CARTESIAN PML TRUNCATION FOR THE HELMHOLTZ EQUATION IS EXPONENTIALLY ACCURATE AT HIGH FREQUENCY

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Abstract. For a wide class of Helmholtz scattering problems (namely, those fitting in the black-box framework of Sjöstrand–Zworski [18]) we prove that the error incurred by approximating the radiation condition by a Cartesian perfectly-matched layer (PML) decreases exponentially in the width of the PML, the strength of the PML scaling, and the frequency.

1. Introduction. Since the work of Berenger [1], perfectly matched layers (PMLs) have become a standard tool in the numerical simulation of frequency-domain wave problems such as the Helmholtz equation. This method approximates the solution of a scattering problem in an unbounded domain by making a complex change of variables in a layer away from the region of interest and truncating the problem with a zero Dirichlet condition.

It has long been understood that for a radial PML, the error in the truncation decreases exponentially with the PML width and the strength of the PML scaling [15, Theorem 2.1], [16, Theorem A], [10, Theorem 5.8], [2, Theorem 3.4]. More recently, [7, Theorem 1.5] proved that the error in the truncation decreases exponentially in the PML width, the strength of the scaling, *and* the frequency.

Cartesian PML is a very popular way of approximating the radiation condition in numerical-analysis applications using rectangular meshes. However, Cartesian PML is more difficult to analyse than radial PML – this is because the damping in the Cartesian PML operator only occurs in one coordinate direction at a time; i.e., a ray moving inside the PML and perpendicular to the direction of the scaling is not damped.

The papers [11, 12, 13] proved that the error in Cartesian PML truncation is exponentially small in the PML width, with then [3] proving that the error is exponentially small in both the PML width and the strength of the scaling.

Regarding the frequency-dependence of the Cartesian PML truncation error: using propagation of singularities (see, e.g., [5, Appendix E]) it is relatively straightforward to show that the error in Cartesian PML truncation (and indeed, truncation with any complex absorption) is super-polynomially small in frequency (i.e., given $N > 0$ there exists C_N such that the error is $\leq C_N k^{-N}$ for all sufficiently large frequencies k). These arguments are written out – and this error bound proved – in the case of scattering by smooth variable coefficients (where these propagation arguments are the least technical) in [6, Theorem 4.7]. In the case of no scattering, and for Cartesian PML where the scaling function is linear at the PML boundary, the error was proved to be exponentially small in the PML width, the scaling strength, and the frequency in [4, Lemma 3.4]. Very recently, this result was extended to the case of scattering by a star-shaped Dirichlet obstacle [20, Theorem 5.6].

The main result of the present paper is informally summarised as the following.

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Informal Theorem 1.1. *Consider a Helmholtz scattering problem fitting in the black-box framework of [18]; recall that this includes scattering by Lipschitz Dirichlet and Neumann obstacles and/or Lipschitz penetrable obstacles [14, §2.2].*

Suppose that the solution operator is polynomially bounded in frequency – as occurs for "most" frequencies by [14, Theorem 3.3] in general, and always for nontrapping scatterers including star-shaped obstacles.

Then, for Cartesian PML truncation where the scaling function is linear at the PML boundary, the error decreases exponentially in the width of the PML, the strength of the scaling, and the frequency.

2. Statement of the main result.

2.1. Recap of the black-box framework. We consider P a (semiclassically scaled) Helmholtz scattering operator in the black-box framework of Sjostrand–Zworski [18]. We give a short recap here, and refer to [5, Chapter 4] for the details. In this framework, $P = -k^{-2}\Delta$ outside a ball and is equal to some self-adjoint operator inside the ball. Black-box operators include scattering by Dirichlet, Neumann, and penetrable obstacles (even for Lipschitz boundaries – see [14, §2.2]), and scattering by inhomogeneous media.

For $i = 1, \ldots, d$, let $R_{\mathrm{bb},i}$ be such that the black box is contained in $Q_{\mathrm{bb}} := \prod_{i=1}^{d}(-R_{\mathrm{bb},i}, R_{\mathrm{bb},i})$. Let

$$\mathcal{H} := \mathcal{H}_0 \oplus L^2(\mathbb{R}^d \setminus Q_{\mathrm{bb}}),$$

where $\mathcal{H}_0$ is a Hilbert space such that $P : \mathcal{H} \to \mathcal{H}$ is an unbounded operator with domain $\mathcal{D}$. (Recall that if $u = (0, u_1)$ with $\operatorname{supp} u_1 \cap \overline{Q_{\mathrm{bb}}} = \emptyset$, then $u \in \mathcal{D} \Leftrightarrow u_1 \in H^2(\mathbb{R}^d \setminus Q_{\mathrm{bb}})$ and, furthermore, $P(0, u_1) = (0, -k^{-2}\Delta u_1)$.) We use the following notation for multiplication operators on $\mathcal{H}$: for $u = (u_1, u_2) \in \mathcal{H}$ and $\chi \in L^\infty(\mathbb{R}^d)$ with $\operatorname{supp}(1-\chi) \cap Q_{\mathrm{bb}} = \emptyset$ we set $\chi u := (u_1, \chi u_2)$.

In addition to the usual black-box assumptions, we require the following unique-continuation-type property:

$$\text{if } u = (u_1, u_2) \in \mathcal{D},\ (P-1)u = 0, \text{ and } u_2 \text{ is compactly supported, then } u = 0 \tag{2.1}$$

(note that this is the case for the scattering examples listed above; see the discussion and references in [8, §4.2]). This unique-continuation property combined with Rellich's theorem (see [5, Theorem 4.17]) implies uniqueness of outgoing solutions to the equation $(P-1)u = g$ for compactly supported $g \in \mathcal{H}$.

We can now define the limiting absorption resolvent $R_P := \lim_{\epsilon \to 0^+}(P - 1 - i\epsilon)^{-1}$ and recall that $\chi R_P \chi : \mathcal{H} \to \mathcal{D}$ [5, Theorem 4.4].

2.2. Definition of the scaled operators. Given $R_{\mathrm{bb},j}$, $j = 1, \ldots, d$, let $R_{\mathrm{bb},j} < R_{\mathrm{st},j} < R_{\mathrm{lin},j} < R_{\mathrm{tr},j}$ (where "bb" stands for "black-box", "st" stands for "start", "lin" stands for "linear", and "tr" stands for "truncation"), and let $Q_\star := \prod_{j=1}^{d}(-R_{\star,j}, R_{\star,j})$ with $\star$ standing for either of the previous subscripts. We consider a Cartesian totally real deformation (see [5, Section 4.5]), Γ, of $\mathbb{R}^d$ given by

$$\gamma_\theta : x \mapsto x + i(\tan\theta)\nabla F(x), \qquad \text{where} \qquad F(x) := \sum_{j=1}^{d} F_j(x_j), \tag{2.2}$$

with $F_j \in C^\infty(\mathbb{R})$, $F_j \equiv 0$ on $[-R_{\mathrm{bb},j}, R_{\mathrm{bb},j}]$ and $F_j'(x) = x$ for $|x| \geq R_{\mathrm{lin},j}$, $\{F_j'' > 0\} = \{|x| > R_{\mathrm{st},j}\}$ and F_j convex. (The notation "lin" is used since when $|x_j| \geq R_{\mathrm{lin},j}$

the scaling/stretching in the jth coordinate is linear by (2.2).) We identify Γ with $\mathbb{R}^d$ using the map γ_θ.

