac{1}{\ell^2}.$$

Hence, $v_{n,\ell}^{D}$ and $v_{j,\ell}^{D}$ are tight as above. $\qquad\square$

Since the boundary measures form tight sequences, extracting subsequences if necessary, we can assume $v_{d,\ell}^{I/D} \rightharpoonup v_d^{I/D}$, $v_{n,\ell}^{I/D} \rightharpoonup v_n^{I/D}$ and $v_{j,\ell}^{I/D} \rightharpoonup v_j^{I/D}$ for some measures $v_d^{I/D}$, and $v_n^{I/D}$, and a complex measure $v_j^{I/D}$. Furthermore, $v_{d,\ell}^{D} = \omega_{\ell,D} \to 0$, and hence $v_{j,\ell}^{D} \to 0$. We also have $\alpha_\ell \to 0$.

Since these measures converge as distributions and $\tilde{\Gamma}_{I,\ell} \to \Gamma_{\mathrm{tr}}^\infty$ in C^∞, the equations from Lemma 2.12 and Theorem 2.15 hold for the limiting measures on $\Gamma_{\mathrm{tr}}^\infty$. (Here, we think of $\tilde{\Gamma}_{I,\ell}$ as a C^∞ graph over $\Gamma_{\mathrm{tr}}^\infty$.) In addition, since $\alpha_\ell \to 0$,

$$\mu(H_p a) = \lim_{\ell \to \infty} \mu_\ell(H_p a) = 0, \qquad a \in C_c^\infty\big(T^* U_\infty \setminus B(0, R^{-1})\big).$$

In addition, (4.27) holds by Lemma 2.12.

We now introduce notation for various billiard flows in the next section. First, let φ_t^ℓ denote the billiard flow on $\mathbb{R}^d \setminus (\Omega_-/R_\ell)$. Then, define

$$\varphi_t^\infty(x, \xi) = \lim_{\ell \to \infty} \varphi_t^\ell(x, \xi), \qquad (x, \xi) \in S^*\big(\mathbb{R}^d \setminus (\Omega_-/R)\big).$$

Note that, the convergence to φ_t^∞ is uniform and, in the case $R < \infty$, $\varphi_t^\infty(x, \xi)$ agrees with the billiard flow on $\mathbb{R}^d \setminus (\Omega_-/R)$ and we identify the two flows.

PROPOSITION 4.10   Suppose that $T < \infty$ and $A \subset S_{U_\ell}^* \mathbb{R}^d$ with

$$\bigcup_{0 \le t \le T} \varphi_t^\ell(A) \cap \tilde{\Gamma}_{I,\ell} = \emptyset.$$

Then,

$$\lim_{\ell \to \infty} \sup_{t \in [0,T]} \big|\mu_\ell\big(\varphi_t^\ell(A)\big) - \mu_\ell(A)\big| = 0$$

Proof. This follow from Theorem 2.15 since

$$\big\|\mu_{D,\ell}^{\mathrm{in}} - \mu_{D,\ell}^{\mathrm{out}}\big\| = 2\big\|\Re v_{j,\ell}^D\big\| \le C\sqrt{\|\omega_{D,\ell}\|} = O(\ell^{-1}),$$

and

$$\big\|\mu_\ell^j\big\| \le C\sqrt{\alpha_\ell} = O(\ell^{-1}).$$

$\square$

Next, we show that μ_∞ is invariant under φ_t^∞ when $R < \infty$.

LEMMA 4.11   Suppose that $R < \infty$ and that $A \subset S_{U_\infty}^* \mathbb{R}^d$ is closed and

$$\bigcup_{0 \le t \le T} \varphi_t^\infty(A) \cap \Gamma_{\mathrm{tr}}^\infty = \emptyset.$$

Then,

$$\mu\big(\varphi_t^\infty(A)\big) = \mu(A).$$

Proof. First, note that since the convergence of φ_t^ℓ to φ_t^∞ is uniform,

$$\lim_{\ell \to \infty} \mathrm{d}\big(\varphi_t^\infty(A), \varphi_t^\ell(A)\big) = 0.$$

Therefore, fixing $\epsilon > 0$, for ℓ large enough,

$$\varphi_t^\ell(A) \subset \{(x, \xi) \,:\, \mathrm{d}(\varphi_T(A), (x, \xi)) < \epsilon\}$$

and

$$\varphi_\ell^{-T}\left(\varphi_t^\infty A\right) \subset \{(x, \xi) \,:\, \mathrm{d}(A, (x, \xi)) < \epsilon\}.$$

Now, for finite times T, μ_ℓ is invariant under φ_t^ℓ up to $o(1)_{\ell \to \infty}$. Combining this with the fact that our assumption on A implies that, for ℓ large enough, φ_t^ℓ does not intersect $\Gamma_{\mathrm{tr},R}$ in $[0, T]$, we have

$$\mu_\ell\left(\varphi_t^\infty(A)\right) = \mu_\ell\big(\varphi_\ell^{-T}\varphi_t^\infty(A)\big) + o(1)_{\ell \to \infty} \le \mu_\ell(\{(x, \xi) \,:\, \mathrm{dist}\,((x, \xi), A) < \epsilon\}) + o(1)_{\ell \to \infty}$$

and

$$\mu_\ell(A) = \mu_\ell\big(\varphi_t^\ell(A)\big) + o(1)_{\ell \to \infty} \le \mu_\ell\left(\{(x, \xi) \,:\, \mathrm{dist}\,\big((x, \xi), \varphi_t^\infty(A)\big) < \epsilon\}\right) + o(1)_{\ell \to \infty}.$$

Sending $\ell \to \infty$ and then $\epsilon \to 0$, we obtain

$$\mu(A) = \mu\left(\varphi_t^\infty(A)\right)$$

as claimed. $\qquad\square$

REMARK. Note that when $R = \infty$, the analogue of Lemma 4.11 is obvious except on the sets $\{\xi = \pm\frac{x}{|x|}\}$ and $\{x = 0\}$ since we can test μ against $H_p a$ away from these sets.

In the case $R = \infty$, we use the following lemmas.

LEMMA 4.12 If $R = \infty$, then $\mu(\{x = 0\} = 0)$.

Proof. Fix $\epsilon > 0$. Since Ω_- is nontrapping and $\Gamma_D \Subset B(0, 1)$, there is $T > 0$ and $c > 0$ such that

$$\bigcup_{\pm t \ge TR_\ell^{-1}} \varphi_t^\ell\big(|x| \le 2R_\ell^{-1}\big) \cap \big(\{|x| \le 3R_\ell^{-1}\} \cup \{|\langle \tfrac{x}{|x|}, \xi\rangle| \le c\}\big) = \emptyset.$$

Thus, for ℓ large enough

$$\varphi_{4\epsilon}^\ell(|x| \le \epsilon) \subset \big\{2\epsilon \le |x| \le 6\epsilon, \, \xi \cdot \tfrac{x}{|x|} > c\big\}.$$

In particular, there is $c > 0$ such that for $j \ne k$, $0 \le j < k < c\epsilon^{-1}$

$$\varphi_{4\epsilon+c^{-1}k}^\ell(\{|x| \le \epsilon\}) \cap \varphi_{4\epsilon+c^{-1}j}^\ell(\{|x| \le \epsilon\}) = \emptyset.$$

Since $\mu_\ell(T^*\mathbb{R}^d) \leq 1$, this implies that

$$\mu_\ell(\{|x| \leq \epsilon\}) \leq C\epsilon + o_{\ell\to\infty}(1),$$

and hence, sending $\ell \to \infty$,

$$\mu(\{|x| \leq \epsilon\}) \leq C\epsilon.$$

Finally, sending $\epsilon \to 0$ proves the claim. $\qquad\square$

LEMMA 4.13 If $R = \infty$ then μ_∞ is invariant under φ_t^∞ away from $\Gamma_{\mathrm{tr}}^\infty$.

Proof. Let

$$A_\pm := \left\{ \pm\xi = \tfrac{x}{|x|} \right\} \cap \left\{ |x| = \tfrac{1}{2M} \right\}.$$

Note that μ_ℓ is invariant under φ_t^ℓ modulo $o_{\ell\to\infty}(1)$. Now, $\widetilde{\Gamma}_{D,\ell} \subset B(0, R_\ell^{-1})$. Since $R_\ell \to \infty$, and Ω_- is nontrapping for $(x,\xi) \in A_-$,

$$\lim_{\ell\to\infty} \sup_{(x,\xi)\in A_-} \mathrm{dist}\left(\varphi_{1/M}^\ell(x,\xi), A_+\right) = 0.$$

Similarly,

$$\lim_{\ell\to\infty} \sup_{(x,\xi)\in A_+} \mathrm{dist}\left(\varphi_{-1/M}^\ell(x,\xi), A_-\right) = 0.$$

Now, for $\delta > 0$ small enough, $-\delta \leq t \leq \delta$ and $\mathrm{dist}\left((x,\xi), A_\pm\right) \leq \delta$, $\varphi_t^\ell(x,\xi) = \varphi_t^\infty(x,\xi)$. In particular, for $B_- \subset A_-$,

$$\mu_\ell\left(\bigcup_{-\delta\leq t\leq\delta} \varphi_t^\infty(B_-)\right) = \mu_\ell\left(\bigcup_{-\delta\leq t\leq\delta} \varphi_t^\ell(B_-)\right) = \mu_\ell\left(\bigcup_{\frac{1}{M}-\delta\leq t\leq\frac{1}{M}+\delta} \varphi_t^\ell(B_-)\right) + o_{\ell\to\infty}(1).$$

Fix $\epsilon > 0$. Then for ℓ large enough,

$$\bigcup_{1/M-\delta\leq t\leq 1/M+\delta} \varphi_t^\ell(B_-) \subset \bigcup_{-\delta\leq t\leq\delta} \varphi_t^\ell\left(\{(x,\xi) : \mathrm{dist}\left((x,\xi), \varphi_{1/M}^\infty(B_-)\right) \leq \epsilon\}\right).$$

In particular,

$$\mu_\ell\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty(B_-)\right) \le \mu_\ell\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\ell\left(\{(x,\xi)\mid \operatorname{dist}\left((x,\xi),\varphi_{1/M}^\infty(B_-)\right)\le\epsilon\}\right)\right) + o(1)_{\ell\to\infty},$$

$$= \mu_\ell\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty\left(\{(x,\xi)\,:\,\operatorname{dist}\left((x,\xi),\varphi_{1/M}^\infty(B_-)\right)\le\epsilon\}\right)\right) + o(1)_{\ell\to\infty},$$

where in the last line we use that $\varphi_t^\ell = \varphi_t^\infty$ on the relevant set. Similarly, for ℓ large enough (depending on ϵ), and $B_+ \subset A_+$

$$\mu_\ell\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty(B_+)\right) \le \mu_\ell\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty\left(\{(x,\xi)\,:\,\operatorname{dist}\left((x,\xi),\varphi_{-1/M}^\infty(B_+)\right)\le\epsilon\}\right)\right) + o(1)_{\ell\to\infty}.$$

Putting $B_+ = \varphi_{1/M}^\infty(B_-)$, sending $\ell \to \infty$ and then $\epsilon \to 0$, we obtain

$$\mu\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty(B_+)\right) \le \mu\left(\bigcup_{-\delta\le t\le\delta}\varphi_{t-1/M}^\infty(B_+)\right) = \mu\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty(B_-)\right)$$

$$\le \mu\left(\bigcup_{-\delta\le t\le\delta}\varphi_{t+1/M}^\infty(B_-)\right) = \mu\left(\bigcup_{-\delta\le t\le\delta}\varphi_t^\infty(B_+)\right),$$

and the claim then follows from the fact that

$$\mu(H_p a) = 0$$

for all $a \in C_c^\infty(T_{U_\infty\setminus\{0\}}^*\mathbb{R}^d)$. □

We now derive our contradiction to prove the bound (4.21), and thus complete the proof of Theorem 4.6. By Lemmas 4.11, 4.12 and 4.13, μ is invariant under φ_t^∞ away from $\Gamma_{\mathrm{tr}}^\infty$. In particular, Lemma 4.8 applies and we obtain that $\mu = 0$, which is a contradiction to (4.34).

5. Proofs of the bounds on the relative error (Theorems 1.6–1.11)

As discussed in § 3, the upper bounds in Theorem 1.7 and in Theorem 1.9 follow from applying Theorem 1.5 to $u - v$ and then using Lemma 3.2. It therefore remains to prove the lower bounds in Theorems 1.6, 1.7, 1.8, 1.10 and 1.11.

5.1 *Existence of defect measures*

LEMMA 5.1 If Ω_- is nontrapping, then Assumption 2.2 holds for u and v the solutions of (2.1) and (2.2), respectively.

Proof. The bound on $\|\chi u\|_{L^2}$ follows from Lemma 3.1; the bound on $\|hD_n u\|_{L^2(\Gamma_D)}$ follows from Corollary 4.3 and that on $\|u\|_{L^2(\Gamma_D)}$ follows from the condition (2.1b) that $u|_{\Gamma_D} = \exp(ix \cdot a/h)$. The

bound on $\|v\|_{L^2}$ follows from Theorem 1.5. The bounds on $\|v\|_{L^2(\Gamma_{\mathrm{tr},R})}$ and $\|hD_n v\|_{L^2(\Gamma_{\mathrm{tr},R})}$ follow from Corollary 4.2, and those for $\|hD_n u\|_{L^2(\Gamma_D)}$ from Corollary 4.3. The bound on $\|v\|_{L^2(\Gamma_D)}$ follows from the condition (2.2b) that $v|_{\Gamma_D} = \exp(ix \cdot a/h)$. $\qquad\square$

REMARK 5.2 (Neumann boundary conditions). We do not consider Neumann boundary conditions on Γ_D because, as far as we know, propagation of measures for Neumann boundary conditions is not available. Indeed, the Neumann boundary condition does not satisfy the uniform Lopatinski–Shapiro condition (see, e.g., (Hörmander, 1985, Part (ii) of Definition 20.1.1, page 233)) and, under Neumann boundary conditions, if u is normalized so that $\|h\partial_n u\|_{L^2(\Gamma_D)}$ is bounded, then $\|u\|_{L^2(\Gamma_D)}$ is typically not uniformly bounded as $h \to 0$ (for example, when Γ_D is the boundary of a ball; see, e.g., (Spence, 2014, Equation 3.31)); therefore Assumption 2.2 does not hold.

5.2   *Reduction to a lower bound on the measure of the incoming set*

LEMMA 5.3   There exists $C_1 > 0$ such that if $\{u_\ell\}_{\ell=1}^\infty$ and $\{v_\ell\}_{\ell=1}^\infty$ are sequences of solutions to (2.1) and (2.2), respectively, such that u_ℓ has a defect measure and v_ℓ has defect measure μ, then

$$\liminf_{\ell\to\infty} \frac{\|u_\ell - v_\ell\|_{L^2(\Omega_R)}}{\|u_\ell\|_{L^2(\Omega_R)}} \geq C_1 \sqrt{\frac{\mu(\mathcal{I})}{R}}, \tag{5.1}$$

and

$$\liminf_{\ell\to\infty} \frac{\|u_\ell - v_\ell\|_{L^2(B(0,2)\setminus\Omega_-)}}{\|u_\ell\|_{L^2(B(0,2)\setminus\Omega_-)}} \geq C_1 \sqrt{\mu\big(\mathcal{I} \cap \big(S^*_{B(0,3/2)}\mathbb{R}^d\big)\big)}, \tag{5.2}$$

where $\mathcal{I}$ is the directly-incoming set defined by (3.3).

Proof.   Let $b \in C_c^\infty(S^*\Omega_R)$ be supported in $\mathcal{I}$ and such that

$$\int |b|^2 \, \mathrm{d}\mu \geq \mu(\mathcal{I})/2.$$

If $\widetilde{\mu}$ is a defect measure of u, then $\widetilde{\mu}(\mathcal{I}) = 0$ by Lemma 3.6. By the definition of defect measures,

$$\lim_{\ell\to\infty} \big\langle b(x, h_\ell D)u_\ell, b(x, h_\ell D)u_\ell \big\rangle = 0,$$

and therefore

$$\begin{aligned}
\mu(\mathcal{I})/2 &\leq \lim_{\ell\to\infty} \big\langle b(x, h_\ell D)v_\ell, b(x, h_\ell D)v_\ell \big\rangle \\
&= \lim_{\ell\to\infty} \big(\langle b(x, h_\ell D)v_\ell, b(x, h_\ell D)v_\ell \rangle + \langle b(x, h_\ell D)u_\ell, b(x, h_\ell D)u_\ell \rangle \big) \\
&\quad - 2 \lim_{\ell\to\infty} \Re \langle b(x, h_\ell D)u_\ell, b(x, h_\ell D)v_\ell \rangle \\
&= \lim_{\ell\to\infty} \big\langle b(x, h_\ell D)(v_\ell - u_\ell), b(x, h_\ell D)(v_\ell - u_\ell) \big\rangle \\
&\lesssim \|u_\ell - v_\ell\|_{L^2(\Omega_R)}^2
\end{aligned}$$

(where the upper bound on $b(x, h_\ell D)$ is independent of $\mathcal{I}$ by (Zworski, 2012, Theorem 5.1)). The bound (5.1) then follows from the upper bound on $\|u_\ell\|_{L^2(\Omega_R)}$ in Lemma 3.1. The estimate (5.2) is proved in the same way by taking b supported in $S^*_{B(0,3)}\mathbb{R}^d$ and such that $\int |b|^2 \, d\mu \geq \mu(\mathcal{I} \cap S^*_{B(0,3/2)}\mathbb{R}^d)/2$. □

COROLLARY 5.4 Let $\{v_\ell\}_{\ell=1}^\infty$, $\{h_\ell\}_{\ell=1}^\infty$, and $\{a_\ell\}_{\ell=1}^\infty$ be sequences such that v_ℓ satisfies (2.2) with $a = a_\ell$ and $\{v_\ell\}_{\ell=1}^\infty$ has defect measure μ.

(i) To prove Theorem 1.6 it is sufficient to prove that there exists $c_0 > 0$ that depends continuously on $\Gamma_{\text{tr},R}$ such that

$$\mu(\mathcal{I}) \geq c_0.$$

(ii) Having proved Theorem 1.6, to prove the lower bound in Theorem 1.7 it is sufficient to prove that there exists $c_1 > 0$ (independent of R) and R_0 such that, for all $R \geq R_0$,

$$\mu(\mathcal{I}) \geq \frac{c_1}{R^{4m_{\text{ord}}-1}}. \tag{5.3}$$

(iii) Having proved Theorem 1.6, to prove Theorem 1.8 it is sufficient to prove that there exists $c_2 > 0$ and $R_0 > 0$ (independent of R) such that, for all $R \geq R_0$,

$$\mu(\mathcal{I}) \geq c_2 R. \tag{5.4}$$

(iv) To prove Theorem 1.10 it is sufficient to prove that there exists $c_3 > 0$ (independent of R) and $R_0 \geq 2$ such that, for all $R \geq R_0$,

$$\mu\big(\mathcal{I} \cap \big(S^*_{B(0,3/2)}\mathbb{R}^d\big)\big) \geq \frac{c_3}{R^{4m_{\text{ord}}}}. \tag{5.5}$$

(v) To prove Theorem 1.11 it is sufficient to prove that there exists $c_4 > 0$ (independent of R) such that, for all $R \geq 2$,

$$\mu\big(\mathcal{I} \cap \big(S^*_{B(0,3/2)}\mathbb{R}^d\big)\big) \geq \frac{c_4}{R^{d-1}}. \tag{5.6}$$

Proof. We prove Part (ii), i.e., the lower bound in (1.14) in Theorem 1.7; the proofs of the other parts are essentially identical and/or simpler.

We first show that it is sufficient to prove that there exists $\widetilde{C}_1 = \widetilde{C}_1(\Omega_-, \mathsf{M}, \mathsf{N})$ and $R_0 = R_0(\Omega_-, \mathsf{M}, \mathsf{N}) > 0$ such that for any $R \geq R_0$, there exists $\widetilde{k}_0(R) > 0$ such that, for any direction a,

$$\frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}} \geq \frac{\widetilde{C}_1}{R^{2m_{\text{ord}}}} \qquad \text{for all } k \geq k_0. \tag{5.7}$$

Indeed, having proved (5.7), we let

$$C_1 := \min\left(\widetilde{C}_1, \ \min_{1 \leq R \leq R_0} \frac{\|u - v\|_{L^2(\Omega_R)}}{\|u\|_{L^2(\Omega_R)}}\right).$$

By Theorem 1.6 and the fact that the constant C in this theorem depends continuously on R, C_1 exists, is > 0, and is independent of k. With this definition of C_1, (5.7) implies that the lower bound in (1.14) holds with $k_0(R) := \widetilde{k}_0(R)$ for $R \geq R_0$, and $k_0(R)$ equal to the respective k_0 from Theorem 1.6 for $1 \leq R \leq R_0$.

We now prove (5.7); seeking a contradiction, suppose that the converse of (5.7) is true; that is, given $C_0 > 0$, for any $\widetilde{R}_0 > 0$ there exists $R \geq \widetilde{R}_0$ and sequences $\{h_\ell\}_{\ell=1}^\infty$, $\{a_\ell\}_{\ell=1}^\infty$ with $h_\ell \to 0$, $|a_\ell| = 1$ such that the solutions u_ℓ and v_ℓ to (2.1) and (2.2) satisfy

$$\frac{\|u_\ell - v_\ell\|_{L^2(\Omega_R)}}{\|u_\ell\|_{L^2(\Omega_R)}} \leq \frac{C_0}{R^{2m_{\mathrm{ord}}}}. \tag{5.8}$$

By extracting subsequences, we can assume that u_ℓ has defect measure $\widetilde{\mu}$ and v_ℓ has defect measure μ by Lemma 5.1.

Setting $\widetilde{R}_0 := R_0$, with R_0 such that (5.3) holds for $R \geq R_0$, and using this lower bound on $\mu(\mathcal{I})$ in (5.1), we have

$$\liminf_{\ell \to \infty} \frac{\|u_\ell - v_\ell\|_{L^2(\Omega_R)}}{\|u_\ell\|_{L^2(\Omega_R)}} \geq \frac{C_1\sqrt{c_1}}{R^{2m_{\mathrm{ord}}}},$$

for all $R \geq \widetilde{R}_0$, which contradicts (5.8) for $C_0 < C_1\sqrt{c_1}$, thus proving the lower bound in Theorem 1.7. $\qquad\square$

5.3 *Outline of the ideas behind rest of the proofs, and the structure of the rest of this section*

By Corollary 5.4, we need to prove lower bounds on the measure of the incoming set $\mu(\mathcal{I})$. We argue by contradiction and assume that $\mu(\mathcal{I})$ is small. The overall plan is the following.

(i) Show that, since $\mu(\mathcal{I})$ is small, mass is created when incoming rays reflect off Γ_D using Lemma 2.20 above.

(ii) Show that there exists a neighbourhood of rays starting from Γ_D that hit $\Gamma_{\mathrm{tr},R}$ directly (i.e., without hitting Γ_D in the meantime) and hit $\Gamma_{\mathrm{tr},R}$ at angles to the normal that are not zero, and not one of the special angles corresponding to the nonzero zeros $\{t_j\}_{j=1}^{m_{\mathrm{vanish}}}$ of $q(t)\sqrt{1-t} - p(t)$ (these conditions are made more precise in Condition 5.9 below).

(iii) Propagate the mass created in Point (i) on the rays constructed in Point (ii) using Part (i) of Corollary 2.17 (to go from mass on Γ_D to mass on $\Gamma_{\mathrm{tr},R}$).

(iv) Show that mass is reflected on $\Gamma_{\mathrm{tr},R}$ using the expression for the reflection coefficient in Corollary 2.19 and the fact that the rays hit $\Gamma_{\mathrm{tr},R}$ away from angles where the reflection coefficient vanishes.

(v) Show that this reflected mass produces mass on $\mathcal{I}$ using Part (ii) of Corollary 2.17 (to go from mass on $\Gamma_{\mathrm{tr},R}$ to mass in Ω_R), contradicting the assumption that $\mu(\mathcal{I})$ is small.

For the quantitative (i.e., explicit-in-R) bounds the goal is to prove a lower bound on $\mu(\mathcal{I})$ that is explicit in R. Therefore, on top of the requirements on the rays in Point (ii) above, we need (a) the angles the rays hit $\Gamma_{\mathrm{tr},R}$ to have certain R-dependence (since this will affect the R-dependence of the reflection coefficient in Point (iv)), and (b) information about when the reflected rays next hit Γ_D.

For the bounds on the relative error in subsets of Ω_R (Theorems 1.10 and 1.11), we also require information about when the rays return to a neighbourhood of Ω_-, since we need information about the defect-measure mass here (more specifically, $\mu(\mathcal{I} \cap S^*_{B(0,3/2)}\mathbb{R}^d)$).

Outline of the rest of § 5.

§ 5.4 contains preliminary results required for the ray arguments. § 5.5 states the condition the rays must satisfy (Condition 5.9) and results constructing rays satisfying this condition (Lemmas 5.10–5.13). § 5.7 proves Lemmas 5.10–5.13. § 5.8 bounds the reflection coefficient (2.48) for rays satisfying Condition 5.9. § 5.9 proves the qualitative (i.e., not explicit in R) lower bound in Theorem 1.6; the steps (i)–(v) above therefore appear in their simplest form in this proof. § 5.10 proves the quantitative (i.e., explicit in R) lower bounds in Theorem 1.7, 1.8, 1.10, 1.11.

