Decompositions of high-frequency Helmholtz solutions via functional calculus, and application to the finite element method

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Abstract

Over the last ten years, results from [48], [49], [22], and [47] decomposing high-frequency Helmholtz solutions into "low"- and "high"-frequency components have had a large impact in the numerical analysis of the Helmholtz equation. These results have been proved for the constant-coefficient Helmholtz equation in either the exterior of a Dirichlet obstacle or an interior domain with an impedance boundary condition.

Using the Helffer–Sjöstrand functional calculus [33], this paper proves analogous decompositions for scattering problems fitting into the black-box scattering framework of Sjöstrand–Zworski [63], thus covering Helmholtz problems with variable coefficients, impenetrable obstacles, and penetrable obstacles all at once.

These results allow us to prove new frequency-explicit convergence results for (i) the *hp*-finite-element method (*hp*-FEM) applied to the variable-coefficient Helmholtz equation in the exterior of an analytic Dirichlet obstacle, where the coefficients are analytic in a neighbourhood of the obstacle, and (ii) the *h*-FEM applied to the Helmholtz penetrable-obstacle transmission problem. In particular, the result in (i) shows that the *hp*-FEM applied to this problem does not suffer from the pollution effect.

1 Introduction

1.1 Context: the results of [48], [49], [22], [47] and their impact on numerical analysis of the Helmholtz equation.

At the heart of the papers [48], [49], [22], and [47] are results that decompose solutions of the high-frequency Helmholtz equation, i.e.,

$$\Delta u + k^2 u = -f \tag{1.1}$$

with k large, into

(i) a component with H^2 regularity, satisfying bounds with improved k-dependence compared to those satisfied by the full Helmholtz solution, and

(ii) an analytic component, satisfying bounds with the same k-dependence as those satisfied by the full Helmholtz solution,

with these components corresponding to the "high"- and "low"-frequency components of the solution. In the rest of this paper, we write this decomposition as $u = u_{H^2} + u_{\mathcal{A}}$.

Such a decomposition was obtained for

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- the Helmholtz equation (1.1) posed in $\mathbb{R}^d$, $d = 2,3$, with compactly-supported f, and with the Sommerfeld radiation condition

$$\frac{\partial u}{\partial r}(x) - \mathrm{i}ku(x) = o\left(\frac{1}{r^{(d-1)/2}}\right) \tag{1.2}$$

as $r := |x| \to \infty$, uniformly in $\widehat{x} := x/r$ [48, Lemma 3.5],

- the Helmholtz exterior Dirichlet problem where the obstacle has analytic boundary [49, Theorem 4.20], and

- the Helmholtz interior impedance problem where the domain is either analytic ($d = 2,3$) [49, Theorem 4.10], [47, Theorem 4.5], or polygonal [49, Theorem 4.10], [22, Theorem 3.2],

in all cases under an assumption that the solution operator grows at most polynomially in k (which has recently been shown to hold, for most frequencies, for a variety of scattering problems in [38]).

These decompositions have had a large impact in the numerical analysis of the Helmholtz equation in that they allow one to prove convergence, explicit in the frequency k, of so-called *hp*-finite-element methods (*hp*-FEM) applied to discretisations of the Helmholtz equation. Recall that the *hp*-FEM approximates solutions of PDEs by piecewise polynomials of degree p on a mesh with meshwidth h and obtains convergence by both decreasing h and increasing p; this is in contrast to the h-FEM where p is fixed and only h decreases.

Indeed, these decompositions were used to prove frequency-explicit convergence of a variety of *hp* methods in [48, 49, 22, 47, 72, 71, 19, 5]. These results about *hp* methods are particularly significant, since they show that, if h and p are chosen appropriately, the FEM solution is uniformly accurate as $k \to \infty$ with the total number of degrees of freedom proportional to k^d; i.e., the *hp*-FEM does not suffer from the so-called pollution effect (i.e. the total number of degrees of freedom needing to be $\gg k^d$) which plagues the h-FEM [2].

These decompositions were also used to prove sharp results about the convergence of h methods with large but fixed p [23], [18], [39]. Furthermore, analogous decompositions and analogous convergence results were obtained for *hp*-boundary-element methods [46], [43], *hp* methods applied to Helmholtz problems with arbitrarily-small dissipation [51] and *hp* methods applied to formulations of the time-harmonic Maxwell equations [50], [54]. This work has also motivated attempts to provide simpler decompositions valid for a variety of variable-coefficient problems [13].

The recent paper [40] obtained the analogous decomposition to that in [48] for the Helmholtz problem in $\mathbb{R}^d$ but now for the variable-coefficient Helmholtz equation

$$\nabla \cdot (A\nabla u) + \frac{k^2}{c^2}u = -f \tag{1.3}$$

with A and $c \in C^\infty$. The goal of the present paper is to obtain decompositions for more-general Helmholtz problems.

1.2 Informal statement of the main results

We show a decomposition of the form $u = u_{H^2} + u_{\mathcal{A}}$ for the solutions of the following three Helmholtz problems.

(P1) The C^∞-variable-coefficient Helmholtz exterior Dirichlet problem where the obstacle has analytic boundary and the coefficients are analytic near the obstacle. The corresponding result, discussed in §1.3 below, is stated as Theorem B, and applied to prove quasi-optimality of the *hp*-FEM in Theorem B1. In particular, Theorem B1 shows that the *hp*-FEM applied to this Helmholtz problem does not suffer from the pollution effect.

(P2) The transmission problem with finite regularity of the interface and the coefficients - that is, the problem of scattering by a penetrable obstacle. This result is discussed in §1.4, where it is stated as Theorem C, and applied to prove quasi-optimality of the h-FEM in Theorem C1.

(P3) The C^∞-variable-coefficient Helmholtz equation in the full space $\mathbb{R}^d$; this situation was studied in [40] and we recover the results of [40] with the more general method presented here; see §1.5 and Theorem D. In §1.6 we discuss the ideas behind both [40] and the present method, and the relationship between them.

We highlight that, just as in the earlier works [48], [49], [22], and [47], u_{H^2} and $u_{\mathcal{A}}$ correspond to "high" and "low" frequencies of the solution, respectively – this is discussed further in the informal discussion in §1.6.

The three results stated outlined above are obtained as applications of a single, more general, albeit abstract result, Theorem A below. This theorem is stated using the black-box framework of Sjöstrand–Zworski [63], and covers Helmholtz problems with variable coefficients, impenetrable obstacles, and penetrable obstacles all at once. We postpone the rigorous statement of Theorem A to §1.7 and give an informal version of it here.

Theorem A′ (Informal statement of our main general result) *Let P be a formally self-adjoint operator with $P = -\Delta$ outside $B(0, R_0)$ ("the black-box"). We assume that $P - k^2$ is well defined and that*

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

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

(H2) one has an estimate quantifying the regularity of P inside $B(0, R_0)$ (i.e., "inside the black-box").

Then, for any $R > R_0$, any solution of $(P - k^2)u = g$ splits as

$$u|_{B(0,R)} = u_{H^2} + u_{\mathcal{A}},$$

where

(i) u_{H^2} satisfies

$$\|u_{H^2}\|_{L^2} + k^{-2}\|P u_{H^2}\|_{L^2} \lesssim \|g\|_{L^2},$$

(ii) $u_{\mathcal{A}}$ 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 $u_{\mathcal{A}}$ away from "the black-box" $B(0, R_0)$ is entire (in the sense of Lemma 1.1(i) below).*

When P is the Dirichlet Laplacian, for example, $\|P u_{H^2}\|_{L^2}$ controls $\|u_{H^2}\|_{H^2}$ by elliptic regularity, and thus the bound in (i) is a bound on $\|u_{H^2}\|_{H^2}$ (hence the notation u_{H^2}).

The paper [39] shows that Assumption (H1) holds in the black-box framework for "most" frequencies (see Part (ii) of Theorem 1.5 for a more precise statement of this). The key point, therefore, to apply this result to specific situations is to check that an estimate of the type (H2) holds. In the three applications to problems (P1), (P2), and (P3) above, this estimate (H2) corresponds to, respectively, a heat-flow estimate, an elliptic estimate, and regularity of the eigenfunctions of the Laplace operator on the torus. Theorem A could be applied to a range of other specific situations, provided an estimate of type (H2) is at hand. For a reader interested in applying Theorem A without going into the details of the proof, §1.7.1 gives a short summary on how to do this.

Before stating the main result applied the problems (P1), (P2), and (P3) above, we record the following lemma about how the bound an analytic function depending on k satisfies dictate the k-dependence of the region of analyticity; we use this below to understand the properties of the $u_{\mathcal{A}}$s in (P1) and (P3).

Lemma 1.1 (k-explicit analyticity) *Let $u \in C^\infty(D)$ be a family of functions depending on k.*
(i) If there exist $C, C_u > 0$, independent of α, such that

$$\|\partial^\alpha u\|_{L^2(D)} \le C_u (Ck)^{|\alpha|} \quad \textit{for all multiindices } \alpha,$$

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

(ii) If there exist $C, C_u > 0$, independent of α, such that

$$\|\partial^\alpha u\|_{L^2(D)} \le C_u (Ck)^{|\alpha|} |\alpha|! \quad \text{for all multiindices } \alpha,$$

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

(iii) If there exist $C, C_u > 0$, independent of α, such that

$$\|\partial^\alpha u\|_{L^2(D)} \le C_u C^{|\alpha|} \max\big\{|\alpha|, k\big\}^{|\alpha|} \quad \text{for all multiindices } \alpha,$$

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

Proof. In each case, 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 Case (iii), see, e.g., [48, Proof of Lemma C.2]; the proofs for the other cases are similar. ∎

1.3 The main result applied to the exterior Dirichlet problem

1.3.1 Background definitions

Definition 1.2 (Exterior Dirichlet problem) *Let $\mathcal{O}_- \subset \mathbb{R}^d$, $d \ge 2$ be a bounded Lipschitz open set such that the open complement $\mathcal{O}_+ := \mathbb{R}^d \setminus \overline{\mathcal{O}_-}$ is connected and such that $\mathcal{O}_- \subset B_{R_0}$. Let $A \in C^{0,1}(\mathcal{O}_+, \mathbb{R}^{d\times d})$ be such that $\operatorname{supp}(I - A) \subset B_{R_1}$, with $R_1 > R_0$, A is symmetric, and there exists $A_{\min} > 0$ such that*

$$\big(A(x)\xi\big) \cdot \overline{\xi} \ge A_{\min}|\xi|^2 \quad \text{for all } x \in \mathcal{O}_+ \text{ and for all } \xi \in \mathbb{C}^d. \tag{1.4}$$

Let $c \in L^\infty(\mathcal{O}_+)$ be such that $\operatorname{supp}(1 - c) \subset B_{R_1}$, and $c_{\min} \le c \le c_{\max}$ with $c_{\min}, c_{\max} > 0$.

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

$$c^2 \nabla \cdot (A\nabla u) + k^2 u = -f \quad \text{in } \mathcal{O}_+, \tag{1.5}$$

$$u = 0 \quad \text{on } \partial\mathcal{O}_+, \tag{1.6}$$

and u satisfies the Sommerfeld radiation condition (1.2).

We highlight from Definition 1.2 that the obstacle $\mathcal{O}_-$ is contained in B_{R_0}, and the variation of the coefficients A and c is contained inside the larger ball B_{R_1}.

We use the standard weighted H^1 norm, $\|\cdot\|_{H^1_k(B_R\cap\mathcal{O}_+)}$, defined by

$$\|u\|^2_{H^1_k(B_R\cap\mathcal{O}_+)} := \|\nabla u\|^2_{L^2(B_R\cap\mathcal{O}_+)} + k^2 \|u\|^2_{L^2(B_R\cap\mathcal{O}_+)}. \tag{1.7}$$

Definition 1.3 ($C_{\rm sol}$) *Given $f \in L^2(\mathcal{O}_+)$ supported in B_R with $R \ge R_1$, let u be the solution of the exterior Dirichlet problem of Definition 1.2. Given $k_0 > 0$, let $C_{\rm sol} = C_{\rm sol}(k, A, c, R, k_0) > 0$ be such that*

$$\|u\|_{H^1_k(B_R\cap\mathcal{O}_+)} \le C_{\rm sol} \|f\|_{L^2(B_R\cap\mathcal{O}_+)} \quad \text{for all } k > 0. \tag{1.8}$$

$C_{\rm sol}$ exists by standard results about uniqueness of the exterior Dirichlet problem and Fredholm theory; see, e.g., [30, §1] and the references therein. How $C_{\rm sol}$ depends on k is crucial to our analysis, and to emphasise this we write $C_{\rm sol} = C_{\rm sol}(k)$. A key assumption in our analysis is that $C_{\rm sol}(k)$ is polynomially bounded in k in the following sense.

Definition 1.4 ($C_{\rm sol}$ is polynomially bounded in k) *Given k_0 and $K \subset [k_0, \infty)$, $C_{\rm sol}(k)$ is polynomially bounded for $k \in K$ if there exists $C > 0$ and $M > 0$ such that*

$$C_{\rm sol}(k) \le Ck^M \text{ for all } k \in K, \tag{1.9}$$

where C and M are independent of k (but depend on k_0 and possibly also on K, A, c, d, R).

There exist C^∞ coefficients A and c such that $C_{\rm sol}(k_j) \geq C_1 \exp(C_2 k_j)$ for $0 < k_1 < k_2 < \ldots$ with $k_j \to \infty$ as $j \to \infty$, see [56], but this exponential growth is the worst-possible, since $C_{\rm sol}(k) \leq c_3 \exp(c_4 k)$ for all $k \geq k_0$ by [6, Theorem 2]. We now recall results on when $C_{\rm sol}(k)$ is polynomially bounded in k.

Theorem 1.5 (Conditions under which $C_{\rm sol}(k)$ is polynomially bounded in k for the exterior Dirichlet problem)
(i) If A and c are C^∞ and nontrapping (i.e. all the trajectories of the generalised bicharacteristic flow defined by the semiclassical principal symbol of (1.5) starting in B_R leave B_R after a uniform time), then $C_{\rm sol}(k)$ is independent of k for all sufficiently large k; i.e., (1.9) holds for all $k \geq k_0$ with $M = 0$.

(ii) If A is $C^{0,1}$ and $c \in L^\infty$ then, given $k_0 > 0$ and $\delta > 0$ there exists a set $J \subset [k_0, \infty)$ with $|J| \leq \delta$ such that

$$C_{\rm sol}(k) \leq C k^{5d/2+1+\varepsilon} \quad \text{for all } k \in [k_0, \infty) \setminus J,$$

for any $\varepsilon > 0$, where C depends on $\delta, \varepsilon, d, k_0$, and A. If both $\mathcal{O}_-$ and A are $C^{1,\sigma}$ for some $\sigma > 0$ then the exponent is reduced to $5d/2 + \varepsilon$.

References for the proof. (i) follows from *either* the results of [52] combined with either [68, Theorem 3]/ [69, Chapter 10, Theorem 2] or [41], *or* [7, Theorem 1.3 and §3]. It has recently been proved that, for this situation, $C_{\rm sol}$ is proportional to the length of the longest trajectory in B_R; see [26, Theorems 1 and 2, and Equation 6.32]. (ii) is proved for $c = 1$ in [38, Theorem 1.1 and Corollary 3.6]; the proof for more-general c follows from Lemma 2.3 below. ∎

1.3.2 Theorem A applied to the exterior Dirichlet problem

Theorem B (Theorem A applied to the exterior Dirichlet problem with analytic $\mathcal{O}_-$ and locally analytic A, c) *Suppose that $\mathcal{O}_-, A, c, R_0$, and R_1 are as in Definition 1.2. In addition, assume that $\mathcal{O}_-$ is analytic, and that A and c are C^∞ everywhere and analytic in B_{R_*} for some $R_0 < R_* < R_1$.*

If $C_{\rm sol}(k)$ is polynomially bounded for $k \in K$ (in the sense of Definition 1.4), then given $f \in L^2(\mathcal{O}_+)$ supported in B_R with $R \geq R_1$, the solution u of the exterior Dirichlet problem is such that there exists $u_{\mathcal{A}} \in C^\infty(B_R \cap \mathcal{O}_+)$, and $u_{H^2} \in H^2(B_R \cap \mathcal{O}_+)$, both with zero Dirichlet trace on $\partial\mathcal{O}_+$, such that

$$u|_{B_R} = u_{\mathcal{A}} + u_{H^2}.$$

Furthermore, there exists C_1, independent of k and α, such that

$$\|\partial^\alpha u_{H^2}\|_{L^2(B_R \cap \mathcal{O}_+)} \leq C_1 k^{|\alpha|-2} \|f\|_{L^2(B_R \cap \mathcal{O}_+)} \quad \text{for all } k \in K \text{ and for all } |\alpha| \leq 2, \tag{1.10}$$

and there exist C_2, C_3, C_4 and C_5, all independent of k and α, and $R_{\rm I}, R_{\rm II}, R_{\rm III}, R_{\rm IV}$ with $R_0 < R_{\rm I} < R_{\rm II} < R_{\rm III} < R_{\rm IV} < R$ such that $u_{\mathcal{A}}$ decomposes as $u_{\mathcal{A}} = u_{\mathcal{A}}^{R_0} + u_{\mathcal{A}}^\infty$, where $u_{\mathcal{A}}^{R_0}$ is analytic in $B_{R_{\rm IV}}$ and has zero Dirichlet trace on $\partial\mathcal{O}_+$, and $u_{\mathcal{A}}^\infty$ is analytic in $(B_{R_{\rm I}})^c$ with, for all $k \in K$ and all α,

$$\|\partial^\alpha u_{\mathcal{A}}^{R_0}\|_{L^2(B_{R_{\rm IV}} \cap \mathcal{O}_+)} \leq C_2 (C_3)^{|\alpha|} \max\left\{|\alpha|^{|\alpha|}, k^{|\alpha|}\right\} k^{-1+M} \|f\|_{L^2(B_R \cap \mathcal{O}_+)}, \tag{1.11}$$

$$\|\partial^\alpha u_{\mathcal{A}}^\infty\|_{L^2((B_{R_{\rm I}})^c \cap \mathcal{O}_+)} \leq C_4 (C_5)^{|\alpha|} k^{|\alpha|-1+M} \|f\|_{L^2(B_R \cap \mathcal{O}_+)}, \tag{1.12}$$

and, for any $N, m > 0$ there exists $C_{N,m} > 0$ so that

$$\|u_{\mathcal{A}}^\infty\|_{H^m(B_{R_{\rm II}} \cap \mathcal{O}_+)} + \|u_{\mathcal{A}}^{R_0}\|_{H^m((B_{R_{\rm III}})^c \cap \mathcal{O}_+)} \leq C_{N,m} k^{-N} \|f\|_{L^2(B_R \cap \mathcal{O}_+)} \text{ for all } k \in K. \tag{1.13}$$

By Parts (iv) and (i) of Lemma 1.1, $u_{\mathcal{A}}^{R_0}$ is analytic in $B_{R_{\rm IV}}$ with k-independent radius of convergence, and $u_{\mathcal{A}}^\infty$ is entire in $(B_{R_{\rm I}})^c$; see Figure 1.1.

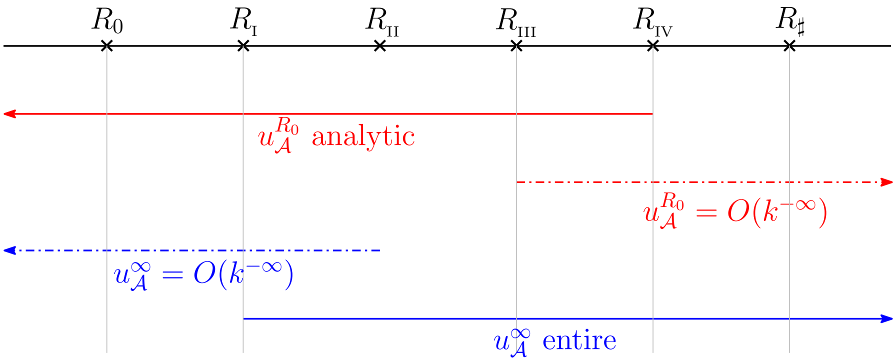

Figure 1.1: The regions where $u_{\mathcal{A}}^{R_0}$ and $u_{\mathcal{A}}^{\infty}$ appearing in Theorem B are analytic, entire, or $O(k^{-\infty})$.

1.3.3 Corollary about frequency-explicit convergence of the *hp*-FEM

As discussed in §1.1, Theorem B implies a frequency-explicit convergence result about the *hp*-FEM applied to the exterior Dirichlet problem; we now give the necessary definitions to state this result. Recall that the FEM is based on the standard variational formulation of the exterior Dirichlet problem: Let

$$H^1_{0,\partial\mathcal{O}_+}(B_R\cap\mathcal{O}_+) := \Big\{ v \in H^1(B_R\cap\mathcal{O}_+) \text{ with } v=0 \text{ on } \partial\mathcal{O}_+\Big\}.$$

Given $R \geq R_1$ and $F \in (H^1_{0,\partial\mathcal{O}_+}(B_R\cap\mathcal{O}_+))^*$,

$$\text{find } u \in H^1_{0,\partial\mathcal{O}_+}(B_R\cap\mathcal{O}_+) \text{ such that } \ a(u,v) = F(v) \ \text{ for all } v \in H^1_{0,\partial\mathcal{O}_+}(B_R\cap\mathcal{O}_+), \tag{1.14}$$

where

$$a(u,v) := \int_{B_R\cap\mathcal{O}_+}\left((A\nabla u)\cdot\overline{\nabla v} - \frac{k^2}{c^2}u\overline{v}\right) - \big\langle \mathrm{DtN}_k(u), v\big\rangle_{\partial B_R}, \tag{1.15}$$

where $\langle\cdot,\cdot\rangle_{\partial B_R}$ denotes the duality pairing on ∂B_R that is linear in the first argument and antilinear in the second, and $\mathrm{DtN}_k : H^{1/2}(\partial B_R) \to H^{-1/2}(\partial B_R)$ is the Dirichlet-to-Neumann map for the equation $\Delta u + k^2 u = 0$ posed in the exterior of B_R with the Sommerfeld radiation condition (1.2); the definition of DtN_k in terms of Hankel functions and polar coordinates (when $d=2$)/spherical polar coordinates (when $d=3$) is given in, e.g., [48, Equations 3.7 and 3.10]. We use later the fact that there exist $C_{\mathrm{DtN}} = C_{\mathrm{DtN}}(k_0R_0)$ such that

$$\big|\big\langle \mathrm{DtN}_k(u), v\rangle_{\partial B_R}\big\rangle\big| \leq C_{\mathrm{DtN}}\, \|u\|_{H^1_k(B_R\cap\mathcal{O}_+)}\, \|v\|_{H^1_k(B_R\cap\mathcal{O}_+)} \tag{1.16}$$

for all $u,v \in H^1_{0,\partial\mathcal{O}_+}(B_R\cap\mathcal{O}_+)$ and for all $k \geq k_0$; see [48, Lemma 3.3].

If $F(v) = \int_{B_R\cap\mathcal{O}_+} fv$, then the solution of the variational problem (1.14) is the restriction to B_R of the solution of the exterior Dirichlet problem of Definition 1.2. If

$$F(v) = \int_{\partial B_R}\big(\partial_n u^I - \mathrm{DtN}_k(u^I)\big)\overline{v}, \tag{1.17}$$

where u^I is a solution of $\Delta u^I + k^2 u^I = 0$ in $B_R\cap\mathcal{O}_+$, then the solution of the variational problem (1.14) is the restriction to $B_R\cap\mathcal{O}_+$ of the sound-soft scattering problem (see, e.g, [9, Page 107]).

