The hp-FEM applied to the Helmholtz equation with PML truncation does not suffer from the pollution effect

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Abstract

We consider approximation of the variable-coefficient Helmholtz equation in the exterior of a Dirichlet obstacle using perfectly-matched-layer (PML) truncation; it is well known that this approximation is exponentially accurate in the PML width and the scaling angle, and the approximation was recently proved to be exponentially accurate in the wavenumber k in [28].

We show that the hp-FEM applied to this problem does not suffer from the pollution effect, in that there exist $C_1, C_2 > 0$ such that if $hk/p \leq C_1$ and $p \geq C_2 \log k$ then the Galerkin solutions are quasioptimal (with constant independent of k), under the following two conditions (i) the solution operator of the original Helmholtz problem is polynomially bounded in k (which occurs for "most" k by [41]), and (ii) *either* there is no obstacle and the coefficients are smooth *or* the obstacle is analytic and the coefficients are analytic in a neighbourhood of the obstacle and smooth elsewhere.

This hp-FEM result is obtained via a decomposition of the PML solution into "high-" and "low-frequency" components, analogous to the decomposition for the original Helmholtz solution recently proved in [29]. The decomposition is obtained using tools from semiclassical analysis (i.e., the PDE techniques specifically designed for studying Helmholtz problems with large k).

Keywords: Helmholtz equation, high frequency, perfectly-matched layer, pollution effect, finite element method, error estimate, semiclassical analysis.

AMS subject classifications: 35J05, 65N12, 65N15, 65N30

1 Introduction and statement of the main results

1.1 Recap of the Helmholtz exterior Dirichlet problem and k-dependence of its solution operator

This paper is primarily concerned with computing solutions of the Helmholtz exterior Dirichlet problem when the wavenumber k is large.

Definition 1.1 (Helmholtz Exterior Dirichlet problem) *Let $\Omega_- \subset B_{R_0} := \{x : |x| < R_0\} \subset \mathbb{R}^d$, $d = 2, 3$, be a bounded open set with C^∞ boundary Γ_D such that $\Omega_+ := \mathbb{R}^d \setminus \overline{\Omega_-}$ is connected. Let $A_{\rm scat} \in C^\infty(\Omega_+, \mathbb{R}^{d\times d})$ be symmetric positive definite, let $c_{\rm scat} \in C^\infty(\Omega_+; \mathbb{R})$ be strictly positive and bounded, and let $A_{\rm scat}$ and $c_{\rm scat}$ be such that there exists $R_{\rm scat} > R_0 > 0$ such that*

$$\overline{\Omega_-} \cup \mathrm{supp}(I - A_{\rm scat}) \cup \mathrm{supp}(1 - c_{\rm scat}) \Subset B_{R_{\rm scat}}.$$

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Given $g \in L^2(\Omega_+)$ with $\operatorname{supp} g \Subset \mathbb{R}^d$ *and $k > 0$, $u \in H^1_{\rm loc}(\Omega_+)$ satisfies the exterior Dirichlet problem if*

$$c_{\rm scat}^2 \nabla \cdot (A_{\rm scat} \nabla u) + k^2 u = -g \quad \text{in } \Omega_+, \qquad u = 0 \quad \text{on } \Gamma_D, \tag{1.1}$$

and u is outgoing *in the sense that u satisfies the Sommerfeld radiation condition*

$$\partial_r u(x) - {\rm i}ku(x) = o\big(r^{-(d-1)/2}\big) \quad \text{as } r := |x| \to \infty, \text{ uniformly in } \widehat{x} := x/r. \tag{1.2}$$

Although the exterior Dirichlet problem makes sense for non-smooth domains and coefficients, our results below require (at least) the smoothness in Definition 1.1, and so we assume this smoothness from the start for simplicity. Let $\|\cdot\|_{H^1_k}$ be the standard weighted H^1 norm

$$\|w\|^2_{H^1_k} := \|\nabla w\|^2_{L^2} + k^2 \|w\|^2_{L^2}. \tag{1.3}$$

Definition 1.2 (Polynomial-boundedness of the solution operator) *Given $k_0 > 0$, $K \subset [k_0, \infty)$, the solution operator of the Helmholtz exterior Dirichlet problem is* polynomially bounded for $k \in K$ *if there exists $M \geq 0$ such that given $R > 0$ there exists $C > 0$ such that given $g \in L^2(\Omega_+)$ with* $\operatorname{supp} g \subset B_R$*, the solution u of the Helmholtz exterior Dirichlet problem satisfies*

$$\|u\|_{H^1_k(B_R \cap \Omega_+)} \leq C k^M \|g\|_{L^2(B_R \cap \Omega_+)} \quad \text{for all } k \in K. \tag{1.4}$$

There exist C^∞ coefficients $A_{\rm scat}$ and $c_{\rm scat}$ and obstacles Ω_- such that the solution operator is *not* polynomially bounded for all k. E.g., [57] gives an example of a $c_{\rm scat} \in C^\infty$ such that the solution operator with this $c_{\rm scat}$ and $A_{\rm scat} \equiv I$ grows exponentially through a sequence $0 < k_1 < k_2 < \ldots$ with $k_j \to \infty$ as $j \to \infty$. Note that this exponential growth is the worst-possible growth of the solution operator by [10, Theorem 2].

Theorem 1.3 (Conditions under which the solution operator is polynomially bounded) *Suppose Ω_-, $A_{\rm scat}$, and $c_{\rm scat}$ are as in Definition 1.1.*

(i) If Ω_-, $A_{\rm scat}$, and $c_{\rm scat}$ are additionally nontrapping (i.e. all the trajectories of the generalised bicharacteristic flow defined by the semiclassical principal symbol of (1.1) starting in B_R leave B_R after a uniform time), then given $k_0 > 0$, (1.4) holds with $M = 0$ and $K = [k_0, \infty)$.

(ii) Given $k_0, \delta, \varepsilon > 0$ there exists a set $J \subset [k_0, \infty)$ with $|J| \leq \delta$ such that (1.4) holds with $M = 5d/2 + \varepsilon$ and $K = [k_0, \infty) \setminus J$.

References for the proof. (i) follows from *either* the results of [56] combined with either [67, Theorem 3] or [46], *or* [11, Theorem 1.3 and §3]. (ii) is proved for $c = 1$ in [41, Theorem 1.1 and Corollary 3.6] and the proof for more-general c follows from combining the results of [41] with [29, Lemma 2.3]; we highlight that, under an additional assumption about the location of resonances, a similar result with a larger M can also be extracted from [65, Proposition 3] by using the Markov inequality. ■

1.2 Truncation of the exterior domain Ω_+ using the exact Dirichlet-to-Neumann map and solution via the hp-FEM

A popular way of solving boundary value problems involving variable-coefficient PDEs, such as the Helmholtz exterior Dirichlet problem of Definition 1.1, is the finite-element method (FEM). When the FEM is used with standard piecewise-polynomial subspaces (i.e., piecewise polynomials of degree p on a mesh with meshwidth h), the exterior domain Ω_+ must be truncated before the FEM can be used.

One truncation option is to introduce $R > R_{\rm scat}$ such that $\operatorname{supp} g \subset B_R$, and then replace Ω_+ by $\Omega_+ \cap B_R$, using as a boundary condition on ∂B_R the exact Dirichlet-to-Neumann (DtN) map for the Helmholtz equation $\Delta u + k^2 u = 0$ in the exterior of B_R with the radiation condition (1.2) (with this map given explicitly, by separation of variables, in terms of Fourier series and Hankel functions). The solution of this truncated problem is then the restriction of the solution of the exterior Dirichlet problem to B_R.

For the exterior Dirichlet problem with exact-DtN-map truncation, there has been a relatively large amount of analysis of the associated FEMs since the initial work of [49, 39]. In particular, for the *hp*-version of the FEM, where accuracy is increased by *both* decreasing h *and* increasing p, the results of [55, Theorem 5.8] (when Γ_D is analytic, $A = I$, and $c = 1$) and [29, Theorem B1] (when Γ_D is analytic and A, c are analytic near Γ_D – see Assumption 1.11 below) show that if the solution operator is polynomially bounded in k as $k \to \infty$ (in the sense of Definition 1.2) then there exist C_1, C_2, and $C_{\rm qo}$ (independent of k, h, and p) such that if

$$\frac{hk}{p} \leq C_1 \quad \text{and} \quad p \geq C_2 \log k$$

then the Galerkin solution u_N exists, is unique, and satisfies

$$\|u - u_N\|_{H^1_k(B_R \cap \Omega_+)} \leq C_{\rm qo} \min_{v_N \in V_N} \|u - v_N\|_{H^1_k(B_R \cap \Omega_+)},$$

where V_N is the *hp* approximation space.

Since the total number of degrees of freedom of the approximation space is proportional to $(p/h)^d$, these results show there is a choice of h and p such that the Galerkin solution is quasioptimal, with quasioptimality constant (i.e. $C_{\rm qo}$) independent of k, and with the total number of degrees of freedom proportional to k^d. The significance of this result is that it is well-known that the h-FEM (where accuracy is increased by decreasing h with p fixed) is *not* quasioptimal with $C_{\rm qo}$ independent of k when the total number of degrees of freedom $\sim k^d$ (i.e., when $h \sim k^{-1}$); see [2]. This feature is known as "the pollution effect" (with the term coined in [38]), and the results of [55, 29] quoted above therefore show that the *hp*-FEM applied to the exterior Dirichlet problem with exact-DtN-map truncation does not suffer from it.

1.3 Truncation of Ω_+ using a PML

Although the solution of the problem truncated with the exact DtN map is the restriction of the solution of the true problem to $\Omega_+ \cap B_R$, the exact DtN map is a non-local operator, and hence expensive to compute. A popular way of truncating in a less-computationally-expensive way is to use a *perfectly-matched layer (PML)*, introduced by [5] (in cartesian coordinates) and [16] (in spherical coordinates). In this paper we consider the following radial PMLs.

Radial PML definition. Let $R_{\rm tr} > R_1 > R_{\rm scat}$ and let $\Omega_{\rm tr} \subset \mathbb{R}^d$ be a bounded Lipschitz open set with $B_{R_{\rm tr}} \subset \Omega_{\rm tr}$. Let $\Omega := \Omega_{\rm tr} \cap \Omega_+$, $\Gamma_{\rm tr} := \partial\Omega_{\rm tr}$, and $0 \leq \theta < \pi/2$. Let

$$P := -c_{\rm scat}^2 \nabla \cdot (A_{\rm scat} \nabla).$$

so that the Helmholtz equation in (1.1) is $(P - k^2)u = g$. The PML method replaces (1.1)-(1.2) by

$$(P_\theta - k^2)v = g \quad \text{in } \Omega, \quad v = 0 \text{ on } \Gamma_D, \quad \text{and} \quad v = 0 \text{ on } \Gamma_{\rm tr}, \tag{1.5}$$

where

$$P_\theta := \begin{cases} P, & r \leq R_1, \\ -\Delta_\theta, & r > R_1, \end{cases} \tag{1.6}$$

where $-\Delta_\theta$ is a second order differential operator that is given in spherical coordinates $(r, \omega) \in [0, \infty) \times S^{d-1}$ by

$$\begin{aligned} \Delta_\theta &= \Big(\frac{1}{1 + {\rm i} f_\theta'(r)} \frac{\partial}{\partial r}\Big)^2 + \frac{d-1}{(r + {\rm i} f_\theta(r))(1 + {\rm i} f_\theta'(r))} \frac{\partial}{\partial r} + \frac{1}{(r + {\rm i} f_\theta(r))^2} \Delta_\omega, \\ &= \frac{1}{(1 + {\rm i} f_\theta'(r))(r + {\rm i} f_\theta(r))^{d-1}} \frac{\partial}{\partial r} \left(\frac{(r + {\rm i} f_\theta(r))^{d-1}}{1 + {\rm i} f_\theta'(r)} \frac{\partial}{\partial r} \right) + \frac{1}{(r + {\rm i} f_\theta(r))^2} \Delta_\omega, \end{aligned} \tag{1.7}$$

with Δ_ω the surface Laplacian on S^{d-1} and $f_\theta(r) \in C^\infty([0, \infty); \mathbb{R})$ given by $f_\theta(r) := f(r) \tan\theta$ for some f satisfying

$$\big\{f(r) = 0\big\} = \big\{f'(r) = 0\big\} = \big\{r \leq R_1\big\}, \qquad f'(r) \geq 0, \qquad f(r) \equiv r \text{ on } r \geq R_2; \tag{1.8}$$

i.e., the scaling "turns on" at $r = R_1$, and is linear when $r \geq R_2$. We emphasize that $R_{\rm tr}$ can be $< R_2$, i.e., we allow truncation before linear scaling is reached. Indeed, $R_2 > R_1$ can be arbitrarily large and therefore, given any bounded interval $[0, R]$ and any function $\widetilde{f} \in C^\infty([0,R])$ satisfying

$$\big\{\widetilde{f}(r) = 0\big\} = \big\{\widetilde{f}'(r) = 0\big\} = \big\{r \leq R_1\big\}, \qquad \widetilde{f}'(r) \geq 0,$$

our results hold for an f with $f|_{[0,R]} = \widetilde{f}$.

Remark 1.4 (Link with other notation used in the literature) *In (1.5)-(1.8) the PML problem is written using notation from the method of complex scaling (see, e.g., [22, §4.5]). In the numerical-analysis literature on PML, the scaled variable is often written as $r(1 + i\widetilde{\sigma}(r))$ with $\widetilde{\sigma}(r) = \sigma_0$ for r sufficiently large, see, e.g., [35, §4], [8, §2]. To convert from our notation, set $\widetilde{\sigma}(r) = f_\theta(r)/r$ and $\sigma_0 = \tan\theta$.*

Remark 1.5 (Smoothness of the PML scaling function f_θ) *We assume that $f_\theta \in C^\infty$ because we need the differential operator $-\Delta_\theta$ to be a semiclassical pseudodifferential operator (with the definition of these recapped in §A). More precisely, we need the operator $\widetilde{Q}_{\hbar,\theta}$, defined by (3.10) in terms of $-\Delta_\theta$, to be a semiclassical pseudodifferential operator. While we could work with pseudodifferential operators with non-smooth symbols, and thus cover f_θ with lower regularity, this would be more technical.*

Accuracy of PML truncation. It is well-known that, for fixed k, the error $\|u - v\|_{H^1_k(B_{R_1}\setminus\Omega)}$ decays exponentially in $R_{\rm tr} - R_1$ and $\tan\theta$ – see [44, Theorem 2.1], [45, Theorem A], [35, Theorem 5.8] (with analogous results for cartesian PMLs in [40, Theorem 5.5], [9, Theorem 5.8]).

It was recently proved in [28] that the error $\|u - v\|_{H^1_k(B_{R_1}\setminus\Omega)}$ also decreases exponentially in k; indeed, the following theorem is a simplified version of [28, Theorems 1.2 and 1.5].

Theorem 1.6 (Radial PMLs are exponentially accurate for k large) *Suppose that $f_\theta \in C^3(0,\infty)$ and the solution operator of exterior Dirichlet problem is polynomially bounded in k (in the sense of Definition 1.2). Given $\epsilon > 0$, there exist $C_1, C_2, k_0 > 0$ such that for all $\theta \geq \epsilon$, $R_{\rm tr} \geq R_1(1+\epsilon)$, and $k \geq k_0$ the following is true.*

Given $g \in L^2(\Omega_+)$ with $\operatorname{supp} g \subset B_{R_1}$, the solution v to (1.5) exists, is unique, and satisfies

$$\|u - v\|_{H^1_k(B_{R_1}\setminus\Omega_-)} \leq C_1 \exp\Big(- C_2 k\big(R_{\rm tr} - R_1(1+\epsilon)\big)\tan\theta\Big)\|g\|_{L^2(\Omega_+)}, \tag{1.9}$$

where u is the solution to the exterior Dirichlet problem of Definition 1.1.

We make four remarks regarding Theorem 1.6.

- The order of the quantifiers in Theorem 1.6 (and also later results in the paper) dictates what the constants depend on; e.g., in Theorem 1.6, C_1, C_2, and k_0 depend on ϵ, but are independent of $R_{\rm tr}, R_1$, and θ.
- A similar bound on the error holds even when the solution operator is *not* polynomially bounded and grows exponentially in k; see [28, Theorems 1.2 and 1.5].
- Results showing exponential decay in k (similar to in (1.9)) for the model problem of $A_{\rm scat} \equiv I, c_{\rm scat} \equiv 1$, and $\Omega_- = \emptyset$ (i.e., no scatterer) were given in [15, Lemma 3.4] for $d = 2$ and [47, Theorem 3.7] for $d = 2, 3$, using the fact that the solution of this problem can be written explicitly via the fundamental solution or separation of variables.
- The exponential decay of the error (1.9) in k is in contrast to truncation with local absorbing boundary conditions (introduced in [48, 23, 24, 4, 3]) which give $O(1)$ relative errors as $k \to \infty$ when approximating the solutions of scattering problems; see [27].

The variational formulation of the PML problem. Given $f_\theta(r)$, let

$$\alpha(r) := 1 + \mathrm{i} f_\theta'(r) \quad \text{and} \quad \beta(r) := 1 + \mathrm{i} f_\theta(r)/r. \tag{1.10}$$

Let

$$A := \begin{cases} A_{\rm scat} & \text{for } r < R_1 \\ HDH^T & \text{for } r \geq R_1, \end{cases} \quad \text{and} \quad \frac{1}{c^2} := \begin{cases} c_{\rm scat}^{-2} & \text{for } r < R_1 \\ \alpha(r)\beta(r)^{d-1} & \text{for } r \geq R_1, \end{cases} \tag{1.11}$$

where, in polar coordinates (r,φ),

$$D = \begin{pmatrix} \beta(r)\alpha(r)^{-1} & 0 \\ 0 & \alpha(r)\beta(r)^{-1} \end{pmatrix} \quad \text{and} \quad H = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} \text{ for } d = 2,$$

and, in spherical polar coordinates (r,φ,ϕ),

$$D = \begin{pmatrix} \beta(r)^2\alpha(r)^{-1} & 0 & 0 \\ 0 & \alpha(r) & 0 \\ 0 & 0 & \alpha(r) \end{pmatrix} \text{ and } H = \begin{pmatrix} \sin\varphi\cos\phi & \cos\varphi\cos\phi & -\sin\phi \\ \sin\varphi\sin\phi & \cos\varphi\sin\phi & \cos\phi \\ \cos\varphi & -\sin\varphi & 0 \end{pmatrix} \text{ for } d = 3.$$

(since $A_{\rm scat} = I$ and $c_{\rm scat}^{-2} = 1$ when $r = R_1$, A and c^{-2} are continuous at $r = R_1$).

Lemma 1.7 (Variational formulation of the PML problem (1.5)) *Given $g \in L^2(\Omega_+)$ with $\operatorname{supp} g \subset B_{R_1}$, the variational formulation of the PML problem (1.5) is*

$$\textit{find } v \in H_0^1(\Omega) \textit{ such that } a(v,w) = G(w) \textit{ for all } w \in H_0^1(\Omega), \tag{1.12}$$

where

$$a(v,w) := \int_\Omega A\nabla v \cdot \overline{\nabla w} - \frac{k^2}{c^2} v\overline{w} \quad \textit{and} \quad G(w) := \int_{B_{R_1}} \frac{g}{c^2}\overline{w}.$$

Proof. With α and β defined by (1.10) (with this notation used by [44, 47]), Δ_θ defined by (1.7) becomes

$$\Delta_\theta = \frac{1}{\alpha(r\beta)^{d-1}}\frac{\partial}{\partial r}\left(\frac{(\beta r)^{d-1}}{\alpha}\frac{\partial}{\partial r}\right) + \frac{1}{(r\beta)^2}\Delta_\omega.$$

Multiplying the PDE in (1.5) by $c_{\rm scat}^{-2}\alpha\beta^{d-1}$, using that $c_{\rm scat} \equiv 1$ for $r \geq R_1$, $\alpha \equiv \beta \equiv 1$ for $r \leq R_1$, and $\operatorname{supp} g \subset B_{R_1}$, and then changing variables to cartesian coordinates, we find that $\nabla\cdot(A\nabla u) + (k^2/c^2)u = -g/c^2$; the variational formulation (1.12) follows. ∎

Remark 1.8 (Plane-wave scattering) *The exterior Dirichlet problem of Definition 1.1 considers the Helmholtz equation with right-hand side g. Another important Helmholtz problem is that of plane-wave scattering; that is, with Ω_-, $A_{\rm scat}$, and $c_{\rm scat}$ as above, given $a \in \mathbb{R}^d$ with $|a| = 1$, let $u^I(x) := \exp(\mathrm{i}kx\cdot a)$ and find $u \in H^1_{\rm loc}(\Omega_+)$ such that*

$$c_{\rm scat}^2\nabla\cdot(A_{\rm scat}\nabla u) + k^2u = 0 \quad \textit{in } \Omega_+, \qquad u = 0 \quad \textit{on } \Gamma_D,$$

and $u^S := u - u^I$ is outgoing (i.e., satisfies (1.2)). Since u itself is not outgoing, it cannot be directly approximated by the solution of a problem with PML truncation. However, let $\chi \in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ be such that $\chi \equiv 1$ for $r \leq R_{\rm scat}$ and $\chi \equiv 0$ for $r \geq R_1$, and let

$$\widetilde{u} := \chi u^I + u^S = u - (1-\chi)u^I \quad \textit{and} \quad g := 2\nabla\chi\cdot\nabla u^I + u^I\Delta\chi.$$

Observe that $\widetilde{u}$ then satisfies the PDE in (1.1), and that the right-hand side g is supported in $R_{\rm scat} \leq r \leq R_1$. Therefore PML truncation can be used to approximate $\widetilde{u}$. Observe further that $\widetilde{u} \equiv u$ for $r \leq R_{\rm scat}$, with this usually the region where one is interested in finding the solution u.

Assumption 1.9 *When $d = 3$, $f_\theta(r)/r$ is nondecreasing.*

Assumption 1.9 is standard in the literature (in the notation described in Remark 1.4 it is that $\widetilde{\sigma}$ is non-decreasing; see, e.g., [8, §2]) and ensures that the matrix A (1.11) satisfies $\Re A > 0$ (in the sense of quadratic forms) for all θ; see Lemma 2.3 and Remark 2.5 below.

1.4 The main result: accuracy of the hp-FEM applied to the Helmholtz exterior Dirichlet problem with PML truncation

Existing results on the accuracy of the FEM applied to Helmholtz problems with PML truncation. Although the FEM with PML truncation is widely used to compute solutions of the Helmholtz exterior Dirichlet problem (and other boundary value problems involving the Helmholtz or Maxwell equations), until now there have been no rigorous k-explicit results guaranteeing the accuracy of the computed solutions of the Helmholtz exterior Dirichlet problem with PML truncation as described in §1.3.

Indeed, the only existing k-explicit results on the accuracy of the FEM applied to Helmholtz problems with PML truncation are the following.

- The result [47, Theorem 4.4] concerns the model problem of $A_{\rm scat} \equiv I, c_{\rm scat} \equiv 1$, and $\Omega_- = \emptyset$ (i.e., no scatterer), and shows that $\|v - v_N\|_{H^1_k(\Omega)}$ is bounded (independently of k) in terms of the data if $hk^{3/2}$ is sufficiently small; this threshold is observed empirically to be sharp when $p = 1$ and is the same threshold that appears for the problem with DtN truncation [42] or a first-order absorbing boundary condition [68]. [1]
- The result [12] considers Ω_- starshaped, $A_{\rm scat} \equiv I$, and $c_{\rm scat} \equiv 1$, and obtains the same thresholds for quasioptimality (for arbitrary fixed $p > 0$) as for both the problem with DtN truncation or a first-order absorbing boundary condition [55]. However, [12] considers scaling functions of the form $f_\theta(r) = r\widetilde{\sigma}/k$ (with $\widetilde{\sigma}$ independent of k), and with such scaling the PML error is not exponentially small in k.
- The result [6, Theorem 6.6.7]/[7, Theorem 5.5] covers the exterior Dirichlet problem with PML truncation, with a Robin boundary condition on $\Gamma_{\rm tr}$, under the assumptions that (i) the PML scaling angle, θ, is sufficiently small and (ii) the solution operator for this problem is polynomially bounded (in the sense of Definition 1.2); we discuss the results of [6, 7] further in §1.8 below.

Statement of the main result. We consider the exterior Dirichlet problem with domain and coefficients satisfying one of the following two assumptions.

Assumption 1.10 *(i)* $\Omega_- = \emptyset$.
(ii) $A_{\rm scat}$ *and* $c_{\rm scat}$ *are as in Definition 1.1.*
(iii) $\Gamma_{\rm tr}$ *is* $C^{1,1}$.

Assumption 1.11 *(i)* $\Omega_-, A_{\rm scat}$, *and* $c_{\rm scat}$ *are as in Definition 1.1.*
(ii) Ω_- *is analytic, and both* $A_{\rm scat}$ *and* $c_{\rm scat}$ *are analytic in* B_{R_*} *for some* $R_0 < R_* < R_1$.
(iii) $\Gamma_{\rm tr}$ *is* $C^{1,1}$.

The reasons we consider these classes of domain and coefficients is explained in §1.8/§4.2 below. We note here that the assumption that $\Gamma_{\rm tr}$ is $C^{1,1}$ ensures that the PML solution is in $H^2(\Omega_{\rm tr})$.

Theorem 1.12 (Quasioptimality of hp-FEM for the exterior Dirichlet problem with PML truncation) *Suppose that* $\Omega_-, A_{\rm scat}, c_{\rm scat}$, *and* $\Omega_{\rm tr}$ *satisfy* either *Assumption 1.10* or *Assumption 1.11. Suppose further that* $\Omega_-, A_{\rm scat}, c_{\rm scat}$, *and* $K \subset [k_0, \infty)$ *are such that the solution operator of the exterior Dirichlet problem is polynomially bounded (in the sense of Definition 1.2). Suppose that the PML scaling function* $f_\theta \in C^\infty$ *and satisfies Assumption 1.9. Let* $(V_N)_{N=0}^\infty$ *be the piecewise-polynomial approximation spaces described in [54, §5], [55, §5.1.1] (where, in particular, the triangulations are quasi-uniform and allow curved elements).*

[1] Since the preprint of the present paper appeared, the preprint [30] generalised the result of [47, Theorem 4.4] to general scattering problems with PML truncation and h-FEM spaces of arbitrary polynomial degree, proving quasi-optimality if $(hk)^p k^{1+M}$ is sufficiently small, where M is as in (1.4), and a bound on the relative error if $(hk)^{2p} k^{1+M}$ is sufficiently small.

Given $\epsilon > 0$, there exist $k_1, C_1, C_2, C_{\rm qo} > 0$ such that the following is true. Given $G \in (H^1_k(\Omega))^*$, for all $k \in K \cap [k_1, \infty)$, $\epsilon \leq \theta \leq \pi/2 - \epsilon$, and $R_{\rm tr} \geq R_1(1+\epsilon)$, the solution v to the PML problem (1.5)/ (1.12) exists and is unique. Furthermore, if

$$\frac{hk}{p} \leq C_1 \quad \text{and} \quad p \geq C_2 \log k, \tag{1.13}$$

then the Galerkin solution v_N of the PML problem (1.12), satisfying

$$a(v_N, w_N) = G(w_N) \quad \text{for all } w_N \in V_N, \tag{1.14}$$

exists, is unique, and satisfies the quasioptimal error bound

$$\|v - v_N\|_{H^1_k(\Omega)} \leq C_{\rm qo} \min_{w_N \in V_N} \|v - w_N\|_{H^1_k(\Omega)}. \tag{1.15}$$

The error on $B_R \cap \Omega_+$ between the true solution u and the Galerkin approximation to the PML solution v_N is then controlled by combining (1.15) with (1.9).

Remark 1.13 (Non-conforming error) *Theorem 1.12 assumes that the domain Ω is triangulated exactly. In practical applications, however, exact triangulations are seldom used, and some analysis of the geometric error is therefore necessary. We ignore this issue here (just as in the previous work on the hp-FEM in [54, 55, 26, 53, 43, 29]), but note that, empirically, at least for the h-FEM, the geometric error caused by using simplicial elements is smaller than the pollution error.*

1.5 The idea behind the hp-FEM result of Theorem 1.12: decompositions of high-frequency Helmholtz solutions

Decomposition of constant-coefficient Helmholtz solutions in [54, 55, 26]. The celebrated papers [54, 55, 26, 53] established a k-explicit convergence theory for the hp-FEM applied to the constant-coefficient Helmholtz equation $\Delta u + k^2 u = -f$. This theory is based on decomposing solutions of this equation as

$$u = u_{\mathcal{A}} + u_{H^2}, \tag{1.16}$$

where

(i) $u_{\mathcal{A}}$ is analytic, and satisfies bounds with the same k-dependence as those satisfied by the full Helmholtz solution, but with explicit k-dependence built into the Cauchy estimates, and

(ii) u_{H^2} has finite regularity (normally H^2), and satisfies bounds with improved k-dependence compared to those satisfied by the full Helmholtz solution.

The papers [54, 55, 26] obtained such a decomposition for a variety of constant-coefficient Helmholtz problems, with the idea of the decomposition that $u_{\mathcal{A}}$ corresponds to the low-frequency components of the solution u (i.e., components with frequencies $\lesssim k$) u_{H^2} corresponds to the high-frequency components of solution (i.e., components with frequencies $\gtrsim k$) – we discuss this "decomposing-via-frequencies" idea further in §1.8.

How the decomposition shows that the hp-FEM does not suffer from the pollution effect under the conditions (1.13). The classic duality argument (originating from ideas introduced in [61] and then refined by [60]) gives a condition for the Galerkin solutions to be quasioptimal in terms of how well solutions of the adjoint problem are approximated by the finite-element space (see §2.1 below and the discussion/references therein). Note that solutions of the adjoint problem for the Helmholtz equation are just complex-conjugates of Helmholtz solutions (see Lemma 2.7 below), so in this argument one only needs to consider approximation of Helmholtz solutions.