5.4 *Preliminary results required for the ray arguments*

Recall that $\mathcal{S}^{d-1}$ denotes the d-dimensional unit sphere. Given $a \in \mathbb{R}^d$ with $|a| = 1$, let $\mathfrak{R}_a : \Gamma_D \to \mathcal{S}^{d-1}$ be defined by

$$\mathfrak{R}_a(x') = \left(\xi_1 = \sqrt{r\left(x', (a_T(x'))^\flat\right)}, \xi' = (a_T(x'))^\flat \right).$$

The definition of the local coordinates in § 2.3 and the fact that $\xi_1 > 0$ imply that

$$\mathfrak{R}_a(x') = \begin{cases} a - 2(n(x') \cdot a)n(x') & \text{if } a \cdot n(x') \leq 0, \\ a & \text{if } a \cdot n(x') \geq 0, \end{cases} \tag{5.9}$$

i.e., $\mathfrak{R}_a(x')$ is the reflection of a from Γ_D if x' is in the illuminated part of Γ_D and $\mathfrak{R}_a(x')$ is just a if x' is in the shadow part of Γ_D.

DEFINITION 5.5 Given $x' \in \Gamma_D$ and $a \in \mathbb{R}^d$ with $|a| = 1$, *the ray emanating from x'* is the ray starting from $\left(x = x', \xi = \mathfrak{R}_a(x')\right)$.

DEFINITION 5.6 The ray emanating from $x' \in \Gamma_D$ is *direct* if the flow along the ray, starting at x', hits $\Gamma_{\mathrm{tr},R}$ before hitting Γ_D.

We now show that there are direct rays emanating from Γ_D in every direction.

LEMMA 5.7 Given $a \in \mathbb{R}^d$ with $|a| = 1$. Let $\Gamma_D^{+,a} \subset \Gamma_D$ denote the set of points x' of Γ_D such that both $a \cdot n(x') \neq 0$ and the ray emanating from x' is direct. Then,

$$\mathfrak{R}_a\left(\Gamma_D^{+,a}\right) = \mathcal{S}^{d-1}.$$

Proof. We first prove that $a \in \mathfrak{R}_a(\Gamma_D^{+,a})$. Without loss of generality $a = (1, 0, \ldots, 0)$. Let $x_0' \in \Gamma_D$ be the point with maximal x_1 coordinate. Then $\mathfrak{R}_a(x_0') = a$ by (5.9), $x_0' \in \Gamma_D^{+,a}$ by the fact it has maximal x_1 coordinate, and so $a \in \mathfrak{R}_a(\Gamma_D^{+,a})$.

We now need to show that, given $\zeta \in \mathcal{S}^{d-1} \setminus \{a\}$, $\zeta \in \mathfrak{R}_a(\Gamma_D^{+,a})$. Let $\mathcal{P}$ be the plane defined by $\mathcal{P} := \mathrm{Span}(a, \zeta)$. Choose a cartesian system of coordinates in which $\mathcal{P} = \{x_3 = \cdots = x_n = 0\}$, $a = (1, 0, \cdots, 0)$, and (x_1, x_2) is right-handed oriented in $\mathcal{P}$. For $\xi \in \mathcal{S}^{d-1}$, let $r_a(\xi) := a - 2(\xi \cdot a)\xi$; i.e., $r_a(\xi)$ is the reflection of a from a boundary with normal ξ. This definition implies that

$$r_a((\cos\omega, \sin\omega, 0, \cdots, 0)) = (\cos(2\omega - \pi), \sin(2\omega - \pi), 0, \cdots, 0),$$
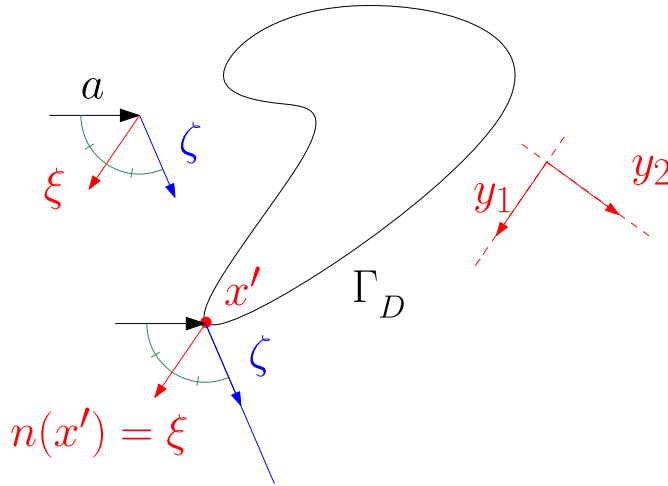
FIG. 6. Illustration of the proof of Lemma 5.7 in the two-dimensional case; i.e., construction of a ray reflecting from Γ_D in an arbitrary direction ζ. The point x' has maximal y_1 coordinate, where the vector ξ defines the y_1 axis, and ξ is defined by $\zeta = a - 2(a \cdot \xi)\xi$.

so that

$$r_a(\mathcal{D}) = \left(\mathcal{S}^{d-1} \cap \mathcal{P}\right) \setminus \{a\}, \text{ where } \mathcal{D} := \left\{(\cos\omega, \sin\omega, 0, \cdots, 0), \ \omega \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right)\right\}.$$

Hence, there exists $\xi \in \mathcal{D}$ such that $r_a(\xi) = \zeta$.

Finally, to show $\zeta \in \mathfrak{R}_a(\Gamma_D^{+,a})$, we need to find $x' \in \Gamma_D^{+,a}$ such that $\mathfrak{R}_a(x') = r_a(\xi)$. Let $(y_1, \cdots, y_d)$ be a cartesian system of coordinates such that $\xi = (y_1 = 1, y_2 = 0, \cdots, y_d = 0)$; see Fig. 6; let x' be a point of Γ_D with maximal y_1 coordinate. By definition, $n(x') = \xi$, and, since $\xi \in \mathcal{D}$, $a \cdot n(x') < 0$. Therefore, $\mathfrak{R}_a(x') = r_a(n(x')) = r_a(\xi) = \zeta$. Since x' has maximal y_1 coordinate in Γ_D, the ray emanating from x' only intersects Γ_D at x', and thus $x' \in \Gamma_D^{+,a}$. □

The following dilation property $\mathfrak{R}_a(x')$ is needed for one of the proofs below (the proof of Lemma 5.13).

LEMMA 5.8 Let $0 < \delta < 1$ and let $\mathcal{C} \subset \Gamma_D^{+,a}$ be uniformly convex (i.e., the second fundamental form is positive definite) and such that, for any $x' \in \mathcal{C}$, $\delta \leq |n(x') \cdot a| \leq 1 - \delta$. Then, there exists $C_{\mathfrak{R}} > 0$ and $\alpha_0 > 0$ such that, for any $x' \in \mathcal{C}$ and any $0 < \alpha \leq \alpha_0$, if $\partial B(x', \alpha) \cap \mathcal{C} \neq \emptyset$ and $\partial B(x', \alpha) \cap \partial \mathcal{C} = \emptyset$, there exists $y' \in \partial B(x', \alpha) \cap \mathcal{C}$ so that

$$|\mathfrak{R}_a(x') - \mathfrak{R}_a(y')| \geq C_{\mathfrak{R}}|x' - y'| = C_{\mathfrak{R}}\alpha.$$

Proof of Lemma 5.8. Let $(\mathsf{x}_1, \cdots, \mathsf{x}_d) =: (\mathsf{x}_1, \mathsf{x}')$ be an Euclidian system of coordinates in which $a = (1, 0, \cdots, 0)$. Since $\mathcal{C}$ is included in $\{\delta \leq |n(x') \cdot a| \leq 1 - \delta\}$, there exists $\mathsf{X} \subset \{\mathsf{x}_1 = 0\}$ and a smooth map $\gamma_{\mathcal{C}} : \mathsf{X} \longrightarrow \mathbb{R}$ such that $\mathcal{C}$ is given by, in this Euclidian system of coordinates

$$\mathcal{C} = \left\{(\gamma_{\mathcal{C}}(\mathsf{x}'), \mathsf{x}') \ : \ \mathsf{x}' \in \mathsf{X}\right\}.$$

First observe that, for $x' = (\gamma_D(\mathrm{x}'), \mathrm{x}') \in \mathcal{C}$ and $y' = (\gamma_D(\mathrm{y}'), \mathrm{y}') \in \mathcal{C}$

$$|x' - y'| \leq |\mathrm{x}' - \mathrm{y}'| + |\gamma_D(\mathrm{x}') - \gamma_D(\mathrm{y}')| \leq \left(1 + \sup_{\mathrm{X}} |\nabla\gamma_{\mathcal{C}}|\right) |\mathrm{x}' - \mathrm{y}'|,$$

and hence

$$C_0|x' - y'| \leq |\mathrm{x}' - \mathrm{y}'| \leq |x' - y'|, \quad \text{where} \quad C_0 := \left(1 + \sup_{\mathrm{X}} |\nabla\gamma_D|\right)^{-1}. \tag{5.10}$$

By the definition of $\mathfrak{R}_a$ (5.9),

$$\mathfrak{R}_a(x') - \mathfrak{R}_a(y') = 2\left(H(x') - H(y')\right), \tag{5.11}$$

$$H(x') := (n(x') \cdot a)n(x') \quad \text{and} \quad n(x') := (1, -\nabla\gamma_D(\mathrm{x}'))/\sqrt{1 + |\nabla\gamma_D(\mathrm{x}')|^2},$$

i.e., $n(x')$ is the outward-pointing normal to Γ_D at $x' = (\gamma_D(\mathrm{x}'), \mathrm{x}') \in \mathcal{C}$.

Given x', our plan is to use Taylor's theorem on H to bound $|\mathfrak{R}_a(x') - \mathfrak{R}_a(y')|$ below, and then choose y' appropriately so that this lower bound is $\geq C_{\mathfrak{R}}|x' - y'|$. We first record that, since $|n(x') \cdot a| \leq 1 - \delta$ and $a = (1, 0, \ldots, 0)$,

$$|\nabla\gamma_{\mathcal{C}}(\mathrm{x}')| \geq (1 - \delta)^{-2} - 1 =: \beta > 0. \tag{5.12}$$

Let H_1 be the component of H in the x_1 direction (i.e., the direction of a), i.e.,

$$H_1(x') = \frac{1}{1 + |\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|^2}. \tag{5.13}$$

Then, using (5.11), Taylor's theorem, (5.13), (5.10) and (5.12), we obtain

$$\frac{1}{2}\left|\mathfrak{R}_a(x') - \mathfrak{R}_a(y')\right| \geq \left|H_1(x') - H_1(y')\right| \geq \left|\nabla H_1(x') \cdot (x' - y')\right| - \sup_{\mathrm{X}}\left|\partial^2 H_1\right|\left|x' - y'\right|^2$$

$$= \left|\left\langle \frac{2\partial^2\gamma_{\mathcal{C}}(\mathrm{x}')\nabla\gamma_{\mathcal{C}}(\mathrm{x}')}{(1 + |\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|^2)^2}, \frac{\mathrm{x}' - \mathrm{y}'}{|\mathrm{x}' - \mathrm{y}'|}\right\rangle\right| |\mathrm{x}' - \mathrm{y}'| - \sup_{\mathrm{X}}\left|\partial^2 H_1\right|\left|x' - y'\right|^2$$

$$= \frac{2|\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|}{(1 + |\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|^2)^2}\left|\left\langle \partial^2\gamma_{\mathcal{C}}(\mathrm{x}')\frac{\nabla\gamma_{\mathcal{C}}(\mathrm{x}')}{|\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|}, \frac{\mathrm{x}' - \mathrm{y}'}{|\mathrm{x}' - \mathrm{y}'|}\right\rangle\right| |\mathrm{x}' - \mathrm{y}'| - \sup_{\mathrm{X}}\left|\partial^2 H_1\right|\left|x' - y'\right|^2$$

$$\geq 2C_1\beta C_0 Q_{\mathcal{C}}\left|\left\langle v, \frac{\mathrm{x}' - \mathrm{y}'}{|\mathrm{x}' - \mathrm{y}'|}\right\rangle\right| |x' - y'| - C_2|x' - y'|^2, \tag{5.14}$$

where

$$v := \left(\partial^2\gamma_{\mathcal{C}}(\mathrm{x}')\frac{\nabla\gamma_{\mathcal{C}}(\mathrm{x}')}{|\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|}\right)\left|\partial^2\gamma_{\mathcal{C}}(\mathrm{x}')\frac{\nabla\gamma_{\mathcal{C}}(\mathrm{x}')}{|\nabla\gamma_{\mathcal{C}}(\mathrm{x}')|}\right|^{-1},$$

and

$$C_1 := \left(1 + \sup_{\mathrm{X}} |\nabla \gamma_{\mathcal{C}}|^2\right)^{-2} > 0, \quad C_2 := \sup_{\mathrm{X}} \left|\partial^2 H_1\right| < \infty, \quad Q_{\mathcal{C}} := \inf_{x' \in \mathrm{X}, |e|=1} \left|\partial^2 \gamma_{\mathcal{C}}(x')e\right| > 0,$$

where $Q_{\mathcal{C}} > 0$ because $\mathcal{C}$ is uniformly convex.

We now claim that, under the assumption that $\partial B(x', \alpha) \cap \mathcal{C} \neq \emptyset$ and $\partial B(x', \alpha) \cap \partial C = \emptyset$, it is always possible to choose $y' \in \mathcal{C}$ so that

$$|x' - y'| = \alpha \quad \text{and} \quad \frac{x' - y'}{|x' - y'|} = v. \tag{5.15}$$

Indeed, for $d \geq 3$, the projection of $\partial B(x', \alpha) \cap \mathcal{C}$ on the hyperplane $\{x_1 = 0\}$ is a closed hypersurface of $\mathbb{R}^{d-1}$ (e.g., for $d = 3$ it is a closed curve). Since x' is in the geometrical interior of this hypersurface, for any $v \in \mathbb{R}^{d-1}$, there exists y' satisfying (5.15). For $d = 2$, the projection of $\partial B(x', \alpha) \cap \mathcal{C}$ on the hyperplane $\{x_1 = 0\}$ equals two points (one on either side of x'); since $v = \pm 1$ in this case, there exists y' satisfying (5.15).

For such a $y' \in \mathcal{C}$ satisfying (5.15), by (5.14),

$$|\mathfrak{R}_a(x') - \mathfrak{R}_a(y')| \geq (2C_1 \beta C_0 Q_{\mathcal{C}} - C_2 \alpha) \alpha;$$

taking $\alpha_0 := C_0 C_1 \beta Q_{\mathcal{C}} / C_2$ gives the result with $C_{\mathfrak{R}} := C_1 \beta C_0 Q_{\mathcal{C}}$.   □

5.5 *Statement of the lemmas constructing the rays*

CONDITION 5.9 Given $\{\psi_j\}_{j=1}^m \in (0, \pi/2]$, there exist $c_{\mathrm{ray},j}, j = 1, \ldots, 5$, such that, given $a \in \mathbb{R}^d$ with $|a| = 1$, there exists $V_D \subset \Gamma_D$ such that

   (i) $\mathrm{vol}(V_D) \geq c_{\mathrm{ray},1}$,

   (ii) $|n(x') \cdot a| \geq c_{\mathrm{ray},2}$ for all $x' \in V_D$,

   (iii) the emanating rays from V_D hit $\Gamma_{\mathrm{tr},R}$ directly and, for each ray, the angle θ the ray makes with the normal satisfies

$$\theta \geq c_{\mathrm{ray},3} \quad \text{and} \quad \min_{j=1,\ldots,m} |\theta - \psi_j| \geq c_{\mathrm{ray},4}, \tag{5.16}$$

   (iv) after hitting $\Gamma_{\mathrm{tr},R}$, the rays travel a distance $\geq c_{\mathrm{ray},5}$ before hitting either $\Gamma_{\mathrm{tr},R}$ or Γ_D again.

The $\{\psi_j\}_{j=1}^m$ in Condition 5.9 are arbitrary angles, but in the proofs below we choose them to be the angles at which the reflection coefficient on $\Gamma_{\mathrm{tr},R}$ (i.e. (2.48)) vanishes, i.e., the angles corresponding to the zeros of $q(t)\sqrt{1-t} - p(t)$ in $(0, 1]$. We set

$$\psi_j := \sin^{-1} \sqrt{t_j} \in (0, \pi/2], \qquad j = 1, \ldots, m_{\mathrm{vanish}}, \tag{5.17}$$

where $\{t_j\}_{j=1}^{m_{\mathrm{vanish}}}$ are defined at the end of § 1.3. Then, when $|\xi'|_g = \sin \psi_j$ for some $j = 1, \ldots, m_{\mathrm{vanish}}$, $\sigma(\mathcal{N})\sqrt{r} - \sigma(\mathcal{D}) = q(t_j)\sqrt{1-t_j} - p(t_j) = 0$.

We now state four lemmas constructing the rays used to prove the different lower bounds on $\mu(\mathcal{I})$ required by Corollary 5.4.

LEMMA 5.10 (The rays for general strictly-convex $\Gamma_{\mathrm{tr},R}$). If $\Gamma_{\mathrm{tr},R}$ is strictly convex, then Condition 5.9 holds with $c_{\mathrm{ray},j} = c_{\mathrm{ray},j}(\Gamma_D, \Gamma_{\mathrm{tr},R})$ for $j = 1, 3, 4, 5$, and $c_{\mathrm{ray},2} = c_{\mathrm{ray},2}(\Gamma_D)$. Furthermore $c_{\mathrm{ray},j}, j = 1, 3, 4, 5$, are continuous in R.

LEMMA 5.11 (The rays for $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$). If $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$ then there exists $R_0 > 0$ such that Condition 5.9 holds for all $R \geq R_0$ with $c_{\mathrm{ray},1}, c_{\mathrm{ray},2}, c_{\mathrm{ray},4}$ independent of R, $c_{\mathrm{ray},3} = \widetilde{c}_3/R$ and $c_{\mathrm{ray},5} = \widetilde{c}_5 R$ with $\widetilde{c}_3, \widetilde{c}_5 > 0$ independent of R. Furthermore,

(iv)$'$ after their first reflection from $\Gamma_{\mathrm{tr},R}$, all of the rays hit $B(0,1)$.

LEMMA 5.12 (The rays for generic $\Gamma_{\mathrm{tr},R}$). If $\Gamma_{\mathrm{tr},R}$ satisfies the assumptions of Theorem 1.8, then Condition 5.9 holds for R sufficiently large with $c_{\mathrm{ray},j}, j = 1, \ldots, 4$, independent of R and $c_{\mathrm{ray},5} = \widetilde{c}_5 R$ with $\widetilde{c}_5 > 0$ independent of R.

LEMMA 5.13 (The rays for when $\Gamma_{\mathrm{tr},R}$ is a smoothed hypercube). Let $\Gamma_{\mathrm{tr},R}$ coincide with the boundary of the hypercube $[-R/2, R/2]^d$ at distance more than ϵ from the corners (as described in the statement of Theorem 1.11).

There exists $\epsilon_0 > 0$ and $M \in \mathbb{Z}^+$ (both dependent on Γ_D, but not on R) such that, if $0 < \epsilon \leq \epsilon_0$ and $R \geq 4$, then Condition 5.9 holds with $c_{\mathrm{ray},2}, c_{\mathrm{ray},3}$, and $c_{\mathrm{ray},4}$ independent of R, $c_{\mathrm{ray},1} = \widetilde{c}_{\mathrm{ray},1}/R^{d-1}$ and $c_{\mathrm{ray},5} = \widetilde{c}_5 R$ with $\widetilde{c}_1, \widetilde{c}_5 > 0$ independent of R, and

(iv)$'$ the emanating rays from V_D hit $\Gamma_{\mathrm{tr},R}$ $N(R) \leq M$ times, each time with an angle θ to the normal satisfying (5.16) without hitting Γ_D in between, and then, after their $N(R)$th reflection, the rays intersect $B(0, 3/2) \setminus B(0, 5/4)$ before hitting either Γ_D or $\Gamma_{\mathrm{tr},R}$ again.

5.6 The ideas used in the proofs of the lemmas constructing the rays

In this subsection, we outline the ideas used in the proofs of Lemmas 5.10–5.12, in the simplest possible case when $\mathsf{M} = \mathsf{N} = 0$ (i.e., the boundary condition on $\Gamma_{\mathrm{tr},R}$ is the impedance boundary condition (1.10)). In this case $m_{\mathrm{vanish}} = 0$ and there are no nonzero angles ψ_j; when such angles exist, mass needs to be excluded in a careful way from the neighbourhoods described below so that the rays avoid these angles. The proof of Lemma 5.13 has a different character to the proofs of Lemmas 5.10–5.12, and so we postpone discussion of the ideas of that proof until the start of the proof itself.

The idea behind the ray construction for general strictly-convex $\Gamma_{\mathrm{tr},R}$ in Lemma 5.10 is as follows. We consider a point x_0' in Γ_D that is the extremum point on Γ_D in the direction of a. The rays emanating from a neighbourhood of this point are rays in the direction a, and thus hit $\Gamma_{\mathrm{tr},R}$ directly. Since $\Gamma_{\mathrm{tr},R}$ is strictly-convex, these rays cannot be normal to $\Gamma_{\mathrm{tr},R}$ at more than one point, see Fig. 7, and thus the required neighbourhood exists.

For the proof of Lemma 5.11, we need in addition to quantify how far from the normal the ray described in the last paragraph hits $\Gamma_{\mathrm{tr},R}$. When $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$, we show that a set of points of volume $c > 0$ can reach $\Gamma_{\mathrm{tr},R}$ with an angle $|\theta| \gtrsim R^{-1}$; see Fig. 8.

For the proof of Lemma 5.12, i.e. when $\Gamma_{\mathrm{tr}}^\infty := \lim_{R \to \infty}(\Gamma_{\mathrm{tr},R}/R)$ is *not* a sphere centred at zero, we recall from Lemma 5.7 that, given any direction, there exists a direct ray emanating from Γ_D in that direction. We need to show that at least one of these rays hits $\Gamma_{\mathrm{tr}}^\infty$ non-normally. Since $\Gamma_{\mathrm{tr}}^\infty$ is not a sphere centred at the origin, there exists $x_0^\infty \in \Gamma_{\mathrm{tr}}^\infty$ with $n_{\Gamma_{\mathrm{tr}}^\infty}(x_0^\infty) \neq x_0^\infty/|x_0^\infty|$. We use Lemma 5.7 to identify a point $x_0' \in \Gamma_D$ such that the ray emanating from x_0' is in the direction $x_0^\infty/|x_0^\infty|$ and does not hit Γ_D again. In the limit $R \to \infty$, the rescaled obstacle Ω_-/R shrinks to the origin; therefore the rays emanating from a neighbourhood of x_0' hit $\Gamma_{\mathrm{tr},R}$ with an angle close to the angle between $x_0^\infty/|x_0^\infty|$ and $n_{\Gamma_{\mathrm{tr}}^\infty}(x_0^\infty)$; this angle is $\geq c > 0$, with c independent of R; see Fig. 9.
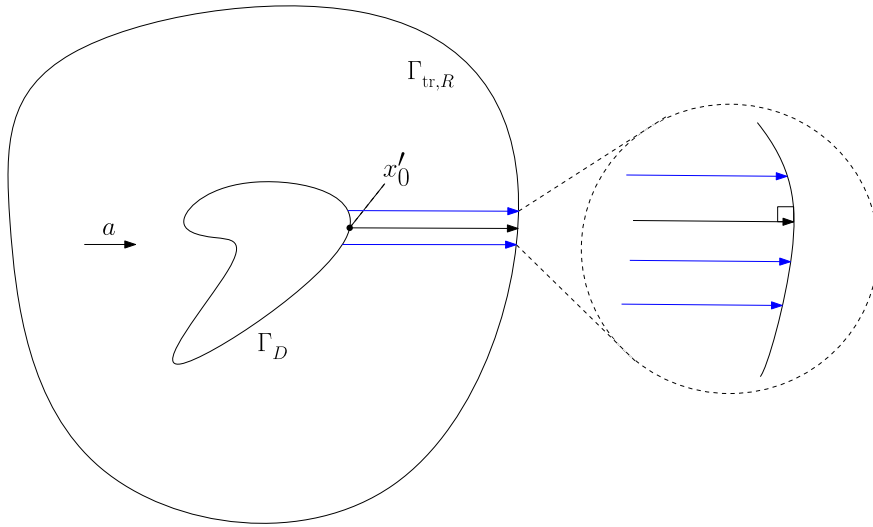
FIG. 7. The rays in Lemma 5.10 (i.e., for general strictly convex $\Gamma_{\mathrm{tr},R}$). Neighbourhoods on Γ_D from which any of the blue rays emanate satisfy Condition 5.9.
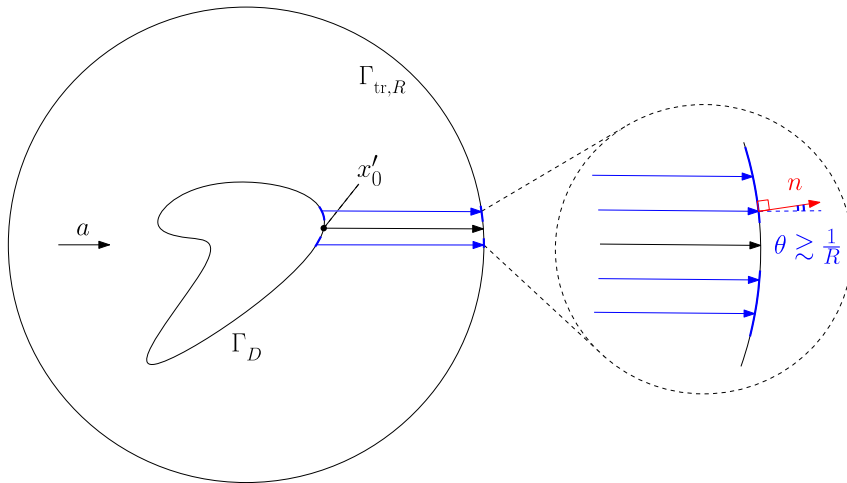

FIG. 8. The rays in Lemma 5.11 (i.e., for $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$). Neighbourhoods on Γ_D from which any of the blue rays emanate satisfy Condition 5.9.