Given a sequence, $\{V_N\}_{N=0}^{\infty}$, of finite-dimensional subspaces of $H^1_{0,\partial\mathcal{O}_+}(B_R\cap\mathcal{O}_+)$, the finite-element method for the variational problem (1.14) is the Galerkin method applied to the variational problem (1.14), i.e.,

$$\text{find } u_N \in V_N \text{ such that } \ a(u_N,v_N) = F(v_N) \ \text{ for all } v_N \in V_N. \tag{1.18}$$

Theorem B1 (Quasioptimality of hp-FEM for the exterior Dirichlet problem) *Let $d = 2$ or 3. Suppose that $\mathcal{O}_-, A, c, R, R_{\rm I}$, and $R_{\rm IV}$ are as in Theorem B. Let $(V_N)_{N=0}^\infty$ be the piecewise-polynomial approximation spaces described in [48, §5], [49, §5.1.1] (where, in particular, the triangulations are quasi-uniform, allow curved elements, and thus fit $B_R \cap \mathcal{O}_+$ exactly). Let u_N be the Galerkin solution defined by (1.18).*

If $C_{\rm sol}(k)$ is polynomially bounded (in the sense of Definition 1.4) for $k \in K \subset [k_0, \infty)$ then there exist $k_1, C_1, C_2 > 0$, depending on A, c, R, and d, but independent of k, h, and p, such that if

$$\frac{hk}{p} \leq C_1 \quad \text{and} \quad p \geq C_2 \log k, \tag{1.19}$$

then, for all $k \in K \cap [k_1, \infty)$, the Galerkin solution exists, is unique, and satisfies the quasioptimal error bound

$$\|u - u_N\|_{H^1_k(B_R\cap\mathcal{O}_+)} \leq C_{\rm qo} \min_{v_N\in V_N} \|u - v_N\|_{H^1_k(B_R\cap\mathcal{O}_+)}, \tag{1.20}$$

with

$$C_{\rm qo} := \frac{2\big(\max\{A_{\max}, c_{\min}^{-2}\} + C_{\rm DtN}\big)}{A_{\min}}. \tag{1.21}$$

Remark 1.6 (The significance of Theorem B1: the hp-FEM does not suffer from the pollution effect) *For finite-dimensional subspaces consisting of piecewise polynomials of degree p on meshes with meshwidth h, the total number of degrees of freedom $\sim (p/h)^d$. Therefore Theorem B1, as well as the results in [48], [49], [22], [47], [40], show that there is a choice of h and p such that the hp-FEM is quasioptimal with the total number of degrees of freedom $\sim k^d$. As highlighted in §1.1, the significance of this is that when the total number of degrees of freedom $\sim k^d$ the h-FEM (i.e., with p fixed) does not satisfy the quasioptimal error estimate (1.20) with $C_{\rm qo}$ independent of k; this is called the* pollution effect *– see [2] and the references therein.*

The results in [48], [49], [22], [47] are for constant-coefficient Helmholtz problems, and those in [40] are for the Helmholtz equation with smooth variable coefficients and no obstacle. Theorem B1 is therefore the first result showing that the hp-FEM applied the Helmholtz exterior Dirichlet problem with variable coefficients does not suffer from the pollution effect.

In the specific case of the plane-wave scattering problem, the recent results of [39, Theorem 9.1 and Remark 9.10] allow us to bound the best approximation error on the right-hand side of (1.20) and obtain a bound on the relative error.

Corollary 1.7 (Bound on the relative error of the Galerkin solution) *Let the assumptions of Theorem B1 hold and, furthermore, let $F(v)$ be given by (1.17) with $u^I(x) = \exp(ikx\cdot a)$ for some $a \in \mathbb{R}^d$ with $|a| = 1$ (so that u is then the solution of the plane-wave scattering problem). Suppose $C_{\rm sol}(k)$ is polynomially bounded (in the sense of Definition 1.4) for $k \in K \subset [k_0, \infty)$. Then there exists $C_3 > 0$, independent of k, h, and p, such that, with k_1, C_1, and C_2 as in Theorem B1, if $hk/p \leq C_1$ and $p \geq C_2 \log k$ then, for all $k \in K \cap [k_1, \infty)$,*

$$\frac{\|u - u_N\|_{H^1_k(B_R\cap\mathcal{O}_+)}}{\|u\|_{H^1_k(B_R\cap\mathcal{O}_+)}} \leq C_{\rm qo} C_3 \frac{hk}{p}\left(1 + \frac{hk}{p}\right), \tag{1.22}$$

with $C_{\rm qo}$ given by (1.21); i.e. the relative error can be made arbitrarily small by making hk/p smaller.

1.4 The main result applied to the transmission problem

1.4.1 Background definitions

Definition 1.8 (Transmission problem (i.e. scattering by a penetrable obstacle)) *Let $\mathcal{O}_- \subset \mathbb{R}^d$, $d \geq 2$ be a bounded Lipschitz open set such that the open complement $\mathcal{O}_+ := \mathbb{R}^d \setminus \overline{\mathcal{O}_-}$ is connected and such that $\mathcal{O}_- \subset B_{R_0}$. Let $A = (A_-, A_+)$ with $A_\pm \in C^{0,1}(\mathcal{O}_\pm, \mathbb{R}^{n\times n})$ be such that $\operatorname{supp}(I - A) \subset B_{R_0}$, A is symmetric, and there exists $A_{\min} > 0$ such that (1.4) holds (with $\mathcal{O}_+$ replaced by $\mathbb{R}^d$). Let $c \in L^\infty(\mathcal{O}_-)$ be such that $c_{\min} \leq c \leq c_{\max}$ with $0 < c_{\min} \leq c_{\max} < \infty$. Let $\beta > 0$.*

Let ν be the unit normal vector field on $\partial\mathcal{O}_-$ pointing from $\mathcal{O}_-$ into $\mathcal{O}_+$, and let $\partial_{\nu,A}$ denote the corresponding conormal derivative defined by, e.g., [44, Lemma 4.3] (recall that this is such that, when $v \in H^2(\mathcal{O}_+)$, $\partial_{\nu,A} v = \nu \cdot \gamma(A\nabla v)$).

Given $f \in L^2(\mathcal{O}_+)$ with $\operatorname{supp} f \Subset \mathbb{R}^d$ and $k > 0$, $u = (u_-, u_+) \in H^1_{\rm loc}(\mathbb{R}^d)$ satisfies the transmission problem if

$$\begin{aligned} c^2\nabla\cdot(A_-\nabla u_-) + k^2 u_- &= -f \qquad \text{in } \mathcal{O}_-, \\ \nabla\cdot(A_+\nabla u_+) + k^2 u_+ &= -f \qquad \text{in } \mathcal{O}_+, \\ u_- = u_+, \quad \partial_{\nu,A_-} u_- &= \beta\partial_{\nu,A_+} u_+ \qquad \text{on } \partial\mathcal{O}_-, \end{aligned} \tag{1.23}$$

and u_+ satisfies the Sommerfeld radiation condition (1.2).

When A_-, A_+, and c are constant, two of the four parameters A_-, A_+, c, and β are redundant. For example, by rescaling u_-, u_+, and f, all such transmission problems can be described by the parameters c and β (with $A_- = A_+ = 1$), as in, e.g., [8], or by the parameters A_- and c (with $A_+ = \beta = 1$); see, e.g., the discussion and examples after [53, Definition 2.3].

The definition of $C_{\rm sol}$ for the transmission problem is almost identical to Definition 1.3, except that the norms in (1.8) are now over B_R (as opposed to $B_R \cap \mathcal{O}_+$) and now $C_{\rm sol}$ depends additionally on β

Theorem 1.9 (Conditions under which $C_{\rm sol}(k)$ is polynomially bounded in k for the transmission problem) *In each of the following conditions we assume that $\mathcal{O}_-$, A, and c are as in Definition 1.8.*

(i) If $\mathcal{O}_-$ is smooth and strictly convex with strictly positive curvature, $A = I$, c is a constant ≥ 1, and $\beta > 0$, then $C_{\rm sol}(k)$ is independent of k for all sufficiently large k; i.e., (1.8) holds for all $k \geq k_0$ with $M = 0$

(ii) If $\mathcal{O}_-$ is Lipschitz and star-shaped, $A = I$, and c is a constant with

$$\frac{1}{c^2} \leq \frac{1}{\beta} \leq 1$$

then $C_{\rm sol}(k)$ is independent of k for all sufficiently large k.

(iii) If $\mathcal{O}_-$ is star-shaped, $\beta = 1$, and both A and c are monotonically non-increasing in the radial direction (in the sense of [30, Condition 2.6]) then $C_{\rm sol}(k)$ is independent of k for all sufficiently large k.

(iv) Under no additional assumptions on $\mathcal{O}_-$, A, and c, given $k_0 > 0$ and $\delta > 0$ there exists a set $J \subset [k_0, \infty)$ with $|J| \leq \delta$ such that

$$C_{\rm sol}(k) \leq C k^{5d/2+1+\varepsilon} \qquad \text{for all } k \in [k_0,\infty) \setminus J,$$

for any $\varepsilon > 0$, where C depends on $\delta, \varepsilon, d, k_0, A, c$, and β.

References for the proof. (i) is proved in [8, Theorem 1.1] (we note that, in fact, a stronger result with A_- variable is also proved there). (ii) is proved in [53, Theorem 3.1]. (iii) is proved in [30, Theorem 2.7]. (iv) is proved for constant c and globally Lipschitz A in [38, Theorem 1.1 and Corollary 3.6]; the proof for these more-general c and A follows from Lemma 2.3 below. ■

1.4.2 Theorem A applied to the transmission problem

Theorem C (Theorem A applied to the transmission problem) *Suppose that $\mathcal{O}_-$, A, c, and β, are as in Definition 1.8 and, additionally, A and c are $C^{2m-2,1}$ and $\mathcal{O}_-$ is $C^{2m-1,1}$ for some integer $m \geq 1$.*

If $C_{\rm sol}(k)$ is polynomially bounded for $k \in K$ (in the sense of Definition 1.4), then given $f \in L^2(\mathbb{R}^d)$ supported in B_R with $R \geq R_0$, the solution u of the transmission problem is such that there exists $u_{\mathcal{A}} = (u_{+,\mathcal{A}}, u_{-,\mathcal{A}}) \in C^\infty(B_R \cap \mathcal{O}_+) \times C^\infty(\mathcal{O}_-)$ and $u_{H^2} = (u_{+,H^2}, u_{-,H^2}) \in H^2(B_R \cap \mathcal{O}_+) \times H^2(\mathcal{O}_-)$, satisfying (1.23), and such that

$$u|_{B_R} = u_{\mathcal{A}} + u_{H^2}.$$

Furthermore there exist $C_1, C_2 > 0$, independent of k but with $C_2 = C_2(m)$, such that

$$\|\partial^\alpha u_{\pm,H^2}\|_{L^2(B_R\cap\mathcal{O}_\pm)} \leq C_1 k^{|\alpha|-2}\|f\|_{L^2(B_R)} \quad \text{for all } k\in K \text{ and for all } |\alpha|\leq 2, \tag{1.24}$$

and

$$\|\partial^\alpha u_{\pm,\mathcal{A}}\|_{L^2(B_R\cap\mathcal{O}_\pm)} \leq C_2(m) k^{|\alpha|-1+M}\|f\|_{L^2(B_R)} \quad \text{for all } k\in K \text{ and for all } |\alpha|\leq 2m. \tag{1.25}$$

1.4.3 Corollary about frequency-explicit convergence of the h-FEM

For simplicity we consider the case where the parameter β in the transmission condition (1.23) equals one; recall from the comments below Definition 1.8 that, at least in the constant-coefficient case, this is without loss of generality. The variational formulation of the transmission problem is then (1.14) with $B_R \cap \mathcal{O}_+$ replaced by B_R and $a(\cdot,\cdot)$ given by (1.15) with c understood as equal to one in $B_R \cap \mathcal{O}_+$

Since the constant C_2 in (1.25) depends on m, we cannot prove a result about the hp-FEM for the transmission problem of Definition 1.8. We therefore consider the h-FEM and prove the first sharp quasioptimality result for this problem (see Remark 1.11 below for more discussion on the novelty of our result).

Assumption 1.10 *$(V_N)_{N=0}^\infty$ is a sequence of piecewise-polynomial approximation spaces on quasi-uniform meshes with mesh diameter h and polynomial degree p. Furthermore, (i) the mesh consists of curved elements that exactly triangulate B_R and $\mathcal{O}_-$, so that each element in the mesh is included in either $\mathcal{O}_-$ or $B_R\cap\mathcal{O}_+$, and (ii) there exists an interpolant operator $I_{h,p}$ such that for all $0\leq j\leq \ell\leq p$, there exists $C(j,\ell,d)>0$ such that*

$$\big|v - I_{h,p}v\big|_{H^j(B_R)} \leq C(j,\ell,d)\, h^{\ell+1-j}\Big(\|v_+\|_{H^{\ell+1}(B_R\cap\mathcal{O}_+)} + \|v_-\|_{H^{\ell+1}(\mathcal{O}_-)}\Big) \tag{1.26}$$

for all $v=(v_+,v_-)\in H^{\ell+1}(B_R\cap\mathcal{O}_+)\times H^{\ell+1}(\mathcal{O}_-)$.

Assumption 1.10 is satisfied by the hp approximation spaces described in [48, §5], [49, §5.1.1] (with (1.26) holding by [48, Theorem B.4], and also by curved Lagrange finite-element spaces in [4] (with (1.26) holding by [4, Theorem 4.1 and Corollary 4.1]).

Theorem C1 (Quasioptimality of h-FEM for the transmission problem) *Let $d=2$ or 3. Suppose that $\beta=1$, A, c, and $\mathcal{O}_-$ are as in Definition 1.8. Given an integer p, if p is odd assume that $\mathcal{O}_-$ is $C^{p,1}$ and both A and c are $C^{p-1,1}$; if p is even, assume that $\mathcal{O}_-$ is $C^{p+1,1}$ and both A and c are $C^{p,1}$.*

Let $(V_N)_{N=0}^\infty$ be a sequence of piecewise-polynomial approximation spaces of degree p satisfying Assumption 1.10 and let u_N be the Galerkin solution defined by (1.18).

If $C_{\rm sol}(k)$ is polynomially bounded (in the sense of Definition 1.4) for $k\in K\subset[k_0,\infty)$ then there exists $C>0$, depending on A, c, R, d, k_0, and p, but independent of k and h, such that if

$$h^p k^{p+1+M} \leq C$$

then, for all $k\in K$, the Galerkin solution exists, is unique, and satisfies the quasioptimal error bound

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

with $C_{\rm qo}$ given by (1.21).

The regularity assumptions in Theorem C1 are optimal with p is odd, but suboptimal when p is even. This is due to Theorem C controlling Sobolev norms of even order of the solution, which is ultimately due to our using powers of the operator (which is of order two) to obtain regularity of the solution (see (4.14) in the proof of Theorem C). For example, when $p=2$ we require $u\in H^3$ in Theorem C1, but we achieve this by requiring that $\mathcal{O}_-$, A, and c are such that $u\in H^4$.

Remark 1.11 (The significance of Theorem C1) *The fact that "$h^p k^{p+1}$ sufficiently small" is a sufficient condition for quasioptimality of the Helmholtz h-FEM in nontrapping situations (i.e. $M = 0$) was proved for a variety of Helmholtz problems for $p = 1$ in [45, Prop. 8.2.7], [31, Theorem 4.5], [26, Theorem 3] (building on the 1-d results of [1, Theorem 3.2], [36, Theorem 3], [35, Theorem 4.13], and [37, Theorem 3.5]) and for $p > 1$ in [48, Corollary 5.6], [49, Remark 5.9], [27, Theorem 5.1], and [13, Theorem 2.15]. Numerical experiments indicate that this condition is also necessary – see, e.g., [13, §4.4].*

Of these existing results, only [13, Theorem 2.15] covers the Helmholtz equation with variable A and c that are also allowed to be discontinuous. However, the results in [13] hold only when an impedance boundary condition is imposed on the truncation boundary (in our case ∂B_R), which is equivalent to approximating the exterior Helmholtz Dirichlet-to-Neumann map by ik. *Furthermore, the proof of [13, Theorem 2.15] uses the impedance boundary condition in an essential way. Indeed, in [13, Proof of Lemma 2.13] the solution is expanded in powers of k, i.e. $u = \sum_{j=0}^{\infty} k^j u_j$, and then on ∂B_R one has $\partial_n u_{j+1} = \mathrm{i} u_j$; this relationship between u_{j+1} and u_j on ∂B_R no longer holds if DtN_k is not approximated by* ik.

The Helmholtz equation with an impedance boundary condition is often used as a model problem for numerical analysis (see, e.g., the references in [25, §1.8]). However, it has recently been shown that, in the limit $k \to \infty$ with the truncation boundary fixed, the error incurred in approximating the Dirichlet-to-Neumann map with ik *is bounded away from zero, independently of k, even in the best-possible situation when the truncation boundary equals ∂B_R for some R; see [25, §1.2]. Therefore, even if one solves the problem truncated with an impedance boundary condition with a high-order method (i.e., p large), the solution of the truncated problem will not be a good approximation to the true scattering problem when k is large.*

1.5 The main result applied to the Helmholtz equation in $\mathbb{R}^d$ with C^∞ coefficients

Theorem A can also be used to recover the main result of [40], namely [40, Theorem 3.1].

Theorem D (The main result of [40] as a corollary of Theorem A) *Assume that $\mathcal{O}_- = \emptyset$ and that A, c are as in Definition 1.2 and are furthermore C^∞. If $C_{\rm sol}(k)$ is polynomially bounded (in the sense of Definition 1.4), then, given $f \in L^2(B_R)$, the solution u of the Helmholtz problem* (1.5), (1.2) *is such that there exists $u_{\mathcal{A}}$, analytic in B_R, and $u_{H^2} \in H^2(B_R)$, such that*

$$u|_{B_R} = u_{\mathcal{A}} + u_{H^2}.$$

Furthermore, there exist C_1, C_2 and C_3, all independent of k and α, such that

$$\|\partial^\alpha u_{H^2}\|_{L^2(B_R)} \leq C_1 k^{|\alpha|-2} \|f\|_{L^2(B_R)} \quad \text{for all } k \in K \text{ and for all } |\alpha| \leq 2, \tag{1.27}$$

and

$$\|\partial^\alpha u_{\mathcal{A}}\|_{L^2(B_R)} \leq C_2 (C_3)^{|\alpha|} k^{|\alpha|-1+M} \|f\|_{L^2(B_R)} \quad \text{for all } k \in K \text{ and for all } \alpha. \tag{1.28}$$

Observe that, by Part (i) of Lemma 1.1, $u_{\mathcal{A}}$ is entire. The decomposition in Theorem D can be used to show that the hp-FEM applied to the Helmholtz equation in $\mathbb{R}^d$ with C^∞ coefficients is quasioptimal (with constant independent of k) if the conditions (1.19) hold; see [40, Theorem 3.4].

1.6 Informal discussion of the ideas behind Theorem A

It is instructive to first recall the ideas behind the results of [48, 49, 22, 47].

How the results of [48, 49, 22, 47] were obtained. The paper [48] considered the Helmholtz equation (1.1) posed in $\mathbb{R}^d$ with the Sommerfeld radiation condition (1.2). The decomposition $u = u_{H^2} + u_{\mathcal{A}}$ was obtained by decomposing the data f in (1.1) into "high-" and "low-" frequency components, with u_{H^2} the Helmholtz solution for the high-frequency component of f, and $u_{\mathcal{A}}$ then the Helmholtz solution for the low-frequency component of f. The frequency cut-offs were defining using the indicator function

$$1_{B_{\lambda k}}(\zeta) := \begin{cases} 1 & \text{for } |\zeta| \leq \lambda\, k, \\ 0 & \text{for } |\zeta| \geq \lambda\, k, \end{cases} \tag{1.29}$$

with λ a free parameter (see [48, Equation 3.31] and the surrounding text). In [48] the frequency cut-off (1.29) was then used with (a) the expression for u as a convolution of the fundamental solution and the data f, and (b) the fact that the fundamental solution is known explicitly for the PDE (1.1) to obtain the appropriate bounds on $u_{\mathcal{A}}$ and u_{H^2} using explicit calculation (involving Bessel and Hankel functions). The decompositions in [49, 22, 47] for the exterior Dirichlet problem and interior impedance problem were obtained using the results of [48] combined with extension operators (to go from problems with boundaries to problems on $\mathbb{R}^d$).

Because the proof technique in [48] does not generalise to the variable-coefficient Helmholtz equation (1.3), until the recent paper [40] there did not exist in the literature analogous decomposition results for the variable-coefficient Helmholtz equation. This was despite the increasing interest in the numerical analysis of (1.3) see, e.g., [11, 3, 13, 28, 55, 31, 26, 39, 29].

The recent results of [40]: the decomposition for the variable-coefficient Helmholtz equation in free space. The paper [40] obtained the analogous decomposition to that in [48] for the Helmholtz problem in $\mathbb{R}^d$ but now for the variable-coefficient Helmholtz equation (1.3) with A and $c \in C^\infty$. This result was obtained again using frequency cut-offs (as in [48]) but now applying them to the solution u as opposed to the data f. Any cut-off function that is zero for $|\zeta| \geq Ck$ is a cutoff to a compactly-supported set in phase space, and hence enjoys analytic estimates. The main difficulty in [40], therefore, was in showing that the high-frequency component u_{H^2} satisfies a bound with one power of k improvement over the bound satisfied by u. This was achieved by choosing the cut-off so that the (scaled) Helmholtz operator $k^{-2}\nabla \cdot (A\nabla) + c^{-2}$ is *semiclassically elliptic* on the support of the high-frequency cut-off. Then, choosing the cut-off function to be smooth (as opposed to discontinuous, as in (1.29)) allowed [40] to use basic facts about the "nice" behaviour of elliptic semiclassical pseudodifferential operators (namely, they are invertible up to a small error) to prove the required bound on u_{H^2}. The expository paper [65] shows that, when $A = I$ and $c = 1$, the arguments in [40] involving pseudodifferential operators reduce to using the Fourier transform, and in this case a frequency cut-off of the form (1.29) can be used.

The frequency decomposition achieved in Theorem A. In this paper, we achieve the desired decomposition into low- and high-frequency pieces in the manner best adapted to the functional analysis of the Helmholtz equation: by using the functional calculus for the Helmholtz operator itself. Recall that once we realise the operator

$$P = -c^2 \nabla \cdot (A\nabla) \tag{1.30}$$

with appropriate domain as a self-adjoint operator (on a space weighted by c^{-2}), the functional calculus for self-adjoint operators allows us to define $\phi(P)$ for a broad class of functions g. In particular, given $k > 0$, we take ϕ a cutoff function on $\mathbb{R}^d$ equal to 1 on $B(0, \mu k)$ for some $\mu > 1$. Then, for fixed k, $(1 - \phi)(P)$ is a high-frequency cutoff and $\phi(P)$ a low-frequency cutoff. We emphasise that working with functions of the operator can be thought of as just the classic idea of using expansions in terms of eigenfunctions of the differential operator. Indeed, in the special case $A = I, c = 1$, these frequency cut-offs are simply Fourier multipliers of the type used in [38].

The novelty of the approach used here is to make the functional calculus approach work in the much more general setting of *semiclassical black-box scattering* introduced by Sjöstrand-Zworski [63], which allows us to treat variable (possibly rough) media, impenetrable obstacles, and penetrable obstacles all at once. We rescale, setting $\hbar = k^{-1}$, and study operators $P_\hbar$ equal to a variable-coefficient Laplacian outside the "black-box" B_{R_0}, and equal to $-\hbar^2\Delta$ outside a larger ball B_{R_1}. We are now interested in functions of $P_\hbar$ of the form $\psi(P_\hbar)$ with $\psi = 1$ in $B(0, \mu)$ and 0 in $(B(0, 2\mu))^c$. After multiplying the solution u by a cut-off function φ that equals one near the black box (since u is only locally L^2), we split

$$\varphi u = \Pi_{\mathrm{High}}(\varphi u) + \Pi_{\mathrm{Low}}(\varphi u)$$

with

$$\Pi_{\text{Low}} \equiv \psi(P_\hbar), \quad \Pi_{\text{High}} \equiv (1-\psi)(P_\hbar),$$

and both pieces again defined by the spectral theorem. We now discuss the two pieces separately.