When applying the classic duality argument to the Helmholtz equation, approximating the Helmholtz solution directly (without any decomposing) and using the sharp bound (in terms of k-dependence) on its H^2 norm results in the condition "hk^2/p sufficiently small" for quasioptimality; this is the sharp condition when $p = 1$ – see, e.g., [38, Figure 8].

The fact that u_{H^2} satisfies a bound one power of k better than that satisfied by u means that the analogue of the condition "hk^2/p sufficiently small" with u replaced by u_{H^2} is the improved "hk/p sufficiently small"; i.e., the first condition in (1.13). Provided that the solution operator is polynomially bounded in the sense of (1.4), the analogue of the condition "hk^2/p sufficiently small" with u replaced by $u_{\mathcal{A}}$ (and using the first $p+1$ derivatives of $u_{\mathcal{A}}$) is essentially

$$k^{1+M}\left(\frac{hk}{\sigma p}\right)^{p} \tag{1.17}$$

sufficiently small (with σ constant); see (2.6) below. With hk/p sufficiently small, (1.17) can be made arbitrarily small if $p/\log k$ is sufficiently large, leading to the second condition in (1.13); note that the analyticity of $u_{\mathcal{A}}$ is crucial here, since it allows us to take p arbitrarily large.

The recent paper [29]: analogous decompositions for very general Helmholtz scattering problems. The recent paper [29] (following [43]) showed that similar decompositions can be obtained for very general Helmholtz scattering problems, namely, those fitting into the so-called "black-box" framework of Sjöstrand–Zworski [63], with this framework including problems where the scattering is caused by variable coefficients, penetrable obstacles, or impenetrable obstacles. For these general Helmholtz solutions, $u_{\mathcal{A}}$ is not necessarily analytic, but the regularity is determined by properties of the scatterer. The paper [29] then showed that, if the domain and coefficients satisfy either Assumptions 1.10 or 1.11, then $u_{\mathcal{A}}$ is analytic (possibly modulo a remainder that is super-algebraically small in k), and then the arguments of [54, 55] can be used to show that the hp-FEM applied to these Helmholtz problems does not suffer from the pollution effect.

The main contribution of the present paper. The main contribution of the present paper is *showing that the decompositions of outgoing Helmholtz solutions obtained in [29] also hold for the corresponding Helmholtz solutions with PML truncation.* Indeed, our main decomposition result for PML solutions, stated informally in the next subsection as Theorem 1.15, and then rigorously in Theorem 4.1, is the exact analogue of the corresponding decomposition result in [29] for outgoing Helmholtz solutions.

The results in [29] that show that $u_{\mathcal{A}}$ is analytic if the domain and coefficients satisfy either Assumption 1.10 or 1.11, then show the corresponding result for the low-frequency components of the PML solution. Thus, exactly as in [29], the arguments of [54, 55] can be used to show that the hp-FEM applied to these PML problems does not suffer from the pollution effect, i.e., Theorem 1.12.

We emphasise that the proof of Theorem 4.1 involves several new technical ideas compared to the proof of the analogous result in [29] for outgoing Helmholtz solutions. These differences arise from the fact that in [29] the notion of "high-frequency" and "low-frequency" components of the solution is defined via the functional calculus for self-adjoint operators (see §1.8 below) but the PML operator is not self-adjoint. To overcome this obstacle, we use (i) the ellipticity of the PML operator in the scaling region and the recent results of [28], (ii) the fact that the functional calculus is pseudolocal (see Lemma 3.5 below), and (iii) the fact that, away from the scatterer and the PML truncation boundary, the functional calculus is pseudodifferential (see Lemma 3.6 below).

Recap of k-explicit analyticity. Before stating informally the main decomposition result for PML solutions (Theorem 1.15), we record the following lemma about how the bound an analytic function depending on k satisfies dictates the k-dependence of the region of analyticity; we use this lemma below to understand the properties of the $v_{\mathcal{A}}$s in Theorems 1.15, 1.16, and 1.17.

Lemma 1.14 (k-explicit analyticity) *With D a bounded open set, let $u \in C^\infty(D)$ be a family of functions depending on k.*

(i) If there exist $C, C_u > 0$ such that, for all multiindices α,

$$\|\partial^\alpha u\|_{L^2(D)} \leq C_u (Ck)^{|\alpha|}.$$

then u is real analytic in D with infinite radius of convergence, i.e., u is entire.

(ii) If there exist $C, C_u > 0$ such that, for all multiindices α,

$$\|\partial^\alpha u\|_{L^2(D)} \leq C_u (Ck)^{|\alpha|} |\alpha|!,$$

then u is real analytic in D with radius of convergence proportional to $(Ck)^{-1}$.

(iii) If there exist $C, C_u > 0$ such that, for all multiindices α,

$$\|\partial^\alpha u\|_{L^2(D)} \leq C_u C^{|\alpha|} \max\big\{|\alpha|, k\big\}^{|\alpha|},$$

then u is real analytic in D with radius of convergence independent of k.

Proof. In each part, we use the Sobolev embedding theorem to obtain a bound on $\|\partial^\alpha u\|_{L^\infty(D)}$, and then sum the remainder in the truncated Taylor series. For this procedure carried out in Part (iii), see, e.g., [54, Proof of Lemma C.2]; the proofs for the other cases are similar. ∎

1.6 Informal statement of the main decomposition result for Helmholtz problems with PML truncation

Theorem 1.15 (Informal statement of the main decomposition result) *Let P be a formally self-adjoint operator with $P = -\Delta$ outside a sufficiently-large ball ("the black box"). Suppose that $P - k^2$ is well defined and that*

(H1) the solution operator associated with $P - k^2$ is polynomially bounded: there exists $M \geq 0$ so that for any $\chi \in C^\infty_{\rm comp}$ and any compactly-supported $g \in L^2$, the outgoing solution of $(P - k^2)u = g$ satisfies

$$\|\chi u\|_{L^2} \lesssim k^{-1+M} \|g\|_{L^2},$$

(H2) one has an estimate quantifying the regularity of P inside the black box.

Let P_θ be defined by (1.6), and let $\Omega_{\rm tr}$ and Ω be as in §1.1. Then any solution of $(P_\theta - k^2)v = g$ in Ω can be written as

$$v = v_{H^2} + v_{\mathcal{A}} + v_{\rm residual}$$

where

(i) v_{H^2} satisfies the same boundary conditions as v and the bound

$$\|v_{H^2}\|_{L^2(\Omega)} + k^{-2}\|P_\theta v_{H^2}\|_{L^2(\Omega)} \lesssim k^{-2}\|g\|_{L^2(\Omega)},$$

(ii) $v_{\mathcal{A}}$ is regular*, with an estimate depending on* both *the regularity of the underlying problem (as measured by (H2))* and *M. In addition, the part of $v_{\mathcal{A}}$ away from the black box is entire (in the sense of Lemma 1.14(i)).*

(iii) $v_{\rm residual}$ is negligible, in the sense that all of its norms are smaller than any algebraic power of k.

Finally, given $\epsilon > 0$, the constants in the bounds on $v_{H^2}, v_{\mathcal{A}}$, and $v_{\rm residual}$ are uniform in θ for $\epsilon \leq \theta \leq \pi/2 - \epsilon$.

We make the following immediate remarks:

- The assumptions in Theorem 1.15 (involving the unscaled operator P) are exactly the same as in the analogue of Theorem 1.15 for outgoing Helmholtz solutions; see [29, Theorem A′]. The conclusions of Theorem 1.15 are essentially the same as those [29, Theorem A′], except with u replaced by v, P replaced by P_θ, and the addition of the "residual" term $v_{\rm residual}$ (the reason why this residual term appears here, but not in [29, Theorem A′], is to make v_{H^2} satisfy the zero Dirichlet boundary condition on $\Gamma_{\rm tr}$ – see the discussion after Theorem 4.1).
- If P is the Dirichlet Laplacian with both Γ_D and $\Gamma_{\rm tr} \in C^{1,1}$ then $\|P_\theta v_{H^2}\|_{L^2}$ controls $\|v_{H^2}\|_{H^2}$ up to $\|v_{H^2}\|_{L^2}$ by elliptic regularity, and thus the bound in (i) is a bound on $\|v_{H^2}\|_{H^2}$ – hence the notation v_{H^2}. (Assumptions 1.10 and 1.11 contain these assumptions on Γ_D and $\Gamma_{\rm tr}$ precisely to ensure this H^2 regularity of v_{H^2}.)

- The paper [41] shows that the assumption (H1) holds in the black-box framework for "most" frequencies (see Part (i) of Theorem 1.3 for a more precise statement of this). Therefore, to apply this result to specific situations, the key point is to check that an estimate of the type (H2) holds; we discuss this further in §4.2.

Transferring the results in [29] for particular Helmholtz solutions to the corresponding Helmholtz solutions with PML truncation. Since (i) the assumptions of Theorem 1.15 (and its precise version Theorem 4.1) are exactly the same (by design) as the assumptions of [29, Theorem A′/Theorem A], and (ii) these assumptions are checked in [29] for the particular Helmholtz problems we are interested in here, analogous decompositions to those in [29] for outgoing Helmholtz solutions then immediately hold for the analogous PML problems. Indeed, [29] proves the decomposition $u = u_{\mathcal{A}} + u_{H^2}$ (1.16) with $u_{\mathcal{A}}$ analytic under Assumptions 1.10 and 1.11, with (H2) corresponding to, respectively, an explicit estimate on the eigenfunctions of the Laplace operator on the torus and an analytic estimate for solutions of the heat equation. The PML analogues of these results then follow immediately and are stated in Theorems 1.16 and 1.17 in the next section.

We highlight that [29] also decomposes the solution of the Helmholtz transmission problem, and thus an analogous result holds for the corresponding PML problem. This result shows only finite-regularity of $v_{\mathcal{A}}$ (as opposed to analyticity), and so gives a (sharp) result about quasioptimality of the h-FEM, but not the hp-FEM. Since we focus on the hp-FEM in the present paper, we do not state this decomposition for the transmission problem with PML truncation (but highlight here that it exists).

1.7 The main decomposition result applied to the Helmholtz exterior Dirichlet problem with PML truncation under Assumptions 1.10 or 1.11

Theorem 1.16 (Decomposition of the PML solution under Assumption 1.10) *Suppose that $\Omega_-, A_{\rm scat}$, $c_{\rm scat}$, and $\Omega_{\rm tr}$ satisfy Assumption 1.10. Suppose further that $A_{\rm scat}$, $c_{\rm scat}$, and $K \subset [k_0,\infty)$ are such that the solution operator is polynomially bounded (in the sense of Definition 1.2).*

Given $\epsilon > 0$, there exist $C_j, j = 1,2,3$, and $k_1 > 0$ such that the following is true. For all $R_{\rm tr} > R_1 + \epsilon$, $B_{R_{\rm tr}} \subset \Omega_{\rm tr} \Subset \mathbb{R}^d$, and $\epsilon < \theta < \pi/2 - \epsilon$, given $g \in L^2(\Omega)$, the solution v of the PML problem (1.5) exists, is unique, and is such that

$$v = v_{H^2} + v_{\mathcal{A}} + v_{\rm residual},$$

where $v_{\mathcal{A}}, v_{H^2}$, and $v_{\rm residual}$ satisfy the following. $v_{H^2} \in H^2(\Omega)\cap H^1_0(\Omega)$ with

$$\|\partial^\alpha v_{H^2}\|_{L^2(\Omega)} \le C_1 k^{|\alpha|-2}\|g\|_{L^2(\Omega)} \quad \text{for all } k \in K\cap[k_1,\infty) \text{ and for all } |\alpha|\le 2. \tag{1.18}$$

$v_{\mathcal{A}}$ satisfies

$$\|\partial^\alpha v_{\mathcal{A}}\|_{L^2(\Omega)} \le C_2(C_3)^{|\alpha|}k^{|\alpha|-1+M}\,\|g\|_{L^2(\Omega)} \quad \text{for all } k \in K\cap[k_1,\infty) \text{ and for all } \alpha \tag{1.19}$$

and is negligible in the scaling region in the sense that for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such

$$\|v_{\mathcal{A}}\|_{\mathcal{H}^m((B_{R_1(1+\epsilon)})^c)} \le C_{N,m}k^{-N}\|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } k \in K\cap[k_1,\infty).$$

Finally $v_{\rm residual}$ is negligible in the sense that for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) so that

$$\|v_{\rm residual}\|_{H^m(\Omega)} \le C_{N,m}k^{-N}\,\|g\|_{L^2(\Omega)} \text{ for all } k \in K\cap[k_1,\infty). \tag{1.20}$$

By Part (i) of Lemma 1.14, $v_{\mathcal{A}}$ in Theorem 1.16 is entire.

Theorem 1.17 (Decomposition of the PML solution under Assumption 1.11) *Suppose that $\Omega_-, A_{\rm scat}$, $c_{\rm scat}$, and $\Omega_{\rm tr}$ satisfy Assumption 1.11. Suppose further that $\Omega_-, A_{\rm scat}$, $c_{\rm scat}$, and*

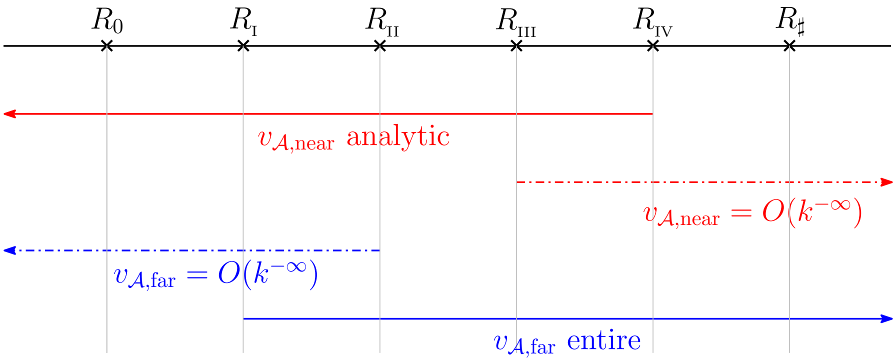

Figure 1.1: The regions where $v_{\mathcal{A},\mathrm{near}}$ and $v_{\mathcal{A},\mathrm{far}}$ appearing in Theorem 1.17 are analytic, entire, or $O(k^{-\infty})$.

$K \subset [k_0,\infty)$ are such that the solution operator is polynomially bounded (in the sense of Definition 1.2).

Given $\epsilon > 0$, there exist $C_j > 0, j = 1,\ldots,5$, and $R_0 < R_{\mathrm{I}} < R_{\mathrm{II}} < R_{\mathrm{III}} < R_{\mathrm{IV}} < R_1$ such that the following is true. For all $R_{\mathrm{tr}} > R_1+\epsilon$, $B_{R_{\mathrm{tr}}} \subset \Omega_{\mathrm{tr}} \Subset \mathbb{R}^d$, and $\epsilon < \theta < \pi/2-\epsilon$, given $g \in L^2(\Omega)$, the solution v of the PML problem (1.5) exists, is unique, and is such that

$$v = v_{H^2} + v_{\mathcal{A}} + v_{\mathrm{residual}}$$

where $v_{\mathcal{A}}, v_{H^2}$, and v_{residual} satisfy the following. $v_{H^2} \in H^2(\Omega)\cap H^1_0(\Omega)$ with

$$\|\partial^\alpha u_{H^2}\|_{L^2(\Omega)} \leq C_1 k^{|\alpha|-2}\|g\|_{L^2(\Omega)} \qquad \text{for all } k \in K\cap[k_1,\infty) \text{ and for all } |\alpha|\leq 2. \tag{1.21}$$

$v_{\mathcal{A}} = v_{\mathcal{A},\mathrm{near}} + v_{\mathcal{A},\mathrm{far}}$, where $v_{\mathcal{A},\mathrm{near}}$ has zero Dirichlet trace on Γ_D, $v_{\mathcal{A},\mathrm{far}}$ has zero Dirichlet trace on Γ_{tr}, and, for all $k \in K\cap[k_1,\infty)$ and all α,

$$\|\partial^\alpha v_{\mathcal{A},\mathrm{near}}\|_{L^2(B_{R_{\mathrm{IV}}}\cap\Omega)} \leq C_2(C_3)^{|\alpha|}\max\left\{|\alpha|^{|\alpha|}, k^{|\alpha|}\right\}k^{-1+M}\,\|g\|_{L^2(\Omega)}, \tag{1.22}$$

$$\|\partial^\alpha v_{\mathcal{A},\mathrm{far}}\|_{L^2((B_{R_{\mathrm{I}}})^c\cap\Omega)} \leq C_4(C_5)^{|\alpha|}k^{|\alpha|-1+M}\,\|g\|_{L^2(\Omega)},$$

and, for any $N,m>0$ there exists $C_{N,m}>0$ (independent of θ) so that

$$\|v_{\mathcal{A},\mathrm{far}}\|_{H^m(B_{R_{\mathrm{II}}}\cap\Omega)} + \|v_{\mathcal{A},\mathrm{near}}\|_{H^m((B_{R_{\mathrm{III}}})^c\cap\Omega)} \leq C_{N,m}k^{-N}\,\|g\|_{L^2(\Omega)} \text{ for all } k\in K\cap[k_1,\infty).$$

Finally v_{residual} is negligible in the sense that for any $N,m>0$ there exists $C_{N,m}>0$ (independent of θ) so that (1.20) holds.

By Parts (iii) and (i) of Lemma 1.14, $v_{\mathcal{A},\mathrm{near}}$ is analytic in $B_{R_{\mathrm{IV}}}$ with k-independent radius of convergence, and $v_{\mathcal{A},\mathrm{far}}$ is entire in $(B_{R_{\mathrm{I}}})^c$; see Figure 1.1.

1.8 The ideas behind the decomposition result of Theorems 1.15, 1.16, and 1.17 and previous decomposition results for Helmholtz problems

Table 1.1 summarises the problems considered and approaches to the decompositions in the papers [54, 55, 26, 43, 29], and the present paper. We now discuss the six main ideas/ingredients used in the proof of Theorem 1.15 (and its precise statement in Theorem 4.1).

Paper	Helmholtz equation	Problem	Freq. cut-offs defined by	Freq. cut-offs applied to	Proof of bound on HF part	Proof of bound on LF part
[54]	$\Delta u + k^2 u = -f$	in $\mathbb{R}^d$ with SRC	Fourier transform on $\mathbb{R}^d$ with sharp cut-off	data	asymptotics of Bessel/Hankel functions	asymptotics of Bessel/Hankel functions
[55]	$\Delta u + k^2 u = -f$	EDP obstacle analytic IIP convex polygon or smooth	as in [54] plus extension operators	data	bounds on cut-offs from [54]	analytic estimate on Helm. solutions with analytic data
[26]	$\Delta u + k^2 u = -f$	IIP convex polygon	as in [54] plus extension operators	data	bounds on cut-offs from [54]	analytic estimate on Helm. solutions with analytic data
[43]	$\nabla\cdot(A\nabla u) + k^2 cu = -f$	in $\mathbb{R}^d$ with SRC A, c smooth	Fourier transform on $\mathbb{R}^d$ smooth cut-off	solution $\times$ spatial cut-off	semiclassical ellip. of Helmholtz on HF	immediate from FT
[29] (general result)	equations that are $\Delta u + k^2 u = 0$ outside large ball	any problem fitting in framework of black-box scattering	functional calculus (i.e., eigenfunction expansion), smooth cut-off	solution $\times$ spatial cut-off	semiclassical ellip. pseudo. prop. of func. calc.	abstract regularity estimate in black box
[29] (specific result)	$\nabla\cdot(A\nabla u) + k^2 cu = -f$	EDP obstacle analytic A, c analytic near obstacle	functional calculus, smooth cut-off	solution $\times$ spatial cut-off	semiclassical ellip. pseudo. prop. of func. calc.	heat-flow estimate
this paper	$\nabla\cdot(A\nabla u) + k^2 cu = -f$ + PML truncation	*either* A, c smooth, no obs. *or* EDP obstacle analytic A, c analytic near obstacle	functional calculus, smooth cut-off	solution $\times$ spatial cut-off supported into PML region	semiclassical ellip. pseudo. prop. of func. calc.	heat-flow estimate

Table 1.1: Summary of the decomposition results in the papers [54, 55, 26, 43, 29] and the present paper. "SRC" stands for "Sommerfeld radiation condition", "EDP" stands for "exterior Dirichlet problem", "IIP" stands for "interior impedance problem", "HF" stands for "high-frequency", and "LF" stands for "low-frequency". To keep the notation concise, we abbreviate $A_{\rm scat}$ and $c_{\rm scat}$ by A and c, respectively.

Ingredient 1: semiclassical ellipticity of the Helmholtz operator on high frequencies. The reason the high-frequency component v_{H^2} satisfies a bound with better k-dependence than the solution v is because *the Helmholtz operator is semiclassically elliptic on frequencies with modulus* $> k$. While this feature was observed in [43] in the variable-coefficient setting, its essence is most easily illustrated in the constant-coefficient setting. With the Fourier transform defined by

$$\mathcal{F}_k\phi(\xi) := \int_{\mathbb{R}^d} \exp\big(-\mathrm{i}kx\cdot\xi\big)\phi(x)\,\mathrm{d}x \tag{1.23}$$

(i.e., the standard Fourier transform with the Fourier variable scaled by k), the constant-coefficient Helmholtz operator is Fourier multiplier with Fourier symbol $|\xi|^2-1$; i.e.,

$$\big((-k^{-2}\Delta-1)v\big)(x) = \mathcal{F}_k^{-1}\Big((|\xi|^2-1)\mathcal{F}_k v(\xi)\Big)(x). \tag{1.24}$$

If $\lambda > 1$ then there exists $C > 0$ such that

$$\big||\xi|^2-1\big| \geq C\langle\xi\rangle^2 \quad \text{ for } |\xi| \geq \lambda;$$

i.e., the Fourier symbol of the constant-coefficient Helmholtz operator is elliptic on $|\xi| > 1$, with this range of ξ corresponding to the standard Fourier variable (i.e., with no scaling by k in (1.23)) having modulus $> k$. The "high-frequency" components of the solution are then defined as those with frequency $> k$, and the "low-frequency" ones defined as those with frequencies $\lesssim k$.

Ingredient 2: semiclassical pseudodifferential operators. The variable-coefficient Helmholtz operator $\nabla\cdot(A_{\rm scat}\nabla) + k^2 c_{\rm scat}$ is no longer a Fourier multiplier (i.e., it cannot be written in the form (1.24)). It is, however, a pseudodifferential operator; indeed, recall that part of the motivation for the development of pseudodifferential operators was to extend Fourier analysis to study variable-coefficient (as opposed to constant-coefficient) PDEs. *Semiclassical* pseudodifferential operators are those defined with Fourier transform defined by (1.23), i.e., with the large parameter k (or small parameter k^{-1}) built in; thus semiclassical pseudodifferential operators are precisely the pseudodifferential operators tailor-made to study problems with a large/small parameter.

The paper [43] uses the "nice" behaviour of elliptic semiclassical pseudodifferential operators (namely, they are invertible up to a small error) to prove the required bound on the high-frequency components of the decomposition for the (non-truncated) Helmholtz equation in $\mathbb{R}^d$ (i.e., $\Omega_- = \emptyset$) with smooth $A_{\rm scat}$ and $c_{\rm scat}$. Note that (i) the polynomial boundedness condition of Definition 1.2 is needed to show that the $O(k^{-\infty})$ error terms in the pseudodifferential calculus acting on the solution are indeed small (which is not guaranteed if the solution operator grows exponentially in k), and (ii) the theory of pseudodifferential operators is the least technical when the symbols are smooth, thus [43] used smooth frequency cut-offs (as opposed to those defined by an indicator function in [54, 55]). [2]

Ingredient 3: frequency cut-offs defined as functions of the operator (i.e., eigenfunction expansion). For problems posed in domains other than $\mathbb{R}^d$, it is difficult to use the Fourier transform to define frequency cut-offs. The papers [55, 26] tackle this issue by using the composition of the frequency cut-offs on $\mathbb{R}^d$ and a suitable extension operator from the domain to $\mathbb{R}^d$. Here, following [29], we instead define frequency cut-offs using the eigenfunctions of the Helmholtz operator considered on a large torus including $\Omega_{\rm tr}$ (and the black box inside it); this approach has the advantage that the frequency cut-offs then commute with the Helmholtz operator used to define them.

More precisely, recall that the functional calculus defines functions of a self-adjoint elliptic operator in terms of eigenfunction expansions. Here we choose the operator to be the so-called *reference operator* in the framework of black-box scattering; this is just the operator $P_\hbar^\sharp :=$

[2] The expository paper [64] shows that a frequency cut-off defined by an indicator function can nevertheless be used in the constant-coefficient case; this is because Fourier multipliers can be formulated without any differentiability requirements on the symbols. The paper [64] gives an alternative proof of the decomposition result in [54] using just elementary properties of the Fourier transform and integration by parts (in particular, without any of the Bessel/Hankel-function asymptotics used in [54]).

$-k^{-2}c_{\rm scat}^2\nabla\cdot(A_{\rm scat}\nabla)$ considered on the torus $\mathbb{T}^d_{R_\sharp}$ with $R_\sharp$ sufficiently large so that the torus contains $\Omega_{\rm tr}$ (see §3.1 below). Then, with $\lambda_j^\sharp$ and $\phi_j^\sharp$ the eigenvalues and eigenfunctions of $P_\hbar^\sharp$ and f a real-valued Borel function,

$$f(P_\hbar^\sharp)v=\sum_j a_j f(\lambda_j^\sharp)\phi_j^\sharp \quad \text{for} \quad v=\sum_j a_j\phi_j^\sharp$$

(see §3.4 below). Given $\psi\in C^\infty_{\rm comp}(\mathbb{R};[0,1])$ with $\operatorname{supp}\psi\subset[-2,2]$ and $\psi\equiv 1$ on $[-1,1]$, we define $\psi_\mu:=\psi(\cdot/\mu)$ and let

$$\Pi_{\rm Low}:=\psi_\mu(P_\hbar^\sharp) \quad \text{and} \quad \Pi_{\rm High}:=(1-\psi_\mu)(P_\hbar^\sharp)=I-\Pi_{\rm Low};$$

see (5.6) and (5.7) below. As mentioned above, a crucial fact about these frequency cut-offs is that they commute with $P_\hbar^\sharp$.

Ingredient 4: introduce a spatial cut-off and use ellipticity of the PML operator in the scaling region. We choose $\varphi_{\rm tr}\in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ such that $\varphi_{\rm tr}\equiv 1$ on $B_{R_1(1+\delta)}$ and $\operatorname{supp}\varphi_{\rm tr}\subset B_{R_1(1+2\delta)}$ for a suitably chosen $\delta>0$. We then decompose v as

$$v=\underbrace{\Pi_{\rm High}(\varphi_{\rm tr}v)}_{=:v_{\rm High}}+\underbrace{\Pi_{\rm Low}(\varphi_{\rm tr}v)}_{=:v_{\rm Low}}+\underbrace{(1-\varphi_{\rm tr})v}_{=:v_{\rm PML}}. \tag{1.25}$$

We then use results from the recent paper [28] to bound $v_{\rm PML}$ in terms of the data with one power better k-dependence than the bound on the solution v; thus $v_{\rm PML}$ can be included in the component v_{H^2} (note that the conditions on $\Gamma_{\rm tr}$ in Assumptions 1.10 and 1.11 ensure that the PML solution is H^2 up to the boundary $\Gamma_{\rm tr}$).

The ingredients used to bound $v_{\rm PML}$ are (i) the fact that, at highest order, the imaginary part of $-k^{-2}\Delta_\theta-1$ has a sign in the scaling region (see, e.g., [28, Equation 4.22], with this behind Lemma 5.4 below) and (ii) a Carleman estimate describing how v propagates in the scaling region (see Lemma 5.5 below).

In bounding $v_{\rm PML}$, it is crucial that $(1-\varphi_{\rm tr})$ (and hence also $(1-\varphi_{\rm tr})v$) is supported only in the PML scaling region $(B_{R_1})^c$. However, the fact that $\operatorname{supp}\varphi_{\rm tr}$ enters the scaling region causes the following issue. When bounding $v_{\rm High}$, we consider

$$(P_\hbar^\sharp-I)\Pi_{\rm High}(\varphi_{\rm tr}v)=\Pi_{\rm High}(P_\hbar^\sharp-I)(\varphi_{\rm tr}v)=\Pi_{\rm High}\Big([P_\hbar^\sharp,\varphi_{\rm tr}]v+\varphi_{\rm tr}(P_\hbar^\sharp-I)v\Big). \tag{1.26}$$

We would now like to say that $(P_\hbar^\sharp-I)v$ equals the data $(P_{\hbar,\theta}-I)v$, but this is not the case since $P_\hbar^\sharp\neq P_{\hbar,\theta}$ on $\operatorname{supp}\varphi_{\rm tr}$ (which enters the scaling region).

The solution is twofold: we first split $v_{\rm High}=\Pi_{\rm High}(\varphi_0 v)+\Pi_{\rm High}(1-\varphi_0)\varphi_{\rm tr}v$ (see (5.28) below), where $\varphi_0\in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ such that $\varphi_0\equiv 1$ on B_{R_0} and $\operatorname{supp}\varphi_0\subset B_{R_1}$, and thus $P_\hbar^\sharp=P_{\hbar,\theta}$ on $\operatorname{supp}\varphi_0$. We argue as above for $\Pi_{\rm High}(\varphi_0 v)$ and then deal with the component $\Pi_{\rm High}(1-\varphi_0)\varphi_{\rm tr}v$, as well as the commutator term in (1.26), using the next ingredient.

Ingredient 5: away from the black box, functions of $P_\hbar^\sharp$ are semiclassical pseudodifferential operators. When bounding $v_{\rm High}$ and $v_{\rm Low}$, we use repeatedly the result that, when f is sufficiently well-behaved and $\chi\in C^\infty(\mathbb{R}^d;[0,1])$ is zero in a neighbourhood of the black box, $\chi f(P_\hbar^\sharp)\chi$ is a pseudodifferential operator (up to a negligible error term); see Lemma 3.6 below. In particular, this result allows us to treat $\Pi_{\rm High}$ and $\Pi_{\rm Low}$ as pseudodifferential operators away from the black box.