5.7 *Proofs of Lemmas* 5.10–5.13

In the proofs of these lemmas we use the notation that $\widehat{(b_1, b_2)}$ is the angle between vectors b_1 and b_2; i.e.,

$$\widehat{(b_1, b_2)} := \cos^{-1}\left(\frac{b_1 \cdot b_2}{|b_1||b_2|}\right),$$
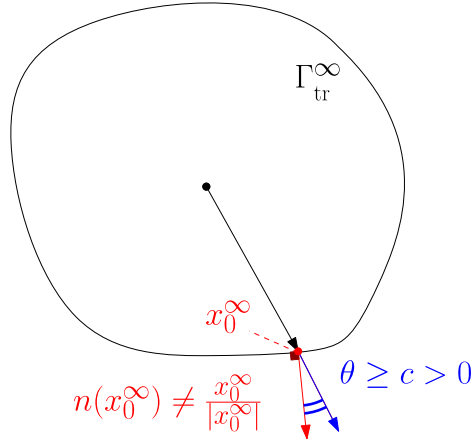
FIG. 9. The rays in Lemma 5.12, i.e., when $\Gamma_{\mathrm{tr}}^\infty$ is not a ball centred at the origin. The figure shows the rescaled domain in the limit $R \to \infty$ (recall that in this limit the obstacle shrinks to the origin).

where the range of $\cos^{-1}$ is $[0, \pi]$.

Proof of Lemma 5.10. Step 1. Construction of direct emanating rays in the direction of a.
Without loss of generality, we assume that $a = (1, 0, \ldots, 0)$. Let $x_0' \in \Gamma_D$ be the point on Γ_D with maximal x_1 coordinate. By translating the obstacle Ω_-, we can assume that $x_0' = 0$. Then, locally near 0, for any $0 < \epsilon \le \epsilon_0(\Gamma_D)$, where ϵ_0 is small enough

$$\Gamma_D \cap B(0, \epsilon) \subset \{(\gamma_D(x'), x') : x' \in B(0, \epsilon) \subset \mathbb{R}^{d-1}\}, \tag{5.18}$$

where $\gamma_D \in C^\infty(\mathbb{R}^{d-1})$ and $\partial \gamma_D(0) = 0$, and $\gamma_D(x') \le 0$. Moreover, for $\epsilon_0 > 0$ small enough and $0 < \epsilon \le \epsilon_0$

$$\Gamma_D \cap \{(x_1, x') : x_1 > \gamma_D(x') \text{ and } x' \in B(0, \epsilon)\} = \emptyset. \tag{5.19}$$

Indeed, if not then there exist $x_n' \to 0$, $(y_n, x_n') \in \Gamma_D$ such that $y_n > \gamma_D(x_n')$. But then, extracting subsequences if necessary, $(y_n, x_n') \to (y, 0) \in \Gamma_D$ and $y \ge \gamma_D(0)$. In particular, by maximality of the x_1 coordinate at x_0', $y = 0$. But, near x_0' (5.18) holds and, in particular, for n large enough, $y_n = \gamma_D(x_n')$, which is a contradiction.

Observe that, shrinking $\epsilon_0 > 0$ if necessary, a is outward-pointing along $\Gamma_D \cap B(0, \epsilon_0)$, and

$$|n(x') \cdot a| \ge c_{\mathrm{ray},2}(\epsilon_0), \text{ for all } x' \in B(0, \epsilon_0), \tag{5.20}$$

where $c_{\mathrm{ray},2}(\epsilon_0) > 0$ depends only on ϵ_0 and hence Γ_D. By (5.9), $\mathfrak{R}_a(x') = a$ for all $x' \in \Gamma_D \cap B(0, \epsilon_0)$, and thus the rays emanating from $\Gamma_D \cap B(0, \epsilon_0)$ are the rays in the x_1 direction; see Fig. 7. By (5.19), these rays hit $\Gamma_{\mathrm{tr},R}$ before hitting Γ_D again. The neighbourhood V_D will be a subset of $B(0, \epsilon_0)$, and thus Point (ii) in Condition 5.9 follows.

Step 2. Parametrization of $\Gamma_{tr,R}$.
Let $\gamma_{tr} : B(0, \epsilon_0) \subset \mathbb{R}^{d-1} \to \mathbb{R}_+$ be such that

$$\Gamma_{tr,R} \cap \{x_1 > 0, |x'| < \epsilon_0\} := \{(\gamma_{tr}(x'), x') \ : \ |x'| < \epsilon_0\};$$

since $\Gamma_{tr,R}$ is strictly convex, this property holds without needing to reduce ϵ_0, and thus ϵ_0 still only depends on Γ_D. The outward-pointing normal to $\Gamma_{tr,R}$ is given by

$$n_{tr}(x') := \frac{(1, -\nabla\gamma_{tr}(x'))}{\sqrt{1 + |\nabla\gamma_{tr}(x')|^2}}.$$

For $x' \in B(0, \epsilon_0) \subset \mathbb{R}^{d-1}$, let $\theta(x') \in [0, \pi/2)$ be the angle between the ray emanating from $(\gamma_D(x'), x')$ and the normal to $\Gamma_{tr,R}$; since $\cos\theta(x') = (1, 0, \ldots 0) \cdot n_{tr}(x')$,

$$\theta(x') = \cos^{-1}\left(\frac{1}{\sqrt{1 + |\nabla\gamma_{tr}(x')|^2}}\right) \in [0, \pi/2). \tag{5.21}$$

We use later the facts, obtained from from (5.21) by direct calculation, that,

$$\tan\theta(x') = |\nabla\gamma_{tr}(x')|, \tag{5.22}$$

and, in $\{\nabla\gamma_{tr}(x') \neq 0\}$,

$$\nabla\theta(x') = \frac{1}{1 + |\nabla\gamma_{tr}(x')|^2}\partial^2\gamma_{tr}(x')\frac{\nabla\gamma_{tr}(x')}{|\nabla\gamma_{tr}(x')|}. \tag{5.23}$$

We also use the following quantities,

$$Q := \inf_{x',|v|=1}\left|\partial^2\gamma_{tr}(x')v\right| \qquad \text{and} \qquad C_k := \sup_{x'}\max_{|\mathbf{k}|=k}\left|\partial^{\mathbf{k}}\gamma_{tr}(x')\right|, \ k = 1, 2, 3. \tag{5.24}$$

Step 3. Avoiding the angle $\psi_i = 0$.
Recall that our goal is to construct $V_D \subset \Gamma_D \cap B(0, \epsilon)$ so that

$$\min_{i=1,\ldots,m} |\theta(x') - \psi_i| \geq C > 0 \quad \text{for all } x' \in V_D,$$

where $\text{vol}(V_D)$ and C depend only on $\Gamma_{tr,R}$. Our plan is to exclude mass from $B(0, \epsilon)$ for each i, taking care that the volume is still bounded below to give Point (i) of Condition 5.9.

Avoiding the angle zero corresponds to obtaining a lower bound on $|\theta(x')|$. By Taylor's theorem,

$$|\nabla\gamma_{tr}(x')| \geq \left|\nabla\gamma_{tr}(0) + \partial^2\gamma_{tr}(0)x'\right| - \widetilde{C}_d C_3 |x'|^2,$$

where C_3 is defined by (5.24), and $\widetilde{C}_d$ depends only on d. By the definition of Q in (5.24),

$$\left|\nabla\gamma_{\mathrm{tr}}(0) + \partial^2\gamma_{\mathrm{tr}}(0)x'\right| = \left|\partial^2\gamma_{\mathrm{tr}}(0)\Big(\big(\partial^2\gamma_{\mathrm{tr}}(0)\big)^{-1}\nabla\gamma_{\mathrm{tr}}(0) + x'\Big)\right| \geq Q\left|\big(\partial^2\gamma_{\mathrm{tr}}(0)\big)^{-1}\nabla\gamma_{\mathrm{tr}}(0) + x'\right|.$$

Suppose that $|(\partial^2\gamma_{\mathrm{tr}}(0))^{-1}\nabla\gamma_{\mathrm{tr}}(0)| \leq \epsilon/3$. Then

$$|\nabla\gamma_{\mathrm{tr}}(x')| \geq \frac{Q\epsilon}{6} - \widetilde{C}_d C_3\epsilon^2 \quad \text{for } x' \in B(0,\epsilon) \setminus B(0,\epsilon/2).$$

On the other hand, if $\left|\big(\partial^2\gamma_{\mathrm{tr}}(0)\big)^{-1}\nabla\gamma_{\mathrm{tr}}(0)\right| \geq \epsilon/3$, then

$$|\nabla\gamma_{\mathrm{tr}}(x')| \geq \frac{Q\epsilon}{6} - \frac{\widetilde{C}_d C_3\epsilon^2}{36} \quad \text{for } x' \in B(0,\epsilon/6).$$

Therefore, in both cases, if $\epsilon \leq Q/(12\widetilde{C}_d C_3)$, then there exists a set W with

$$\mathrm{vol}(W) \leq \max(2^{-d}, 1 - 6^{-d})\,\mathrm{vol}(B(0,\epsilon)) = (1 - 6^{-d})\,\mathrm{vol}(B(0,\epsilon)), \tag{5.25}$$

such that

$$|\nabla\gamma_{\mathrm{tr}}(x')| \geq \frac{Q\epsilon}{12} \quad \text{for all } x' \in B(0,\epsilon) \setminus W.$$

Therefore, for $x' \in B(0,\epsilon) \setminus W$, by (5.21)

$$1 - \frac{\theta(x')^2}{2} \leq \cos\theta(x') \leq 1 - \frac{|\nabla\gamma_{\mathrm{tr}}(x')|^2}{2} \leq 1 - \frac{Q^2\epsilon^2}{288},$$

and we conclude that

$$\text{if } 0 < \epsilon \leq \min\left(\frac{Q}{12\widetilde{C}_d C_3}, \epsilon_0\right), \quad \text{then } \theta(x') \geq \frac{Q\epsilon}{12} \quad \text{for all } x' \in B(0,\epsilon) \setminus W. \tag{5.26}$$

Step 4. Avoiding the angles ψ_i.
Given ψ_i, let $x_i' \in \overline{B(0,\epsilon)} \subset \mathbb{R}^{d-1}$ be such that

$$|\theta(x_i') - \psi_i| = \min_{x' \in \overline{B(0,\epsilon)}} |\theta(x') - \psi_i|, \tag{5.27}$$

i.e., x_i' is the point in $\overline{B(0,\epsilon)}$ where $\theta(x')$ is closest to ψ_i. Let

$$\psi_{\min} := \min_{j=1,\dots,m} \psi_j > 0. \tag{5.28}$$

In the following we use the notation $[a, b]$ for the line segment between a and b, i.e.,

$$[a, b] := \{ta + (1 - t)b, \ t \in [0, 1]\},$$

and $\langle \cdot, \cdot \rangle$ denotes the Euclidean inner product on $\mathbb{R}^d$.

The main idea of the rest of this step is the following: $|\theta(x') - \psi_i|$ is, by definition, smallest at x_i', and will be smallest when the minimum in (5.28) is attained, i.e., $\theta(x_i') = \psi_i$; in this case, the idea is for the size of the neighbourhood of x_i' that we exclude to be dictated by using Taylor's theorem

$$
\begin{aligned}
|\theta(x') - \theta(x_i')| &\geq |\nabla \theta(x_i') \cdot (x' - x_i')| - \sup_{y' \in [x', x_i']} \max_{|\mathbf{k}| = 2} |\partial^{\mathbf{k}} \theta(y')| |x' - x_i'|^2 \\
&= \frac{1}{1 + |\nabla \gamma_{\mathrm{tr}}(x_i')|^2} \left| \left\langle \partial^2 \gamma_{\mathrm{tr}}(x_i') \frac{\nabla \gamma_{\mathrm{tr}}(x_i')}{|\nabla \gamma_{\mathrm{tr}}(x_i')|}, x' - x_i' \right\rangle \right| - \sup_{y' \in [x', x_i']} \max_{|\mathbf{k}| = 2} |\partial^{\mathbf{k}} \theta(y')| |x' - x_i'|^2,
\end{aligned}
\tag{5.29}
$$

where the requirement that the right-hand side is bounded below determines the size of the excluded neighbourhood. The issues we then have to deal with are (a) $\theta(x_i')$ is not necessarily equal to ψ_i, and (b) $|\gamma_{\mathrm{tr}}'(x')| = \tan \theta(x')$ is zero when $\theta(x') = 0$, and then the second-order term in (5.29) blows up.

To deal with Point (b), we first consider points in $B(0, \epsilon)$ where the second-order term in (5.29) does not blow up. Let

$$Z_i := \left\{ x' \in B(0, \epsilon) \ : \ \theta(y') \geq \theta_0 \text{ for all } y' \in [x', x_i'] \right\}, \tag{5.30}$$

where θ_0 will be chosen later in the proof (when dealing with the points not in Z_i). By (5.22), for any $x' \in B(0, \epsilon) \cap Z_i$, $|\nabla \gamma_{\mathrm{tr}}(y')| \geq \tan(\theta_0) > 0$ for $y' \in [x', x_i']$. Recalling the definitions (5.24), and using (5.29) and (5.23), we have

$$\left| \theta(x') - \theta\left(x_i'\right) \right| \geq D_1 Q \left| \left\langle v_i, \frac{x' - x_i'}{|x' - x_i'|} \right\rangle \right| |x' - x_i'| - D_3 |x' - x_i'|^2, \tag{5.31}$$

where

$$D_1 := \left(1 + C_1^2\right)^{-1}, \qquad D_3 := C_3 + C_1 C_2^2 + \frac{C_2^2}{|\tan(\theta_0)|}, \tag{5.32}$$

and the unit vector v_i is defined by

$$v_i := \left(\partial^2 \gamma_{\mathrm{tr}}\left(x_i'\right) \frac{\nabla \gamma_{\mathrm{tr}}\left(x_i'\right)}{|\nabla \gamma_{\mathrm{tr}}\left(x_i'\right)|} \right) \left| \partial^2 \gamma_{\mathrm{tr}}\left(x_i'\right) \frac{\nabla \gamma_{\mathrm{tr}}\left(x_i'\right)}{|\nabla \gamma_{\mathrm{tr}}\left(x_i'\right)|} \right|^{-1}. \tag{5.33}$$

Let

$$W_i(\eta, \delta) := B\left(x_i', \eta \epsilon\right) \cup \left\{ \left| \left\langle \frac{x' - x_i'}{|x' - x_i'|}, v_i \right\rangle \right| \leq \delta \right\},$$

where $\eta < 1$; then (5.31) implies that

$$\left|\theta(x') - \theta\left(x_i'\right)\right| \geq \left(D_1 Q \delta \eta - 4D_3 \epsilon\right)\epsilon \quad \text{for all } x' \in \left(B(0,\epsilon) \cap Z_i\right) \setminus W_i.$$

We now deal with Point (a) above (i.e., that $\theta(x_i')$ is not necessarily equal to ψ_i). If $|\theta(x_i') - \psi_i| > \alpha$, for α to be fixed later, then, by (5.27),

$$|\theta(x') - \psi_i| \geq \left|\theta\left(x_i'\right) - \psi_i\right| > \alpha \quad \text{for all } x' \in B(0,\epsilon). \tag{5.34}$$

If $|\theta(x_i') - \psi_i| \leq \alpha$, then

$$|\theta(x') - \psi_i| \geq \left|\theta(x') - \theta\left(x_i'\right)\right| - \alpha$$

and then

$$|\theta(x') - \psi_i| \geq \left(D_1 Q \delta \eta - 4D_3 \epsilon\right)\epsilon - \alpha \text{ for all } x' \in \left(B(0,\epsilon) \cap Z_i\right) \setminus W_i. \tag{5.35}$$

Combining (5.34) and (5.35), we have

$$\min_{i=1,\ldots,m} |\theta(x') - \psi_i| \geq \min\left(\left(D_1 Q \delta \eta - 4D_3 \epsilon\right)\epsilon - \alpha, \alpha\right) \text{ for all } x' \in \left(B(0,\epsilon) \cap Z_i\right) \setminus \bigcup_{i=1}^{m} W_i(\eta,\delta); \tag{5.36}$$

recall that we still have the freedom to choose θ_0, η, δ, and α.

We now deal with the case $x' \in B(0,\epsilon) \setminus Z_i$; the idea here is the following: Z_i consists of points x' such that every point on $[x', x_i']$ has $\theta \geq \theta_0$, i.e., θ bounded below. If $\theta(x') < \theta_0$, and we chose θ_0 appropriately, then $|\theta(x')|$ can be small compared to $|\psi_i|$, and thus $|\theta(x') - \psi_i|$ can be bounded below. Indeed, let $\theta_0 := \psi_{\min}/2$; if $\theta(x') < \psi_{\min}/2$, then

$$|\theta(x') - \psi_i| \geq |\psi_i| - |\theta(x')| \geq \frac{1}{2}\psi_{\min}. \tag{5.37}$$

We now need to consider $x' \in B(0,\epsilon) \setminus Z_i$ with $\theta(x') \geq \psi_{\min}/2$. The sequence of ideas here is that (i) by the definition of Z_i, there is a point, x_t', in $[x', x_i']$ with $\theta(x_t') < \psi_{\min}/2$, (ii) the argument in (5.37) applies at x_t', (iii) $|x' - x_t'| \leq \epsilon$, which is small, (iv) x_t' can be chosen so that $|\nabla \gamma_{\mathrm{tr}}| \neq 0$ on $[x', x_t']$ and then $|\theta(x') - \theta(x_t')|$ can also be made small. The detail is as follows: let

$$t_i(x') := \inf\left\{t \in [0,1] : \left|\nabla\gamma_{\mathrm{tr}}\left((1-t)x' + tx_i'\right)\right| < \left|\tan(\psi_{\min}/2)\right|\right\};$$

the set on the right-hand side is not empty by (5.22) and the definition of Z_i (5.30). Let $x_t' := (1 - t_i(x'))x' + t_i(x')x_i'$. This definition implies that $\nabla\gamma_{\mathrm{tr}}(y') \neq 0$ for $y' \in [x', x_t']$. Therefore, using the mean-value theorem and (5.23), we have

$$\left|\theta(x') - \theta\left(x_t'\right)\right| \leq \sup_{y' \in [x', x_t']} |\nabla\theta(y')| \left|x' - x_t'\right| \leq 2C_2 \epsilon.$$

Using this together with (5.37), we obtain

$$|\theta(x') - \psi_i| \geq |\theta\left(x'_t\right) - \psi_i| - |\theta(x') - \theta\left(x'_t\right)| \geq \frac{1}{2}\psi_{\min} - 2C_2\epsilon. \tag{5.38}$$

Collecting both cases (5.37) and (5.38), we obtain that

$$\text{if } 0 < \epsilon \leq \min\left(\frac{\psi_{\min}}{4C_2}, \epsilon_0\right), \quad \text{then } |\theta(x') - \psi_i| \geq \frac{1}{4}\psi_{\min} \quad \text{for all } x' \in B(0, \epsilon) \setminus Z_i. \tag{5.39}$$

Putting (5.36) and (5.39) together, we find that if

$$\widetilde{V}_D := B(0, \epsilon) \setminus \bigcup_{i=1}^{m} W_i(\eta, \delta), \tag{5.40}$$

and

$$0 < \epsilon \leq \min\left(\frac{\psi_{\min}}{4C_2}, \epsilon_0\right),$$

then

$$\min_{i=1,\dots,m} |\theta(x') - \psi_i| \geq \min\left((D_1 Q \delta \eta - 4D_3\epsilon)\epsilon - \alpha, \alpha, \frac{1}{4}\psi_{\min}\right) \text{ for all } x' \in \widetilde{V}_D. \tag{5.41}$$

We now tune $\eta > 0$ and $\delta > 0$ to make the volume of $\widetilde{V}_D$ big enough, and conclude the step by selecting suitable $\epsilon > 0$ and $\alpha > 0$. From the definition (5.40),

$$\text{vol}\left(\widetilde{V}_D\right) \geq \text{vol}\left(B(0, \epsilon)\right) - \sum_{i=1}^{m}\left(\text{vol}\left(B(x'_i, \eta\epsilon)\right) + \text{vol}\left(\mathcal{C}_i \cap B(0, \epsilon)\right)\right),$$

$$\geq \text{vol}\left(B(0, \epsilon)\right) - \sum_{i=1}^{m}\left(\text{vol}\left(B(x'_i, \eta\epsilon)\right) + \text{vol}\left(\mathcal{C}_i \cap B(x'_i, 2\epsilon)\right)\right), \tag{5.42}$$

where

$$\mathcal{C}_i := \left\{x' : \left|\left\langle \frac{x' - x'_i}{|x' - x'_i|}, v_i \right\rangle\right| \leq \delta\right\} = \left\{x' : \cos^{-1}\delta \leq \widehat{\left(\frac{x' - x'_i}{|x' - x'_i|}, v_i\right)} \leq \pi - \cos^{-1}\delta\right\}.$$

Observe that $\mathcal{C}_i$ is the complement of a double cone, rotationally symmetric around the axis v_i (recall that v_i defined by (5.33) depends on x'_i and not x'); therefore, $\text{vol}(\mathcal{C}_i)$ decreases as $\delta \to 0$. By integrating in

hyperspherical coordinates centered at x_i with axis v_i, and comparing $\mathrm{vol}(\mathcal{C}_i \cap B(x_i', 2\epsilon))$ to $\mathrm{vol}(B(x_i', 2\epsilon))$, we have

$$\mathrm{vol}\left(\mathcal{C}_i \cap B(x_i', 2\epsilon)\right) \leq \left(\frac{\pi - 2\cos^{-1}\delta}{2\pi}\right) \mathrm{vol}\left(B(x_i', 2\epsilon)\right) = \frac{2^d}{\pi}\left(\frac{\pi}{2} - \cos^{-1}\delta\right)\mathrm{vol}\left(B(0,\epsilon)\right).$$

Using this in (5.42), we have

$$\mathrm{vol}\left(\widetilde{V}_D\right) \geq \mathrm{vol}\left(B(0,\epsilon)\right) - \sum_{i=1}^{m}\left(\mathrm{vol}\left(B(x_i', \eta\epsilon)\right) + \frac{2^d}{\pi}\left(\frac{\pi}{2} - \cos^{-1}\delta\right)\mathrm{vol}\left(B(0,\epsilon)\right)\right)$$

$$\geq \left(1 - m\eta^d - m\frac{2^d}{\pi}\left(\frac{\pi}{2} - \cos^{-1}\delta\right)\right)\mathrm{vol}\left(B(0,\epsilon)\right). \tag{5.43}$$

We now fix both $\delta > 0$ and $\eta > 0$ to be sufficiently small such that

$$0 < \frac{\pi}{2} - \cos^{-1}\delta \leq \frac{\pi}{2^d m}\frac{10^{-d}}{2}, \qquad 0 < \eta^d \leq \frac{1}{m}\frac{10^{-d}}{2};$$

then (5.43) implies that

$$\mathrm{vol}\left(\widetilde{V}_D\right) \geq (1 - 10^{-d})\,\mathrm{vol}\left(B(0,\epsilon)\right) > 0. \tag{5.44}$$

To conclude this step, we now restrict ϵ so that $0 < \epsilon \leq (D_1 Q\delta\eta)/(8D_3)$ and then set $\alpha := D_1 Q\delta\eta\epsilon/4$; then (5.41) implies that if

$$0 < \epsilon \leq \min\left(\frac{D_1 Q\delta\eta}{8D_3}, \frac{\psi_{\min}}{4C_2}, \epsilon_0\right) \tag{5.45}$$

then

$$\min_{i=1,\dots,m}|\theta(x') - \psi_i| \geq \frac{1}{4}\min\left(D_1 Q\delta\eta\epsilon, \psi_{\min}\right) \quad \text{for all } x' \in \widetilde{V}_D. \tag{5.46}$$

Step 5. Conclusion.
Combining the result of Step 3 (5.26) and the result of Step 4 (5.45)–(5.46), we see that if

$$0 \leq \epsilon \leq \min\left(\frac{Q}{12\widetilde{C}_d C_3}, \epsilon_0, \frac{D_1 Q\delta\eta}{8D_3}, \frac{\psi_{\min}}{4C_2}\right),$$

then

$$\theta(x') \geq \frac{Q\epsilon}{12} \quad \text{and} \quad \min_{i=1,\dots,m}|\theta(x') - \psi_i| \geq \min\left(\frac{D_1 Q\delta\eta\epsilon}{4}, \frac{\psi_{\min}}{4}\right) \quad \text{for all } x' \in \widetilde{V}_D \setminus W.$$

We then let

$$\epsilon = \epsilon_1 := \min\left(\frac{D_1 Q \delta \eta}{8 D_3}, \frac{Q}{12 \widetilde{C}_d C_3}, \frac{\psi_{\min}}{4 C_2}, \epsilon_0\right), \tag{5.47}$$

so that

$$\min_{i=1,\ldots,m} |\theta(x') - \psi_i| \geq Q^2 \times \min\left(\frac{D_1 \delta \eta}{4}, \frac{\psi_{\min}}{4 Q \epsilon_0}\right) \times \min\left(\frac{D_1 \delta \eta}{8 D_3}, \frac{1}{12 \widetilde{C}_d C_3}, \frac{\psi_{\min}}{4 Q C_2}, \frac{\epsilon_0}{Q}\right),$$

$$\text{for all } x' \in \widetilde{V}_D \setminus W,$$

where, by (5.44) and (5.25)

$$\text{vol}\left(\widetilde{V}_D \setminus W\right) \geq (6^{-d} - 10^{-d}) \,\text{vol}\left(B(0, \epsilon_1)\right).$$

Points (i) and (iii) in Condition 5.9 then hold with

$$V_D := \widetilde{V}_D \setminus W, \qquad c_{\mathrm{ray},1} := (6^{-d} - 10^{-d}) \,\text{vol}\left(B(0, \epsilon_1)\right),$$

$$c_{\mathrm{ray},3} := \frac{Q}{12} \min\left(\frac{D_1 Q \delta \eta}{8 D_3}, \frac{Q}{12 \widetilde{C}_d C_3}, \frac{\psi_{\min}}{4 C_2}, \epsilon_0\right), \tag{5.48}$$

and

$$c_{\mathrm{ray},4} := Q^2 \times \min\left(\frac{D_1 \delta \eta}{4}, \frac{\psi_{\min}}{4 Q \epsilon_0}\right) \times \min\left(\frac{D_1 \delta \eta}{8 D_3}, \frac{1}{12 \widetilde{C}_d C_3}, \frac{\psi_{\min}}{4 Q C_2}, \frac{\epsilon_0}{Q},\right). \tag{5.49}$$

Since Q, C_2, C_3, D_1 and D_3 (defined by (5.24) and (5.32)) all depend continuously on γ_{tr}, and γ_{tr} depends continuously on R, $c_{\mathrm{ray},1}, c_{\mathrm{ray},3}$, and $c_{\mathrm{ray},4}$ depend continuously on R. The constant $c_{\mathrm{ray},5}$ depends on $c_{\mathrm{ray},3}, c_{\mathrm{ray},4}$ $\Gamma_{\mathrm{tr},R}$, and Γ_D, and thus also depends continuously on R. □

Before proving Lemma 5.11, we prove the following simple lemma.