We wish to analyze $\Pi_{\text{High}}\varphi u$ by using the semiclassical ellipticity of $P_\hbar - 1$ on its support in phase space. The latter notion would be well-defined if Π_{High} were globally a pseudodifferential operator. In the broad context of the black-box theory, though, while the function $\psi(P_\hbar)$ is well-defined as an abstract operator on a Hilbert space, its *structure* is much less manifest than it would be for the flat Laplacian in Euclidean space. Not much can be said in any generality about Π_{High} on the black-box, but this is unnecessary in any event: we use an abstract ellipticity argument based on the Borel functional calculus, with the ellipticity in question now amounting to the bounded invertibility of $P_\hbar - 1$ on the range of Π_{High}, which just follows from the boundedness of the function $(\lambda-1)^{-1}(1-\psi(\lambda))$. However, we do additionally need to understand the commutator of Π_{High} with the localiser φ. Fortunately, we are able to use the Helffer–Sjöstrand approach to the functional calculus [33] to describe this commutator explicitly. The method of [33] is a powerful tool for obtaining the structure theorem that a decently-behaved function of a self-adjoint elliptic differential operator is, as one might hope, in fact a pseudodifferential operator [17, Chapter 8] (a result originally due to Strichartz [67] in the setting of the homogeneous pseudodifferential calculus and Helffer–Robert [32] in the semiclassical setting used here). Additionally, Davies [15] later pointed out that in fact the same method affords a novel proof of the functional calculus formulation of the spectral theorem itself. Here, we use some refinements of Sjöstrand [62] to learn that *away* from the black-box we can in fact treat Π_{High} as a pseudodifferential operator (see Lemma 2.8), and hence deal with $[\Pi_{\text{High}}, \varphi]$ as an element of the pseudodifferential calculus, solving it away by once again using ellipticity (this time in the context of pseudodifferential operators) together with our polynomial resolvent estimate.

While the analysis of $\Pi_{\text{High}}\varphi u$ is insensitive to the contents of the black-box, our study of the low-frequency piece $\Pi_{\text{Low}}\varphi u$ necessarily entails "opening" the black-box and studying the local question of elliptic or parabolic estimates within it. Intuitively the compact support in the spectral parameter of the spectral measure of P applied to $\Pi_{\text{Low}}\varphi u$ should imply that strong elliptic estimates hold, but knowing Cauchy-type estimates on high derivatives is dependent on analyticity of the underlying problem. We therefore make the abstract regularity hypothesis (1.34) locally near the black-box, which allows us to estimate the part of $\Pi_{\text{Low}} u$ spatially localised near its content. The remaining part living in $\mathbb{R}^d$ is then given, thanks to Sjöstrand [62] again, by a Fourier multiplier up to negligible terms, and hence enjoys the analytic estimate (1.41) thanks to the properties of the Fourier transform, as used in [40].

If, for instance, P is given by (1.30) exterior to a C^∞ obstacle with Dirichlet boundary condition, we know by the functional calculus that $P^m\Pi_{\text{Low}}\varphi u$ is bounded for all $m \in \mathbb{N}$. This yields elliptic estimates which allow us to estimate all derivatives of $\Pi_{\text{Low}}\varphi u$ up to the obstacle, but the resulting estimates on $\partial^\alpha \Pi_{\text{Low}} u$ grow non-optimally in α; see Corollary 4.2 and Theorem C. Such estimates, which indeed are the only ones we have been able to obtain in the case of penetrable obstacles, suffice for applications to the h-FEM but are far from optimal in dealing with hp-FEM. In the boundary case we therefore use a stronger property of $\Pi_{\text{Low}}\varphi u$: we can run the *backward heat equation* on $\Pi_{\text{Low}}\varphi u$ for as long as we like and obtain L^2 estimates on the result. If the boundary is analytic then known heat kernel estimates (see [21]) yield satisfactory Cauchy-type estimates on $\partial^\alpha \Pi_{\text{Low}}\varphi u$; see Corollary 4.1 and Theorem B.

1.7 Statement of the main result in the black-box setting

The following theorem (Theorem A) obtains the decomposition $u = u_{H^2} + u_{\mathcal{A}}$ in the framework of black-box scattering introduced by Sjöstrand–Zworski in [63]. In this framework, the operator $P_\hbar$, where $\hbar := k^{-1}$ is the semiclassical parameter [1] , is a variable-coefficient Helmholtz operator outside B_{R_0} (the ball of radius R_0 and centre zero) for some $R_0 > 0$, but is not specified inside this ball (i.e., inside the "black box"). In particular, this framework includes the Helmholtz exterior Dirichlet and transmission problems, and Theorems B and C above are Theorem A is specialised to those settings.

[1]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 §1.1 and used in Theorems B1 and C1.

The theorem is stated using notation from the black-box framework, recapped in §2. The only non-standard concept we use is that of a *black-box differentiation operator*, which is a family of operators agreeing with differentiation outside the black-box (see Definition 2.2 below).

To understand the statement of the following theorem, the reader not familiar with black box scattering should read it with the following identifications, which always hold away from the black box, and, with suitable interpretation, continue to hold inside it in the examples considered below: the Hilbert space $\mathcal{H}$ is L^2, the operator $P_\hbar$ is $-\hbar^2\Delta$, and the subspace $\mathcal{D}\subset\mathcal{H}$ is the domain of $P_\hbar$. The superscript $\sharp$ denotes the corresponding object compactified onto a large reference torus $\mathbb{T}^d_{R_\sharp}:=\mathbb{R}^d\,/\,(2R_\sharp\mathbb{Z})^d$, so that $P^\sharp_\hbar$ is $-\hbar^2\Delta$, on the torus, and $\mathcal{D}^{\sharp,m}_\hbar$ the domain of $(P^\sharp_\hbar)^m$, with norms weighted in the standard way with $\hbar$ (see (A.2) below, and compare to (1.7)). Finally, the notation $\lesssim$ indicates that the omitted constant is independent of $\hbar$ and α and

$$C_0(\mathbb{R}):=\Big\{f\in C(\mathbb{R})\colon\ \lim_{\lambda\to\pm\infty}f(\lambda)=0\Big\}. \tag{1.31}$$

Theorem A (The decomposition in the black-box setting) *Let $P_\hbar$ be a semiclassical black-box operator on $\mathcal{H}$ (in the sense of Definition 2.1). Then 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 $\mathcal{D}_{\rm out}\subset\mathcal{D}_{\rm loc}$ and $M>0$ such that for any $\chi\in C^\infty_{\rm comp}(\mathbb{R}^d)$ equal to one near B_{R_0}, there exists $C>0$ such that if $v\in\mathcal{D}_{\rm out}$ is a solution to $(P_\hbar-1)v=\chi g$, then*

$$\|\chi v\|_{\mathcal{H}}\leq C\hbar^{-M-1}\|g\|_{\mathcal{H}}\quad \text{for all } \hbar\in\mathfrak{H}. \tag{1.32}$$

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

$$\mathcal{E}(P^\sharp_\hbar)=E+O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar\to\mathcal{D}^{\sharp,\infty}_\hbar}, \tag{1.33}$$

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 $(D(\alpha))_{\alpha\in\mathfrak{A}}$,

$$\|\rho D(\alpha)Ev\|_{\mathcal{H}^\sharp}\leq C_{\mathcal{E}}(\alpha,\hbar)\|v\|_{\mathcal{H}^\sharp}\quad \text{for all } v\in\mathcal{D}^{\sharp,\infty}_\hbar \text{ and } \hbar\in\mathfrak{H}, \tag{1.34}$$

for some $C_{\mathcal{E}}(\alpha,\hbar)>0$.

Given $R>0$ such that $R_0<R<R_\sharp$, if $g\in\mathcal{H}$ is compactly supported in B_R and $u\in\mathcal{D}_{\rm out}$ satisfies

$$(P_\hbar-1)u=g, \tag{1.35}$$

then there exists $u_{H^2}\in\mathcal{D}^\sharp$ and $u_{\mathcal{A}}\in\mathcal{D}^{\sharp,\infty}_\hbar$ such that

$$u|_{B_R}=\big(u_{H^2}+u_{\mathcal{A}}\big)|_{B_R}. \tag{1.36}$$

Furthermore, u_{H^2} satisfies

$$\|u_{H^2}\|_{\mathcal{H}^\sharp}+\big\|P^\sharp_\hbar u_{H^2}\big\|_{\mathcal{H}^\sharp}\lesssim\|g\|_{\mathcal{H}}\quad \text{for all } \hbar\in\mathfrak{H}, \tag{1.37}$$

and for any $\widetilde{R}>0$ with $R_0<\widetilde{R}<R_\sharp$, there exist $R_{\rm I},R_{\rm II},R_{\rm III},R_{\rm IV}$ with $R_0<R_{\rm I}<R_{\rm II}<R_{\rm III}<R_{\rm IV}<\widetilde{R}$ such that $u_{\mathcal{A}}$ decomposes as

$$u_{\mathcal{A}}=u^{R_0}_{\mathcal{A}}+u^\infty_{\mathcal{A}}, \tag{1.38}$$

where $u^{R_0}_{\mathcal{A}}\in\mathcal{D}^\sharp$ is regular near the black-box and negligible away from it, in the sense that

$$\|D(\alpha)u^{R_0}_{\mathcal{A}}\|_{\mathcal{H}^\sharp(B_{R_{\rm IV}})}\lesssim C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in[-\Lambda,\Lambda]}\big|\mathcal{E}(\lambda)^{-1}\big|\,\hbar^{-M-1}\|g\|_{\mathcal{H}}\quad \text{for all } \hbar\in\mathfrak{H} \text{ and } \alpha\in\mathfrak{A}, \tag{1.39}$$

and, for any $N,m>0$ there exists $C_{N,m}>0$ such that

$$\|u^{R_0}_{\mathcal{A}}\|_{\mathcal{D}^{\sharp,m}_\hbar((B_{R_{\rm III}})^c)}\leq C_{N,m}\hbar^N\|g\|_{\mathcal{H}}\quad \text{for all } \hbar\in\mathfrak{H} \tag{1.40}$$

and $u_{\mathcal{A}}^\infty$ is entire away from the black-box and negligible near it, in the sense that for some $\lambda > 1$

$$\|\partial^\alpha u_{\mathcal{A}}^\infty\|_{\mathcal{H}^\sharp((B_{R_{\rm I}})^c)} \lesssim \lambda^{|\alpha|}\hbar^{-|\alpha|-M-1}\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A}, \tag{1.41}$$

and, for any $N, m > 0$ there exists $C_{N,m} > 0$ such that

$$\|u_{\mathcal{A}}^\infty\|_{\mathcal{D}_\hbar^{\sharp,m}(B_{R_{\rm II}})} \le C_{N,m}\hbar^N\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H}. \tag{1.42}$$

In addition, 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 (1.33)), then the functions $u_{\mathcal{A}}, u_{\mathcal{A}}^\infty, u_{\mathcal{A}}^{R_0}, u_{H^2}$ are all independent of $\mathcal{E}$, and all the implicit constants above are independent of $\mathcal{E}$ as well.

Finally, if $\rho = 1$, the decomposition (1.36) can be constructed in such a way that instead of (1.38)–(1.42), $u_{\mathcal{A}}$ satisfies the global regularity estimate

$$\|D(\alpha)u_{\mathcal{A}}\|_{\mathcal{H}^\sharp} \lesssim C_{\mathcal{E}}(\alpha,\hbar) \sup_{\lambda\in[-\Lambda,\Lambda]} \left|\mathcal{E}(\lambda)^{-1}\right| \hbar^{-M-1}\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A}; \tag{1.43}$$

here as well, if $\mathcal{E}(P_\hbar^\sharp) = E$, then the functions $u_{\mathcal{A}}, u_{H^2}$ and all the above estimates do not depend on $\mathcal{E}$.

Point 1 in Theorem A is the assumption that the solution operator is polynomially bounded in $\hbar$. In the black-box setting, [38] 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 1.5 and Part (iv) of Theorem 1.9). 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 [66, Proposition 3] by using the Markov inequality.)

Point 2 in Theorem A is a regularity assumption that depends on the contents of the black box. We later refer to (1.34) 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 cutoff ρ in (1.34) is needed when the black box contains, e.g., an analytic obstacle and the operator inside has analytic coefficients; indeed the analyticity estimates that we use for (1.34) in this case cannot hold in the transition region outside the black box, where the coefficients cannot be analytic.

Regarding u_{H^2}: comparing (1.32) and (1.37), and recalling that in the nontrapping case (1.32) holds with $M = 0$, we see that u_{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 (i) in §1.1 of the results of [48, 49, 22, 47], and is a consequence of the semiclassical ellipticity of $P_\hbar - 1$ on high-frequencies (discussed in §1.6). The regularity of u_{H^2} depends on the domain of the operator ($u_{H^2} \in \mathcal{D}^\sharp$) but not on any other features of the black box (in particular, not on the regularity estimate (1.34)).

Regarding $u_{\mathcal{A}}$: $u_{\mathcal{A}}$ is in the domain of arbitrary powers of the operator ($u_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$) and so is smooth in an abstract sense. $u_{\mathcal{A}}$ is split further into two parts: $u_{\mathcal{A}}^{R_0}$ and $u_{\mathcal{A}}^\infty$, with $u_{\mathcal{A}}^{R_0}$ regular near the black-box and negligible away from it, and $u_{\mathcal{A}}^\infty$ entire away from the black-box and negligible near it; Figure 1.1 illustrates this set up (with "$u_{\mathcal{A}}^{R_0}$ analytic" replaced by "$u_{\mathcal{A}}^{R_0}$ regular"). Comparing (1.32) and (1.39)/(1.41), we see that, in the regions where they are not negligible, $u_{\mathcal{A}}^{R_0}$ and $u_{\mathcal{A}}^\infty$ satisfy bounds with the same $\hbar$-dependence as u, but with improved regularity. These properties are the analogue of the property (ii) in §1.1 of the results of [48], [49], [22], [47]. In particular, the regularity of $u_{\mathcal{A}}$ depends on the regularity inside the black-box (from (1.34)), and, for the exterior Dirichlet problem with analytic obstacle and coefficients analytic in a neighbourhood of the obstacle, $u_{\mathcal{A}}$ is analytic.

1.7.1 How to use Theorem A

To apply Theorem A to a scattering problem not discussed in this paper, the steps are the following.

1. Check that the problem fits in the black-box scattering framework of Sjöstrand–Zworski [63].

2. Check that a polynomial bound on the solution operator (1.32) holds.

3. Show a "low-frequency" estimate of type (1.34) for the corresponding compactified problem.

Concerning Point 1: the black-box framework is specifically designed to include most scattering problems. Examples treated in the literature include scattering by a Lipschitz Dirichlet or Neumann obstacle (Lemma 2.3, [39, §2.2]), by a Lipschitz penetrable obstacle (Lemma 2.4, [39, §2.2]), by a compactly supported potential, by elliptic compactly supported perturbations of the Laplacian, and scattering on finite volume surface (see for example [20, §4.1] for these three last problems). For problems not already covered in the literature, of the conditions in §2.1, the condition on the growth of eigenvalues for the compactified operator (BB5) will be the main non-trivial assumption to check (for examples of checking this assumption, see, e.g., §B, [39, Appendix A]).

Concerning Point 2: as mentioned below Theorem A, this assumption holds for any $M > 5d/2$ and for most frequencies by [39]. For nontrapping problems, one expects (1.32) to hold with $M = 0$ and $\mathfrak{H} = (0, h_0]$ (see, e.g., Theorem 1.5 below and the references therein).

Therefore, the key step in applying Theorem A is Point 3: show a "low-frequency" estimate of type (1.34) for the corresponding compactified problem (i.e., the same problem, but considered in a large reference torus). This estimate dictates the regularity estimate on the component $u_{\mathcal{A}}$, hence, the better the estimate, the better the decomposition. In practical applications, the operator $D(\alpha)$ in (1.34) will be nothing but differentiation $D(\alpha) := \partial^\alpha$. The two main considerations are then the following.

3-a. Understand if one needs $\rho = 1$, or ρ vanishing away from the scatterer. If one aims for an analytic-type estimate, because the problem under consideration has constant coefficients outside a compact set, it cannot typically be analytic everywhere, and one needs to take ρ vanishing away from the scatterer. For lower-regularity estimates, one can use a global estimate, i.e., with $\rho = 1$.

3-b. Choose the operator E and the function $\mathcal{E}$. In the first instance, one can ignore the flexibility given by the error term and aim for $E = \mathcal{E}(P^\sharp_\hbar)$. The function $\mathcal{E}$ is then dictated by the type of estimate used. For example:

   - $\mathcal{E}(\lambda) = \mathrm{e}^{-|\lambda|}$ corresponds to a heat-flow estimate (see the proof of Corollary 4.1),
   - $\mathcal{E}(\lambda) = \sqrt{1+\lambda^2}^{-L}$, $L \geq 1$ corresponds to an elliptic estimate (see the proof of Corollary 4.2),
   - $\mathcal{E} \in C^\infty_{\mathrm{comp}}$ with $\mathcal{E} = 1$ in $[-M, M]$ corresponds to an estimate on the eigenfunctions of the compactified operator (see the proof of Theorem D in §4.3).

   An example where the error term in $\mathcal{E}(P^\sharp_\hbar) = E + O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}$ gives more flexibility is the proof of Theorem D, where the error term is used to take advantage of the regularity of the eigenfunctions of $-\Delta$ on the torus, instead of those of the variable-coefficient operator.

   On the other hand, the fact that if $\mathcal{E}(P^\sharp_\hbar) = E$ (i.e., with no $O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}$ remainder in (1.33)) then the decomposition is independent of $\mathcal{E}$, allows us to use a *family* of $\mathcal{E}$'s in (1.33) and hence a family of estimates as (1.34). This feature allows us to tune the choice of $\mathcal{E}$, depending on $\hbar$ and α, to get the best possible estimate; this procedure is used in the proof of Theorem B using Corollary 4.1, using a heat-flow estimate with a time depending on $\hbar$ and α.

   Finally, note that Theorem A assumes that $\mathcal{E} \in C_0(\mathbb{R})$, but this is not essential. We could replace $\mathcal{E}$ with an element of C^∞_{comp} by extending the functions above smoothly from $\{\lambda \geq 0\}$ to $\{\lambda < 0\}$ and multiplying by a cut-off; this is possible since the spectrum of $P^\sharp_\hbar$ is in $[0, \infty)$.

1.8 Outline of the rest of the paper

Section 2 recalls the black-box framework and sets up the associated functional calculus. Section 3 proves Theorem A. Section 4 proves Theorems B and C (i.e., Theorem A specialised to the exterior Dirichlet and transmission problems), and Theorem D. Section 5 proves Theorems B1 and C1 (i.e., the convergence results for the hp-FEM for the exterior Dirichlet problem and the h-FEM for the transmission problem). Appendix A recalls results about semiclassical pseudodifferential operators on the torus. Appendix B proves a subsidiary result used to prove Lemma 2.4.

2 Recap of the black-box framework

2.1 Abstract framework

We now briefly recap the abstract framework of *black-box scattering* introduced in [63]; for more details, see the comprehensive presentation in [20, Chapter 4]. A brief overview of black-box scattering with an emphasis on the counting of resonances is contained in [38, §2].

We emphasise that here 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 [20, Chapter 4] (although the operator still agrees with $-\hbar^2\Delta$ outside a sufficiently large ball).

The Hilbert-space decomposition

Let $\mathcal{H}$ be an 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. 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 $C_1 > 0$

$$\sum_{|\alpha|=2} a_{\hbar,\alpha}(x)\xi^\alpha \geq C_1|\xi|^2 \quad \text{for all } x \in \mathbb{R}^d, \tag{2.1}$$

(ii) for some $R_1 > R_0$

$$\sum_{|\alpha|\leq 2} a_{\hbar,\alpha}(x)\xi^\alpha = |\xi|^2 \quad \text{for } |x| \geq R_1,$$

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

$$Q_\hbar := \sum_{|\alpha|\leq 2} a_{\hbar,\alpha}(x)(\hbar D_x)^\alpha \tag{2.2}$$

(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 (2.8) 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 [20, 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

$$\mathcal{D}_{\mathrm{loc}} := \Big\{ u \in \mathcal{H}_{R_0} \oplus L^2_{\mathrm{loc}}(\mathbb{R}^d\backslash B_{R_0}) \ : \ \text{if } \chi \in C^\infty_{\mathrm{comp}}(\mathbb{R}^d),\ \chi|_{B_{R_0}} = 1 \\ \text{then } (\mathbf{1}_{B_{R_0}} u, \chi \mathbf{1}_{\mathbb{R}^d\backslash B_{R_0}} u) \in \mathcal{D} \Big\}. \tag{2.3}$$

The reference operator $P_\hbar^\sharp$

Let $R_\sharp > R_1$, and let $\mathbb{T}^d_{R_\sharp} := \mathbb{R}^d \,/\, (2R_\sharp\mathbb{Z})^d$; we work with $[-R_\sharp, R_\sharp]^d$ as a fundamental domain for this torus. Let

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

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

$$\mathcal{D}^\sharp := \Big\{u \in \mathcal{H}^\sharp : \ \text{ if } \chi \in C^\infty_{\rm comp}(B_{R_\sharp}),\ \chi = 1 \text{ near } B_{R_0},\ \text{then } (\mathbf{1}_{B_{R_0}}u, \chi\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}}u) \in \mathcal{D}, \\ \text{and } (1-\chi)\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}}u \in H^2(\mathbb{T}^d_{R_\sharp})\Big\}, \tag{2.4}$$

and, for any χ as in (2.4) and $u \in \mathcal{D}^\sharp$,

$$P_\hbar^\sharp u := P_\hbar(\mathbf{1}_{B_{R_0}}u, \chi\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}}u) + Q_\hbar\big((1-\chi)\mathbf{1}_{\mathbb{T}^d_{R_\sharp}\backslash B_{R_0}}u\big), \tag{2.5}$$

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 an operator acting on the torus $\mathbb{T}^d_{R_\sharp}$ (see Appendix A for a review of semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_\sharp}$). We record for later the fact that (2.1), (2.2), and the uniform boundedness of $a_{\hbar,\alpha}(x)$ with respect to $\hbar$ imply that there exist $C_1, C_2 > 0$ such that

$$C_1|\xi|^2 \le q_\hbar \le C_2|\xi|^2 \quad \text{for sufficiently large } \xi. \tag{2.6}$$

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 $P_\hbar^\sharp$ 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 2.1. The resolvent $(P_\hbar^\sharp + i)^{-1}$ is compact (see [20, Lemma 4.11]), and hence the spectrum of $P_\hbar^\sharp$, denoted by $\operatorname{Sp} P_\hbar^\sharp$, is discrete (i.e., countable and with no accumulation point).

We assume that the eigenvalues of $P_\hbar^\sharp$ satisfy the *polynomial growth of eigenvalues condition*

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

for some $d^\sharp \ge d$ and $N(P_\hbar^\sharp, I)$ is the number of eigenvalues of $P_\hbar^\sharp$ 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 2.1 (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).*

We define a family of black-box differentiation operators as a family of operators agreeing with differentiation outside the black-box (note that there is no notion of derivative inside the black-box itself).

Definition 2.2 (Black-box differentiation operator) *$(D(\alpha))_{\alpha\in\mathfrak{A}}$ is a family of black-box differentiation operators on $\mathcal{D}_\hbar^{\sharp,\infty}$ (defined by (2.12) below) if $\mathfrak{A}$ is a family of d–multi-indices, and for any α and any $v \in C^\infty_{\rm comp}(\mathbb{T}^d_{R_\sharp}\backslash\overline{B_{R_0}})$,*

$$D(\alpha)v = \partial^\alpha v.$$

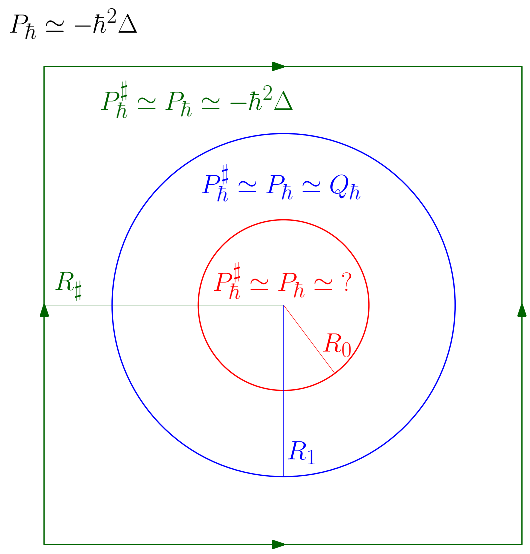

Figure 2.1: The black-box setting. The symbol $\simeq$ is used to denote equality in the sense of (BB2) and (2.5).

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 $L^2(\mathbb{T}^d_{R_\sharp})$ essentially supported outside B_{R_0},
- the elements of $L^2(\mathbb{R}^d)$ essentially 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 essentially supported in $[-R_\sharp, R_\sharp]^d \backslash B_{R_0}$.