The context of this result, due to Sjöstrand [62], is the following: in the setting of the homogeneous pseudodifferential calculus, Strichartz [66] proved that a well-behaved function of a self-adjoint elliptic differential operator is a pseudodifferential operator. Helffer–Robert [33] proved the corresponding result in the semiclassical setting (see, e.g., the account [19, Chapter 8]), with this result using the Helffer–Sjöstrand approach to the functional calculus [34]. In the setting of black-box scattering, we cannot expect such a result to hold everywhere, because we don't know what's inside the black box. However, thanks to Sjöstrand [62] this pseudodifferential property holds when localised away from the black box.

Ingredient 6: regularity estimates inside the black box. While the analysis of v_{High} is insensitive to the contents of the black-box (see Ingredient 3) understanding the properties of the low-frequency piece v_{Low} necessarily involves "opening" the black box. Intuitively, the fact that the spectral parameter in $\Pi_{\mathrm{Low}}(\varphi_{\mathrm{tr}}v)$ is compactly supported indicates that strong elliptic estimates should hold, but knowing that v_{Low} is analytic is dependent on the coefficients and domain inside the black box.

The abstract result Theorem 4.1 contains the abstract regularity hypothesis (4.4). The choices of this hypothesis to prove Theorems 1.16 and 1.17 are discussed in §4.2 (after the statement of Theorem 4.1), but we highlight here that bound (1.19) on v_{Low} in Theorem 1.16 is proved using explicit calculation involving the eigenvalues of $-\Delta$ on the torus, and the bound (1.22) on v_{Low} in Theorem 1.17 is proved using heat equation bounds from [25]. Indeed, for the latter, because of the compact support of the spectral parameter in Π_{Low}, we can run the *backward heat equation* on $\Pi_{\mathrm{Low}}(\varphi_{\mathrm{tr}}v)$ for as long as we like and obtain L^2 estimates on the result. If the boundary and coefficients are analytic then known heat kernel estimates yield the necessary Cauchy-type estimates on $\partial^\alpha \Pi_{\mathrm{Low}}(\varphi_{\mathrm{tr}}v)$; see Corollary 6.1 and Theorem 6.2 below.

Discussion of the recent results [6, 7] that extend the approach of [54, 55, 26] to variable-coefficient problems. The recent thesis [6] is an extension of the approach of [54, 55, 26] to variable-coefficient Helmholtz problems. Since the preprint of the present paper appeared, the results of [6] appeared as the preprint [7]. We make the following three remarks comparing and contrasting the approach of [6, 7] (following [54, 55, 26]) and the approach of [43]/[29]/the present paper.

1. *(Boundary conditions.)* The approach of [6, 7] in principle covers a variety of boundary conditions. For example, [7, Theorem 5.5] proves an analogous result to Theorem 1.12 for the PML problem with an impedance boundary condition on Γ_{tr} under (i) assumptions about the coefficients and domain discussed in Point 2 below, (ii) the assumption that the solution operator of the PML problem is polynomially bounded in k, and (iii) the assumption that the PML scaling angle θ is sufficiently small. Theorem 5.3 below (from [28]) verifies the assumption (ii) for truncation with a Dirichlet boundary condition (under the assumptions on the scaling function in §1.3) and this result also holds for truncation with an impedance boundary condition (indeed, the boundary condition on Γ_{tr} enters the analysis in [28] via [28, Lemma 4.4], and this lemma – relying on integration by parts near Γ_{tr} – goes through as before provided the impedance parameter has the correct sign).

   We note that truncation via the exact DtN map, which is the easiest boundary condition to deal with in the approach of [43]/[29]/the present paper, is the most difficult boundary condition to deal with in the approach of [6]. Indeed, the decomposition for the DtN map required in the latter approach is proved using results about boundary integral operators from [52] (see [6, Lemma 6.5.12 and its proof in §6.9]).

2. *(Assumptions on the coefficients/domain.)* As in [54, 55, 26], the frequency cut-offs in [6, 7] are applied to the data; $v_{\mathcal{A}}$ is then the solution of a Helmholtz problem with (piecewise) analytic data, and one needs (piecewise) analytic coefficients (where the pieces are separated by analytic surfaces) and an analytic domain to get that $v_{\mathcal{A}}$ is analytic [6, Lemma 6.5.8]. In contrast, the approach in [43]/[29]/the present paper can deal with smooth coefficients (everywhere when $\Omega_- = \emptyset$, and away from the obstacle in the general case) as a result of applying the cut-offs to the solution itself.

3. *(Bound on the high-frequency part.)* In [6, 7], the semiclassical ellipticity of the Helmholtz operator on high frequencies – although not explicitly mentioned – is again behind the improved bound on v_{H^2} compared to v. Indeed, with S_k^- the solution operator to the Helmholtz equation $(\Delta + k^2)v = -f$ and S_k^+ the solution operator to $(\Delta - k^2)v = f$, [6, Page 98] writes "we will later see that S_k^- and S_k^+ act very similar on high-frequency data" (with "later" referring to [6, Remark 6.3.7]).

1.9 Outline of the rest of the paper

Section 2 proves the *hp*-FEM convergence result of Theorem 1.12 using Theorems 1.16 and 1.17, as discussed in §1.5, this follows closely the arguments in [54, 55, 43, 29] and so, for brevity, quotes several results from these papers without proof.

Section 3 recalls the framework of black-box scattering, and sets up the associated functional calculus; this section is similar to [29, §2] (and refers to that for some of the proofs) except that it now has to deal with both the (unscaled) operator P and the scaled operator P_θ, whereas [29, §2] only deals with P.

Section 4 states the main decomposition result for Helmholtz solutions in the black-box framework with PML truncation (Theorem 4.1), with this result then proved in Section 5.

Section 6 shows how Theorems 1.16 and 1.17 follow from Theorem 4.1 – by design, these proofs are essentially identical to the proofs in [29] of the analogous results for outgoing Helmholtz solutions; we therefore give a sketch of the main steps.

Appendix A recalls results about semiclassical pseudodifferential operators on the torus.

2 Proof of Theorem 1.12 using Theorems 1.16 and 1.17

2.1 Overview

The two ingredients for the proof of Theorem 1.12 are

- Lemma 2.9, which is the classic duality argument giving a condition for quasioptimality to hold in terms of how well the solution of the adjoint problem is approximated by the finite-element space (measured by the quantity $\eta(V_N)$ defined by (2.5)), and
- Lemma 2.10 that bounds $\eta(V_N)$ using the decomposition from Theorem 1.17.

Regarding Lemma 2.9: this argument came out of ideas introduced in [61], was formalised in its present form in [60], and has been used extensively in the analysis of the Helmholtz FEM; see, e.g., [1, 20, 51, 37, 60, 54, 55, 69, 68, 21, 13, 47, 14, 12, 32, 31, 43].

Regarding Lemma 2.10: given the decomposition in Theorem 1.17, the bound on $\eta(V_N)$ when Assumption 1.11 is satisfied is identical to the corresponding proof of [29, Lemma 5.5] (which is also very similar to the proof of [54, Theorem 5.5]).

The main work in this section is therefore recalling that the PML variational formulation (1.12) satisfies a Gårding inequality and therefore fits in the framework of Lemma 2.9.

2.2 The sesquilinear form $a(\cdot,\cdot)$ is continuous and satisfies a Gårding inequality

In the following lemma $(\cdot,\cdot)_2$ and $\|\cdot\|_2$ denote, respectively, the Euclidean inner product and associated norm on $\mathbb{C}^d$.

Lemma 2.1 *Given $A_{\rm scat}$ and $c_{\rm scat}$ as in Definition 1.1, a scaling function $f(r)$ satisfying (1.8), and $\epsilon>0$ there exist $A_{\max}$ and $c_{\max}$ such that, for all $\epsilon\leq\theta\leq\pi/2-\epsilon$, $x\in\Omega$, and $\xi,\zeta\in\mathbb{C}^d$,*

$$|(A(x)\xi,\zeta)_2|\leq A_{\max}\|\xi\|_2\|\zeta\|_2 \qquad \textit{and} \qquad \frac{1}{|c(x)|^2}\geq\frac{1}{(c_{\max})^2}.$$

Proof. This follows from the definitions of A and c in (1.11), the definitions of α and β in (1.10), and the fact that $f_\theta(r):=f(r)\tan\theta$. ∎

Corollary 2.2 (Continuity of $a(\cdot,\cdot)$) *If $C_{\rm cont}:=\max\{A_{\max},c_{\min}^{-2}\}$, then*

$$|a(v,w)|\leq C_{\rm cont}\,\|v\|_{H^1_k(\Omega)}\,\|w\|_{H^1_k(\Omega)} \qquad \textit{for all } v,w\in H^1_0(\Omega).$$

Proof. This follows by the Cauchy-Schwarz inequality and the definition of $\|\cdot\|_{H^1_k(\Omega)}$ (1.3). ∎

Lemma 2.3 *Suppose that Assumption 1.9 holds when $d = 3$. With A defined by (1.11), given $\epsilon > 0$ there exists $A_{\min} > 0$ such that, for all $\epsilon \leq \theta \leq \pi/2 - \epsilon$,*

$$\Re\big(A(x)\xi, \xi\big)_2 \geq A_{\min}\|\xi\|_2^2 \quad \text{for all } \xi \in \mathbb{C}^d \text{ and } x \in \Omega_+.$$

Corollary 2.4 ($a(\cdot,\cdot)$ satisfies a Gårding inequality)

$$\Re a(w,w) \geq A_{\min}\|w\|^2_{H^1_k(\Omega)} - \big(A_{\min} + (c_{\min})^{-2}\big)k^2\|w\|^2_{L^2(\Omega)} \quad \text{for all } w \in H^1_0(\Omega). \tag{2.1}$$

Proof of Lemma 2.3. By assumption, $A_{\rm scat}(x)$ is symmetric positive definite for all $x \in \Omega$ with $r \leq R_1$. We therefore only need to consider the region $r \geq R_1$

Let $\eta := H^T\xi$; since H is orthogonal, $\|\eta\|_2 = \|\xi\|_2$. Then $\Re(A\xi,\xi)_2 = \Re(D\eta,\eta)_2$. Explicit calculation from the definition of D shows that

$$\Re D = \begin{pmatrix} \frac{1+r^{-1}f_\theta f_\theta'}{1+(f_\theta')^2} & 0 \\ 0 & \frac{1+r^{-1}f_\theta f_\theta'}{1+r^{-2}f_\theta^2} \end{pmatrix}, \ d=2, \quad \text{and} \quad \Re D = \begin{pmatrix} \frac{1-r^{-2}f_\theta^2+2r^{-1}f_\theta' f_\theta}{1+f_\theta^2} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ d=3. \tag{2.2}$$

We now claim that there exists $C > 0$ (depending on $\tan\theta$) such that

$$\Re(D(x)\eta,\eta)_2 = (\Re D(x)\eta,\eta)_2 \geq C\|\eta\|_2^2 \quad \text{for all } \eta \in \mathbb{C}^d \text{ and } r \geq R_1; \tag{2.3}$$

the result then follows since $\tan\theta$ depends continuously on θ and is bounded above and below (with bounds depending on ϵ) for $\epsilon \leq \theta \leq \pi/2 - \epsilon$.

When $d = 2$, (2.3) follows immediately from (2.2) and the fact that both $r^{-1}f_\theta$ and f_θ' are non-negative. When $d = 3$, (2.3) follows if we can show that $r^{-1}f_\theta(r) \leq f_\theta'(r)$ for all $r \geq R_1$, which in turn follows from Assumption 1.9 since $f_\theta'(r) = f_\theta(r)/r + r(f_\theta(r)/r)'$. ∎

Remark 2.5 (Assumption 1.9 and Lemma 2.3) *Without assumptions on $f_\theta(r)$ additional to (1.8) (such as Assumption 1.9) the eigenvalues of the matrix D will not all lie in a half plane. Indeed, α (defined in (1.10)) lies in the first quadrant of the complex plane for all $\theta \in [0,\pi/2]$. Explicit calculation shows that*

$$\frac{\beta^2}{\alpha} = \big(1+(f_\theta')^2\big)^{-1}\left[1 - \left(\frac{f_\theta}{r}\right)^2 + \frac{2f_\theta f_\theta'}{r} + \mathrm{i}\left(\frac{2f_\theta}{r} + f_\theta'\left(\left(\frac{f_\theta}{r}\right)^2 - 1\right)\right)\right].$$

If $f_\theta(r)/r$ is small compared to both 1 and $f_\theta'(r)$ (which can occur when the scaling "turns on" sufficiently quickly at a large R_1)

$$\frac{\beta^2}{\alpha} \approx \big(1+(f_\theta')^2\big)^{-1}\left[1 + \frac{2f_\theta f_\theta'}{r} - \mathrm{i}f_\theta'\right]$$

and so is in the fourth quadrant of the complex plane. If, in addition, $f_\theta'(r)$ is large compared to 1, then $3\pi/2 \leq \arg(\beta^2/\alpha) \leq 7\pi/8$.

If there exists $r^* \in (R_1, R_2)$ such that $f_\theta'(r^*)$ is small then

$$\frac{\beta^2}{\alpha} \approx 1 - \left(\frac{f_\theta}{r}\right)^2 + \mathrm{i}\frac{2f_\theta}{r}.$$

Suppose, furthermore, that $f_\theta(r^*) > r^*\tan\theta$. Then if $\tan\theta > 1$ (i.e., $\theta > \pi/4$), then when $r = r^*$, β^2/α lies in the second quadrant of the complex plane. Furthermore, as $\theta \to \pi/2$, the argument of β^2/α tends to π.

Therefore, for an $f_\theta(r)$ combining the two types of behaviour above, β^2/α and α are not contained in the same half plane for all $R_1 \leq r \leq R_2$ and $\epsilon \leq \theta \leq \pi/2 - \epsilon$.

2.3 The standard duality argument

Definition 2.6 (Adjoint solution operator $\mathcal{S}^*$) *Given $f \in L^2(\Omega)$, let $\mathcal{S}^* f$ be defined as the solution of the variational problem*

$$\text{find } \mathcal{S}^* f \in H_0^1(\Omega) \text{ such that } a(v, \mathcal{S}^* f) = \int_\Omega v\, \overline{f} \text{ for all } v \in H_0^1(\Omega). \tag{2.4}$$

The conditions for quasioptimality below are formulated in terms of $\mathcal{S}^*$. However, we record immediately in the following lemma that $\mathcal{S}^* f$ is just the complex-conjugate of a solution of the PML variational problem (1.12).

Lemma 2.7 (The adjoint solution is the complex conjugate of a Helmholtz solution) *With $\mathcal{S}^*$ is defined by (2.4),*

$$a(\overline{\mathcal{S}_k^* f}, w) = \int_\Omega \overline{f}\, \overline{w} \qquad \text{for all } w \in H_0^1(\Omega).$$

Proof. By the definitions of $a(\cdot,\cdot)$ and the coefficients A and c^{-2} (1.11), and the facts that H is real and D is diagonal (and hence symmetric), $a(\overline{v}, w) = a(\overline{w}, v)$ for all $v, w \in H_0^1(\Omega)$; the result then follows from the definition of $\mathcal{S}_k^*$ (2.4). ∎

Definition 2.8 ($\eta(V_N)$) *Given a sequence $(V_N)_{N=0}^\infty$ of finite-dimensional subspaces of $H_0^1(\Omega)$, let*

$$\eta(V_N) := \sup_{0 \neq f \in L^2(\Omega)} \min_{w_N \in V_N} \frac{\|S^* f - w_N\|_{H_k^1(\Omega)}}{\|f\|_{L^2(\Omega)}}. \tag{2.5}$$

Lemma 2.9 (Conditions for quasioptimality) *If*

$$k\,\eta(V_N) \leq \frac{1}{C_{\mathrm{cont}}} \sqrt{\frac{A_{\max}}{2(A_{\min} + c_{\min}^{-2})}},$$

then the Galerkin equations (1.14) have a unique solution which satisfies

$$\|v - v_N\|_{H_k^1(\Omega)} \leq \frac{2C_{\mathrm{cont}}}{A_{\min}} \left(\min_{w_N \in V_N} \|v - w_N\|_{H_k^1(\Omega)} \right).$$

References for the proof. This is based on the Gårding inequality (2.1); see, e.g., [54, Theorem 4.3] (when $A \equiv I$ and $c \equiv 1$) or [43, Lemma 6.4] (for general A and c). ∎

2.4 The bound on $\eta(V_N)$ obtained using Theorems 1.16 and 1.17

Lemma 2.10 (Bound on $\eta(V_N)$ under Assumption 1.10 or 1.11) *Suppose that $\Omega_-, A_{\mathrm{scat}}$, and c_{scat} satisfy* either *Assumption 1.10* or *1.11. Suppose further that $\Omega_-, A_{\mathrm{scat}}$, c_{scat}, and $K \subset [k_0, \infty)$ are such that the solution operator of the exterior Dirichlet problem is polynomially bounded (in the sense of Definition 1.2).*

Given $N > 0$ there exist

- *$k_1, C_1, C_2, \sigma > 0$, all independent of k, h, p, and N, and*
- *$C_N > 0$, independent of k, h, p,*

such that, for $k \in K \cap [k_1, \infty)$,

$$k\,\eta(V_N) \leq C_1 \frac{hk}{p}\left(1 + \frac{hk}{p}\right) + C_2 k^M \left(\left(\frac{h}{h+\sigma}\right)^p + k\left(\frac{hk}{\sigma p}\right)^p \right) + C_N k^{1-N}. \tag{2.6}$$

Proof. The proof of the bound (2.6) using Theorems 1.16/1.17 is identical to the proof of [29, Lemma 5.5], which uses the results [54, Theorem 5.5] and [55, Proposition 5.3]. The only difference between the present set up and [29, Lemma 5.5] is that here we have $v = v_{H^2} + v_{\mathcal{A}} + v_{\mathrm{residual}}$, whereas [29, Lemma 5.5] only has $v = v_{H^2} + v_{\mathcal{A}}$. The term v_{residual}, however, can be approximated by zero giving a term of the form $C_N k^{1-N}$ (other terms of this form arise, exactly as in the proof of [29, Lemma 5.5], from approximating in the regions where they are negligible *either* $v_{\mathcal{A},\mathrm{far}}$ and $v_{\mathcal{A},\mathrm{near}}$ in Theorem 1.17 *or* $v_{\mathcal{A}}$ in Theorem 1.16). ∎

2.5 Proof of Theorem 1.12 from the bound on $\eta(V_N)$

The existence of the solution v to the variational problem (1.12) follows from [28, Theorem 1.6]. Indeed, this result proves existence and uniqueness of the PML solution for k is sufficiently large when $G(w) = \int_\Omega g\,\overline{w}$ for $g \in L^2(\Omega)$. Existence and uniqueness of the PML solution for $G \in (H_k^1(\Omega))^*$ follows from existence and uniqueness for L^2 right-hand sides since the problem is Fredholm (via the Gårding inequality (2.1)).

To prove existence of the Galerkin solution v_N to (1.14) under the conditions (1.13), we combine Lemmas 2.9 and 2.10 Indeed, the bound on $k\,\eta(V_N)$ (2.6) holds by Lemma 2.10. We choose $N > 1$, and then increase $k_1 > 0$ (if necessary) so that

$$C_N k^{1-N} \leq \frac{1}{2C_{\rm cont}}\sqrt{\frac{A_{\min}}{2\big(A_{\min}+c_{\min}^{-2}\big)}} \quad \text{for all } k \geq k_1.$$

After using this bound in (2.6), we see that the conditions (1.13) with C_1 sufficiently small and C_2 sufficiently large then ensure that $k\,\eta(V_N)$ is sufficiently small (independent of k), and the result follows from Lemma 2.9.

3 The black-box framework and functional calculus

3.1 Recap of the black-box framework

Let $\hbar := k^{-1}$ be the semiclassical parameter; in the literature, the semiclassical parameter is often denoted by h, but we use $\hbar$ to avoid a notational clash with the meshwidth of the FEM appearing in §1 and §2.

In this subsection, we briefly recap the abstract framework of *black-box scattering* introduced in [63]; for more details, see the comprehensive presentation in [22, Chapter 4]. In fact, we use the approach of [62, §2], where the black-box operator is a variable-coefficient Laplacian (with smooth coefficients) outside the black box, and not the Laplacian $-\hbar^2\Delta$ itself as in [22, Chapter 4] (although the operator still agrees with $-\hbar^2\Delta$ outside a sufficiently large ball).

The operator $P_\hbar$. Let $\mathcal{H}$ be a Hilbert space with an orthogonal decomposition

$$\mathcal{H} = \mathcal{H}_{R_0} \oplus L^2(\mathbb{R}^d\backslash B_{R_0}, \omega(x)\mathrm{d}x), \tag{BB1}$$

where the weight-function $\omega : \mathbb{R}^d \to \mathbb{R}$ is measurable and $\mathrm{supp}(1-\omega)$ is compact in $\mathbb{R}^d$. We call $\mathcal{H}_{R_0}$ the "black box". We emphasise that, although standard examples of the subspace $\mathcal{H}_{R_0}$ are $L^2(B_{R_0})$ or $L^2(B_{R_0}\cap\Omega_+)$ (see §3.2 below), $\mathcal{H}_{R_0}$ need only be an abstract Hilbert space; see the discussion at the end of [22, §4.1]. Let $\mathbf{1}_{B_{R_0}}$ and $\mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}}$ denote the corresponding orthogonal projections. Let $P_\hbar$ be a family in $\hbar$ of self adjoint operators $\mathcal{H} \to \mathcal{H}$ with domain $\mathcal{D} \subset \mathcal{H}$ independent of $\hbar$ (so that, in particular, $\mathcal{D}$ is dense in $\mathcal{H}$). Outside the black box $\mathcal{H}_{R_0}$, we assume that $P_\hbar$ equals $Q_\hbar$ defined as follows. We assume that, for any multi-index $|\alpha| \leq 2$, there exist functions $a_{\hbar,\alpha} \in C^\infty(\mathbb{R}^d)$, uniformly bounded with respect to $\hbar$, independent of $\hbar$ for $|\alpha| = 2$, and such that (i) for some $C_1 > 0$

$$\sum_{|\alpha|=2} a_{\hbar,\alpha}(x)\xi^\alpha \geq C_1|\xi|^2 \quad \text{for all } x \in \mathbb{R}^d \tag{3.1}$$

(where $\xi^\alpha := \xi_1^{\alpha_1}\ldots\xi_d^{\alpha_d}$), (ii) for some $R_{\rm scat} > R_0$

$$\sum_{|\alpha|\leq 2} a_{\hbar,\alpha}(x)\xi^\alpha = |\xi|^2 \quad \text{for } |x| \geq R_{\rm scat},$$

and (iii) the operator $Q_\hbar$ defined by

$$Q_\hbar := \sum_{|\alpha|\leq 2} a_{\hbar,\alpha}(x)(\hbar D_x)^\alpha \tag{3.2}$$

(where $D := -\mathrm{i}\partial$) is formally self-adjoint on $L^2(\mathbb{R}^d, \omega(x)\mathrm{d}x)$.

We require the operator $P_\hbar$ to be equal to $Q_\hbar$ outside the black box $\mathcal{H}_{R_0}$ in the sense that

$$\mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}}(P_\hbar u) = Q_\hbar(u|_{\mathbb{R}^d\backslash B_{R_0}}) \quad \text{for } u \in \mathcal{D}, \quad \text{and} \quad \mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}}\mathcal{D} \subset H^2(\mathbb{R}^d\backslash B_{R_0}). \tag{BB2}$$

We further assume that if, for some $\varepsilon > 0$,

$$v \in H^2(\mathbb{R}^d) \quad \text{and} \quad v|_{B_{R_0+\varepsilon}} = 0, \quad \text{then} \quad v \in \mathcal{D}, \tag{BB3}$$

(with the restriction to $B_{R_0+\epsilon}$ defined in terms of the projections in (BB2); see also (3.7) below) and that

$$\mathbf{1}_{B_{R_0}}(P_\hbar + \mathrm{i})^{-1} \text{ is compact from } \mathcal{H} \to \mathcal{H}. \tag{BB4}$$

Under these assumptions, the semiclassical resolvent $R(z,\hbar) := (P_\hbar - z)^{-1} : \mathcal{H} \to \mathcal{D}$ is meromorphic for $\operatorname{Im} z > 0$ and extends to a meromorphic family of operators of $\mathcal{H}_{\mathrm{comp}} \to \mathcal{D}_{\mathrm{loc}}$ in the whole complex plane when d is odd and in the logarithmic plane when d is even [22, Theorem 4.4]; where $\mathcal{H}_{\mathrm{comp}}$ and $\mathcal{D}_{\mathrm{loc}}$ are defined by

$$\mathcal{H}_{\mathrm{comp}} := \Big\{ u \in \mathcal{H} \ : \ \mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}} u \in L^2_{\mathrm{comp}}(\mathbb{R}^d\backslash B_{R_0}) \Big\},$$

(where L^2_{comp} denotes compactly-supported L^2 functions) and

$$\mathcal{D}_{\mathrm{loc}} := \Big\{ u \in \mathcal{H}_{R_0} \oplus L^2_{\mathrm{loc}}(\mathbb{R}^d\backslash B_{R_0}) : \text{ if } \chi \in C^\infty_{\mathrm{comp}}(\mathbb{R}^d),\ \chi|_{B_{R_0}} \equiv 1 \text{ then } (\mathbf{1}_{B_{R_0}} u, \chi \mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}} u) \in \mathcal{D} \Big\}.$$

The reference operator $P^\sharp_\hbar$. We now define the so-called *reference operator* using the torus $\mathbb{T}^d_{R_\sharp} := \mathbb{R}^d / (2R_\sharp\mathbb{Z})^d$ for some $R_\sharp > 0$ such that $\operatorname{supp}(1-\omega) \subset B_{R_\sharp}$. We work with $[-R_\sharp, R_\sharp]^d$ as a fundamental domain for this torus. The black-box framework by itself requires that $R_\sharp > R_{\mathrm{scat}}$; for simplicity we take $R_\sharp > \operatorname{diam}(\Omega_{\mathrm{tr}})$, so that $\Omega_{\mathrm{tr}} \subset [-R_\sharp, R_\sharp]^d$ (where we assume, without loss of generality, the origin is inside Ω_{tr}). [3]

Let

$$\mathcal{H}^\sharp := \mathcal{H}_{R_0} \oplus L^2(\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}, \omega(x)\mathrm{d}x),$$

and let $\mathbf{1}_{B_{R_0}}$ and $\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}}$ denote the corresponding orthogonal projections. We define

$$\begin{aligned}\mathcal{D}^\sharp := \Big\{ u \in \mathcal{H}^\sharp : \ \text{ if } \chi \in C^\infty_{\mathrm{comp}}(B_{R_\sharp}),\ \chi = 1 \text{ near } B_{R_0},\ \text{then } (\mathbf{1}_{B_{R_0}} u, \chi \mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}} u) \in \mathcal{D}, \\ \text{and } (1-\chi)\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}} u \in H^2(\mathbb{T}^d_{R_\sharp}) \Big\},\end{aligned} \tag{3.3}$$

and, for any χ as in (3.3) and $u \in \mathcal{D}^\sharp$,

$$P^\sharp_\hbar u := P_\hbar(\mathbf{1}_{B_{R_0}} u, \chi \mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}} u) + Q_\hbar\big((1-\chi)\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}} u\big), \tag{3.4}$$

where we have identified functions supported in $B(0,R_\sharp)\backslash B(0,R_0) \subset \mathbb{T}^d_{R_\sharp}\backslash B(0,R_0)$ with the corresponding functions on $\mathbb{R}^d\backslash B(0,R_0)$ – see the paragraph on notation below.

Let $q_\hbar \in S^2(\mathbb{T}^d_{R_\sharp})$ denote the principal symbol of $Q_\hbar$ as a semiclassical pseudodifferential operator acting on the torus $\mathbb{T}^d_{R_\sharp}$ (see Appendix A for a review of semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_\sharp}$); i.e.,

$$q_\hbar(x,\xi) = \sum_{|\alpha|\le 2} a_{\hbar,\alpha}(x)\xi^\alpha.$$

We record for later the fact that (3.1), (3.2), and the uniform boundedness of $a_{\hbar,\alpha}(x)$ with respect to $\hbar$ imply that there exist $C_1, C_2 > 0$ such that

$$C_1|\xi|^2 \le q_\hbar(x,\xi) \le C_2|\xi|^2 \quad \text{for sufficiently large } \xi \text{ and all } x. \tag{3.5}$$

[3] In fact, we could modify the arguments below to work for $R_\sharp > R_1$ only, since we just need $\operatorname{supp}\varphi_{\mathrm{tr}}$ contained inside $B_{R_\sharp}$.

The idea behind these definitions is that we have glued our black box into a torus instead of $\mathbb{R}^d$, and then defined on the torus an operator $P^\sharp_\hbar$ that can be thought of as $P_\hbar$ in $\mathcal{H}_{R_0}$ and $Q_\hbar$ in $(\mathbb{R}/2R_\sharp\mathbb{Z})^d\backslash B_{R_0}$; see Figure 3.1. The resolvent $(P^\sharp_\hbar + i)^{-1}$ is compact (see [22, Lemma 4.11]), and hence the spectrum of $P^\sharp_\hbar$, denoted by $\mathrm{Sp}\, P^\sharp_\hbar$, is discrete (i.e., countable and with no accumulation point).

We assume that the eigenvalues of $P^\sharp_\hbar$ satisfy the *polynomial growth of eigenvalues condition*

$$N\big(P^\sharp_\hbar, [-C,\lambda]\big) = O(\hbar^{-d^\sharp}\lambda^{d^\sharp/2}), \tag{BB5}$$

for some $d^\sharp \geq d$, where $N(P^\sharp_\hbar, I)$ is the number of eigenvalues of $P^\sharp_\hbar$ in the interval I, counted with their multiplicity. When $d^\sharp = d$, the asymptotics (BB5) correspond to a Weyl-type upper bound, and thus (BB5) can be thought of as a weak Weyl law.

We summarise with the following definition.