Let

$$\Delta_\theta := \sum_{j=1}^{d} \left(\frac{1}{1 + i(\tan\theta) F_j''(x_j)} \partial_{x_j} \right)^2,$$

and let

$$P_{\theta,\mathrm{free}} - 1 := -k^{-2}\Delta_\theta - 1;$$

i.e., $P_{\theta,\mathrm{free}} - 1$ is the free, scaled Helmholtz operator. Let $(P_\theta - 1)$ be the operator P deformed to Γ, and let $(P_\theta^D - 1)$ be the Dirichlet realization of $P_\theta - 1$ on Q_{tr} More precisely, let

$$\mathcal{H}(Q_{\mathrm{tr}}) := \mathcal{H}_0 \oplus L^2(Q_{\mathrm{tr}} \setminus Q_{\mathrm{bb}}),$$

$$\mathcal{D}(Q_{\mathrm{tr}}) := \Big\{ u \in \mathcal{H}(Q_{\mathrm{tr}}) \,:\, \text{for all}\, \chi \in C_c^\infty(Q_{\mathrm{st}}),\, \chi \equiv 1 \text{ on } Q_{\mathrm{bb}}, \chi u \in \mathcal{D},$$
$$(1-\chi)u \in H_0^1(Q_{\mathrm{tr}}),\, -\Delta_\theta((1-\chi)u) \in L^2(Q_{\mathrm{tr}}) \Big\},$$

and then define

$$P_\theta^D u := P(\chi u) + (-k^{-2}\Delta_\theta)((1-\chi)u)$$

so that $P_\theta^D : \mathcal{H}(Q_{\mathrm{tr}}) \to \mathcal{H}(Q_{\mathrm{tr}})$ with domain $\mathcal{D}(Q_{\mathrm{tr}})$ and norm

$$\|u\|^2_{\mathcal{D}(Q_{\mathrm{tr}})} = \|u\|^2_{\mathcal{H}(Q_{\mathrm{tr}})} + \|P_\theta u\|^2_{\mathcal{H}(Q_{\mathrm{tr}})}, \qquad u \in \mathcal{D}(Q_{\mathrm{tr}}). \tag{2.3}$$

2.3. The main result.

THEOREM 2.1 (Exponential accuracy of Cartesian PML truncation). *Let* $\chi \in C_c^\infty(Q_{\mathrm{st}})$ *with* $\mathrm{supp}(1-\chi) \cap Q_{\mathrm{bb}} = \emptyset$*, and suppose that there are* $\mathcal{J} \subset (0,\infty)$ *and* $M > 0$ *such that for all* $k_0 > 0$*, there is* $C > 0$ *such that for* $k \in \mathcal{J}$*,* $k \geq k_0$

$$\|\chi R_P \chi\|_{\mathcal{H}\to\mathcal{H}} \leq C k^M.$$

Then, for all $\delta, \epsilon > 0$ *there are* $C, c, k_1 > 0$ *such that for* $R_{\mathrm{st},i} + \epsilon < R_{\mathrm{lin}}$*,* $R_{\mathrm{lin}} + \epsilon < R_{\mathrm{tr},i}$*, for all* $\theta \in [\delta, \pi/2 - \delta]$*, and all* $k \in \mathcal{J}$ *with* $k \geq k_1$*,* $(P_\theta^D - 1)^{-1} : \mathcal{H}(Q_{\mathrm{tr}}) \to \mathcal{D}(Q_{\mathrm{tr}})$ *exists with*

$$\big\|\chi\big(R_P - (P_\theta^D - 1)^{-1}\big)\chi\big\|_{\mathcal{H}(Q_{\mathrm{tr}})\to\mathcal{D}(Q_{\mathrm{tr}})} \leq C \exp\big(-ck\tan\theta \min_i\{R_{\mathrm{tr},i} - R_{\mathrm{st},i}\}\big). \tag{2.4}$$

We emphasise that, in the case of scattering by Dirichlet, Neumann, and penetrable Lipschitz obstacles and scattering by variable coefficients, for all $k_0 > 0$, there is $C > 0$ such that for $k > k_0$,

$$\|u\|^2_{H^1_k} := \|u\|^2_{L^2} + \|k^{-1}\nabla u\|^2_{L^2} \leq C\|u\|^2_{\mathcal{D}(Q_{\mathrm{tr}})};$$

i.e., (2.4) controls the k-weighted H^1 error.

Overview of the proof. Let $g \in \mathcal{H}$, χ a cutoff supported in the unscaled region Q_{st}, and consider u_θ, u_θ^D the solutions of

$$(P_\theta - 1)u_\theta = (P_\theta^D - 1)u_\theta^D = \chi g.$$

By the well-known property that u_θ equals the scattering solution $R_P\chi g$ in the unscaled region (see Theorem 4.1 below), it suffices to show that u_θ and u_θ^D agree up to exponentially small errors in the unscaled region.

To bound the error $E := \psi u_\theta - u_\theta^D$ (where $\operatorname{supp}\chi \subset \{\psi \equiv 1\} \subset \operatorname{supp}\psi \subset Q_{\rm tr}$), we observe that it satisfies the PDE

$$(P_\theta^D - 1)E = [P_\theta, \psi]u_\theta = [P_\theta, \psi]\phi u_\theta$$

for some cutoff $\phi \equiv 0$ near the black-box and $\phi \equiv 1$ outside of $Q_{\rm st}$. We now use the fact that any Helmholtz solution away from the scatterer can be written in terms of the free resolvent. Indeed,

$$(P_{\theta,\rm free} - 1)\phi u_\theta = (\phi\chi g + [P_{\theta,\rm free}, \phi]u_\theta) =: \tilde{g} \qquad \Longrightarrow \qquad \phi u_\theta = (P_{\theta,\rm free} - 1)^{-1}\widetilde{g}\,,$$

and thus

$$E = (P_\theta^D - 1)^{-1}[P_\theta, \psi](P_{\theta,\rm free} - 1)^{-1}\widetilde{g}.$$

Importantly, $\widetilde{g}$ is supported in the unscaled region, and $[P_\theta, \psi]$ is supported near the truncation boundary.

Theorem 2.1 then follows from two additional properties.

1. Exponential decay of $\chi_1(P_{\theta,\rm free}-1)^{-1}\chi_2$ with respect to the distance between the supports of χ_1 and χ_2.
2. An estimate on $(P_\theta^D - 1)^{-1}$ of the form $\|(P_\theta^D - 1)^{-1}\| \leq Ck^M$.

Property 1 follows from the decaying behaviour of the free Green's function in the complex-scaled coordinates (see Lemma 3.6).

Property 2 follows by first bounding $(P_\theta^D - 1)^{-1}$ in terms of $(P_\theta - 1)^{-1}$ (see Lemma 4.2), and then bounding the latter in terms of $\chi R_P \chi$ (see Lemma 5.2), which is polynomially bounded by assumption. This first bound requires an estimate on $(P_{\theta,\rm free} - 1)^{-1}$ (see Theorem 3.1).

The bound on $(P_\theta^D - 1)^{-1}$ in terms of $(P_\theta - 1)^{-1}$ follows from an a priori estimate on solutions to

$$(P_\theta^D - 1)u = g$$

in a neighborhood of the truncation boundary. For radial PMLs, this type of estimate follows easily from coercivity of the quadratic on functions supported near the truncation boundary (see [7, Lemma 4.4]). However, because Cartesian PMLs are not coercive near the truncation boundary (coercivity only occurs in the "corners" of the scaling region), this estimate is now more delicate and relies on a propagation of semiclassical singularities argument. Namely, at any point (x, ξ) in phase space with x near the truncation boundary, *either* the semiclassical symbol of the operator is non-zero – and hence the operator is elliptic –*or* the backward Hamiltonian trajectory escapes to a region of ellipticity in finite time; see Figure 2.1.

Remark 2.2. *We highlight that the only places where the Cartesian structure of the PML is used in the above arguments are (i) to bound $(P_{\theta,\rm free} - 1)^{-1}$, (ii) to prove the exponential estimate on the free Green's kernel, and (iii) to prove the a priori estimate near the truncation boundary. In particular, in any scaling where one can establish these two estimates one can prove exponential error bounds for the PML problem.*

Why we assume that F_i' is linear near the PML boundary. The principal symbol of the scaled operator P_θ has a nonpositive imaginary part; see (3.3) below. For such an operator, the relevant propagation of singularities results in the semiclassical calculus for domains with a boundary have not yet been written down in the literature. Indeed, such propagation of singularities results in the semiclassical calculus have been proved (i) on manifolds without boundary for operators with symbols whose imaginary parts are single-signed [5, Theorem E.47] and (ii) on manifolds with boundary for P [19].