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

$$\chi v := (\alpha \mathbf{1}_{B_{R_0}} v, \chi \mathbf{1}_{\mathbb{R}^d \backslash B_{R_0}} v) \in \mathcal{H}. \tag{2.7}$$

(for example, using this notation, the requirements on u in the definition of $\mathcal{D}^\sharp$ 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

$$v|_{B_R} := \big(\mathbf{1}_{B_{R_0}} v, (\mathbf{1}_{\mathbb{R}^d \backslash B_{R_0}} v)|_{B_R}\big) \in \mathcal{H}_{R_0} \oplus L^2(B_R \backslash B_{R_0}), \tag{2.8}$$

and, if $v \in \mathcal{H}^\sharp$,

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

Futhermore, we say that $g \in \mathcal{H}$ is compactly supported in B_R if $g = \chi_0 g$ for some $\chi_0 \in C^\infty_{\rm comp}(\mathbb{R}^d)$ equal to one near B_{R_0} and supported in B_R.

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

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

and

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

2.2 Scattering problems fitting in the black-box framework

The two following lemmas show that both scattering by Dirichlet obstacles with variable coefficients and scattering by penetrable obstacles fit in the black-box framework. For other examples of scattering problems fitting in the black-box framework, see [20, §4.1].

Lemma 2.3 (Scattering by a Dirichlet Lipschitz obstacle fits in the black-box framework) *Let $\mathcal{O}_-, A, c, R_0$, and R_1 be as in Definition 1.2. Then the family of operators*

$$P_\hbar v := -\hbar^2 c^2 \nabla \cdot \big(A\nabla v\big)$$

with the domain

$$\mathcal{D}_D := \Big\{ v \in H^1(\mathcal{O}_+),\ \nabla \cdot \big(A\nabla v\big) \in L^2(\mathcal{O}_+),\ v = 0 \text{ on } \partial\mathcal{O}_+ \Big\}$$

is a semiclassical black-box operator (in the sense of Definition 2.1) with $\omega = c^{-2}$, $Q_\hbar = -\hbar^2 c^2 \nabla \cdot (A\nabla)$, and

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

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

Proof. The non-semiclassically-scaled version of this lemma was proved for $c = 1$ in [38, Lemma 2.1]. The proof of (BB2), (BB3), and (BB4) is essentially the same in the present semiclassically-scaled setting. The bound (BB5) follows from comparing the counting function for $P^\sharp_\hbar$ to the counting function for the problem with $c = 1$ by a similar argument to [38, Lemma B.2]/Appendix B, and then using the result for the problem with $c = 1$ proven in [38, Lemma B.1]. ∎

Lemma 2.4 (Scattering by a penetrable Lipschitz obstacle fits in the black-box framework) *Let $\mathcal{O}_-, A$, c, β, and R_0 be as in Definition 1.8. Let ν be the unit normal vector field on $\partial\mathcal{O}_-$ pointing from $\mathcal{O}_-$ into $\mathcal{O}_+$, and let $\partial_{\nu,A}$ the corresponding conormal derivative from either $\mathcal{O}_-$ or $\mathcal{O}_+$. Let*

$$\mathcal{H}_{R_0} = L^2\big(\mathcal{O}_-, c(x)^{-2}\beta^{-1}\mathrm{d}x\big) \oplus L^2\big(B_{R_0}\backslash\overline{\mathcal{O}_-}\big),$$

so that

$$\mathcal{H} = L^2\big(\mathcal{O}_-; c(x)^{-2}\beta^{-1}\mathrm{d}x\big) \oplus L^2\big(B_{R_0}\backslash\overline{\mathcal{O}_-}\big) \oplus L^2\big(\mathbb{R}^d\backslash B_{R_0}\big).$$

Let

$$\begin{aligned}\mathcal{D} :=\Big\{ v = (v_1, v_2, v_3) \quad &\text{where} \quad v_1 \in H^1(\mathcal{O}_-), \quad \nabla \cdot (A_-\nabla v_1) \in L^2(\mathcal{O}_-),\\ &v_2 \in H^1\big(B_{R_0} \setminus \overline{\mathcal{O}_-}\big), \quad \nabla \cdot (A_+\nabla v_2)) \in L^2\big(B_{R_0} \setminus \overline{\mathcal{O}_-}\big),\\ &v_3 \in H^1\big(\mathbb{R}^d \setminus \overline{B_{R_0}}\big), \quad \Delta v_3 \in L^2\big(\mathbb{R}^d \setminus \overline{B_{R_0}}\big),\\ &v_1 = v_2 \quad \text{and} \quad \partial_{\nu,A_-} v_1 = \beta\, \partial_{\nu,A_+} v_2 \quad \text{on } \partial\mathcal{O}_-, \text{ and}\\ &v_2 = v_3 \quad \text{and} \quad \partial_\nu v_2 = \partial_\nu v_3 \quad \text{on } \partial B_{R_0} \qquad \Big\}\end{aligned} \tag{2.9}$$

(observe that the conditions on v_2 and v_3 on ∂B_{R_0} in the definition of $\mathcal{D}$ are such that $(v_2, v_3) \in H^1(\mathbb{R}^d \setminus \overline{\mathcal{O}_-})$ and $\nabla \cdot (A_+\nabla(v_2, v_3)) \in L^2(\mathbb{R}^d \setminus \overline{\mathcal{O}_-})$). Then the family of operators

$$P_\hbar v := -\hbar^2\Big(c^2\nabla \cdot (A_-\nabla v_1), \nabla \cdot (A_+\nabla v_2), \Delta v_3\Big),$$

defined for $v = (v_1, v_2, v_3)$, is a semiclassical black-box operator (in the sense of Definition 2.1) on $\mathcal{H}$, with $Q_\hbar = -\hbar^2\Delta$, and any $R_1 > R_0$. Furthermore, the corresponding reference operator $P^\sharp_\hbar$ satisfies (BB5) with $d^\sharp = d$.

Proof. The non-semiclassically-scaled version of this lemma was proved for $c = 1$ in [38, Lemma 2.3]. The proof of (BB2), (BB3), and (BB4) is essentially the same in the present semiclassically-scaled setting. The proof of the bound (BB5) is similar to the the analogous proof for $c = 1$ and A Lipschitz in [38, Lemma B.1]; for completeness we include the proof in §B. ∎

Remark 2.5 *Lemma 2.3 has the obstacle $\mathcal{O}_-$ in the black box (i.e., in B_{R_0}) but not all the variation of the coefficients A and c (which are contained in $B_{R_1} \supset B_{R_0}$). In contrast, Lemma 2.4 has* both *the obstacle $\mathcal{O}_-$* and *all the variation of the coefficients A and c in the black box. The transmission problem also fits in the black-box framework with some of the variation of the coefficients outside the black box (i.e., in B_{R_1}), but we do not need this formulation to prove Theorem C.*

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

The operator $P_\hbar^\sharp$ on the torus with domain $\mathcal{D}^\sharp$ is self-adjoint with compact resolvent [20, Lemma 4.11], hence we can describe the Borel functional calculus [57, 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

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

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

$$f(P_\hbar^\sharp)(v) := \sum a_j f(\lambda_j^\sharp) \phi_j^\sharp. \tag{2.10}$$

For f a bounded Borel function, $f(P^\sharp)$ 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 $(P_\hbar^\sharp)^m$ equipped with the norm

$$\|v\|_{\mathcal{D}_\hbar^{\sharp,m}} := \|v\|_{\mathcal{H}^\sharp} + \|(P_\hbar^\sharp)^m v\|_{\mathcal{H}^\sharp}, \tag{2.11}$$

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 define also the partial norms, for $k > 0$, $\|v\|_{\mathcal{D}_\hbar^{\sharp,m}(B)} := \|v\|_{\mathcal{H}^\sharp(B)} + \|(P_\hbar^\sharp)^m v\|_{\mathcal{H}^\sharp(B)}$, where $B = B_r$ or $B = B_r^c$ with $R_0 \leq r \leq R_\sharp$. In addition, we let

$$\mathcal{D}_\hbar^{\sharp,\infty} := \bigcap_{m \geq 0} \mathcal{D}_\hbar^{\sharp,m}, \tag{2.12}$$

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 [16, Pages 23 and 24]; see also [57, Theorem VIII.5].

Theorem 2.6 *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 $\|f(P_\hbar^\sharp)\|_{\mathcal{L}(\mathcal{H}^\sharp)} \leq \sup_{\lambda\in\mathbb{R}} |f(\lambda)|$.*
4. *If f has disjoint support from $\operatorname{Sp} P_\hbar^\sharp$, then $f(P_\hbar^\sharp) = 0$.*

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 [33], [16, §2.2] (which can also be used to prove the spectral theorem to begin with; see [15]).

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 $|f^{(r)}(x)| \leq C_r (1 + |x|^2)^{(\beta - r)/2}$.

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

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

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

$$f(P_\hbar^\sharp) := -\frac{1}{\pi} \int_{\mathbb{C}} \frac{\partial \widetilde{f}}{\partial \bar{z}} (P_\hbar^\sharp - z)^{-1} \, \mathrm{d}x \mathrm{d}y, \tag{2.13}$$

where $\mathrm{d}x\mathrm{d}y$ is the Lebesgue measure on $\mathbb{C}$. The integral on the right-hand side of (2.13) converges; see, e.g., [15, Lemma 1], [16, 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 [15, Theorems 2-5], [16, Lemmas 2.2.4-2.2.7].

When P is a self-adjoint elliptic semiclassical differential operator on a compact manifold, the Helffer–Sjöstrand construction can be used to show that $f(P)$ is a pseudodifferential operator [33]. Here, in the presence of a black box, it can instead be used to show that, modulo residual errors, $f(P_\hbar^\sharp)$ agrees with $f(Q_\hbar)$ on the region of the torus outside the black box, with the latter being a pseudodifferential operator. Furthermore, the operator wavefront set of $f(Q_\hbar)$ can be seen to be included in the support of $f \circ q_\hbar$. We now state these results, obtained originally in [62].

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

$$\|E_\infty\|_{\mathcal{D}_\hbar^{\sharp,-m} \to \mathcal{D}_\hbar^{\sharp,m}} \le C_{N,m} \hbar^N \tag{2.14}$$

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

Lemma 2.7 *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*

$$\psi_1 f(P_\hbar^\sharp) \psi_2 = O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty} \to \mathcal{D}_\hbar^{\sharp,\infty}}. \tag{2.15}$$

Proof. In the usual case of 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., (2.15) with $f(w) := (w - z)^{-1}$)) with (2.13) 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 following sense. 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 2.8 *Suppose $f \in C^\infty_{\mathrm{comp}}(\mathbb{R})$ is independent of $\hbar$. If $\chi \in C^\infty(\mathbb{T}^d_{R_\sharp})$ is equal to zero near B_{R_0}, then,*

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

Furthermore, $f(Q_\hbar) \in \Psi^{-\infty}(\mathbb{T}^d_{R_\sharp})$ with

$$\mathrm{WF}_\hbar \, f(Q_\hbar) \subset \operatorname{supp} f \circ q_\hbar.$$

Proof. By [62, Lemma 4.2 and the subsequent two paragraphs],

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

The results of Helffer-Robert [32] (see the account in [59]) imply that $f(Q_\hbar)$ is a pseudodifferential operator on $\mathbb{T}^d_{R_\sharp}$. It remains to show that $\mathrm{WF}_\hbar \, f(Q_\hbar) \subset \operatorname{supp} f \circ q_\hbar$. To do so, let K_ϵ be defined for $\epsilon > 0$ by

$$K_\epsilon := \Big\{ z \in T^*\mathbb{T}^d_{R_\sharp} \ : \ \operatorname{dist}(q_\hbar(z), \operatorname{supp} f) \le \epsilon \Big\}.$$

We show that $\mathrm{WF}_\hbar \, f(Q_\hbar) \subset K_\epsilon$ for any $\epsilon > 0$, from which the result follows. To do so, let $b \in C^\infty(T^*\mathbb{T}^d_{R_\sharp})$ be such that $b = 1$ on $(K_\epsilon)^c$, and $\operatorname{supp} b \subset (K_{\epsilon/2})^c$, and let $B := \mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(b)$. It suffices to show that $Bf(Q_\hbar) = O(\hbar^\infty)_{\Psi^{-\infty}}$. Indeed, if this is the case, then $\mathrm{WF}_\hbar\, Bf(Q_\hbar) = \emptyset$ by (A.7). Then, by (A.8) and (A.9), $\mathrm{WF}_\hbar\, f(Q_\hbar) \subset \mathrm{WF}_\hbar(I-B)f(Q_\hbar) \subset \mathrm{WF}_\hbar(I-B) \subset K_\epsilon$.

It therefore remains to prove that $Bf(Q_\hbar) = O(\hbar^\infty)_{\Psi^{-\infty}}$. Let $g \in C^\infty(\mathbb{R})$ be such that $g = 0$ on $\operatorname{supp} f$ and $g = 1$ on $q_\hbar((K_{\epsilon/2})^c)$; such a g exists since, by the definition of $K_{\epsilon/2}$, $\operatorname{dist}(\operatorname{supp} f, q_\hbar((K_{\epsilon/2})^c)) \geq \epsilon/2 > 0$. This definition then implies that $g \circ q_\hbar = 1$ on $(K_{\epsilon/2})^c$. By Part 1 of Theorem 2.6,

$$g(Q_\hbar)f(Q_\hbar) = (gf)(Q_\hbar) = 0. \tag{2.16}$$

By [59] again, $g(Q_\hbar)$ is a pseudodifferential operator with principal symbol $g \circ q_\hbar$, which is one on $(K_{\epsilon/2})^c$ and hence on $\mathrm{WF}_\hbar\, B$. Therefore, by the microlocal elliptic parametrix, Theorem A.2, there exists a pseudodifferential operator S such that $B = Sg(Q_\hbar) + O(\hbar^\infty)_{\Psi^{-\infty}}$. Using this and (2.16), we obtain that

$$Bf(Q_\hbar) = Sg(Q_\hbar)f(Q_\hbar) + O(\hbar^\infty)_{\Psi^{-\infty}} = O(\hbar^\infty)_{\Psi^{-\infty}},$$

and the proof is complete. ■

3 Proof of Theorem A (the main result in the black-box framework)

The decomposition (1.36) is defined in §3.1 (and illustrated schematically in Figures 3.1 and 3.3). The estimates (1.37) and (1.39)–(1.43) are proved in §3.2 and 3.3 respectively.

3.1 The decomposition

Let $\varphi \in C^\infty_{\mathrm{comp}}(\mathbb{R}^d)$ be equal to one in B_R and supported in $B_{R_\sharp}$. For $v \in \mathcal{H}$, we define

$$M_\varphi v := \varphi v,$$

where the multiplication is in the sense of (2.7). Let $u \in \mathcal{D}_{\mathrm{out}}$ be solution to

$$(P_\hbar - 1)u = g,$$

and let

$$w := M_\varphi u.$$

We view w as an element of $\mathcal{H}^\sharp$ and work in the torus $\mathbb{T}^d_{R_\sharp}$.

We now define our frequency cut-offs. By (2.1), there exists $\widetilde{\mu} > 1$ and $c_{\mathrm{ell}} > 0$ such that

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

Therefore, by (2.6), there exists $\mu > 1$ such that

$$q_\hbar(x,\xi) \geq \mu \quad \text{implies that } \langle \xi \rangle^{-2}(q_\hbar(x,\xi) - 1) \geq c_{\mathrm{ell}} > 0. \tag{3.1}$$

Let $\psi \in C^\infty_{\mathrm{comp}}(\mathbb{R})$ be such that

$$\psi = \begin{cases} 1 \text{ in } B(0,2), \\ 0 \text{ in } (B(0,4))^c. \end{cases} \tag{3.2}$$

We now fix $\frac{1}{2} \leq \mu' \leq \frac{\mu}{2}$, and define

$$\psi_\mu := \psi\left(\frac{\cdot}{\mu}\right), \qquad \psi_{\mu'} := \psi\left(\frac{\cdot}{\mu'}\right). \tag{3.3}$$

These definitions imply that

$$(1-\psi_{\mu'})(1-\psi_\mu) = (1-\psi_{\mu'}) \tag{3.4}$$

(since $4\mu' \leq 2\mu$), and

$$1 \notin \operatorname{supp}(1-\psi_{\mu'}) \tag{3.5}$$

(since $2\mu' \geq 1$). Let

$$\Lambda := 5\mu \tag{3.6}$$

(note that, by (3.1), both μ and Λ only depend on $q_\hbar$), and observe that

$$\operatorname{supp} \psi_\mu \subset [-\Lambda, \Lambda]. \tag{3.7}$$

We define, by the Borel functional calculus for $P_\hbar^\sharp$ (Theorem 2.6), in $\mathcal{L}(\mathcal{H}^\sharp)$

$$\Pi_{\text{Low}} := \psi_\mu(P_\hbar^\sharp), \tag{3.8}$$

and additionally

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

By (3.4) and the fact the Borel functional calculus is an algebra homomorphism (Part 1 of Theorem 2.6),

$$\Pi'_{\text{High}}\Pi_{\text{High}} = \Pi_{\text{High}}. \tag{3.9}$$

By Part 3 of Theorem 2.6, the operators $\Pi_{\text{Low}}, \Pi_{\text{High}}$, and Π'_{High} are bounded on $\mathcal{H}^\sharp$, with

$$\|\Pi_{\text{Low}}\|_{\mathcal{L}(\mathcal{H}^\sharp)},\ \|\Pi_{\text{High}}\|_{\mathcal{L}(\mathcal{H}^\sharp)},\ \|\Pi'_{\text{High}}\|_{\mathcal{L}(\mathcal{H}^\sharp)} \leq 1, \tag{3.10}$$

and they commute with $P_\hbar^\sharp$ by Part 1 of Theorem 2.6.

Since $u \in \mathcal{D}_{\text{loc}}$ (defined by (2.3)), the definition of $\mathcal{D}^\sharp$ (2.4), (BB2), and the fact that φ is compactly supported imply that $w \in \mathcal{D}^\sharp$. By the definition of ψ_μ (3.3), (2.10), and the fact that $\operatorname{Sp} P_\hbar^\sharp$ is discrete, $\Pi_{\text{Low}} w$ projects non-trivially only on a finite number of eigenspaces of $P_\hbar^\sharp$, and thus $\Pi_{\text{Low}} w \in \mathcal{D}_\hbar^{\sharp,\infty}$. Therefore $\Pi_{\text{High}} w = w - \Pi_{\text{Low}} w \in \mathcal{D}^\sharp$. We now define

$$u_{\text{High}} := \Pi_{\text{High}} w \in \mathcal{D}^\sharp, \quad u_{\text{Low}} := \Pi_{\text{Low}} w \in \mathcal{D}_\hbar^{\sharp,\infty}. \tag{3.11}$$

We show in §3.3 below that we can split u_{Low} as

$$u_{\text{Low}} = u_{\mathcal{A}} + u_\epsilon, \tag{3.12}$$

where $u_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ satisfies (1.38)–(1.42) (or (1.43) if $\rho = 1$), and that u_{High} and u_ϵ satisfy

$$\|u_{\text{High}}\|_{\mathcal{H}^\sharp} + \left\|P_\hbar^\sharp u_{\text{High}}\right\|_{\mathcal{H}^\sharp} \lesssim \|g\|_{\mathcal{H}}, \tag{3.13}$$

and

$$\|u_\epsilon\|_{\mathcal{H}^\sharp} + \left\|P_\hbar^\sharp u_\epsilon\right\|_{\mathcal{H}^\sharp} \lesssim \|g\|_{\mathcal{H}}, \tag{3.14}$$

and we then define

$$u_{H^2} := u_{\text{High}} + u_\epsilon$$

so that the decomposition (1.36), (1.37) and (1.38)–(1.42) (or (1.43) if $\rho = 1$) holds. Our splitting strategy is summed-up in Figure 3.1; with an overview of the splitting of the low-frequency component u_{Low} in Figure 3.3.

In §3.2 we prove the estimate (3.13) for u_{High}. In §3.3 we prove that the decomposition (3.12) holds, with $u_{\mathcal{A}}$ satisfying (1.38)–(1.42) (or (1.43) if $\rho = 1$) and u_ϵ satisfying (3.14) We highlight that all the arguments from now on consider $\hbar \in \mathfrak{H}$.

3.2 Proof of the bound (3.13) on u_{High} (the high-frequency component)

We proceed in three steps: we first use the abstract information we have about $P_\hbar^\sharp$ to bound $\Pi_{\text{High}} w$ by $\|g\|_{\mathcal{H}}$ modulo a commutator term living away from the black box B_{R_0}. We then use Lemmas 2.7 and 2.8 to show that this commutator is given, up to negligible terms, by the semiclassical pseudodifferential calculus on the torus $\mathbb{T}^d_{R_\sharp}$. Finally, we work in the torus and use the semiclassical elliptic-parametrix construction (Theorem A.2) to estimate this commutator, seen as a semiclassical pseudodifferential operator on $\mathbb{T}^d_{R_\sharp}$.

