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 [52], [53], [26], and [51] 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 [36], this paper proves analogous decompositions for scattering problems fitting into the black-box scattering framework of Sjöstrand–Zworski [67], thus covering Helmholtz problems with variable coefficients, impenetrable obstacles, and penetrable obstacles all at once.

In particular, these results allow us to prove new frequency-explicit convergence results for (i) the $hp$-finite-element method applied to the variable coefficient Helmholtz equation in the exterior of a Dirichlet obstacle, when the obstacle and coefficients are analytic, and (ii) the $h$-finite-element method applied to the Helmholtz penetrable-obstacle transmission problem.

1 Introduction

1.1 Context: the results of [52], [53], [26], [51] and their impact on numerical analysis of the Helmholtz equation.

At the heart of the papers [52], [53], [26], and [51] are results that decompose solutions of the high-frequency Helmholtz equation, i.e.,

$$\Delta u + k^2 u = -f$$  \hspace{1cm} (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 $u = u_{H^2} + u_A$.

Such a decomposition was obtained for

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

$$\frac{\partial u}{\partial r}(x) -iku(x) = o\left(\frac{1}{r^{(d-1)/2}}\right)$$  \hspace{1cm} (1.2)

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as $r := |x| \to \infty$, uniformly in $\widehat{x} := x/r$ [52, Lemma 3.5],

- the Helmholtz exterior Dirichlet problem where the obstacle has analytic boundary [53, Theorem 4.20], and

- the Helmholtz interior impedance problem where the domain is either analytic ($d = 2, 3$) [53, Theorem 4.10], [51, Theorem 4.5], or polygonal [53, Theorem 4.10], [26, 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 [42]).

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 [52], [53], [26], [51], [75], [74], [21], [7]. 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 $h$-FEM with large but fixed $p$ [27], [20], [41]. Furthermore, analogous decompositions and analogous convergence results were obtained for $hp$-boundary-element methods [50], [46], $hp$ methods applied to Helmholtz problems with arbitrarily-small dissipation [55] and $hp$ methods applied to formulations of the time-harmonic Maxwell equations [54], [58]. This work has also motivated attempts to provide simpler decompositions valid for a variety of variable-coefficient problems [15].

Our recent paper [43] obtained the analogous decomposition to that in [52] for the Helmholtz problem in $\mathbb{R}^d$ but now for the variable-coefficient Helmholtz equation

$$\nabla \cdot (A \nabla u) + \frac{k^2}{c^2} u = -f$$  \hspace{1cm} (1.3)$$

with $A$ and $c \in C^\infty$. The goal of the present paper is to obtain decompositions for more-general Helmholtz problems. This is achieved in Theorem 1.1 below, and in §1.5 we show how the results of [43] follow as a corollary of Theorem 1.1. In §1.6 we discuss the ideas behind both [43] and Theorem 1.1, and the relationship between them.

### 1.2 Statement of the main result

The following theorem (Theorem 1.1) obtains the decomposition $u = u_{H^2} + u_A$ in the framework of black-box scattering introduced by Sjöstrand–Zworski in [67]. In this framework, the operator $P_h$, where $h := k^{-1}$ is the semiclassical parameter \footnote{The semiclassical parameter is often denoted by $h$, but we use $h$ to avoid a notational clash with the meshwidth of the FEM appearing in §1.1 and used in Theorems 1.7 and 1.14 below}, 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 Theorem 1.1 is specialised to these settings in Theorems 1.6 and 1.12, respectively.

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 $H$ is $L^2$; the subspace $\mathcal{D}$ is $H^2$ (i.e. the domain of the Laplacian) and $\mathcal{D}^k = H^{2k}$; the operator $P_h$ is $-h^2 \Delta$. The superscript $\mathcal{Z}$ denotes the corresponding object compactified onto a large reference torus.
Theorem 1.1 (The decomposition in the black-box setting) Let \( P_h \) 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 \( h_0 > 0 \), there exists \( H \subset (0, h_0) \) such that the following two assumptions hold.

1. There exists \( D_{\text{out}} \subset D_{\text{loc}} \) and \( M > 0 \) such that for any \( \chi \in C_c^\infty(\mathbb{R}^d) \) equal to one near \( B_{R_0} \), there exists \( C > 0 \) such that if \( v \in D_{\text{out}} \) is a solution to \((P_h-1)v = \chi g\), then
   \[
   \|\chi v\|_\mathcal{H} \leq C h^{-M-1} \|g\|_\mathcal{H} \quad \text{for all } h \in H.
   \] (1.4)

2. There exists \( E \in C_0(\mathbb{R}) \) that is nowhere zero on \([-\Lambda, \Lambda]\) and such that \( E(P_h^*) = \mathcal{E}_0 + O(h^\infty)_{P_h^*} \rightarrow D^\infty_+ \) and \( \rho \in C^\infty(\mathcal{T}_{R_h}^h) \) equal to one near \( B_{R_0} \), such that, for some \( \alpha \)-family of black-box differentiation operators \((D(\alpha))_{\alpha \in \mathcal{A}}\),
   \[
   \|\rho D(\alpha)^0 E_0^v\|_\mathcal{H} \leq C_{E}(\alpha, h)\|v\|_\mathcal{H} \quad \text{for all } v \in D_0^\infty \text{ and } h \in H,
   \] (1.5)
   for some \( C_{E}(\alpha, h) > 0 \).