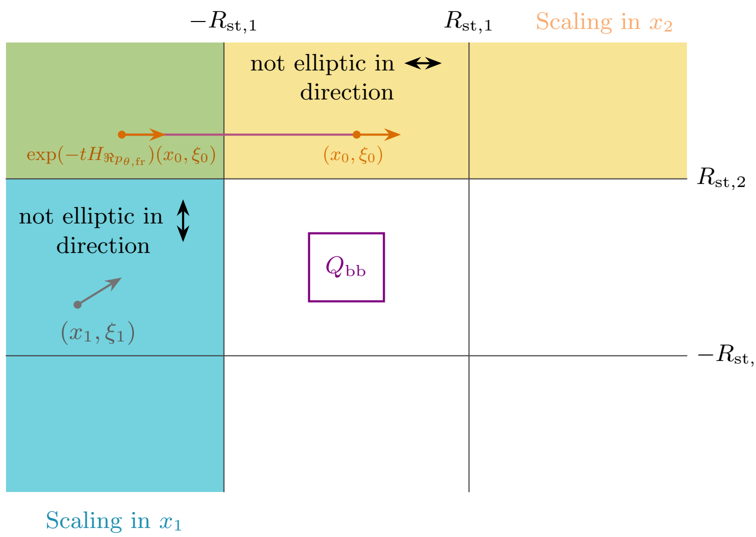

FIG. 2.1. *Sketch of the main argument used to prove an a priori estimate for solutions of the Cartesian PML problem near the truncation boundary.* (x_1,ξ_1) *is a point of phase-space where the problem is elliptic and hence estimates are available without propagation. In contrast,* (x_0,ξ_0) *is a point where the problem is not elliptic, but from any such point, the backward Hamiltonian flow associated to the real part of the symbol of* $P_\theta - 1$ *will eventually reach a corner (i.e., a point of ellipticity)*

The assumption in §2.2 that $F_i'(x) = x$ for $|x| \geq R_{\mathrm{lin},i}$ allows us to use a reflection argument (similar to that used for the Cartesian PML analyses in 2-d in [3, Proof of Theorem 5.5], [4, Lemma 3.4]) to extend the solution past ∂Q_{tr} and use the propagation results of (i) above, i.e., bypassing the issue of propagation up to the boundary. Once the relevant propagation results are written down in the literature, this assumption can be removed.

3. Results about the free complex-scaled resolvent. With

$$\mathcal{F}_k(u)(\xi) := \int_{\mathbb{R}^d} e^{-ik\langle \xi, x\rangle} u(x)dx, \tag{3.1}$$

define for $s \in \mathbb{R}$

$$\|u\|^2_{H^s_k(\mathbb{R}^d)} := \frac{k^d}{(2\pi)^d} \int_{\mathbb{R}^d} (1+|\xi|^2)^s |\mathcal{F}_k(u)(\xi)|^2 d\xi.$$

THEOREM 3.1 (Bound on the free scaled resolvent). *Given* $\delta > 0$ *and* $s \in \mathbb{R}$, *there exists* $C > 0$ *and* $k_0 > 0$ *such that for all* $k \geq k_0$ *and* $\theta \in [\delta, \frac{\pi}{2} - \delta]$,

$$\left\|(P_{\theta,\mathrm{free}} - 1)^{-1}\right\|_{H^s_k(\mathbb{R}^d)\to H^{s+2}_k(\mathbb{R}^d)} \leq Ck.$$

REMARK 3.2. *[20, Theorem 3.6] proves an* $L^2 \to L^2$ *bound analogous to that in Theorem 3.1 for the case of a piecewise-linear scaling function. The analogue of Theorem 3.1 for radial PML is [7, Theorem 3.2].*

To prove Theorem 3.1, and also other results below, we use the following facts about the adjoint of $-\Delta_\theta$. Let

$$\widetilde{\Delta}_\theta := \det(I + i(\tan\theta)F''(x))\Delta_\theta = \prod_{j=1}^{d}(1 + i(\tan\theta)F_j''(x_j))\Delta_\theta.$$

Then, by a simple calculation,

$$(\widetilde{\Delta}_\theta)^* = J\widetilde{\Delta}_\theta J,$$

where J is the action of complex conjugate; i.e., $Jv = \overline{v}$. Therefore

$$(\Delta_\theta)^* = J\det(I + i(\tan\theta)F''(x))\Delta_\theta J(\det(I - i(\tan\theta)F''(x)))^{-1}. \tag{3.2}$$

To prove Theorem 3.1 we use semiclassical propagation results (i.e., PDE bounds describing how behaviour of Helmholtz solutions are dictated by the behaviour of the rays) from [5, Appendix E] and [21]. Note that here we use the small parameter k^{-1}, but [5, 21] denote the small parameter by h.

The semiclassical principal symbol of $P_{\theta,\mathrm{free}}$ is

$$p_{\theta,\mathrm{fr}}(x,\xi) := \sigma(P_{\theta,\mathrm{fr}}) = \sum_{i=1}^{d}\left(\frac{\xi_i}{1 + i\tan\theta F_i''(x_i)}\right)^2.$$

Observe that

$$\begin{aligned} \Re p_{\theta,\mathrm{fr}}(x,\xi) &= \sum_{i=1}^{d}\frac{(1 - (\tan\theta F_i''(x_i))^2)\xi_i^2}{\big(1 + (\tan\theta F_i''(x_i))^2\big)^2}, \\ \Im p_{\theta,\mathrm{fr}}(x,\xi) &= \sum_{i=1}^{d}\frac{-2\tan\theta F_i''(x_i)\xi_i^2}{\big(1 + (\tan\theta F_i''(x_i))^2\big)^2} \le 0. \end{aligned} \tag{3.3}$$

Before proceeding to estimate the free resolvent, we need a dynamical fact about the rays associated to $P_{\theta,\mathrm{fr}}$ (more precisely, the Hamiltonian flow of $\Re p_{\theta,\mathrm{fr}}$).

Lemma 3.3 (Uniform escape of the rays to ellipticity). *Let $\delta > 0$. Then there are $T > 0$, $\mu > 0$ such that for all $\theta \in [\delta, \frac{\pi}{2} - \delta]$, $(x_0, \xi_0) \in T^*\mathbb{R}^d$ with $|p_{\theta,\mathrm{fr}}(x_0,\xi_0) - 1| \le \mu$, there is $0 \le t \le T$ such that*

$$|p_{\theta,\mathrm{fr}}(\exp(-tH_{\Re p_{\theta,\mathrm{fr}}}(x_0,\xi_0)) - 1| \ge \mu.$$

Proof. Define

$$p_\theta^i := \frac{1 - (\tan\theta F_i''(x_i))^2}{(1 + (\tan\theta F_i''(x_i))^2)^2}\xi_i^2.$$

Then, since $\{p_\theta^i, \Re p_{\theta,\mathrm{fr}}\} = 0$, p_θ^i is preserved by the Hamiltonian flow for $\Re p_{\theta,\mathrm{fr}}$.

Define $(x(t),\xi(t)) := \exp(tH_{\Re p_{\theta,\mathrm{fr}}})(x_0,\xi_0)$. Let

$$T_0 := -\sup\big\{t \le 0 \,:\, |p_{\theta,\mathrm{fr}}(x(t),\xi(t)) - 1| \ge \mu\big\}.$$

Then,

$$\partial_t(x_i\xi_i) = 2p_\theta^i + \frac{2\tan^2\theta F_i''(x_i)(3 - (\tan\theta F_i''(x_i))^2)F_i'''(x_i)}{(1 + (\tan\theta F_i''(x_i))^2)^3}\xi_i^2 x_i. \tag{3.4}$$

Observe that on $|p_{\theta,\mathrm{fr}} - 1| \le \mu$,

$$0 \le F_i''(x_i)\xi_i^2 \le C_\delta |\Im(p_{\theta,\mathrm{fr}} - 1)| = O_\delta(\mu) \qquad \Longrightarrow \qquad \Re p_{\theta,\mathrm{fr}}(x_0,\xi_0) = 1 + O_\delta(\mu).$$

Therefore, there is i such that

$$p_\theta^i(x_0,\xi_0) = p_\theta^i(x(t),\xi(t)) \ge \frac{1}{d} + O_\delta(\mu) \qquad \Longrightarrow \qquad |\xi_i(t)| \ge c + O_\delta(\sqrt{\mu})$$