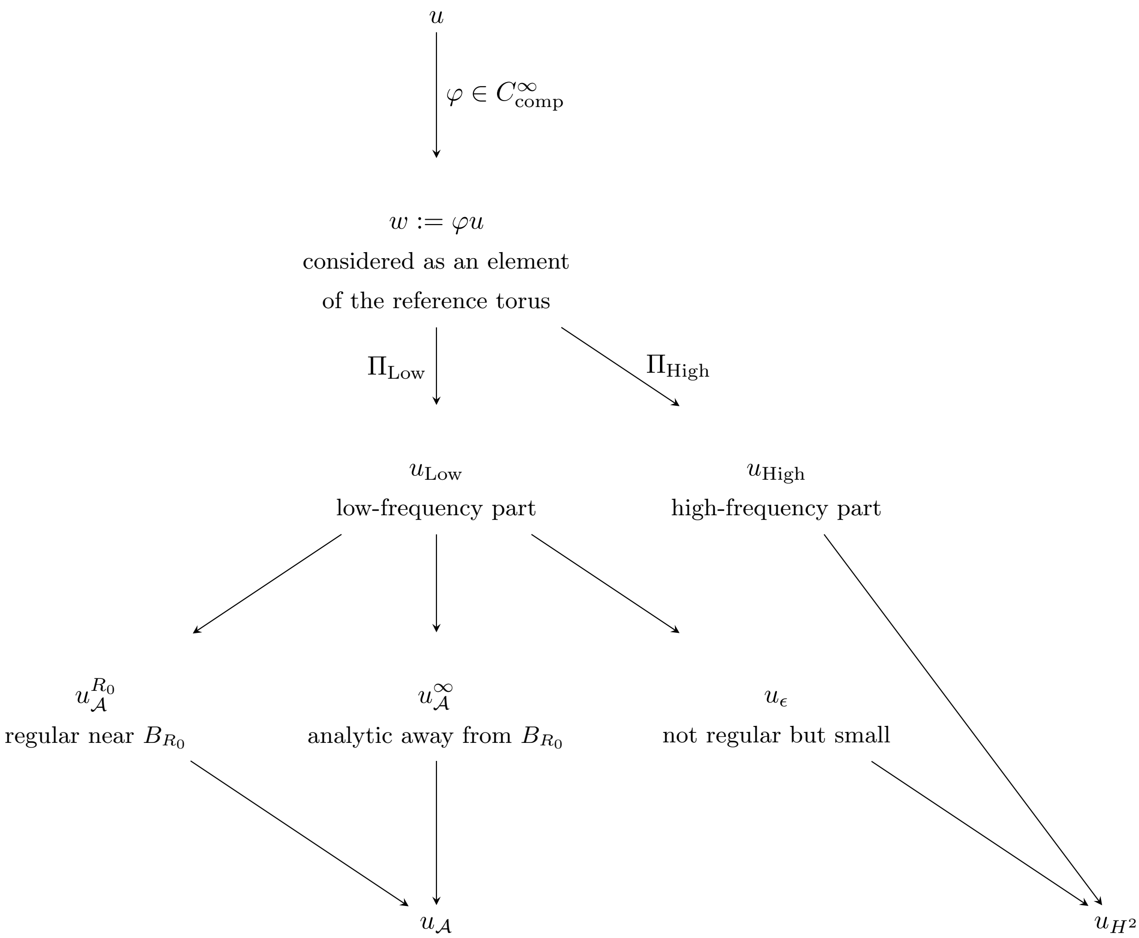

Figure 3.1: Splitting of the Helmholtz solution

Step 1: An abstract estimate in $\mathcal{H}^\sharp$

Since $\Pi_{\rm High}$ commutes with $P_\hbar^\sharp$,

$$\begin{aligned}(P_\hbar^\sharp-1)(\Pi_{\rm High}w)&=\Pi_{\rm High}(P_\hbar^\sharp-1)(w)\\&=\Pi_{\rm High}(P_\hbar-1)(w)=\Pi_{\rm High}\varphi g+\Pi_{\rm High}[P_\hbar,M_\varphi]u=\Pi_{\rm High}\varphi g+\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u,\end{aligned}\tag{3.15}$$

where we used the fact that we can replace $P_\hbar^\sharp$ by $P_\hbar$ (and vice versa) on ${\rm supp}\varphi\subset B_{R_0}$ by (BB2) and (2.5)). For $\lambda\in\mathbb{R}$, let

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

where f is in $C_0(\mathbb{R})$ by (3.5). Using (3.9), the fact that the Borel calculus in an algebra homomorphism (Part 1 of Theorem 2.6), and finally (3.15), we get

$$\Pi_{\rm High}w=\Pi'_{\rm High}\Pi_{\rm High}w=f(P_\hbar^\sharp)(P_\hbar^\sharp-1)\Pi_{\rm High}w=f(P_\hbar^\sharp)\big(\Pi_{\rm High}\varphi g+\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u\big).\tag{3.16}$$

Since f is in $C_0(\mathbb{R})$, $f(P_\hbar^\sharp)$ is uniformly bounded from $\mathcal{H}^\sharp\to\mathcal{H}^\sharp$ by Part 3 of Theorem 2.6. Combining this fact with (3.16), we obtain

$$\|\Pi_{\rm High}w\|_{\mathcal{H}^\sharp}\lesssim\|\Pi_{\rm High}\varphi g\|_{\mathcal{H}^\sharp}+\Big\|\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u\Big\|_{\mathcal{H}^\sharp}.$$

Writing $P_\hbar^\sharp\Pi_{\rm High}w=\Pi_{\rm High}w+(P_\hbar^\sharp-1)\Pi_{\rm High}w$ and using (3.15) again, we obtain

$$\|\Pi_{\rm High}w\|_{\mathcal{H}^\sharp}+\Big\|P_\hbar^\sharp\Pi_{\rm High}w\Big\|_{\mathcal{H}^\sharp}\lesssim\|\Pi_{\rm High}\varphi g\|_{\mathcal{H}^\sharp}+\Big\|\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u\Big\|_{\mathcal{H}^\sharp}.$$

Hence, by (3.10)

$$\begin{aligned}\|\Pi_{\rm High}w\|_{\mathcal{H}^\sharp}+\Big\|P_\hbar^\sharp\Pi_{\rm High}w\Big\|_{\mathcal{H}^\sharp}&\lesssim\|\varphi g\|_{\mathcal{H}^\sharp}+\Big\|\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u\Big\|_{\mathcal{H}^\sharp}\\&\lesssim\|g\|_{\mathcal{H}}+\Big\|\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u\Big\|_{\mathcal{H}^\sharp}.\end{aligned}\tag{3.17}$$

Step 2: Viewing $\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]$ as a semiclassical pseudodifferential operator on $\mathbb{T}^d_{R_\sharp}$

To prove (3.13) from (3.17), it therefore remains to bound the commutator term $\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]u$. Since $[P_\hbar^\sharp,M_\varphi]$ lives away from $\mathcal{H}_{R_0}$, we consider the high-frequency cut-off *in terms of the semiclassical pseudodifferential calculus* thanks to Lemma 2.8.

Since φ is compactly supported in $B_{R_\sharp}$ and equal to one near B_{R_0}, in $\mathcal{H}^\sharp$ we can write $[P_\hbar^\sharp,M_\varphi]$ as (using the notation in §2.1)

$$[P_\hbar^\sharp,M_\varphi]=(0,[Q_\hbar,\varphi])=(0,\phi[Q_\hbar,\varphi]\phi)=(0,[Q_\hbar,\varphi]\phi)\tag{3.18}$$

where $\phi\in C^\infty_{\rm comp}(\mathbb{R}^d)$ is supported in $B_{R_\sharp}$, equal to zero near B_{R_0}, and such that

$$\phi=1\text{ near }\operatorname{supp}\nabla\varphi.\tag{3.19}$$

Let $\chi\in C^\infty_c(\mathbb{R}^d)$ be supported in $B_{R_\sharp}$, equal to zero near B_{R_0}, and equal to one near $\operatorname{supp}\phi$. Using Lemma 2.7 (i.e., the pseudo-locality of the functional calculus) with $\psi_1=1-\chi$ and $\psi_2=\chi\varphi$, we obtain that

$$\begin{aligned}\Pi_{\rm High}[P_\hbar^\sharp,M_\varphi]&=\chi\Pi_{\rm High}\chi\phi[P_\hbar^\sharp,M_\varphi]\phi+O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}\\&=\chi\Pi_{\rm High}\chi[P_\hbar^\sharp,M_\varphi]\phi+O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}},\end{aligned}\tag{3.20}$$

where we used the last equality in (3.18) to obtain the second line. By Lemma 2.8 with $f(P_\hbar^\sharp)=\psi_\mu(P_\hbar^\sharp)=\Pi_{\rm Low}$, there exists $\Pi_{\rm Low}^\Psi\in\Psi^{-\infty}(\mathbb{T}^d_{R_\sharp})$ such that

$$\chi\Pi_{\rm Low}\chi=\chi\Pi^\Psi_{\rm Low}\chi+O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}\quad\text{ and }\quad{\rm WF}_\hbar\,\Pi^\Psi_{\rm Low}\subset\operatorname{supp}\psi_\mu\circ q_\hbar.$$

Hence, taking $\Pi^{\Psi}_{\rm High} := I - \Pi^{\Psi}_{\rm Low} \in \Psi^0_\hbar(\mathbb{T}^d_{R_\sharp})$,

$$\chi \Pi_{\rm High}\chi = \chi \Pi^{\Psi}_{\rm High}\chi + O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar} \quad \text{ and } \quad \mathrm{WF}_\hbar\, \Pi^{\Psi}_{\rm High} \subset \mathrm{supp}(1-\psi_\mu)\circ q_\hbar; \tag{3.21}$$

in other words, modulo negligible terms, $\chi\Pi_{\rm High}\chi$ is a high-frequency cut-off defined from the semiclassical pseudodifferential calculus. We here emphasise that, since χ is supported in $B_{R_\sharp}$ and vanishes near B_{R_0}, $\chi\Pi^{\Psi}_{\rm High}\chi$ can be seen *both* as an element of $\mathcal{L}(\mathcal{H}^\sharp)$ *and* of $\Psi^0_\hbar(\mathbb{T}^d_{R_\sharp})$. By (3.20) and (3.21), for any N and any m,

$$\big\|\Pi_{\rm High}[P^\sharp_\hbar, M_\varphi]u\big\|_{\mathcal{H}^\sharp} \le \big\|\chi\Pi^{\Psi}_{\rm High}\chi[P^\sharp_\hbar, M_\varphi]\phi u\big\|_{\mathcal{H}^\sharp} + C_{N,m}\hbar^N\big\|[P^\sharp_\hbar, M_\varphi]\phi u\big\|_{\mathcal{D}^{\sharp,-m}_\hbar} + C'_N\hbar^N\big\|\widetilde{\phi}u\big\|_{\mathcal{H}^\sharp},$$

with $\widetilde{\phi}$ compactly supported in $B_{R_\sharp}\backslash B_{R_0}$ and equal to one on $\mathrm{supp}\,\phi$. Taking $m = 1$, then $N = M+1$ and using the resolvent estimate (1.32) we get

$$\begin{aligned}\big\|\Pi_{\rm High}[P^\sharp_\hbar, M_\varphi]u\big\|_{\mathcal{H}^\sharp} &\le \big\|\chi\Pi^{\Psi}_{\rm High}\chi[P^\sharp_\hbar, M_\varphi]\phi u\big\|_{\mathcal{H}^\sharp} + C''_{M+1}\hbar^{M+1}\big\|\widetilde{\phi}u\big\|_{\mathcal{H}^\sharp}\\ &= \big\|\chi\Pi^{\Psi}_{\rm High}\chi[P^\sharp_\hbar, M_\varphi]\phi u\big\|_{\mathcal{H}^\sharp} + C''_{M+1}\hbar^{M+1}\big\|\widetilde{\phi}u\big\|_{\mathcal{H}}\\ &\lesssim \big\|\chi\Pi^{\Psi}_{\rm High}\chi[P^\sharp_\hbar, M_\varphi]\phi u\big\|_{\mathcal{H}^\sharp} + \big\|g\big\|_{\mathcal{H}}.\end{aligned} \tag{3.22}$$

Finally, by the definition of $P^\sharp_\hbar$ (2.5) and the fact that ϕ equals zero near B_{R_0},

$$\big\|\chi\Pi^{\Psi}_{\rm High}\chi[P^\sharp_\hbar, M_\varphi]\phi u\big\|_{\mathcal{H}^\sharp} = \big\|\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi]\phi u\big\|_{L^2(\mathbb{T}^d_{R_\sharp})},$$

hence by (3.22),

$$\big\|\Pi_{\rm High}[P^\sharp_\hbar, M_\varphi]u\big\|_{\mathcal{H}^\sharp} \lesssim \big\|\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi]\phi u\big\|_{L^2(\mathbb{T}^d_{R_\sharp})} + \|g\|_{\mathcal{H}}. \tag{3.23}$$

Step 3: A semiclassical elliptic estimate in $\mathbb{T}^d_{R_\sharp}$

Combining (3.17) and (3.23), we see that to prove (1.37) we only need to bound $\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi]\phi u$ in $L^2(\mathbb{T}^d_{R_\sharp})$. To do this, we use the semiclassical parametrix construction given by Theorem A.2.

Lemma 3.1 *The operator $Q_\hbar - 1$ is semiclassically elliptic on the semiclassical wavefront set of $\hbar^{-1}\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi]$.*

Proof. By (A.9), (A.11), (3.21) and the support properties of ψ_μ given by (3.2), (3.3),

$$\mathrm{WF}_\hbar(\hbar^{-1}\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi]) \subset \mathrm{WF}_\hbar\,\Pi^{\Psi}_{\rm High} \subset \mathrm{supp}(1-\psi_\mu)\circ q_\hbar \subset \{q_\hbar \ge \mu\}.$$

But, on $\{q_\hbar \ge \mu\}$, by definition of μ (3.1),

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

and the proof is complete. ∎

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

$$\mathrm{WF}_\hbar\, S \subset \mathrm{WF}_\hbar\left(\hbar^{-1}\Pi^{\Psi}_{\rm High}[Q_\hbar - 1, \varphi]\right), \tag{3.24}$$

and such that

$$\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi] = \hbar S(Q_\hbar - 1) + R.$$

We apply both sides of this identity to ϕu and then use (BB2) and the fact that ϕ is equal to zero near B_{R_0} and supported in $B_{R_\sharp}$; the result is that

$$\chi\Pi^{\Psi}_{\rm High}\chi[Q_\hbar - 1, \varphi]\phi u = \hbar S(Q_\hbar - 1)\phi u + R\phi u$$

$$
\begin{aligned}
&= \hbar S(P_\hbar - 1)\phi u + R\phi u \\
&= \hbar S\phi(P_\hbar - 1)u + \hbar S[P_\hbar - 1, \phi]u + R\phi u \\
&= \hbar S\phi(P_\hbar - 1)u + \hbar S[Q_\hbar - 1, \phi]u + R\phi u. \qquad (3.25)
\end{aligned}
$$

The following lemma combined with (A.10) shows that

$$
S[Q_\hbar - 1, \phi] = O(\hbar^\infty)_{\Psi^{-\infty}}. \qquad (3.26)
$$

Lemma 3.2

$$
\mathrm{WF}_\hbar\, S \cap \mathrm{WF}_\hbar[Q_\hbar - 1, \phi] = \emptyset.
$$

Proof. By (3.24) and the definition of $Q_\hbar$ (2.2),

$$
\mathrm{WF}_\hbar\, S \subset \mathrm{WF}_\hbar[Q_\hbar - 1, \varphi] \subset (\operatorname{supp} \nabla\varphi) \times \mathbb{R}^d
$$

Similarly,

$$
\mathrm{WF}_\hbar[Q_\hbar - 1, \phi] \subset (\operatorname{supp} \nabla\phi) \times \mathbb{R}^d,
$$

Now, by (3.19), $\operatorname{supp} \nabla\varphi$ and $\operatorname{supp} \nabla\phi$ are disjoint, and the result follows. ∎

Therefore, by (3.25), (3.26) and the definition of $O(\hbar^\infty)_{\Psi^{-\infty}}$ (A.4), for any N, there exists $C_N, C'_N > 0$ such that

$$
\begin{aligned}
\|\chi\Pi^\Psi_{\mathrm{High}}\chi[Q_\hbar - 1, \varphi]\phi u\|_{L^2(\mathbb{T}^d_{R_\sharp})} &\leq \hbar\|S\phi(P_\hbar - 1)u\|_{L^2(\mathbb{T}^d_{R_\sharp})} + C_N\hbar^N\|\widetilde{\phi}u\|_{L^2(\mathbb{T}^d_{R_\sharp})} + C'_N\hbar^N\|\phi u\|_{L^2(\mathbb{T}^d_{R_\sharp})} \\
&= \hbar\|S\phi(P_\hbar - 1)u\|_{L^2(\mathbb{T}^d_{R_\sharp})} + C_N\hbar^N\|\widetilde{\phi}u\|_{\mathcal{H}} + C'_N\hbar^N\|\phi u\|_{\mathcal{H}},
\end{aligned}
$$

where $\widetilde{\phi}$ is compactly supported in $B_{R_\sharp}\backslash B_{R_0}$ and equal to one on $\operatorname{supp}\phi$. Taking $N := M+1$ and using the resolvent estimate (1.32), we then obtain that

$$
\begin{aligned}
\|\chi\Pi^\Psi_{\mathrm{High}}\chi[Q_\hbar - 1, \varphi]\phi u\|_{L^2(\mathbb{T}^d_{R_\sharp})} &\lesssim \hbar\|S\phi(P_\hbar - 1)u\|_{L^2(\mathbb{T}^d_{R_\sharp})} + \hbar\|g\|_{\mathcal{H}} \\
&\lesssim \hbar\|\phi(P_\hbar - 1)u\|_{L^2(\mathbb{T}^d_{R_\sharp})} + \hbar\|g\|_{\mathcal{H}}, \qquad (3.27)
\end{aligned}
$$

where we used in the second line the fact 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. Now, since ϕ is equal to zero near B_{R_0} and supported in $B_{R_\sharp}$, we get

$$
\|\phi(P_\hbar - 1)u\|_{L^2(\mathbb{T}^d_{R_\sharp})} = \|\phi(P_\hbar - 1)u\|_{\mathcal{H}} = \|\phi g\|_{\mathcal{H}} \leq \|g\|_{\mathcal{H}}.
$$

Thus, (3.27) implies that

$$
\|\chi\Pi^\Psi_{\mathrm{High}}\chi[Q_\hbar - 1, \varphi]\phi u\|_{L^2(\mathbb{T}^d_{R_\sharp})} \lesssim \hbar\|g\|_{\mathcal{H}}.
$$

Combining this last estimate with (3.17) and (3.23) we conclude that

$$
\|\Pi_{\mathrm{High}} w\|_{\mathcal{H}^\sharp} + \left\|P^\sharp_\hbar \Pi_{\mathrm{High}} w\right\|_{\mathcal{H}^\sharp} \lesssim \|g\|_{\mathcal{H}};
$$

hence (3.13) holds.

3.3 Decomposition (3.12) of u_{Low}, and proof of the bounds (1.39)–(1.43) and (3.14) (the low-frequency component)

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

$$
\mathcal{E}(P^\sharp_\hbar) = E + E_\infty, \qquad (3.28)
$$

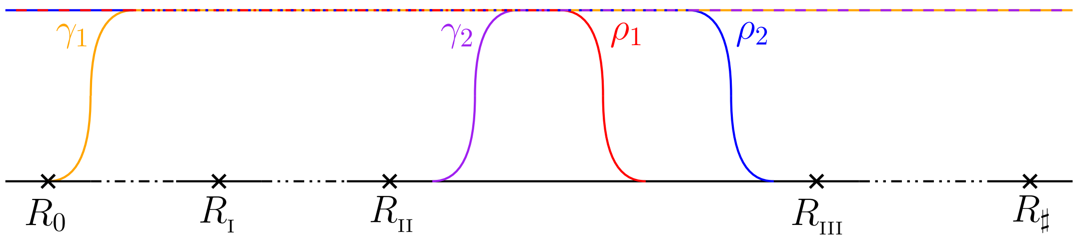

Figure 3.2: The cut-off functions $\rho_1, \rho_2, \gamma_1, \gamma_2$. ρ_1 is used in §3.3.2, ρ_2 in §3.3.3, and γ_1 and γ_2 in §3.3.4.

and the low-frequency estimate (1.34) holds. By (3.7) (a consequence of the definition of the constant Λ (3.6)), $\mathcal{E}$ is nowhere zero on the support of ψ_μ; therefore the function $\psi_\mu/\mathcal{E}$ is well-defined and in $C_0(\mathbb{R})$. The definition of $\Pi_{\rm Low}$ (3.8) and Part 1 of Theorem 2.6 imply that

$$\Pi_{\rm Low} = \psi_\mu(P_\hbar^\sharp) = \mathcal{E}(P_\hbar^\sharp)\left(\frac{1}{\mathcal{E}}\psi_\mu\right)(P_\hbar^\sharp) = E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right) + E_\infty \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right). \tag{3.29}$$

Then, by Part 3 of Theorem 2.6 and the fact that $E_\infty = O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}$,

$$E_\infty \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right) = O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}. \tag{3.30}$$

3.3.1 The decomposition (3.12) of $u_{\rm Low}$ when $\rho = 1$

We first assume that $\rho = 1$ and we show the decomposition (3.12), together with the bound (1.43) on $u_{\mathcal{A}}$ and the bound (3.14) on u_ϵ. In this case, we let

$$u_{\mathcal{A}} := E \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right) w \quad \text{and} \quad u_\epsilon := E_\infty \circ \left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right) w,$$

so that (3.12) holds by (3.28) and (3.8). Moreover, since both $u_{\mathcal{A}}$ and u_ϵ involve compactly-supported functions of $P_\hbar^\sharp$, by the reasoning immediately above (3.11), both $u_{\mathcal{A}}$ and u_ϵ are in $\mathcal{D}_\hbar^{\sharp,\infty}$. Then, using (in this order) the low-frequency estimate (1.34), Part 3 of Theorem 2.6, and finally the resolvent estimate (1.32), we get

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

thus (1.43) holds. In addition, the bound (3.14) on u_ϵ follows from (3.30) together with the resolvent estimate (1.32).

3.3.2 The decomposition (3.12) of $u_{\rm Low}$ when $\rho \neq 1$

We now tackle the general case (i.e., $\rho \neq 1$). Given R_0 and $\widetilde{R}$, let $R_{\rm I}, R_{\rm II}, R_{\rm III}, R_{\rm IV}$, be such that $R_0 < R_{\rm I} < R_{\rm II} < R_{\rm III} < R_{\rm IV} < \widetilde{R}$ and $\rho = 1$ near $B_{R_{\rm IV}}$. In addition, let $\rho_1 \in C^\infty(\mathbb{T}^d_{R_\sharp})$ be equal to one near B_{R_0} and such that $\operatorname{supp}(1-\rho_1) \subset (B_{R_{\rm II}})^c$ and $\operatorname{supp}\rho_1 \Subset B_{R_{\rm III}}$ (see Figure 3.2).

Using the decomposition (3.29) of $\Pi_{\rm Low}$, we decompose $u_{\rm Low} = \Pi_{\rm Low}w$ as

$$\begin{aligned}u_{\rm Low} &= \Pi_{\rm Low}\rho_1 w + \Pi_{\rm Low}(1-\rho_1)w\\ &= E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w + E_\infty\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w + \Pi_{\rm Low}(1-\rho_1)w,\end{aligned} \tag{3.31}$$

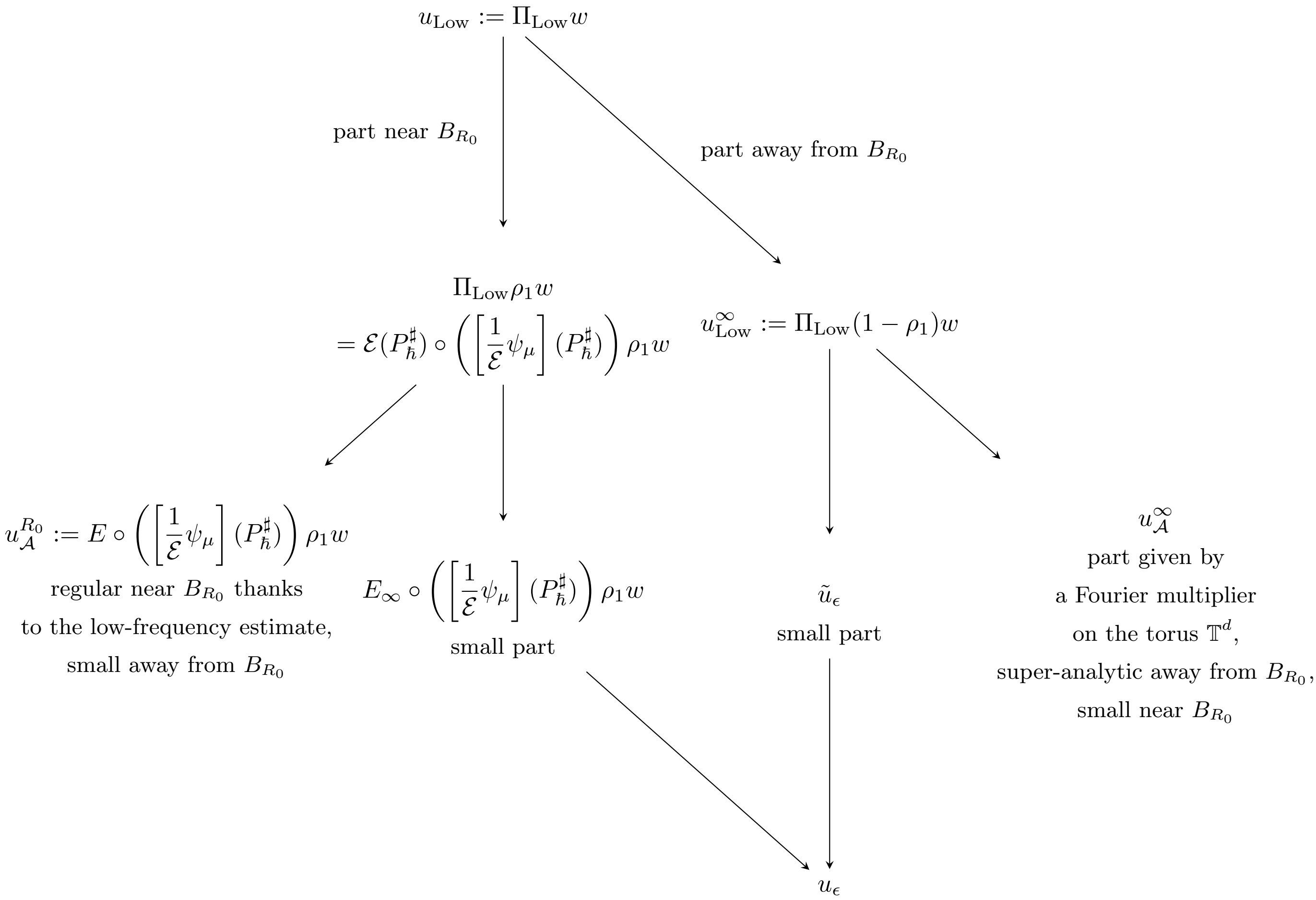

Figure 3.3: The splitting of u_{Low}

and we define

$$u_{\mathcal{A}}^{R_0} := E \circ \left(\left[\frac{1}{\mathcal{E}} \psi_\mu \right] (P_\hbar^\sharp) \right) \rho_1 w \quad \text{and} \quad u_{\mathrm{Low}}^\infty := \Pi_{\mathrm{Low}}(1-\rho_1) w. \tag{3.32}$$

We now claim that $u_{\mathcal{A}}^{R_0} \in \mathcal{D}^\sharp$; indeed, this follows from (3.31), since both Π_{Low} and $([\frac{1}{\mathcal{E}}\psi_\mu])(P_\hbar^\sharp)$ map into $\mathcal{D}^\sharp$, and $E_\infty : \mathcal{D}^\sharp \to \mathcal{D}^\sharp$ (by (2.14)).