Then, given \( R > 0 \) such that \( R_0 < R < R_1 \), if \( g \in \mathcal{H} \) is compactly supported in \( B_R \) and \( u \in D_{\text{out}} \) satisfies
   \[
   (P_h-1)u = g,
   \] (1.6)
then there exists \( u_{H^2} \in D^I \) and \( u_A \in D_0^\infty \) such that
   \[
   u|_{B_R} = (u_{H^2} + u_A)|_{B_R}.
   \] (1.7)
Furthermore, \( u_{H^2} \) satisfies
   \[
   \|u_{H^2}\|_{HI} + \|P_h^0 u_{H^2}\|_{HI} \lesssim \|g\|_\mathcal{H} \quad \text{for all } h \in H,
   \] (1.8)
and for any \( \tilde{R} > 0 \) with \( R_0 < \tilde{R} < R_1 \), there exist \( R_i, R_{hi}, R_{iv}, R_{0i} \) with \( R_0 < R_i < R_{hi} < R_{iv} < R_{1} < \tilde{R} \) such that \( u_A \) decomposes as
   \[
   u_A = u_{A}^{R_0} + u_{A}^{\infty},
   \] (1.9)
where \( u_{A}^{R_0} \) is regular near the black-box and negligible away from it, in the sense that
   \[
   \|D(\alpha)u_{A}^{R_0}\|_{H^\alpha(B_{R_0})} \lesssim C_{E}(\alpha, h)h^{-M-1}\|g\|_\mathcal{H} \quad \text{for all } h \in H \text{ and } \alpha \in \mathcal{A},
   \] (1.10)
and, for any \( N, m > 0 \) there exists \( C_{N,m} > 0 \) such that
   \[
   \|u_{A}^{R_0}\|_{D_h^m((B_{R_0})^c)} \leq C_{N,m} h^N \|g\|_\mathcal{H} \quad \text{for all } h \in H \text{ and } \alpha \in \mathcal{A},
   \] (1.11)
and \( u_{A}^{\infty} \) is regular away from the black-box and negligible near it, in the sense that for some \( \lambda > 1 \)
   \[
   \|
   \partial^\alpha u_{A}^{\infty}\|_{H^\alpha((B_{R_0})^c)} \lesssim \lambda^{\alpha} h^{-\alpha-\lambda-M-1}\|g\|_\mathcal{H} \quad \text{for all } h \in H \text{ and } \alpha \in \mathcal{A},
   \] (1.12)
and, for any \( N, m > 0 \) there exists \( C_{N,m} > 0 \) such that
   \[
   \|u_{A}^{\infty}\|_{D_h^m((B_{R_0})^c)} \leq C_{N,m} h^N \|g\|_\mathcal{H} \quad \text{for all } h \in H \text{ and } \alpha \in \mathcal{A}.
   \] (1.13)
In addition, if \( \rho = 1 \), the decomposition (1.7) can be constructed in such a way that instead of (1.9)--(1.13), \( u_A \) satisfies the global regularity estimate
   \[
   \|D(\alpha)u_A\|_{H^\alpha} \lesssim C_{E}(\alpha, h)h^{-M-1}\|g\|_\mathcal{H} \quad \text{for all } h \in H \text{ and } \alpha \in \mathcal{A}.
   \] (1.14)
Finally, the omitted constants in (1.8) and (1.10)--(1.14) are independent of \( h \) and \( \alpha \).
Point 1 in Theorem 1.1 is the assumption that the solution operator is polynomially bounded in $h$. In the setting of impenetrable-obstacle problems, this assumption holds with $M = 0$ and $H = (0, h_0)$ when the problem is nontrapping (see Theorem 1.5 below and the references therein). In the black-box setting, [42] proved that this assumption always holds with $M > 5d/2$ and the complement of the set $\hat{H}$ having arbitrarily-small measure (we note that, under an additional assumption about the location of resonances, a similar result with a larger $M$ can also be extracted from [69, Proposition 3] by using the Markov inequality).

Point 2 in Theorem 1.1 is a regularity assumption that depends on the contents of the black box. We later refer to (1.5) as the “low-frequency estimate”, since the fact that $\mathcal{F}$ is nowhere zero on $[-\Lambda, \Lambda]$ means that it bounds low-frequency components. The cutoff $\rho$ in (1.5) 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 (1.5) in this case cannot hold in the transition region outside the black box, where the coefficients cannot be analytic.

Regarding $u_{H^2}$: comparing (1.4) and (1.8), we see that $u_{H^2}$ satisfies a bound with better $h$-dependence than that satisfied by $u$; this is the analogue of the property (i) in §1.1 of the results of [52], [53], [26], [51]. The regularity of $u_{H^2}$ depends on the domain of the operator ($u_{H^2} \in \mathcal{D}^\delta$) but not on any other features of the black box (in particular, not on the regularity estimate (1.5)).

Regarding $u_A$: $u_A$ is in the domain of arbitrary powers of the operator ($u_A \in \mathcal{D}^{1,\infty}_H$) and so is smooth in an abstract sense. $u_A$ is split further into two parts: $u_A^{R_0}$ regular near the black-box and negligible away from it, and $u_A^\infty$ regular away from the black-box and negligible near it; see Figure 1.1. Comparing (1.4) and (1.10)/(1.12), we see that, in the regions where they are not negligible, $u_A^{R_0}$ and $u_A^\infty$ satisfy bounds with the same $h$-dependence as $u$, but with improved regularity. These properties are the analogue of the property (ii) in §1.1 of the results of [52], [53], [26], [51]. In particular, the regularity of $u_A$ depends on the regularity inside the black-box (from (1.5)), and, for the exterior Dirichlet problem with analytic obstacle and coefficients analytic in a neighbourhood of the obstacle, $u_A$ is analytic.

### 1.3 The main result applied to the exterior Dirichlet problem

#### 1.3.1 Background definitions

**Definition 1.2 (Exterior Dirichlet problem)** Let $\mathcal{O}_- \subset \mathbb{R}^d$, $d \geq 2$ 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 $A \in C^{0,1}(\mathcal{O}_+, \mathbb{R}^{n \times n})$ be such that $\text{supp}(I - A) \subset B_{R_1}$, with $R_1 > R_0$, $A$ is symmetric, and there exists $A_{\min} > 0$ such that

\[ (A(x)\xi) \cdot \xi \geq A_{\min}|\xi|^2 \quad \text{for all } x \in \mathcal{O}_+ \text{ and all } \xi \in \mathbb{C}^d. \quad (1.15) \]

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

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Figure 1.1: The regions where $u_A^{R_0}$ and $u_A^\infty$ appearing in Theorem 1.1 are regular, analytic, or $O(h^\infty)$. Recall from (1.9) that $u_A = u_A^{R_0} + u_A^\infty$. 
Given $f \in L^2(\Omega_+)$ with $\text{supp} f \subseteq \mathbb{R}^d$ and $k > 0$, $u \in H^1_{\text{loc}}(\Omega_+)$ satisfies the exterior Dirichlet problem if
\begin{align}
e^2 \nabla \cdot (A \nabla u) + k^2 u &= -f \quad \text{in } \Omega_+, \\
u &= 0 \quad \text{on } \partial \Omega_+, \tag{1.16}
\end{align}
and $u$ satisfies the Sommerfeld radiation condition (1.2).

We highlight from Definition 1.2 that the obstacle $\Omega_-$ 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, $\| \cdot \|_{H^1_k(B_R \cap \Omega_+)}$, defined by
\begin{equation}
\| u \|_{H^1_k(B_R \cap \Omega_+)}^2 = \| \nabla u \|_{L^2(B_R \cap \Omega_+)}^2 + k^2 \| u \|_{L^2(B_R \cap \Omega_+)}^2. \tag{1.18}
\end{equation}

**Definition 1.3 (\textit{C}_{\text{sol}})** Given $f \in L^2(\Omega_+)$ supported in $B_R$ with $R \geq R_1$, let $u$ be the solution of the exterior Dirichlet problem of Definition 1.2. Given $k_0 > 0$, let $C_{\text{sol}} = C_{\text{sol}}(k, A, c, R, k_0) > 0$ be such that
\begin{equation}
\| u \|_{H^1_k(B_R \cap \Omega_+)} \leq C_{\text{sol}} \| f \|_{L^2(B_R \cap \Omega_+)} \quad \text{for all } k > 0. \tag{1.19}
\end{equation}

$C_{\text{sol}}$ exists by standard results about uniqueness of the exterior Dirichlet problem and Fredholm theory; see, e.g., [33, §1] and the references therein. How $C_{\text{sol}}$ depends on $k$ is crucial to our analysis, and to emphasise this we write $C_{\text{sol}} = C_{\text{sol}}(k)$. A key assumption in our analysis is that $C_{\text{sol}}(k)$ is polynomially bounded in $k$ in the following sense.