Hence, if $t \le 0$ and $|x_i(t)| \ge R_{\mathrm{lin},i}$, we have

$$\Im p_{\theta,\mathrm{fr}} \le -c < 0$$

which implies $t \le -T_0$. In particular, for $-T_0 \le t \le 0$, $|x_i| \le R_{\mathrm{lin},i}$ and hence using this in (3.4) along with Gronwall's inequality, for $-T_0 \le t \le 0$,

$$x_i(t)\xi_i(t) \le \Big(-\frac{2}{d} + O_\delta(\mu^{1/2})\Big)|t| + x_i(0)\xi_i(0).$$

But then, using again that $c \le |\xi_i(t)| \le C$, and $|x_i(t)| \le R_{\mathrm{lin},i}$, for $-T_0 \le t \le 0$,

$$R_{\mathrm{lin},i} \ge |x_i(-T_0)| \ge C\bigg(\Big(\frac{2}{d} - O_\delta(\mu^{1/2})\Big)|T_0| - R_{\mathrm{lin},i}\bigg),$$

which implies that $|T_0| \le C R_{\mathrm{lin},i}$, completing the proof. ∎

Recall (from, e.g., [21, §9.3]) that

$$S^m(\mathbb{R}^{2d}) := \Big\{ a \in C^\infty(\mathbb{R}^{2d}) \,:\, \forall \alpha,\beta \in \mathbb{N}^d,\ \sup_{\substack{(x,\xi)\in\mathbb{R}^{2d}\\ k>1}} \langle \xi\rangle^{-m+|\beta|} |\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| < \infty \Big\},$$

where $\langle \xi \rangle := (1+|\xi|^2)^{1/2}$. Furthermore, for $u \in \mathcal{S}'$ and $a \in S^m$, we define

$$\mathrm{Op}_k(a)u(x) := \frac{k^d}{(2\pi)^d} \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{ik\langle x-y,\xi\rangle} a(x,\xi) u(y) dy d\xi.$$

Lemma 3.4 (Elliptic estimate). *Let $\mu, \delta, N, k_0 > 0$, $s \in \mathbb{R}$ and $a \in S^0$ with* $\operatorname{supp} a \subset \{|p_{\theta,\mathrm{fr}} - 1| \ge \mu\}$. *Then there is $C > 0$ such that for all $\theta \in [\delta, \frac{\pi}{2} - \delta]$, $u \in \mathcal{S}'(\mathbb{R}^d)$ with $(P_{\theta,\mathrm{free}} - 1)u \in H_k^s(\mathbb{R}^d)$, and $k \ge k_0$,*

$$\|\mathrm{Op}_k(a)u\|_{H_k^{s+2}} \le C\|(P_{\theta,\mathrm{free}} - 1)u\|_{H_k^s} + C_N k^{-N}\|u\|_{H_k^{-N}}.$$

Proof. Observe that for all $\mu > 0$, there is $c > 0$ such that

$$\big\{|p_{\theta,\mathrm{fr}-1} - 1| \ge \mu\big\} \subset \big\{|p_{\theta,\mathrm{fr}} - 1| \ge c\langle\xi\rangle^2\big\}.$$

Hence, the lemma follows from the elliptic estimate for semiclassical pseudodifferential operators (see e.g. the proof of [5, Theorem E.33] together with [21, Theorem 9.5]). ∎

Lemma 3.5 (Propagation estimate). *Let $k_0 > 0$, there is $\mu > 0$ such that for all $\delta, N > 0$ and $a \in S^0$ with* $\operatorname{supp} a \subset \{|p_{\theta,\mathrm{fr}} - 1| \le \mu\}$, *there is $C > 0$ such that for all $\theta \in [\delta, \frac{\pi}{2} - \delta]$, $u \in \mathcal{S}'(\mathbb{R}^d)$ with $(P_{\theta,\mathrm{free}} - 1)u \in H_k^{-N}(\mathbb{R}^d)$, and $k \ge k_0$,*

$$\|\mathrm{Op}_k(a)u\|_{H_k^N(\mathbb{R}^d)} \le Ck\|(P_{\theta,\mathrm{free}} - 1)u\|_{H_k^{-N}(\mathbb{R}^d)} + C_N k^{-N}\|u\|_{H_k^{-N}(\mathbb{R}^d)}.$$

Proof. It will be convenient in this proof to work with pseudodifferential operators whose kernels are supported in a unit neighborhood of the diagonal. To do this, we fix $\psi \in C_c^\infty([-1,1])$ with $\operatorname{supp}(1-\psi)\cap[-1/2,1/2]=\emptyset$, and write for $b\in S^\infty$, and $u\in\mathcal{S}'$,

$$\widetilde{\operatorname{Op}}_k(b)u(x) := \frac{k^d}{(2\pi)^d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} e^{ik\langle x-y,\xi\rangle} b(x,\xi)\psi(|x-y|)u(y)dyd\xi.$$

By integration by parts in ξ (see [21, Theorem 9.6]),

$$\|(\operatorname{Op}_k(a)-\widetilde{\operatorname{Op}}_k(a))u\|_{H_k^N} \le C_N k^{-N}\|u\|_{H_k^{-N}}.$$

Therefore, it is sufficient to estimate $\widetilde{\operatorname{Op}}_k(a)u$. For this, let $\chi\in C_c^\infty(B(0,4\sqrt{d});[0,1])$ such that $\sum_{n\in\mathbb{Z}^d}\chi(x-n)\equiv 1$ and define

$$a_n := a(x,\xi)\chi_n(x), \qquad \chi_n(x):=\chi(x-n).$$

Then, by [5, Theorem E.47] together with locality of $P_{\theta,\mathrm{free}}$ and Lemma 3.3 there are $C>0$, $b_n, b_n'\in C_c^\infty(\mathbb{R}^{2d})$, $\phi_n\in C_c^\infty(\mathbb{R}^d)$ with $\operatorname{supp} b_n\subset\{|p_{\theta,\mathrm{fr}}-1|\ge c\langle\xi\rangle^2,\ |x-n|\le C\}$, $\operatorname{supp} b_n'\subset\{|x-n|\le C\}$, $\operatorname{supp}\phi_n\subset\{|x-n|\le C\}$ such that

$$\begin{aligned}
&\|\widetilde{\operatorname{Op}}_k(a_n)u\|_{L^2}\\
&\quad\le Ck\|\widetilde{\operatorname{Op}}_k(b_n')(P_{\theta,\mathrm{free}}-1)u\|_{H_k^{-1}} + C\|\widetilde{\operatorname{Op}}_k(b_n)u\|_{L^2} + C_N k^{-N}\|\phi_n u\|_{H_k^{-N}}\\
&\quad\le Ck\|\phi_n(P_{\theta,\mathrm{free}}-1)u\|_{H_k^{-N}} + C\|\widetilde{\operatorname{Op}}_k(b_n)u\|_{L^2} + C_N k^{-N}\|\phi_n u\|_{H_k^{-N}}.
\end{aligned}$$

Next, using the elliptic estimate (see, e.g., the proof of [5, Theorem E.33] together with [21, Theorem 9.5]) and locality of $P_{\theta,\mathrm{free}}$ to control $\widetilde{\operatorname{Op}}_k(b_n)u$, we obtain

$$\|\widetilde{\operatorname{Op}}_k(a_n)u\|_{L^2}\le Ck\|\phi_n(P_{\theta,\mathrm{free}}-1)u\|_{H_k^{-N}} + C_N k^{-N}\|\phi_n u\|_{H_k^{-N}}. \tag{3.5}$$

Now, we estimate

$$\|\widetilde{\operatorname{Op}}_k(a)u\|_{H_k^N}^2 \le C\|\widetilde{\operatorname{Op}}_k(a)u\|_{L^2}^2 + C_N k^{-N}\|u\|_{H_k^{-N}}^2. \tag{3.6}$$