LEMMA 5.14 If $\Gamma_{\mathrm{tr},R} = \partial B(0, R)$, then the emanating rays from Γ_D hit $\Gamma_{\mathrm{tr},R}$ directly with an angle to the normal θ satisfying $\theta < R^{-1}$.

Proof. Since $\Omega_- \subset B(0, 1)$, any ray starting from Ω_- hits $\Gamma_{\mathrm{tr},R} = \partial B(0, R)$ with an angle to the normal θ satisfying $\tan \theta \leq 1/R$. Since $\theta < \tan \theta$, the result follows. □

Proof of Lemma 5.11. We first observe that Point (iv)′ follows from the same argument used to prove Lemma 5.14; this implies that $c_{\mathrm{ray},5} = \widetilde{c}_5 R$ with $\widetilde{c}_5$ independent of R.

The fact that $c_{\mathrm{ray},2}$ is independent of R follows from the proof of Lemma 5.10; see (5.20). By direct calculation from the definitions (5.24), (5.32), using the fact that $\gamma_{\mathrm{tr}}(x') = \sqrt{R^2 - |x'|^2} + c$ where c is a constant, we obtain that

$$Q \sim R^{-1}, \ C_1 \sim 1, \ C_2 \sim R^{-1}, \ C_3 \sim R^{-2}, \text{ and thus } D_1 \sim 1, \ D_3 \sim R^{-2}.$$

Using these asymptotics in (5.47), (5.48) and (5.49), we find that $c_{\text{ray},1}$ is independent of R and $c_{\text{ray},3} \sim R^{-1}$ (observe that the first minimum in (5.49) ~ 1 and the second minimum $\sim R$).

These arguments from the proof of Lemma 5.10 also show that $c_{\text{ray},4} \sim R^{-1}$, but we now show that in fact $c_{\text{ray},4} \sim 1$ for R sufficiently large. By Lemma 5.14, all the rays from V_D hit $\Gamma_{\text{tr},R}$ with angles $< 1/R$. Therefore, if $R \geq 2/\psi_{\min}$, then $|\theta - \psi_j| \geq \psi_{\min}/2$ for all j. □

REMARK 5.15 (Lemma 5.11 when $\mathsf{M} = \mathsf{N} = 0$). Recall that when $\mathsf{M} = \mathsf{N} = 0$, then $m_{\text{vanish}} = 0$, inspecting the proof of Lemma 5.11, we see that the result then holds with $c_{\text{ray},4} = 0$ and $R_0 = 1$.

Proof of Lemma 5.12. For $0 < \delta < 1$, let $\Psi = \{0, \psi_1, \ldots, \psi_m\}$ and

$$V_{\text{tr}}^{\infty}(\delta) := \left\{ x^{\infty} \in \Gamma_{\text{tr}}^{\infty}, \; : \; n(x^{\infty}) \text{ exists and } \min_{\psi \in \Psi} \left| \widehat{\left(n(x^{\infty}), \frac{x^{\infty}}{|x^{\infty}|}\right)} - \psi \right| > \delta \right\}.$$

We now claim that there exists $\delta_0 < 1$ such that $V_{\text{tr}}^{\infty}(\delta_0)$ is nonempty. Indeed, first observe that the map

$$\left\{ x \in \Gamma_{\text{tr}}^{\infty} \; : \; n(x) \text{ exists} \right\} \to \mathbb{R} \quad \text{given by} \quad x \mapsto \widehat{\left(n(x), \frac{x}{|x|}\right)} = \left\langle n(x), \frac{x}{|x|} \right\rangle$$

is continuous. The only way for this map to be constant is for $\Gamma_{\text{tr}}^{\infty}$ to be a sphere centred at the origin, and this is ruled out by assumption. Since $\Gamma_{\text{tr},R}/R \to \Gamma_{\text{tr}}^{\infty}$ in $C^{0,1}$, $\Gamma_{\text{tr}}^{\infty}$ is Lipschitz, and the set $\{ x \in \Gamma_{\text{tr}}^{\infty} : n(x) \text{ exists} \}$ has full $(d-1)$ dimensional (i.e., surface) measure. Therefore, the image of the map contains an interval, and the claim follows. We note for later that $V_{\text{tr}}^{\infty}(\delta_0)$ is open in $\Gamma_{\text{tr}}^{\infty}$.

Let $x_0^{\infty} \in V_{\text{tr}}^{\infty}(\delta_0)$. By Lemma 5.7, there exists $x_0' \in \Gamma_D^{+,a}$ such that

$$\mathfrak{R}_a(x_0') = \frac{x_0^{\infty}}{|x_0^{\infty}|};$$

see Fig. 10. For $x' \in \Gamma_D$, let $x_R' \in \Gamma_{\text{tr},R}$ denote the point where the ray emanating from x' first hits $\Gamma_{\text{tr},R}$; we use later the fact that this definition implies that

$$\frac{(x_0')_R - x_0'}{|(x_0')_R - x_0'|} = \frac{x_0^{\infty}}{|x_0^{\infty}|}. \tag{5.50}$$

The neighbourhood V_D in Condition 5.9 will be $\Gamma_D \cap B(0, \epsilon)$ for ϵ sufficiently small, independent of R, and this ensures that Point (i) holds with $c_{\text{ray},1}$ independent of R. Let $\epsilon > 0$ be small enough so that $\Gamma_D \cap B(x_0', \epsilon) \subset \Gamma_D^{+,a}$; this ensures that Point (ii) holds with $c_{\text{ray},2}$ independent of R.

We now show that Point (iii) of Condition 5.9 holds with $c_{\text{ray},3}$ and $c_{\text{ray},4}$ independent of R. Let $W_{\text{tr},\epsilon}^{\infty} \subset \Gamma_{\text{tr}}^{\infty}$ be defined by

$$W_{\text{tr},\epsilon}^{\infty} := \lim_{R \to \infty} \left\{ \frac{(x')_R}{R} \; : \; x' \in \Gamma_D \cap B(x_0', \epsilon) \right\}; \tag{5.51}$$

this limit exists $W_{\text{tr},\epsilon}^{\infty}$ is the limit of subsets of $\Gamma_{\text{tr},R}/R$ and $\Gamma_{\text{tr},R}/R \to \Gamma_{\text{tr}}^{\infty}$ as $R \to \infty$. We claim that it is sufficient to prove that $W_{\text{tr},\epsilon}^{\infty} \subset V_{\text{tr}}^{\infty}(\delta_0)$ for ϵ sufficiently small (independent of R). This shows the analogue of Point (iii) in Condition 5.9 with $\Gamma_{\text{tr},R}$ replaced by $\Gamma_{\text{tr}}^{\infty}$; i.e., that the emanating rays
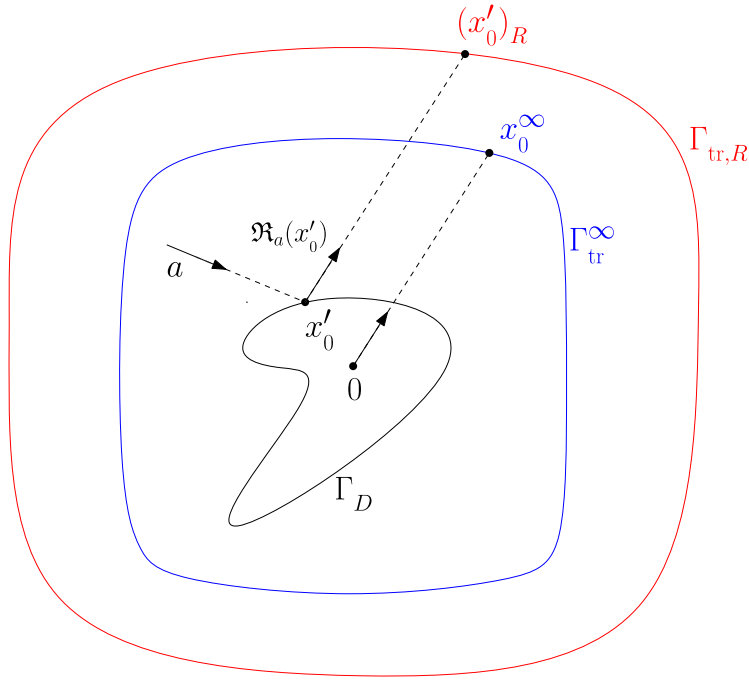
FIG. 10. The points and rays used in the proof of Lemma 5.12.

from points in V_D hit Γ_{tr}^∞ directly with an angle θ to the normal satisfying (5.16) with $c_{ray,3}$ and $c_{ray,4}$ independent of R. Point (iii) for $\Gamma_{tr,R}$ with R sufficiently large then follows since $W_{tr,\epsilon}^\infty$ is the limit of subsets of $\Gamma_{tr,R}/R$, and $\Gamma_{tr,R}/R \to \Gamma_{tr}^\infty$ as $R \to \infty$.

We now claim that to prove that $W_{tr,\epsilon}^\infty \subset V_{tr}^\infty(\delta_0)$ for ϵ sufficiently small (independent of R) it is sufficient to show that $x_0^\infty \in W_{tr,\epsilon}^\infty$ for all $\epsilon > 0$. Indeed, if this is the case then $\cap_{\epsilon>0} W_{tr,\epsilon}^\infty = \{x_0^\infty\}$. Then, since (i) $V_{tr}^\infty(\delta_0)$ is open in Γ_{tr}^∞ and contains x_0^∞, and (ii) $W_{tr,\epsilon_1}^\infty \subseteq W_{tr,\epsilon_2}^\infty$ for $\epsilon_1 \leq \epsilon_2$, there exists $\epsilon_0 > 0$ such that $W_{tr,\epsilon}^\infty \subset V_{tr}^\infty(\delta_0)$ for all $\epsilon \leq \epsilon_0$.

We now show that $x_0^\infty \in W_{tr,\epsilon}^\infty$ for all $\epsilon > 0$. We do this by showing that $(x_0')_{R_k}/R_k \to x_0^\infty$ for a sequence $R_k \to \infty$, and then the result follows from (5.51). Observe that the inclusions (1.18) imply that $|x_R'| \leq MR$, for any $x' \in \Gamma_D$, and thus $(x_0')_R/R$ is bounded as $R \to \infty$. Therefore, there exists a sequence $R_k \to \infty$ and $y \in \Gamma_{tr}^\infty$ such that $(x_0')_{R_k}/R_k \to y$, and thus also

$$\frac{(x_0')_{R_k}}{|(x_0')_{R_k}|} \to \frac{y}{|y|} \quad \text{as } R_k \to \infty. \tag{5.52}$$

By simple geometry, as $R \to \infty$,

$$\frac{(x_0')_R}{|(x_0')_R|} = \frac{(x_0')_R - x_0'}{|(x_0')_R - x_0'|} + O(R^{-1}) = \frac{x_0^\infty}{|x_0^\infty|} + O(R^{-1}),$$

by (5.50). Comparing this to (5.52), and using the uniqueness of the limit, we see that $y/|y| = x_0^\infty/|x_0^\infty|$. Since $\Gamma_{\mathrm{tr}}^\infty$ is convex, and thus star-shaped, $y = x_0^\infty$, and the proof that $x_0^\infty \in W_{\mathrm{tr},\epsilon}^\infty$ for all $\epsilon > 0$ is complete; this completes the proof that Point (iii) of Condition 5.9 holds with $c_{\mathrm{ray},3}$ and $c_{\mathrm{ray},4}$ independent of R.

Finally, we show that Point (iv) of Condition 5.9 holds for R sufficiently large with $c_{\mathrm{ray},5} = \widetilde{c}_5 R$ with $\widetilde{c}_5 > 0$ independent of R. Since $\Omega_- \subset B(0,1)$ and Ω_R satisfies the inclusions (1.18), after hitting $\Gamma_{\mathrm{tr},R}$, a ray must travel a distance $\sim R$ before hitting Γ_D. Therefore, we only need to show that, after hitting $\Gamma_{\mathrm{tr},R}$, a ray must travel a distance $\sim R$ before hitting $\Gamma_{\mathrm{tr},R}$ again. Since $\Gamma_{\mathrm{tr},R}/R$ tends to a limit as $R \to \infty$, this result follows if the rays first hit $\Gamma_{\mathrm{tr},R}$ with angle to the normal θ satisfying $|\theta - \pi/2| \geq c > 0$, with c independent of R, which is the case because $\Omega_- \subset B(0,1)$ and Ω_R satisfies the inclusions (1.18). $\quad\square$

Proof of Lemma 5.13. The overall plan is to select a ray emanating from Γ_D that returns to $B(0,1)$ after multiple reflections from the sides of the hypercube $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$. We do this by identifying $\mathbb{R}^d$ with $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$ by reflection through the lines

$$(x)_j = \frac{R}{2} + nR \quad \text{for } n \in \mathbb{Z} \text{ and}$$

$$, j = 1, \ldots, d$$

(where $(x)_j$ denotes the jth component of the vector $x \in \mathbb{R}^d$); under this identification the corners of the hypercube correspond to the points $(R/2 + R\mathbb{Z})^d$. Since $\Gamma_{\mathrm{tr},R}$ coincides with the boundary of the hypercube $[-R/2, R/2]^d$ only at distance more than ϵ from the corners, we need to make sure that the selected ray avoids these neighbourhoods of the corners; hence the requirement that $\epsilon \leq \epsilon_0(\Omega_-)$ in the statement of the result. We highlight that the constant C in the bound then depends only on the dynamics of the rays, and hence is independent of ϵ.

Step 0: Preliminary notation and results. This argument involves three domains, and three associated flows. The first domain is Ω_R, with associated generalized bicharacteristic flow φ_t (as defined in § 2.3). The second domain is $\widehat{\Omega}_R := \left[-\frac{R}{2}, \frac{R}{2}\right]^d \setminus \overline{\Omega_{R-}}$, and we denote the generalized bicharacteristic flow on $\widehat{\Omega}_R$ by $\widehat{\varphi}_t$. The third domain is the hypercube $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$, and we denote the generalized bicharacteristic flow on $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$ by $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}$.

By the definition (5.9) of $\mathfrak{R}_a$, if both x' and y' are in the illuminated part of Γ_D (i.e., $a \cdot n(x') < 0$), then there exists $C_0 > 0$ (depending on the Lipschitz constant of n) such that

$$|\mathfrak{R}_a(x') - \mathfrak{R}_a(y')| \leq C_0 |x' - y'|, \tag{5.53}$$

i.e., $\mathfrak{R}_a$ is Lipschitz.

We record for later use that, since $\Omega_- \subset B(0,1)$ and $R \geq 4$,

$$\mathrm{dist}\left(\Gamma_D, \partial\left(\left[-\frac{R}{2}, \frac{R}{2}\right]^d\right)\right) \geq \frac{R}{2} - 1 \geq \frac{R}{4}. \tag{5.54}$$

Finally, let $\mathcal{D}$ be a nonempty, uniformly-convex open subset of $\Gamma_D^{+,a}$ in which $n(x') \cdot a < 0$ (such a $\mathcal{D}$ exists, since Lemma 5.7 implies that $\Gamma_D^{+,a} \cap \{n(x') \cdot a < 0\}$ is not everywhere flat). Shrinking $\mathcal{D}$ if

necessary, we can assume that

$$\text{there exists} \quad 0 < \nu < 1 \text{ such that} \quad \nu \le |n(x') \cdot a| \le 1 - \nu \quad \text{for all } x' \in \mathcal{D}; \tag{5.55}$$

this implies that the first assumption of Lemma 5.8 holds with $\mathcal{C} = \mathcal{D}$. The neighbourhood V_D we construct will be a subset of $\mathcal{D}$.

Step 1: Bounding the distance between projections of the flow on $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$.

For $(x_j, \xi_j) \in S^*B(0,1), j = 1, 2$, since $\varphi_t^{\mathbb{R}^d}(x_j, \xi_j) = x_j + 2t\xi_j$,

$$\left| \pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_1, \xi_1) - \pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_2, \xi_2) \right| \le |x_1 - x_2| + 2t|\xi_1 - \xi_2|. \tag{5.56}$$

We now show that the same inequality holds for the flow on $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$; i.e., that for $(x_j, \xi_j) \in S^*B(0,1)$, $j = 1, 2$,

$$\left| \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_1, \xi_1) - \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_2, \xi_2) \right| \le |x_1 - x_2| + 2t|\xi_1 - \xi_2|. \tag{5.57}$$

To prove (5.57), we compare $\left| \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_1, \xi_1) - \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_2, \xi_2) \right|$ with $\left| \pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_1, \xi_1) - \pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_2, \xi_2) \right|$ by using the relationship between the two flows $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}$ and $\varphi_t^{\mathbb{R}^d}$.

First, observe that, since

$$\left| \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_1, \xi_1) - \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_2, \xi_2) \right| \le \text{diam} \left[-\frac{R}{2}, \frac{R}{2}\right]^d = \sqrt{d}R,$$

we can assume that

$$|x_1 - x_2| + 2t|\xi_1 - \xi_2| \le \sqrt{d}R.$$

Therefore, there exists $\ell = (\ell_1, \cdots \ell_d) \in \mathbb{Z}^d$ and $\iota = (\iota_1, \cdots, \iota_d) \in \{-1, 0, 1\}^d$ such that

$$\begin{cases} \pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_1, \xi_1) \in \left(\left[-\frac{R}{2}, \frac{R}{2}\right]^d + \ell R \right), \\ \pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_2, \xi_2) \in \left(\left[-\frac{R}{2}, \frac{R}{2}\right]^d + (\ell + \iota) R \right); \end{cases} \tag{5.58}$$

i.e., after time t, the free-space rays from (x_1, ξ_1) and (x_2, ξ_2) are either in the same hypercube or in adjacent hypercubes. We use the following notation for the components of $\varphi_t^{\mathbb{R}^d}(x_j, \xi_j), j = 1, 2$:

$$\pi_{\mathbb{R}^d} \varphi_t^{\mathbb{R}^d}(x_j, \xi_j) := \left(z_j^1, \cdots, z_j^d \right) \in \mathbb{R}^d. \tag{5.59}$$

Now, observe that by (5.58) and the relationship between $\varphi_t^{\left[-\frac{R}{2},\frac{R}{2}\right]^d}$ and $\varphi_t^{\mathbb{R}^d}$,

$$
\begin{cases}
\pi_{\mathbb{R}^d}\varphi_t^{\left[-\frac{R}{2},\frac{R}{2}\right]^d}(x_1,\xi_1) &= \left(\text{par}(\ell_1)\left(z_1^1-\ell_1 R\right),\cdots,\text{par}(\ell_d)\left(z_1^d-\ell_d R\right)\right),\\
\pi_{\mathbb{R}^d}\varphi_t^{\left[-\frac{R}{2},\frac{R}{2}\right]^d}(x_2,\xi_2) &= \left(\text{par}(\ell_1+\iota_1)\left(z_2^1-(\ell_1+\iota_1)R\right),\cdots,\text{par}(\ell_d+\iota_d)\left(z_2^d-(\ell_d+\iota_d)R\right)\right),
\end{cases}
\tag{5.60}
$$

where

$$
\text{par}(\ell) := \begin{cases} 1 & \text{if } \ell \text{ is even},\\ -1 & \text{if } \ell \text{ is odd}. \end{cases}
$$

Let $i \in \{1,\cdots,d\}$. We first assume that $\iota_i = 1$; then

$$
\left|\text{par}(\ell_j)\left(z_1^i-\ell_i R\right)-\text{par}(\ell_i+\iota_i)\left(z_2^i-(\ell_i+\iota_i)R\right)\right| = \left|\left(z_1^i-\ell_i R\right)+\left(z_2^i-\ell_i R\right)-R\right|.
\tag{5.61}
$$

Since $\iota = 1$, $z_1^i-\ell_i R \in \left[-\frac{R}{2},\frac{R}{2}\right]$, $z_2^i-\ell_i R \in \left[\frac{R}{2},\frac{3R}{2}\right]$, and hence $z_2^i \geq z_1^i$. Now, because $z_1^i-\ell_i R \leq R/2$,

$$
\left(z_1^i-\ell_i R\right)+\left(z_2^i-\ell_i R\right)-R \leq \left(z_2^i-\ell_i R\right)-\left(z_1^i-\ell_i R\right) = z_2^i-z_1^i = \left|z_1^i-z_2^i\right|.
\tag{5.62}
$$

Similarly, since $z_2^i-\ell_i R \geq R/2$,

$$
-\left(z_1^i-\ell_i R\right)-\left(z_2^i-\ell_i R\right)+R \leq \left(z_2^i-\ell_i R\right)-\left(z_1^i-\ell_i R\right) = z_2^i-z_1^i = \left|z_1^i-z_2^i\right|.
\tag{5.63}
$$

Then, combining (5.61), (5.62) and (5.63), we have that, for $i \in \{1,\cdots,d\}$ with $\iota_i = 1$,

$$
\left|\text{par}(\ell_j)\left(z_1^i-\ell_i R\right)-\text{par}(\ell_i+\iota_i)\left(z_2^i-(\ell_i+\iota_i)R\right)\right| \leq \left|z_1^i-z_2^i\right|.
\tag{5.64}
$$

If $\iota_i = -1$, the proof of (5.64) follows in a very similar way; if $\iota_i = 0$, it is straightforward to check that (5.64) holds with equality. Hence, (5.64) holds for any $i \in \{1,\cdots,d\}$. Recalling the notation (5.59), we therefore obtain from (5.60) and (5.64) that

$$
\left|\pi_{\mathbb{R}^d}\varphi_t^{\left[-\frac{R}{2},\frac{R}{2}\right]^d}(x_1,\xi_1)-\pi_{\mathbb{R}^d}\varphi_t^{\left[-\frac{R}{2},\frac{R}{2}\right]^d}(x_2,\xi_2)\right| \leq \left|\pi_{\mathbb{R}^d}\varphi_t^{\mathbb{R}^d}(x_1,\xi_1)-\pi_{\mathbb{R}^d}\varphi_t^{\mathbb{R}^d}(x_2,\xi_2)\right|,
$$

and (5.57) follows from (5.56).

Step 2: Selecting a periodic ray. Let $\mathfrak{F}$ be the finite set of unit vectors forming an angle belonging to Ψ to one of the elements $(\pm e_i)_{1\leq i\leq d}$, where $(e_i)_{1\leq i\leq d}$ denote the unit vectors in cartesian coordinates. With $\mathcal{D}$ as in Step 0, $\mathfrak{R}_a(\mathcal{D})$ contains a nonempty open subset of $\mathcal{S}^{d-1}$ by Lemma 5.7, and therefore

contains a vector of the form

$$\xi_0 = \frac{(p_1, \cdots, p_d)}{|p|}, \quad p_i \in \mathbb{Z} \quad \text{and} \quad \xi_0 \notin \mathfrak{F}$$

(since vectors of this form are dense in $\mathcal{S}^{d-1}$). Let $x_0' \in \mathcal{D}$ be such that $\mathfrak{R}_a(x_0') = \xi_0$.

We identify $\mathbb{R}^d$ with $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$ as described above. Then, given any $q_1, \ldots, q_d \in \mathbb{Z}$,

$$(x_1, \ldots, x_d) + 2R(q_1, \ldots, q_d) \equiv (x_1, \ldots, x_d); \tag{5.65}$$

the factor of two is because one reflection changes the parity.

The trajectory starting from (x_0', ξ_0) and evolving according to the flow $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}$ can be identified with the trajectory in $\mathbb{R}^d$

$$x_0' + 2t\xi_0 = x_0' + 2t\frac{(p_1, \ldots, p_d)}{|p|};$$

therefore, by (5.65), the former trajectory is periodic, with period at most $R|p|$. Thus, there exists $t > 0$ such that $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d} \in B(0, 11/8)$; let $T(R)$ be the infimum of such ts. Therefore,

$$T(R) \leq R|p|, \tag{5.66}$$

and

$$\pi_{\mathbb{R}^d}\left(\widehat{\varphi}_{T(R)}(x_0', \xi_0)\right) \in \partial B\left(0, \frac{11}{8}\right). \tag{5.67}$$

Since $\Omega_- \subset B(0, 1)$, the flows $\widehat{\varphi}_t$ and $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}$ acting on (x_0', ξ_0) agree up to (at least) time $T(R)$; i.e.,

$$\widehat{\varphi}_t(x_0', \xi_0) = \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_0', \xi_0) \quad \text{for all } 0 \leq t \leq T(R). \tag{5.68}$$

Furthermore, since $\xi_0 \notin \mathfrak{F}$, the flows $\widehat{\varphi}_t$ and $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}$ acting on (x_0', ξ_0) never hit $\partial\left(\left[-\frac{R}{2}, \frac{R}{2}\right]^d\right)$ at an angle belonging to Ψ.