**Definition 1.4 (\textit{C}_{\text{sol}} \text{ is polynomially bounded in } k** Given $k_0$ and $K \subset [k_0, \infty)$, $C_{\text{sol}}(k)$ is polynomially bounded for $k \in K$ if there exists $C > 0$ and $M > 0$ such that
\begin{equation}
C_{\text{sol}}(k) \leq Ck^M \quad \text{for all } k \in K, \tag{1.20}
\end{equation}
where $C$ and $M$ are independent of $k$ (but depend on $k_0$ and possibly also on $K, A, c, d, R$).

There exist $C^\infty$ coefficients $A$ and $c$ such that $C_{\text{sol}}(k_j) \geq C_1 \exp(C_2k_j)$ for $0 < k_1 < k_2 < \ldots$ with $k_j \to \infty$ as $j \to \infty$, see [60], but this exponential growth is the worst-possible, since $C_{\text{sol}}(k) \leq c_3 \exp(c_4 k)$ for all $k \geq k_0$ by [8, Theorem 2]. We now recall results on when $C_{\text{sol}}(k)$ is polynomially bounded in $k$.

**Theorem 1.5 (Conditions under which \textit{C}_{\text{sol}}(k) \text{ is polynomially bounded in } k \text{ for the exterior Dirichlet problem)**

(i) If $A$ and $c$ are $C^\infty$ and nontrapping (i.e., all the trajectories of the generalised bicharacteristic flow defined by the semiclassical principal symbol of (1.16) starting in $B_R$ leave $B_R$ after a uniform time), then $C_{\text{sol}}(k)$ is independent of $k$ for all sufficiently large $k$; i.e., (1.20) 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
\begin{equation}
C_{\text{sol}}(k) \leq Ck^{5d/2 + 1 + \varepsilon} \quad \text{for all } k \in [k_0, \infty) \setminus J, \tag{1.21}
\end{equation}
for any $\varepsilon > 0$, where $C$ depends on $\delta, \varepsilon, d, k_0$, and $A$. If both $\Omega_-$ 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 [56] combined with either [71, Theorem 3] or [72, Chapter 10, Theorem 2] or [44], or [9, Theorem 1.3 and §3]. It has recently been proved that, for this situation, $C_{\text{sol}}$ is proportional to the length of the longest trajectory in $B_R$; see [29, Theorems 1 and 2, and Equation 6.32]. (ii) is proved for $c = 1$ in [42, Theorem 1.1 and Corollary 3.6]; the proof for more-general $c$ follows from Lemma 2.3 below.
1.3.2 Theorem 1.1 applied to the exterior Dirichlet problem

Theorem 1.6 (Theorem 1.1 applied to the exterior Dirichlet problem with analytic $A, c$, and $O$) Suppose that $O, A, c, R_0$, and $R_3$ are as in Definition 1.2. In addition, assume that $O$ is analytic, and that $A$ and $c$ are $C^\infty$ everywhere and analytic in $B_{R_3}$ for some $R_0 < R_3 < R_1$.

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

$$u|_{B_R} = u_A + u_{H^2}.$$  

Furthermore, there exist $C_1$, independent of $k$ and $\alpha$, such that

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

and there exist $C_2, C_3, C_4$ and $C_5$, all independent of $k$ and $\alpha$, and $R_1, R_3, R_{\text{iv}}, R_{\text{iv}}$ with $R_0 < R_1 < R_3 < R_{\text{iv}} < R_{\text{iv}} < \tilde{R}$ such that $u_A$ decomposes as $u_A = u_{A}^{R_0} + u_{A}^{\infty}$, where $u_{A}^{R_0}$ is analytic in $B_{R_{\text{iv}}}$ and $u_{A}^{\infty}$ is analytic in $(B_{R_1})^c$ with

$$\|\partial^\alpha u_{A}^{R_0}\|_{L^2(B_{R_{\text{iv}}} \cap O_+)} \leq C_2 (C_4) |\alpha| |k_\alpha|^{-1+M} \|f\|_{L^2(B_R \cap O_+)} \quad \text{for all } k \in K \text{ and for all } \alpha,$$

$$\|\partial^\alpha u_{A}^{\infty}\|_{L^2((B_{R_1})^c \cap O_+)} \leq C_4 (C_5) |\alpha| |k_\alpha|^{-1+M} \|f\|_{L^2(B_R \cap O_+)} \quad \text{for all } k \in K \text{ and for all } \alpha,$$

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

$$\|u_{A}^{\infty}\|_{H^N(B_{R_1} \cap O_+)} + \|u_{A}^{R_0}\|_{H^N((B_{R_{\text{iv}}})^c \cap O_+)} \leq C_{N,m} k^{-N} \|f\|_{L^2(B_R \cap O_+)} \quad \text{for all } k \in K \text{ and for all } \alpha.$$  

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

As discussed in §1.1, Theorem 1.6 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: given $R \geq R_3$ and $F \in (H^1(B_R \cap O_+))^*$,

$$\text{find } u \in H^1(B_R \cap O_+) \text{ such that } a(u, v) = F(v) \quad \text{for all } v \in H^1(B_R \cap O_+),$$

where

$$a(u, v) := \int_{B_R \cap O_+} \left( (A \nabla u) \cdot \nabla v - \frac{k^2}{c^2} u v \right) - \langle \text{DtN}_k(u), v \rangle_{\partial B_R}$$

(1.26)

where $\langle \cdot, \cdot \rangle_{\partial B_R}$ denotes the duality pairing on $\partial B_R$ that is linear in the first argument and antilinear in the second, and $\text{DtN}_k : H^{1/2}(\partial B_R) \to H^{-1/2}(\partial B_R)$ 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 $\text{DtN}_k$ in terms of Hankel functions and polar coordinates (when $d = 2$)/spherical polar coordinates (when $d = 3$) is given in, e.g., [52, Equations 3.7 and 3.10]. We use later the fact that there exist $C_{\text{DIN}} = C_{\text{DIN}}(k_0 R_0)$ such that

$$\left| \langle \text{DtN}_k(u), v \rangle_{\partial B_R} \right| \leq C_{\text{DIN}} \|u\|_{H^1(B_R \cap O_+)} \|v\|_{H^1(B_R \cap O_+)}$$

(1.27)

for all $u, v \in H^1(B_R \cap O_+)$ and for all $k \geq k_0$; see [52, Lemma 3.3].