We decompose u_{Low}^∞ in §3.3.4 below as

$$u_{\mathrm{Low}}^\infty = u_{\mathcal{A}}^\infty + \widetilde{u}_\epsilon \tag{3.33}$$

with $u_{\mathcal{A}}^\infty \in \mathcal{D}^\sharp$, (see (3.42) below) and then define

$$u_{\mathcal{A}} := u_{\mathcal{A}}^{R_0} + u_{\mathcal{A}}^\infty \in \mathcal{D}^\sharp \quad \text{and} \quad u_\epsilon := \widetilde{u}_\epsilon + E_\infty \circ \left(\left[\frac{1}{\mathcal{E}} \psi_\mu \right] (P_\hbar^\sharp) \right) \rho_1 w \tag{3.34}$$

(with the first definition implying (1.38)). These definitions imply that $u_{\mathrm{Low}} = u_{\mathcal{A}} + u_\epsilon$, i.e., that (3.12) holds. To complete the proof, we now need to show that the bounds (1.39) and (1.40) on $u_{\mathcal{A}}^{R_0}$, the bounds (1.41) and (1.42) on $u_{\mathcal{A}}^\infty$, and the bound (3.14) on u_ϵ all hold. This decomposition of u_{Low} and the ideas behind it are summed-up in Figure 3.3.

3.3.3 Proof of (1.39) and (1.40) for the localised term $u_{\mathcal{A}}^{R_0}$.

Using (in this order) the definition of $u_{\mathcal{A}}^{R_0}$ (3.32), the fact that $\rho = 1$ on $B_{R_{\rm IV}}$, the low-frequency estimate (1.34), Part 3 of Theorem 2.6, and finally the resolvent estimate (1.32) we obtain

$$\begin{aligned}\|D(\alpha)u_{\mathcal{A}}^{R_0}\|_{\mathcal{H}^\sharp(B_{R_{\rm IV}})} &= \left\|D(\alpha)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w\right\|_{\mathcal{H}^\sharp(B_{R_{\rm IV}})} \leq \left\|\rho D(\alpha)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w\right\|_{\mathcal{H}^\sharp}\\ &\leq C_{\mathcal{E}}(\alpha,\hbar)\left\|\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w\right\|_{\mathcal{H}^\sharp} \leq C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\|w\|_{\mathcal{H}^\sharp}\\ &= C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\|w\|_{\mathcal{H}} \lesssim C_{\mathcal{E}}(\alpha,\hbar)\sup_{\lambda\in\mathbb{R}}\left|\frac{1}{\mathcal{E}(\lambda)}\psi_\mu(\lambda)\right|\hbar^{-M-1}\|g\|_{\mathcal{H}};\end{aligned}$$

thus (1.39) holds, where the $\sup_{\lambda\in\mathbb{R}}$ becomes $\sup_{\lambda\in[-\Lambda,\Lambda]}$ because of the support property (3.7) of ψ_μ.

Let $\rho_2 \in C^\infty(\mathbb{T}^d_{R_\sharp})$ be supported in $B_{R_{\rm III}}$ and such that $\rho_2 = 1$ on $\operatorname{supp}\rho_1$ (see Figure 3.2). By (3.28), Part 1 of Theorem 2.6, and the pseudo-locality of the functional calculus (Lemma 2.7),

$$\begin{aligned}(1-\rho_2)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 &= (1-\rho_2)\mathcal{E}(P_\hbar^\sharp)\left(\frac{1}{\mathcal{E}}\psi_\mu\right)(P_\hbar^\sharp)\rho_1 + O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}\\ &= (1-\rho_2)\Pi_{\rm Low}\rho_1 + O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}} = O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}.\end{aligned} \tag{3.35}$$

On the other hand, since $\rho_2 = 0$ on $B^c_{R_{\rm III}}$,

$$\begin{aligned}\|u_{\mathcal{A}}^{R_0}\|_{\mathcal{D}^{m,\sharp}((B_{R_{\rm III}})^c)} &= \left\|(1-\rho_2)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w\right\|_{\mathcal{D}^{m,\sharp}((B_{R_{\rm III}})^c)}\\ &\leq \left\|(1-\rho_2)E\circ\left(\left[\frac{1}{\mathcal{E}}\psi_\mu\right](P_\hbar^\sharp)\right)\rho_1 w\right\|_{\mathcal{D}^{m,\sharp}}.\end{aligned}$$

Combining this with (3.35) and then using the resolvent estimate (1.32), we obtain (1.40).

3.3.4 The term away from the black-box $u_{\rm Low}^\infty$.

Step 1: obtaining the decomposition (3.33) and the bound (3.14) on u_ϵ. Let $\gamma_1 \in C^\infty(\mathbb{T}^d_{R_\sharp})$ be equal to zero near B_{R_0}, and such that $\gamma_1 = 1$ near $(B_{R_{\rm I}})^c$. Since $\operatorname{supp}(1-\gamma_1)$ and $\operatorname{supp}(1-\rho_1)$ are disjoint (see Figure 3.2), by the pseudo-locality of the functional calculus given by Lemma 2.7,

$$\begin{aligned}\Pi_{\rm Low}(1-\rho_1) &= \gamma_1\Pi_{\rm Low}(1-\rho_1) + O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}\\ &= \gamma_1\Pi_{\rm Low}\gamma_1(1-\rho_1) + O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}.\end{aligned}$$

Therefore, by Lemma 2.8,

$$\Pi_{\rm Low}(1-\rho_1) = \gamma_1\Pi_L^\Psi\gamma_1(1-\rho_1) + O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}, \tag{3.36}$$

where $\Pi^\Psi_{\rm Low} \in \Psi^\infty(\mathbb{T}^d_{R_\sharp})$ and

$$\operatorname{WF}_\hbar \Pi^\Psi_{\rm Low} \subset \operatorname{supp}\psi_\mu\circ q_\hbar. \tag{3.37}$$

By (2.6), since ψ_μ is compactly supported, there exists $\lambda > 1$ such that

$$\operatorname{supp}\psi_\mu\circ q_\hbar \subset \mathbb{T}^d_{R_\sharp}\times B\left(0,\frac{\lambda}{2}\right). \tag{3.38}$$

Now, let $\widetilde{\varphi} \in C^\infty_{\rm comp}$ be compactly supported in $B(0,\lambda^2)$ and equal to one on $B(0,\lambda^2/4)$. By (3.38) and (3.37) together with (A.11), $\operatorname{WF}_\hbar\left(1-\operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\right)\cap\operatorname{WF}_\hbar\left(\Pi^\Psi_{\rm Low}\right) = \emptyset$. Therefore, by (A.10), as operators on the torus,

$$\Pi^\Psi_{\rm Low} = \operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi^\Psi_{\rm Low} + E_1, \tag{3.39}$$

where $E_1 = O(\hbar^\infty)_{\Psi^{-\infty}}$. Since $\gamma_1 = 0$ near B_{R_0}, by the definitions of $P^\sharp$ (2.5), $\|\cdot\|_{\mathcal{D}^{\sharp,m}_\hbar}$ (2.11), and $\|\cdot\|_{H^{2m}_\hbar(\mathbb{T}^d_{R^\sharp})}$ (A.2),

$$\|\gamma_1 w\|_{\mathcal{D}^{\sharp,m}_\hbar} \lesssim_m \|\gamma_1 w\|_{H^{2m}_\hbar(\mathbb{T}^d_{R^\sharp})} \lesssim_m \|\gamma_1 w\|_{\mathcal{D}^{\sharp,m}_\hbar} \qquad \text{for all } w \in \mathcal{D}^{\sharp,m}_\hbar, \tag{3.40}$$

and thus $\gamma_1 E_1 \gamma_1 = O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}$. Therefore, combining this with (3.39) and (3.36), we obtain that

$$\Pi_{\rm Low}(1-\rho_1) = \gamma_1 \operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^\Psi \gamma_1(1-\rho_1) + E_2, \tag{3.41}$$

where $E_2 = O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}$. We let

$$u_{\mathcal{A}}^\infty := \gamma_1 \operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^\Psi \gamma_1(1-\rho_1)w \quad \text{ and } \quad \widetilde{u}_\epsilon := E_2 w; \tag{3.42}$$

observe that $u_{\mathcal{A}}^\infty \in \mathcal{D}^\sharp$ because of the presence of γ_1 at the start of the expression. The decomposition (3.33) then holds by (3.41) and (3.32). The bound (3.14) on u_ϵ follows directly from the definition of u_ϵ (3.34), together with (3.30), the fact that $E_2 = O(\hbar^\infty)_{\mathcal{D}^{\sharp,-\infty}_\hbar \to \mathcal{D}^{\sharp,\infty}_\hbar}$, and the resolvent estimate (1.32).

Step 2: proving that $u_{\mathcal{A}}^\infty$ is regular in $(B_{R_{\rm I}})^c$ (i.e., the bound (1.41)). By the definition of $u_{\mathcal{A}}^\infty$ (3.42) and the fact that $\gamma_1 = 1$ on $(B_{R_{\rm I}})^c$,

$$\begin{aligned}\|\partial^\alpha u_{\mathcal{A}}^\infty\|_{\mathcal{H}((B_{R_{\rm I}})^c)} &= \left\|\partial^\alpha \operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^\Psi \gamma_1(1-\rho_1)w\right\|_{\mathcal{H}((B_{R_{\rm I}})^c)} \\ &\le \left\|\partial^\alpha \operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^\Psi \gamma_1(1-\rho_1)w\right\|_{L^2(\mathbb{T}^d_{R_\sharp})}. \end{aligned}\tag{3.43}$$

We now bound the right-hand side of (3.43). By Lemma A.3, $\operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))$ is given as a Fourier multiplier on the torus (defined by (A.12)), i.e.,

$$\operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2)) = \widetilde{\varphi}(-\hbar^2\Delta). \tag{3.44}$$

Let $v \in L^2(\mathbb{T}^d_{R_\sharp})$ be arbitrary, and let $\widehat{v}(j)$ be the Fourier coefficients of v. By (A.12),

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

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

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

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

$$\begin{aligned}\|\partial^\alpha\widetilde{\varphi}(-\hbar^2\Delta)v\|^2_{L^2(\mathbb{T}^d_{R_\sharp})} &= \sum_{j\in\mathbb{Z}^d,\ |j|\le\frac{\lambda}{R_\sharp\hbar\pi}} \left|\widehat{v}(j)\widetilde{\varphi}(\hbar^2|j|^2\pi^2/R_\sharp^2)\left(\frac{\mathrm{i}\pi j}{R_\sharp}\right)^\alpha\right|^2 \\ &\le \lambda^{2|\alpha|}\hbar^{-2|\alpha|}\sum_{j\in\mathbb{Z}^d}|\widehat{v}(j)|^2 \\ &= \lambda^{2|\alpha|}\hbar^{-2|\alpha|}\|v\|^2_{L^2(\mathbb{T}^d_{R_\sharp})}.\end{aligned}\tag{3.45}$$

We now use (3.45) with

$$v := \Pi_L^{\Psi}\gamma_1(1-\rho_1)w,$$

and combine the resulting estimate with (3.43) and (3.44). Using the fact that $\Pi_L^{\Psi} \in \Psi^{\infty}(\mathbb{T}^d_{R_\sharp})$, $\gamma_1 = 0$ near B_{R_0}, and the resolvent estimate, we get

$$\begin{aligned}\|\partial^\alpha u_{\mathcal{A}}^{\infty}\|_{\mathcal{H}((B_{R_{\rm I}})^c)} &\leq \lambda^{|\alpha|}\hbar^{-|\alpha|}\|\Pi_L^{\Psi}\gamma_1(1-\rho_1)w\|_{L^2(\mathbb{T}^d_{R_\sharp})} \lesssim \lambda^{|\alpha|}\hbar^{-|\alpha|}\|\gamma_1(1-\rho_1)w\|_{L^2(\mathbb{T}^d_{R_\sharp})}\\ &= \lambda^{|\alpha|}\hbar^{-|\alpha|}\|\gamma_1(1-\rho_1)w\|_{\mathcal{H}} \leq \lambda^{|\alpha|}\hbar^{-|\alpha|}\hbar^{-M-1}\|g\|_{\mathcal{H}};\end{aligned}$$

hence (1.41) holds.

Step 3: proving that $u_{\mathcal{A}}^{\infty}$ is negligible in $B_{R_{\rm II}}$ (i.e., the bound (1.42)). It therefore remains to show (1.42). Let $\gamma_2 \in C^{\infty}(\mathbb{T}^d_{R_\sharp})$ be equal to zero on $B_{R_{\rm II}}$ and such that $\gamma_2 = 1$ on $\operatorname{supp}(1-\rho_1)$; see Figure 3.2. Since $\operatorname{supp}(1-\gamma_2)$ and $\operatorname{supp}(1-\rho_1)$ are disjoint, using (A.9) and (A.11)

$$\mathrm{WF}_\hbar\Big((1-\gamma_2)\operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^{\Psi}\Big) \cap \mathrm{WF}_\hbar(1-\rho_1) = \emptyset.$$

Then, by (A.10),

$$(1-\gamma_2)\operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^{\Psi}(1-\rho_1) = O(\hbar^\infty)_{\Psi^{-\infty}}$$

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 (3.40), we find

$$(1-\gamma_2)\gamma_1\operatorname{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\Pi_L^{\Psi}\gamma_1(1-\rho_1) = O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}} \tag{3.46}$$

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

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

Then (1.42) follows from combining this last equation with the definition of $u_{\mathcal{A}}^{\infty}$ (3.42), (3.46), and the resolvent estimate (1.32).

3.3.5 Showing that the decomposition is independent of $\mathcal{E}$ when $E_\infty = 0$.

When $E_\infty = 0$, $u_{\mathcal{A}}^{R_0} = \Pi_{\rm Low}\rho_1 w$ (by (3.31)), and $u_\epsilon = \widetilde{u}_\epsilon$ (by (3.34)); see Figure 3.3. The decomposition, and bounds thereon, is hence independent of $\mathcal{E}$.

The proof of Theorem A is now complete.

4 Proofs of Theorems B, C, and D (i.e., the application of Theorem A to the Dirichlet, transmission, and full-space problems)

Theorem D is proved by directly verifying the assumptions of Theorem A. Theorems B and C are proved using the following two corollaries of Theorem A. In the first corollary (Corollary 4.1), the low-frequency estimate (1.34) comes from a heat-flow estimate, and in the second (Corollary 4.2) from an elliptic-regularity estimate.

Corollary 4.1 *Let $P_\hbar$ be a semiclassical black-box operator on $\mathcal{H}$ satisfying the polynomial resolvent estimate (1.32) 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 2.2), 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,*

$$\left\|\rho D(\alpha)\mathrm{e}^{-tP_\hbar^\sharp}\right\|_{\mathcal{H}^\sharp\to\mathcal{H}^\sharp} \leq C(\alpha,t,\hbar) \quad \text{for all } \alpha\in\mathfrak{A},\ t\in I(\hbar,\alpha),\ \hbar\in\mathfrak{H}. \tag{4.1}$$

Then, if $R > 0$ is such that $R_0 < R < R_\sharp$, $g \in \mathcal{H}$ is compactly supported in B_R, and $u(\hbar) \in \mathcal{D}_{\rm out}$ satisfies (1.35), there exist $u_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$ and $u_{H^2} \in \mathcal{D}^\sharp$ such that u decomposes as (1.36). Furthermore, u_{H^2} satisfies (1.37) and there exists $R_{\rm I}, R_{\rm II}, R_{\rm III}, R_{\rm IV}$, and $R_\sharp$, with $R_0 < R_{\rm I} < R_{\rm II} < R_{\rm III} < R_{\rm IV} < R_\sharp$, such that $u_{\mathcal{A}}$ decomposes as $u_{\mathcal{A}} = u_{\mathcal{A}}^{R_0} + u_{\mathcal{A}}^{\infty}$ with, for some $\Lambda > 0$ and $\lambda > 1$,

$$\|D(\alpha)u_{\mathcal{A}}^{R_0}\|_{\mathcal{H}^\sharp(B_{R_{\rm IV}})} \lesssim \inf_{t\in I(\hbar,\alpha)} C(\alpha,\hbar,t)\mathrm{e}^{\Lambda t}\,\hbar^{-M-1}\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A}, \tag{4.2}$$

$$\|\partial^\alpha u_{\mathcal{A}}^{\infty}\|_{\mathcal{H}^\sharp((B_{R_{\rm I}})^c)} \lesssim \lambda^{|\alpha|}\hbar^{-|\alpha|-M-1}\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A}, \tag{4.3}$$

and, for any $N, m > 0$ there exists $C_{N,m} > 0$ such that

$$\|u_{\mathcal{A}}^{\infty}\|_{\mathcal{D}_\hbar^{\sharp,m}(B_{R_{\rm II}})} + \|u_{\mathcal{A}}^{R_0}\|_{\mathcal{D}_\hbar^{\sharp,m}((B_{R_{\rm III}})^c)} \leq C_{N,m}\hbar^N\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A}. \tag{4.4}$$

In addition, if $\rho = 1$, the decomposition (1.36) can be constructed in such a way that instead of (4.2)–(4.4), $u_{\mathcal{A}}$ satisfies the global regularity estimate

$$\|D(\alpha)u_{\mathcal{A}}\|_{\mathcal{H}^\sharp} \lesssim \inf_{t\in I(\hbar,\alpha)} C(\alpha,\hbar,t)\mathrm{e}^{\Lambda t}\,\hbar^{-M-1}\|g\|_{\mathcal{H}} \quad \text{for all } \hbar \in \mathfrak{H} \text{ and } \alpha \in \mathfrak{A}. \tag{4.5}$$

Finally, the omitted constants in (4.2), (4.3), and (4.5) are independent of $\hbar$ and α.

Proof. 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 2.6, $\mathrm{e}^{-tP_\hbar^\sharp} = \mathcal{E}_t(P_\hbar^\sharp)$. Such an $\mathcal{E}_t$ is in $C_0(\mathbb{R})$, never vanishes, and satisfies (1.34) with $E_t := \mathcal{E}_t(P_\hbar^\sharp)$ and $C_{\mathcal{E}_t}(\alpha,\hbar) := C(\alpha,\hbar,t)$ by (4.1). From Theorem A, we therefore obtain the above decomposition $u_{\mathcal{A}}, u_{\mathcal{A}}^{R_0}, u_{\mathcal{A}}^{\infty}, u_{H^2}$. Since $\mathcal{E}_t(P_\hbar^\sharp) = E_t$, by the final part of Theorem A, the decomposition is constructed independently of $\mathcal{E}_t$, and hence independently of t. The result then follows, with the infimum in t in (4.2) coming from (1.39) and the fact that this estimate in valid for any $t \in I(\hbar,\alpha)$. ■

Corollary 4.2 *Let $P_\hbar$ be a semiclassical black-box operator on $\mathcal{H}$ satisfying the polynomial resolvent estimate* (1.32) *in $\mathfrak{H} \subset (0,\hbar_0]$. Assume further that, for some α-family of black-box differentiation operators $(D(\alpha))_{\alpha\in\mathfrak{A}}$ (in the sense of Definition 2.2), there exists $L > 0$ and $0 < L(\alpha) \leq L$ such that the following elliptic-regularity estimate holds,*

$$\|D(\alpha)w\|_{\mathcal{H}^\sharp} \leq \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha,\hbar)\big\|(P_\hbar^\sharp)^\ell w\big\|_{\mathcal{H}^\sharp} \quad \text{for all } \alpha \in \mathfrak{A},\ w \in \mathcal{D}_\hbar^{\sharp,\infty},\ \text{and } \hbar \in \mathfrak{H}, \tag{4.6}$$

for some $C_\ell(\alpha,\hbar) > 0$, $\ell = 0,\ldots,L(\alpha)$.

Then, if $R_0 < R < R_\sharp$, $g \in \mathcal{H}$ is compactly supported in B_R and $u(\hbar) \in \mathcal{D}_{\rm out}$ satisfies (1.35), there exists $u_{\mathcal{A}} \in \mathcal{D}_\hbar^{\sharp,\infty}$, $u_{H^2} \in \mathcal{D}^\sharp$ such that u can be written as (1.36), u_{H^2} satisfies (1.37), and $u_{\mathcal{A}}$ satisfies

$$\|D(\alpha)u_{\mathcal{A}}\|_{\mathcal{H}^\sharp} \lesssim \bigg(\sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha,\hbar)\bigg)\hbar^{-M-1}\|g\|_{\mathcal{H}} \quad \text{for all } \alpha \in \mathfrak{A} \text{ and } \hbar \in \mathfrak{H}, \tag{4.7}$$

where the omitted constant is independent of $\hbar$ and α.

Proof. Let $\rho := 1$, $\mathcal{E}(\lambda) := \langle\lambda\rangle^{-L}$ and $C_{\mathcal{E}}(\alpha,\hbar) := \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha,\hbar)$. We now need to show that the bound (4.6) implies that the bound (1.34) holds with these choices of $\mathcal{E}$ and $C_{\mathcal{E}}$. Given $v \in D_\hbar^{\sharp,\infty}$, let $w := \langle P_\hbar^\sharp\rangle^{-L}v \in D_\hbar^{\sharp,\infty}$. The bound (4.6) implies that

$$\Big\|\rho D(\alpha)\langle P_\hbar^\sharp\rangle^{-L}v\Big\|_{\mathcal{H}^\sharp} \leq \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha,\hbar)\big\|(P_\hbar^\sharp)^\ell\langle P_\hbar^\sharp\rangle^{-L}v\big\|_{\mathcal{H}^\sharp} \quad \text{for all } \alpha \in \mathfrak{A} \text{ and } \hbar \in \mathfrak{H}. \tag{4.8}$$

Since $\langle\lambda\rangle^{-L}\lambda^\ell \leq 1$, by Part 3 of Theorem 2.6, the term in brackets on the right-hand side of (4.8) is bounded by $C_{\mathcal{E}}(\alpha,\hbar)\|v\|_{H^\sharp}$, and then (1.34) follows. The result (4.7) then follows from the bound (1.43) in Theorem A. ■

4.1 Proof of Theorem B

Let $\hbar := k^{-1}$, $g := \hbar^2 f$, and define $\mathcal{H}$ and $P_\hbar$ as in Lemma 2.3, so that $P_\hbar$ is a semiclassical black-box operator on $\mathcal{H}$. The assumption that $C_{\rm sol}(k)$ is polynomially bounded means that (1.32) holds with

$$\mathfrak{H} := \big\{\hbar : \hbar = k^{-1} \text{ with } k \in K\big\}. \tag{4.9}$$

The plan is to apply Corollary 4.1, showing that the heat-flow estimate (4.1) is satisfied using the following theorem.

Theorem 4.3 (Heat-equation estimate from [21]) *Suppose that $\mathcal{O}_-, A, c, R_0$, and R_1 are as in Definition 1.2. In addition, assume that $\mathcal{O}_-$ is analytic, and that A and c are C^∞ everywhere and analytic in B_{R_*} for some $R_0 < R_* < R_1$. Let $P^\sharp_\hbar$ denote the associated black-box reference operator on the torus (as described in §2.1).*

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

$$\Big\|\rho \partial^\alpha \mathrm{e}^{t\hbar^{-2}P^\sharp_\hbar}\Big\|_{L^2\to L^2} \le \exp(t^{-\tau})|\alpha|!\, C^{|\alpha|} t^{(\tau-1)|\alpha|/2}. \tag{4.10}$$

Note that the operator $\mathrm{e}^{t\hbar^{-2}P^\sharp_\hbar}$ is just the variable coefficient heat operator for time t.