Finally, observe that a length R of a ray can be reflected at most twice. Therefore, since the length of $\varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_0', \xi_0)$ for $t \in [0, T(R)]$ is at most $2R|p|$, if $M := \lceil 4|p| \rceil$, then the number of reflections of this ray for $t \in [0, T(R)]$, $N(R)$, is bounded by M, i.e.,

$$N(R) \leq \lceil 4|p| \rceil. \tag{5.69}$$

Step 3: The neighbourhood V_D on Γ_D. The neighbourhood $V_D = V_D(R)$ is chosen later in the proof as a subset of

$$V_1(R) := \Gamma_D \cap B\left(x_0', \frac{\delta_1}{R}\right), \tag{5.70}$$

where $\delta_1 > 0$ (independent of R) is small enough so that, for all $R \geq 1$,

$$\begin{cases}
V_1(R) \subset \mathcal{D}, \\
\text{for all } x' \in V_1(R), \quad |n(x') \cdot a| \geq \frac{1}{2}|n(x_0') \cdot a|, \\
\text{for all } x' \in V_1(R), \quad \min_{\mathfrak{f} \in \mathfrak{F}} |\mathfrak{R}_a(x') - \mathfrak{f}| \geq \frac{1}{2} \min_{\mathfrak{f} \in \mathfrak{F}} |\xi_0 - \mathfrak{f}|.
\end{cases} \tag{5.71}$$

Since the neighbourhood V_D will be a subset of $V_1(R)$, the second condition in (5.71) implies that Part (ii) of Condition 5.9 holds with $c_{\mathrm{ray},2} := |n(x_0') \cdot a|/2$, which is positive since $x_0' \in \mathcal{D}$, and the third condition in (5.71) implies that Part (iii) of Condition 5.9 holds with $c_{\mathrm{ray},3} > 0$.

By (5.57), the fact that $\xi_0 = \mathfrak{R}_a(x_0')$, (5.53) and (5.66), we have, for any $x' \in V_1(R)$ and any $0 \leq t \leq T(R)$

$$\left| \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_0', \xi_0) - \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x', \mathfrak{R}_a(x')) \right| \leq |x_0' - x'| + 2T(R)|\mathfrak{R}_a(x_0') - \mathfrak{R}_a(x')|,$$

$$\leq \left(1 + 2R|p|C_0\right)|x_0' - x'|,$$

$$\leq \left(1 + 2|p|C_0\right)R|x_0' - x'|. \tag{5.72}$$

Therefore, if $\delta_1 \leq (16(1 + 2C_0|p|))^{-1}$, then

$$\left| \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x_0', \xi_0) - \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x', \mathfrak{R}_a(x')) \right| \leq \frac{1}{16} \tag{5.73}$$

for all $x' \in V_1(R)$ and for all $0 \leq t \leq T(R)$. Combining (5.73), (5.67) and (5.68), we have

$$\pi_{\mathbb{R}^d}\left(\widehat{\varphi}_{T(R)}(x', \xi_0)\right) \in B\left(0, \frac{23}{16}\right) \setminus B\left(0, \frac{21}{16}\right) \quad \text{for all } x' \in V_1(R); \tag{5.74}$$

and

$$\widehat{\varphi}_t(x', \mathfrak{R}_a(x')) = \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x', \mathfrak{R}_a(x')) \quad \text{for all } x' \in V_1(R) \text{ and for all } 0 \leq t \leq T(R). \tag{5.75}$$

Step 4: Avoiding the corners. Under the identification of $\left[-\frac{R}{2}, \frac{R}{2}\right]^d$ with $\mathbb{R}^d$, the corners of the hypersquare correspond to $(R/2 + R\mathbb{Z})^d$. Given $x' \in V_1(R)$, each point on the ray $x' + 2t\mathfrak{R}_a(x')$ for $0 \leq t \leq T(R)$ has a corner that is closest; we let $Q_\alpha(x')$ denote the subset of these corners that are a

distance $\leq \alpha$ away. More precisely,

$$Q_\alpha(x') := \left\{ q \in (R/2 + R\mathbb{Z})^d \ : \ \text{there exists } 0 \leq t \leq T \text{ such that}\right.$$

$$\left. \text{dist}\left(x' + 2t\mathfrak{R}_a(x'), (R/2 + R\mathbb{Z})^d\right) = \text{dist}\left(x' + 2t\mathfrak{R}_a(x'), q\right) \leq \alpha \right\}.$$

We then order the elements of $Q_\alpha(x')$ with the closest first; i.e., $Q_\alpha(x') = \{q_1(x'), \ldots, q_{m(x')}(x')\}$ with $\text{dist}(x', q_i)$ nondecreasing with i.

We now prove that if $\delta_1 \leq (4(1 + 2|p|C_0))^{-1}$, then

$$Q_{1/4}(x') \subset Q_{1/2}(x'_0) \quad \text{for all } x' \in V_1(R). \tag{5.76}$$

To prove this, observe that, for $0 \leq t \leq T(R)$, by (5.66) and (5.53) (in a similar way to as in (5.72)),

$$\text{dist}\left(x' + 2t\mathfrak{R}_a(x'), x'_0 + 2t\mathfrak{R}_a(x'_0)\right) \leq |x' - x'_0| + 2t|\mathfrak{R}_a(x') - \mathfrak{R}_a(x'_0)|,$$
$$\leq \left(1 + 2|p|C_0\right) R|x' - x'_0| \leq \delta_1 \left(1 + 2|p|C_0\right)$$

if $x' \in V_1(R)$. Therefore, if $\delta_1 \leq (4(1 + 2|p|C_0))^{-1}$, the distance between the rays is $< 1/4$. If $q_i \in Q_{1/4}(x')$ then, since $R \geq 1$, q_i is at most distance $1/2$ away from a point on the ray $x'_0 + 2t\mathfrak{R}_a(x'_0)$, and thus $q_i \in Q_{1/2}(x'_0)$.

It turns out that we will not need to restrict δ_1 further in the proof; we therefore set

$$\delta_1 := \frac{1}{16(1 + 2C_0|p|)}, \tag{5.77}$$

and observe that this satisfies the requirements imposed on δ_1 earlier in the proof (to ensure that (5.73) and (5.76) hold).

We now select one set of corners to work with for all $x' \in V_1(R)$. Let $Q := Q_{1/2}(x'_0) = (q_1, \ldots q_m)$. By (5.76),

$$\left((R/2 + R\mathbb{Z})^d \setminus Q\right) \subset \left((R/2 + R\mathbb{Z})^d \setminus Q_{1/4}(x')\right) \quad \text{for all } x' \in V_1(R),$$

so that

$$\text{dist}\left(x' + 2t\mathfrak{R}_a(x'), (R/2 + R\mathbb{Z})^d \setminus Q\right) \geq 1/4 \quad \text{for all } x' \in V_1(R). \tag{5.78}$$

Furthermore, since $R \geq 4$, the number of corners within distance $1/2$ of the ray is less than or equal to the number of reflections, i.e.,

$$m \leq N(R). \tag{5.79}$$

We now iteratively construct $x'_i \in V_1(R)$, $i = 1, \ldots, m$, such that the ray $x'_i + 2t\mathfrak{R}_a(x'_i)$ for $0 \leq t \leq T(R)$ is at least a distance η_i from $(q_1, \ldots, q_i)$ where $\eta_i > 0$, $i = 0, \ldots, m$, are defined below (see (5.86))

and, in particular, have the property that $\eta_i > \eta_{i+1}$, $i = 0, \ldots m-1$. Given x'_i, if $\mathrm{dist}(x'_i + 2t\mathfrak{R}_a(x'_i), q_{i+1}) \geq \eta_{i+1}$, we set $x'_{i+1} := x'_i$. Otherwise, first observe that, for $0 \leq t \leq R/16$,

$$\mathrm{dist}\left(x' + 2t\mathfrak{R}_a(x'), q_{i+1}\right) \geq R/8 \geq 1/2, \tag{5.80}$$

by (5.54) and the fact that $R \geq 4$; we can therefore restrict attention to $t \geq R/16$. Let $\lambda_i > 0$, to be fixed later. We first assume that there exists $x'_{i+1} \in V_1(R)$ so that, with $C_\mathfrak{R}$ the constant associated to $\mathcal{D}$ by Lemma 5.8,

$$|x'_{i+1} - x'_i| = \lambda_i \quad \text{and} \quad \left|\mathfrak{R}_a(x'_{i+1}) - \mathfrak{R}_a(x'_i)\right| \geq C_\mathfrak{R}\lambda_i; \tag{5.81}$$

we later use Lemma 5.8 to show that such an x'_{i+1} exists once the value of λ_i has been fixed. By, respectively, the triangle inequality, the convexity of $V_1(R) \subset \mathcal{D}$, (5.81), and the fact that we are dealing with the case that $\mathrm{dist}(x'_i + 2t\mathfrak{R}_a(x'_i), q_{i+1}) < \eta_{i+1}$, we have that, for $R/16 \leq t \leq T(R)$,

$$
\begin{aligned}
\mathrm{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'), q_{i+1}\right) &\geq \mathrm{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'_{i+1}), x'_i + 2t\mathfrak{R}_a(x'_i)\right) - \mathrm{dist}\left(x'_i + 2t\mathfrak{R}_a(x'_i), q_{i+1}\right), \\
&\geq \mathrm{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'_{i+1}), x'_{i+1} + 2t\mathfrak{R}_a(x'_i)\right) - \mathrm{dist}\left(x'_i + 2t\mathfrak{R}_a(x'_i), q_{i+1}\right), \\
&= 2t|\mathfrak{R}_a(x'_{i+1}) - \mathfrak{R}_a(x'_i)| - \mathrm{dist}\left(x'_i + 2t\mathfrak{R}_a(x'_i), q_{i+1}\right), \\
&\geq 2tC_\mathfrak{R}\lambda_i - \eta_{i+1}, \\
&\geq \frac{C_\mathfrak{R}R}{8}\lambda_i - \eta_{i+1}. \tag{5.82}
\end{aligned}
$$

Having bounded the distance from the ray to q_{i+1}, we now bound the distance to q_j for $j = 0, \ldots, i$. By, respectively, the triangle inequality, (5.53), and (5.66), for $j = 0, \ldots, i$ and $0 \leq t \leq T(R)$,

$$
\begin{aligned}
\mathrm{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'), q_j\right) &\geq \mathrm{dist}\left(x'_i + 2t\mathfrak{R}_a(x'_i), q_j\right) - \mathrm{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'_{i+1}), x'_i + 2t\mathfrak{R}_a(x'_i)\right) \\
&\geq \eta_i - \left(1 + 2tC_0\right)|x' - x'_i|, \\
&\geq \eta_i - R\left(1 + 2C_0|p|\right)\lambda_i. \tag{5.83}
\end{aligned}
$$

The two inequalities (5.82) and (5.83) imply that if η_i and η_{i+1} satisfy

$$\frac{16\eta_{i+1}}{C_\mathfrak{R}} = \frac{\eta_i - \eta_{i+1}}{(1 + 2C_0|p|)}, \tag{5.84}$$

and λ_i is defined by

$$\lambda_i := \frac{16\eta_{i+1}}{RC_\mathfrak{R}} = \frac{\eta_i - \eta_{i+1}}{R(1 + 2C_0|p|)}, \tag{5.85}$$

then

$$\mathrm{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'_{i+1}), q_{i+1}\right) \geq \eta_{i+1} \quad \text{for all } R/16 \leq t \leq T(R)$$

and

$$\text{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x'_{i+1}), q_j\right) \geq \eta_{i+1} \quad \text{for } j = 0, \dots, i, \text{ and for all } 0 \leq t \leq T(R).$$

This last two inequalities, combined with (5.80), imply that

$$\text{dist}\left(x'_{i+1} + 2t\mathfrak{R}_a(x_{i+1}), q_j\right) \geq \eta_{i+1} \quad \text{for } j = 0, \dots, i+1, \text{ and for all } 0 \leq t \leq T(R)$$

as required. We observe for use later that (5.84) implies that

$$\eta_{i+1} = \frac{\eta_i}{1 + \frac{16}{C_\mathfrak{R}}\left(1 + 2C_0|p|\right)} \quad \text{so that} \quad \eta_j := \eta_0 \left(\frac{1}{1 + \frac{16}{C_\mathfrak{R}}\left(1 + 2C_0|p|\right)}\right)^j, \quad j = 0, \dots, m. \quad (5.86)$$

Since the value of $\lambda_i > 0$ has been fixed by (5.85), it remains to show that there exists $x'_{i+1} \in V_1(R)$ satisfying (5.81). We now use the freedom we have in choosing η_0 to ensure that the can use Lemma 5.8 to construct such an x'_{i+1}. Recall that we chose $\mathcal{D}$ so that the assumptions of Lemma 5.8 hold; let α_0 be the associated constant. We impose the condition that

$$\sum_{j=0}^{m-1} \lambda_j \leq \min\left(\frac{\delta_1}{2R}, \alpha_0\right), \qquad \text{i.e.,} \quad \eta_0 \frac{16}{C_\mathfrak{R}} \sum_{j=1}^{m-2} \left(\frac{1}{1 + \frac{16}{C_\mathfrak{R}}\left(1 + 2C_0|p|\right)}\right)^j \leq \min\left(\frac{\delta_1}{2}, 4\alpha_0\right), \tag{5.87}$$

where we have used the definitions of λ_j (5.85) and η_j (5.86) and the fact that $R \geq 4$. Observe that (5.87) is a condition that η_0 is sufficiently small (recall that δ_1 has been fixed by (5.77)).

The rationale behind imposing (5.87) is as follows; recalling the definition of $V_1(R)$ (5.70), we see that $\sum_{j=0}^{m-1} \lambda_j \leq \delta_1/2$ implies that $x'_i \in V_1(R)$ for $i = 1, \dots, m$. The first inequality in (5.87) implies that $\lambda_i \leq \alpha_0$, for all i, and, since $V_1(R) \subset \mathcal{D}$ (by (5.71)),

$$\partial B(x'_i, \lambda_i) \cap \mathcal{D} \neq \emptyset \quad \text{and} \quad \partial B(x'_i, \lambda_i) \cap \partial \mathcal{D} = \emptyset.$$

These relations combined with (5.55) imply that the assumptions of Lemma 5.8 are satisfied with $\mathcal{D} = \mathcal{C}$. This lemma therefore implies that there exists $x'_{i+1} \in \mathcal{D}$ satisfying (5.81), for all $i = 1, \dots, m$.

In summary, we have proved that the ray $x'_m + t\mathfrak{R}_a(x'_m)$, $0 \leq t \leq T(R)$, is a distance at least η_m from any of the corners $q_1, \dots, q_m$, and a distance at least $1/4$ from any of the other corners by (5.78).

Let $\eta_{\lceil 4|p| \rceil}$ be defined by the second equation in (5.86) with $j = \lceil 4|p| \rceil$ and with η_0 fixed to satisfy (5.87). By (5.79) and (5.69), $m \leq N(R) \leq \lceil 4|p| \rceil$ so that $\eta_m \geq \eta_{\lceil 4|p| \rceil}$. Therefore, with

$$\epsilon_0 := \frac{1}{2} \min\left(\eta_{\lceil 4|p| \rceil}, \frac{1}{4}\right),$$

the ray $x'_m + t\mathfrak{R}_a(x'_m)$, $0 \leq t \leq T(R)$ is a distance at least $2\epsilon_0 > 0$ from any corner. By (5.86) and (5.87), $\eta_{\lceil 4|p| \rceil}$ (and hence ϵ_0) depends on C_0, $C_\mathfrak{R}$, α_0, and $|p|$, and hence only on Γ_D.

Step 5: Putting everything together. By combining the results of Step 4 with the results (5.74) and (5.75) of Step 3, we have

$$
\begin{cases}
\widehat{\varphi}_t(x'_m, \mathfrak{R}_a(x'_m)) = \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x'_m, \mathfrak{R}_a(x'_m)) & \text{for all } 0 \le t \le T(R), \\
\text{dist}\left(\widehat{\varphi}_t(x'_m, \mathfrak{R}_a(x'_m)), \left(\frac{R}{2} + R\mathbb{Z}\right)^d\right) \ge 2\epsilon_0 & \text{for all } 0 \le t \le T(R), \quad \text{and} \\
\pi_{\mathbb{R}^d}\left(\widehat{\varphi}_{T(R)}(x'_m, \xi_0)\right) \in B\left(0, \frac{23}{16}\right) \setminus B\left(0, \frac{21}{16}\right).
\end{cases}
\tag{5.88}
$$

We now define the neighbourhood V_D (the neighbourhood of rays in the statement of the lemma) as a neighbourhood of x'_m. Indeed, we let

$$
V_D := \Gamma_D \cap B\left(x'_m, \frac{\delta}{R}\right)
$$

with $\delta > 0$ chosen sufficiently small; if $\delta > 0$ is independent of R, then this implies that $\text{vol}(V_D) \ge \widetilde{c}_{\text{ray},1}/R^{d-1}$ for some $\widetilde{c}_{\text{ray},1} > 0$ independent of R; i.e., that Point (i) of Condition 5.9 holds.

We first choose $\delta > 0$ sufficiently small so that $V_D \subset V_1(R)$; since δ_1 (5.77) is independent of R, δ can be chosen to be independent of R. As discussed below (5.71), the inclusion $V_D \subset V_1(R)$ ensures that Points (ii) and (iii) of Condition 5.9 hold.

Point (iv) in the statement of the result will follow if we can show that, for all $x' \in V_D$,

$$
\begin{cases}
\widehat{\varphi}_t(x_m, \mathfrak{R}_a(x_m)) = \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x', \mathfrak{R}_a(x')) & \text{for all } 0 \le t \le T(R), \\
\text{dist}\left(\widehat{\varphi}_t(x', \mathfrak{R}_a(x')), \left(\frac{R}{2} + R\mathbb{Z}\right)^d\right) \ge \epsilon_0 & \text{for all } 0 \le t \le T(R), \quad \text{and} \\
\pi_{\mathbb{R}^d}\left(\widehat{\varphi}_{T(R)}(x', \xi_0)\right) \in B\left(0, \frac{47}{32}\right) \setminus B\left(0, \frac{41}{32}\right).
\end{cases}
\tag{5.89}
$$

Indeed, the second property in (5.89) (missing the corners) implies that all three flows are the same when applied to $(x_m, \mathfrak{R}_a(x_m))$ for $0 \le t \le T(R)$, i.e.,

$$
\varphi_t(x_m, \mathfrak{R}_a(x_m)) = \widehat{\varphi}_t(x_m, \mathfrak{R}_a(x_m)) = \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x', \mathfrak{R}_a(x')) \quad \text{for all } 0 \le t \le T(R).
$$

We now obtain (5.89) from (5.88). By (5.57), (5.53) and (5.66) (in a similar way to as in (5.72)), for any $x' \in V(R)$ and any $0 \le t \le T(R)$,

$$
\left| \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x'_m, \mathfrak{R}_a(x_m)) - \pi_{\mathbb{R}^d} \varphi_t^{\left[-\frac{R}{2}, \frac{R}{2}\right]^d}(x', \mathfrak{R}_a(x')) \right| \le \left(1 + 2C_0|p|\right) R|x'_m - x'|,
$$

so that (5.89) follows as long as

$$
\delta \le \min\left(\frac{1}{32\left(1 + C_0|p|\right)}, \frac{\epsilon_0}{\left(1 + 2C_0|p|\right)} \right).
$$

Since $\delta > 0$ is independent of R, Point (i) of Condition 5.9 holds with $c_{\mathrm{ray},1} = \widetilde{c}_{\mathrm{ray},1}/R$, with $\widetilde{c}_{\mathrm{ray},1}$ independent of R, and the proof is complete. □

5.8   *Bounding below the reflection coefficient* (2.48) *for rays satisfying Condition* 5.9

In the follow result, we use the subscripts D and tr on $\mathcal{H}$ to denote the hyperbolic set on Γ_D and $\Gamma_{\mathrm{tr},R}$, respectively.

LEMMA 5.16 (Lower bound on the reflection coefficient for general $\Gamma_{\mathrm{tr},R}$). Let $\mathcal{V}_{\mathrm{tr}} \subset \mathcal{H}_{\mathrm{tr}}$. Given $(x', \xi') \in \mathcal{V}_{\mathrm{tr}}$, let

$$\theta(x', \xi') := \sin^{-1}\left(|\xi'|_g\right) \in [0, \pi/2); \tag{5.90}$$

observe that θ is well-defined since $r(x', \xi') := 1 - |\xi'|_g^2 > 0$ on $\mathcal{H}_{\mathrm{tr}}$.

Let $\{\psi_j\}_{j=1}^{m_{\mathrm{vanish}}}$ be defined be (5.17). Suppose that

$$\theta \geq c_3 \quad \text{and} \quad \min_{j=1,\dots,m} |\theta - \psi_j| \geq c_4, \tag{5.91}$$

and $\mathcal{N}$ and $\mathcal{D}$ satisfy Assumption 1.4 with *either* $\mathsf{M} = \mathsf{N}$ *or* $\mathsf{M} = \mathsf{N} + 1$. Then there exists $C_{\mathrm{ref}} = C_{\mathrm{ref}}(\mathsf{M}, \mathsf{N}) > 0$ such that

$$\left| \frac{\sqrt{r}\sigma(\mathcal{N}) - \sigma(\mathcal{D})}{\sqrt{r}\sigma(\mathcal{N}) + \sigma(\mathcal{D})} \right| \geq C_{\mathrm{ref}} \min\left(|c_3|^{2m_{\mathrm{ord}}}, |c_4|^{m_{\mathrm{mult}}}\right) \quad \text{on } \mathcal{V}_{\mathrm{tr}}. \tag{5.92}$$

We make three remarks.

- The rationale behind the definition of θ (5.90) is that later we apply it to sets $\mathcal{V}_{\mathrm{tr}}$ whose elements are of the form $\pi_{\Gamma_{\mathrm{tr},R}}(x, \xi)$ where $(x, \xi) \in S^*_{\overline{\Omega_R}}\mathbb{R}^d$ (so that $|\xi| = 1$). In this case, θ is the angle the vector ξ makes with the normal to $\Gamma_{\mathrm{tr},R}$.

- We have denoted the constants in (5.91) by c_3 and c_4 since we later apply this lemma with $c_3 = c_{\mathrm{ray},3}$ and $c_4 = c_{\mathrm{ray},4}$.

- We highlight that C_{ref} only depends on M and N, and not on $\Gamma_{\mathrm{tr},R}$.

Proof of Lemma 5.16. By Assumption 1.4,

$$\sigma(\mathcal{N})(x', \xi')\sqrt{r(x', \xi')} - \sigma(\mathcal{D})(x', \xi') = q\left(|\xi'|_g^2\right)\sqrt{1 - |\xi'|_g^2} - p\left(|\xi'|_g^2\right). \tag{5.93}$$

Since $\mathcal{N}$ and $\mathcal{D}$ satisfy Assumption 1.4 with *either* $\mathsf{M} = \mathsf{N}$ *or* $\mathsf{M} = \mathsf{N} + 1$, Part (a) of Lemma 4.4 implies that there exists $C_1 = C_1(\mathsf{M}, \mathsf{N}) > 0$ such that $|\sqrt{r}\sigma(\mathcal{N}) + \sigma(\mathcal{D})| \geq C_1$ on $\mathcal{V}_{\mathrm{tr}}$.

By the definitions in § 1.3 of $p(t), q(t), m_{\mathrm{ord}}, \{t_j\}_{j=1}^{m_{\mathrm{vanish}}}$ and m_{mult}, there exists $C_2 = C_2(\mathsf{M}, \mathsf{N}) > 0$ such that

$$\left|q(t)\sqrt{1 - t} - p(t)\right| \geq C_1 \min\left(|t|^{m_{\mathrm{ord}}}, \left(\min_{j=1,\dots,m_{\mathrm{vanish}}} |t - t_j|\right)^{m_{\mathrm{mult}}}\right) \quad \text{for all } t \in [0, 1]. \tag{5.94}$$

Since $\sin x \geq 2x/\pi$ for $x \in [0, \pi/2]$ and there exists $C_2 = C_2(\psi_{\min}) > 0$ such that $|\sin^2 \theta - \sin^2 \psi_j| \geq C_2 |\theta - \psi_j|$ for $j = 1, \ldots, m_{\text{vanish}}$, the inequalities in (5.91) imply that

$$|\xi'|_g^2 \geq (c_3)^2 \left(\frac{2}{\pi}\right)^2 \quad \text{and} \quad \min_{j=1,\ldots,m_{\text{vanish}}} \left| |\xi'|_g^2 - t_j \right| \geq C_2 c_4.$$

The bound (5.92) then follows from combining these bounds with (5.93) and (5.94). $\qquad \square$

5.9 *Proof of Theorem* 1.6 *(the qualitative lower bound)*

Similar to above, we use the subscripts D and tr on $\mathcal{H}$ (and subsets of it) to denote the hyperbolic set on Γ_D and $\Gamma_{\text{tr},R}$, respectively; we use analogous notation for boundary measures.