Then, using the support properties of ϕ_n, and (3.5), we have

$$\begin{aligned}
\Big\|\sum_{n\in\mathbb{Z}^d}\widetilde{\operatorname{Op}}_k(a_n)u\Big\|_{L^2}^2 &= \sum_{n,n'}\langle\widetilde{\operatorname{Op}}_k(a_n)u,\widetilde{\operatorname{Op}}_k(a_{n'})u\rangle_{L^2}\\
&=\sum_{|n-n'|\le C}\langle\widetilde{\operatorname{Op}}_k(a_n)u,\widetilde{\operatorname{Op}}_k(a_{n'})u\rangle_{L^2}\\
&\le C\sum_n\|\widetilde{\operatorname{Op}}_k(a_n)u\|_{L^2}^2\\
&\le C\sum_n k^2\|\phi_n(P_{\theta,\mathrm{free}}-1)u\|_{H_k^{-N}}^2 + C_N k^{-N}\|\phi_n u\|_{H_k^{-N}}^2\\
&\le Ck^2\|(P_{\theta,\mathrm{free}}-1)u\|_{H_k^{-N}}^2 + C_N k^{-N}\|u\|_{H_k^{-N}}^2. \qquad (3.7)
\end{aligned}$$

Combining (3.6) with (3.7) completes the proof. ∎

Proof of Theorem 3.1. Let μ be as in Lemma 3.5 and $a \in S^0$ with $\operatorname{supp} a \subset \{|p_{\theta,\mathrm{fr}} - 1| \le \mu\}$ and $\operatorname{supp}(1-a) \subset \{|p_{\theta,\mathrm{fr}} - 1| \ge \frac{\mu}{2}\}$. Then, Lemmas 3.5 and 3.4 imply, respectively, that

$$\|\mathrm{Op}_k(a)u\|_{H_k^N} \le Ck\|(P_{\theta,\mathrm{free}} - 1)u\|_{H_k^{-N}} + C_N k^{-N}\|u\|_{H_k^{-N}}$$

and

$$\|\mathrm{Op}_k(1-a)u\|_{H_k^{s+2}} \le C\|(P_{\theta,\mathrm{free}} - 1)u\|_{H_k^s} + C_N k^{-N}\|u\|_{H_k^{-N}}.$$

Hence, for k large enough,

$$\|u\|_{H_k^{s+2}} \le Ck\|(P_{\theta,\mathrm{free}} - 1)u\|_{H_k^s}.$$

An identical argument but applied to $P^*_{\theta,\mathrm{free}}$ (using the relation (3.2)) implies

$$\|u\|_{H_k^{-s}} \le Ck\|(P^*_{\theta,\mathrm{free}} - 1)u\|_{H_k^{-s-2}},$$

and hence that $(P_{\theta,\mathrm{free}} - 1)$ is invertible with the required estimate. $\square$

LEMMA 3.6 (Decay estimates for the free complex-scaled resolvent). *Given $\delta, \epsilon, C_0, k_0 > 0$ there exists $C, \widetilde{c} > 0$ such that the following is true. Let $\chi_1, \chi_2 \in C^\infty(\mathbb{R}^d; [0,1])$ with $\operatorname{supp} \chi_1 \subset Q_{\mathrm{tr}} \setminus Q_{\mathrm{lin}}$ $\operatorname{supp} \chi_2 \subset Q_{\mathrm{st}}$, and*

$$\|\partial^\alpha \chi_i\|_{L^\infty} \le C_0, \qquad |\alpha| \le 2, \quad i = 1, 2.$$

Then for $R_{\mathrm{st}} + \epsilon < R_{\mathrm{lin}}$, $k > k_0$, $\theta \in [\delta, \pi/2 - \delta]$,

$$\big\|\chi_1(P_{\theta,\mathrm{free}} - 1)^{-1}\chi_2\big\|_{L^2(\mathbb{R}^d)\to H_k^2(\mathbb{R}^d)} \le C\exp\big(-\widetilde{c}k\tan\theta\,\mathrm{dist}(\operatorname{supp}\chi_1, \operatorname{supp}\chi_2)\big).$$

To prove Lemma 3.6, we use the following lemma.

LEMMA 3.7. *Suppose that $u, v \in \mathbb{R}^d$ with $\langle u, v\rangle \ge 0$ and $u \ne 0$. Then (with the principal branch of the square root),*

$$\Im\Big(\Big(\sum_{j=1}^d (u_j + iv_j)^2\Big)^{1/2}\Big) \ge \frac{\langle u, v\rangle}{|u|}.$$

Proof. To keep the notation concise, we denote $\sum_{j=1}^d (u_j + iv_j)^2$ by $\langle u + iv, u + iv\rangle$ (i.e., the inner product on $\mathbb{R}^d$ is extended to $\mathbb{C}^d$ bilinearly). Let p, q be such that

$$p + iq := \langle u + iv, u + iv\rangle^{1/2} \quad \text{so that} \quad (p + iq)^2 = |u|^2 - |v|^2 + 2i\langle u, v\rangle. \tag{3.8}$$

Now $q \ge 0$ since $\langle u, v\rangle \ge 0$, and $p \ge 0$ from the principal branch of the square root.

We need to prove that $q \ge \langle u, v\rangle/|u|$. Taking the imaginary part of the second equation in (3.8) we see that $pq = \langle u, v\rangle$, so it is enough to show that $p \le |u|$. Taking the real part of the second equation in (3.8) and combining it with the equality $p^2 + q^2 = |\langle u + iv, u + iv\rangle|$, we obtain that

$$p^2 = \frac{|\langle u + iv, u + iv\rangle| + |u|^2 - |v|^2}{2}.$$

By the Cauchy–Schwarz inequality,

$$|\langle u + iv, u + iv\rangle|^2 = (|u|^2 - |v|^2)^2 + 4\langle u, v\rangle^2 \le (|u|^2 - |v|^2)^2 + 4|u|^2|v|^2$$

$$= (|u|^2 + |v|^2)^2.$$

Hence

$$p^2 \le \frac{|u|^2 + |v|^2 + |u|^2 - |v|^2}{2} = |u|^2$$

and the proof is complete. □

Proof of Lemma 3.6. By the explicit expression for the fundamental solution,

$$\big((P_{\theta,\mathrm{free}} - 1)^{-1} f\big)(x) = \int_{\mathbb{R}^d} G_k(\gamma_\theta(x) - \gamma_\theta(y)) f(y) \prod_{j=1}^{d} (1 + i(\tan\theta) F_j''(y_j))\, dy$$

where

(3.9)

$$G_k(z) := \frac{ik^2}{4}\left(\frac{k}{2\pi\rho(z)}\right)^{\nu} H_\nu^{(1)}(kr(z)), \quad r(z) := \Big(\sum_{j=1}^{d} z_j^2\Big)^{1/2}, \quad \text{and } \nu := (d-2)/2.$$

By the Schur test (see, e.g., [9, §I.1]) or the Riesz-Thorin interpolation theorem (see, e.g., [9, Theorem 1.34]),

$$\begin{aligned}
&\|\chi_1(P_{\theta,\mathrm{free}} - 1)^{-1}\chi_2\|_{L^2\to L^2}\\
&\quad\le \Big(\mathrm{esssup}_{x\in\mathbb{R}^d} \int_{\mathbb{R}^d} \big|\chi_1(x) G_k(\gamma_\theta(x) - \gamma_\theta(y))\chi_2(y)\big|\, dy\Big)^{1/2}\\
&\qquad\qquad \times \Big(\mathrm{esssup}_{y\in\mathbb{R}^d} \int_{\mathbb{R}^d} \big|\chi_1(x) G_k(\gamma_\theta(x) - \gamma_\theta(y))\chi_2(y)\big|\, dx\Big)^{1/2}.
\end{aligned}$$

Now

$$H_\nu^{(1)}(t) = \sqrt{\frac{2}{\pi t}} \exp\Big(i\Big(t - \frac{\pi\nu}{2} - \frac{\pi}{4}\Big)\Big)\Big(1 + \mathcal{O}\Big(\frac{1}{t}\Big)\Big) \quad \text{as } |t| \to \infty \tag{3.10}$$

for $-\pi + \delta \le \arg t \le \pi - \delta$; see, e.g., [17, §10.17(i)]). Therefore given $c > 0$ there exists $C > 0$ such that if $\Im r(z) \ge c$ then

$$|G_k(z)| \le C k^{\frac{d+1}{2}} |r(z)|^{-\frac{d-1}{2}} \exp(-k\Im r(z)).$$

With γ_θ defined by (2.2), by direct calculation

$$\gamma_\theta(x) - \gamma_\theta(y) = (x - y) + i(\tan\theta)\big(\nabla F(x) - \nabla F(y)\big).$$