If $F(v) = \int_{B_R \cap O_+} f v$, then the solution of the variational problem (1.25) is the restriction to $B_R$ of the solution of the exterior Dirichlet problem of Definition 1.2. If

$$F(v) = \int_{\partial B_R} (\partial_n u' - \text{DtN}_k(u')) \nu,$$

(1.28)

where $u'$ is a solution of $\Delta u' + k^2 u' = 0$ in $B_R \cap O_+$, then the solution of the variational problem (1.25) is the restriction to $B_R \cap O_+$ of the sound-soft scattering problem (see, e.g, [11, Page 107]).
Given a sequence, \( \{ V_N \}_{N=0}^{\infty} \) of finite-dimensional subspaces of \( H^1(B_R \cap \Omega_+^c) \), the finite-element method for the variational problem (1.25) is the Galerkin method applied to the variational problem (1.25), i.e.,

\[
\text{find } u_N \in V_N \text{ such that } a(u_N, v_N) = F(v_N) \text{ for all } v_N \in V_N. \tag{1.29}
\]

**Theorem 1.7 (Quasioptimality of hp-FEM for the exterior Dirichlet problem)** Let \( d = 2 \) or 3. Suppose that \( \Omega_-, \Omega_+, A, c, R, R_1, \) and \( R_\infty \) are as in Theorem 1.6. Let \( \{ V_N \}_{N=0}^{\infty} \) be the piecewise-polynomial approximation spaces described in [52], [53], [5.1.1] (where, in particular, the triangulations are quasi-uniform, allow curved elements, and thus fit \( B_R \cap \Omega_+ \) exactly); assume further that the triangulations fit \( B_R \) and \( B_\infty \) exactly, and let \( u_N \) be the Galerkin solution defined by (1.29).

If \( C_{\text{sol}}(k) \) 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

\[
hk \leq C_1 \quad \text{and} \quad p \geq C_2 \log k,
\]

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

\[
\| u - u_N \|_{H^1(B_R \cap \Omega_+^c)} \leq C_{q_0} \min_{v_N \in V_N} \| u - v_N \|_{H^1(B_R \cap \Omega_+^c)},
\]

with

\[
C_{q_0} := \frac{2(\max\{A_{\text{max}}, c_{\text{min}}^{-2}\} + C_{\text{DN}})}{A_{\text{min}}},
\]

**Remark 1.8 (The significance of Theorem 1.7)** For finite-dimensional subspaces consisting of piecewise polynomials of degree \( p \) on meshes with meshwidth \( h \), the total number of degrees of freedom \( \sim (p/h)^d \). The results about Helmholtz hp-FEM in [52], [53], [26], [51], [43] show quasioptimality of the hp-FEM under the slightly weaker condition than (1.30), namely

\[
\frac{hk}{p} \leq C_1 \quad \text{and} \quad p \geq C_2 \log k,
\]

for \( C_1 \) sufficiently small and \( C_2 \) sufficiently large (but both independent of \( k, h, \) and \( p \)). These results then 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 mentioned in §1.1, the significance of this is that the h-FEM (i.e., with \( p \) fixed) is not quasioptimal with \( C_{q_0} \), independent of \( k \) when the total number of degrees of freedom \( \sim k^d \); this is called the pollution effect – see [2] and the references therein.

Theorem 1.7 shows that there is a choice of \( h \) and \( p \) such that the hp-FEM applied to the exterior Dirichlet problem of Definition 1.2 (with the obstacle and coefficients analytic) is quasioptimal with the total number of degrees of freedom \( \sim (k \log k)^d \).

Although this result is \( (\log k)^d \) away from proving that the hp-FEM applied to the exterior Dirichlet problem does not suffer from the pollution effect, it is nevertheless the first frequency-explicit result about the convergence of the hp-FEM applied the exterior Dirichlet problem (with the obstacle and coefficients analytic). Our understanding is that the sharp result will be proved in the forthcoming paper [5] announced in [6].

In the specific case of the plane-wave scattering problem, the recent results of [41, Theorem 9.1 and Remark 9.10] allow us to bound the best approximation error on the right-hand side of (1.31) and obtain a bound on the relative error.

**Corollary 1.9 (Bound on the relative error of the Galerkin solution)** Let the assumptions of Theorem 1.7 hold and, furthermore, let \( F(v) \) be given by (1.28) with \( u^j(x) = \exp(ikx \cdot a) \) for some \( a \in \mathbb{R}^d \) with \( |a| = 1 \) (so that \( u \) is then the solution of the plane-wave scattering problem). If \( C_{\text{sol}}(k) \) 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 1.7, if (1.30) holds, then, for all \( k \in K \cap [k_1, \infty) \),

\[
\frac{\| u - u_N \|_{H^1(B_R \cap \Omega_+^c)}}{\| u \|_{H^1(B_R \cap \Omega_+^c)}} \leq C_{q_0} C_3 \frac{C_1}{C_2 \log k} \left(1 + \frac{C_1}{C_2 \log k}\right),
\]

with \( C_{q_0} \) given by (1.32); i.e. the relative error can be made arbitrarily small by making \( C_1 \) smaller.
1.4 The main result applied to the transmission problem

1.4.1 Background definitions

Definition 1.10 (Transmission problem (i.e. scattering by a penetrable obstacle)) Let $O_- \subset \mathbb{R}^d$, $d \geq 2$ be a bounded Lipschitz open set such that the open complement $O_+ := \mathbb{R}^d \setminus O_-$ is connected and such that $O_- \subset B_{R_0}$. Let $A = (A_-, A_+)$ with $A_\pm \in C^{0,1}(\mathbb{R}^d_\pm, \mathbb{R}^{n \times n})$ be such that $\text{supp}(I - A) \subset B_{R_0}$, $A$ is symmetric, and there exists $A_{\text{min}} > 0$ such that (1.15) holds (with $O_+$ replaced by $\mathbb{R}^d$). Let $c \in L^\infty(O_-)$ be such that $c_{\text{min}} \leq c \leq c_{\text{max}}$ with $0 < c_{\text{min}} \leq c_{\text{max}} < \infty$. Let $\beta > 0$.

Let $v$ be the unit normal vector field on $\partial O_-$ pointing from $O_-$ into $O_+$, and let $\partial_{v,A} u$ denote the corresponding conormal derivative defined by, e.g., [47, Lemma 4.3] (recall that this is such that, when $v \in H^2(O_+)$, $\partial_{v,A} u = v \cdot \gamma(A \nabla u)$).

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

$$c^2 \nabla \cdot (A_- \nabla u_-) + k^2 u_- = -f \quad \text{in } O_-,$$

$$\nabla \cdot (A_+ \nabla u_+) + k^2 u_+ = -f \quad \text{in } O_+,$$

$$u_- = u_+, \quad \partial_{v,A} u_- = \beta \partial_{v,A} u_+ \quad \text{on } \partial O_-,$$  \hspace{1cm} (1.35)

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 $\beta$ are redundant. For example, by rescaling $u_-, u_+$, and $f$, all such transmission problems can be described by the parameters $c$ and $\beta$ (with $A_- = A_+ = 1$), as in, e.g., [10], or by the parameters $A_-$ and $c$ (with $A_+ = \beta = 1$); see, e.g., the discussion and examples after [57, Definition 2.3].