Proof of Theorem 1.6. By Part (i) of Corollary 5.4, we only need to show that $\mu(\mathcal{I}) > 0$. We now follow the steps outlined in § 5.3; seeking a contradiction, we assume that $\mu(\mathcal{I}) = 0$. The inequality (2.44) from Point (ii) of Corollary 2.17 implies that $\mu_D^{\text{in}} = 0$. Therefore, (2.26) implies that

$$\mu_D^{\text{out}} = 2\sqrt{r(x', \xi')}\, v_{d,D}$$

and Lemma 2.20 therefore gives that

$$\mu_D^{\text{out}} = 2\sqrt{r(x', \xi')}\, d\text{vol}(x') \otimes \delta_{\xi' = (a_{T(x')})^\flat}. \tag{5.95}$$

Given M and N, let $\{\psi_j\}_{j=1}^{m_{\text{vanish}}}$ be defined by (5.17); i.e., $\{\psi_j\}_{j=1}^{m_{\text{vanish}}}$ is the set of nonzero angles at which the reflection coefficient (2.48) vanishes. Let the set $V_D \subset \Gamma_D$ be given by Lemma 5.10; i.e., the rays emanating from V_D are nontangent to Γ_D and hit $\Gamma_{\text{tr},R}$ directly and at angles bounded away from $\{0, \psi_1, \ldots, \psi_{m_{\text{vanish}}}\}$. Let

$$\mathcal{V}_D := \left\{ \left(x', (a_{T(x')})^\flat\right),\ x' \in V_D \right\} \subset \mathcal{H}_D.$$

By (5.95), $\mu_D^{\text{out}}(\mathcal{V}_D) > 0$. Therefore, using the equality (2.42) from Point (i) of Corollary 2.17 and the fact that $r > 0$ on $\mathcal{H}$,

$$\left(2\sqrt{r}\mu_{\text{tr}}^{\text{in}}\right)(\mathcal{V}_{\text{tr}}) = \left(2\sqrt{r}\mu_D^{\text{out}}\right)(\mathcal{V}_D) > 0, \tag{5.96}$$

where

$$\mathcal{V}_{\text{tr}} := \bigcup_{q \in \mathcal{V}_D} \pi_{\Gamma_{\text{tr},R}}\left(\varphi_{t^{\text{out}}(q)}\left(p^{\text{out}}(q)\right)\right) \subset \mathcal{H}_{\text{tr}},$$

where t^{out} and p^{out} are defined in (2.38) and (2.37), respectively, and $\pi_{\Gamma_{\text{tr},R}}$ equals $\pi_{\partial M}$ restricted to $T_{\Gamma_{\text{tr},R}}^* \mathbb{R}^d$; observe that $\sup_{q \in \mathcal{V}_D} t^{\text{out}}(q) < \infty$ since $\Gamma_{\text{tr},R}$ is (strictly) convex.

Corollary 2.19 then implies that

$$(2\sqrt{r}\mu^{\text{out}})(\mathcal{V}_{\text{tr}}) = \left|\frac{\sqrt{r}\sigma(\mathcal{N}) - \sigma(\mathcal{D})}{\sqrt{r}\sigma(\mathcal{N}) + \sigma(\mathcal{D})}\right|^2 (2\sqrt{r}\mu^{\text{in}})(\mathcal{V}_{\text{tr}}),$$

where we have used the fact that $|\sigma(\mathcal{N})| > 0$ on $\mathcal{V}_{\text{tr}}$ by Corollary 4.5.

Since the rays emanating from V_D hit $\Gamma_{\text{tr},R}$ directly and at angles bounded away from $\{0, \psi_1, \ldots, \psi_k\}$, Lemma 5.16 implies that $(2\sqrt{r}\mu^{\text{out}})(\mathcal{V}_{\text{tr}}) \geq C(2\sqrt{r}\mu^{\text{in}})(\mathcal{V}_{\text{tr}})$ for $C > 0$. Combining this inequality with (5.96), we have $(2\sqrt{r}\mu^{\text{out}})(\mathcal{V}_{\text{tr}}) > 0$. By the inequality (2.43) in Point (ii) of Corollary 2.17, $\mu(\mathcal{I}) > 0$, which is the desired contradiction.

Finally, the fact that C in Theorem 1.8 depends continuously on $\Gamma_{\text{tr},R}$ follows from the fact that $c_{\text{ray},j}, j = 1, \ldots, 4$, depend continuously on $\Gamma_{\text{tr},R}$, and C_{ref} in Lemma 5.16 is independent of $\Gamma_{\text{tr},R}$. □

5.10 *Proof of the lower bounds in Theorem 1.7, Theorem 1.8, Theorem 1.9, Theorem 1.10, and Theorem 1.11*

Recall from Corollary 5.4 that to prove the lower bounds in Theorems 1.7, 1.8, 1.10 and 1.11, we only need to bound $\mu(\mathcal{I})$ and $\mu\big(\mathcal{I} \cap S^*_{B(0,3/2)}\big)$ below; the following lemma provides the necessary lower bounds.

LEMMA 5.17 (i) Suppose Condition 5.9 holds for $R \geq R_0$ with $c_{\text{ray},2}$ independent of R and $c_{\text{ray},5} \geq \widetilde{c}_5 R$ with $\widetilde{c}_5 > 0$ independent of R. Then, there exists $C > 0$ such that, for all $R \geq R_0$,

$$\mu(\mathcal{I}) \geq CR\big(\min\big(|c_{\text{ray},3}|^{2m_{\text{ord}}}, |c_{\text{ray},4}|^{m_{\text{mult}}}\big)\big)^2 c_{\text{ray},1}. \tag{5.97}$$

(ii) If, in addition, there exists $N_{\text{ref}} \geq 1$ such that, for the interior billiard flow in Ω_R, these rays are reflected on $\Gamma_{\text{tr},R}$ N_{ref} times, without being reflected on Γ_D in between, and after their N_{ref}th reflection all of these rays intersect $B(0, 3/2) \setminus B(0, 5/4)$ without being reflected before, then

$$\mu\big(\mathcal{I} \cap S^*_{B(0,3/2)}\mathbb{R}^d\big) \geq C\big(\min\big(|c_{\text{ray},3}|^{2m_{\text{ord}}}, |c_{\text{ray},4}|^{m_{\text{mult}}}\big)\big)^2 c_{\text{ray},1}. \tag{5.98}$$

Proof of (i). As in the proof of Theorem 1.6, we argue by contradiction and follow the steps in § 5.3. Suppose that Condition 5.9 holds for $R \geq R_0$, but, for any $\epsilon > 0$, there exists $R \geq R_0$ such that

$$\mu(\mathcal{I}) \leq \epsilon R\big(\min\big(|c_{\text{ray},3}|^{2m_{\text{ord}}}, |c_{\text{ray},4}|^{m_{\text{mult}}}\big)\big)^2 c_{\text{ray},1}. \tag{5.99}$$

Let

$$\mathcal{V}_D := \big\{\big(x', (a_{T(x')})^\flat\big) \in T^*\Gamma_D, \, x' \in V_D\big\} \subset \mathcal{H}_D. \tag{5.100}$$

We now claim that

$$\mu(\mathcal{I}) \geq \left(\frac{\delta}{M}\right) R\,(2\sqrt{r}\mu^{\text{in}})(\mathcal{V}_D) \quad \text{for all } R \geq 1. \tag{5.101}$$

Indeed, Part (ii) of Corollary 2.17 implies that

$$\mu(\mathcal{I}) \geq \text{dist}(\Gamma_{\text{tr},R}, \Omega_-)(2\sqrt{r}\mu^{\text{in}})(\mathcal{V}_D),$$

and then to prove (5.101) we only need to show that

$$\text{dist}(\Gamma_{\text{tr},R}, \Omega_-) \geq \left(\frac{\delta}{M}\right) R. \tag{5.102}$$

Let $\delta = \text{dist}(\Omega_-, \partial B(0,1))$. Then, since $\widetilde{\Omega}_R \supset B(0, M^{-1}R) \cup B(0,1)$ and $\Omega_- \subset B(0,1)$, if $R \geq M$,

$$\text{dist}(\Gamma_{\text{tr},R}, \Omega_-) \geq \left(M^{-1}R - 1 + \delta\right) = \left(M^{-1} - \frac{(1-\delta)}{R}\right) R \geq \left(\frac{\delta}{M}\right) R$$

and then (5.102) follows for $R \geq M$. On the other hand, if $R \leq M$, then

$$\text{dist}(\Gamma_{\text{tr},R}, \Omega_-) \geq \delta \geq \left(\frac{\delta}{M}\right) R,$$

and then (5.102) follows for $R \leq M$.

Combining (5.99) and (5.101), we have

$$(2\sqrt{r}\mu^{\text{in}})(\mathcal{V}_D) \leq \epsilon \frac{M}{\delta} \left(\min\left(|c_{\text{ray},3}|^{2m_{\text{ord}}}, |c_{\text{ray},4}|^{m_{\text{mult}}}\right)\right)^2 c_{\text{ray},1}. \tag{5.103}$$

We now use Lemmas 2.12 and 2.20 to obtain a lower bound on $\mu^{\text{out}}(\mathcal{V}_D)$. The two equations in (2.25) imply that

$$\mu^{\text{out}} = \sqrt{r}v_d + \frac{1}{\sqrt{r}}v_n - \mu^{\text{in}} \tag{5.104}$$

(see (2.32)). By Lemma 2.20 and Part (i) of Condition 5.9,

$$v_d(\mathcal{V}_D) = \text{vol}(V_D) \geq c_{\text{ray},1}. \tag{5.105}$$

By the assumption that Condition 5.9 holds (with $c_{\text{ray},2}$ independent of R), $|n(x') \cdot a| \geq c_{\text{ray},2} > 0$ on V_D. By the definitions of V_D (5.100) and $r(x', \xi')$ (1.7), $r(x', (a_{T(x')})^\flat = |n(x') \cdot a|$ for $x' \in V_D$), and thus $r \geq c_{\text{ray},2} > 0$ on $\mathcal{V}_D$. Combining (5.104) with (5.105) and (5.103), and using the facts that v_n is nonnegative and $c_{\text{ray},3}, c_{\text{ray},4} \leq \pi/2$, we have

$$(2\sqrt{r}\mu^{\text{out}})(\mathcal{V}_D) \geq 2rv_d(\mathcal{V}_D) - (2\sqrt{r}\mu^{\text{in}})(\mathcal{V}_D)$$

$$\geq 2\sqrt{c_{\text{ray},2}} \left(\sqrt{c_{\text{ray},2}} - \epsilon \frac{M}{\delta} \left(\frac{\pi}{2}\right)^{\max(2m_{\text{ord}}, m_{\text{mult}})}\right) c_{\text{ray},1}.$$

If

$$\epsilon \leq \frac{\sqrt{c_{\mathrm{ray},2}}}{2} \frac{\delta}{M} \left(\frac{2}{\pi}\right)^{\max(2m_{\mathrm{ord}}, m_{\mathrm{mult}})} \tag{5.106}$$

(observe that, since $c_{\mathrm{ray},2}$ is assumed independent of R, this upper bound on ϵ is independent of R), then

$$(2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_D) \geq c_{\mathrm{ray},2}\, c_{\mathrm{ray},1}.$$

We now use Corollary 2.17 to propagate this lower bound on Γ_D to a lower bound on $\Gamma_{\mathrm{tr},R}$. Indeed, Part (i) of Corollary 2.17 then implies that

$$(2\sqrt{r}\mu^{\mathrm{in}})(\mathcal{V}_{\mathrm{tr}}) = (2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_D) \geq c_{\mathrm{ray},2}\, c_{\mathrm{ray},1}, \tag{5.107}$$

where

$$\mathcal{V}_{\mathrm{tr}} := \bigcup_{q \in \mathcal{V}_D} \pi_{\Gamma_{\mathrm{tr},R}}\big(\varphi_{t^{\mathrm{out}}(q)}\big(p^{\mathrm{out}}(q)\big)\big) \subset \mathcal{H}_{\mathrm{tr}},$$

where t^{out} and p^{out} are defined in (2.38) and (2.37), respectively, and $\pi_{\Gamma_{\mathrm{tr},R}}$ equals $\pi_{\partial M}$ restricted to $T^*_{\Gamma_{\mathrm{tr},R}}\mathbb{R}^d$.

Combining Corollary 2.19, Lemma 5.16, and Point (iii) of Condition 5.9, we have

$$\mu^{\mathrm{out}}(\mathcal{V}_{\mathrm{tr}}) = \left|\frac{\sqrt{r}\sigma(\mathcal{N}) - \sigma(\mathcal{D})}{\sqrt{r}\sigma(\mathcal{N}) + \sigma(\mathcal{D})}\right|^2 \mu^{\mathrm{in}}(\mathcal{V}_{\mathrm{tr}}) \geq \big(C_{\mathrm{ref}} \min\big(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\big)\big)^2 \mu^{\mathrm{in}}(\mathcal{V}_{\mathrm{tr}}). \tag{5.108}$$

Finally, using Part (ii) of Corollary 2.17 with Point (iv) of Condition 5.9, and then using (5.108) and (5.107), we have,

$$\begin{aligned}\mu(\mathcal{I}) &\geq \widetilde{c}_5\, R\, (2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_{\mathrm{tr}}) \geq \widetilde{c}_5\, R\, (2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_{\mathrm{tr}})\\ &\geq \widetilde{c}_5\, R\, \big(C_{\mathrm{ref}} \min\big(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\big)\big)^2 c_{\mathrm{ray},2}\, c_{\mathrm{ray},1}.\end{aligned} \tag{5.109}$$

We now restrict ϵ so that, in addition to satisfying (5.106), ϵ satisfies

$$\epsilon < \widetilde{c}_5\, \big(C_{\mathrm{ref}}\big)^2 c_{\mathrm{ray},2}$$

(observe that, since $\widetilde{c}_5$ and $c_{\mathrm{ray},2}$ are assumed independent of R, this upper bound is independent of R). Thus, ϵ can be chosen sufficiently small (independent of R) such that (5.109) contradicts (5.99), which is the desired contradiction.

Proof of (ii). If the assumption of (ii) holds, then our contradiction argument also assumes that for all $\epsilon > 0$ there exists $R \geq R_0$ such that

$$\mu(\mathcal{I} \cap S^*_{B(0,3/2)}\mathbb{R}^d) \leq \epsilon\big(\min\big(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\big)\big)^2 c_{\mathrm{ray},1}. \tag{5.110}$$

Applying Part (i) of Corollary 2.17 $N_{\mathrm{ref}} - 1$ more times and using (5.108), we construct $\mathcal{V}_{\mathrm{tr}}^1, \ldots, \mathcal{V}_{\mathrm{tr}}^{N_{\mathrm{ref}}} \subset T^* \Gamma_{\mathrm{tr},R}$, satisfying

$$\mathcal{V}_{\mathrm{tr}}^1 := \mathcal{V}_{\mathrm{tr}}, \qquad (2\sqrt{r}\mu^{\mathrm{in}})(\mathcal{V}_{\mathrm{tr}}^{j+1}) = (2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_{\mathrm{tr}}^j),$$

$$(2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_{\mathrm{tr}}^j) \geq \left(C_{\mathrm{ref}} \min\left(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\right)\right)^2 (2\sqrt{r}\mu^{\mathrm{in}})(\mathcal{V}_{\mathrm{tr}}^j), \qquad (5.111)$$

and so that for any $q \in \mathcal{V}_{\mathrm{tr}}^{N_{\mathrm{ref}}}$, $\left\{\varphi_t^{\mathbb{R}^d}(p^{\mathrm{out}}(q))\right\}_{t\geq 0}$ intersects $B(0, \frac{3}{2}) \setminus B(0, \frac{5}{4})$ before hitting Γ_D or $\Gamma_{\mathrm{tr},R}$. Therefore, by (5.111) and (5.107)

$$(2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_{\mathrm{tr}}^N) \geq \left(C_{\mathrm{ref}} \min\left(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\right)\right)^{2N_{\mathrm{ref}}} c_{\mathrm{ray},2}\, c_{\mathrm{ray},1}. \qquad (5.112)$$

Finally, since any ray entering $B(0, \frac{3}{2}) \setminus B(0, \frac{5}{4})$ spends a time at least $\frac{1}{2}(\frac{3}{2} - \frac{5}{4}) = \frac{1}{8}$ in this annulus, Part (ii) of Corollary 2.17 implies that

$$\mu\left(\mathcal{I} \cap S_{B(0,3/2)\setminus B(0,5/4)}^* \mathbb{R}^d\right) \geq \frac{1}{8}(2\sqrt{r}\mu^{\mathrm{out}})(\mathcal{V}_{\mathrm{tr}}^{N_{\mathrm{ref}}})$$

$$\geq \frac{1}{8}\left(C_{\mathrm{ref}} \min\left(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\right)\right)^{2N_{\mathrm{ref}}} c_{\mathrm{ray},2}\, c_{\mathrm{ray},1}, \qquad (5.113)$$

where we have used (5.112). Therefore, if

$$\epsilon < (C_{\mathrm{ref}})^{2N_{\mathrm{ref}}} c_{\mathrm{ray},2},$$

then (5.113) contradicts (5.110), which is the desired contradiction. (Observe that, similar to in Part (i), the upper bound on ϵ is independent of R since $c_{\mathrm{ray},2}$ and C_{ref} are independent of R.) □

Proof of the lower bounds in Theorems 1.7, 1.8, 1.10 *and* 1.11. The lower bounds will follow from combining Corollary 5.4, Lemma 5.17, and the ray constructions in Lemmas 5.10–5.13.

For Theorem 1.8 (for generic $\Gamma_{\mathrm{tr},R}$), Lemma 5.12 implies that the assumptions of Part (i) of Lemma 5.17 are satisfied with $c_{\mathrm{ray},1}, c_{\mathrm{ray},3}, c_{\mathrm{ray},4}$ independent of R, and R_0 sufficiently large; the required lower bound (5.4) on $\mu(\mathcal{I})$ then follows by inserting this (lack of) R-dependence into (5.97).

For the lower bound in Theorem 1.7 (for $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$), Lemma 5.11 implies that the assumptions of Part (i) of Lemma 5.17 are satisfied with $c_{\mathrm{ray},1}, c_{\mathrm{ray},4}$ independent of R, $c_{\mathrm{ray},3} = \widetilde{c}_3/R$ with $\widetilde{c}_3 > 0$ independent of R, and R_0 sufficiently large. The required lower bound (5.3) $\mu(\mathcal{I})$ then follows by inserting these R-dependences into (5.97), and observing that, for R sufficiently large,

$$\min\left(|c_{\mathrm{ray},3}|^{2m_{\mathrm{ord}}}, |c_{\mathrm{ray},4}|^{m_{\mathrm{mult}}}\right) = \left|\frac{\widetilde{c}_3}{R}\right|^{2m_{\mathrm{ord}}}. \qquad (5.114)$$

For Theorem 1.10 (i.e., the local error for $\Gamma_{\mathrm{tr},R} = \partial B(0,R)$), Point (iv)′ in Lemma 5.11 implies that the assumptions of Part (ii) of Lemma 5.17 are satisfied $N_{\mathrm{ref}} = 1$ and R_0 sufficiently large. The required lower bound on $\mu(\mathcal{I} \cap S_{B(0,3/2)}^* \mathbb{R}^d)$ (5.5) then follows from (5.98) using (5.114) and the fact that $c_{\mathrm{ray},1}$ is independent of R. The fact that the result holds with $R_0 = 2$ when $\mathsf{M} = \mathsf{N} = 0$ follows from Remark 5.15.

Finally, for Theorem 1.11 (i.e., the local error for the hypercube), Lemma 5.13 implies that the assumptions of Part (ii) of Lemma 5.17 are satisfied with $c_{\mathrm{ray},3}, c_{\mathrm{ray},4}$ independent of R, $c_{\mathrm{ray},1} = \widetilde{c}_1/R^{d-1}$ with $\widetilde{c}_1$ independent of R, and $R_0 = 4$. The required lower bound on $\mu(\mathcal{I} \cap S^*_{B(0,3/2)}\mathbb{R}^d)$ (5.6) then follows from (5.98) by inserting these R-dependences. □

6. Proof of the trace bounds (Theorem 4.1)

6.1 *Strategy of the proof*

To illustrate some of the main ideas, consider the BVP (4.1) with $\mathcal{N} = \mathcal{D} = I$, $\overline{M}$ compact, and the boundary condition imposed on the whole of ∂M, i.e.,

$$\begin{cases} (-h^2 \Delta - 1)u = hf & \text{in } M \\ hD_n u - u = g & \text{on } \Gamma := \partial M. \end{cases} \tag{6.1}$$

In the notation of Theorem 4.1, we have $m_{0,i} = m_{1,i} = 0$, and the bounds (4.7) and (4.8) in the case $\ell_i = 0$ are that

$$\|u\|_{L^2(\Gamma)} + \|hD_n u\|_{L^2(\Gamma)} \le C\left(\|u\|_{L^2(M)} + \|f\|_{L^2(M)} + \|g\|_{L^2(\Gamma)}\right) \tag{6.2}$$

and

$$\|u\|_{H^1_h(M)} \le C\left(\|u\|_{L^2(M)} + h\|f\|_{L^2(M)} + \|g\|_{L^2(\Gamma)}\right). \tag{6.3}$$

We now show how to obtain these bounds; pairing the PDE in (6.1) with u and integrating by parts, we have

$$h^2 \|\nabla u\|^2_{L^2(M)} - \|u\|^2_{L^2(M)} - h\langle f, u\rangle_{L^2(M)} = hi\|u\|^2_{L^2(\Gamma)} + h\langle g, u\rangle_{L^2(\Gamma)}. \tag{6.4}$$

Taking the imaginary part of (6.4), we find that

$$\|u\|^2_{L^2(\Gamma)} \le \|g\|^2_{L^2(\Gamma)} + \|f\|^2_{L^2(M)} + \|u\|^2_{L^2(M)}. \tag{6.5}$$

Taking the real part of (6.4) and adding $2\|u\|^2_{L^2(M)}$ to both sides of the resulting equation, we find that

$$\|u\|^2_{H^1_h(M)} \le \frac{5}{2}\|u\|^2_{L^2(M)} + \frac{h^2}{2}\|f\|^2_{L^2(M)} + \frac{h^2}{2}\|u\|^2_{L^2(\Gamma)} + \frac{1}{2}\|g\|^2_{L^2(\Gamma)}. \tag{6.6}$$

Combining the inequality (6.5) with the boundary condition in (6.1), we obtain the first result (6.2). Then, using (6.5) in (6.6), we obtain the second result (6.3).

The proof of Theorem 4.1 follows similar steps; indeed, the two main ingredients are (i) bounds on the traces in terms of the data and H^1_h norms of u, and (ii) a bound the H^1_h norm of u in term of the traces and the data. The bound in (ii) is obtained by considering $\Re\langle(-h^2\Delta_g - 1)u, u\rangle_{L^2(M)}$ and integrating by parts, similar to above, with the inequality (6.19) the generalization of the inequality (6.6). The bounds in (i) are obtained by considering $\Im\langle(-h^2\Delta_g-1)u, u\rangle_{L^2(M)}$, similar to above, but also $\Im\langle(-h^2\Delta_g-1)u, hD_\nu u\rangle_{L^2(M)}$

(with Lemma 2.6 above considering a general commutator, and Lemma 6.1 specializing to the case of a normal derivative).

The additional complications for the bounds in (i) are because we need to consider the cases where $\mathcal{D}$ and $\mathcal{N}$ are both elliptic (Lemma 6.2), where $\mathcal{D}$ is small and $\mathcal{N}$ elliptic (Lemma 6.3), and where $\mathcal{D}$ is elliptic and $\mathcal{N}$ small (Lemma 6.4), These three cases are considered in § 6.2, and then in § 6.3 we show that, under the assumptions (4.3)–(4.5), the bounds in these three cases cover all of $T^*\Gamma$.

6.2 A priori *estimates*

We begin by proving some *a-priori* estimates for (4.1). As usual, we work near Γ where M is locally given by $x_1 > 0$, as in § 2.3. We repeatedly use the integration by parts result in Lemma 2.6.

LEMMA 6.1 If u solves (4.1), then, for all $\epsilon > 0$ and for all ℓ,

$$\|hD_{x_1}u\|_{H_h^\ell(\Gamma_i)} \leq C\big(\|u\|_{H_h^{\ell+1}(\Gamma_i)} + \|u\|_{H_h^{\ell+1}(M)} + \epsilon^{-1}\|f\|_{H_h^\ell(M)} + \epsilon\|u\|_{H_h^1(M)}\big).$$

Proof. Let $\chi \in C_c^\infty((-2\delta, 2\delta); [0, 1])$ with $\chi \equiv 1$ on $[-\delta, \delta]$. Let

$$B_1(x, hD_{x'}) := \chi(x_1)\langle hD_{x'}\rangle^{2\ell} \quad \text{and} \quad B_0(x, hD_{x'}) := \frac{1}{2}hD_{x_1}B_1 = \frac{h}{2i}\chi'(x_1)\langle hD_{x'}\rangle^{2\ell}.$$

Then (2.11) holds, and B satisfies the assumption of Lemma 2.6; since $B_0|_{x_1=0} = 0$, (2.12) implies that

$$\frac{i}{h}\langle[P, B]u, u\rangle_{L^2(M)} + \frac{2}{h}\Im\langle Pu, Bu\rangle_{L^2(M)} = \langle h(B_1a_1 - \overline{a_1}B_1)hD_{x_1}u, u\rangle_{L^2(\Gamma_i)}$$
$$+ \langle B_1(R - ha_0)u, u\rangle_{L^2(\Gamma_i)} + \langle B_1hD_{x_1}u, hD_{x_1}u\rangle_{L^2(\Gamma_i)}. \quad (6.7)$$

Now, observe that

$$[P, B] = h(\widetilde{B}_2(hD_{x_1})^2 + \widetilde{B}_1hD_{x_1} + \widetilde{B}_0),$$

where

$$\widetilde{B}_2 \in C_c^\infty((\delta, 2\delta); \Psi^{2\ell}(\Gamma_i)), \quad \widetilde{B}_1 \in C_c^\infty((\delta, 2\delta); \Psi^{2\ell+1}(\Gamma_i)), \quad \widetilde{B}_0 \in C_c^\infty((-2\delta, 2\delta); \Psi^{2\ell+2}(\Gamma_i)).$$

In particular, by boundary elliptic regularity, we have

$$\big\|[P, B]u\big\|_{H_h^s(M)} \leq C_sh\big(\|Pu\|_{H_h^{s+2\ell}(M)} + \|u\|_{H_h^{s+2\ell}(M)}\big).$$

Therefore,

$$\left| \langle B_1(1 - R)u, u\rangle_{L^2(\Gamma_i)} + \langle B_1hD_{x_1}u, hD_{x_1}u\rangle_{L^2(\Gamma_i)} \right|$$
$$\leq Ch\|u\|_{H_h^\ell(\Gamma_i)}^2 + C\|u\|_{H_h^\ell(M)}^2 + C\epsilon^{-1}\|f\|_{H_h^\ell}^2 + \epsilon\|u\|_{H_h^1(M)}^2,$$

and hence

$$\|hD_{x_1}u\|^2_{H_h^\ell} \le C\|u\|^2_{H_h^{\ell+1}(\Gamma_i)} + C\|u\|^2_{H_h^\ell(M)} + C\epsilon^{-1}\|f\|^2_{H_h^\ell} + \epsilon\|u\|^2_{H_h^1(M)}.$$

$\square$

REMARK. When $\ell = 0$ the bound in Lemma 6.1 is valid for Lipschitz domains and goes back to Nečas; see (Nečas, 1967, §5.1.2), (McLean, 2000, Theorem 4.24 (i)).