By convexity of F, $\langle \nabla F(x) - \nabla F(y), x - y\rangle \ge 0$. Therefore, by Lemma 3.7, with $u = x - y$ and $v = (\tan\theta)(\nabla F(x) - \nabla F(y))$,

$$\Im\Big(\sum_{j=1}^{d} (\gamma_\theta(x) - \gamma_\theta(y))_j^2\Big)^{1/2} \ge (\tan\theta)\Big\langle \frac{x-y}{|x-y|}, \nabla F(x) - \nabla F(y)\Big\rangle. \tag{3.11}$$

Since $\operatorname{supp}\chi_1 \subset Q_{\mathrm{tr}} \setminus Q_{\mathrm{lin}}$ and $\operatorname{supp}\chi_2 \subset Q_{\mathrm{st}}$, for $x \in \operatorname{supp}\chi_1$ and $y \in \operatorname{supp}\chi_2$, there is i such that $|x_i - y_i| \ge c|x - y|$ and $|x_i| > R_{\mathrm{lin},i}$ and $|y_i| \le R_{\mathrm{st},i}$ and hence, using that $D_x^2 F = \mathrm{diag}(F_i''(x_i))$ and $F_i''(x_i) \ge 0$, we obtain

$$\Big\langle \frac{x-y}{|x-y|}, \nabla F(x) - \nabla F(y)\Big\rangle = |x - y| \int_0^1 \big\langle D_x^2 F(sx + (1-s)y)\tfrac{x-y}{|x-y|}, \tfrac{x-y}{|x-y|}\big\rangle ds$$

$$\geq c|x-y|\int_0^1 F_i''(sx_i+(1-s)y_i)ds$$
$$= c|x-y|\frac{F_i'(x_i)-F_i'(y_i)}{x_i-y_i} = c|x-y|\frac{x_i}{x_i-y_i} \geq c'|x-y|.$$

The result then follows after using elliptic regularity for $P_{\theta,\mathrm{free}}$. ∎

4. Results about the complex-scaled resolvent.

THEOREM 4.1 (Agreement away from scaling). *If $\chi \in C_c^\infty(Q_{\mathrm{st}})$ with* $\operatorname{supp}(1-\chi)\cap Q_{\mathrm{bb}} = \emptyset$*, then*

$$\chi(P_\theta-1)^{-1}\chi = \chi R_P\chi.$$

Proof. This is proved for the case of scattering by a Dirichlet obstacle in [11, Proposition IX.2], [3, Proof of Theorem 5.4]. For completeness we give the (short) proof here in the black-box setting.

Given $g\in\mathcal{H}$, let $u\in\mathcal{D}$ solve $(P_\theta-1)u=\chi g$. We first show that away from the black-box u can be written as a solution to the free complex-scaled problem. Let $\phi\in C^\infty(\mathbb{R}^d;[0,1])$ be such that $\operatorname{supp}\phi\cap\operatorname{supp}(P_\theta-(-k^{-2}\Delta_\theta))=\emptyset$ and $\operatorname{supp}(\nabla\phi)\subset Q_{\mathrm{st}}$. Then

$$\begin{aligned}(P_{\theta,\mathrm{free}}-1)\phi u = (P_\theta-1)\phi u = \phi\chi g+[P_\theta,\phi]u &= \phi\chi g+[-k^{-2}\Delta_\theta,\phi]u\\ &= \phi\chi g+[-k^{-2}\Delta,\phi]u.\end{aligned}$$

so that

$$\phi u = (P_{\theta,\mathrm{free}}-1)^{-1}\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big). \tag{4.1}$$

Let $\tilde\phi\in C^\infty(\mathbb{R}^d;[0,1])$ with $\operatorname{supp}(1-\tilde\phi)\cap\operatorname{supp}\phi=\emptyset$ and $\operatorname{supp}\tilde\phi\subset\mathbb{R}^d\setminus Q_{\mathrm{bb}}$ and $\tilde\chi_j\in C_c^\infty(Q_{\mathrm{st}}))$, $j=1,2$ with $\operatorname{supp}(1-\tilde\chi_j)\cap\operatorname{supp}\chi = \operatorname{supp}(1-\tilde\chi_1)\cap\operatorname{supp}\nabla\phi = \operatorname{supp}(1-\tilde\chi_2)\cap\operatorname{supp}\nabla\widetilde{\phi} = \operatorname{supp}\tilde\chi_2\cap\operatorname{supp}\phi=\emptyset$

Observe that

$$(P_{\theta,\mathrm{free}}-1)^{-1}\tilde\chi_1 := (-k^{-2}\Delta_\theta-1)^{-1}\tilde\chi_1 = \big(R_{P_{\mathrm{free}}}\tilde\chi_1\big)|_\Gamma;$$

in the last equality, we mean the analytic continuation of $R_{P_{\mathrm{free}}}\tilde\chi_1$ to $\mathbb{C}^d$ (away from $\operatorname{supp}\tilde\chi_1$), restricted to Γ. Hence, since $\Gamma=\mathbb{R}^d$ on $\operatorname{supp}\tilde\chi_2$, we obtain

$$\tilde\chi_2(P_{\theta,\mathrm{free}}-1)^{-1}\tilde\chi_1 = \tilde\chi_2(-k^{-2}\Delta-1)^{-1}\tilde\chi_1|_\Gamma = \tilde\chi_2R_{P_{\mathrm{free}}}\tilde\chi_1.$$

In particular, by (4.1),

$$\begin{aligned}0=\tilde\chi_2\phi u &= \tilde\chi_2(P_{\theta,\mathrm{free}}-1)^{-1}\tilde\chi_1\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big)\\ &= \tilde\chi_2R_{P_{\mathrm{free}}}\tilde\chi_1\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big).\end{aligned}\tag{4.2}$$

Now define

$$\tilde u := (1-\phi)u+\tilde\phi R_{P_{\mathrm{free}}}\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big)$$

and observe that

$$\begin{aligned}(P-1)\tilde u &= (P-1)(1-\phi)u+(P-1)\tilde\phi R_{P_{\mathrm{free}}}\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big)\\ &= (P-1)(1-\phi)u+(P_{\mathrm{free}}-1)\tilde\phi R_{P_{\mathrm{free}}}\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big)\\ &= \chi g+[-k^{-2}\Delta,\tilde\phi]\tilde\chi_2R_{P_{\mathrm{free}}}\widetilde{\chi_1}\big(\phi\chi g+[-k^{-2}\Delta,\phi]u\big)\end{aligned}$$

$$= \chi g,$$

where we used (4.2) in the last line. Since $\tilde{u}$ is outgoing, the result now follows from uniqueness of outgoing solutions to $(P-1)u = \chi g$ (see (2.1)). ∎

LEMMA 4.2 (Bounding the complex-scaled resolvent in terms of the resolvent). *Given $\delta > 0$ there exists $k_0 > 0$ such that the following is true. Given $\chi \in C_c^\infty(Q_{\rm st})$ with* $\operatorname{supp}(1-\chi) \cap Q_{\rm bb} = \emptyset$, *there exists $C > 0$ such that for all $\theta \in [\delta, \frac{\pi}{2} - \delta]$, and $k \geq k_0$, $(P_\theta - 1)^{-1} : \mathcal{H} \to \mathcal{D}$ exists and satisfies*

$$\|(P_\theta - 1)^{-1}\|_{\mathcal{H}\to\mathcal{D}} \leq C\|\chi R_P \chi\|_{\mathcal{H}\to\mathcal{H}}.$$

Proof. Given Theorem 4.1, the proof of Lemma 4.2 under the assumption that $(P_\theta - 1)^{-1} : \mathcal{H} \to \mathcal{D}$ exists is identical to the proof of the analogue of this result for radial PML in [7, Proof of Lemma 3.3] – the only difference is that the appropriate cut-off functions in [7, Proof of Lemma 3.3], whose support properties are defined via balls, must now have support properties defined via suitable hyperrectangles.