The definition of $C_{\text{sol}}$ for the transmission problem is almost identical to Definition 1.3, except that the norms in (1.19) are now over $B_R$ (as opposed to $B_R \cap O_+$) and now $C_{\text{sol}}$ depends additionally on $\beta$.

Theorem 1.11 (Conditions under which $C_{\text{sol}}(k)$ is polynomially bounded in $k$ for the transmission problem) In each of the following conditions we assume that $O_-, A$, and $c$ are as in Definition 1.10.

(i) If $O_-$ is smooth and strictly convex with strictly positive curvature, $A = I$, $c$ is a constant $\leq 1$, and $\beta > 0$, then $C_{\text{sol}}(k)$ is independent of $k$ for all sufficiently large $k$; i.e., (1.19) holds for all $k \geq k_0$ with $M = 0$.

(ii) If $O_-$ is Lipschitz and star-shaped, $A = I$, and $c$ is a constant with $c^2 \leq \beta \leq 1$.

(iii) If $O_-$ is star-shaped, $\beta = 1$, and both $A$ and $c$ are monotonically non-increasing in the radial direction (in the sense of [33, Condition 2.6]).

(iv) Given $k_0 > 0$ and $\delta > 0$ there exists a set $J \subset [k_0, \infty)$ with $|J| \leq \delta$ such that

$$C_{\text{sol}}(k) \leq C k^{5d/2 + 1 + \varepsilon} \quad \text{for all } k \in [k_0, \infty) \setminus J,$$  \hspace{1cm} (1.36)

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

References for the proof. (i) is proved in [10, Theorem 1.1] (we note that, in fact, a stronger result with $A_-$ variable is also proved there). (ii) is proved in [57, Theorem 3.1]. (iii) is proved in [33, Theorem 2.7]. (iv) is proved for constant $c$ and globally Lipschitz $A$ in [42, 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 1.1 applied to the transmission problem

Theorem 1.12 (Theorem 1.1 applied to the transmission problem) Suppose that $O_-, A, c$, and $\beta$, are as in Definition 1.10 and, additionally, $A$ and $c$ are $C^{2m-2,1}$ and $O_-$ is $C^{2m-1,1}$.

If $C_{\text{sol}}(k)$ 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
Furthermore there exists \( u_A = (u_+,A; u_-,A) \in C^\infty(B_R \cap O_+) \times C^\infty(O_-) \) and \( u_{HZ} = (u_+,HZ; u_-,HZ) \in H^2(B_R \cap O_+) \times H^2(O_-) \), satisfying (1.35), and such that

\[
u|_{B_R} = u_A + u_{HZ}.
\]

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

\[
\|\partial^\alpha u_\pm,H \|_{L^2(B_R \cap O_\pm)} \leq C_1 k^{\|\alpha\| - 2} \|f\|_{L^2(B_R)} \quad \text{for all } k \in K \text{ and for all } |\alpha| \leq 2, \tag{1.37}
\]

and

\[
\|\partial^\alpha u_\pm,A \|_{L^2(B_R \cap O_\pm)} \leq C_2(m) k^{\|\alpha\| - 1 + \ell} \|f\|_{L^2(B_R)} \quad \text{for all } k \in K \text{ and for all } |\alpha| \leq 2m. \tag{1.38}
\]

### 1.4.3 Corollary about frequency-explicit convergence of the \( h \)-FEM

For simplicity we consider the case where the parameter \( \beta \) in the transmission condition (1.35) equals one; recall from the comments below Definition 1.10 that, at least in the constant-coefficient case, this is without loss of generality. The variational formulation of the transmission problem is then (1.25) with \( B_R \cap O_+ \) replaced by \( B_R \) and \( a(\cdot, \cdot) \) given by (1.26) with \( c \) understood as equal to one in \( B_R \cap O_+ \).

Since the constant \( C_2 \) in (1.38) depends on \( m \), we cannot prove a result about the \( hp \)-FEM for the transmission problem of Definition 1.10. We therefore consider the \( h \)-FEM and prove the first sharp quasioptimality result for this problem (see Remark 1.15 below for more discussion on the novelty of our result).

**Assumption 1.13** \( (V_N)^{\infty}_{N=0} \) 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 \( O_- \), so that each element in the mesh is included in either \( O_- \) or \( B_R \cap O_+ \), 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

\[
\|v - I_{h,p}v\|_{H^j(B_R)} \leq C(j, \ell, d) h^{\ell + 1 - j} \left( \|v_+\|_{H^{\ell+1}(B_R \cap O_+)} + \|v_-\|_{H^{\ell+1}(O_-)} \right) \tag{1.39}
\]

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

Assumption 1.13 is satisfied by the \( hp \) approximation spaces described in \([52, \S 5] \), \([53, \S 5.1.1] \) (with (1.39) holding by \([52, \text{Theorem B.4}] \), and also by curved Lagrange finite-element spaces in \([4] \) (with (1.39) holding by \([4, \text{Theorem 4.1 and Corollary 4.1}] \)).

**Theorem 1.14 (Quasioptimality of \( h \)-FEM for the transmission problem)** Let \( d = 2 \) or 3. Suppose that \( \beta = 1 \), \( A, c, \) and \( O_- \) are as in Definition 1.10. Given an integer \( p \), if \( p \) is odd assume that \( O_- \) is \( C^{p-1} \) and both \( A \) and \( c \) are \( C^{p-1,1} \); if \( p \) is even, assume that \( O_- \) is \( C^{p+1,1} \) and both \( A \) and \( c \) are \( C^p \).

Let \((V_N)^{\infty}_{N=0}\) be a sequence of piecewise-polynomial approximation spaces of degree \( p \) satisfying Assumption 1.13 and let \( u_N \) be the Galerkin solution defined by (1.29).

If \( C_{\text{sol}}(k) \) 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

\[
h^p k^p + M \leq C
\]

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

\[
\|u - u_N\|_{H^j(B_R)} \leq C_{qo} \min_{v_N \in V_N} \|u - v_N\|_{H^j(B_R)},
\]

with \( C_{qo} \) given by (1.32).

The regularity assumptions in Theorem 1.14 are optimal with \( p \) is odd, but suboptimal when \( p \) is even. This is due to Theorem 1.12 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 (4.11) in the proof of Theorem 1.12). For example, when \( p = 2 \) we require \( u \in H^2 \) in Theorem 1.14, but we achieve this by requiring that \( O_- \), \( A \), and \( c \) are such that \( u \in H^4 \).
Remark 1.15 (The significance of Theorem 1.14) 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 [48, Prop. 8.2.7], [34, Theorem 4.5], [29, Theorem 3] (building on the 1-d results of [1, Theorem 3.2], [39, Theorem 3], [38, Theorem 4.13], and [40, Theorem 3.5]) and for \( p > 1 \) in [52, Corollary 5.6], [53, Remark 5.9], [30, Theorem 5.1], and [15, Theorem 2.15]. Numerical experiments indicate that this condition is also necessary – see, e.g., [15, §4.4].