Definition 3.1 (Semiclassical black-box operator) *We say that a family of self-adjoint operators $P_\hbar$ on a Hilbert space $\mathcal{H}$, with dense domain $\mathcal{D}$, independent of $\hbar$, is a semiclassical black-box operator if $(P_\hbar, \mathcal{H})$ satisfies (BB1), (BB2), (BB3), (BB4), (BB5).*

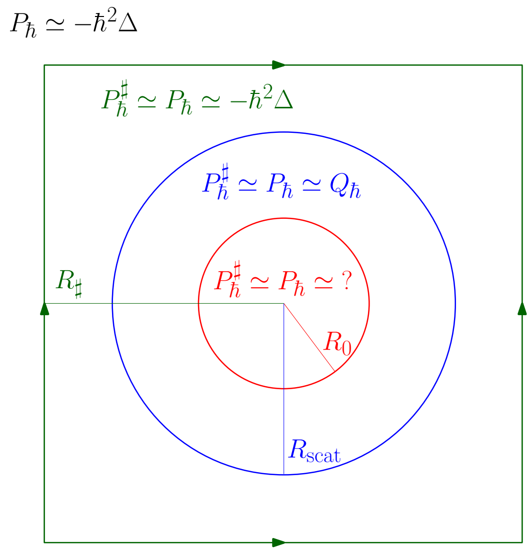

Figure 3.1: The black-box setting. The symbol $\simeq$ is used to denote equality in the sense of (BB2) and (3.4).

Notation. We identify in the natural way:

- the elements of $\{0\} \oplus L^2(\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}) \subset \mathcal{H}^\sharp$,
- the elements of $L^2(\mathbb{T}^d_{R_\sharp}\backslash B_{R_0})$,
- the elements of $L^2(\mathbb{T}^d_{R_\sharp})$ supported outside B_{R_0},
- the elements of $L^2(\mathbb{R}^d)$ supported in $[-R_\sharp, R_\sharp]^d\backslash B_{R_0}$,
- and the elements of $\{0\} \oplus L^2(\mathbb{R}^d\backslash B_{R_0}) \subset \mathcal{H}$ whose orthogonal projection onto $L^2(\mathbb{R}^d\backslash B_{R_0})$ is supported in $[-R_\sharp, R_\sharp]^d\backslash B_{R_0}$.

If $v \in \mathcal{H}$ and $\chi \in C^\infty_{\mathrm{comp}}(\mathbb{R}^d)$ is equal to some constant α on a neighbourhood of B_{R_0}, we *define*

$$\chi v := (\alpha \mathbf{1}_{B_{R_0}} v, \chi \mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}} v) \in \mathcal{H}. \tag{3.6}$$

(for example, using this notation, the requirements on u in the definition of $\mathcal{D}^\sharp$ (3.3) are $\chi u \in \mathcal{D}$ and $(1-\chi)u \in H^2(\mathbb{T}^d_{R_\sharp})$ for χ equal to 1 near B_{R_0}). If $v \in \mathcal{H}$ and $R > R_0$, we define

$$v|_{B_R} := \big(\mathbf{1}_{B_{R_0}} v, (\mathbf{1}_{\mathbb{R}^d\setminus B_{R_0}} v)|_{B_R\setminus B_{R_0}}\big) \in \mathcal{H}_{R_0} \oplus L^2(B_R\setminus B_{R_0}), \tag{3.7}$$

(where the restriction of $\mathbf{1}_{\mathbb{R}^d\setminus B_{R_0}} v$ to $B_R \setminus B_{R_0}$ is restriction in the standard sense, since $\mathbf{1}_{\mathbb{R}^d\setminus B_{R_0}} v \in L^2(\mathbb{R}^d \setminus B_{R_0})$) and, if $v \in \mathcal{H}^\sharp$,

$$v|_{B_R} := \big(\mathbf{1}_{B_{R_0}} v, (\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\setminus B_{R_0}} v)|_{B_R\setminus B_{R_0}}\big) \in \mathcal{H}_{R_0} \oplus L^2(B_R\setminus B_{R_0}).$$

Finally, if $R_0 \leq r \leq R_\sharp$, we define the partial norms

$$\|u\|_{\mathcal{H}^\sharp(B_r)} = \|u\|_{\mathcal{H}(B_r)} := \|u\|_{\mathcal{H}_{R_0}\oplus L^2(B_r\setminus B_{R_0})}, \qquad \|u\|_{\mathcal{H}^\sharp(B_r^c)} := \|\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\setminus B_{R_0}} u\|_{L^2(\mathbb{T}^d_{R_\sharp}\setminus B_r)}$$

and

$$\|u\|_{\mathcal{H}(B_r^c)} := \|\mathbf{1}_{\mathbb{R}^d\setminus B_{R_0}} u\|_{L^2(\mathbb{R}^d\setminus B_r)}.$$

3.2 Scattering problems fitting in the black-box framework

A wide variety of scattering problems fit in the black-box framework; see [22, §4.1], [29, §2.2]. The present paper only uses that the exterior Dirichlet problem of Definition 1.1 fits in this framework.

Lemma 3.2 (Scattering by a Dirichlet obstacle in the black-box framework) *Let $\Omega_-, A_{\rm scat}, c_{\rm scat}, R_0$, and $R_{\rm scat}$ be as in Definition 1.1. Then the family of operators*

$$P_\hbar v := -\hbar^2 c_{\rm scat}^2 \nabla\cdot\big(A_{\rm scat}\nabla v\big) \quad \text{with the domain} \quad \mathcal{D} := H^2(\Omega_+)\cap H^1_0(\Omega_+)$$

is a semiclassical black-box operator (in the sense of Definition 3.1) with $\omega = c_{\rm scat}^{-2}$, $Q_\hbar = -\hbar^2 c_{\rm scat}^2\nabla\cdot(A_{\rm scat}\nabla)$, and

$$\mathcal{H}_{R_0} = L^2\big(B_{R_0}\cap\Omega_+; c_{\rm scat}^{-2}(x)\mathrm{d}x\big) \quad \text{so that} \quad \mathcal{H} = L^2\big(\Omega_+; c_{\rm scat}^{-2}(x)\mathrm{d}x\big).$$

Furthermore the corresponding reference operator $P^\sharp_\hbar$ satisfies (BB5) with $d^\sharp = d$.

Proof. In [29, Lemma 2.3] the result is proved for Lipschitz Ω_- and $A_{\rm scat}$ and $c \in L^\infty$ with domain

$$\Big\{v \in H^1(\Omega_+),\ \nabla\cdot\big(A_{\rm scat}\nabla v\big) \in L^2(\Omega_+),\ v = 0 \text{ on } \partial\Omega_+\Big\};$$

by elliptic regularity, this domain equals $H^2(\Omega_+)\cap H^1_0(\Omega_+)$ when Ω_- and $A_{\rm scat}$ are smooth. ■

3.3 The scaled operator $P_{\hbar,\theta}$ and its truncation

The scaled operator $P_{\hbar,\theta}$. With $\chi \in C^\infty_{\rm comp}(B_{R_1})$ equal to 1 on B_{R_0}, we define the scaled operator

$$P_{\hbar,\theta} u := P_\hbar(\chi u) + (-\hbar^2\Delta_\theta)((1-\chi)u), \tag{3.8}$$

where Δ_θ is defined by (1.7) Although the domain and range of $P_{\hbar,\theta}$ strictly involve the scaled manifold (see [22, Definition 4.31], [27, Equation A.3]), they can be naturally identified with $\mathcal{D}$ and $\mathcal{H}$, respectively.

Truncation of the scaled operator (i.e., PML truncation). For the PML truncation, just as in §1.3, we let $\Omega_{\rm tr} \subset \mathbb{R}^d$ be a bounded Lipschitz open set with $B_{R_{\rm tr}} \subset \Omega_{\rm tr}$. Just as for $P_{\hbar,\theta}$ on the whole exterior domain, the domain and range of $P_{\hbar,\theta}$ on the truncated domain strictly involve the scaled manifold (see [28, §A.3]). However, we can naturally identify them with the following:

$$\begin{aligned}
\mathcal{H}(\Omega_{\rm tr}) &:= \mathcal{H}_{R_0} \oplus L^2(\Omega_{\rm tr}\setminus B_{R_0}),\\
\mathcal{D}(\Omega_{\rm tr}) &:= \Big\{u \in \mathcal{H}(\Omega_{\rm tr}) \ :\ \text{if } \chi \in C^\infty_{\rm comp}(B_{R_1}) \text{ with } \chi\equiv 1 \text{ near } B_{R_0} \text{ then}\\
&\qquad\qquad \chi u \in \mathcal{D},\ (1-\chi)u \in H^1_0(\Omega_{\rm tr}),\ -\Delta_\theta((1-\chi)u) \in L^2(\Omega_{\rm tr})\Big\}.
\end{aligned}$$

Remark 3.3 (A different choice of reference operator) *Instead of defining the reference operator $P_\hbar^\sharp$ using the torus $\mathbb{T}^d_{R_\sharp}$, we could instead define $P_\hbar^\sharp$ using a large ball or hypercube with zero Dirichlet boundary conditions; see [22, Remark on Page 236]. We could therefore define the reference operator $P_\hbar^\sharp$ on the domain $\Omega_{\rm tr}$ used for the PML truncation, which would have the advantage that the domain of $P_\hbar^\sharp$ could be naturally identified with the domain of $P_{\hbar,\theta}$. We choose not to do this, however, since our arguments extensively use pseudodifferential operators defined on the torus $\mathbb{T}^d_{R_\sharp}$, and part of our proof of the decomposition of Theorem 1.15/4.1 involve explicit computation with the eigenvalues of the Laplacian on $\mathbb{T}^d_{R_\sharp}$; see §5.4.6.*

Definition of a suitable scaled operator on the torus. Fix $\delta > 0$ so that $R_1 + 4\delta < R_{\rm tr}$. In the course of the proof of the main result, we need a operator defined on $\mathbb{T}^d_{R_\sharp}$ and equal to $P_{\hbar,\theta}$ on $B_{R_1(1+3\delta)} \setminus B_{R_0}$. We therefore let $-\widetilde{\Delta}_\theta$ be defined by (1.7) with f_θ replaced by a non-negative function $\widetilde{f}_\theta \in C^\infty([0,\infty);\mathbb{R})$ such that

$$\widetilde{f}_\theta(r) = f_\theta(r) \quad \text{for } r \leq R_1 + 3\delta \quad \text{and} \quad \widetilde{f}(r) = 0 \quad \text{for } r \geq R_1 + 4\delta; \tag{3.9}$$

i.e., $-\widetilde{\Delta}_\theta = -\Delta_\theta$ for $r \leq R_1 + 3\delta$ and $-\widetilde{\Delta}_\theta = -\Delta$ for $r \geq R_1 + 4\delta$ (so that the coefficients of $-\widetilde{\Delta}_\theta$ are periodic on the torus $\mathbb{T}^d_{R_\sharp}$). Define the operator $\widetilde{Q}_{\hbar,\theta}$ on $H^2(\mathbb{T}^d_{R_\sharp})$ by

$$\widetilde{Q}_{\hbar,\theta} u = Q_\hbar\big(\psi u\big) + (-\hbar^2\widetilde{\Delta}_\theta)\big((1-\psi)u\big), \tag{3.10}$$

where $\psi \in C^\infty_{\rm comp}(B_{R_1})$ with $\psi \equiv 1$ on $B_{R_{\rm scat}}$ (we use a tilde in the notation to denote that $\widetilde{Q}_{\hbar,\theta}$ is not just the natural scaling of $Q_\hbar$). Let $\widetilde{q}_{\hbar,\theta} \in S^2(\mathbb{T}^d_{R_\sharp})$ denote the principal symbol of $\widetilde{Q}_{\hbar,\theta}$ as a semiclassical pseudodifferential operator acting on the torus $\mathbb{T}^d_{R_\sharp}$ (see §A).

3.4 A black-box functional calculus for $P_\hbar^\sharp$

The Borel functional calculus. The operator $P_\hbar^\sharp$ on the torus with domain $\mathcal{D}^\sharp$ is self-adjoint with compact resolvent [22, Lemma 4.11], hence we can describe the Borel functional calculus [58, Theorem VIII.6] for this operator explicitly in terms of the orthonormal basis of eigenfunctions $\phi_j^\sharp \in \mathcal{H}^\sharp$ (with eigenvalues $\lambda_j^\sharp$, appearing with multiplicity and depending on $\hbar$): for f a real-valued Borel function on $\mathbb{R}$, $f(P_\hbar^\sharp)$ is self-adjoint with domain

$$\mathcal{D}_f := \Big\{ \sum a_j \phi_j^\sharp \in \mathcal{H}^\sharp \ : \ \sum \big|f(\lambda_j^\sharp) a_j\big|^2 < \infty \Big\},$$

and if $v = \sum a_j \phi_j^\sharp \in \mathcal{D}_f$ then

$$f(P_\hbar^\sharp)(v) := \sum a_j f(\lambda_j^\sharp)\phi_j^\sharp.$$

For f a bounded Borel function, $f(P_\hbar^\sharp)$ is a bounded operator, hence in this case we can dispense with the definition of the domain and allow f to be complex-valued.

For $m \geq 1$, we then define $\mathcal{D}_\hbar^{\sharp,m}$ as the domain of $(P_\hbar^\sharp)^m$, i.e.,

$$\mathcal{D}_\hbar^{\sharp,m} := \Big\{ v \in \mathcal{H}^\sharp \ : \ (P_\hbar^\sharp)^\ell v \in \mathcal{D}^\sharp,\ \ell = 0,\ldots,m-1 \Big\},$$

equipped with the norm

$$\|v\|_{\mathcal{D}_\hbar^{\sharp,m}} := \|v\|_{\mathcal{H}^\sharp} + \|(P_\hbar^\sharp)^m v\|_{\mathcal{H}^\sharp}, \tag{3.11}$$

and $\mathcal{D}_\hbar^{\sharp,-m}$ as its dual (note that, in the exterior of the black box, the regularity imposed in the definition of $\mathcal{D}_\hbar^{\sharp,m}$ is that of periodic functions on the torus with $2m$ derivatives in L^2). We also define the partial norms, for $m > 0$,

$$\|v\|_{\mathcal{D}_\hbar^{\sharp,m}(B)} := \|v\|_{\mathcal{H}^\sharp(B)} + \|(P_\hbar^\sharp)^m v\|_{\mathcal{H}^\sharp(B)},$$

where B equals one of B_r or $(B_r)^c$ (with $R_0 \le r \le R_\sharp$) or $\Omega_{\rm tr}$. In addition, we let

$$\mathcal{D}_\hbar^{\sharp,\infty} := \bigcap_{m\ge 0} \mathcal{D}_\hbar^{\sharp,m}, \tag{3.12}$$

so that $v \in \mathcal{D}_\hbar^{\sharp,\infty}$ iff $(P_\hbar^\sharp)^m v \in \mathcal{D}_\hbar^\sharp$ for all $m \in \mathbb{Z}^+$.

The following theorem is proved in [18, Pages 23 and 24]; see also [58, Theorem VIII.5].

Theorem 3.4 *The Borel functional calculus enjoys the following properties.*

1. $f \to f(P_\hbar^\sharp)$ *is a $\star$-algebra homomorphism.*
2. *for $z \notin \mathbb{R}$, if $r_z(w) := (w-z)^{-1}$ then $r_z(P^\sharp) = (P_\hbar^\sharp - z)^{-1}$.*
3. *If f is bounded, $f(P_\hbar^\sharp)$ is a bounded operator for all $\hbar$, with $\|f(P_\hbar^\sharp)\|_{\mathcal{L}(\mathcal{H}^\sharp)} \le \sup_{\lambda\in\mathbb{R}} |f(\lambda)|$.*
4. *If f has disjoint support from $\operatorname{Sp} P_\hbar^\sharp$, then $f(P_\hbar^\sharp) = 0$.*

The Helffer–Sjöstrand construction. In describing the *structure* of the operators produced by the functional calculus, at least for well-behaved functions f, it is useful to recall the Helffer–Sjöstrand construction of the functional calculus [34], [18, §2.2] (which can also be used to prove the spectral theorem to begin with; see [17]).

We say that $f \in \mathcal{A}$ if $f \in C^\infty(\mathbb{R})$ and there exists $\beta < 0$, such that, for all $r > 0$, there exists $C_r > 0$ such that $|f^{(r)}(x)| \le C_r(1+|x|^2)^{(\beta-r)/2}$.

Let $\tau \in C^\infty(\mathbb{R})$ be such that $\tau(s) = 1$ for $|s| \le 1$ and $\tau(s) = 0$ for $|s| \ge 2$. Finally, let $\mathfrak{n} \ge 1$. We define an $\mathfrak{n}$-almost-analytic extension of f, denoted by $\widetilde{f}$, by

$$\widetilde{f}(z) := \left(\sum_{m=0}^{\mathfrak{n}} \frac{1}{m!}\big(\partial^m f(\operatorname{Re} z)\big)\,(\mathrm{i}\operatorname{Im} z)^m\right) \tau\left(\frac{\operatorname{Im} z}{\langle \operatorname{Re} z\rangle}\right)$$

(observe that $\widetilde{f}(z) = f(z)$ if z is real). For $f \in \mathcal{A}$, we define

$$f(P_\hbar^\sharp) := -\frac{1}{\pi}\int_{\mathbb{C}} \frac{\partial \widetilde{f}}{\partial \bar{z}} (P_\hbar^\sharp - z)^{-1}\, \mathrm{d}x\mathrm{d}y, \tag{3.13}$$

where $\mathrm{d}x\mathrm{d}y$ is the Lebesgue measure on $\mathbb{C}$. The integral on the right-hand side of (3.13) converges; see, e.g., [17, Lemma 1], [18, Lemma 2.2.1]. This definition can be shown to be independent of the choices of $\mathfrak{n}$ and τ, and to agree with the operators defined by the Borel functional calculus for $f \in \mathcal{A}$; see [17, Theorems 2-5], [18, Lemmas 2.2.4-2.2.7].

Pseudodifferential properties of the functional calculus. We say that $E_\infty \in \mathcal{L}(\mathcal{H}^\sharp)$ is $O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}$ if, for any $N > 0$ and any $m > 0$, there exists $C_{N,m} > 0$ such that

$$\|E_\infty\|_{\mathcal{D}_\hbar^{\sharp,-m}\to\mathcal{D}_\hbar^{\sharp,m}} \le C_{N,m}\hbar^N$$

(compare to (A.4) below). Operators in the functional calculus are pseudo-local in the following sense.

Lemma 3.5 (Pseudolocality) *Suppose $f \in \mathcal{A}$ is independent of $\hbar$, and $\psi_1, \psi_2 \in C^\infty(\mathbb{T}^d_{R_\sharp})$ are constant near B_{R_0}. If ψ_1 and ψ_2 have disjoint supports, then*

$$\psi_1 f(P_\hbar^\sharp)\psi_2 = O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}. \tag{3.14}$$

Proof. On a smooth manifold with boundary, this result follows from the fact that $f(P_\hbar^\sharp)$ is a pseudodifferential operator, and hence pseudo-local. Here, it follows from combining the corresponding result about the resolvent [62, Lemma 4.1] (i.e., (3.14) with $f(w) := (w-z)^{-1}$)) with (3.13) and then integrating (as discussing in a slightly different context in [62, Paragraph after proof of Lemma 4.2]). ∎

Furthermore, we can show from [62, §4] that, modulo a negligible term, away from the black box the functional calculus is given by the semiclassical pseudodifferential calculus in the sense of our next lemma. The following lemma uses the notion of semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_\sharp}$ (including the concept of the *operator wavefront set* $\mathrm{WF}_\hbar$), recapped in Appendix A.

Lemma 3.6 (Pseudodifferential properties away from the black box) *If $f \in C^\infty_{\mathrm{comp}}(\mathbb{R})$ is independent of $\hbar$ and $\chi \in C^\infty(\mathbb{T}^d_{R_\sharp})$ is equal to zero near B_{R_0}, then $f(Q_\hbar) \in \Psi^{-\infty}_\hbar(\mathbb{T}^d_{R_\sharp})$ with*

$$\chi f(P^\sharp_\hbar)\chi = \chi f(Q_\hbar)\chi + O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}. \tag{3.15}$$

References for the proof. The relation (3.15) follows from [62, Lemma 4.2 and the subsequent two paragraphs] (similar to in the proof of Lemma 3.6). The result [33, Théorème 4.1] (see also [59, Théorème III-11], [19, Theorem 8.7]) imply that $f(Q_\hbar)$ is a pseudodifferential operator on $\mathbb{T}^d_{R_\sharp}$. ∎

3.5 Black-box differentiation operator

Finally, we define the (non-standard) notion of a family of black-box differentiation operators as a family of operators agreeing with differentiation outside the black box (note that there is no a priori notion of derivative inside the black box itself).

Definition 3.7 (Black-box differentiation operator) *$(D(\alpha))_{\alpha\in\mathfrak{A}}$ is a family of black-box differentiation operators on $\mathcal{D}^{\sharp,\infty}_\hbar$ (defined by (3.12)) if $\mathfrak{A}$ is a family of d–multi-indices, and for any α and any $v \in C^\infty_{\mathrm{comp}}(\mathbb{T}^d_{R_\sharp}\backslash\overline{B_{R_0}})$, $D(\alpha)v = \partial^\alpha v$.*

4 The main decomposition result in the black-box setting

4.1 The precise statement of Theorem 1.15

In addition to the black-box notation introduced in §3, we use the notation that

$$C_0(\mathbb{R}) := \Big\{ f \in C(\mathbb{R})\colon \lim_{\lambda\to\pm\infty} f(\lambda) = 0 \Big\}. \tag{4.1}$$

Theorem 4.1 (The decomposition in the black-box setting) *Let $P_\hbar$ be a semiclassical black-box operator on $\mathcal{H}$ (in the sense of Definition 3.1). There exists $\Lambda > 0$ such that the following holds. Suppose that, for some $\hbar_0 > 0$, there exists $\mathfrak{H} \subset (0, \hbar_0]$ such that the following two assumptions hold.*

1. *There exists $M \geq 0$ such that for any $\chi \in C^\infty_{\mathrm{comp}}(\mathbb{R}^d)$ equal to one near B_{R_0}, there exists $C > 0$ such that if $u \in \mathcal{D}$ is an outgoing solution to $(P_\hbar - I)u = \chi g$, then*

$$\|\chi u\|_{\mathcal{H}} \leq C\hbar^{-1-M}\|\chi g\|_{\mathcal{H}} \quad \textit{for all } \hbar \in \mathfrak{H}. \tag{4.2}$$

2. *There exists $\mathcal{E} \in C_0(\mathbb{R})$ that is nowhere zero on $[-\Lambda, \Lambda]$ such that*

$$\mathcal{E}(P^\sharp_\hbar) = E + O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}, \tag{4.3}$$

where E has the following property: there exists $\rho \in C^\infty(\mathbb{T}^d_{R_\sharp})$ equal to one near B_{R_0}, such that, for some α-family of black-box differentiation operators $(D(\alpha))_{\alpha\in\mathfrak{A}}$ and for some $C_{\mathcal{E}}(\alpha,\hbar) > 0$,

$$\|\rho D(\alpha)Ew\|_{\mathcal{H}^\sharp} \leq C_{\mathcal{E}}(\alpha,\hbar)\|w\|_{\mathcal{H}^\sharp} \quad \textit{for all } w \in \mathcal{D}^{\sharp,\infty}_\hbar \textit{ and } \hbar \in \mathfrak{H}. \tag{4.4}$$

Given $\epsilon > 0$, there exist $\hbar_1 > 0$, $C_j > 0$, $j = 1, 2, 3$, and $\lambda > 1$ such that for all $R_{\rm tr} > (1+\epsilon)R_1$, $B_{R_{\rm tr}} \subset \Omega_{\rm tr} \Subset \mathbb{R}^d$, $\epsilon < \theta < \pi/2 - \epsilon$, all $g \in \mathcal{H}(\Omega_{\rm tr})$, and all $\hbar \in \mathfrak{H} \cap (0, \hbar_1]$, the following holds. The solution $v \in \mathcal{D}(\Omega_{\rm tr})$ to

$$(P_{\hbar,\theta} - I)v = g \quad \text{on } \Omega_{\rm tr} \quad \text{ and } \quad v = 0 \quad \text{on } \Gamma_{\rm tr} \tag{4.5}$$

exists and is unique and there exists $v_{H^2} \in \mathcal{D}(\Omega_{\rm tr})$, $v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$, and $v_{\rm residual} \in \mathcal{D}_\hbar^{\sharp,\infty}$ such that

$$v = v_{H^2} + v_{\mathcal{A}} + v_{\rm residual} \tag{4.6}$$

and $v_{H^2}, v_{\mathcal{A}}$, and $v_{\rm residual}$ satisfy the following properties. The component $v_{H^2} \in \mathcal{D}(\Omega_{\rm tr})$ satisfies

$$\|v_{H^2}\|_{\mathcal{H}(\Omega_{\rm tr})} + \left\|P_{\hbar,\theta} v_{H^2}\right\|_{\mathcal{H}(\Omega_{\rm tr})} \leq C_1 \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1]. \tag{4.7}$$

There exist $R_{\rm I}, R_{\rm II}, R_{\rm III}, R_{\rm IV}$ with $R_0 < R_{\rm I} < R_{\rm II} < R_{\rm III} < R_{\rm IV} < R_1$ such that $v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ decomposes as

$$v_{\mathcal{A}} = v_{\mathcal{A},\rm near} + v_{\mathcal{A},\rm far}, \tag{4.8}$$

where $v_{\mathcal{A},\rm near} \in \mathcal{D}^\sharp$ is regular near the black box and negligible away from it, in the sense that

$$\|D(\alpha) v_{\mathcal{A},\rm near}\|_{\mathcal{H}^\sharp(B_{R_{\rm IV}})} \leq C_2 C_{\mathcal{E}}(\alpha, \hbar) \sup_{\lambda \in [-\Lambda,\Lambda]} \left|\mathcal{E}(\lambda)^{-1}\right| \hbar^{-1-M} \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \tag{4.9}$$

for all $\hbar \in \mathfrak{H} \cap (0, \hbar_1], \alpha \in \mathfrak{A}$, and, for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such that

$$\|v_{\mathcal{A},\rm near}\|_{\mathcal{D}_\hbar^{\sharp,m}((B_{R_{\rm III}})^c)} \leq C_{N,m} \hbar^N \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1] \tag{4.10}$$

and $v_{\mathcal{A},\rm far} \in \mathcal{D}(\Omega_{\rm tr})$ is entire away from the black box and negligible near it, in the sense that

$$\|\partial^\alpha v_{\mathcal{A},\rm far}\|_{\mathcal{H}^\sharp((B_{R_{\rm I}})^c)} \leq C_3 \lambda^{|\alpha|} \hbar^{-|\alpha|-1-M} \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1] \text{ and } \alpha \in \mathfrak{A}, \tag{4.11}$$

and, for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such that

$$\|v_{\mathcal{A},\rm far}\|_{\mathcal{D}_\hbar^{\sharp,m}(B_{R_{\rm II}})} \leq C_{N,m} \hbar^N \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1]. \tag{4.12}$$

Finally, $v_{\rm residual} \in \mathcal{D}_\hbar^{\sharp,\infty}$ is negligible in the sense that for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such that

$$\|v_{\rm residual}\|_{\mathcal{D}_\hbar^{\sharp,m}(\Omega_{\rm tr})} \leq C_{N,m} \hbar^N \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1]. \tag{4.13}$$

In addition, if $\rho = 1$ in (4.4), then the decomposition (4.6) can be constructed in such a way that instead of (4.8)–(4.12), $v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ satisfies the global regularity estimate

$$\|D(\alpha) v_{\mathcal{A}}\|_{\mathcal{H}^\sharp} \lesssim C_{\mathcal{E}}(\alpha, \hbar) \sup_{\lambda \in [-\Lambda,\Lambda]} \left|\mathcal{E}(\lambda)^{-1}\right| \hbar^{-1-M} \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A} \tag{4.14}$$

and is negligible in the scaling region in the sense that for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such

$$\|v_{\mathcal{A}}\|_{\mathcal{D}_\hbar^{\sharp,m}((B_{R_1(1+\epsilon)})^c)} \leq C_{N,m} \hbar^N \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1]. \tag{4.15}$$

Finally, If $\mathcal{E}(P_\hbar^\sharp) = E$ (i.e., with no $O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty} \to \mathcal{D}_\hbar^{\sharp,\infty}}$ remainder in (4.3)), then the functions v_{H^2}, $v_{\mathcal{A}}$, $v_{\mathcal{A},\rm near}$, and $v_{\mathcal{A},\rm far}$ are all independent of $\mathcal{E}$, and all the constants in the bounds above are independent of $\mathcal{E}$ as well.

4.2 Discussion of Theorem 4.1

The first assumption (involving (4.2)). This assumption is that the solution operator is polynomially bounded in $\hbar$. In the black-box setting, [41] proved that this assumption always holds with $M > 5d/2$ and $\{\hbar^{-1} : \hbar \in \mathfrak{H}\}^c$ having arbitrarily small measure in $\mathbb{R}^+$ (see Part (ii) of Theorem 1.3). The solution operator is then polynomially bounded because $\mathfrak{H}$ excludes (inverse) frequencies close to resonances. (Under an additional assumption about the location of resonances, a similar result with a larger M can also be extracted from [65, Proposition 3] by using the Markov inequality.) For nontrapping problems, one expects (4.2) to hold with $M = 0$ and $\mathfrak{H} = (0, h_0]$ (see Theorem 1.3 and the references therein).

The second assumption (involving (4.3) and (4.4)). This assumption is a regularity assumption that depends on the contents of the black box. We later refer to (4.4) as the "low-frequency estimate", since the fact that $\mathcal{E}$ is nowhere zero on $[-\Lambda, \Lambda]$ means that it bounds low-frequency components. The cut-off ρ in (4.4) is needed when the black box contains, e.g., an analytic obstacle and the operator inside has analytic coefficients and we want to show that Ew is analytic inside the black box.