To demonstrate that $(P_\theta - 1)^{-1} : \mathcal{H} \to \mathcal{D}$ exists, we repeat the argument above for the adjoint $(P_\theta^* - 1) : \mathcal{H} \to \mathcal{D}^*$, and then use the fact that an operator is invertible if and only if both the operator and its adjoint are bounded below. ∎

5. Results about the truncated complex-scaled resolvent.

LEMMA 5.1 (Estimate near PML boundary using propagation and reflection). *Given $\epsilon, \delta, C_0 > 0$ there exists $k_0 > 0$ such that given $N > 0$ there exists $C > 0$ such that the following is true. Let $R_{{\rm st},i} + \epsilon < R_i < R_{{\rm tr},i}$ and let $U := Q_{\rm tr} \setminus \prod_{i=1}^d (-R_i, R_i)$ and $\psi \in C_c^\infty(\overline{U})$ with*

$$\|\partial^\alpha \psi\|_{L^\infty} \leq C_0, \qquad |\alpha| \leq 2.$$

Then for all $\theta \in [\delta, \pi/2 - \delta]$, all $k \geq k_0$ and all $u \in \mathcal{D}(Q_{\rm tr})$ with $u = 0$ on $\partial Q_{\rm tr}$

$$\|\psi u\|_{\mathcal{D}(Q_{\rm tr})} \leq C\Big(k\|(P_\theta^D - 1)u\|_{\mathcal{H}(Q_{\rm tr})} + k^{-N}\|u\|_{\mathcal{H}(Q_{\rm tr})}\Big), \tag{5.1}$$

and for all $v \in \mathcal{H}(Q_{\rm tr})$

$$\|\psi v\|_{\mathcal{H}(Q_{\rm tr})} \leq C\Big(k\|(P_\theta^D - 1)^* v\|_{\mathcal{D}^*(Q_{\rm tr})} + k^{-N}\|v\|_{\mathcal{H}(Q_{\rm tr})}\Big). \tag{5.2}$$

Proof. To prove (5.1), let $f := (P_\theta^D - 1)u \in \mathcal{H}(Q_{\rm tr})$. By [6, Lemma 3.6], since $R_{{\rm tr},i} > R_{{\rm lin},i}$, we may extend u to a solution $\tilde{u}$ to

$$(P_\theta - 1)\tilde{u} = \tilde{f}$$

in a neighborhood, V, of $\partial Q_{\rm tr}$ with $U \Subset V$, where $\tilde{f} \in L^2(V)$ is an appropriate reflection of f across $\partial Q_{\rm tr}$ and hence $\|\tilde{f}\|_{L^2(V)} \leq C\|f\|_{\mathcal{H}}$.

We now apply the propagation and elliptic estimates of [5, Theorem E.47, Theorem E.33]. To do this, we first show that for any $(x,\xi) \in T^*U$ with $p_{\theta,{\rm fr}}(x,\xi) = 1$ the backward Hamiltonian trajectory for $\Re p_{\theta,{\rm fr}}$ encounters $p_{\theta,{\rm fr}} \neq 1$ before exiting T^*V. Once we have proved this, the result follows directly by applying to $\tilde{u}$ [5, Theorem E.47] near points where $p_{\theta,{\rm fr}} - 1 = 0$ and [5, Theorem E.33] otherwise.

To prove the dynamical statement, observe that for any $j = 1, \ldots, d$ and $(x,\xi) \in T^*U$, with $x_j > R_{{\rm st},j}$ and $p_{\theta,{\rm fr}}(x,\xi) = 1$, we have $\xi_j = 0 \Rightarrow \partial_{\xi_j}\Re p_{\theta,{\rm fr}} = 0$ and hence x_j is constant along the Hamiltonian trajectory of $\Re p_{\theta,{\rm fr}}$ until the trajectory meets $p_{\theta,{\rm fr}} \neq 1$. This implies that such trajectories remain inside V until they either encounter $p_{\theta,\mathrm{fr}} \neq 1$ or exit V. To see that the former happens notice that $\sum_{i\neq j} \xi_i^2 > c > 0$ and hence there is i with $|\xi_i| > 0$, $F_i''(x_i) = 0$. This implies that x_i increases (or decreases) and ξ_i is constant along the Hamiltonian flow for $\Re p_{\theta,\mathrm{fr}}$ until $F_i''(x_i) \neq 0$. Since $F_i''(x_i) \neq 0$, $\xi_i \neq 0$ implies $p_{\theta,\mathrm{fr}}(x_i,\xi_i) \neq 1$ and $F_i''(x_i) > 0$ for $|x_i| > R_{\mathrm{st},i}$ this implies that the backward trajectory for $\Re p_{\theta,\mathrm{free}}$ meets $p_{\theta,\mathrm{fr}} \neq 1$ before exiting V.

For (5.2), the procedure is the same except that we set $f := (P_\theta^D - 1)^* v \in \mathcal{D}^*(Q_{\mathrm{tr}})$. Then, in a neighborhood, V, of ∂Q_{tr},

$$(P_\theta - 1)^* \tilde{v} = \tilde{f}$$

where $\tilde{f}$ in $H^{-2}(V)$ and $\|\tilde{f}\|_{H_k^{-2}(V)} \leq C\|f\|_{\mathcal{D}^*}$ (see the proof of [6, Lemma 3.2]). The estimate then follows in the same way except that we follow trajectories of $\Re p_{\theta,\mathrm{fr}}$ forward. ∎

Lemma 5.2 (Bounding the truncated complex-scaled resolvent in terms of the resolvent). *Suppose that there exists $\chi \in C_c^\infty(Q_{\mathrm{st}})$ with $\mathrm{supp}(1-\chi) \cap Q_{\mathrm{bb}} = \emptyset$, $\mathcal{J} \subset (0,\infty)$, and $M > 0$ such that for $k_0 > 0$ and there is $C_0 > 0$ such that for all $k \in \mathcal{J}$, $k \geq k_0$*

$$\|\chi R_P \chi\|_{\mathcal{H}\to\mathcal{D}} \leq C_0 k^M.$$

Given $\delta, \epsilon > 0$ there exists $C > 0$ and $k_1 \geq k_0 > 0$ such that for $R_{\mathrm{st},i} + \epsilon < R_{\mathrm{tr},i}$, $\theta \in [\delta, \pi/2 - \delta]$, and all $k \in \mathcal{J}$ with $k \geq k_1$,

$$\|(P_\theta^D - 1)^{-1}\|_{\mathcal{H}(Q_{\mathrm{tr}})\to\mathcal{D}(Q_{\mathrm{tr}})} \leq C\|\chi R_P \chi\|_{\mathcal{H}\to\mathcal{D}}.$$

Proof. Let $(P_\theta^D - 1)u = g$ and $(P_\theta^D - 1)^* v = g$. Recall that an operator is invertible if and only if both the operator and its adjoint are bounded below. By this and Lemma 4.2, it is sufficient to prove that

$$\|u\|_{\mathcal{D}(Q_{\mathrm{tr}})} \leq C\|(P_\theta - 1)^{-1}\|_{\mathcal{H}\to\mathcal{D}}\|g\|_{\mathcal{H}(Q_{\mathrm{tr}})} \tag{5.3}$$

and

$$\|v\|_{\mathcal{H}(Q_{\mathrm{tr}})} \leq C\|(P_\theta^* - 1)^{-1}\|_{\mathcal{D}^*\to\mathcal{H}}\|g\|_{\mathcal{D}^*(Q_{\mathrm{tr}})}. \tag{5.4}$$

Let U be as in Lemma 5.1 and let $\chi \in C_c^\infty(Q_{\mathrm{tr}})$ with $\mathrm{supp}\,\partial\chi \subset U$ and $\mathrm{supp}(1-\chi) \cap Q_{\mathrm{bb}} = \emptyset$. By (5.1), given $N > M + 1$, there exists $C > 0$ such that

$$\|(1-\chi)u\|_{\mathcal{D}(Q_{\mathrm{tr}})} \leq C\Big(k\|g\|_{\mathcal{H}(Q_{\mathrm{tr}})} + k^{-N}\|u\|_{\mathcal{H}(Q_{\mathrm{tr}})}\Big). \tag{5.5}$$