References for the proof of Theorem 4.3. When $\tau = 1$, (4.10) is essentially [21, Theorem 1.1], and when $\tau = 0$, (4.10) is a more-standard heat-equation estimate [21, Equation 1.5], attributed there to [24, Part 3, §3].

Indeed, the bound with $\tau = 1$ follows from [21, Lemma 2.7] with the choice of their parameter θ equal to 1 (via an argument using Sobolev embedding in time, as discussed immediately before [21, Lemma 2.7]). The bound with $\tau = 0$ follows from [21, Lemma 2.7] with $\theta = t$ (since $\sigma = 1$ for the heat equation in the notation of [21, §2]), as highlighted in [21, Remark 2.8]. The bound for general $\tau \in [0,1]$ then follows from [21, Lemma 2.7] with $\theta = t^{1-\tau}$.

The main difference between the set up of [21] and the hypotheses of Theorem 4.3 is that [21] works on a bounded domain with Dirichlet boundary conditions, whereas Theorem 4.3 works on the torus with a Dirichlet obstacle inside. However, these global considerations only enter the arguments in [21] in deriving time-analyticity estimates of the heat semi group in [21, Lemma 2.1], and these estimates hold equally well on the torus with a Dirichlet obstacle. ∎

As in Corollary 4.1, we choose ρ to be equal to one near B_{R_0}, and further assume that ρ is supported in $B_{(R_0+R_*)/2}$ (i.e., in a region where A and c are known to be analytic). Given $\hbar \in \mathfrak{H}$ and a multi-index α, let $\tau = \tau(\hbar,\alpha) \in [0,1]$, depending only on $\hbar$ and α, to be fixed later. By letting $t \mapsto t\hbar^2$ in Theorem 4.3, we see that the heat-flow estimate (4.1) is satisfied with $D(\alpha) := \partial^\alpha$,

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

note that the heat-flow given by the functional calculus, appearing in (4.1), is indeed the solution of the heat equation; see, e.g., [57, Theorem VIII.7].

We can therefore apply Corollary 4.1 with an arbitrary $R_\sharp > R$, and we obtain $u_{H^2} \in \mathcal{D}^\sharp$ and $u_{\mathcal{A}} \in \mathcal{D}^{\sharp,\infty}_\hbar$ with $u_{\mathcal{A}} = u^{R_0}_{\mathcal{A}} + u^\infty_{\mathcal{A}}$ satisfying (1.36), (1.37), (1.38), and the bounds (4.2)–(4.4). Observe that u_{H^2} and $u_{\mathcal{A}}$ satisfy the Dirichlet boundary condition (1.6) since they are in $\mathcal{D}^\sharp$ (2.4).

The low-frequency bounds (4.3)–(4.4) give directly the low-frequency bound away from the obstacle (1.12) and the error bound (1.13). The rest of the proof therefore consists in obtaining the low-frequency bound near the obstacle (1.11) from (4.2) and the high-frequency bound (1.10) from (1.37).

To obtain (1.11), by (4.2), we only have to show that, for some $\tau \in [0,1]$ and $\mathcal{C} > 0$,

$$\inf_{t\in(0,\hbar^{-2}]}\left(\exp\big[(\hbar^2 t)^{-\tau} + \Lambda t\big]|\alpha|!\, C^{|\alpha|\left(\hbar^2 t\right)^{(\tau-1)|\alpha|/2}}\right) \le \mathcal{C}^{|\alpha|}\max\big\{|\alpha|^{|\alpha|}, \hbar^{-|\alpha|}\big\}. \tag{4.11}$$

We first prove (4.11) when $|\alpha| \ge \hbar^{-1}$, i.e., when the max on the right equals $\mathcal{C}^{|\alpha|}\alpha^{|\alpha|}$. If $\tau = 1$ and $t = \hbar^{-1}$, then the quantity in the infimum on the left-hand side of (4.11) equals

$$\exp\big[(1+\Lambda)\hbar^{-1}\big]|\alpha|!\, C^{|\alpha|} \le (\widetilde{C})^{|\alpha|}|\alpha|^{|\alpha|}$$

(by Stirling's formula) as required.

To prove (4.11) when $|\alpha| \le \hbar^{-1}$, we seek to choose t and τ such that

$$(\hbar^2 t)^{(\tau-1)|\alpha|/2} = \hbar^{-|\alpha|}|\alpha|^{-|\alpha|} \quad \text{and} \quad t = (\hbar^2 t)^{-\tau}. \tag{4.12}$$

Under the second equality in (4.12), the left-hand side of the first equality becomes $\hbar^{-|\alpha|}t^{-|\alpha|}$; we therefore let $t = |\alpha|$, which is allowed since $|\alpha| \le \hbar^{-1} \le \hbar^{-2}$. We now choose τ such that the second equality in (4.12) holds; i.e.,

$$\tau = \frac{\log|\alpha|}{\log(\hbar^{-2}|\alpha|^{-1})}.$$

When $1 \le |\alpha| \le \hbar^{-1}$, $0 \le \tau \le 1$, and so this choice of τ is allowed. Under the equalities in (4.12), the quantity in the infimum on the left-hand side of (4.11) equals

$$\exp\big[(1+\Lambda)|\alpha|\big]|\alpha|!C^{|\alpha|}\hbar^{-|\alpha|}|\alpha|^{-|\alpha|} \le (\widetilde{C})^{|\alpha|}\hbar^{-|\alpha|},$$

which is the right-hand side of (4.11) when $|\alpha| \le \hbar^{-1}$. We have therefore proved (4.11), and thus the low-frequency bound near the obstacle (1.11).

We now complete the proof by proving the high-frequency bound (1.10). The bound (1.37) implies that

$$\|u_{H^2}\|_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + k^{-2}\|\nabla\cdot(A\nabla u_{H^2})\|_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} \lesssim k^{-2}\|f\|_{L^2(B_R\cap\mathcal{O}_+)},$$

and then Green's first identity (see, e.g., [44, Lemma 4.3]) and the fact that A satisfies (1.4) imply that

$$\|u_{H^2}\|_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + k^{-1}\|\nabla u_{H^2}\|_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + k^{-2}\|\nabla\cdot(A\nabla u_{H^2})\|_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} \lesssim k^{-2}\|f\|_{L^2(B_R\cap\mathcal{O}_+)}; \tag{4.13}$$

see, e.g., [30, Lemma 3.10]. That is, (1.10) holds for $|\alpha| = 0$ and 1. To obtain (1.10) for $|\alpha| = 2$, we combine (4.13) with the H^2 regularity result of, e.g., [44, Part (i) of Theorem 4.18, pages 137-138], applied with $\Omega_1 = B_R \cap \mathcal{O}_+$ and $\Omega_2 = B_{(R+R_\sharp)/2} \cap \mathcal{O}_+$. Finally, the fact that $u^{R_0}_{\mathcal{A}}$ is analytic in $B_{R_{\rm IV}}$ and $u^\infty_{\mathcal{A}}$ is analytic in $(B_{R_{\rm I}})^c$ follows from Lemma 1.1 and the bounds (1.11) and (1.12), respectively.

4.2 Proof of Theorem C

The plan is to apply Corollary 4.2. Let $\hbar := k^{-1}$, $g := \hbar^2 f$, and define $\mathcal{H}$ and $P_\hbar$ as in Lemma 2.3. By Lemma 2.3, $P_\hbar$ is a semiclassical black-box operator on $\mathcal{H}$.

The assumption that $C_{\rm sol}(k)$ is polynomially bounded means that (1.32) holds with H given by (4.9) and thus we only need to show that the regularity estimate (4.6) is satisfied for appropriate $D(\alpha), C_\ell(\alpha,\hbar)$, and $L(\alpha)$.

We claim that for n even with $n \le 2m$

$$\|w\|_{H^n(\mathcal{O}_-)\oplus H^n(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} \le \sum_{\ell=0}^{n/2}\widetilde{C}_\ell(n)\left\|(\nabla\cdot(A\nabla))^\ell w\right\|_{L^2(\mathcal{O}_-)\oplus L^2(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} \qquad \text{for all } w \in \mathcal{D}^{\sharp,\infty}_\hbar, \tag{4.14}$$

where $\widetilde{C}_\ell(n)$ also depends on $\mathcal{O}_-, A$, and c. If (4.14) holds, then the regularity estimate (4.6) is satisfied with (i) $D(\alpha) := (\partial^\alpha|_{\mathcal{O}_-}, \partial^\alpha|_{\mathcal{O}_+})$, (ii) $\mathfrak{A}$ consisting of multi-indices α such that $|\alpha|$ is even and $|\alpha| \le 2m$, (iii) $L(\alpha) := |\alpha|/2$, and (iv)

$$C_\ell(\alpha,\hbar) := \hbar^{-2\ell}\widetilde{C}_\ell(|\alpha|). \tag{4.15}$$

We assume that (4.14) holds, and show how the result of the theorem follows from Corollary 4.2. Applying this corollary, we obtain $u_{H^2}, u_{\mathcal{A}}$ satisfying (1.36), (1.37), and (4.7). Observe that u_{H^2}

and $u_{\mathcal{A}}$ satisfy the transmission conditions (1.23) since they are in $\mathcal{D}^\sharp$. By (4.15), there exists $C_2 = C_2(m) > 0$ such that, for $|\alpha| \le 2m$,

$$\sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha, \hbar) \le C_2(m) \hbar^{-|\alpha|}.$$

The low-frequency bound (4.7) therefore gives (1.25) for all $\alpha \in \mathfrak{A}$, i.e., for all α with $|\alpha|$ even and $\le 2m$. The bound (1.25) then holds for all α with $|\alpha| \le 2m$ by interpolation (see, e.g., [44, Theorem B.8], [10, §4.2]). Finally, (1.24) follows from the high-frequency estimate (1.37), together with Green's identity and (4.14) applied with $n = 2$ (similar to the end of the proof of Theorem B).

We therefore only need to prove (4.14). The two ingredients to do this are the regularity result

$$\|v\|_{H^{n+2}(\mathcal{O}_-)\oplus H^{n+2}(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} \lesssim \|\nabla\cdot(A\nabla v)\|_{H^n(\mathcal{O}_-)\oplus H^n(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} + \|v\|_{H^1(\mathcal{O}_-)\oplus H^1(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} \tag{4.16}$$

for all integers $n \le 2m-2$, and the bound

$$\|v\|_{H^1(\mathcal{O}_-)\oplus H^1(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} \lesssim \|\nabla\cdot(A\nabla v)\|_{L^2(\mathcal{O}_-)\oplus L^2(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} + \|v\|_{L^2(\mathcal{O}_-)\oplus L^2(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)}, \tag{4.17}$$

where both bounds are valid for all $v \in \mathcal{D}^\sharp$, and the omitted constants in both depend on $A, c,$ and β.

The bound (4.17) is proved using Green's first identity (see, e.g., [44, Lemma 4.3]), the fact that v satisfies the transmission conditions in (2.9), and the fact that A satisfies (1.4); see, e.g., [30, Lemma 3.10] for an analogous bound in $\mathbb{R}^d$ for the case $\beta = 1$.

Regarding (4.16): standard elliptic regularity results imply that, given Ω_1, Ω_2 with $\mathcal{O}_- \Subset \Omega_1 \Subset \Omega_2 \Subset B_{R^\sharp}$,

$$\begin{aligned}\|v\|_{H^{n+2}(\mathcal{O}_-)\oplus H^{n+2}(\Omega_1\cap\mathcal{O}_+)} &\lesssim \|\nabla\cdot(A\nabla v)\|_{H^n(\mathcal{O}_-)\oplus H^n(\Omega_2\cap\mathcal{O}_+)} + \|v\|_{H^1(\mathcal{O}_-)\oplus H^1(\Omega_2\cap\mathcal{O}_+)}\\ &\le \|\nabla\cdot(A\nabla v)\|_{H^n(\mathcal{O}_-)\oplus H^n(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)} + \|v\|_{H^1(\mathcal{O}_-)\oplus H^1(\mathbb{T}^d_{R_\sharp}\cap\mathcal{O}_+)},\end{aligned} \tag{4.18}$$

for all $v \in \mathcal{D}^\sharp$ and integers $n \le 2m-2$, where the omitted constant depends on A, c, β; see, e.g., [44, Theorem 4.20], [14, Theorem 5.2.1, Part (i)]. Since the torus is compact (and is thus covered by a finite number of Ω_1s), (4.18) holds with the left-hand side replaced by $\|v\|_{H^{n+2}(\mathcal{O}_-)\oplus H^{n+2}(\mathcal{O}_+\cap\mathbb{T}^d_{R_\sharp})}$ and (4.16) follows.

We now use (4.16) and (4.17) to prove (4.14) by induction. The bound (4.14) with $n = 2$ follows from combining (4.16) with $n = 0$ and $v = w$ and (4.17) with $v = w$ (observe that choosing $v = w$ in both is allowed since $w \in \mathcal{D}^\sharp$). We now assume that we have proved (4.14) for n even and $n \le 2q$ for some $0 \le q \le m-1$; i.e.,

$$\|w\|_{H^{2q}} \lesssim \sum_{\ell=0}^{q} \left\|(\nabla\cdot(A\nabla))^\ell w\right\|_{L^2} \qquad \text{for all } w \in \mathcal{D}^{\sharp,\infty}_\hbar, \tag{4.19}$$

where we have omitted the q-dependent constants and the domains of the norms for brevity.

Applying (4.16) with $n = 2q$ and $v = w$, we have

$$\|w\|_{H^{2q+2}} \lesssim \|\nabla\cdot(A\nabla w)\|_{H^{2q}} + \|w\|_{H^1} \tag{4.20}$$

(again omitting the domains of the norms for brevity). The desired bound (4.14) with $n = 2q+2$ then follows by using in (4.20) the inequality (4.19) with w replaced by $\nabla\cdot(A\nabla w)$ (which is allowed since $w \in \mathcal{D}^{\sharp,\infty}_\hbar$ implies that $P^\sharp_\hbar w \in \mathcal{D}^{\sharp,\infty}_\hbar$ by (2.12)), and then using (4.17) with $v = w$.

4.3 Proof of Theorem D

Let $\hbar := k^{-1}$, $g := \hbar^2 f$, and define $\mathcal{H}$ and $P_\hbar$ as in Lemma 2.3 with $\mathcal{O}_- = \emptyset$. By Lemma 2.3, $P_\hbar$ is a semiclassical black-box operator on $\mathcal{H}$. The reference operator is given by $P^\sharp_\hbar = -\hbar^2 c^2 \nabla\cdot(A\nabla)$, acting on the torus $\mathbb{T}^d_{R_\sharp}$.

The assumption that $C_{\rm sol}(k)$ is polynomially bounded means that the bound (1.32) holds with H given by (4.9); i.e., the assumption in Point 1 of Theorem A is satisfied.

We now construct $\mathcal{E}$ and E satisfying the assumptions in Point 2 of Theorem A. Let $\Lambda>0$ be as in Theorem A, 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 [32] (see the account in [59]) imply that $\mathcal{E}(P_\hbar^\sharp)=\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla)\big)$ is a pseudo-differential operator on the torus $\mathbb{T}^d_{R_\sharp}$. Then, the same argument as in the proof of Lemma 2.8 shows that

$$\mathrm{WF}_\hbar\,\mathcal{E}\big(-\hbar^2c^2\nabla\cdot(A\nabla)\big)\subset\operatorname{supp}\mathcal{E}\circ q,$$

where $q(x,\xi)=c(x)^2\langle A(x)\xi,\xi\rangle$ is the semi-classical principal symbol of $-\hbar^2c^2\nabla\cdot(A\nabla)$. Hence, since $\mathcal{E}$ is compactly supported and A satisfies (1.4), there exists $\Lambda_0>0$ such that

$$\mathrm{WF}_\hbar\,\mathcal{E}\big(-\hbar^2c^2\nabla\cdot(A\nabla)\big)\subset\mathbb{T}^d_{R_\sharp}\times B\left(0,\frac{\Lambda_0}{2}\right). \tag{4.21}$$

Let $\widetilde{\varphi}\in C^\infty_{\rm comp}$ be compactly supported in $B(0,\Lambda_0^2)$ and equal to one on $B(0,\Lambda_0^2/4)$. By (4.21) and (A.11), $\mathrm{WF}_\hbar\left(1-\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\right)\cap\mathrm{WF}_\hbar\,\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla)\big)=\emptyset$, therefore

$$\mathcal{E}\big(-\hbar^2c^2\nabla\cdot(A\nabla)\big)=\mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(\widetilde{\varphi}(|\xi|^2))\mathcal{E}\big(-\hbar^2c^2\nabla\cdot(A\nabla)\big)+O(\hbar^\infty)_{\Psi^{-\infty}}.$$

Then, by Lemma A.3,

$$\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla)\big)=\widetilde{\varphi}(-\hbar^2\Delta)\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla)\big)+O(\hbar^\infty)_{\Psi^{-\infty}}. \tag{4.22}$$

We now define

$$E:=\widetilde{\varphi}(-\hbar^2\Delta)\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla v)\big), \tag{4.23}$$

and thus (4.22) implies that

$$\mathcal{E}(P_\hbar^\sharp)=E+O(\hbar^\infty)_{\mathcal{D}_\hbar^{\sharp,-\infty}\to\mathcal{D}_\hbar^{\sharp,\infty}}.$$

We now need to show that a low-frequency estimate of the form (1.34) is satisfied. Since $\widetilde{\varphi}$ is compactly supported in $B(0,\Lambda_0^2)$, the definition of E (4.23) and the same argument used to show the bound (3.45) imply that

$$\|\partial^\alpha Ev\|_{L^2(\mathbb{T}^d_{R_\sharp})}\leq\Lambda_0^{|\alpha|}\hbar^{-|\alpha|}\|\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla v)\big)v\|_{L^2(\mathbb{T}^d_{R_\sharp})}\quad\text{for all }v\in L^2(\mathbb{T}^d_{R_\sharp})\text{ and multi-indices }\alpha.$$

Then, since $\mathcal{E}(-\hbar^2c^2\nabla\cdot\big(A\nabla)\big)\in\Psi^{-\infty}(\mathbb{T}^d_{R_\sharp})$, there exists $C>0$ such that

$$\|\partial^\alpha Ev\|_{L^2(\mathbb{T}^d_{R_\sharp})}\leq C\Lambda_0^{|\alpha|}\hbar^{-|\alpha|}\|v\|_{L^2(\mathbb{T}^d_{R_\sharp})}\qquad\text{for all }v\in L^2(\mathbb{T}^d_{R_\sharp})\text{ and multi-indices }\alpha.$$

Therefore, the assumption in Point 2 of Theorem A is satisfied with $D(\alpha):=\partial^\alpha$, $C_{\mathcal{E}}(\alpha,\hbar):=C\Lambda_0^{|\alpha|}\hbar^{-|\alpha|}$ and $\rho=1$. The result then follows from Theorem A; indeed, the bound (1.28) follows immediately from (1.43), and (1.27) follows from (1.37) after using Green's identity and elliptic regularity in the same way as at the end of the proof of Theorem B – see (4.13) and the surrounding text.

5 Proofs of Theorems B1 and C1 and Corollary 1.7 (the frequency-explicit results about the convergence of the FEM)

5.1 Recap of FEM convergence theory

The two ingredients for the proof of Theorems B1 and C1 are

- Lemma 5.4, which is the standard 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 (5.4)), and
- Lemma 5.5 that bounds $\eta(V_N)$ using the decomposition from Theorems B and C.

Regarding Lemma 5.4: this argument came out of ideas introduced in [61], was then formalised in [60], and has been used extensively in the analysis of the Helmholtz FEM; see, e.g., [1, 36, 45, 60, 48, 49, 72, 70, 18, 12, 42, 13, 27, 31, 26, 40].

Before stating Lemma 5.4 we need to introduce some notation. Let $C_{\rm cont} = C_{\rm cont}(A, c^{-2}, R, k_0)$ be the *continuity constant* of the sesquilinear form $a(\cdot,\cdot)$ (defined in (1.15)) in the norm $\|\cdot\|_{H^1_k(B_R\cap\mathcal{O}_+)}$; i.e.

$$|a(u,v)| \leq C_{\rm cont}\, \|u\|_{H^1_k(B_R\cap\mathcal{O}_+)}\, \|v\|_{H^1_k(B_R\cap\mathcal{O}_+)} \qquad \text{for all } u,v\in H^1(B_R\cap\mathcal{O}_+).$$

By the Cauchy-Schwarz inequality and (1.16),

$$C_{\rm cont} \leq \max\{A_{\max}, c_{\min}^{-2}\} + C_{\rm DtN}. \tag{5.1}$$

The following definitions are stated for the sesquilinear form of the Dirichlet problem (1.15). For the sesquilinear form of the transmission problem with the transmission parameter $\beta = 1$, one only needs to replace $B_R\cap\mathcal{O}_+$ by B_R and define c to be equal to one in $B_R\cap\mathcal{O}_+$.

Definition 5.1 (The adjoint sesquilinear form $a^*(\cdot,\cdot)$) *The adjoint sesquilinear form, $a^*(u,v)$, to the sesquilinear form $a(\cdot,\cdot)$ defined in* (1.15) *is given by*

$$a^*(u,v) := \overline{a(v,u)} = \int_{B_R\cap\mathcal{O}_+}\left((A\nabla u)\cdot\overline{\nabla v} - \frac{k^2}{c^2}u\overline{v}\right) - \big\langle u, {\rm DtN}_k(v)\big\rangle_{\partial B_R}.$$

Definition 5.2 (Adjoint solution operator $\mathcal{S}^*$) *Given $f\in L^2(B_R\cap\mathcal{O}_+)$, let $\mathcal{S}^*f$ be defined as the solution of the variational problem*

$$\text{find } \mathcal{S}^*f\in H^1(B_R\cap\mathcal{O}_+) \quad \text{such that} \quad a^*(\mathcal{S}^*f, v) = \int_{B_R\cap\mathcal{O}_+} f\,\overline{v} \quad \text{for all } v\in H^1(B_R\cap\mathcal{O}_+). \tag{5.2}$$

Green's second identity applied to solutions of the Helmholtz equation satisfying the Sommerfeld radiation condition (1.2) implies that $\big\langle {\rm DtN}_k\psi, \overline{\phi}\big\rangle_{\partial B_R} = \big\langle {\rm DtN}_k\phi, \overline{\psi}\big\rangle_{\partial B_R}$ for all $\phi,\psi\in H^{1/2}(\partial B_R)$ (see, e.g., [64, Lemma 6.13]); thus $a(\overline{v},u) = a(\overline{u},v)$ and so the definition (5.2) implies that

$$a(\overline{\mathcal{S}^*f}, v) = (\overline{f}, v)_{L^2(B_R)} \qquad \text{for all } v\in H^1(B_R\cap\mathcal{O}_+). \tag{5.3}$$

Definition 5.3 ($\eta(V_N)$) *Given a sequence $(V_N)_{N=0}^\infty$ of finite-dimensional subspaces of let*

$$\eta(V_N) := \sup_{0\neq f\in L^2(B_R\cap\mathcal{O}_+)}\ \min_{v_N\in V_N} \frac{\|S^*f - v_N\|_{H^1_k(B_R\cap\mathcal{O}_+)}}{\|f\|_{L^2(B_R\cap\mathcal{O}_+)}}. \tag{5.4}$$

Lemma 5.4 (Conditions for quasioptimality) *If*

$$k\,\eta(V_N) \leq \frac{1}{C_{\rm cont}}\sqrt{\frac{A_{\min}}{2\big(n_{\max}+A_{\min}\big)}},$$

then the Galerkin equations (1.18) *have a unique solution which satisfies*

$$\|u-u_h\|_{H^1_k(B_R\cap\mathcal{O}_+)} \leq \frac{2C_{\rm cont}}{A_{\min}}\left(\min_{v_N\in V_N}\|u-v_N\|_{H^1_k(B_R\cap\mathcal{O}_+)}\right).$$

References for the proof. See, e.g., [40, Lemma 6.4]. ■

The following two lemmas are proved in the next subsections.