To prove Theorem 1.16, we choose $\mathcal{E} \in C^\infty_{\rm comp}(\mathbb{R}^d)$ with $\mathcal{E} \equiv 1$ on $[-\Lambda, \Lambda]$, and $\rho \equiv 1$; the low-frequency estimate (4.4) then corresponds to a bound on the eigenfunctions of $P^\sharp_\hbar$. By using the flexibility to write $\mathcal{E}(P^\sharp_\hbar)$ as $E + O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}$, we can actually obtain the low-frequency estimate (4.4) from a bound on the eigenfunctions of $-\Delta$ on the torus, instead of those of the variable-coefficient operator; see §6.2.

To prove Theorem 1.17, we choose $\mathcal{E}(\lambda) = {\rm e}^{-t|\lambda|}$, corresponding to a heat-flow estimate; see §6.3. Since $E_\infty = 0$, the decomposition is independent of $\mathcal{E}$, and this allows us to use a *family* of $\mathcal{E}$s, depending on t, and hence a family of estimates as (4.4). This feature allows us to tune the choice of the parameter t, depending on $\hbar$ and α, to get the best possible estimate on $v_{\mathcal{A},\rm near}$ in (4.9).

The component v_{H^2}. Comparing (4.2) and (4.7), and recalling that in the nontrapping case (4.2) holds with $M = 0$, we see that v_{H^2} satisfies a bound that is better, by at least one power of $\hbar$, than the bound satisfied by u; this is the analogue of the property (ii) in §1.5 of the results of [54, 55, 26, 53], and is a consequence of the semiclassical ellipticity of $P_\hbar - 1$ on high-frequencies (as discussed in §1.8). The regularity of v_{H^2} depends on the domain of the operator but not on any other features of the black box (in particular, not on the regularity estimate (4.4)).

The component $v_\mathcal{A}$. $v_\mathcal{A}$ is in the domain of arbitrary powers of the operator ($v_\mathcal{A} \in \mathcal{D}^{\sharp,\infty}_\hbar$) and so is smooth in an abstract sense. $v_\mathcal{A}$ is split further into two parts: $v_{\mathcal{A},\rm near}$ and $v_{\mathcal{A},\rm far}$, with $v_{\mathcal{A},\rm near}$ regular near the black box and negligible away from it, and $v_{\mathcal{A},\rm far}$ entire away from the black box and negligible near it; Figure 1.1 illustrates this set up (with "$v_{\mathcal{A},\rm near}$ analytic" replaced by "$v_{\mathcal{A},\rm near}$ regular"). Comparing (4.2) and (4.9)/(4.11), we see that, in the regions where they are not negligible, $v_{\mathcal{A},\rm near}$ and $v_{\mathcal{A},\rm far}$ satisfy bounds with the same $\hbar$-dependence as u, but with improved regularity. These properties are the analogue of the property (i) in §1.5 of the results of [54], [55], [26], [53]. In particular, the regularity of $u_\mathcal{A}$ depends on the regularity inside the black box (from (4.4)), and, for the exterior Dirichlet problem with analytic obstacle and coefficients analytic in a neighbourhood of the obstacle, $u_\mathcal{A}$ is analytic.

The boundary conditions satisfied by each component. On *both* $\Gamma_{\rm tr}$ *and* on any boundaries in the interior of the black box, each of the main components v_{H^2}, $v_{\mathcal{A},\rm far}$, and $v_{\mathcal{A},\rm near}$ *either* satisfies the same boundary condition as the PML solution v *or* is negligible in a neighbourhood of that boundary. Indeed, both v_{H^2} and $v_{\mathcal{A},\rm far} \in \mathcal{D}(\Omega_{\rm tr})$, and thus satisfy the same boundary conditions as v in both the black box and on $\Gamma_{\rm tr}$. The component $v_{\mathcal{A},\rm near} \in \mathcal{D}^{\sharp,\infty}_\hbar$, and thus satisfies the same boundary condition(s) (if any) as the PML solution v in the black box; furthermore, by (4.10), $v_{\mathcal{A},\rm near}$ is negligible near $\Gamma_{\rm tr}$. This discussion was all for the case $\rho \neq 1$ in (4.4) (where $v_\mathcal{A}$ is split into $v_{\mathcal{A},\rm far}$ and $v_{\mathcal{A},\rm near}$). When $\rho = 1$ in (4.4), $v_\mathcal{A} \in \mathcal{D}^{\sharp,\infty}_\hbar$, and thus satisfies the same boundary condition(s) (if any) as the PML solution v in the black box, and is negligible itself in a neighbourhood of $\Gamma_{\rm tr}$ by (4.15) and the fact that $R_{\rm tr} > R_1(1+\epsilon)$.

These facts about the boundary conditions are important when using the decomposition of Theorem 1.17 (obtained from the general decomposition in Theorem 4.1) in proving Theorem 1.12 about the *hp*-FEM. Indeed, Lemma 2.9 reduces proving quasioptimality of the Galerkin solution to determining how well v is approximated by the sequence of finite-element spaces $(V_N)_{N=0}^\infty$, with each $V_N \subset \mathcal{D}(\Omega_{\rm tr})$ (i.e., the spaces have the boundary conditions for v "built in"). Via the decomposition $v = v_{H^2} + v_\mathcal{A}$, we then seek to determine how well v_{H^2} and $v_\mathcal{A}$ are approximated in these spaces – hence why we care about the boundary conditions.

The error term $v_{\rm residual}$. The reason the negligible error term $v_{\rm residual}$ appears in the decomposition (4.6) is so that v_{H^2} satisfies the zero Dirichlet boundary condition on $\Gamma_{\rm tr}$, the importance of which is highlighted above. Note that if we did not care about v_{H^2} satisfying this boundary condition, we could include $v_{\rm residual}$ in v_{H^2}.

Comparison with the analogous result for the (non-truncated) Helmholtz solution in [29, Theorem A]. By design, the assumptions of Theorem 4.1 are exactly the same as the assumptions in the analogue of Theorem 4.1 for the non-truncated Helmholtz problem, i.e., [29, Theorem A]. The conclusions of Theorem 4.1 are essentially the same as those of [29, Theorem A], except for the fact that the decomposition has the residual term $v_{\rm residual}$; as discussed in the previous paragraph, the reason for this is that we want v_{H^2} to satisfy the zero Dirichlet boundary condition on $\Gamma_{\rm tr}$ (which is not present for the non-truncated Helmholtz problem).

5 Proof of Theorem 4.1

The decomposition (4.6) is defined in §5.1 (and illustrated schematically in Figures 5.1 and 5.4). The estimates (4.7) and (4.9)–(4.14) are proved in §5.3 and 5.4 respectively.

In this proof, we shorten the notation $O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}$ to $O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}$ to keep expressions compact.

5.1 The decomposition

Definition of the frequency cut-offs. Let $\psi\in C^\infty_{\rm comp}(\mathbb{R};[0,1])$ be such that $\operatorname{supp}\psi\subset[-2,2]$ and $\psi\equiv 1$ on $[-1,1]$. For $\mu,\mu'>0$, let

$$\psi_\mu := \psi\left(\frac{\cdot}{\mu}\right) \qquad \text{and} \qquad \psi_{\mu'} := \psi\left(\frac{\cdot}{\mu'}\right). \tag{5.1}$$

We now assume that $\mu>2$ and choose μ' as a function of μ so that

$$(1-\psi_{\mu'})(1-\psi_\mu) = (1-\psi_\mu) \qquad \text{and} \qquad 1\notin \operatorname{supp}(1-\psi_{\mu'}); \tag{5.2}$$

these two conditions are ensured if $1\le\mu'\le\mu/2$ (hence the assumption that $\mu>2$).

Choice of the parameter μ. We now impose additional conditions on μ. By (3.5), there exists μ_0 such that if $\mu\ge\mu_0$, then

$$\big\{(x,\xi)\,:\,|q_\hbar(x,\xi)|\ge\mu\big\} = \big\{(x,\xi)\,:\,q_\hbar(x,\xi)\ge\mu\big\}. \tag{5.3}$$

We then choose $\mu\ge\max\{\mu_0,\mu_1\}$, where μ_1 is given by the following lemma.

Lemma 5.1 (Semiclassical ellipticity of $Q_\hbar$ and $\widetilde{Q}_{\hbar,\theta}$ for μ large enough) *Given $\epsilon>0$, there exists $\mu_1>2$ and $c_{\rm ell}>0$ such that if $\mu\ge\mu_1$ then the following hold.*

(i) If $q_\hbar(x,\xi)\ge\mu$, then

$$\langle\xi\rangle^{-2}(q_\hbar(x,\xi)-1)\ge c_{\rm ell}>0 \tag{5.4}$$

(i.e., $Q_\hbar-1$ is semiclassically elliptic in this region of phase space).

(ii) If $\epsilon\le\theta\le\pi/2-\epsilon$, $x\in B_{R_1(1+3\delta)}\setminus B_{R_0}$, and $q_\hbar(x,\xi)\ge\mu$, then

$$\langle\xi\rangle^{-2}\big|\widetilde{q}_{\hbar,\theta}(x,\xi)-1\big|\ge c_{\rm ell}>0.$$

(i.e., $\widetilde{Q}_{\hbar,\theta}-1$ defined by (3.10) is semiclassically elliptic in this region of phase space).

Proof. In each part we show that there exists a μ_1 such that the conclusion holds, and set the final constant μ to be the maximum of the two.

(i) By the lower bound in (3.5), there exists $\widetilde{\mu}>1$ and $c_{\rm ell}>0$ such that

$$|\xi|\ge\widetilde{\mu} \quad \text{implies that } \langle\xi\rangle^{-2}(q_\hbar(x,\xi)-1)\ge c_{\rm ell}>0.$$

The lower bound (3.5) also ensures that there exists $\mu>1$ such that $q_\hbar(x,\xi)\ge\mu$ implies that $|\xi|\ge\widetilde{\mu}$, and thus (5.4) holds.

(ii) Recall from §3.3 that $\widetilde{Q}_{\hbar,\theta} = Q_\hbar$ on $B_{R_{\rm scat}}$ and $\widetilde{Q}_{\hbar,\theta} = -\hbar^2\Delta_\theta$ on $B_{R_1(1+3\delta)} \setminus B_{R_{\rm scat}}$. Therefore, by [22, Theorem 4.32], given $\epsilon > 0$, there exist $C_1, C_2 > 0$ such that

$$C_1|\xi|^2 \leq \big|\widetilde{q}_{\hbar,\theta}(x,\xi)\big| \leq C_2|\xi|^2$$

for all $x \in B_{R_1(1+3\delta)} \setminus B_{R_{\rm scat}}$, for all ξ, and for $\epsilon \leq \theta \leq \pi/2-\epsilon$. The result then follows in a similar way to the proof of Part (i). ∎

Let

$$\Lambda := 2\mu \quad \text{so that} \quad \operatorname{supp}\psi_\mu \subset [-\Lambda, \Lambda]. \tag{5.5}$$

Note that both μ and Λ only depend on $q_\hbar$ and $\{\widetilde{q}_{\hbar,\theta}\}_{\epsilon\leq\theta\leq\pi/2-\epsilon}$.

The frequency cut-offs. We define, using the Borel functional calculus for $P_\hbar^\sharp$ (Theorem 3.4),

$$\Pi_{\rm Low} := \psi_\mu(P_\hbar^\sharp), \tag{5.6}$$

and additionally

$$\Pi_{\rm High} := (1-\psi_\mu)(P_\hbar^\sharp) = I - \Pi_{\rm Low} \quad \text{and} \quad \Pi'_{\rm High} := (1-\psi_{\mu'})(P_\hbar^\sharp). \tag{5.7}$$

By the first property in (5.2) and the fact the Borel functional calculus is an algebra homomorphism (Part 1 of Theorem 3.4),

$$\Pi'_{\rm High}\Pi_{\rm High} = \Pi_{\rm High}. \tag{5.8}$$

By Part 3 of Theorem 3.4, the operators $\Pi_{\rm Low}, \Pi_{\rm High}$, and $\Pi'_{\rm High}$ are bounded on $\mathcal{H}^\sharp$, with

$$\|\Pi_{\rm Low}\|_{\mathcal{L}(\mathcal{H}^\sharp)},\ \|\Pi_{\rm High}\|_{\mathcal{L}(\mathcal{H}^\sharp)},\ \|\Pi'_{\rm High}\|_{\mathcal{L}(\mathcal{H}^\sharp)} \leq 1, \tag{5.9}$$

and they commute with $P_\hbar^\sharp$ by Part 1 of Theorem 3.4.

By the definition of ψ_μ (5.1), $\langle t\rangle^m\psi_\mu(t)$ is a bounded function for all m, and thus $\Pi_{\rm Low} : \mathcal{D}^\sharp \to \mathcal{D}_\hbar^{\sharp,\infty}$. Then, $\Pi_{\rm High} := I - \Pi_{\rm Low} : \mathcal{D}^\sharp \to \mathcal{D}^\sharp$.

Definition of the decomposition. Let v be the solution of (4.5). Given $\epsilon > 0$, fix $\delta > 0$ so that $R_1(1+4\delta) < R_1(1+\epsilon)$; the condition that $R_1(1+\epsilon) < R_{\rm tr}$ implies that $R_1(1+4\delta) < R_{\rm tr}$ (which is what we assumed in §3.3). Let $\varphi_{\rm tr} \in C^\infty_{\rm comp}(\mathbb{R}^d; [0,1])$ be such that $\varphi_{\rm tr} \equiv 1$ on $B_{R_1(1+\delta)}$ and $\operatorname{supp}\varphi_{\rm tr} \subset B_{R_1(1+2\delta)}$. After writing

$$v = \varphi_{\rm tr}v + (1-\varphi_{\rm tr})v,$$

we then treat $\varphi_{\rm tr}v$ as an element of $\mathcal{D}^\sharp$ and let

$$v_{\rm High} := \Pi_{\rm High}(\varphi_{\rm tr}v) \in \mathcal{D}^\sharp, \quad v_{\rm Low} := \Pi_{\rm Low}(\varphi_{\rm tr}v) \in \mathcal{D}_\hbar^{\sharp,\infty}, \quad v_{\rm PML} := (1-\varphi_{\rm tr})v \in \mathcal{D}(\Omega_{\rm tr}), \tag{5.10}$$

so that

$$v = (v_{\rm High} + v_{\rm Low}) + v_{\rm PML}. \tag{5.11}$$

Remark 5.2 *The parentheses in (5.11) are present because, strictly speaking, one cannot add* either $v_{\rm Low}$ *and* $v_{\rm PML}$ or $v_{\rm High}$ *and* $v_{\rm PML}$ *individually, since* $v_{\rm Low}, v_{\rm High} \in \mathcal{D}^\sharp$ *are functions on the torus and* $v_{\rm PML} \in \mathcal{D}(\Omega_{\rm tr})$ *is a function on* $\Omega_{\rm tr}$*. However, by construction,* $v_{\rm High} + v_{\rm Low}$ *is identically zero on* $\overline{(\Omega_{\rm tr})^c}$*, and hence can be thought of as an element of* $\mathcal{D}(\Omega_{\rm tr})$ *by restriction. Similar sums, e.g., (5.17), arise below, but we omit the parentheses.*

We show below that, given $\epsilon > 0$, there exist $\hbar_1 > 0$, $C > 0$ such that, for all $R_{\rm tr} > R_1(1+\epsilon)$, $B_{R_{\rm tr}} \subset \Omega_{\rm tr} \Subset \mathbb{R}^d$ with Lipschitz boundary, $\epsilon < \theta < \pi/2-\epsilon$, all $g \in \mathcal{H}(\Omega_{\rm tr})$, and all $\hbar \in \mathfrak{H} \cap (0, \hbar_1]$,

$$\|v_{\rm High}\|_{\mathcal{H}(\Omega_{\rm tr})} + \|P_{\hbar,\theta}v_{\rm High}\|_{\mathcal{H}(\Omega_{\rm tr})} \leq C\|g\|_{\mathcal{H}(\Omega_{\rm tr})}, \tag{5.12}$$

and

$$\|v_{\rm PML}\|_{\mathcal{H}(\Omega_{\rm tr})} + \|P_{\hbar,\theta}v_{\rm PML}\|_{\mathcal{H}(\Omega_{\rm tr})} \leq C\|g\|_{\mathcal{H}(\Omega_{\rm tr})}, \tag{5.13}$$

When $\rho = 1$ in the assumption (4.4), we show that

$$v_{\rm Low} = v_{\mathcal{A}} + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} \varphi_{\rm tr} v, \tag{5.14}$$

with $v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ satisfying (4.14) and (4.15). Otherwise, we show that

$$v_{\rm Low} = v_{\mathcal{A},\rm near} + v_{\mathcal{A},\rm far} + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} \varphi_{\rm tr} v, \tag{5.15}$$

where $v_{\mathcal{A},\rm near}$ and $v_{\mathcal{A},\rm far}$ satisfy (4.9)-(4.12), $v_{\mathcal{A},\rm near} \in \mathcal{D}_\hbar^{\sharp,\infty}$, and $v_{\mathcal{A},\rm far} \in \mathcal{D}(\Omega_{\rm tr})$.

The idea now is to let v_{H^2} equal $v_{\rm High} + v_{\rm PML}$, and then the decomposition (4.6) would hold by (5.11) and (5.14)/(5.15). However, we want v_{H^2} to be in $\mathcal{D}(\Omega_{\rm tr})$, which is not guaranteed since, although $v_{\rm PML} \in \mathcal{D}(\Omega_{\rm tr})$ (as noted above), $v_{\rm High}$ need not be in $\mathcal{D}(\Omega_{\rm tr})$. We therefore let $\widetilde{\varphi}_{\rm tr} \in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ be such that $\widetilde{\varphi}_{\rm tr} \equiv 1$ on a neighbourhood of $\operatorname{supp} \varphi_{\rm tr}$ and such that $\operatorname{supp} \widetilde{\varphi}_{\rm tr} \subset B_{R_1+3\delta}$. Then, by the definitions of $v_{\rm High}$ (5.10) and $\Pi_{\rm High}$ (5.7) and Lemma 3.5,

$$v_{\rm High} = \widetilde{\varphi}_{\rm tr} v_{\rm High} + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} \varphi_{\rm tr} v. \tag{5.16}$$

We then set

$$v_{H^2} := \widetilde{\varphi}_{\rm tr} v_{\rm High} + v_{\rm PML},$$

so that, by (5.11), (5.15), and (5.16),

$$v = v_{H^2} + v_{\mathcal{A}} + v_{\rm residual} \quad \text{where} \quad v_{\rm residual} = O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} \varphi_{\rm tr} v. \tag{5.17}$$

The bound (4.13) on $v_{\rm residual}$ (which completes the proof) follows from the result of [28] (recapped in Theorem 5.3 below) that v inherits the polynomial bound on the resolvent enjoyed by u (4.2).

This decomposition strategy is summed-up in Figure 5.1; with an overview of the decomposition of the low-frequency component $v_{\rm Low}$ in Figure 5.4.

Organisation of the rest of the proof. In §5.2 we prove the bound (5.13) on $v_{\rm PML}$. In §5.3 we prove the bound (5.12) on $v_{\rm High}$. In §5.4 we prove that the decomposition (5.15) holds, with $v_{\mathcal{A},\rm near}$ and $v_{\mathcal{A},\rm far}$ satisfying (4.9)-(4.12).

In the rest of the proof we assume that $\hbar \in \mathfrak{H}$ and we omit the quantifiers and the explicit statement that the bounds hold uniformly for $R_{\rm tr} > R_1(1+\epsilon)$ and $\epsilon < \theta < \pi/2 - \epsilon$. We use the notation $\lesssim$ in bounds to indicate that the omitted constant is independent of $\hbar$.

5.2 The component near the PML boundary

In this subsection we prove that the bound (5.13) on $v_{\rm PML}$ holds. We first recap results from [28] about PML truncation.

5.2.1 Recap of three results from [28]

The first result is a special case of the result from [28, Theorem 1.6] that the solution operator of the PML problem "inherits" the $\hbar$-dependence of the solution operator of the original (nontruncated) Helmholtz problem.

Theorem 5.3 (Simplified version of [28, Theorem 1.6]) *Suppose Point 1 in Theorem 4.1 holds; i.e., the solution operator of the black-box problem is polynomially bounded for $\hbar \in \mathfrak{H}$. Given $\epsilon > 0$, there exist $C, \hbar_0 > 0$ such that the following holds. For all $R_{\rm tr} > R_1(1+\epsilon)$, $B_{R_{\rm tr}} \subset \Omega_{\rm tr} \Subset \mathbb{R}^d$ with Lipschitz boundary, $\epsilon < \theta < \pi/2 - \epsilon$, all $g \in \mathcal{H}$ with $\operatorname{supp} g \subset \Omega_{\rm tr}$, and all $\hbar \in \mathfrak{H} \cap [0, \hbar_0]$, the solution v to*

$$(P_{\hbar,\theta} - I)v = g \text{ in } \Omega_{\rm tr} \quad \text{and} \quad v = 0 \text{ on } \Gamma_{\rm tr}$$

(i.e., (4.5)) exists, is unique, and satisfies

$$\|v\|_{\mathcal{H}(\Omega_{\rm tr})} + \|P_{\hbar,\theta} v\|_{\mathcal{H}(\Omega_{\rm tr})} \le C\hbar^{-1-M} \|g\|_{\mathcal{H}(\Omega_{\rm tr})}. \tag{5.18}$$

The next result is an elliptic estimate on the PML solution near the boundary (proved using the structure of $-\Delta_\theta$ in the scaling region).

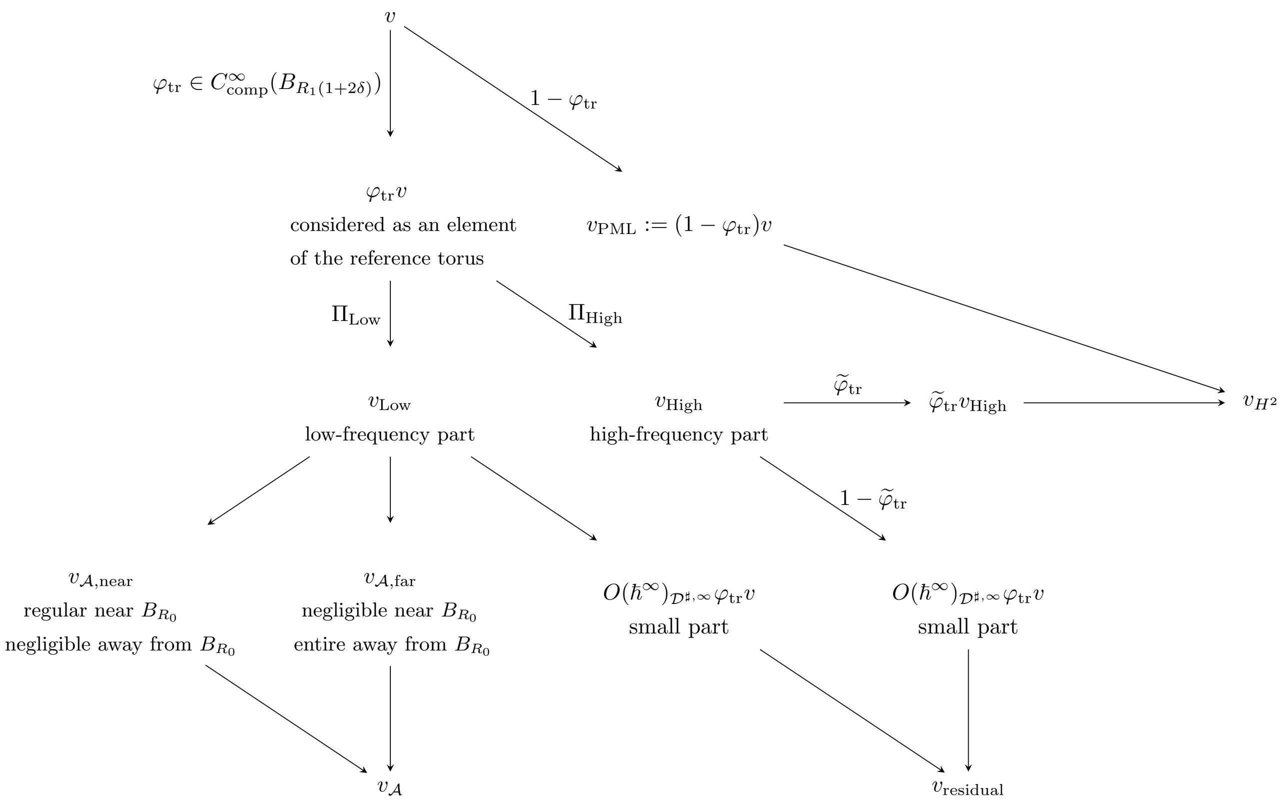

Figure 5.1: Decomposition of the PML solution described in §5.1 (when $\rho \neq 1$ in (4.4))

Lemma 5.4 (Estimate on the PML solution near the boundary [28, Lemma 4.4]) *For any $\varepsilon > 0$, there exists $\hbar_0 > 0$ and $C > 0$ so that for any $\varepsilon < \theta < \pi/2 - \varepsilon$, $R_{\mathrm{tr}} > R_1(1+\varepsilon)$, $B_{R_1} \Subset \Omega_{\mathrm{tr}} \subset \mathbb{R}^d$ with Lipschitz boundary, if v is supported in $\Omega_{\mathrm{tr}} \setminus B_{R_1+\varepsilon}$ and $v = 0$ on Γ_{tr}, then, for all $0 < \hbar \le \hbar_0$,*

$$\|v\|_{H^1_\hbar(\Omega_{\mathrm{tr}})} \le C\|(P_{\hbar,\theta} - I)v\|_{L^2(\Omega_{\mathrm{tr}})}. \tag{5.19}$$

The final result is a Carleman estimate describing how solutions of $(-\hbar^2\Delta_\theta - 1)v = f$ propagate in the scaling region.

Lemma 5.5 (Simplified version of [28, Lemma 4.2, Equation 4.6]) *Given $\varepsilon > 0$ there exist $C_j > 0, j = 1,2,3,$ and $\hbar_0 > 0$ such that, for all $\varepsilon \le \theta \le \pi/2 - \varepsilon$ and $0 < \hbar < \hbar_0$,*

$$\|v\|_{H^1_\hbar(\Omega_{\mathrm{tr}}\setminus B_{R_1+\varepsilon})} \le C_1\|(-\hbar^2\Delta_\theta - 1)v\|_{L^2(\Omega_{\mathrm{tr}}\setminus B_{R_1})} + C_2\exp(-C_3\hbar^{-1})\|v\|_{H^1_\hbar(B_{R_1+\varepsilon}\setminus B_{R_1})}. \tag{5.20}$$

5.2.2 Proof of the bound (5.13) on v_{PML}

Since $v_{\mathrm{PML}} := (1-\varphi_{\mathrm{tr}})v$,

$$(P_{\hbar,\theta} - I)v_{\mathrm{PML}} = (P_{\hbar,\theta} - I)(1-\varphi_{\mathrm{tr}})v = (1-\varphi_{\mathrm{tr}})g + [P_{\hbar,\theta}, \varphi_{\mathrm{tr}}]v, \tag{5.21}$$

and the fact that $\varphi_{\mathrm{tr}} \equiv 1$ on $B_{R_1+\delta}$ implies that $\operatorname{supp} v_{\mathrm{PML}} \subset \Omega_{\mathrm{tr}} \setminus B_{R_1+\delta}$. Thus, applying Lemma 5.4 with $\varepsilon = \min\{\epsilon, \delta\}$, we see that the bound (5.19) implies that

$$\|v_{\mathrm{PML}}\|_{H^1_\hbar(\Omega_{\mathrm{tr}}\setminus B_{R_1+\delta})} \lesssim \big\|(P_{\hbar,\theta} - I)v_{\mathrm{PML}}\big\|_{L^2(\Omega_{\mathrm{tr}})} \lesssim \|g\|_{\mathcal{H}(\Omega_{\mathrm{tr}})} + \big\|[P_{\hbar,\theta}, \varphi_{\mathrm{tr}}]v\big\|_{L^2(\Omega_{\mathrm{tr}})}.$$

Now, by direct computation and the fact that $\operatorname{supp}\nabla\varphi_{\mathrm{tr}} \subset B_{R_1+2\delta} \setminus B_{R_1+\delta}$,

$$\big\|[P_{\hbar,\theta}, \varphi_{\mathrm{tr}}]v\big\|_{L^2(\Omega_{\mathrm{tr}})} \lesssim \hbar\|v\|_{H^1_\hbar(B_{R_1+2\delta}\setminus B_{R_1+\delta})}, \tag{5.22}$$

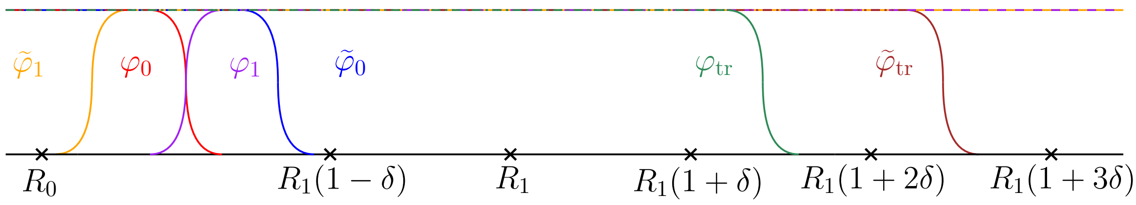

Figure 5.2: The cut-off functions $\varphi_0, \widetilde{\varphi}_0, \varphi_1, \widetilde{\varphi}_1, \varphi_{\rm tr}$, and $\widetilde{\varphi}_{\rm tr}$ described at the start of §5.3.

so that

$$\|v_{\rm PML}\|_{H^1_\hbar(\Omega_{\rm tr}\setminus B_{R_1+\delta})} \lesssim \|g\|_{\mathcal{H}(\Omega_{\rm tr})} + \hbar\|v\|_{H^1_\hbar(B_{R_1+2\delta}\setminus B_{R_1+\delta})}. \tag{5.23}$$

Using (5.21) again, we have

$$\|P_{\hbar,\theta}v_{\rm PML}\|_{\mathcal{H}(\Omega_{\rm tr})} \lesssim \|g\|_{\mathcal{H}(\Omega_{\rm tr})} + \big\|[P_{\hbar,\theta},\varphi_{\rm tr}]v\big\|_{L^2(\Omega_{\rm tr})} + \|v_{\rm PML}\|_{L^2(\Omega_{\rm tr})},$$

and combining this with (5.22) and (5.23) (and recalling that $\operatorname{supp} v_{\rm PML} \subset \Omega_{\rm tr}\setminus B_{R_1+\delta}$) we find that

$$\|v_{\rm PML}\|_{\mathcal{H}(\Omega_{\rm tr})} + \|P_{\hbar,\theta}v_{\rm PML}\|_{\mathcal{H}(\Omega_{\rm tr})} \lesssim \|g\|_{\mathcal{H}(\Omega_{\rm tr})} + \hbar\|v\|_{H^1_\hbar(B_{R_1+2\delta}\setminus B_{R_1+\delta})}. \tag{5.24}$$

Our plan is to use the Carleman estimate (5.20) to bound this last term in terms of $\|g\|_{\mathcal{H}(\Omega_{\rm tr})}$. We first claim that (5.18) implies that

$$\|v\|_{H^1_\hbar(B_{R_1+\delta}\setminus B_{R_1})} \lesssim \hbar^{-1-M}\|g\|_{\mathcal{H}(\Omega_{\rm tr})}; \tag{5.25}$$

indeed, this follows by the combination of (i) the fact that $P_{\hbar,\theta} = -\hbar^2\Delta_\theta$ for $R \geq R_1$, (ii) the fact that $-\Delta_\theta$ is elliptic (by, e.g., [22, Theorem 4.32]), (iii) elliptic regularity (to obtain control of the $H^2_\hbar$ norm of v), and then (iv) interpolation (to obtain control of the $H^1_\hbar$ norm of v). Then, the combination of (5.20) (with $\varepsilon = \min\{\epsilon,\delta\}$) and (5.25) implies that

$$\|v\|_{H^1_\hbar(B_{R_1+2\delta}\setminus B_{R_1+\delta})} \lesssim \Big(1+\exp(-C_3\hbar^{-1})\hbar^{-1-M}\Big)\|g\|_{\mathcal{H}(\Omega_{\rm tr})}.$$

Combining this last inequality with (5.24) and reducing $\hbar_0$ if necessary, the result (5.13) follows.