We now show a bound where $\mathcal{D}$ and $\mathcal{N}$ are both elliptic.

LEMMA 6.2 Suppose that $\mathrm{WF}_h(E) \subset \mathrm{Ell}(\mathcal{D}) \cap \mathrm{Ell}(\mathcal{N})$. Then for any $B' \in \Psi^0$ with

$$\mathrm{WF}_h(E) \cap \mathrm{WF}_h(\mathrm{Id} - B') = \emptyset, \qquad \mathrm{WF}_h(B') \subset \mathrm{Ell}(\mathcal{N}) \cap \mathrm{Ell}(\mathcal{D})$$

there exist $C > 0$ and $h_0 > 0$ such that for any $\epsilon > 0, 0 < h < h_0$,

$$\|Eu\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|EhD_{x_1}u\|_{H_h^{\ell+m_1}(\Gamma_i)}$$

$$\le C\left(\|u\|_{H_h^{\frac{2\ell+m_1+m_0+1}{2}}(M)} + \|u\|_{L^2(M)} + \|f\|_{H_h^{\frac{2\ell+m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)}\right)$$

$$+ \epsilon\left(\|B'u\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|B'hD_{x_1}u\|_{H_h^{\ell+m_1}(\Gamma_i)}\right) + C\epsilon^{-1}\|B'g_i\|_{H_h^\ell(\Gamma_i)}$$

$$+ O\left(h^\infty\left(\|u\|_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)}\right)\right).$$

Proof. Let $B_0 \in \Psi^{\ell_0}(\Gamma_i)$ self-adjoint with $\mathrm{WF}_h(b_0(x', hD_{x'})) \subset \mathrm{WF}_h(E)$. Let $B' \in \Psi^0(\Gamma_i)$ with

$$\mathrm{WF}_h(E) \subset \mathrm{Ell}(B') \subset \mathrm{WF}_h(B') \subset \mathrm{Ell}(\mathcal{N}) \cap \mathrm{Ell}(\mathcal{D}).$$

We can assume without loss of generality that B' is microlocally the identity in a neighbourhood of $\mathrm{WF}_h(E)$. Next, let $B_1 = 0$ and $\mathcal{N}^{-1}$ and $\mathcal{D}^{-1}$ denote microlocal inverses for $\mathcal{N}$ and $\mathcal{D}$ on $\mathrm{WF}_h(B')$. Then, by Lemma 2.6,

$$\left|\langle B_0 hD_{x_1}u, u\rangle_{L^2(\Gamma_i)} + \langle h\overline{a_1}B_0 u, u\rangle_{L^2(\Gamma_i)} + \langle B_0 u, hD_{x_1}u\rangle_{L^2(\Gamma_i)}\right|$$
$$\le |2\langle f, Bu\rangle_{L^2(M)}| + h^{-1}|\langle [P, B]u, u\rangle_{L^2(M)}|.$$

First, note that

$$[P, B] = h(\widetilde{B}_1 hD_{x_1} + \widetilde{B}_2),$$

where

$$\widetilde{B}_1 \in C_c^\infty\big((\delta, 2\delta); \Psi^{\ell_0}(\Gamma_i)\big), \qquad \widetilde{B}_2 \in C_c^\infty\big((-2\delta, 2\delta); \Psi^{\ell_0+1}(\Gamma_i)\big).$$

In particular, by boundary elliptic regularity, for all $s \in \mathbb{R}$,

$$\|[P, B]\|_{H_h^s(M)} \leq C_s h \Big(\|Pu\|_{H_h^{s+\ell_0-1}(M)} + \|u\|_{H_h^{s+\ell_0+1}(M)} + \|u\|_{L^2(M)} \Big).$$

Therefore,

$$\Big| \langle B_0 h D_{x_1} u, u \rangle_{L^2(\Gamma_i)} + \langle h \overline{a_1} B_0 u, u \rangle_{L^2(\Gamma_i)} + \langle B_0 u, h D_{x_1} u \rangle_{L^2(\Gamma_i)} \Big|$$

$$\leq C \left(\|f\|_{H_h^{\frac{\ell_0-1}{2}}(M)} + \|u\|_{H_h^{\frac{\ell_0+1}{2}}(M)} + \|u\|_{L^2(M)} + \|f\|_{L^2(M)} \right) \left(\|u\|_{H_h^{\frac{\ell_0+1}{2}}(M)} + \|u\|_{L^2(M)} \right).$$

Now, using (4.1),

$$\langle B_0 h D_{x_1} u, u \rangle_{L^2(\Gamma_i)} = \langle B_0 \mathcal{N}^{-1}(\mathcal{D}u + g_i), u \rangle_{L^2(\Gamma_i)} + O\Big(h^\infty \Big(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)}^2 \Big) \Big)$$

and

$$\langle B_0 u, h D_{x_1} u \rangle_{L^2(\Gamma_i)} = \langle B_0 u, \mathcal{N}^{-1}(\mathcal{D}u + g_i) \rangle_{L^2(\Gamma_i)} + O\Big(h^\infty \Big(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)}^2 \Big) \Big).$$

In particular, letting $B' \in \Psi^0$ with $\mathrm{WF}_h(B_0) \subset \mathrm{Ell}(B')$,

$$\Big| \langle [(\mathcal{N}^{-1}\mathcal{D})^* B_0 + B_0(\mathcal{N}^{-1}\mathcal{D})]u, u \rangle_{L^2(\Gamma_i)} \Big|$$

$$\leq C \left(\|f\|_{H_h^{\frac{\ell_0-1}{2}}(M)} + \|f\|_{L^2(M)} + \|u\|_{H_h^{\frac{\ell_0+1}{2}}(M)} + \|u\|_{L^2(M)} \right) \left(\|u\|_{H_h^{\frac{\ell_0+1}{2}}(M)} + \|u\|_{L^2(M)} \right)$$

$$+ O(h) \|B'u\|_{H_h^{\frac{\ell_0}{2}}(\Gamma_i)}^2 + \epsilon \|B'u\|_{H_h^{\frac{m_0-m_1+\ell_0}{2}}(\Gamma_i)}^2 + C\epsilon^{-1} \|B'g_i\|_{H_h^{\frac{\ell_0-m_1-m_0}{2}}(\Gamma_i)}^2$$

$$+ O\Big(h^\infty \Big(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)}^2 + \|g\|_{H_h^{-N}(\Gamma_i)}^2 \Big) \Big).$$

Now, choose $b_0(x', h D_{x'}) \in \Psi^{m_1-m_0+2\ell}$ self adjoint (i.e., $\ell_0 = m_1 - m_0 + 2\ell$) such that B_0 is elliptic on $\mathrm{WF}_h(E)$. Then, since $\mathcal{D}$ and $\mathcal{N}$ have real-valued symbols and $-\mathcal{N}^{-1}\mathcal{D}$ is elliptic on $\mathrm{WF}_h(E)$,

$$-\Re \langle B_0 \mathcal{N}^{-1}\mathcal{D}u, u \rangle \geq C \|Eu\|_{H_h^\ell(\Gamma_i)}^2 - Ch \|B'u\|_{H_h^{\frac{\ell-1}{2}}(\Gamma_i)}^2 - O(h^\infty) \|u\|_{H_h^{-N}(M)}^2,$$

and

$$\|Eu\|_{H_h^\ell}^2 \le C\left(\|f\|_{H_h^{\frac{m_1-m_0+2\ell-1}{2}}(M)} + \|f\|_{L^2(M)} + \|u\|_{H_h^{\frac{m_1-m_0+2\ell+1}{2}}(M)} + \|u\|_{L^2(M)}\right)$$
$$\times\left(\|u\|_{H_h^{\frac{m_1-m_0+2\ell+1}{2}}(M)} + \|u\|_{L^2(M)}\right)$$
$$+ O(h)\|B'u\|_{H_h^{\frac{m_1-m_0+2\ell}{2}}(\Gamma_i)}^2 + \epsilon\|B'u\|_{H_h^\ell(\Gamma_i)}^2 + C\epsilon^{-1}\|B'g_i\|_{H_h^{k-m_0}(\Gamma_i)}^2$$
$$+ O\left(h^\infty\left(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)}^2 + \|g\|_{H_h^{-N}(\Gamma_i)}^2\right)\right). \tag{6.8}$$

Let $E' \in \Psi^0$ with

$$\mathrm{WF}_h(E) \cap \mathrm{WF}_h(\mathrm{Id} - E') = \emptyset, \qquad \mathrm{WF}_h(E') \subset \mathrm{Ell}(B') \cap \mathrm{Ell}(\mathcal{N}) \cap \mathrm{Ell}(\mathcal{D}).$$

By (6.8),

$$\|E'u\|_{H_h^\ell(\Gamma_i)}^2 \le C\left(\|u\|_{H_h^{\frac{m_1-m_0+2\ell+1}{2}}(M)}^2 + \|u\|_{L^2(M)}^2 + C\left(\|f\|_{H_h^{\frac{m_1-m_0+2\ell-1}{2}}(M)}^2 + \|f\|_{L^2(M)}^2\right)\right)$$
$$+ O(h)\|B'u\|_{H_h^{\frac{2\ell-m_0+m_1}{2}}(\Gamma_i)}^2 + \epsilon\|B'u\|_{H_h^\ell(\Gamma_i)}^2 + C\epsilon^{-1}\|B'g_i\|_{H_h^{k-m_0}(\Gamma_i)}^2$$
$$+ O\left(h^\infty\left(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)}^2 + \|g\|_{H_h^{-N}(\Gamma_i)}^2\right)\right).$$

Let $\mathcal{N}^{-1}$ denote a microlocal inverse for $\mathcal{N}$ on $\mathrm{WF}_h(B')$. Then,

$$EhD_{x_1}u = E\left(\mathcal{N}^{-1}(-\mathcal{D}E'u + B'g_i)\right) + O\left(h^\infty\|u\|_{H_h^{-N}(\Gamma_i)}\right)_{H_h^N},$$

so

$$\|EhD_{x_1}u\|_{H_h^\ell(\Gamma_i)} \le C\|E'u\|_{H_h^{\ell+m_0-m_1}} + \|B'g_i\|_{H_h^{k-m_1}} + O\left(h^\infty\|u\|_{H_h^{-N}(\Gamma_i)}\right).$$

In particular,

$$\|EhD_{x_1}u\|_{H_h^\ell}^2 \le C\left(\|u\|_{H_h^{\frac{m_0-m_1+2\ell+1}{2}}(M)}^2 + \|u\|_{L^2(M)}^2 + \|f\|_{H_h^{\frac{m_0-m_1+2\ell-1}{2}}(M)}^2 + \|f\|_{L^2(M)}^2\right)$$
$$+ O(h)\|B'u\|_{H_h^{\frac{2\ell+m_0-m_1}{2}}(\Gamma_i)}^2 + \epsilon\|B'hD_{x_1}u\|_{H_h^\ell(\Gamma_i)}^2 + C\epsilon^{-1}\|B'g_i\|_{H_h^{k-m_1}(\Gamma_i)}^2$$
$$+ O\left(h^\infty\left(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)}^2 + \|g\|_{H_h^{-N}(\Gamma_i)}^2\right)\right).$$

$\square$

We now consider $\mathcal{D}$ small and $\mathcal{N}$ elliptic:

LEMMA 6.3 Let $K \Subset T^*\Gamma_i$. Then for all $\eta > 0$ there is $\delta_0 > 0$ and $C > 0$ such that for all $0 < \delta < \delta_0$, $E \in \Psi^0$ with

$$\mathrm{WF}_\mathrm{h}(E) \subset K \cap \mathrm{Ell}(\mathcal{N}) \cap \left\{ |\sigma(\mathcal{D})| < \delta\langle\xi\rangle^{m_0} \right\} \cap \left\{ |R(x', \xi')| > \eta \right\}, \tag{6.9}$$

and $B' \in \Psi^0$ with

$$\mathrm{WF}_\mathrm{h}(E) \cap \mathrm{WF}_\mathrm{h}(\mathrm{Id} - B') = \emptyset, \qquad \mathrm{WF}_\mathrm{h}(B') \subset \mathrm{Ell}(\mathcal{N}) \cap \left\{ |\sigma(\mathcal{D})| < \delta\langle\xi\rangle^{m_0} \right\},$$

there is $h_0 > 0$ small enough such that for all $0 < h < h_0$ and $0 < \epsilon < 1$

$$\|Eu\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|EhD_{x_1}u\|_{H_h^{\ell+m_1}(\Gamma_i)}$$

$$\leq C(\epsilon + h)\|B'u\|_{H_h^{\ell+m_0}(\Gamma_i)} + C(\epsilon^{-1} + 1)\|B'g\|_{H_h^\ell(\Gamma_i)}$$

$$+ C\|u\|_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1}\left(\|f\|_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)} \right) + C\epsilon\|u\|_{H_h^1(M)}$$

$$+ O\left(h^\infty \left(\|u\|_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)} \right) \right). \tag{6.10}$$

Moreover, if $m_0 \leq m_1 + 1$ (6.10) holds with $K = T^*\Gamma_i$

Proof. Throughout the proof, we take $b_1(x', hD_{x'})$ self-adjoint with $b_1 \in \Psi^{2(k+m_0-1)}$ if $m_0 \leq m_1 + 1$ and $b_1 \in \Psi^{\mathrm{comp}}$ otherwise. We assume that

$$\mathrm{WF}_\mathrm{h}(E) \subset \mathrm{Ell}(b_1(x', hD_{x'})) \subset \mathrm{WF}_\mathrm{h}(b_1(x', hD_{x'})) \subset \mathrm{Ell}(\mathcal{N}) \cap \left\{ |\sigma(\mathcal{D})| < \delta\langle\xi\rangle^{m_0} \right\}.$$

As in Lemma 6.1, let $\chi \in C_c^\infty((-2\delta, 2\delta); [0, 1])$ with $\chi \equiv 1$ on $[-\delta, \delta]$. Let

$$B_1(x, hD_{x'}) := \chi(x_1)b_1(x', hD_{x'}) \quad \text{and} \quad B_0(x', hD_{x'}) := \frac{1}{2}hD_{x_1}B_1. \tag{6.11}$$

Then (2.11) holds, and B satisfies the assumption of Lemma 2.6; since $B_0|_{x_1=0} = 0$, (2.12) implies that (6.7) holds.

Since $\mathcal{N}$ is elliptic on $\mathrm{WF}_\mathrm{h} B'$, there exists $\mathcal{N}^{-1} \in \Psi^{-m_1}$ a microlocal inverse for $\mathcal{N}$ on $\mathrm{WF}_\mathrm{h}(B')$; that is, for any $\widetilde{B}$ with $\mathrm{WF}_\mathrm{h}(\widetilde{B}) \subset \{B' \equiv \mathrm{Id}\}$,

$$\widetilde{B}hD_{x_1}u = \widetilde{B}\mathcal{N}^{-1}(\mathcal{D}B'u + B'g) + O(h^\infty)_{\Psi^{-\infty}}g + O(h^\infty)_{\Psi^{-\infty}}u + O(h^\infty)_{\Psi^{-\infty}}hD_{x_1}u. \tag{6.12}$$

and hence, using the fact that we are working with compactly microlocalized operators on Γ to see that all $H_h^s(\Gamma_i)$ norms are equivalent up to h^∞ remainders, we have

$$
\begin{aligned}
&\left|\langle B_1 R u, u\rangle_{L^2(\Gamma_i)} + \langle B_1 h D_{x_1} u, h D_{x_1} u\rangle_{L^2(\Gamma_i)}\right| \\
&\quad \leq C h \|B' u\|^2_{H_h^{\ell+m_0}(\Gamma_i)} + C h \|B' g\|^2_{H_h^\ell(\Gamma_i)} + \left|i h^{-1}\langle [P, B] u, u\rangle_{L^2(M)} + 2\Im\langle f, B u\rangle_{L^2(M)}\right| \\
&\qquad + O\left(h^\infty\left(\|u\|^2_{H_h^{-N}(\Gamma_i)} + \|h D_{x_1} u\|^2_{H_h^{-N}(\Gamma_i)} + \|g\|^2_{H_h^{-N}(\Gamma_i)}\right)\right).
\end{aligned}
\tag{6.13}
$$

Now, observe that

$$
[P, B] = h\left(\widetilde{B}_2 (h D_{x_1})^2 + \widetilde{B}_1 h D_{x_1} + \widetilde{B}_0\right),
$$

where

$$
\widetilde{B}_2 \in C_c^\infty((\delta, 2\delta); \Psi^{2(k+m_0-1)}(\Gamma_i)), \quad \widetilde{B}_1 \in C_c^\infty((\delta, 2\delta); \Psi^{2(k+m_0)-1}(\Gamma_i)),
$$
$$
\widetilde{B}_0 \in C_c^\infty((-2\delta, 2\delta); \Psi^{2(k+m_0)}(\Gamma_i)).
$$

In particular, by boundary elliptic regularity as before, we have

$$
\|[P, B] u\|_{H_h^s(M)} \leq C_s h\left(\|P u\|_{H_h^{s+2(k+m_0)}(M)} + \|u\|_{H_h^{s+2(k+m_0)}(M)} + \|u\|_{L^2(M)}\right),
$$

so by (6.12) and (6.13),

$$
\begin{aligned}
&\left|\langle B_1 R u, u\rangle_{L^2(\Gamma_i)} + \langle B_1 \mathcal{N}^{-1}\mathcal{D} u, \mathcal{N}^{-1}\mathcal{D} u\rangle_{L^2(\Gamma_i)}\right| \\
&\quad \leq C(\epsilon + h)\|B' u\|^2_{H_h^{\ell+m_0}(\Gamma_i)} + C(\epsilon^{-1} + 1)\|B' g\|^2_{H_h^\ell(\Gamma_i)} \\
&\qquad + C\|u\|^2_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1}\left(\|f\|^2_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|^2_{L^2(M)}\right) + C\epsilon\|u\|^2_{H_h^1(M)} \\
&\qquad + O\left(h^\infty\left(\|u\|^2_{H_h^{-N}(\Gamma_i)} + \|h D_{x_1} u\|^2_{H_h^{-N}(\Gamma_i)} + \|g\|^2_{H_h^{-N}(\Gamma_i)}\right)\right).
\end{aligned}
\tag{6.14}
$$

If $m_0 > m_1 + 1$, we assume that $b_1 \in S^{\text{comp}}$. Therefore, for all (m_0, m_1)

$$
B_1 R + (\mathcal{N}^{-1}\mathcal{D})^* B_1 \mathcal{N}^{-1}\mathcal{D} \in \Psi^{2(\ell+m_0)},
$$

for our choice of B_1. Next, since $\mathcal{D}$ is elliptic on $\{R = 0\}$, for any $K \subset T^*\Gamma_i$ compact, there exists $\delta_0 > 0$ small enough such that

$$
\inf\left\{\langle \xi'\rangle^{-2}\left|\sigma(\mathcal{N}^{-1}\mathcal{D})(x', \xi')\right|^2 + R(x', \xi')\right| \text{ where } |\sigma(\mathcal{D})(x', \xi')| \leq \delta_0\langle \xi'\rangle^{m_0}, (x', \xi') \in K\right\} \geq c_K > 0.
$$

Moreover, if $m_0 \leq m_1 + 1$, then there is $\delta_0 > 0$ small enough such that

$$\inf \left\{ \langle \xi' \rangle^{-2} \left| \sigma(\mathcal{N}^{-1}\mathcal{D})(x', \xi') \right|^2 + R(x, \xi) \right| \text{ where } |\sigma(\mathcal{D})(x', \xi')| \leq \delta_0 \langle \xi' \rangle^{m_0}, \, (x', \xi') \in T^*\Gamma_i \right\} \geq c > 0.$$

In particular, since R is real-valued, there is $B_1 \in \Psi^{2(k+m_0-1)}$ self adjoint, elliptic on $\mathrm{WF}_h(E)$, such that

$$\sigma\big(B_1 R + (\mathcal{N}^{-1}\mathcal{D})^* B_1 \mathcal{N}^{-1}\mathcal{D}\big)(x', \xi') \geq c \langle \xi' \rangle^{2(k+m_0)}, \qquad (x', \xi') \in \mathrm{WF}_h(E).$$

In particular, then the sharp Gårding inequality (Zworski, 2012, Theorem 9.11) gives

$$\|Eu\|^2_{H_h^{\ell+m_0}(\Gamma_i)} \leq C \big\langle \big(B_1 R + (\mathcal{N}^{-1}\mathcal{D})\big)^* B_1 \mathcal{N}^{-1}\mathcal{D}\big)u, u \big\rangle_{L^2(\Gamma_i)} + Ch\|B'u\|^2_{H_h^{\ell+m_0-\frac{1}{2}}} + O(h^\infty)\|u\|^2_{H_h^{-N}(\Gamma_i)},$$

and we obtain from (6.14),

$$\begin{aligned}
\|Eu\|^2_{H_h^{\ell+m_0}(\Gamma_i)} \leq \ & C(\epsilon + h)\|B'u\|^2_{H_h^{\ell+m_0}(\Gamma_i)} + C(\epsilon^{-1} + 1)\|B'g\|^2_{H_h^\ell(\Gamma_i)} \\
& + C\|u\|^2_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1}\left(\|f\|^2_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|^2_{L^2(M)}\right) + C\epsilon\|u\|^2_{H_h^1(M)} \\
& + O\Big(h^\infty\Big(\|u\|^2_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|^2_{H_h^{-N}(\Gamma_i)} + \|g\|^2_{H_h^{-N}(\Gamma_i)}\Big)\Big).
\end{aligned}$$

Next, we write, as above,

$$EhD_{x_1}u = E\mathcal{N}^{-1}(\mathcal{D}E'u + E'g) + O(h^\infty)_{\Psi^{-\infty}}g + O(h^\infty)_{\Psi^{-\infty}}u + O(h^\infty)_{\Psi^{-\infty}}hD_{x_1}u$$

to obtain

$$\begin{aligned}
\|EhD_{x_1}u\|^2_{H_h^{\ell+m_1}(\Gamma_i)} \leq \ & C\|E'u\|_{H_h^{\ell+m_0}(\Gamma_i)} + C\|E'g\|_{H_h^\ell(\Gamma_i)} \\
& + O\Big(h^\infty\Big(\|u\|_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)}\Big)\Big),
\end{aligned}$$

and this finishes the proof. $\qquad\qquad\square$

Finally, we consider the case $\mathcal{D}$ elliptic and $\mathcal{N}$ small.

LEMMA 6.4 For all $K \Subset T^*\Gamma_i$, there is $\delta_0 > 0$ and $C > 0$ such that for all $0 < \delta < \delta_0$, $E \in \Psi^0$ with

$$\mathrm{WF}_h(E) \subset K \cap \mathrm{Ell}(\mathcal{D}) \cap \big\{|\sigma(\mathcal{N})| < \delta \langle \xi \rangle^{m_1}\big\}, \tag{6.15}$$

and $B' \in \Psi^0$ with

$$\mathrm{WF}_h(E) \cap \mathrm{WF}_h(I - B') = \emptyset, \qquad \mathrm{WF}_h(B') \subset \mathrm{Ell}(\mathcal{D}) \cap \big\{|\sigma(\mathcal{N})| < \delta \langle \xi \rangle^{m_1}\big\},$$

there is $h_0 > 0$ small enough such that have for $0 < h < h_0$ and $0 < \epsilon < 1$,

$$
\|EhD_{x_1}u\|_{H_h^{\ell+m_1}(\Gamma_i)} + \|Eu\|_{H_h^{\ell+m_0}(\Gamma_i)}
$$

$$
\leq C\epsilon \|B'hD_{x_1}\|_{H_h^{\ell+m_1}(\Gamma_i)} + C\epsilon^{-1}\|B'g\|_{H_h^{\ell}(\Gamma_i)}
$$

$$
+ C\|u\|_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1}\left(\|f\|_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)}\right) + C\epsilon\|u\|_{H_h^1(M)}
$$

$$
+ O\left(h^\infty\left(\|u\|_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)}\right)\right). \tag{6.16}
$$

Moreover, if $m_1 + 1 \leq m_0$, then (6.16) holds with $K = T^*\Gamma_i$.