Of these existing results, only [15, Theorem 2.15] covers the Helmholtz equation with variable \( A \) and \( c \) that are also allowed to be discontinuous. However, the results in [15] hold only when an impedance boundary condition is imposed on the truncation boundary (in our case \( \partial B_R \)), which is equivalent to approximating the exterior Helmholtz Dirichlet-to-Neumann map by \( i k \). Furthermore, the proof of [15, Theorem 2.15] uses the impedance boundary condition in an essential way. Indeed, in [15, 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 \( \partial B_R \) one has \( \partial_n u_{j+1} = i u_j \); this relationship between \( u_{j+1} \) and \( u_j \) on \( \partial B_R \) no longer holds if \( \text{DtN}_k \) is not approximated by \( i k \).

The Helmholtz equation with an impedance boundary condition is often used as a model problem for numerical analysis (see, e.g., the references in [28, §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 \( i k \) is bounded away from zero, independently of \( k \), even in the best-possible situation when the truncation boundary equals \( \partial B_R \) for some \( R \); see [28, §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 \( C^\infty \) coefficients

Theorem 1.1 can also be used to recover the main result of [43], namely [43, Theorem 3.1].

Theorem 1.16 (The main result of [43] as a corollary of Theorem 1.1) Assume that \( O_\| = \emptyset \) and that \( A, c \) are as in Definition 1.2 and are furthermore \( C^\infty \). If \( C_{\text{eq}}(k) \) 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 (1.16), (1.2) is such that there exists \( u_A, \) analytic in \( B_R \), and \( u_{H^2} \in H^2(B_R) \), such that

\[
\| \partial^\alpha u_{\text{H}^2} \|_{L^2(B_R)} \leq C_1 k^{\|\alpha\|_2 - 2} \| f \|_{L^2(B_R)} \quad \text{for all } k \in K \text{ and for all } |\alpha| \leq 2,
\]

(1.40)

and

\[
\| \partial^\alpha u_A \|_{L^2(B_R)} \leq C_2 (C_{\|})^{\|\alpha\|} k^{\|\alpha\|-1+M} \| f \|_{L^2(B_R)} \quad \text{for all } k \in K \text{ and for all } \alpha.
\]

(1.41)

The decomposition in Theorem 1.16 can be used to show that the \( h^p \)-FEM applied to the Helmholtz equation in \( \mathbb{R}^d \) with \( C^\infty \) coefficients is quasioptimal (with constant independent of \( k \)) if the conditions (1.33) hold; see [43, Theorem 3.4]. The reason \( k \)-independent quasioptimality holds here under the conditions (1.33) as opposed to (1.30) (with the former being weaker, as discussed in Remark 1.8) is that the right-hand side of the bound (1.41) does not contain the \(|\alpha|!\) present on the right-hand side of (1.22).

1.6 Informal discussion of the ideas behind Theorem 1.1

It is instructive to first recall the ideas behind the results of [52], [53], [26], and [51].
How the results of [52], [53], [26], and [51] were obtained. The paper [52] considered the Helmholtz equation (1.1) posed in $\mathbb{R}^d$ with the Sommerfeld radiation condition (1.2). The decomposition $u = u_{H} + u_{A}$ was obtained by decomposing the data $f$ in (1.1) into “high-” and “low-” frequency components, with $u_{H}$ the Helmholtz solution for the high-frequency component of $f$, and $u_{A}$ then the Helmholtz solution for the low-frequency component of $f$. The frequency cut-offs were defining using the indicator function

$$1_{B,\lambda_k}(\xi) := \begin{cases} 1 & \text{for } |\xi| \leq \lambda k, \\ 0 & \text{for } |\xi| \geq \lambda k, \end{cases}$$

with $\lambda$ a free parameter (see [52, Equation 3.31] and the surrounding text). In [52] the frequency cut-off (1.42) was then used with (a) the expression for $u$ as a convolution of a 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 $u_{A}$ and $u_{H}$ using explicit calculation (involving Bessel and Hankel functions). The decompositions in [53], [26], [51] for the exterior Dirichlet problem and interior impedance problem were obtained using the results of [52] combined with extension operators (to go from problems with boundaries to problems on $\mathbb{R}^d$).

Because the proof technique in [52] does not generalise to the variable-coefficient Helmholtz equation (1.3), until the recent paper [43] 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., [13], [3], [15], [31], [59], [34], [29], [41], [32].

The recent results of [43]: the decomposition for the variable-coefficient Helmholtz equation in free space. The paper [43] obtained the analogous decomposition to that in [52] 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 [52]) but now applying them to the solution $u$ as opposed to the data $f$. Any cut-off function that is zero for $|\xi| \geq Ck$ is a cutoff to a compactly-supported set in phase space, and hence enjoys analytic estimates. The main difficulty in [43], therefore, was in showing that the high-frequency component $u_{H}$ 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 (1.42)) allowed [43] 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 $u_{H}$.

The frequency decomposition achieved in Theorem 1.1. 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

$$P = -c^2 \nabla \cdot (A \nabla)$$

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 $g(P)$ for a broad class of functions $g$. In particular, given $k > 0$, we are interested in taking $g$ a cutoff function of the real axis equal to 1 on $B(0, \mu k)$ for some $\mu > 1$. Then for fixed $k$, $(1 - g)(P)$ is a high-frequency cutoff and $g(P)$ a low-frequency cutoff; in the special case $A = I, c = 1$, these are simply Fourier multipliers of the type used in [42].

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 [67], 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 $(B(0, 2\mu))^c$. We split

$$u = \Pi_H u + \Pi_L u$$
with
\[ \Pi_L \equiv \psi(P_h), \quad \Pi_H u \equiv (1 - \psi)(P_h), \]
and both pieces again defined by the spectral theorem. We now discuss the two pieces separately.

We wish to analyze \( \Pi_H u \) by using the semiclassical ellipticity of \( P_h - 1 \) on its support in phase space. The latter notion would be well-defined if \( \Pi_H \) were globally a pseudodifferential operator. In the broad context of the black-box theory, though, while the function \( \psi(P_h) \) 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 \( \Pi_H \) 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 amounting to the bounded invertibility of \( P_h - 1 \) on the range of \( \Pi_H \), which just follows from the boundedness of the function \( (\lambda - 1)^{-1}(1 - \psi(\lambda)) \). Since our outgoing solution \( u \) is only locally \( L^2 \), however, we do additionally need to understand the commutator of \( \Pi_H \) with a localiser \( \varphi \) that equals one near the black-box. Fortunately, we are able to use the Helffer–Sjöstrand approach to the functional calculus \cite{36} to describe this commutator explicitly. The method of \cite{36} 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 \cite[Chapter 8]{19} (a result originally due to Strichartz \cite{70} in the setting of the homogeneous pseudodifferential calculus and Helffer–Robert \cite{35} in the semiclassical setting used here). Additionally, Davies \cite{17} 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 \cite{66} to learn that \textit{away} from the black-box we can in fact treat \( \Pi_H \) as a pseudodifferential operator (see Lemma 2.8), and hence deal with \( [\Pi_H, \varphi] \) 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 \( \Pi_H u \) is insensitive to the contents of the black-box, our study of the low frequency piece \( \Pi_L u \) 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 \( \Pi_L u \) 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 \( (1.5) \) locally near the black-box, which allows us to estimate the part of \( \Pi_L u \) spatially localised near its content. The remaining part living in \( \mathbb{R}^d \) is then given, thanks to Sjöstrand \cite{66} again, by a Fourier multiplier up to negligible terms, and hence enjoys the analytic estimate \( (1.12) \) thanks to the properties of the Fourier transform, as used in \cite{43}.