5.3 Proof of the bound (5.12) on $v_{\rm High}$ (the high-frequency component)

Decomposing into parts that are "near to" or "far from" the black box. Let $\varphi_0, \widetilde{\varphi}_0 \in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ be such that $\varphi_0 \equiv 1$ near B_{R_0} and $\widetilde{\varphi}_0 \equiv 1$ in a neighbourhood of $\operatorname{supp}\varphi_0$, with $\operatorname{supp}\varphi_0 \subset \operatorname{supp}\widetilde{\varphi}_0 \subset B_{R_1(1-\delta)}$, so that, in particular,

$$P^\sharp_\hbar = P_\hbar = P_{\hbar,\theta} \quad \text{on the supports of } \varphi_0 \text{ and } \widetilde{\varphi}_0. \tag{5.26}$$

In addition, let $\varphi_1 := 1-\varphi_0$ and let $\widetilde{\varphi}_1 \in C^\infty(\mathbb{R}^d;[0,1])$ be supported away from the black box B_{R_0} and such that $\widetilde{\varphi}_1 \equiv 1$ in a neighbourhood of $\operatorname{supp}\varphi_1$. Finally, let $\widetilde{\varphi}_{\rm tr} \in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ be as in §5.1; i.e., equal to one on the support of $\varphi_{\rm tr}$ and so that $\operatorname{supp}\widetilde{\varphi}_{\rm tr} \subset B_{R_1(1+3\delta)}$; see Figure 5.2. (Observe then that a tilde denotes a function with larger support than the corresponding function without the tilde.)

These definitions imply the following support properties

$$\operatorname{supp}(1-\widetilde{\varphi}_{\rm tr})\cap\operatorname{supp}\varphi_{\rm tr} = \emptyset,\ \operatorname{supp}(1-\widetilde{\varphi}_0)\cap\operatorname{supp}\varphi_0 = \emptyset,\ \text{ and }\ \operatorname{supp}(1-\widetilde{\varphi}_1)\cap\operatorname{supp}\varphi_1 = \emptyset. \tag{5.27}$$

Starting from the definition $v_{\rm High} := \Pi_{\rm High}\varphi_{\rm tr}v$ (5.10), using that $\varphi_0+\varphi_1 = 1$, the first and third support properties in (5.27), Lemma 3.5, and that $\varphi_0\varphi_{\rm tr} = \varphi_0$, we obtain that

$$\begin{aligned} v_{\rm High} = \Pi_{\rm High}\varphi_0\varphi_{\rm tr}v + \Pi_{\rm High}\varphi_1\varphi_{\rm tr}v &= \Pi_{\rm High}\varphi_0\varphi_{\rm tr}v + \widetilde{\varphi}_1\Pi_{\rm High}\varphi_1\varphi_{\rm tr}v + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\varphi_{\rm tr}v \\ &= \Pi_{\rm High}\varphi_0\varphi_{\rm tr}v + \widetilde{\varphi}_{\rm tr}\widetilde{\varphi}_1\Pi_{\rm High}\varphi_1\varphi_{\rm tr}v + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\widetilde{\varphi}_{\rm tr}v \\ &= \Pi_{\rm High}\varphi_0 v + \widetilde{\varphi}_{\rm tr}\widetilde{\varphi}_1\Pi_{\rm High}\varphi_1\varphi_{\rm tr}v + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\widetilde{\varphi}_{\rm tr}v \\ &=: v_{\rm High,near} + v_{\rm High,far} + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\widetilde{\varphi}_{\rm tr}v. \end{aligned} \tag{5.28}$$

Remark 5.6 (The decomposition of $v_{\rm High}$) *This decomposition of $v_{\rm High}$ into "near" and "far" components is different from the non-truncated case in [29]. The reason we do it is we want the function to which $\Pi_{\rm High}$ is applied in $v_{\rm High,near}$ to be supported away from the scaling region (i.e., supported where $P^\sharp_\hbar = P_{\hbar,\theta}$) – see (5.31) below. The component $v_{\rm High,far}$ can then be dealt with via Lemma 3.6 (since it involves cut-offs supported away from the black box) and semiclassical ellipticity; see Step 4 below.*

Overview of the rest of the proof of (5.12). We proceed in four steps; Steps 1-3 obtain the bound

$$\|v_{\rm High,near}\|_{\mathcal{H}^\sharp} + \big\|P_{\hbar,\theta}v_{\rm High,near}\big\|_{\mathcal{H}^\sharp} \lesssim \|g\|_{\mathcal{H}(\Omega_{\rm tr})}, \tag{5.29}$$

on $v_{\rm High,near}$ and are the analogues of Steps 1-3 in [29, §3.2] that deal with $u_{\rm High}$ (although Step 1 is more involved because of the presence of the two operators $P^\sharp_\hbar$ and $P_{\hbar,\theta}$ as opposed to just $P^\sharp_\hbar$). Step 4 obtains the bound

$$\|v_{\rm High,far}\|_{\mathcal{H}^\sharp} + \big\|P_{\hbar,\theta}v_{\rm High,far}\big\|_{\mathcal{H}^\sharp} \lesssim \|g\|_{\mathcal{H}(\Omega_{\rm tr})}, \tag{5.30}$$

on $v_{\rm High,far}$ using ideas from Steps 2 and 3 (in a simplified setting).

Step 1: An abstract argument in $\mathcal{H}^\sharp$ to bound $v_{\rm High,near}$. Since $\Pi_{\rm High}$ commutes with $P^\sharp_\hbar$ (by Part 1 of Theorem 3.4) and $P^\sharp_\hbar = P_{\hbar,\theta}$ on $\operatorname{supp}\varphi_0 \subset B_{R_0}$,

$$\begin{aligned}(P^\sharp_\hbar - I)\Pi_{\rm High}(\varphi_0 v) &= \Pi_{\rm High}(P^\sharp_\hbar - I)(\varphi_0 v)\\ &= \Pi_{\rm High}(P_{\hbar,\theta} - I)(\varphi_0 v) = \Pi_{\rm High}\varphi_0 g + \Pi_{\rm High}[P_{\hbar,\theta},\varphi_0]v = \Pi_{\rm High}\varphi_0 g + \Pi_{\rm High}[P^\sharp_\hbar,\varphi_0]v.\end{aligned} \tag{5.31}$$

(Note that, strictly speaking, we should be writing the commutator $[P_{\hbar,\theta},\varphi_0]$ as $[P_{\hbar,\theta}, M_{\varphi_0}]$, where multiplication is defined in the black-box setting by (3.6); however, we abuse this notation slightly for simplicity.) For $\lambda \in \mathbb{R}$, let

$$f(\lambda) := (\lambda-1)^{-1}(1-\psi_{\mu'})(\lambda),$$

and observe that $f \in C_0(\mathbb{R})$ (defined by (4.1)) by the second property in (5.2). Using (5.8), the fact that the Borel calculus is an algebra homomorphism (Part 1 of Theorem 3.4), and finally (5.31), we get

$$\Pi_{\rm High}(\varphi_0 v) = \Pi'_{\rm High}\Pi_{\rm High}(\varphi_0 v) = f(P^\sharp_\hbar)(P^\sharp_\hbar - I)\Pi_{\rm High}(\varphi_0 v) = f(P^\sharp_\hbar)\big(\Pi_{\rm High}\varphi_0 g + \Pi_{\rm High}[P^\sharp_\hbar,\varphi_0]u\big). \tag{5.32}$$

Since $f \in C_0(\mathbb{R})$, $f(P^\sharp_\hbar)$ is uniformly bounded from $\mathcal{H}^\sharp \to \mathcal{H}^\sharp$ by Part 3 of Theorem 3.4. Combining this fact with (5.32), we obtain

$$\|\Pi_{\rm High}(\varphi_0 v)\|_{\mathcal{H}^\sharp} \lesssim \|\Pi_{\rm High}(\varphi_0 g)\|_{\mathcal{H}^\sharp} + \big\|\Pi_{\rm High}[P^\sharp_\hbar,\varphi_0]v\big\|_{\mathcal{H}^\sharp}.$$

Writing $P^\sharp_\hbar\Pi_{\rm High} = \Pi_{\rm High} + (P^\sharp_\hbar - I)\Pi_{\rm High}$ and using (5.31) again, we obtain

$$\|\Pi_{\rm High}(\varphi_0 v)\|_{\mathcal{H}^\sharp} + \big\|P^\sharp_\hbar\Pi_{\rm High}(\varphi_0 v)\big\|_{\mathcal{H}^\sharp} \lesssim \|\Pi_{\rm High}(\varphi_0 g)\|_{\mathcal{H}^\sharp} + \big\|\Pi_{\rm High}[P^\sharp_\hbar,\varphi_0]v\big\|_{\mathcal{H}^\sharp}.$$

Hence, by (5.9)

$$\begin{aligned}\|v_{\rm High,near}\|_{\mathcal{H}^\sharp} + \big\|P^\sharp_\hbar v_{\rm High,near}\big\|_{\mathcal{H}^\sharp} &\lesssim \|\varphi g\|_{\mathcal{H}^\sharp} + \big\|\Pi_{\rm High}[P^\sharp_\hbar,\varphi_0]v\big\|_{\mathcal{H}^\sharp}\\ &\lesssim \|g\|_{\mathcal{H}(\Omega_{\rm tr})} + \big\|\Pi_{\rm High}[P^\sharp_\hbar,\varphi_0]v\big\|_{\mathcal{H}^\sharp}.\end{aligned} \tag{5.33}$$

We now seek to convert the $\|P^\sharp_\hbar v_{\rm High,near}\|_{\mathcal{H}^\sharp}$ on the left-hand side of this last bound into $\|P_{\hbar,\theta}v_{\rm High,near}\|_{\mathcal{H}^\sharp}$ using that $P^\sharp_\hbar = P_{\hbar,\theta}$ on $\operatorname{supp}\varphi_0$ and pseudolocality of the functional calculus. With $\widetilde{\varphi}_0 \in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ defined as above, the definition of $v_{\rm High,near}$ (5.28), the second support property in (5.27), and Lemma 3.5 then imply that

$$v_{\rm High,near} = \widetilde{\varphi}_0\Pi_{{\rm High},\theta}(\varphi_0 v) + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}\varphi_0 v.$$

By (5.26) and a further use of Lemma 3.5,

$$\begin{aligned}P_{\hbar,\theta}v_{\text{High,near}} &= P_{\hbar,\theta}\widetilde{\varphi}_0\Pi_{\text{High},\theta}(\varphi_0 v) + P_{\hbar,\theta}O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\widetilde{\varphi}_0 v\\ &= P_\hbar^\sharp\widetilde{\varphi}_0\Pi_{\text{High},\theta}(\varphi_0 v) + P_{\hbar,\theta}O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\varphi_0 v\\ &= P_\hbar^\sharp\Pi_{\text{High},\theta}(\varphi_0 v) + P_\hbar^\sharp O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\varphi_0 v + P_{\hbar,\theta}O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\varphi_0 v\\ &= P_\hbar^\sharp v_{\text{High,near}} + P_\hbar^\sharp O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\varphi_0 v + P_{\hbar,\theta}O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\varphi_0 v.\end{aligned}$$

Therefore, by the resolvent estimate (5.18) and the bound (5.33),

$$\begin{aligned}\|v_{\text{High,near}}\|_{\mathcal{H}^\sharp} + \big\|P_{\hbar,\theta}v_{\text{High,near}}\big\|_{\mathcal{H}^\sharp} &\lesssim \|v_{\text{High,near}}\|_{\mathcal{H}^\sharp} + \big\|P_\hbar^\sharp v_{\text{High,near}}\big\|_{\mathcal{H}^\sharp} + \|g\|_{\mathcal{H}(\Omega_{\text{tr}})}\\ &\lesssim \|g\|_{\mathcal{H}(\Omega_{\text{tr}})} + \big\|\Pi_{\text{High}}[P_\hbar^\sharp,\varphi_0]v\big\|_{\mathcal{H}^\sharp}.\end{aligned}\tag{5.34}$$

Step 2: Viewing $\Pi_{\text{High}}[P_\hbar^\sharp,\varphi_0]$ as a semiclassical pseudodifferential operator on $\mathbb{T}^d_{R_\sharp}$. To prove (5.29) from (5.34), it therefore remains to bound the commutator term $\Pi_{\text{High}}[P_\hbar^\sharp,\varphi_0]u$. Since $[P_\hbar^\sharp,\varphi_0]$ is supported away from B_{R_0}, we can write the high-frequency cut-off in terms of a semiclassical pseudodifferential operator thanks to Lemma 3.6.

Recall that φ_0 is compactly supported in B_{R_1} and equal to one near B_{R_0}, Let $\phi \in C^\infty_{\text{comp}}(\mathbb{R}^d;[0,1])$ be supported in B_{R_1}, equal to zero near B_{R_0}, and such that

$$\phi \equiv 1 \quad \text{near} \quad \operatorname{supp}\nabla\varphi_0.\tag{5.35}$$

Then, since $P_\hbar^\sharp = Q_\hbar$ on $\operatorname{supp}\varphi_0$,

$$[P_\hbar^\sharp,\varphi_0] = [Q_\hbar,\varphi_0] = [Q_\hbar,\varphi_0]\phi = \phi[Q_\hbar,\varphi_0] = \phi[Q_\hbar,\varphi_0]\phi.\tag{5.36}$$

Let $\chi \in C^\infty_{\text{comp}}(\mathbb{R}^d)$ be supported in B_{R_1}, equal to zero near B_{R_0}, and equal to one near $\operatorname{supp}\phi$. Using (5.36) and Lemma 3.5 with $\psi_1 = 1-\chi$ and $\psi_2 = \chi\phi = \phi$, we obtain that

$$\begin{aligned}\Pi_{\text{High}}[P_\hbar^\sharp,\varphi_0] = \Pi_{\text{High}}\phi[Q_\hbar,\varphi_0]\phi &= \chi\Pi_{\text{High}}\chi\phi[Q_\hbar,\varphi_0]\phi + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\\ &= \chi\Pi_{\text{High}}\chi[Q_\hbar,\varphi_0]\phi + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}.\end{aligned}\tag{5.37}$$

Lemma 3.6 with $f(P_\hbar^\sharp) = \psi_\mu(P_\hbar^\sharp) = \Pi_{\text{Low}}$ implies that $\Pi^\Psi_{\text{Low}} := \psi_\mu(Q_\hbar) \in \Psi_\hbar^{-\infty}(\mathbb{T}^d_{R_\sharp})$ satisfies

$$\chi\Pi_{\text{Low}}\chi = \chi\Pi^\Psi_{\text{Low}}\chi + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}.$$

Hence, taking $\Pi^\Psi_{\text{High}} := I - \Pi^\Psi_{\text{Low}} = (1-\psi_\mu)(Q_\hbar) \in \Psi^0_\hbar(\mathbb{T}^d_{R_\sharp})$,

$$\chi\Pi_{\text{High}}\chi = \chi\Pi^\Psi_{\text{High}}\chi + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\tag{5.38}$$

i.e., modulo negligible terms, $\chi\Pi_{\text{High}}\chi$ is a high-frequency cut-off defined from the semiclassical pseudodifferential calculus. We here emphasise that, since χ is supported in B_{R_1} and vanishes near B_{R_0}, $\chi\Pi^\Psi_{\text{High}}\chi$ can be seen as an element of *both* $\mathcal{L}(\mathcal{H}^\sharp)$ *and* $\Psi^0_\hbar(\mathbb{T}^d_{R_\sharp})$.

Lemma 5.7 *With $\Pi^\Psi_{\text{Low}} := \psi_\mu(Q_\hbar)$ and $\Pi^\Psi_{\text{High}} := (1-\psi_\mu)(Q_\hbar)$,*

$$\operatorname{WF}_\hbar \Pi^\Psi_{\text{Low}} \subset q_\hbar^{-1}\big(\operatorname{supp}\psi_\mu\big) = \{|q_\hbar| \le 2\mu\}\tag{5.39}$$

and

$$\operatorname{WF}_\hbar \Pi^\Psi_{\text{High}} \subset q_\hbar^{-1}\big(\operatorname{supp}(1-\psi_\mu)\big) = \{|q_\hbar| \ge \mu\}.\tag{5.40}$$

Reference for the proof. See [29, Lemma 3.1], where this is proved using Lemma 3.6. ∎

Now, by (5.37) and (5.38), for any N and any m,

$$\big\|\Pi_{\text{High}}[P_\hbar^\sharp,\varphi_0]v\big\|_{\mathcal{H}^\sharp} \le \big\|\chi\Pi^\Psi_{\text{High}}\chi[Q_\hbar,\varphi_0]\phi v\big\|_{\mathcal{H}^\sharp} + C_{N,m}\hbar^N\big\|[Q_\hbar,\varphi_0]\phi v\big\|_{\mathcal{D}_\hbar^{\sharp,-m}} + C'_N\hbar^N\big\|\widetilde{\phi}v\big\|_{\mathcal{H}^\sharp},$$

with $\widetilde{\phi}$ compactly supported in $B_{R_1}\backslash B_{R_0}$ and equal to one on $\operatorname{supp}\phi$. Taking $m=1$, then $N=M+1$ and using the resolvent estimate (5.18) we get

$$\begin{aligned}\big\|\Pi_{\rm High}[P_\hbar^\sharp,\varphi_0]v\big\|_{\mathcal{H}^\sharp} &\leq \big\|\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v\big\|_{\mathcal{H}^\sharp} + C''_{M+1}\hbar^{M+1}\big\|\widetilde{\phi}v\big\|_{\mathcal{H}}\\ &\lesssim \big\|\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v\big\|_{\mathcal{H}^\sharp} + \big\|g\big\|_{\mathcal{H}},\\ &= \big\|\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v\big\|_{\mathcal{H}^\sharp} + \big\|g\big\|_{\mathcal{H}}. \end{aligned} \tag{5.41}$$

Step 3: A semiclassical elliptic estimate in $\mathbb{T}^d_{R_\sharp}$. Combining (5.34) and (5.41), we see that to prove (5.29) we only need to bound $\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v$ in $L^2(\mathbb{T}^d_{R_\sharp})$. To do this, we use the semiclassical elliptic parametrix construction given by Theorem A.2.

Lemma 5.8 *The operator $Q_\hbar-1$ is semiclassically elliptic on* $\mathrm{WF}_\hbar(\hbar^{-1}\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0])$.

Proof. By (A.8), (A.10), (5.40), and (5.3),

$$\mathrm{WF}_\hbar\left(\hbar^{-1}\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\right)\subset \mathrm{WF}_\hbar\,\Pi^\Psi_{\rm High}\subset\{q_\hbar\geq\mu\}.$$

But, on $\{q_\hbar\geq\mu\}$, by definition of μ (5.4), $\langle\xi\rangle^{-2}(q_\hbar(x,\xi)-1)\geq c_{\rm ell}>0$, and the proof is complete. ■

Since $\hbar^{-1}\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\in\Psi^1_\hbar(\mathbb{T}^d_{R_\sharp})$ by Theorem A.1, we can therefore apply the elliptic parametrix construction given by Theorem A.2 with $A=\hbar^{-1}\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar-1,\varphi_0]$, $B=Q_\hbar-1$, and $\ell=1$, $m=2$. Hence, there exists $S\in\Psi^{-1}_\hbar(\mathbb{T}^d_{R_\sharp})$ and $R=O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}$ with

$$\mathrm{WF}_\hbar\,S\subset\mathrm{WF}_\hbar\left(\hbar^{-1}\Pi^\Psi_{\rm High}[Q_\hbar,\varphi_0]\right)\quad\text{ and }\quad\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]=\hbar S(Q_\hbar-1)+R. \tag{5.42}$$

We apply both sides of this identity to ϕv and then use that ϕ is equal to zero near B_{R_0} and supported in B_{R_1}, and thus $Q_\hbar=P_\hbar=P_{\hbar,\theta}$ on $\operatorname{supp}\phi$; the result is that

$$\begin{aligned}\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v=\hbar S(Q_\hbar-1)\phi v+R\phi v&=\hbar S\phi(Q_\hbar-1)v+\hbar S[Q_\hbar,\phi]v+R\phi v\\ &=\hbar S\phi g+\hbar S[Q_\hbar,\phi]v+R\phi v.\end{aligned}\tag{5.43}$$

The following lemma combined with (A.9) shows that

$$S[Q_\hbar,\phi]=O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}. \tag{5.44}$$

Lemma 5.9 $\mathrm{WF}_\hbar\,S\cap\mathrm{WF}_\hbar[Q_\hbar,\phi]=\emptyset$.

Proof. By (5.42) and the definition of $Q_\hbar$ (3.2),

$$\mathrm{WF}_\hbar\,S\subset\mathrm{WF}_\hbar[Q_\hbar,\varphi_0]\subset\big\{(x,\xi)\,:\,x\in\operatorname{supp}\nabla\varphi_0,\ \xi\in\mathbb{R}^d\big\}.$$

Similarly,

$$\mathrm{WF}_\hbar[Q_\hbar,\phi]\subset\big\{(x,\xi)\,:\,x\in\operatorname{supp}\nabla\phi_0,\ \xi\in\mathbb{R}^d\big\}.$$

Now, by (5.35), $\operatorname{supp}\nabla\varphi_0$ and $\operatorname{supp}\nabla\phi$ are disjoint, and the result follows. ■

Therefore, by (5.43), (5.44) and the definition of $O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}$ (A.4), for any N, there exists $C_N,C'_N>0$ such that

$$\begin{aligned}\|\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v\|_{L^2(\mathbb{T}^d_{R_\sharp})}&\lesssim\hbar\|S\phi g\|_{L^2(\mathbb{T}^d_{R_\sharp})}+C_N\hbar^N\|\widetilde{\phi}v\|_{L^2(\mathbb{T}^d_{R_\sharp})}+C'_N\hbar^N\|\phi v\|_{L^2(\mathbb{T}^d_{R_\sharp})}\\ &\lesssim\hbar\|S\phi g\|_{L^2(\mathbb{T}^d_{R_\sharp})}+C_N\hbar^N\|\widetilde{\phi}v\|_{\mathcal{H}}+C'_N\hbar^N\|\phi v\|_{\mathcal{H}},\end{aligned}$$

where $\widetilde{\phi}$ is compactly supported in $B_{R_1}\backslash B_{R_0}$ and equal to one on $\operatorname{supp}\phi$. Taking $N:=M+1$, using the resolvent estimate (5.18), and then using that $S\in\Psi^{-1}(\mathbb{T}^d_{R_\sharp})\subset\Psi^0(\mathbb{T}^d_{R_\sharp})$ together with Part (iii) of Theorem A.1, we obtain that

$$\|\chi\Pi^\Psi_{\rm High}\chi[Q_\hbar,\varphi_0]\phi v\|_{L^2(\mathbb{T}^d_{R_\sharp})}\lesssim\hbar\|S\phi g\|_{L^2(\mathbb{T}^d_{R_\sharp})}+\hbar\|g\|_{\mathcal{H}(\Omega_{\rm tr})}\lesssim\hbar\|\phi g\|_{L^2(\mathbb{T}^d_{R_\sharp})}+\hbar\|g\|_{\mathcal{H}(\Omega_{\rm tr})}\lesssim\hbar\|g\|_{\mathcal{H}}.$$

Combining this last estimate with (5.34) and (5.41) we obtain the desired bound (5.29) on $v_{\rm High,near}$.

Step 4: Obtaining the bound (5.30) on $v_{\rm High,far}$ using the ideas from Steps 2 and 3. We now show that

$$v_{\rm High,far} := \widetilde{\varphi}_{\rm tr}\widetilde{\varphi}_1\Pi_{\rm High}\varphi_1\varphi_{\rm tr}v = \widetilde{\varphi}_{\rm tr}\widetilde{\varphi}_1\Pi_{\rm High}\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\varphi_1\varphi_{\rm tr}v \tag{5.45}$$

satisfies the bound (5.30). Since $\widetilde{\varphi}_1$ is supported away from B_{R_0}, exactly as in Step 2, $\Pi^\Psi_{\rm Low} := \psi_\mu(Q_\hbar) \in \Psi^{-\infty}_\hbar(\mathbb{T}^d_{R_\sharp})$ and $\Pi^\Psi_{\rm High} := (1-\psi_\mu)(Q_\hbar) \in \Psi^0_\hbar(\mathbb{T}^d_{R_\sharp})$ satisfy

$$\widetilde{\varphi}_1\Pi_{\rm Low}\widetilde{\varphi}_1 = \widetilde{\varphi}_1\Pi^\Psi_{\rm Low}\widetilde{\varphi}_1 + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} \quad \text{and} \quad \widetilde{\varphi}_1\Pi_{\rm High}\widetilde{\varphi}_1 = \widetilde{\varphi}_1\Pi^\Psi_{\rm High}\widetilde{\varphi}_1 + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}. \tag{5.46}$$

Now, by (5.45), (5.46), and the facts that $\widetilde{\varphi}_{\rm tr}\varphi_{\rm tr} = \varphi_{\rm tr}$ and $\widetilde{\varphi}_1\varphi_1 = \varphi_1$,

$$v_{\rm High,far} = \widetilde{\varphi}_{\rm tr}\widetilde{\varphi}_1\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}v + O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar\to\mathcal{D}^{\sharp,\infty}_\hbar}\varphi_{\rm tr}v.$$

Lemma 5.10 *The operator $\widetilde{Q}_{\hbar,\theta} - 1$ is semiclassically elliptic on* $\mathrm{WF}_\hbar(\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr})$.