Proof. Throughout the proof, we take $b_1(x', hD_{x'})$ self-adjoint with $b_1 \in \Psi^{2(k+m_0)}$ if $m_1 + 1 \leq m_0$ and $b_1 \in \Psi^{\text{comp}}$ otherwise. We assume that

$$
\mathrm{WF}_h(E) \subset \mathrm{Ell}(b_1(x', hD_{x'})) \subset \mathrm{WF}_h(b_1(x', hD_{x'})) \subset \mathrm{Ell}(\mathcal{D}) \cap \left\{|\sigma(\mathcal{N})| < \delta\langle\xi\rangle^{m_1}\right\}.
$$

Let B_1 and B_0 be defined by (6.11).

Since $\mathcal{D}$ is elliptic on $\mathrm{WF}_h(B')$, there exists $\mathcal{D}^{-1} \in \Psi^{-m_0}$ a microlocal inverse for $\mathcal{D}$ on $\mathrm{WF}_h(B')$; that is, for any B with $\mathrm{WF}_h(B) \subset \{B' \equiv \mathrm{Id}\}$,

$$
Bu = -B\mathcal{D}^{-1}(\mathcal{N}hD_{x_1}B'u - B'g) + O(h^\infty)_{\Psi^{-\infty}}g + O(h^\infty)_{\Psi^{-\infty}}u + O(h^\infty)_{\Psi^{-\infty}}hD_{x_1}u. \tag{6.17}
$$

Arguing as in the proof of Lemma 6.3, we obtain the analogue of (6.14) with $B_1 \in \Psi^{2(k+m_1)}(\Gamma_i)$, namely

$$
\left|\langle B_1 R\mathcal{D}^{-1}\mathcal{N}hD_{x_1}u, \mathcal{D}^{-1}\mathcal{N}hD_{x_1}u\rangle_{L^2(\Gamma_i)} + \langle B_1 hD_{x_1}u, hD_{x_1}u\rangle_{L^2(\Gamma_i)}\right|
$$

$$
\leq C(\epsilon + h)\|B'hD_{x_1}\|^2_{H_h^{\ell+m_1}(\Gamma_i)} + C(\epsilon^{-1} + 1)\|B'g\|^2_{H_h^{\ell}(\Gamma_i)}
$$

$$
+ C\|u\|^2_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1}\left(\|f\|^2_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|^2_{L^2(M)}\right) + C\epsilon\|u\|^2_{H_h^1(M)}
$$

$$
+ O\left(h^\infty\left(\|u\|^2_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|^2_{H_h^{-N}(\Gamma_i)} + \|g\|^2_{H_h^{-N}(\Gamma_i)}\right)\right).
$$

If $m_0 < m_1 + 1$, we assume that $b_1 \in S^{\text{comp}}$. Therefore, for all (m_0, m_1)

$$
\left(\mathcal{D}^{-1}\mathcal{N}\right)^* B_1(1 - R)\mathcal{D}^{-1}\mathcal{N} + B_1 \in \Psi^{2(\ell+m_1)}
$$

for our choice of B_1. Now, any $K \subset T^*\Gamma_i$ compact, there is $\delta_0 > 0$ small enough such that

$$
\inf\left\{\left|1 + \left|\sigma(\mathcal{D}^{-1}\mathcal{N})(x',\xi')\right|^2 R(x',\xi')\right| \text{ where } |\sigma(\mathcal{N})(x',\xi')| \leq \delta_0\langle\xi'\rangle^{m_1}, (x',\xi') \in K\right\} \geq c_K > 0.
$$

Moreover, if $m_0 \leq m_1 + 1$, then there is $\delta_0 > 0$ small enough such that

$$\inf\left\{\left|1 + \left|\sigma(\mathcal{D}^{-1}\mathcal{N})(x',\xi')\right|^2 R(x',\xi')\right| \text{ where } |\sigma(\mathcal{N})(x',\xi')| \leq \delta_0\langle\xi'\rangle^{m_1}, (x',\xi') \in T^*\Gamma_i\right\} \geq c > 0.$$

Therefore, choosing B_1 with non-negative symbol such that B_1 is elliptic on $\mathrm{WF}_\mathrm{h}(E)$, we have

$$\Re\sigma\left((\mathcal{D}^{-1}\mathcal{N})^*B_1 R\mathcal{D}^{-1}\mathcal{N} + B_1\right)(x',\xi') \geq c, \qquad (x',\xi') \in \mathrm{WF}_\mathrm{h}(E).$$

In particular,

$$\|EhD_{x_1}u\|^2_{H_h^{\ell+m_1}(\Gamma_i)} \leq C\big(((\mathcal{D}^{-1}\mathcal{N})^*B_1 R\mathcal{D}^{-1}\mathcal{N} + B_1)hD_{x_1}u, hD_{x_1}u\big)_{L^2(\Gamma_i)}$$
$$+ Ch\|B'u\|^2_{H_h^{\ell+m_1-\frac{1}{2}}} + O(h^\infty)\|hD_{x_1}u\|^2_{H_h^{-N}(\Gamma_i)}.$$

Therefore,

$$\|EhD_{x_1}u\|^2_{H_h^{\ell+m_1}(\Gamma_i)} \leq C(\epsilon+h)\|B'hD_{x_1}\|^2_{H_h^{\ell+m_1}(\Gamma_i)} + C(\epsilon^{-1}+1)\|B'g\|^2_{H_h^\ell(\Gamma_i)}$$
$$+ C\|u\|^2_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1}\left(\|f\|^2_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|^2_{L^2(M)}\right)$$
$$+ C\epsilon\|u\|^2_{H_h^1(M)} + O\left(h^\infty\left(\|u\|^2_{H_h^{-N}(\Gamma_i)} + \|hD_{x_1}u\|^2_{H_h^{-N}(\Gamma_i)} + \|g\|^2_{H_h^{-N}(\Gamma_i)}\right)\right).$$

Then, using (6.17) again the second claim follows. $\qquad\qquad\square$

6.3 *Proof of Theorem* 4.1

Throughout this section we assume that (4.2) holds. In particular, the union of the elliptic sets for $A_{0,i}$ and $A_{1,i}$ covers $T^*\Gamma_i$ and $A_{0,i}$ is elliptic on $S^*\Gamma_i$.

Proof. We start by briefly considering the conditions (4.3)–(4.5) separately. Suppose first that (4.3) holds. Then, fixing $\delta_0 > 0$, such that Lemmas 6.3 and 6.4 with $K = T^*\Gamma_i$ hold, there exist $E_0 \in \Psi^0$ satisfying (6.9) and $E_1 \in \Psi^0$ satisfying (6.15) (both with $K = T^*\Gamma_i$) such that

$$\{\sigma(\mathcal{D}) = 0\} \subset \mathrm{Ell}(E_0), \qquad \{\sigma(\mathcal{N}) = 0\} \subset \mathrm{Ell}(E_1), \qquad T^*\Gamma_i \subset \mathrm{Ell}(E_0) \cup \mathrm{Ell}(E_1).$$

Next, if (4.4) holds, there exists $K_2 \Subset T^*\Gamma_i$ such that

$$K_2 \cup \mathrm{Ell}(\mathcal{N}) \supset T^*\Gamma_i.$$

Fixing $\delta_0 > 0$, such that Lemma 6.3 holds with $K = T^*\Gamma_i$ and 6.4 holds with $K = K_2$, there exist $E_0 \in \Psi^0$ satisfying (6.9) with $K = T^*\Gamma_i$ and $E_1 \in \Psi^{\mathrm{comp}}$ satisfying (6.15) with $K = K_2$ such that

$$\{\sigma(\mathcal{D}) = 0\} \subset \mathrm{Ell}(E_0), \qquad \{\sigma(\mathcal{N}) = 0\} \subset \mathrm{Ell}(E_1), \qquad T^*\Gamma_i \subset \mathrm{Ell}(E_0) \cup \mathrm{Ell}(E_1).$$

Finally, if (4.5) holds, there exists $K_3 \subset T^* \Gamma_i$ such that

$$K_3 \cup \mathrm{Ell}(\mathcal{D}) \supset T^* \Gamma_i.$$

Fixing $\delta_0 > 0$, such that Lemma 6.3 holds with $K = K_3$ and 6.4 holds with $K = T^* \Gamma_i$, there exist $E_0 \in \Psi^{\mathrm{comp}}$ satisfying (6.9) with $K = K_3$ and $E_1 \in \Psi^0$ satisfying (6.15) with $K = T^* \Gamma_i$ such that

$$\{\sigma(\mathcal{D}) = 0\} \subset \mathrm{Ell}(E_0), \qquad \{\sigma(\mathcal{N}) = 0\} \subset \mathrm{Ell}(E_1), \qquad T^* \Gamma_i \subset \mathrm{Ell}(E_0) \cup \mathrm{Ell}(E_1).$$

In particular, in all cases, there exist $h_0 > 0$, $E_0, E_1, E_2 \in \Psi^0$ such that for $0 < h < h_0$, the estimates of Lemma 6.3 hold for $E_0^* E_0$, those for (6.4) hold for $E_1^* E_1$, and those of Lemma 6.2 hold for $E_2^* E_2$ such that

$$T^* \Gamma_i \subset \mathrm{Ell}(E_0) \cup \mathrm{Ell}(E_1) \cup \mathrm{Ell}(E_2).$$

Therefore, by Lemma 6.3

$$\|E_0^* E_0 u\|_{H_h^{\ell+m_0}} + \|E_0^* E_0 h D_{x_1} u\|_{H_h^{\ell+m_1}}$$

$$\leq C(\epsilon + h) \|u\|_{H_h^{\ell+m_0}(\Gamma_i)} + C(\epsilon^{-1} + 1) \|g\|_{H_h^\ell(\Gamma_i)}$$

$$+ C \|u\|_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1} \left(\|f\|_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)} \right) + C\epsilon \|u\|_{H_h^1(M)}$$

$$+ O\left(h^\infty \left(\|u\|_{H_h^{-N}(\Gamma_i)} + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)} \right) \right).$$

Similarly, by Lemma 6.4

$$\|E_1^* E_1 u\|_{H_h^{\ell+m_0}} + \|E_1^* E_1 h D_{x_1} u\|_{H_h^{\ell+m_1}}$$

$$\leq C\epsilon \|h D_{x_1}\|_{H_h^{\ell+m_1}(\Gamma_i)} + C\epsilon^{-1} \|g\|_{H_h^\ell(\Gamma_i)}$$

$$+ C \|u\|_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + C\epsilon^{-1} \left(\|f\|_{H_h^{\ell+\frac{m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)} \right) + C\epsilon \|u\|_{H_h^1(M)}$$

$$+ O\left(h^\infty \left(\|u\|_{H_h^{-N}(\Gamma_i)} + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)} \right) \right).$$

Finally, using Lemma 6.2,

$$
\begin{aligned}
&\|E_2^* E_2 u\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|E_2^* E_2 h D_{x_1} u\|_{H_h^{\ell+m_1}(\Gamma_i)} \\
&\quad \leq C\left(\|u\|_{H_h^{\frac{2\ell+m_1+m_0+1}{2}}(M)} + \|u\|_{L^2(M)} + \|f\|_{H_h^{\frac{2\ell+m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)} \right) \\
&\qquad + \epsilon\left(\|u\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|h D_{x_1} u\|_{H_h^{\ell+m_1}(\Gamma_i)} \right) + C\epsilon^{-1} \|g_i\|_{H_h^\ell(\Gamma_i)} \\
&\qquad + O\left(h^\infty \left(\|u\|_{H_h^{-N}(\Gamma_i)} + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)} + \|g\|_{H_h^{-N}(\Gamma_i)} \right) \right).
\end{aligned}
$$

Since

$$
T^* \Gamma_i \subset \mathrm{Ell}\left(E_0^* E_0 + E_1^* E_1 + E_2^* E_2 \right),
$$

we have all together

$$
\begin{aligned}
&\|u\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|h D_{x_1} u\|_{H_h^{\ell+m_1}(\Gamma_i)} \\
&\quad \leq C\left(\|u\|_{H_h^{\ell+\frac{m_1+m_0+1}{2}}(M)} + \|u\|_{L^2(M)} + \epsilon \|u\|_{H_h^1(M)} + \|f\|_{H_h^{\frac{k+m_1+m_0-1}{2}}(M)} + \|f\|_{L^2(M)} \right) \\
&\qquad + \epsilon\left(\|u\|_{H_h^{\ell+m_0}(\Gamma_i)} + \|h D_{x_1} u\|_{H_h^{\ell+m_1}(\Gamma_i)} \right) + C\epsilon^{-1} \|g_i\|_{H_h^\ell(\Gamma_i)}.
\end{aligned}
\tag{6.18}
$$

Finally, observe that

$$
\Re \langle -h^2 \Delta u, u \rangle_{L^2(M)} = \|h \nabla u\|_{L^2(M)}^2 + h \sum_i \Re \langle h \partial_\nu u, u \rangle_{L^2(\Gamma_i)}.
$$

Letting $\psi \in \Psi^{\mathrm{comp}}$ with $\mathcal{D}$ elliptic on $\mathrm{WF}_h(\psi)$ and $\mathcal{N}$ elliptic on $\mathrm{supp}\,\mathrm{WF}_h(\mathrm{Id} - \psi)$, we have

$$
\begin{aligned}
|\Re \langle h \partial_\nu u, u \rangle_{L^2(\Gamma_i)}| &= \left| \Re i \left(\langle h D_\nu u, \psi u \rangle_{L^2(\Gamma_i)} + \langle (\mathrm{Id} - \psi) h D_\nu u, u \rangle_{L^2(\Gamma_i)} \right) \right| \\
&= \left| \Re i \left(\langle h D_\nu u, -\psi \mathcal{D}^{-1}(\mathcal{N} h D_n u - g) \rangle_{L^2(\Gamma_i)} + \langle (\mathrm{Id} - \psi)\mathcal{N}^{-1}(g + \mathcal{D} u), u \rangle_{L^2(\Gamma_i)} \right) \right| \\
&\qquad + O(h^\infty)\left(\|u\|_{H_h^{-N}(\Gamma_i)}^2 + \|h D_{x_1} u\|_{H_h^{-N}(\Gamma_i)}^2 \right) \\
&\leq Ch \|h D_\nu u\|_{H_h^{-N}(M)}^2 + h^{-1} \|g\|_{H_h^{-m_0-s}(\Gamma_i)}^2 + h \|u\|_{H_h^{\frac{m_0-m_1-1}{2}}(\Gamma_i)}^2 + h \|u\|_{H_h^s(\Gamma_i)}^2.
\end{aligned}
$$

Therefore, for any s,

$$\|u\|^2_{H^1_h(M)} \leq \frac{1}{2}h^2\|f\|^2_{L^2(M)} + \frac{5}{2}\|u\|^2_{L^2(M)}$$

$$+ C\left(\sum_i h^2\|hD_n u\|^2_{H^{-N}_h(\Gamma_i)} + h^2\|u\|^2_{H^{\max\left(s,\frac{m_0-m_1-1}{2}\right)}_h(\Gamma_i)} + \|g_i\|^2_{H^{-m_{1,i}-s}_h(\Gamma_i)}\right). \qquad (6.19)$$

Using this in (6.18) and taking

$$-\frac{m_{0,i}+m_{1,i}}{2} \leq \ell_i \leq \frac{1}{2} - \frac{m_{0,i}+m_{1,i}}{2}, \quad s_i = -\ell_i - m_{1,i}, \qquad (6.20)$$

we obtain

$$\sum_i \|u\|_{H^{\ell_i+m_{0,i}}_h(\Gamma_i)} + \|hD_{x_1}u\|_{H^{\ell_i+m_{1,i}}_h(\Gamma_i)}$$

$$\leq C\|u\|_{L^2(M)} + C(\epsilon^{-1}+\epsilon h)\|f\|_{L^2(M)}$$

$$+ \sum_i \epsilon^{-1}\|g\|_{H^{\ell_i}_h(\Gamma_i)} + C\epsilon\left(\|u\|_{H^{\ell+m_{0,i}}_h(\Gamma_i)} + \|hD_{x_1}u\|_{H^{\ell+m_{1,i}}_h(\Gamma_i)}\right)$$

$$+ \sum_i \left(h\|hD_n u\|_{H^{-N}_h(\Gamma_i)} + h\|u\|_{H^{\max\left(-m_{1,i}-\ell_i,\frac{m_{0,i}-m_{1,i}-1}{2}\right)}_h(\Gamma_i)}\right).$$

Shrinking ϵ such that $C\epsilon < 1/2$ and taking h_0 small enough such that $Ch_0 \leq \frac{1}{2}$, the proof is complete since the inequality (4.6) (i.e., the first inequality in (6.20)) implies that the terms on the right can be absorbed into the left.

The final inequality in Theorem 4.1 follows from combining the result of Lemma 6.1 (with $\ell = -s$) with (4.8). □

Acknowledgements

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Appendix A. Semiclassical pseudodifferential operators and notation

We review the notation and definitions for semiclassical pseudodifferential operators on $\mathbb{R}^d$ and refer the reader to Appendix E in Dyatlov & Zworski (2019) and Chapter 14 in Zworski (2012) for details of how to adapt these definitions to manifolds.

Before we introduce these objects, we recall the notion of *semiclassical Sobolev spaces* H_h^s; these are the standard Sobolev spaces H^s with a norm weighted with h. We say that $u \in H_h^s(\mathbb{R}^d)$ if

$$\|\langle \xi \rangle^s \mathcal{F}_h(u)(\xi)\|_{L^2} < \infty, \quad \text{where} \quad \langle \xi \rangle := (1 + |\xi|^2)^{\frac{1}{2}} \quad \text{and} \quad \mathcal{F}_h(u)(\xi) := \int_{\mathbb{R}^d} e^{-\frac{i}{h}\langle y, \xi \rangle} u(y) \, dy$$

is the *semiclassical Fourier transform*.

We next introduce the notion of symbols. We say that $a \in C^\infty(T^*\mathbb{R}^d)$ is a symbol of order m if

$$\left| \partial_x^\alpha \partial_\xi^\beta a(x, \xi) \right| \leq C_{\alpha\beta} \langle \xi \rangle^m,$$

and write $a \in S^m(T^*\mathbb{R}^d)$. Throughout this section we fix $\chi_0 \in C_c^\infty(\mathbb{R})$ to be identically 1 near 0. We then say that an operator $A : C_c^\infty(\mathbb{R}^d) \to \mathcal{D}'(\mathbb{R}^d)$ is a semiclassical pseudodifferential operator of order m, and write $A \in \Psi^m(\mathbb{R}^d)$, if A can be written as

$$Au(x) = \frac{1}{(2\pi h)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{\frac{i}{h}\langle x - y, \xi \rangle} a(x, \xi) \chi_0(|x - y|) u(y) \, dy \, d\xi + E, \tag{A.1}$$

where $a \in S^m(T^*\mathbb{R}^d)$ and $E = O(h^\infty)_{\Psi^{-\infty}}$, where an operator $E = O(h^\infty)_{\Psi^{-\infty}}$ if for all $N > 0$ there exists $C_N > 0$ such that

$$\|E\|_{H_h^{-N}(\mathbb{R}^d) \to H_h^N(\mathbb{R}^d)} \leq C_N h^N.$$

We also define

$$\Psi^{-\infty} := \bigcap_m \Psi^m, \qquad S^{-\infty} := \bigcap_m S^m, \qquad \Psi^\infty := \bigcup_m \Psi^m, \qquad S^\infty := \bigcup_m S^m.$$

We say that $a \in S^{\text{comp}}$ if $a \in S^{-\infty}$ and a is compactly supported, and we say that $A \in \Psi^{\text{comp}}$ if $A \in \Psi^{-\infty}$ and can be written in the form (A.1) with $a \in S^{\text{comp}}$. We use the notation $a(x, hD_x)$ for the operator A in (A.1) with $E = 0$.

We recall that there exists a map

$$\sigma_m : \Psi^m \to S^m/hS^{m-1}$$

called the *principal symbol map* and such that the sequence

$$0 \to hS^{m-1} \xrightarrow{\text{Op}_h} \Psi^m \xrightarrow{\sigma} S^m/hS^{m-1} \to 0$$

is exact where $\text{Op}_h(a) = a(x, hD)$. Moreover,

$$\sigma(AB) = \sigma(A)\sigma(B), \qquad \sigma(A^*) = \overline{\sigma}(A), \qquad \sigma(-ih^{-1}[A, B]) = \{\sigma(A), \sigma(B)\}, \tag{A.2}$$

where $\{\cdot, \cdot\}$ denotes the Poisson bracket; see Proposition E.17 in Dyatlov & Zworski (2019).

A.1   *Wavefront sets and elliptic sets*

To introduce a notion of wavefront set that respects both decay in h as well as smoothing properties of pseudodifferential operators, we introduce the set

$$\overline{T^*\mathbb{R}^d} := T^*\mathbb{R}^d \sqcup (\mathbb{R}^d \times S^{d-1}),$$

where $\sqcup$ denotes disjoint union and we view $\mathbb{R}^d \times S^{d-1}$ as the 'sphere at infinity' in each cotangent fiber (see also Dyatlov & Zworski, 2019, §E.1.3, for a more systematic approach where $\overline{T^*\mathbb{R}^d}$ is introduced as

the fiber-radial compactification of $T^*\mathbb{R}^d$). We endow $\overline{T^*\mathbb{R}^d}$ with the usual topology near points $(x_0, \xi_0) \in T^*\mathbb{R}^d$ and define a system of neighbourhoods of a point $(x_0, \xi_0) \in \mathbb{R}^d \times S^{d-1}$ to be

$$U_\epsilon := \left\{ (x, \xi) \in T^*\mathbb{R}^d \,\middle|\, |x - x_0| < \epsilon, |\xi| > \epsilon^{-1}, \left| \frac{\xi}{\langle\xi\rangle} - \xi_0 \right| < \epsilon \right\}$$

$$\sqcup \left\{ (x, \xi) \in \mathbb{R}^d \times S^{d-1} \,:\, |x - x_0| < \epsilon., \, |\xi - \xi_0| < \epsilon \right\}.$$

We now say that a point $(x_0, \xi_0) \in \overline{T^*\mathbb{R}^d}$ is not in the wavefront set of an operator $A \in \Psi^m$, and write $(x_0, \xi_0) \notin \mathrm{WF}_\mathrm{h}(A)$, if there exists a neighbourhood U of (x_0, ξ_0) such that A can be written as in (A.1) with

$$\sup_{(x,\xi) \in U} \left| \partial_x^\alpha \partial_\xi^\beta a(x, \xi) \langle\xi\rangle^N \right| \leq C_{\alpha\beta N} h^N.$$

We define the elliptic set of a pseudodifferential operator $A \in \Psi^m$ as follows. We say that $(x_0, \xi_0) \in \overline{T^*\mathbb{R}^d}$ is in the elliptic set of A, and write $(x_0, \xi_0) \in \mathrm{Ell}(A)$, if there exists a neighbourhood U of (x_0, ξ_0) such that A can be written as in (A.1) with

$$\inf_{(x,\xi) \in U} |a(x, \xi) \langle\xi\rangle^{-m}| \geq c > 0.$$

Next, we define the wavefront of a family of distributions u_h, depending on h. We say that u_h is *tempered* if for all $\chi \in C_c^\infty(\mathbb{R}^d)$ there exists $N > 0$ such that

$$\|\chi u\|_{H_h^{-N}} < \infty.$$

For a tempered family of functions, u_h we say that $(x_0, \xi_0) \in \overline{T^*\mathbb{R}^d}$ is not in the wavefront set of u_h and write $(x_0, \xi_0) \notin \mathrm{WF}_\mathrm{h}(u_h)$ if there exists $A \in \Psi^0$ with $(x_0, \xi_0) \in \mathrm{Ell}(A)$ such that for all N there is $C_N > 0$ such that

$$\|Au_h\|_{H_h^N} \leq C_N h^N.$$

A.2 *Bounds for pseudodifferential operators*

We next review some bounds for pseudodifferential operators acting on Sobolev spaces.

LEMMA A1. (Dyatlov & Zworski, 2019, Propositions E.19 and E.24) (Zworski, 2012, Theorem 8.10) Suppose that $A \in \Psi^m$. Then,

$$\|Au\|_{H_h^s} \leq C\|u\|_{H_h^{s+m}}.$$

Moreover, if $A = a(x, hD) \in \Psi^0$, then there exists $C > 0$ such that

$$\|A\|_{L^2 \to L^2} \leq \sup |a| + Ch^{\frac{1}{2}}.$$

Finally, we recall the elliptic parametrix construction (see e.g., Dyatlov & Zworski, 2019, Proposition E.32).

LEMMA A2. Suppose that $A \in \Psi^{m_1}$ and $B \in \Psi^{m_2}$ with $\mathrm{WF}_\mathrm{h}(A) \subset \mathrm{Ell}(B)$. Then there exist $E_1, E_2 \in \Psi^{m_1 - m_2}$ such that

$$A = E_1 B + O(h^\infty)_{\Psi^{-\infty}}, \qquad A = BE_2 + O(h^\infty)_{\Psi^{-\infty}}.$$

A.3 *Tangential pseudodifferential operators*

It will sometimes be convenient to have families of pseudodifferential operators, depending on one of the position variables. In this case, as in § 2.3, we write $x = (x_1, x') \in \mathbb{R}^d$ and $\xi = (\xi_1, \xi')$ for the corresponding dual variables. We then consider families $A \in C_c^\infty(I_{x_1}; \Psi^m(\mathbb{R}^{d-1}))$, that is, smooth functions in x_1 valued in pseudodifferential operators of order m and write $A = a(x, hD_{x'})$ for some $a \in C_c^\infty(I_{x_1}; S^m(\mathbb{R}^{d-1}))$.