If, for instance, \( P \) is given by \( (1.43) \) exterior to a \( C^\infty \) obstacle with Dirichlet boundary condition, we know by the functional calculus that \( P^m \Pi_L u \) is bounded for all \( m \in \mathbb{N} \). This yields elliptic estimates which allow us to estimate all derivatives of \( \Pi_L u \) up to the obstacle, but the resulting estimates on \( \partial^\alpha \Pi_L u \) grow non-optimally in \( \alpha \); see Corollary 4.2 and Theorem 1.12. 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 \( \Pi_L u \) : we can run the \textit{backward heat equation} on \( \Pi_L u \) for as long as we like and obtain \( L^2 \) estimates on the result. If the boundary is analytic then known heat kernel estimates \cite{25} yield satisfactory Cauchy-type estimates on \( \partial^\alpha \Pi_L u ; \) see Corollary 4.1 and Theorem 1.6.

### 1.7 Outline of the rest of the paper

The organization of the paper is as follows. Section 2 recalls the black-box framework and sets up the associated functional calculus. Section 3 proves Theorem 1.1. Section 4 proves Theorems 1.6 and 1.12 (i.e., Theorem 1.1 specialised to the exterior Dirichlet and transmission problems), and Theorem 1.16. Section 5 proves Theorems 1.7 and 1.14 (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 and Appendix C prove subsidiary results used to prove Lemma 2.4 and Theorem 1.6, respectively.
2 Recap of the black-box framework

2.1 Abstract framework

We now briefly recap the abstract framework of black-box scattering introduced in [67]; for more details, see the comprehensive presentation in [22, Chapter 4]. A brief overview of black-box scattering with an emphasis on the counting of resonances is contained in [42, §2].

We emphasise that here we use the approach of [66, §2], where the black-box operator is a variable-coefficient Laplacian (with smooth coefficients) outside the black-box, and not the Laplacian $-\hbar^2 \Delta$ itself as in [22, Chapter 4] (although the operator still agrees with $-\hbar^2 \Delta$ outside a sufficiently large ball).

The Hilbert-space decomposition

Let $\mathcal{H}$ be an Hilbert space with an orthogonal decomposition

$$\mathcal{H} = \mathcal{H}_{R_0} \oplus L^2(\mathbb{R}^d \setminus B_{R_0}, \omega(x)dx),$$

where the weight-function $\omega : \mathbb{R}^d \to \mathbb{R}$ is measurable. Let $1_{B_{R_0}}$ and $1_{\mathbb{R}^d \setminus B_{R_0}}$ denote the corresponding orthogonal projections. Let $P_h$ be a family in $h$ of self-adjoint operators $\mathcal{H} \to \mathcal{H}$ with domain $\mathcal{D} \subset \mathcal{H}$ independent of $h$ (so that, in particular, $\mathcal{D}$ is dense in $\mathcal{H}$). Outside the black-box $\mathcal{H}_{R_0}$, we assume that $P_h$ equals $Q_h$ defined as follows. We assume that, for any multi-index $|\alpha| \leq 2$, there exist functions $a_{h,\alpha} \in C^\infty(\mathbb{R}^d)$, uniformly bounded with respect to $h$, independent of $h$ for $|\alpha| = 2$, and such that (i) for some $C_1 > 0$

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

(ii) for some $R_1 > R_0$

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

and (iii) the operator $Q_h$ defined by

$$Q_h := \sum_{|\alpha| \leq 2} a_{h,\alpha}(x)(hD_x)^\alpha$$

is formally self-adjoint on $L^2(\mathbb{R}^d, \omega(x)dx)$.

We require the operator $P_h$ to be equal to $Q_h$ outside the black-box $\mathcal{H}_{R_0}$ in the sense that

$$1_{\mathbb{R}^d \setminus B_{R_0}} P_h u = Q_h(1_{\mathbb{R}^d \setminus B_{R_0}} u) \quad \text{for } u \in \mathcal{D}, \quad \text{and} \quad 1_{\mathbb{R}^d \setminus B_{R_0}} \mathcal{D} \subset H^2(\mathbb{R}^d \setminus B_{R_0}).$$

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

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

(with the restriction to $B_{R_0 + \varepsilon}$ defined in terms of the projections in (BB2); see also (2.8) below) and that

$$1_{B_{R_0}} (P_h + i)^{-1} \text{ is compact from } \mathcal{H} \to \mathcal{H}.$$  

Under these assumptions, the semiclassical resolvent

$$R(z, h) := (P_h - z)^{-1} : \mathcal{H} \to \mathcal{D}$$

is meromorphic for Re $z > 0$ and extends to a meromorphic family of operators of $\mathcal{H}_{\text{comp}} \to \mathcal{D}_{\text{loc}}$ in the whole complex plane when $n$ is odd and in the logarithmic plane when $n$ is even [22, Theorem 4.4]; where $\mathcal{H}_{\text{comp}}$ and $\mathcal{D}_{\text{loc}}$ are defined by

$$\mathcal{H}_{\text{comp}} := \left\{ u \in \mathcal{H} : 1_{\mathbb{R}^d \setminus B_{R_0}} u \in L^2_{\text{comp}}(\mathbb{R}^d \setminus B_{R_0}) \right\},$$

and

$$\mathcal{D}_{\text{loc}} := \left\{ u \in \mathcal{H}_{R_0} \oplus L^2_{\text{loc}}(\mathbb{R}^d \setminus B_{R_0}) : \text{ if } \chi \in C^\infty_c(\mathbb{R}^d), \chi|_{B_{R_0}} = 1 \right. \left. \text{ then } (1_{B_{R_0}} u, \chi 1_{\mathbb{R}^d \setminus B_{R_0}} u) \in \mathcal{D} \right\}.$$
The reference operator $P^d_h$