Proof. First recall that $\mathrm{supp}(\varphi_1\varphi_{\rm tr}) \subset \mathrm{supp}(\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}) \subset B_{R_1(1+3\delta)} \setminus B_{R_0}$. Using this property, along with (A.8), (A.10), (5.40), and (5.3), we find that

$$\begin{aligned}\mathrm{WF}_\hbar(\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}) &\subset \Big\{(x,\xi)\,:\, x \in B_{R_1(1+3\delta)} \setminus B_{R_0}\Big\} \cap \mathrm{WF}_\hbar\,\Pi^\Psi_{\rm High}\\ &\subset \Big\{(x,\xi)\,:\, x \in B_{R_1(1+3\delta)} \setminus B_{R_0}\Big\} \cap \big\{(x,\xi)\,:\, q_\hbar(x,\xi) \geq \mu\big\}.\end{aligned}$$

By Lemma 5.1, $\widetilde{Q}_{\hbar,\theta} - 1$ is semiclassically elliptic on the set on the right-hand side of the last displayed inclusion, and the proof is complete. ∎

We now apply Theorem A.2 with $A = \widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}$, $B = \widetilde{Q}_{\hbar,\theta} - 1$, $\ell = 0$, and $m = 2$; observe that the assumptions of Theorem A.2 are then satisfied by Lemma 5.10. Hence, there exists $\widetilde{S} \in \Psi^{-2}_\hbar(\mathbb{T}^d_{R_\sharp})$ and $\widetilde{R} = O(\hbar^\infty)_{\Psi^{-\infty}_\hbar}$ with

$$\mathrm{WF}_\hbar\,\widetilde{S} \subset \mathrm{WF}_\hbar(\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}) \quad \text{and} \quad \widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr} = \widetilde{S}(\widetilde{Q}_{\hbar,\theta} - 1) + \widetilde{R}. \tag{5.47}$$

We now apply the equality in (5.47) to $\widetilde{\chi}v$ where $\widetilde{\chi} \in C^\infty_{\rm comp}(\mathbb{R}^d;[0,1])$ is such that $\widetilde{\chi} \equiv 1$ on a neighbourhood of $\mathrm{supp}(\varphi_1\varphi_{\rm tr})$ and $\mathrm{supp}\,\widetilde{\chi} \subset B_{R_1(1+3\delta)} \setminus B_{R_0}$; thus

$$\begin{aligned}\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}v &= \widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}\widetilde{\chi}v\\ &= \widetilde{S}(\widetilde{Q}_{\hbar,\theta} - 1)\widetilde{\chi}v + \widetilde{R}\widetilde{\chi}v = \widetilde{S}\widetilde{\chi}(\widetilde{Q}_{\hbar,\theta} - 1)v + \widetilde{S}[\widetilde{Q}_{\hbar,\theta},\widetilde{\chi}]v + \widetilde{R}\widetilde{\chi}v.\end{aligned}$$

By construction $\widetilde{Q}_{\hbar,\theta} = P_{\hbar,\theta}$ on $B_{R_1(1+3\delta)} \setminus B_{R_0}$ (see (3.10) and (3.9)); thus $\widetilde{\chi}(\widetilde{Q}_{\hbar,\theta} - 1)v = \widetilde{\chi}g$ and

$$\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}v = \widetilde{S}\widetilde{\chi}g + \widetilde{S}[\widetilde{Q}_{\hbar,\theta},\widetilde{\chi}]v + \widetilde{R}\widetilde{\chi}v. \tag{5.48}$$

Arguing exactly as in Lemma 5.9, using (5.47) and the fact that $\mathrm{supp}\,\nabla\widetilde{\chi} \cap \mathrm{supp}(\varphi_1\varphi_{\rm tr}) = \emptyset$, we find that

$$\mathrm{WF}_\hbar\,\widetilde{S} \cap \mathrm{WF}_\hbar[\widetilde{Q}_{\hbar,\theta},\widetilde{\chi}] = \emptyset \quad \text{and thus} \quad \widetilde{S}[\widetilde{Q}_{\hbar,\theta},\widetilde{\chi}] = O(\hbar^\infty)_{\Psi^{-\infty}_\hbar}.$$

Using this in (5.48) and then taking the $H^2_\hbar(\mathbb{T}^d_{R_\sharp})$ norm, using the definitions of $O(\hbar^\infty)_{\Psi^{-\infty}_\hbar}$ and $O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}$, we obtain that, given $N > 0$ there exists $C_N > 0$ such that

$$\big\|\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}v\big\|_{H^2_\hbar(\mathbb{T}^d_{R_\sharp})} \lesssim \big\|\widetilde{S}\widetilde{\chi}g\big\|_{H^2_\hbar(\mathbb{T}^d_{R_\sharp})} + C_N\hbar^N\big\|\widetilde{\chi}_{\rm alt}v\big\|_{L^2(\mathbb{T}^d_{R_\sharp})}$$

where $\widetilde{\chi}_{\rm alt}$ is compactly supported in $B_{R_\sharp} \setminus B_{R_0}$ and equal to one on a neighbourhood of $\mathrm{supp}\,\widetilde{\chi}$. By Part (iii) of Theorem A.1, and the fact that $\widetilde{S} \in \Psi^{-2}_\hbar(\mathbb{T}^d_{R_\sharp})$,

$$\big\|\widetilde{\varphi}_1\widetilde{\varphi}_{\rm tr}\Pi^\Psi_{\rm High}\varphi_1\varphi_{\rm tr}v\big\|_{H^2_\hbar(\mathbb{T}^d_{R_\sharp})} \lesssim \|g\|_{\mathcal{H}^\sharp} + C_N\hbar^N\|v\|_{\mathcal{H}(\Omega_{\rm tr})}.$$

The bound (5.30) on $v_{\rm High,far} := \widetilde{\varphi}_{\rm tr}\widetilde{\varphi}_1\Pi_{\rm High}\varphi_1\varphi_{\rm tr}v$ then follows by combining this last inequality with the resolvent estimate (5.18).

5.4 Proof of the decomposition (5.15) of $v_{\rm Low}$ (the low-frequency component) and associated bounds on $v_{\mathcal{A},\rm near}$ and $v_{\mathcal{A},\rm far}$

5.4.1 Decomposing $\Pi_{\rm Low}$ using Assumption 2 in Theorem 4.1

By Assumption 2 in Theorem 4.1, there exists $E_\infty = O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}$ with

$$\mathcal{E}(P_\hbar^\sharp) = E + E_\infty, \tag{5.49}$$

and the low-frequency estimate (4.4) holds. By (5.5) (a consequence of the definition of the constant Λ (5.5)), $\mathcal{E}$ is nowhere zero on the support of ψ_μ; therefore the function $\psi_\mu/\mathcal{E}$ is well-defined and in $C_0(\mathbb{R})$ (defined by (4.1)). The definition of $\Pi_{\rm Low}$ (5.6) and Part 1 of Theorem 3.4 imply that

$$\Pi_{\rm Low} = \psi_\mu(P_\hbar^\sharp) = \mathcal{E}(P_\hbar^\sharp)\left(\frac{1}{\mathcal{E}}\psi_\mu\right)(P_\hbar^\sharp) = E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right) + E_\infty \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right). \tag{5.50}$$

Then, by Part 3 of Theorem 3.4 and the fact that $E_\infty = O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}$,

$$E_\infty \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right) = O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}. \tag{5.51}$$

5.4.2 The decomposition (5.14) of $v_{\rm Low}$ when $\rho = 1$ in (4.4)

We first assume that $\rho = 1$ and establish the decomposition (5.14), together with the bounds (4.14) and (4.15) on $u_{\mathcal{A}}$. In this case, we let

$$v_{\mathcal{A}} := E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\varphi_{\rm tr} v, \tag{5.52}$$

so that (5.14) holds by (5.50) and (5.51). Moreover, since $v_{\mathcal{A}}$ involves a compactly-supported function of $P_\hbar^\sharp$, by the reasoning below (5.9), $v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$. Then, using (in this order) the low-frequency estimate (4.4), Part 3 of Theorem 3.4, and finally the resolvent estimate (5.18), we get

$$\begin{aligned}
\|D(\alpha)v_{\mathcal{A}}\|_{\mathcal{H}^\sharp} &= \left\|D(\alpha)E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\varphi_{\rm tr} v\right\|_{\mathcal{H}^\sharp} \leq C_{\mathcal{E}}(\alpha,\hbar)\left\|\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\varphi_{\rm tr} v\right\|_{\mathcal{H}^\sharp}\\
&\leq C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\|\varphi_{\rm tr} v\|_{\mathcal{H}^\sharp} = C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\|\varphi_{\rm tr} v\|_{\mathcal{H}(\Omega_{\rm tr})}\\
&\lesssim C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\hbar^{-1-M}\|g\|_{\mathcal{H}(\Omega_{\rm tr})};
\end{aligned}$$

thus (4.14) holds. To establish (4.15), observe that

$$\|v\|_{\mathcal{D}_\hbar^{\sharp,m}((B_{R_1(1+\epsilon)})^c)} \leq \left\|(1-\widetilde{\varphi}_{\rm tr})v\right\|_{\mathcal{D}_\hbar^{\sharp,m}}, \tag{5.53}$$

since $\widetilde{\varphi}_{\rm tr} \equiv 0$ on $(B_{R_1(1+\epsilon)})^c$. Then by (5.49), (5.51), Part 1 of Theorem 3.4, pseudo-locality of the functional calculus (Lemma 3.5), and the first support property in (5.27),

$$\begin{aligned}
(1-\widetilde{\varphi}_{\rm tr})E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\varphi_{\rm tr} &= (1-\widetilde{\varphi}_{\rm tr})\mathcal{E}(P_\hbar^\sharp)\left(\frac{1}{\mathcal{E}}\psi_\mu\right)(P_\hbar^\sharp)\varphi_{\rm tr} + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}\\
&= (1-\widetilde{\varphi}_{\rm tr})\psi_\mu(P_\hbar^\sharp)\varphi_{\rm tr} + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty} = O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}.
\end{aligned}$$

The bound (4.15) then follows by combining this with (5.53) and the resolvent estimate (5.18).

Remark 5.11 (The decomposition is independent of $\mathcal{E}$ if $E_\infty = 0$) *The last part of Theorem 4.1 is the claim that when $E_\infty = 0$, the decomposition is independent of E. To establish this in the case $\rho = 1$, observe that (5.52) and (5.50) imply that if $E_\infty = 0$, then $v_{\mathcal{A}} = v_{\rm Low} = \psi_\mu(P_\hbar^\sharp)\varphi_{\rm tr} v$ (which is independent of $\mathcal{E}$).*

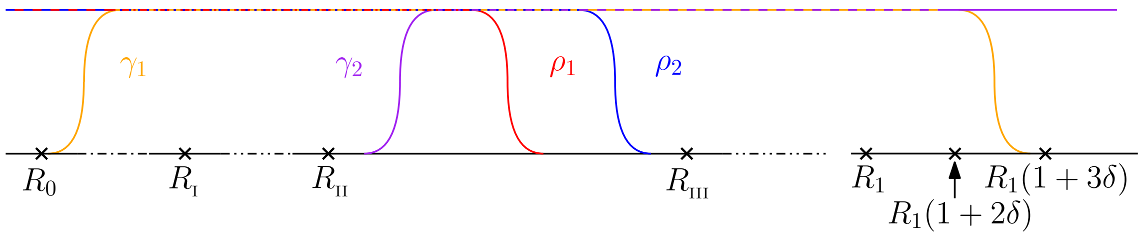

Figure 5.3: The cut-off functions $\rho_1, \rho_2, \gamma_1, \gamma_2$ defined at the start of §5.4.

5.4.3 Cut-off functions for the case $\rho \neq 1$

We first define the cut-off functions used to bound v_{Low}, displayed in Figure 5.3. Whereas the cut-off functions used in the bound on v_{High} (in §5.3) were denoted φ, ϕ, and χ (sometimes with tildes), in this section we use the notation ρ_j and γ_j, $j = 1, 2$. Recall that ρ is the cut-off function in the assumption (4.4).

Given R_0, R_1, and ρ, let $R_{\text{I}}, R_{\text{II}}, R_{\text{III}}, R_{\text{IV}}$, be such that $R_0 < R_{\text{I}} < R_{\text{II}} < R_{\text{III}} < R_{\text{IV}} < R_1$ and $\rho = 1$ on a neighbourhood of $B_{R_{\text{IV}}}$.

Let $\rho_1 \in C^\infty_{\text{comp}}(\mathbb{T}^d_{R_\sharp}; [0,1])$ be such that $\operatorname{supp}(1-\rho_1) \subset (B_{R_{\text{II}}})^c$ and $\operatorname{supp}\rho_1 \Subset B_{R_{\text{III}}}$ Let $\rho_2 \in C^\infty_{\text{comp}}(\mathbb{T}^d_{R_\sharp}; [0,1])$ be supported in $B_{R_{\text{III}}}$ and such that $\rho_2 \equiv 1$ on $\operatorname{supp}\rho_1$, i.e.,

$$\operatorname{supp}(1-\rho_2) \cap \operatorname{supp}\rho_1 = \emptyset. \tag{5.54}$$

Let $\gamma_1 \in C^\infty(\mathbb{T}^d_{R_\sharp}; [0,1])$ be such that $\gamma_1 \equiv 0$ on a neighbourhood of B_{R_0}, such that $\gamma_1 \equiv 1$ on a neighbourhood of $B_{R_1(1+2\delta)} \setminus B_{R_{\text{I}}}$, and $\gamma_1 \equiv 0$ on $(B_{R_1(1+3\delta)})^c$. A key feature of this definition is that

$$\operatorname{supp}(1-\gamma_1) \cap \operatorname{supp}\big((1-\rho_1)\varphi_{\text{tr}}\big) = \emptyset. \tag{5.55}$$

Finally, let $\gamma_2 \in C^\infty(\mathbb{T}^d_{R_\sharp}; [0,1])$ be equal to zero on $B_{R_{\text{II}}}$ and such that $\gamma_2 \equiv 1$ on $\operatorname{supp}(1-\rho_1)$; i.e.,

$$\operatorname{supp}(1-\gamma_2) \cap \operatorname{supp}\big(1-\rho_1\big) = \emptyset. \tag{5.56}$$

5.4.4 Decomposing into parts that are "near to" or "far from" the black box when $\rho \neq 1$

We split v_{Low} in the following way, using the pseudo-locality of the functional calculus (i.e., Lemma 3.5) and the support properties (5.54) and (5.55),

$$\begin{aligned} v_{\text{Low}} := \psi_\mu(P^\sharp_\hbar)\varphi_{\text{tr}}v &= \psi_\mu(P^\sharp_\hbar)\rho_1\varphi_{\text{tr}}v + \psi_\mu(P^\sharp_\hbar)(1-\rho_1)\varphi_{\text{tr}}v \\ &= \psi_\mu(P^\sharp_\hbar)\rho_1\varphi_{\text{tr}}v + \gamma_1\psi_\mu(P^\sharp_\hbar)(1-\rho_1)\varphi_{\text{tr}}v + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}\varphi_{\text{tr}}v \\ &=: v_{\text{Low,near}} + v_{\text{Low,far}} + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}\varphi_{\text{tr}}v. \end{aligned}$$

We now split $v_{\text{Low,near}}$ and $v_{\text{Low,far}}$ further, with this decomposition summarised in Figure 5.4. We highlight that the arguments from here on are identical to the corresponding arguments in [29] (in [29, §3.3.3-§3.3.4]).

5.4.5 The part near the black box $v_{\text{Low,near}}$

By (5.50), and (5.51), along with the fact that $\rho_1\varphi_{\text{tr}} = \rho_1$,

$$v_{\text{Low,near}} = \psi_\mu(P^\sharp_\hbar)\rho_1 v = E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P^\sharp_\hbar)\right)\rho_1 v + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}\varphi_{\text{tr}}v =: v_{\mathcal{A},\text{near}} + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}\varphi_{\text{tr}}v. \tag{5.57}$$

Since $v_{\mathcal{A},\text{near}}$ involves a compactly-supported function of $P^\sharp_\hbar$ by the reasoning below (5.9) $v_{\mathcal{A},\text{near}}$ is in $\mathcal{D}^{\sharp,\infty}_\hbar$.

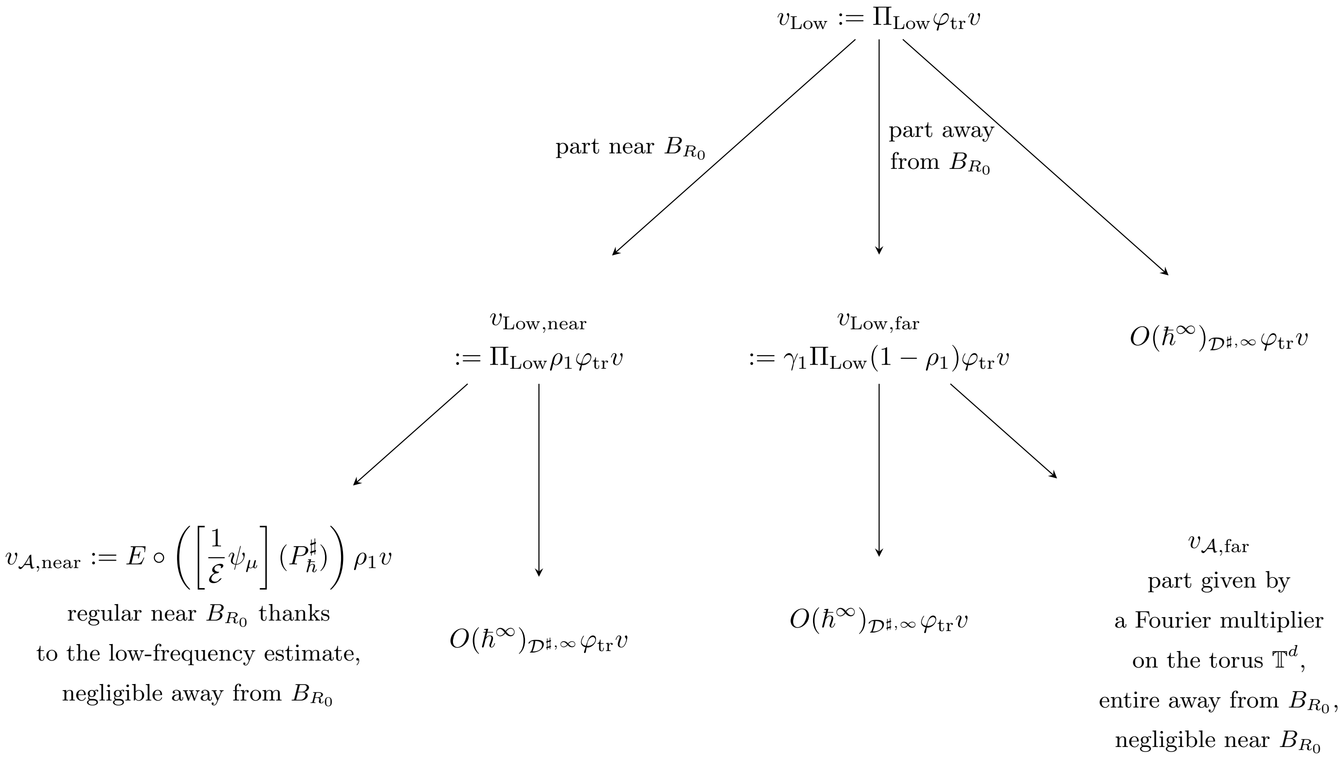

Figure 5.4: The decomposition of v_{Low} when $\rho \neq 1$, described in §5.4.4-§5.4.6

Remark 5.12 (The decomposition is independent of $\mathcal{E}$ if $E_\infty = 0$) *The last part of Theorem 4.1 is the claim that the decomposition is independent of $\mathcal{E}$ if $E_\infty = 0$. To establish this when $\rho \neq 1$, observe that the only part of the definition of the decomposition where $\mathcal{E}$ enters is in the decomposition $v_{\mathrm{Low,near}} = v_{\mathcal{A},\mathrm{near}} + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}v$. Furthermore, if $E_\infty = 0$, then, by (5.50) and (5.57), we can define $v_{\mathcal{A},\mathrm{near}} := \psi_\mu(P_\hbar^\sharp)\rho_1 v$ (which is independent of $\mathcal{E}$) and have $v_{\mathrm{Low,near}} = v_{\mathcal{A},\mathrm{near}}$.*

Proof of (4.9) and (4.10) for $v_{\mathcal{A},\mathrm{near}}$. Using (in this order) the definition of $v_{\mathcal{A},\mathrm{near}}$ (5.57), the fact that $\rho = 1$ on $B_{R_{\mathrm{IV}}}$, the low-frequency estimate (4.4), Part 3 of Theorem 3.4, and finally the resolvent estimate (5.18) we obtain

$$\begin{aligned}\|D(\alpha)v_{\mathcal{A},\mathrm{near}}\|_{\mathcal{H}^\sharp(B_{R_{\mathrm{IV}}})} &\leq \left\|\rho D(\alpha)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 v\right\|_{\mathcal{H}^\sharp} \leq C_{\mathcal{E}}(\alpha,\hbar)\left\|\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 v\right\|_{\mathcal{H}^\sharp}\\ &\leq C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\|\rho_1 v\|_{\mathcal{H}(\Omega_{\mathrm{tr}})}\\ &\lesssim C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\hbar^{-1-M}\|g\|_{\mathcal{H}(\Omega_{\mathrm{tr}})};\end{aligned}$$

thus (4.9) holds, where the $\sup_{\lambda\in\mathbb{R}}$ becomes $\sup_{\lambda\in[-\Lambda,\Lambda]}$ because of the support property (5.5) of ψ_μ.

The proof of (4.10) is very similar to the proof of (4.15) above. Since $\rho_2 \equiv 0$ on $(B_{R_{\mathrm{III}}})^c$,

$$\|v_{\mathcal{A},\mathrm{near}}\|_{\mathcal{D}^{m,\sharp}((B_{R_{\mathrm{III}}})^c)} \leq \left\|(1-\rho_2)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 v\right\|_{\mathcal{D}^{m,\sharp}}. \tag{5.58}$$

By (5.49), Part 1 of Theorem 3.4, pseudo-locality of the functional calculus (Lemma 3.5), and the support property (5.54),

$$(1-\rho_2)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 = (1-\rho_2)\mathcal{E}(P_\hbar^\sharp)\left(\frac{1}{\mathcal{E}}\psi_\mu\right)(P_\hbar^\sharp)\rho_1 + O(\hbar^\infty)_{\mathcal{D}^\sharp,\infty}$$

$$= (1-\rho_2)\psi_\mu(P^\sharp_\hbar)\rho_1 + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} = O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}.$$

Combining this with (5.58) and then using the resolvent estimate (5.18), we obtain (4.10).

5.4.6 The term away from the black box $v_{\mathrm{Low,far}}$.

We now study

$$v_{\mathrm{Low,far}} := \gamma_1 \Pi_{\mathrm{Low}}(1-\rho_1)\varphi_{\mathrm{tr}} v \tag{5.59}$$

which is in $\mathcal{D}^{\sharp,\infty}_\hbar$ by the fact that $\Pi_{\mathrm{Low}} : \mathcal{D}^\sharp \to \mathcal{D}^{\sharp,\infty}_\hbar$ (see §5.1) and the smoothness and support properties of γ_1 (see §5.4.3).

Step 1: expressing $v_{\mathrm{Low,far}}$ in terms of $v_{\mathcal{A},\mathrm{far}}$ Since $\mathrm{supp}(1-\gamma_1)$ and $\mathrm{supp}(1-\rho_1)$ are disjoint (see Figure 5.3), the pseudo-locality of the functional calculus given by Lemma 3.5 implies that

$$\gamma_1\Pi_{\mathrm{Low}}(1-\rho_1) = \gamma_1\Pi_{\mathrm{Low}}\gamma_1(1-\rho_1) + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}.$$

Therefore, by Lemma 3.6 (and exactly as in §5.3), $\Pi^\Psi_{\mathrm{Low}} := \psi_\mu(Q_\hbar) \in \Psi^\infty_\hbar(\mathbb{T}^d_{R_\sharp})$ with

$$\gamma_1\Pi_{\mathrm{Low}}(1-\rho_1) = \gamma_1\Pi^\Psi_{\mathrm{Low}}\gamma_1(1-\rho_1) + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}, \tag{5.60}$$

and, by (5.39), $\mathrm{WF}_\hbar\, \Pi^\Psi_{\mathrm{Low}} \subset \{|q_\hbar| \le 2\mu\}$. Therefore, by (3.5), there exists $\lambda > 1$ such that

$$\mathrm{WF}_\hbar\, \Pi^\Psi_{\mathrm{Low}} \subset \Big\{(x,\xi)\,:\, x\in\mathbb{T}^d_{R_\sharp},\ \xi\in B_{\lambda/2}\Big\}. \tag{5.61}$$

Now, let $\widetilde{\varphi} \in C^\infty_{\mathrm{comp}}(\mathbb{R}^d;[0,1])$ be supported in $[-\lambda^2,\lambda^2]$ and equal to one on $[-\lambda^2/4,\lambda^2/4]$. By (A.10) and (5.61), $\mathrm{WF}_\hbar\big(1-\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\big)\cap\mathrm{WF}_\hbar\big(\Pi^\Psi_{\mathrm{Low}}\big)=\emptyset$. Therefore, by (A.9), as operators on the torus,

$$\Pi^\Psi_{\mathrm{Low}} = \mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\mathrm{Low}} + O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}. \tag{5.62}$$

Since $\gamma_1 = 0$ on a neighbourhood of B_{R_0}, by the definitions of $P^\sharp$ (3.4), $\|\cdot\|_{\mathcal{D}^{\sharp,m}_\hbar}$ (3.11), and $\|\cdot\|_{H^{2m}_\hbar(\mathbb{T}^d_{R^\sharp})}$ (A.2), given $m>0$ there exists $C_j(m)>0$, $j=1,2$, such that

$$C_1(m)\,\|\gamma_1 w\|_{\mathcal{D}^{\sharp,m}_\hbar} \le \|\gamma_1 w\|_{H^{2m}_\hbar(\mathbb{T}^d_{R^\sharp})} \le C_2(m)\,\|\gamma_1 w\|_{\mathcal{D}^{\sharp,m}_\hbar} \qquad \text{for all } w\in\mathcal{D}^{\sharp,m}_\hbar, \tag{5.63}$$

and thus $\gamma_1 O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}\gamma_1 = O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}$. Therefore, combining this with (5.62) and (5.60), we obtain that

$$\gamma_1\Pi_{\mathrm{Low}}(1-\rho_1) = \gamma_1\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\mathrm{Low}}\gamma_1(1-\rho_1) + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}. \tag{5.64}$$

We let

$$v_{\mathcal{A},\mathrm{far}} := \gamma_1\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\mathrm{Low}}\gamma_1(1-\rho_1)\varphi_{\mathrm{tr}}v, \tag{5.65}$$

so that the combination of (5.59), (5.64), and (5.65) implies that

$$v_{\mathrm{Low,far}} = v_{\mathcal{A},\mathrm{far}} + O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}}\varphi_{\mathrm{tr}}v.$$

Observe that $v_{\mathcal{A},\mathrm{far}} \in \mathcal{D}(\Omega_{\mathrm{tr}})$ because of the presence of γ_1 at the start of the expression (which causes $v_{\mathcal{A},\mathrm{far}}$ to be zero on Γ_{tr}).

Step 2: proving that $v_{\mathcal{A},\mathrm{far}}$ is regular in $(B_{R_{\mathrm{I}}})^c$ (i.e., the bound (4.11)). By the definition of $v_{\mathcal{A},\mathrm{far}}$ (5.65) and the fact that $\gamma_1 = 1$ on $(B_{R_{\mathrm{I}}})^c$,

$$\begin{aligned}\|\partial^\alpha v_{\mathcal{A},\mathrm{far}}\|_{\mathcal{H}((B_{R_{\mathrm{I}}})^c)} &= \Big\|\partial^\alpha\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\mathrm{Low}}\gamma_1(1-\rho_1)\varphi_{\mathrm{tr}}v\Big\|_{\mathcal{H}((B_{R_{\mathrm{I}}})^c)}\\ &\le \Big\|\partial^\alpha\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\mathrm{Low}}\gamma_1(1-\rho_1)\varphi_{\mathrm{tr}}v\Big\|_{L^2(\mathbb{T}^d_{R_\sharp})}.\end{aligned} \tag{5.66}$$

We now bound the right-hand side of (5.66). By Lemma A.3, $\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))$ is given as a Fourier multiplier on the torus (defined by (A.11)), i.e.,

$$\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2)) = \widetilde{\varphi}(-\hbar^2\Delta). \tag{5.67}$$

Let $w \in L^2(\mathbb{T}^d_{R_\sharp})$ be arbitrary, and let $\widehat{w}(j)$ be the Fourier coefficients of w. By (A.11),

$$\widetilde{\varphi}(-\hbar^2\Delta)w = \sum_{j\in\mathbb{Z}^d} \widehat{w}(j)\widetilde{\varphi}(\hbar^2|j|^2\pi^2/R_\sharp^2)e_j,$$

where the normalised eigenvectors e_j are defined by (A.1). Hence, for any multi-index α,

$$\partial^\alpha\widetilde{\varphi}(-\hbar^2\Delta)w = \sum_{j\in\mathbb{Z}^d} \widehat{w}(j)\widetilde{\varphi}(\hbar^2|j|^2\pi^2/R_\sharp^2)\left(\frac{\mathrm{i}\pi j}{R_\sharp}\right)^\alpha e_j = \sum_{j\in\mathbb{Z}^d,\ |j|\le\frac{\lambda R_\sharp}{\hbar\pi}} \widehat{w}(j)\widetilde{\varphi}(\hbar^2|j|^2\pi^2/R_\sharp^2)\left(\frac{\mathrm{i}\pi j}{R_\sharp}\right)^\alpha e_j,$$

since $\widetilde{\varphi}$ is supported in $B(0,\lambda^2)$. Therefore

$$\begin{aligned}\|\partial^\alpha\widetilde{\varphi}(-\hbar^2\Delta)w\|^2_{L^2(\mathbb{T}^d_{R_\sharp})} &= \sum_{j\in\mathbb{Z}^d,\ |j|\le\frac{\lambda R_\sharp}{\hbar\pi}} \left|\widehat{w}(j)\widetilde{\varphi}(\hbar^2|j|^2\pi^2/R_\sharp^2)\left(\frac{\mathrm{i}\pi j}{R_\sharp}\right)^\alpha\right|^2 \\ &\le \lambda^{2|\alpha|}\hbar^{-2|\alpha|}\sum_{j\in\mathbb{Z}^d}|\widehat{w}(j)|^2 = \lambda^{2|\alpha|}\hbar^{-2|\alpha|}\|w\|^2_{L^2(\mathbb{T}^d_{R_\sharp})}.\end{aligned} \tag{5.68}$$

We now use (5.68) with

$$w := \Pi^\Psi_{\rm Low}\gamma_1(1-\rho_1)\varphi_{\rm tr}v,$$

and combine the resulting estimate with (5.66) and (5.67). Using the fact that $\Pi^\Psi_{\rm Low}\in\Psi^\infty(\mathbb{T}^d_{R_\sharp})$, $\gamma_1 = 0$ on a neighbourhood of B_{R_0}, and the resolvent estimate (5.18), we get

$$\begin{aligned}\|\partial^\alpha v_{\mathcal{A},\rm far}\|_{\mathcal{H}((B_{R_{\rm I}})^c)} &\le \lambda^{|\alpha|}\hbar^{-|\alpha|}\|\Pi^\Psi_{\rm Low}\gamma_1(1-\rho_1)\varphi_{\rm tr}v\|_{L^2(\mathbb{T}^d_{R_\sharp})} \lesssim \lambda^{|\alpha|}\hbar^{-|\alpha|}\|\gamma_1(1-\rho_1)\varphi_{\rm tr}v\|_{L^2(\mathbb{T}^d_{R_\sharp})} \\ &= \lambda^{|\alpha|}\hbar^{-|\alpha|}\|\gamma_1(1-\rho_1)\varphi_{\rm tr}v\|_{\mathcal{H}} \le \lambda^{|\alpha|}\hbar^{-|\alpha|}\hbar^{-1-M}\|g\|_{\mathcal{H}(\Omega_{\rm tr})};\end{aligned}$$

hence (4.11) holds.

Step 3: proving that $v_{\mathcal{A},\rm far}$ is negligible in $B_{R_{\rm II}}$ (i.e., the bound (4.12)). It therefore remains to show (4.12).