Lemma 5.5 (Bound on $\eta(V_N)$ for the exterior Dirichlet problem) *Let $d = 2$ or 3. Suppose that $\mathcal{O}_-, A, c, R, R_{\mathrm{I}}$, and R_{IV} are as in Theorem B. Let $(V_N)_{N=0}^{\infty}$ be the piecewise-polynomial approximation spaces described in [48, §5], [49, §5.1.1].*

Given $k_0 > 0$ and $N > 0$ there exist

- *$\mathcal{C}_1, \mathcal{C}_2, \sigma > 0$, depending on A, c, R, d, and k_0, but independent of k, h, p, and N, and*
- *C_N depending on A, c, R, d, k_0, and N, but independent of k, h, p,*

such that

$$k\,\eta(V_N) \leq \mathcal{C}_1 \frac{hk}{p}\left(1 + \frac{hk}{p}\right) + \mathcal{C}_2 k^M \left(\left(\frac{h}{h+\sigma}\right)^p + k\left(\frac{hk}{\sigma p}\right)^p\right) + C_N k^{1-N} \qquad \text{for all } k \geq k_0. \quad (5.5)$$

Lemma 5.6 (Bound on $\eta(V_N)$ for the transmission problem) *Let $d = 2$ or 3 and let $\beta = 1$. Suppose that A, c, and $\mathcal{O}_-$ are as in Definition 1.8 and, given an integer p, satisfy the regularity assumptions in Theorem C1. Let $(V_N)_{N=0}^{\infty}$ be a sequence of piecewise-polynomial approximation spaces of degree p satisfying Assumption 1.10.*

Given $k_0 > 0$, there exist $\widetilde{\mathcal{C}}_1, \widetilde{\mathcal{C}}_2$, depending on A, c, R, d, k_0, and p, but independent of k and h, such that

$$k\,\eta(V_N) \leq \big(1 + hk\big)\Big(\widetilde{\mathcal{C}}_1 hk + \widetilde{\mathcal{C}}_2\, k^{M+1}(hk)^p\Big) \qquad \text{for all } k \geq k_0. \quad (5.6)$$

Proof of Theorems B1/C1 assuming Lemmas 5.5/5.6. Theorem C1 follows immediately by combining Lemmas 5.4 and 5.6 and the inequality (5.1).

Theorem B1 follows in a similar way (and is essentially the same as the proof of [49, Theorem 5.8]), except that we first choose $N > 1$, and then let $k_1 > 0$ be such that

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

Theorem B1 then follows by using this bound in (5.5) and then combining the resulting inequality with Lemma 5.4 and the inequality (5.1). ∎

5.2 Proof of Lemma 5.5

Given $f \in L^2(B_R \cap \mathcal{O}_+)$, let $v = \mathcal{S}^* f$. By (5.3) and Theorem B, $v = v_{H^2} + v_{\mathcal{A}}$, where v_{H^2} and $v_{\mathcal{A}}$ satisfy the bounds (1.10)–(1.13) with u replaced by v.

The proof of Lemma 5.5 is very similar to the proofs of [48, Theorem 5.5] and [49, Proposition 5.3] (covering the constant-coefficient Helmholtz equation in, respectively, $\mathbb{R}^d$ and the exterior of an analytic Dirichlet obstacle).

The only difference is that in [48], [49] the function $v_{\mathcal{A}}$ is analytic on the whole of $B_R \cap \mathcal{O}_+$, whereas here $v_{\mathcal{A}} = v_{\mathcal{A}}^{R_0} + v_{\mathcal{A}}^{\infty}$ with $v_{\mathcal{A}}^{R_0}$ and $v_{\mathcal{A}}^{\infty}$ analytic in subsets of the domain and $O(k^{-\infty})$ in the complements of these subsets; see (1.11)-(1.13) and Figure 1.1. The consequence is that $C_N k^{1-N}$ appears on the right-hand side of (5.5), but this term is not present on the right-hand sides of the analogous bounds in [48, Theorem 5.5] and [49, Proposition 5.3 and Equation 5.11]. Since this term can be made arbitrarily-small for k sufficiently large, the only consequence is that Lemma 5.5 and Theorem B1 are valid for k sufficiently large (as opposed to for all $k \geq k_0$ with k_0 arbitrary).

Exactly as in the proof of [48, Theorem 5.5], there exists $\mathcal{C}_3 > 0$ (dependent only on the constants in [48, Assumption 5.2] defining the element maps from the reference element) such that

$$\min_{w_N \in V_N} \|v - w_N\|_{H^1_k(B_R \cap \mathcal{O}_+)} \leq \mathcal{C}_3 \frac{h}{p}\left(1 + \frac{hk}{p}\right)|v|_{H^2(B_R \cap \mathcal{O}_+)}, \quad (5.7)$$

for all $v \in H^2(B_R \cap \mathcal{O}_+)$; recall that this result follows from the polynomial-approximation result of [48, Theorem B.4] and the definition (1.7) of the norm $\|\cdot\|_{H^1_k}$. Applying the bound (5.7) to v_{H^2} and using (1.10) with $|\alpha| = 2$, we obtain

$$\min_{w_N \in V_N} \|v_{H^2} - w_N\|_{H^1_k(B_R \cap \mathcal{O}_+)} \leq \mathcal{C}_3\, C_1 \frac{h}{p}\left(1 + \frac{hk}{p}\right)\|f\|_{L^2(B_R \cap \mathcal{O}_+)};$$

we then let $\mathcal{C}_1 := C_1\,\mathcal{C}_3$.

To prove (5.5), therefore, we only need to show that

$$\min_{w_N\in V_N} \|v_{\mathcal{A}} - w_N\|_{H^1_k(B_R\cap\mathcal{O}_+)} \leq \left(\mathcal{C}_2\, k^M \left(\left(\frac{h}{h+\sigma}\right)^p + k\left(\frac{hk}{\sigma p}\right)^p\right) + C_N k^{-N}\right) \|f\|_{L^2(B_R\cap\mathcal{O}_+)}, \tag{5.8}$$

for some $\mathcal{C}_2 > 0$ independent of k, h, p, and N and some $C_N > 0$ independent of k, h, and p. Recall the regions where $v_{\mathcal{A}}^{R_0}$ and $v_{\mathcal{A}}^{\infty}$ are analytic (see Figure 1.1). Given V_N, choose D_1 such that (i) D_1 is a union of elements of the triangulation associated with V_N and (ii) $B_{R_{\mathrm{III}}} \Subset D_1 \Subset B_{R_{\mathrm{IV}}}$. Thus, by (1.13),

$$\begin{aligned}\min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{R_0} - w_N\right\|_{H^1_k(B_R\cap\mathcal{O}_+)} &\leq \min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{R_0} - w_N\right\|_{H^1_k(D_1\cap\mathcal{O}_+)} + \left\|v_{\mathcal{A}}^{R_0}\right\|_{H^1_k(B_R\cap(D_1)^c)}\\ &\leq \min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{R_0} - w_N\right\|_{H^1_k(D_1\cap\mathcal{O}_+)} + C_N' k^{-N} \|f\|_{L^2(B_R\cap\mathcal{O}_+)}\end{aligned}$$

for some $C_N' > 0$ independent of k, h, and p. Similarly, with D_2 a union of elements of the triangulation and such that $B_{R_{\mathrm{I}}} \Subset D_2 \Subset B_{R_{\mathrm{II}}}$,

$$\min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{\infty} - w_N\right\|_{H^1_k(D_2\cap\mathcal{O}_+)} \leq \min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{\infty} - w_N\right\|_{H^1_k(B_R\cap(D_2)^c)} + C_N'' k^{-N} \|f\|_{L^2(B_R\cap\mathcal{O}_+)}$$

for some $C_N'' > 0$, independent of k, h, and p. To prove (5.8), therefore, we only need to show that

$$\min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{R_0} - w_N\right\|_{H^1_k(D_1\cap\mathcal{O}_+)} \leq \frac{\mathcal{C}_2}{2}\, k^M \left(\left(\frac{h}{h+\sigma}\right)^p + k\left(\frac{hk}{\sigma p}\right)^p\right) \|f\|_{L^2(B_R\cap\mathcal{O}_+)} \tag{5.9}$$

and

$$\min_{w_N\in V_N} \left\|v_{\mathcal{A}}^{\infty} - w_N\right\|_{H^1_k(B_R\cap(D_2)^c)} \leq \frac{\mathcal{C}_2}{2}\, k^M \left(\left(\frac{h}{h+\sigma}\right)^p + k\left(\frac{hk}{\sigma p}\right)^p\right) \|f\|_{L^2(B_R\cap\mathcal{O}_+)}, \tag{5.10}$$

for some $\mathcal{C}_2 > 0$, independent of k, h, p, and N. Note that (i) we introduced D_1 and D_2 so that the domains on which $v_{\mathcal{A}}^{R_0}$ and $v_{\mathcal{A}}^{\infty}$ are approximated in (5.9) and (5.10) are exactly triangulated by the mesh, and (ii) for the approximation (5.9), it is important that $v_{\mathcal{A}}^{R_0} = 0$ on $\partial\mathcal{O}^+$, since the space V_N has this zero Dirichlet boundary condition imposed.

The bounds (5.9) and (5.10) then follow from [49, Proposition 5.3] (which uses [48, Theorem 5.5]); the key point is that $v_{\mathcal{A}}^{\infty}$ and $v_{\mathcal{A}}^{R_0}$ satisfy the same type of bound – namely that in Part (iii) of Lemma 1.1 – as $u_{\mathcal{A}}$ in [49] (see the second displayed equation in [49, Theorem 4.20], and note that α in [49] equals our M).

5.3 Proof of Lemma 5.6

Given $f \in L^2(B_R)$, let $v = \mathcal{S}^* f$. By (5.3) and Theorem C, $v = v_{H^2} + v_{\mathcal{A}}$, where v_{H^2} and $v_{\mathcal{A}}$ satisfy the bounds (1.24) and (1.25) with u replaced by v.

By the definition of the H^1_k norm (1.7) and the bound (1.26), there exists $C_{\mathrm{int}} = C_{\mathrm{int}}(\ell, d) > 0$ such that

$$\min_{w_N\in V_N} \|w - w_N\|_{H^1_k(B_R)} \leq C_{\mathrm{int}}(\ell, d)\big(1 + hk\big)h^\ell \Big(\|w_+\|_{H^{\ell+1}(B_R\cap\mathcal{O}_+)} + \|w_-\|_{H^{\ell+1}(\mathcal{O}_-)}\Big) \tag{5.11}$$

for all $w = (w_+, w_-) \in H^{\ell+1}(B_R \cap \mathcal{O}_+) \times H^{\ell+1}(\mathcal{O}_-)$. Applying (5.11) with $\ell = 1$ to v_{H^2} and using (1.24) with $|\alpha| = 2$, we obtain that

$$\min_{w_N\in V_N} \|v_{H_2} - w_N\|_{H^1_k(B_R)} \leq C_{\mathrm{int}}(1, d)\big(1 + hk\big)\, h\, C_1 \|f\|_{L^2(B_R)}. \tag{5.12}$$

Let $C_{\mathrm{Sob}}(p, d)$ be such that

$$\text{if} \quad \|\partial^\alpha v\|_{L^2} \leq C \quad \text{for all } \alpha \text{ with } |\alpha| \leq p, \quad \text{then } \|v\|_{H^{p+1}} \leq C_{\mathrm{Sob}}(p, d)\, C;$$

i.e., C_{Sob} depends only on the normalisations in the definition of $\|\cdot\|_{H^{p+1}}$.

The regularity assumptions on $\mathcal{O}_-$, A, and c and the regularity results of, e.g., [44, Theorem 4.20], [14, Theorem 5.2.1, Part (i)] imply that $u_{\pm,\mathcal{A}} \in H^{p+1}$ for p odd and H^{p+2} for p even. For p odd we apply Theorem C with $m = (p+1)/2$ and for p even with $m = (p+2)/2$. In both cases, we apply (5.11) with $\ell = p$ to $v_{\mathcal{A}} = (v_{\mathcal{A},+}, v_{\mathcal{A},-})$ and use (1.25) with $|\alpha| = p+1$ to obtain that

$$\min_{w_N \in V_N} \|v_{\mathcal{A}} - w_N\|_{H^1_k(B_R)} \leq C_{\rm int}(p)\big(1 + hk\big)\, h^p\, C_{\rm Sob}(p,d)\, C_2(p)\, k^{p+M}\, \|f\|_{L^2(B_R)}\,. \tag{5.13}$$

The bound on $\eta(V_N)$ in (5.6) then follows from combining (5.12) and (5.13), with $\widetilde{\mathcal{C}}_1 := C_{\rm int}(1,d)C_1$ and $\widetilde{\mathcal{C}}_2 := C_{\rm int}(p,d)C_{\rm Sob}(p,d)C_2$.

5.4 Proof of Corollary 1.7

If u is the solution of the plane-wave scattering problem, then

$$|u|_{H^2(B_R)} \leq C_{\rm osc} k\, \|u\|_{H^1_k(B_R)} \tag{5.14}$$

by [39, Theorem 9.1 and Remark 9.10], where $C_{\rm osc}$ depends on A, c, d, and R, but is independent of k. The combination of (5.14) and (5.7) then imply that

$$\min_{v_N \in V_N} \|u - v_N\|_{H^1_k(B_R)} \leq \mathcal{C}_3 C_{\rm osc} \frac{hk}{p}\left(1 + \frac{hk}{p}\right) \|u\|_{H^1_k(B_R)}\,. \tag{5.15}$$

Combining (1.20), (5.15), and (1.19), we obtain the result (1.22) with $C_6 := \mathcal{C}_3 C_{\rm osc}$.

A Semiclassical pseudodifferential operators on the torus

Recall that for $R_\sharp > 0$ we defined the torus

$$\mathbb{T}^d_{R_\sharp} := \mathbb{R}^d/(2R_\sharp\mathbb{Z})^d.$$

This appendix reviews the material about semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_\sharp}$ used in §3.2, and appearing in Lemma 2.8, with our default references being [73] and [20, 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

$$\widehat{f}(j) := \int_{\mathbb{T}^d_{R_\sharp}} f(x)\overline{e_j}(x)\, dx,$$

where $j \in \mathbb{Z}^d$ and the integral is over the cube of side $2R_\sharp$, and where the Fourier basis given by the L^2-normalized functions

$$e_j(x) = (2R_\sharp)^{-d/2} \exp\big({\rm i}\pi j \cdot x/R_\sharp\big) \tag{A.1}$$

for $j \in \mathbb{Z}^d$. The Fourier inversion formula is then

$$f = \sum_{j \in \mathbb{Z}^d} \widehat{f}(j) e_j.$$

The action of the operator $(\hbar D)^\alpha$ on the torus is therefore

$$(\hbar D)^\alpha f = \sum_{j \in \mathbb{Z}^d} (\hbar j)^\alpha \widehat{f}(j) e_j.$$

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

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

and use the norm

$$\|u\|^2_{H^m_\hbar(\mathbb{T}^d_{R_\sharp})} := \sum |\widehat{f}(j)|^2 \langle \hbar j\rangle^{2m}; \tag{A.2}$$

see [73, §8.3], [20, §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 semiclassical Fourier transform: let the semiclassical Fourier transform $\mathcal{F}_\hbar$ (see [73, §3.3]) on the torus be defined for $\hbar > 0$ by

$$\mathcal{F}_\hbar \phi(\xi) := \int_{\mathbb{T}^d_{R_\sharp}} \exp\big(-\mathrm{i}x\cdot\xi/\hbar\big)\phi(x)\,\mathrm{d}x,$$

and for a function on $\mathbb{R}^d$, we set

$$\|u\|^2_{H^m_\hbar(\mathbb{R}^d)} := (2\pi\hbar)^{-d}\int_{\mathbb{R}^d} \langle\xi\rangle^m |\mathcal{F}_\hbar u(\xi)|^2\,\mathrm{d}\xi.$$

We note for later use that the inverse semiclassical Fourier transform has a pre-factor of $(2\pi\hbar)^{-d}$ in this normalisation.

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,

$$\overline{T}^*\mathbb{T}^d_{R_\sharp} := \mathbb{R}^d \times B^d,$$

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 [20, §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 $a = (a_\hbar)_{0<\hbar\le\hbar_0}$, 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

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

where $C_{\alpha,\beta}$ does not depend on $\hbar$; see [73, p. 207], [20, §E.1.2].

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

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

[73, §4.1] [20, Page 543]. The integral in (A.3) need not converge, and can be understood *either* as an oscillatory integral in the sense of [73, §3.6], [34, §7.8], *or* as an iterated integral, with the y integration performed first; see [20, 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 [73, §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 simply 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., [73, §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 [73, Theorem 8.10], [20, 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 $A = O(\hbar^\infty)_{\Psi^{-\infty}}$ 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 $a \in S^m$,

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

see [73, Page 213], [20, 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 $A = \mathrm{Op}_\hbar^{\mathbb{T}^d_{R_\sharp}}(a) \in \Psi_\hbar^m$, 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 [73, Page 194], [20, 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 $\hbar$.

Three properties of the semiclassical operator wavefront set that we use in §3.2 are

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

(see [20, E.2.2]),

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

(see [20, E.2.4]),

$$\mathrm{WF}_\hbar(AB) \subset \mathrm{WF}_\hbar A \cap \mathrm{WF}_\hbar B, \tag{A.9}$$

(see [73, §8.4], [20, E.2.5]),

$$\mathrm{WF}_\hbar(A) \cap \mathrm{WF}_\hbar(B) = \emptyset \quad \text{implies that} \quad AB = O(\hbar^\infty)_{\Psi^{-\infty}}, \tag{A.10}$$

(by, e.g., (A.9) together with [20, E.2.3]), and

$$\mathrm{WF}_\hbar \big(\mathrm{Op}_\hbar(a)\big) \subset \operatorname{supp} a \tag{A.11}$$

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

Ellipticity. We say that $B \in \Psi_\hbar^m$ 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 [20, Proposition E.32]) [2] *Let $A \in \Psi_\hbar^\ell(\mathbb{T}^d_{R_\sharp})$ and $B \in \Psi_\hbar^m(\mathbb{T}^d_{R_\sharp})$ be such that B is elliptic on $\mathrm{WF}_\hbar(A)$. Then there exist $S, S' \in \Psi_\hbar^{\ell-m}(\mathbb{T}^d_{R_\sharp})$ such that*

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

with

$$\mathrm{WF}_\hbar S \subset \mathrm{WF}_\hbar A, \qquad \mathrm{WF}_\hbar S' \subset \mathrm{WF}_\hbar A.$$

Functional Calculus. The main properties of the functional calculus in the black-box context are recalled in §2.3; 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

$$f(-\hbar^2\Delta)v = \sum_{j \in \mathbb{Z}^d} \widehat{v}(j) f(\hbar^2 |j|^2 \pi^2 / R_\sharp^2) e_j. \tag{A.12}$$

It is reassuring to discover that indeed it 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 *For $f \in S^m(\mathbb{R}^1)$ (i.e., f is a function of only one variable),*

$$f(-\hbar^2\Delta) = \mathrm{Op}_\hbar f(|\xi|^2).$$

[2] We highlight that working in a compact manifold allows us to dispense with the proper-support assumption appearing in [40, §4], [20, Proposition E.32, Theorem E.33].

Proof. First note that for $v \in C^\infty(\mathbb{T}^d_{R_\sharp})$,

$$
\begin{aligned}
v &= \sum \widehat{v}(j) e_j \\
&= (2R_\sharp)^{-d/2} \int_{\mathbb{R}^d} \sum_{j\in\mathbb{Z}^d} \widehat{v}(j)\delta(\xi - \hbar\pi j/R_\sharp)\exp(\mathrm{i}\xi x/\hbar)\,\mathrm{d}\xi \\
&= (2\pi\hbar)^d (2R_\sharp)^{-d/2} \mathcal{F}_\hbar^{-1} \sum_{j\in\mathbb{Z}^d} \widehat{v}(j)\delta(\xi - \hbar\pi j/R_\sharp).
\end{aligned} \tag{A.13}
$$

Thus, if we take the semiclassical Fourier transform of v, regarded as a periodic function,

$$
\mathcal{F}_\hbar v(\xi) = (2\pi\hbar)^d (2R_\sharp)^{-d/2} \sum_{j\in\mathbb{Z}^d} \widehat{v}(j)\delta(\xi - \hbar\pi j/R_\sharp).
$$

Consequently,

$$
\begin{aligned}
\mathcal{F}_\hbar\big[f(-\hbar^2\Delta)v\big](\xi) &= (2\pi\hbar)^d (2R_\sharp)^{-d/2} \sum_{j\in\mathbb{Z}^d} f(\hbar^2\pi^2|j|^2/R_\sharp^2)\widehat{v}(j)\delta(\xi - \hbar\pi j/R_\sharp) \\
&= (2\pi\hbar)^d (2R_\sharp)^{-d/2} \sum_{j\in\mathbb{Z}^d} f(|\xi|^2)\widehat{v}(j)\delta(\xi - \hbar\pi j/R_\sharp) \\
&= f(|\xi|^2)\mathcal{F}_\hbar[v](\xi),
\end{aligned}
$$

by (A.13), from which

$$
f(-\hbar^2\Delta)v = \mathrm{Op}_\hbar f(|\xi|^2)(v).
$$

∎

B Proof of (BB5) for the transmission problem

By the min-max principle for self-adjoint operators with compact resolvent (see, e.g., [58, Page 76, Theorem 13.1])

$$
\lambda_n = \inf_{X\in\Phi_n(\mathcal{D}^\sharp)} \sup_{u\in X} \frac{\langle P^\# u, u\rangle_{\beta,c}}{\|u_+\|^2_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + \beta^{-1}\|u_-/c\|^2_{L^2(\mathcal{O}_-)}}, \tag{B.1}
$$

where $(\lambda_n)_{n\geq 1}$ denotes the ordered eigenvalues of $P^\#$, $\mathcal{D}^\sharp$ is the domain of $P^\#$ defined by (2.4) (with $\mathcal{D}$ given by (2.9)), $\Phi_n(\mathcal{D}^\sharp)$ the set of all n-dimensional subspaces of $\mathcal{D}^\sharp$, and $\langle\cdot,\cdot\rangle_{\beta,c}$ is the scalar product defined implicitly by the norm in the denominator (which is the norm in Lemma 2.4).

By Green's identity and the definition of $\mathcal{D}^\sharp$,

$$
\langle P^\# u, u\rangle_{\beta,c} = \hbar^2\langle A_+\nabla u_+, \nabla u_+\rangle_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + \beta^{-1}\hbar^2\langle A_-\nabla u_-, \nabla u_-\rangle_{L^2(\mathcal{O}_-)}. \tag{B.2}
$$

Furthermore,

$$
\frac{\langle A_+\nabla u_+, \nabla u_+\rangle_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + \beta^{-1}\langle A_-\nabla u_-, \nabla u_-\rangle_{L^2(\mathcal{O}_-)}}{\|u_+\|^2_{L^2(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)} + \beta^{-1}\|u_-/c\|^2_{L^2(\mathcal{O}_-)}} \geq \frac{\min\big((A_+)_{\min},\, \beta^{-1}(A_-)_{\min}\big)}{\max\big(1,\, \beta^{-1}(c_{\min})^{-2}\big)} \frac{\|\nabla u\|^2_{L^2(\mathbb{T}^d_{R_\sharp})}}{\|u\|^2_{L^2(\mathbb{T}^d_{R_\sharp})}}. \tag{B.3}
$$

The definition of $\mathcal{D}^\sharp$ implies that

$$
\mathcal{D}^\sharp \subset \big\{(u_1,u_2)\in H^1(\mathbb{T}^d_{R_\sharp}\setminus\mathcal{O}_-)\oplus H^1(\mathcal{O}_-) \text{ such that } u_1 = u_2 \text{ on } \partial\mathcal{O}_-\big\} = H^1(\mathbb{T}^d_{R_\sharp}). \tag{B.4}
$$

Using (B.2), (B.3), and (B.4) in (B.1), we have

$$
\lambda_n \geq \frac{\min\big((A_+)_{\min},\, \beta^{-1}(A_-)_{\min}\big)}{\max\big(1,\, \beta^{-1}(c_{\min})^{-2}\big)} \left(\inf_{X\in\Phi_n(H^1(\mathbb{T}^d_{R_\sharp}))} \sup_{u\in X} \frac{\hbar^2\|\nabla u\|^2_{L^2(\mathbb{T}^d_{R_\sharp})}}{\|u\|^2_{L^2(\mathbb{T}^d_{R_\sharp})}} \right).
$$

The result then follows from the min-max principle for the eigenvalues of the Laplacian on the torus.

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