On the other hand, since $\chi \in C_c^\infty(Q_{\mathrm{tr}})$,

$$\chi u = (P_\theta - 1)^{-1}\Big(\chi g + [-k^{-2}\Delta_\theta, \chi]u\Big)$$

so that, since $\mathrm{supp}\,\partial\chi \subset U$,

$$\begin{aligned}\|\chi u\|_{\mathcal{D}} &\leq C\|(P_\theta - 1)^{-1}\|_{\mathcal{H}\to\mathcal{D}}\Big(\|g\|_{\mathcal{H}(Q_{\mathrm{tr}})} + k^{-1}\|u\|_{H_k^1(U)}\Big)\\ &\leq C\|(P_\theta - 1)^{-1}\|_{\mathcal{H}\to\mathcal{D}}\Big(\|g\|_{\mathcal{H}(Q_{\mathrm{tr}})} + k^{-N}\|u\|_{\mathcal{H}(Q_{\mathrm{tr}})}\Big),\end{aligned} \tag{5.6}$$

where we have used (5.1) again in the last line. By adding (5.5) and (5.6) and using that $\|(P_\theta - 1)^{-1}\|_{\mathcal{H}\to\mathcal{D}}$ is both polynomially bounded and bounded below by ck (see, e.g., [7, Remark 3.4]) we obtain that

$$\|u\|_{\mathcal{H}(Q_{\mathrm{tr}})} \leq C\|(P_\theta - 1)^{-1}\|_{\mathcal{H}\to\mathcal{D}}\|g\|_{\mathcal{H}(Q_{\mathrm{tr}})}.$$

The bound (5.3) then follows from the definition of $\|\cdot\|_{\mathcal{D}(Q_{\mathrm{tr}})}$ (2.3).

Repeating this argument for the adjoint problem using (5.2) instead of (5.1) proves (5.4), and the proof is complete. ∎

6. Proof of Theorem 2.1. By Theorem 4.1, it is sufficient to prove that, for $\chi \in C_c^\infty(Q_{\rm st})$ with $\operatorname{supp}(1-\chi)\cap Q_{\rm bb} = \emptyset$,

$$\big\|\chi\big((P_\theta^D-1)^{-1}-(P_\theta-1)^{-1}\big)\chi\big\|_{\mathcal{H}\to\mathcal{D}} \le C\exp\big(-ck(\tan\theta)\min_i\{R_{{\rm tr},i}-R_{{\rm st},i}\}\big). \tag{6.1}$$

Given $g\in L^2$ with $\operatorname{supp} g\subset \Omega_{\rm tr}$, let $u\in\mathcal{D}$ solve

$$(P_\theta-1)u=\chi g.$$

As in the proof of Theorem 4.1, u can be written as a solution to the free complex-scaled problem: let $\phi\in C^\infty(\mathbb{R}^d;[0,1])$ be such that $\operatorname{supp}\phi\cap\operatorname{supp}(P_\theta-(-k^{-2}\Delta_\theta))=\emptyset$ and $\operatorname{supp}(\nabla\phi)\subset Q_{\rm st}$. By (4.1),

$$\phi u=(P_{\theta,{\rm free}}-1)^{-1}\big(\phi\chi g+[-k^{-2}\Delta_\theta,\phi]u\big). \tag{6.2}$$

The idea of the proof is now to show that if ψ is a cut-off function supported in $Q_{\rm tr}$ with $\psi\equiv 1$ except in a small neighborhood of $\partial Q_{\rm tr}$ then ψu is a good approximation to $(P_\theta^D-1)^{-1}\chi g$. Furthermore, the commutator in this difference is supported near $\partial Q_{\rm tr}$, and thus the error decreases exponentially via the expression (4.1) and the bounds on $(P_{\theta,{\rm free}}-1)^{-1}$ in Lemma 3.6.

In more detail, let $\psi\in C_c^\infty(Q_{\rm tr})$ with $\operatorname{supp}(1-\psi)\cap\operatorname{supp}\chi=\emptyset$ and $\operatorname{supp}(1-\psi)\cap\prod_{i=1}^d(-R_{{\rm tr},i}+\epsilon,R_{{\rm tr},i}-\epsilon)=\emptyset$ and $\operatorname{supp}\partial\psi\cap\operatorname{supp}(1-\phi)=\emptyset$. Then ψu satisfies $\psi u|_{\partial Q_{\rm tr}}=0$ and

$$\begin{aligned}(P_\theta-1)\psi u&=\psi\chi g+[-k^{-2}\Delta_\theta,\psi]u\\&=\chi g+[-k^{-2}\Delta_\theta,\psi]\phi u\\&=\chi g+[-k^{-2}\Delta_\theta,\psi](P_{\theta,{\rm free}}-1)^{-1}\big(\phi\chi g+[-k^{-2}\Delta_\theta,\phi]u\big).\end{aligned}$$

Let $\widetilde{\chi}\in C_c^\infty(\mathbb{R}^d)$ with $\operatorname{supp}\widetilde{\chi}\subset Q_{\rm st}$ with $\operatorname{supp}(1-\widetilde{\chi})\cap(\operatorname{supp}\chi\cup\operatorname{supp}\nabla\phi)=\emptyset$ and let $\widetilde{\phi}\in C_c^\infty(Q_{\rm tr};[0,1])$ with $\operatorname{supp}\widetilde{\phi}\cap\prod_{i=1}^d(-R_{{\rm tr},i}+\epsilon,R_{{\rm tr},i}-\epsilon)=\emptyset$ and $\operatorname{supp}(1-\widetilde{\phi})\cap\operatorname{supp}\nabla\psi=\emptyset$. Then

$$\begin{aligned}&(P_\theta^D-1)^{-1}\chi g-\psi u\\&=-(P_\theta^D-1)^{-1}[-k^{-2}\Delta_\theta,\psi](P_{\theta,{\rm free}}-1)^{-1}\big(\phi\chi g+[-k^{-2}\Delta_\theta,\phi]u\big)\\&=-(P_\theta^D-1)^{-1}[-k^{-2}\Delta_\theta,\psi]\widetilde{\phi}(P_{\theta,{\rm free}}-1)^{-1}\widetilde{\chi}\big(\phi\chi g+[-k^{-2}\Delta_\theta,\phi](P_\theta-1)^{-1}\chi g\big).\end{aligned}$$

By the combination of Lemmas 4.2 and 5.2, $(P_\theta^D-1)^{-1}$ is polynomially bounded. We now apply Lemma 3.6 to bound $\|\widetilde{\phi}(P_{\theta,{\rm free}}-1)^{-1}\widetilde{\chi}\|_{L^2\to H_k^2}$. By the definitions of $\widetilde{\phi}$ and $\widetilde{\chi}$, for $\epsilon>0$ small enough,

$$\operatorname{dist}(\operatorname{supp}\widetilde{\phi},\operatorname{supp}\widetilde{\chi})\ge\min_i\{R_{{\rm tr},i}-R_{{\rm st},i}-\epsilon\}\ge\frac{1}{2}\min_i\{R_{{\rm tr},i}-R_{{\rm st},i}\}.$$

Therefore, by Lemma 3.6, given $\delta,k_0>0$ there exist $C,\tilde{c}>0$ such that for all $\theta\in[\delta,\pi/2-\delta]$, and all $k\ge k_0$,

$$\big\|\widetilde{\phi}(P_{\theta,{\rm free}}-1)^{-1}\widetilde{\chi}\big\|_{L^2(\mathbb{R}^d)\to H_k^2(\mathbb{R}^d)}\le C\exp\big(-\tilde{c}k\tan\theta\min_i\{R_{{\rm tr},i}-R_{{\rm st},i}\}\big)$$

and the proof is complete.

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ChatGPT version 5.6 Sol was used in the writing of Lemma 3.7, and version 6 Astra was used to proofread the document and create Figure 2.1. The authors assume responsibility for all content.

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