By (A.8), (A.10), and the support property (5.56),

$$\mathrm{WF}_\hbar\left((1-\gamma_2)\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\rm Low}\right)\cap\mathrm{WF}_\hbar(1-\rho_1) = \emptyset.$$

Then, by (A.9),

$$(1-\gamma_2)\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\rm Low}(1-\rho_1) = O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}$$

as a pseudo-differential operator on the torus. Multiplying by γ_1 on the right and on the left, and then using the fact that $\gamma_1 = 0$ on B_{R_0} and the norm equivalence (5.63), we find

$$(1-\gamma_2)\gamma_1\,\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\rm Low}\gamma_1(1-\rho_1) = O(\hbar^\infty)_{\mathcal{D}^{\sharp,\infty}} \tag{5.69}$$

as an element of $\mathcal{L}(\mathcal{H}^\sharp)$. On the other hand, since $\gamma_2 = 0$ on a neighbourhood of $B_{R_{\rm II}}$,

$$\|v_{\mathcal{A},\rm far}\|_{\mathcal{D}_\hbar^{\sharp,m}(B_{R_{\rm II}})} = \|(1-\gamma_2)v_{\mathcal{A},\rm far}\|_{\mathcal{D}_\hbar^{\sharp,m}(B_{R_{\rm II}})}.$$

Then (4.12) follows from combining this last equation with the definition of $u^\infty_{\mathcal{A}}$ (5.65), (5.69), and the resolvent estimate (5.18).

The proof of Theorem 4.1 is now complete.

6 Proofs of Theorems 1.16 and 1.17

These proofs follow very closely the proofs of [29, Theorem D] and [29, Theorem B], i.e., the analogous decompositions for outgoing Helmholtz solutions; this is because (as highlighted after Theorem 4.1) the assumptions of Theorem 4.1 are (by design) the same as the assumptions of the abstract decomposition result in [29, Theorem A]. For completeness, we sketch here the ideas behind these proofs.

6.1 Set-up common to both proofs

Let $\hbar := k^{-1}$ and define $\mathcal{H}$ and $P_\hbar$ as in Lemma 3.2 with $\Omega_- = \emptyset$. By Lemma 3.2, $P_\hbar$ is a semiclassical black-box operator on $\mathcal{H}$. The reference operator is given by $P_\hbar^\sharp = -\hbar^2 c_{\rm scat}^2 \nabla \cdot (A_{\rm scat}\nabla)$. Let

$$\mathfrak{H} := \big\{ \hbar : \hbar = k^{-1} \text{ with } k \in K \big\}. \tag{6.1}$$

The assumption that the solution operator is polynomially bounded (in the sense of Definition 1.2) means that the bound (4.2) holds with $\mathfrak{H}$ given by (6.1); i.e., the assumption in Point 1 of Theorem 4.1 is satisfied. Define $P_{\hbar,\theta}$ by (3.8). In this notation, the PML problem (1.5) becomes $(P_{\hbar,\theta} - I)v = \hbar^2 g$.

6.2 Sketch proof of Theorem 1.16

We now construct $\mathcal{E}$ and E satisfying the assumptions in Point 2 of Theorem 4.1 under Assumption 1.10. Let $\Lambda > 0$ be as in Theorem 4.1, and let $\mathcal{E} \in C^\infty_{\rm comp}(\mathbb{R})$ be such that $\mathcal{E} = 1$ in $[-\Lambda, \Lambda]$, and $\mathcal{E} = 0$ outside $[-2\Lambda, 2\Lambda]$. The results of Helffer-Robert [33] imply that $\mathcal{E}(P_\hbar^\sharp) = \mathcal{E}(-\hbar^2 c_{\rm scat}^2 \nabla \cdot \big(A_{\rm scat}\nabla)\big)$ is a pseudo-differential operator on $\mathbb{T}^d_{R_\sharp}$ (see the discussion in §1.8 under the paragraph "Ingredient 5"). Then, arguing as in Step 1 in §5.4.6, we obtain that there exists $\Lambda_0 > 0$ such that

$$\mathcal{E}(P_\hbar^\sharp) = \mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\mathcal{E}(P_\hbar^\sharp) + O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}.$$

with $\widetilde{\varphi} \in C^\infty_{\rm comp}(\mathbb{R}^d; [0,1])$ supported in $B(0, \Lambda_0^2)$ and equal to one on $B(0, \Lambda_0^2/4)$. By Lemma A.3,

$$\mathcal{E}(P_\hbar^\sharp) = \widetilde{\varphi}(-\hbar^2\Delta)\mathcal{E}(P_\hbar^\sharp) + O(\hbar^\infty)_{\Psi_\hbar^{-\infty}},$$

so that

$$\text{if} \quad E := \widetilde{\varphi}(-\hbar^2\Delta)\mathcal{E}(P_\hbar^\sharp) \quad \text{then} \quad \mathcal{E}(P_\hbar^\sharp) = E + O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty} \to \mathcal{D}_\hbar^{\sharp,\infty}}. \tag{6.2}$$

We now need to show that an estimate of the form (4.4) is satisfied. Since $\widetilde{\varphi}$ is compactly supported in $B(0, \Lambda_0^2)$, the definition of E (6.2) and the same argument used to show the bound (5.68) imply that

$$\|\partial^\alpha E v\|_{L^2(\mathbb{T}^d_{R_\sharp})} \leq \Lambda_0^{|\alpha|}\hbar^{-|\alpha|}\|\mathcal{E}(P_\hbar^\sharp v)\|_{L^2(\mathbb{T}^d_{R_\sharp})}$$

for all $v \in L^2(\mathbb{T}^d_{R_\sharp})$ and multi-indices α. Then, since $\mathcal{E}(P_\hbar^\sharp) \in \Psi_\hbar^{-\infty}(\mathbb{T}^d_{R_\sharp})$, Part (iii) of Theorem A.1 implies that there exists $C > 0$ such that

$$\|\partial^\alpha E v\|_{L^2(\mathbb{T}^d_{R_\sharp})} \leq C\Lambda_0^{|\alpha|}\hbar^{-|\alpha|}\|v\|_{L^2(\mathbb{T}^d_{R_\sharp})}$$

for all $v \in L^2(\mathbb{T}^d_{R_\sharp})$ and multi-indices α. Therefore, the assumption in Point 2 of Theorem 4.1 is satisfied with $D(\alpha) := \partial^\alpha$, $C_{\mathcal{E}}(\alpha, \hbar) := C\Lambda_0^{|\alpha|}\hbar^{-|\alpha|}$ and $\rho = 1$.

The bound (1.19) on $v_{\mathcal{A}}$ follows immediately from (4.14). The bound (1.18) on v_{H^2} follows from (4.7) after using (i) Green's identity and Lemma 2.3 to obtain a bound on the H^1 semi-norm, and then (ii) Lemma 2.3 and H^2 regularity by [50, Theorem 4.18].

6.3 Sketch proof of Theorem 1.17

Theorem 1.17 is based on the following result, which is Theorem 4.1 specialised to the case when the regularity estimate inside the black box comes from a heat flow estimate.

Corollary 6.1 *Let $P_\hbar$ be a semiclassical black-box operator on $\mathcal{H}$ satisfying the polynomial resolvent estimate (4.2) in $\mathfrak{H} \subset (0, \hbar_0]$. Assume further that (i) $P_\hbar^\sharp \geq a(\hbar) > 0$ for some $a(\hbar) > 0$, and (ii) for some α-family of black-box differentiation operators $(D(\alpha))_{\alpha \in \mathfrak{A}}$ (Definition 3.7), there exists $\rho \in C^\infty(\mathbb{T}^d_{R_\sharp})$ equal to one near B_{R_0} such that, for some family of subsets $I(\hbar, \alpha) \subset [0, +\infty)$, the following localised heat-flow estimate holds,*

$$\left\| \rho D(\alpha) \mathrm{e}^{-tP_\hbar^\sharp} \right\|_{\mathcal{H}^\sharp \to \mathcal{H}^\sharp} \leq C(\alpha, t, \hbar) \quad \text{for all } \alpha \in \mathfrak{A},\ t \in I(\hbar, \alpha),\ \hbar \in \mathfrak{H}. \tag{6.3}$$

Given $\epsilon > 0$, there exist $\hbar_1 > 0$, $C_j > 0$, $j = 1, 2, 3$, and $\lambda > 1$ such that for all $R_{\rm tr} > (1+\epsilon)R_1$, $B_{R_{\rm tr}} \subset \Omega_{\rm tr} \Subset \mathbb{R}^d$ with Lipschitz boundary, $\epsilon < \theta < \pi/2 - \epsilon$, all $g \in \mathcal{H}(\Omega_{\rm tr})$, and all $\hbar \in \mathfrak{H} \cap (0, \hbar_1]$, the following holds. The solution $v \in \mathcal{D}(\Omega_{\rm tr})$ to

$$(P_{\hbar,\theta} - I)v = g \quad \text{on } \Omega_{\rm tr} \qquad \text{and} \qquad v = 0 \quad \text{on } \Gamma_{\rm tr}$$

exists and is unique and there exists $v_{H^2} \in \mathcal{D}(\Omega_{\rm tr}), v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ and $v_{\rm residual} \in \mathcal{D}_\hbar^{\sharp,\infty}$ such that

$$v = v_{H^2} + v_{\mathcal{A}} + v_{\rm residual}$$

and $v_{H^2}, v_{\mathcal{A}}$, and $v_{\rm residual}$ satisfy the following properties. The component $v_{H^2} \in \mathcal{D}(\Omega_{\rm tr})$ satisfies (4.7). There exist $R_{\rm I}, R_{\rm II}, R_{\rm III}, R_{\rm IV}$ with $R_0 < R_{\rm I} < R_{\rm II} < R_{\rm III} < R_{\rm IV} < R_1$ such that $v_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ decomposes as

$$v_{\mathcal{A}} = v_{\mathcal{A},\rm near} + v_{\mathcal{A},\rm far},$$

where $v_{\mathcal{A},\rm near} \in \mathcal{D}^\sharp$ is regular near the black box and negligible away from it, in the sense that

$$\|D(\alpha) v_{\mathcal{A},\rm near}\|_{\mathcal{H}^\sharp(B_{R_{\rm IV}})} \leq C_2 \left(\inf_{t \in I(\hbar,\alpha)} C(\alpha, \hbar, t) \mathrm{e}^{\Lambda t} \right) \hbar^{-1-M} \|g\|_{\mathcal{H}(\Omega_{\rm tr})} \quad \text{for all } \hbar \in \mathfrak{H} \cap (0, \hbar_1], \alpha \in \mathfrak{A}, \tag{6.4}$$

and, for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such that (4.10) holds and $v_{\mathcal{A},\rm far} \in \mathcal{D}(\Omega_{\rm tr})$ is entire away from the black box and negligible near it, in the sense that (4.11) holds and, for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such that (4.12) holds. Finally, $v_{\rm residual} \in \mathcal{D}_\hbar^{\sharp,\infty}$ is negligible in the sense that for any $N, m > 0$ there exists $C_{N,m} > 0$ (independent of θ) such that (4.13) holds.

The proof of Corollary 6.1 is identical to the proof of [29, Corollary 4.1]; since the proof is so short, however, we include it for completeness.

Proof of Corollary 6.1. For $\alpha \in \mathfrak{A}$ and $\hbar \in \mathfrak{H}$, let $t \in I(\hbar, \alpha)$, and $\mathcal{E}_t(\lambda) := \mathrm{e}^{-t|\lambda|}$. Since $P_\hbar^\sharp \geq a(\hbar) > 0$, $\operatorname{Sp} P_\hbar^\sharp \subset [a(\hbar), \infty)$. Therefore, by Parts 4 and 3 of Theorem 3.4, $\mathrm{e}^{-tP_\hbar^\sharp} = \mathcal{E}_t(P_\hbar^\sharp)$. Such an $\mathcal{E}_t$ is in $C_0(\mathbb{R})$, never vanishes, and satisfies (4.4) with $E_t := \mathcal{E}_t(P_\hbar^\sharp)$ and $C_{\mathcal{E}_t}(\alpha, \hbar) := C(\alpha, \hbar, t)$ by (6.3). From Theorem 4.1, we therefore obtain the above decomposition $v_{\mathcal{A}}, v_{\mathcal{A},\rm near}, v_{\mathcal{A},\rm far}, v_{H^2}$. Since $\mathcal{E}_t(P_\hbar^\sharp) = E_t$ (i.e., $E_\infty = 0$), by the final part of Theorem 4.1, the decomposition is constructed independently of $\mathcal{E}_t$, and hence independently of t. The result then follows, with the infimum in t in (6.4) coming from (4.9) and the fact that this estimate in valid for any $t \in I(\hbar, \alpha)$. ∎

Theorem 1.17 is proved using Corollary 6.1 with the following heat-flow estimate as (6.3).

Theorem 6.2 (Heat equation estimate from [25]) *Suppose that Assumption 1.11 holds with $A_{\rm scat}$ and $c_{\rm scat}$ analytic in B_{R_*} for some $R_0 < R_* < R_{\rm scat}$. Let $P_\hbar^\sharp$ denote the associated black-box reference operator on the torus (as described in §3.1).*

Given $\rho \in C^\infty_{\rm comp}(\mathbb{R}^d; [0,1])$ with $\operatorname{supp} \rho \subset B_{R_*}$, there exists $C > 0$ such that for all $t \in (0,1]$ and for all $\tau \in [0,1]$

$$\left\| \rho \partial^\alpha \mathrm{e}^{t\hbar^{-2} P_\hbar^\sharp} \right\|_{L^2 \to L^2} \leq \exp(t^{-\tau}) |\alpha|!\, C^{|\alpha|} t^{(\tau-1)|\alpha|/2}. \tag{6.5}$$

References for the proof of Theorem 6.2. Since the operator $e^{t\hbar^{-2}P_\hbar^\sharp}$ is just the variable coefficient heat operator for time t, the estimate (6.5) can be extracted from the heat equation bounds in [25, Theorem 1.1 and Lemma 2.7]; see [29, Proof of Theorem 4.3] for more detail. ∎

We therefore apply Corollary 6.1 to the specific set up in §6.1, noting that the heat-flow estimate (6.3) is then satisfied with $D(\alpha) := \partial^\alpha$,

$$C(\alpha,\hbar,t) := \exp\big((\hbar^2 t)^{-\tau}\big)|\alpha|!\, C^{|\alpha|}\big(\hbar^2 t\big)^{(\tau-1)|\alpha|/2}, \qquad \text{and} \qquad I(\hbar,\alpha) := (0,\hbar^{-2}]$$

(the heat-flow given by the functional calculus, appearing in (6.3), is indeed the solution of the heat equation; see, e.g., [58, Theorem VIII.7]).

To obtain Theorem 1.17 from Corollary 6.1, we then only need to show that (i) v_{H^2} satisfies (1.21), and (ii) $v_{\mathcal{A},\mathrm{near}}$ satisfies (1.22). The proof of (i) is identical to the proof that v_{H^2} in Theorem 1.16 satisfies (1.18). For (ii), we carefully choose t and τ as functions of $|\alpha|$ and $\hbar$ to obtain (1.22); for the details, see [29, §4.1].

A Semiclassical pseudodifferential operators on the torus

Recall that for $R_\sharp > 0$, $\mathbb{T}^d_{R_\sharp} := \mathbb{R}^d/(2R_\sharp\mathbb{Z})^d$. This appendix reviews the material about semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_\sharp}$ used in §5.3-§5.4, and appearing in Lemma 3.6, with our default references being [70] and [22, Appendix E].

Semiclassical Sobolev spaces. We consider functions or distributions on the torus as periodic functions or distributions on $\mathbb{R}^d$. To eliminate confusion between Fourier series and integrals, for $f \in L^2(\mathbb{T}^d_{R_\sharp})$ we define the Fourier coefficients for $j \in \mathbb{Z}^d$

$$\widehat{f}(j) := \int_{\mathbb{T}^d_{R_\sharp}} f(x)\overline{e_j}(x)\,\mathrm{d}x, \qquad \text{where} \qquad e_j(x) = (2R_\sharp)^{-d/2}\exp\big(\mathrm{i}\pi j\cdot x/R_\sharp\big). \tag{A.1}$$

The Fourier inversion formula and the action of the operator $(\hbar D)^\alpha$ on the torus are then, respectively,

$$f = \sum_{j\in\mathbb{Z}^d}\widehat{f}(j)e_j \qquad \text{and} \qquad (\hbar D)^\alpha f = \sum_{j\in\mathbb{Z}^d}(\hbar\pi j/R_\sharp)^\alpha \widehat{f}(j)e_j.$$

We work on the spaces defined by the boundedness of these operators, namely

$$H^m_\hbar(\mathbb{T}^d_{R_\sharp}) := \Big\{u\in L^2(\mathbb{T}^d_{R_\sharp}),\ \langle j\rangle^m\widehat{f}(j)\in\ell^2(\mathbb{Z}^d)\Big\}, \qquad \|u\|^2_{H^m_\hbar(\mathbb{T}^d_{R_\sharp})} := \sum\langle\hbar j\rangle^{2m}|\widehat{f}(j)|^2, \tag{A.2}$$

where $\langle j\rangle := (1+|j|^2)^{1/2}$; see [70, §8.3], [22, §E.1.8]. In this appendix, we abbreviate $H^m_\hbar(\mathbb{T}^d_{R_\sharp})$ to $H^m_\hbar$ and $L^2(\mathbb{T}^d_{R_\sharp})$ to L^2.

Since these spaces are defined for positive integer m by boundedness of $(hD)^\alpha$ with $|\alpha| = m$ (and can be extended to $m\in\mathbb{R}$ by interpolation and duality), they agree with localized versions of the corresponding spaces on $\mathbb{R}^d$ defined by the semiclassical Fourier transform

$$\mathcal{F}_\hbar u(\xi) := \int_{\mathbb{R}^d}\exp\big(-\mathrm{i}x\cdot\xi/\hbar\big)u(x)\,\mathrm{d}x \qquad \text{and} \qquad \|u\|^2_{H^m_\hbar(\mathbb{R}^d)} := (2\pi\hbar)^{-d}\int_{\mathbb{R}^d}\langle\xi\rangle^m|\mathcal{F}_\hbar u(\xi)|^2\,\mathrm{d}\xi.$$

Phase space. The set of all possible positions x and momenta (i.e. Fourier variables) ξ is denoted by $T^*\mathbb{T}^d_{R_\sharp}$; this is known informally as "phase space". Strictly, $T^*\mathbb{T}^d_{R_\sharp} := \mathbb{T}^d_{R_\sharp}\times(\mathbb{R}^d)^*$, but for our purposes, we can consider $T^*\mathbb{T}^d_{R_\sharp}$ as $\{(x,\xi): x\in\mathbb{T}^d_{R_\sharp},\xi\in\mathbb{R}^d\}$. We also use the analogous notation for $T^*\mathbb{R}^d$ where appropriate.

To deal uniformly near fiber-infinity with the behavior of functions on phase space, we also consider the *radial compactification* in the fibers of this space, $\overline{T}^*\mathbb{T}^d_{R_\sharp} := \mathbb{T}^d\times B^d$, where B^d denotes the closed unit ball, considered as the closure of the image of $\mathbb{R}^d$ under the radial compactification map $\mathsf{RC}:\xi\mapsto\xi/(1+\langle\xi\rangle)$; see [22, §E.1.3]. Near the boundary of the ball, $|\xi|^{-1}\circ\mathsf{RC}^{-1}$ is a smooth function, vanishing to first order at the boundary, with $(|\xi|^{-1}\circ \mathsf{RC}^{-1}, \widehat{\xi}\circ \mathsf{RC}^{-1})$ thus furnishing local coordinates on the ball near its boundary. The boundary of the ball should be considered as a sphere at infinity consisting of all possible *directions* of the momentum variable. Where appropriate (e.g., in dealing with finite values of ξ only), we abuse notation by dropping the composition with RC from our notation and simply identifying $\mathbb{R}^d$ with the interior of B^d.

Symbols, quantisation, and semiclassical pseudodifferential operators. A symbol on $\mathbb{R}^d$ is a function on $T^*\mathbb{R}^d$ that is also allowed to depend on $\hbar$, and thus can be considered as an $\hbar$-dependent family of functions. Such a family $a = (a_\hbar)_{0<\hbar\leq\hbar_0}$, with $a_\hbar \in C^\infty(\mathbb{R}^d)$, is a *symbol of order* m on the $\mathbb{R}^d$, written as $a \in S^m(\mathbb{R}^d)$, if for any multi-indices α, β

$$|\partial_x^\alpha \partial_\xi^\beta a(x,\xi)| \leq C_{\alpha,\beta}\langle\xi\rangle^{m-|\beta|} \quad \text{for all } (x,\xi)\in T^*\mathbb{R}^d \text{ and for all } 0<\hbar\leq\hbar_0,$$

where $C_{\alpha,\beta}$ does not depend on $\hbar$; see [70, p. 207], [22, §E.1.2].

For $a \in S^m(\mathbb{R}^d)$, we define the *semiclassical quantisation* of a on $\mathbb{R}^d$, denoted by $\mathrm{Op}_\hbar(a)$

$$\big(\mathrm{Op}_\hbar(a)v\big)(x) := (2\pi\hbar)^{-d}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \exp\big(\mathrm{i}(x-y)\cdot\xi/\hbar\big)\, a(x,\xi) v(y)\,\mathrm{d}y\mathrm{d}\xi; \tag{A.3}$$

[70, §4.1] [22, Page 543]. The integral in (A.3) need not converge, and can be understood *either* as an oscillatory integral in the sense of [70, §3.6], [36, §7.8], *or* as an iterated integral, with the y integration performed first; see [22, Page 543]. It can be shown that for any symbol a, $\mathrm{Op}_\hbar(a)$ preserves Schwartz functions, and extends by duality to act on tempered distributions [70, §4.4]

We use below that if $a = a(\xi)$ depends only on ξ, then $\mathrm{Op}_\hbar(a) = \mathcal{F}_\hbar^{-1} M_a \mathcal{F}_\hbar$, where M_a denotes multiplication by a; i.e., in this case $\mathrm{Op}_\hbar(a)$ is just a Fourier multiplier on $\mathbb{R}^d$.

We now return to considering the torus: if $a(x,\xi) \in S^m(\mathbb{R}^d)$ and is periodic, and if v is a distribution on the torus, we can view v as a periodic (hence, tempered) distribution on $\mathbb{R}^d$, and define

$$\big(\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(a)v\big) = \big(\mathrm{Op}_\hbar(a)v\big),$$

since the right side is again periodic; for details see, e.g., [70, §5.3.1].

If A can be written in the form above, i.e. $A = \mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(a)$ with $a \in S^m$, we say that A is a *semiclassical pseudodifferential operator of order* m on the torus and we write $A \in \Psi_\hbar^m(\mathbb{T}^d_{R_\sharp})$; furthermore that we often abbreviate $\Psi_\hbar^m(\mathbb{T}^d_{R_\sharp})$ to $\Psi_\hbar^m$ in this Appendix. We use the notation $a \in \hbar^l S^m$ if $\hbar^{-l}a \in S^m$; similarly $A \in \hbar^l\Psi_\hbar^m$ if $\hbar^{-l}A \in \Psi_\hbar^m$.

Theorem A.1 (Composition and mapping properties of semiclassical pseudodifferential operators [70, Theorem 8.10], [22, Proposition E.17 and Proposition E.19]) *If $A \in \Psi_\hbar^{m_1}$ and $B \in \Psi_\hbar^{m_2}$, then*

(i) $AB \in \Psi_\hbar^{m_1+m_2}$,

(ii) $[A,B] \in \hbar\Psi_\hbar^{m_1+m_2-1}$,

(iii) For any $s\in\mathbb{R}$, A is bounded uniformly in $\hbar$ as an operator from $H_\hbar^s$ to $H_\hbar^{s-m_1}$.

Residual class. We say that $A = O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}$ if, for any $s>0$ and $N\geq 1$, there exists $C_{s,N}>0$ such that

$$\|A\|_{H_\hbar^{-s}\to H_\hbar^s} \leq C_{N,s}\hbar^N; \tag{A.4}$$

i.e. $A \in \Psi_\hbar^{-\infty}$ and furthermore all of its operator norms are bounded by any algebraic power of $\hbar$.

Principal symbol $\sigma_\hbar$. Let the quotient space $S^m/\hbar S^{m-1}$ be defined by identifying elements of S^m that differ only by an element of $\hbar S^{m-1}$. For any m, there is a linear, surjective map $\sigma_\hbar^m : \Psi_\hbar^m \to S^m/\hbar S^{m-1}$, called the *principal symbol map*, such that, for $a\in S^m$,

$$\sigma_\hbar^m\big(\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(a)\big) = a \mod \hbar S^{m-1}; \tag{A.5}$$

see [70, Page 213], [22, Proposition E.14] (observe that (A.5) implies that $\ker(\sigma_\hbar^m) = \hbar\Psi_\hbar^{m-1}$).

When applying the map $\sigma_\hbar^m$ to elements of $\Psi_\hbar^m$, we denote it by $\sigma_\hbar$ (i.e. we omit the m dependence) and we use $\sigma_\hbar(A)$ to denote one of the representatives in S^m (with the results we use then independent of the choice of representative).

Operator wavefront set $\mathrm{WF}_\hbar$. We say that $(x_0,\zeta_0)\in \overline{T}^*\mathbb{T}^d_{R_\sharp}$ is *not* in the *semiclassical operator wavefront set* of $A=\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(a)\in\Psi^m_\hbar$, denoted by $\mathrm{WF}_\hbar A$, if there exists a neighbourhood U of (x_0,ζ_0) such that for all multi-indices α,β and all $N\geq 1$ there exists $C_{\alpha,\beta,U,N}>0$ (independent of $\hbar$) such that, for all $0<\hbar\leq\hbar_0$,

$$|\partial_x^\alpha\partial_\xi^\beta a(x,\xi)|\leq C_{\alpha,\beta,U,N}\hbar^N\langle\xi\rangle^{-N}\quad\text{ for all }(x,\mathsf{RC}(\xi))\in U. \tag{A.6}$$

For $\zeta_0=\mathsf{RC}(\xi_0)$ in the interior of B^d, the factor $\langle\xi\rangle^{-N}$ is moot, and the definition merely says that outside its semiclassical operator wavefront set an operator is the quantization of a symbol that vanishes faster than any algebraic power of $\hbar$; see [70, Page 194], [22, Definition E.27]. For $\zeta_0\in\partial B^d=S^{d-1}$, by contrast, the definition says that the symbol decays rapidly in a conic neighborhood of the direction ζ_0, in addition to decaying in $\hbar$.

Properties of the semiclassical operator wavefront set that we use in §5.3 and §5.4 are

$$\mathrm{WF}_\hbar A=\emptyset\quad\text{ if and only if }\quad A=O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}, \tag{A.7}$$

(see [22, E.2.3]),

$$\mathrm{WF}_\hbar(AB)\subset\mathrm{WF}_\hbar A\cap\mathrm{WF}_\hbar B, \tag{A.8}$$

(see [70, §8.4], [22, E.2.5]),

$$\mathrm{WF}_\hbar(A)\cap\mathrm{WF}_\hbar(B)=\emptyset\quad\text{ implies that }\quad AB=O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}, \tag{A.9}$$

(as a consequence of (A.7) and (A.8)), and

$$\mathrm{WF}_\hbar\big(\mathrm{Op}_\hbar(a)\big)\subset\operatorname{supp}a \tag{A.10}$$

(since $(\operatorname{supp}a)^c\subset(\mathrm{WF}_\hbar(\mathrm{Op}_\hbar(a)))^c$ by (A.6)).

Ellipticity. We say that $B\in\Psi^m_\hbar$ is *elliptic* at $(x_0,\zeta_0)\in\overline{T}^*\mathbb{T}^d_{R_\sharp}$ if there exists a neighborhood U of (x_0,ζ_0) and $c>0$, independent of $\hbar$, such that

$$\langle\xi\rangle^{-m}\big|\sigma_\hbar(B)(x,\xi)\big|\geq c\quad\text{ for all }(x,\mathsf{RC}(\xi))\in U\text{ and for all }0<\hbar\leq\hbar_0.$$

A key feature of elliptic operators is that they are microlocally invertible; this is reflected in the following result.

Theorem A.2 (Elliptic parametrix [22, Proposition E.32]) [4] *Let $A\in\Psi^\ell_\hbar(\mathbb{T}^d_{R_\sharp})$ and $B\in\Psi^m_\hbar(\mathbb{T}^d_{R_\sharp})$ be such that B is elliptic on $\mathrm{WF}_\hbar(A)$. Then there exist $S,S'\in\Psi^{\ell-m}_\hbar(\mathbb{T}^d_{R_\sharp})$ such that*

$$A=BS+O(\hbar^\infty)_{\Psi_\hbar^{-\infty}}=S'B+O(\hbar^\infty)_{\Psi_\hbar^{-\infty}},$$

with $\mathrm{WF}_\hbar S\subset\mathrm{WF}_\hbar A$ and $\mathrm{WF}_\hbar S'\subset\mathrm{WF}_\hbar A$.

Functional Calculus. The main properties of the functional calculus in the black-box context are recalled in §3.4; here we record a simple result that we need about functions of the flat Laplacian.

For f a Borel function, the operator $f(-\hbar^2\Delta)$ is defined on smooth functions on the torus (and indeed on distributions if f has polynomial growth) by the functional calculus for the flat Laplacian, i.e., by the Fourier multiplier

$$f(-\hbar^2\Delta)v=\sum_{j\in\mathbb{Z}^d}\widehat{v}(j)f(\hbar^2|j|^2\pi^2/R_\sharp^2)e_j. \tag{A.11}$$

The following lemma shows that $f(-\hbar^2\Delta)$ is precisely the quantization of $f(|\xi|^2)$; since our quantization procedure was defined in terms of Fourier transform rather than Fourier series, this is not obvious a priori.

Lemma A.3 ([29, Lemma A.3]) *For $f\in S^m(\mathbb{R}^1)$ (i.e., f is a function of only one variable), $f(-\hbar^2\Delta)=\mathrm{Op}_\hbar f(|\xi|^2)$.*

[4] We highlight that working in a compact manifold allows us to dispense with the proper-support assumption appearing in [43, §4], [22, Proposition E.32, Theorem E.33].

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