Let $R_4 > R_1$, and let $\mathbb{T}^d_{R_1} := \mathbb{R}^d / (2R_4\mathbb{Z})^d$; we work with $[-R_4, R_4]^d$ as a fundamental domain for this torus. Let

$$\mathcal{H}^d := \mathcal{H}_{R_0} \oplus L^2(\mathbb{T}^d_{R_1} \setminus B_{R_0}),$$

and let $1_{B_{R_0}}$ and $1_{\mathbb{T}^d_{R_1} \setminus B_{R_0}}$ denote the corresponding orthogonal projections. We define

$$\mathcal{D}^d := \left\{ u \in \mathcal{H}^d : \begin{array}{l}
\text{if } \chi \in C_0^\infty(B_{R_0}), \chi = 1 \text{ near } B_{R_0}, \text{ then } (1_{B_{R_0}} u, \chi 1_{\mathbb{T}^d_{R_1} \setminus B_{R_0}} u) \in \mathcal{D},
\text{and } (1 - \chi) 1_{\mathbb{T}^d_{R_1} \setminus B_{R_0}} u \in H^2(\mathbb{T}^d_{R_1})\end{array}\right\},$$

(2.4)

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

$$P^d_h u := P_h (1_{B_{R_0}} u, \chi 1_{\mathbb{T}^d_{R_1} \setminus B_{R_0}} u) + Q_h ((1 - \chi) 1_{\mathbb{T}^d_{R_1} \setminus B_{R_0}} u),$$

(2.5)

where we have identified functions supported in $B(0, R_4) \setminus B(0, R_0) \subset \mathbb{T}^d_{R_1} \setminus B(0, R_0)$ with the corresponding functions on $\mathbb{R}^d \setminus B(0, R_0)$; see the paragraph on notation below.

Let $q_h \in S^2(\mathbb{T}^d_{R_1})$ denote the principal symbol of $Q_h$ as an operator acting on the torus $\mathbb{T}^d_{R_1}$ (see Appendix A for a review of semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_1}$). We record for later the fact that (2.1), (2.2), and the uniform boundedness of $a_h(x)$ with respect to $h$ imply that there exist $C_1, C_2 > 0$ such that

$$C_1 |\xi|^2 \leq q_h \leq C_2 |\xi|^2 \quad \text{for sufficiently large } \xi.$$

(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 $P^d_h$ that can be thought of as $P_h$ in $\mathcal{H}_{R_0}$ and $Q_h$ in $(\mathbb{R}/R_4\mathbb{Z})^d \setminus B_{R_0}$; see Figure 2.1. The resolvent $(P^d_h + i)^{-1}$ is compact (see [22, Lemma 4.11]), and hence the spectrum of $P^d_h$, denoted by $\text{Sp} P^d_h$, is discrete (i.e., countable and with no accumulation point).

We assume that the eigenvalues of $P^d_h$ satisfy the polynomial growth of eigenvalues condition

$$N(P^d_h, [-C, \lambda]) = O(h^{-d^2/2}),$$

(BB5)

for some $d^2 \geq n$ and $N(P^d_h, I)$ is the number of eigenvalues of $P^d_h$ in the interval $I$, counted with their multiplicity. When $d^2 = d$, 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 $P_h$ on a Hilbert space $\mathcal{H}$, with dense domain $\mathcal{D}$, independent of $h$, is a semiclassical black-box operator if $(P_h, \mathcal{H})$ 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.

Definition 2.2 (Black-box differentiation operator) $(D(\alpha))_{\alpha \in \mathbb{N}}$ is a family of black-box differentiation operators on $\mathcal{D}^{1, \infty}$ if $\mathcal{A}$ is a family of $d$-multi-indices, and for any $\alpha$ and any $v \in L^2(\mathbb{T}^d_{R_1} \setminus B_{R_0})$,

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

Notation

We identify in the natural way:

- the elements of $\{0\} \oplus L^2(\mathbb{T}^d_{R_1} \setminus B_{R_0}) \subset \mathcal{H}^d$,
- the elements of $L^2(\mathbb{T}^d_{R_1} \setminus B_{R_0})$. 

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\[
\begin{align*}
P_h & \simeq -h^2 \Delta \\
\end{align*}
\]

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

- the elements of \( L^2(\mathbb{T}_R^d) \) essentially supported outside \( B_{R_0} \),
- the elements of \( L^2(\mathbb{R}^d) \) essentially supported in \([-R_1, R_1]^d \setminus B_{R_0}\),
- and the elements of \( \{0\} \oplus L^2(\mathbb{R}^d \setminus B_{R_0}) \subset \mathcal{H} \) whose orthogonal projection onto \( L^2(\mathbb{R}^d \setminus B_{R_0}) \) is essentially supported in \([-R_1, R_1]^d \setminus B_{R_0}\).

If \( v \in \mathcal{H} \) and \( \chi \in C^\infty(\mathbb{R}^d) \) is equal to some constant \( \alpha \) near \( B_{R_0} \), we define
\[
\chi v := (\alpha 1_{B_{R_0}}, \chi 1_{\mathbb{R}^d \setminus B_{R_0}} v) \in \mathcal{H}. \quad (2.7)
\]

(For example, using this notation, the requirements on \( u \) in the definition of \( \mathcal{D}^\varepsilon \) are \( \chi u \in \mathcal{D} \) and \( (1 - \chi)u \in H^2(\mathbb{T}_R^d) \)).

If \( v \in \mathcal{H} \) and \( R > R_0 \), we define
\[
v|_{B_R} := (1_{B_{R_0}}, (1_{\mathbb{R}^d \setminus B_{R_0}} v)|_{B_R}) \in \mathcal{H}_{R_0} \oplus L^2(B_R \setminus B_{R_0}), \quad (2.8)
\]
and, if \( v \in \mathcal{H}^d \),
\[
v|_{B_R} := (1_{B_{R_0}}, (1_{\mathbb{T}_{R}^d \setminus B_{R_0}} v)|_{B_R}) \in \mathcal{H}_{R_0} \oplus L^2(B_R \setminus B_{R_0}).
\]

Furthermore, we say that \( g \in \mathcal{H} \) is compactly supported in \( B_R \) if \( g = \chi_0 g \) for some \( \chi_0 \in C_c^\infty(\mathbb{R}^d) \) equal to one near \( B_{R_0} \) and supported in \( B_R \).

Finally, if \( R_0 \leq r \leq R_0 \), we define the partial norms
\[
\|u\|_{\mathcal{H}(B_r)} := \|u\|_{\mathcal{H}(B_r)} := \|u\|_{\mathcal{H}(B_R) \oplus L^2(B_R \setminus B_{R_0})}, \quad \|u\|_{\mathcal{H}^d(B_r)} := \|1_{\mathbb{T}^d_{R_0} \setminus B_{R_0}} u\|_{L^2(\mathbb{T}^d_{R_0} \setminus B_r)}
\]
and
\[
\|u\|_{\mathcal{H}(B_r)} := \|1_{\mathbb{R}^d \setminus B_{R_0}} u\|_{L^2(\mathbb{R}^d \setminus B_r)}.
\]

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 [22, §4.1].
Lemma 2.3 (Scattering by a Dirichlet Lipschitz obstacle fits in the black-box framework) Let $O_-, A, c, R_0$, and $R_1$ and be as in Definition 1.2. Then the family of operators

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

with the domain

$$D_D := \left\{ v \in H^1(O_+), \nabla \cdot (A \nabla v) \in L^2(O_+), v = 0 \text{ on } \partial O_+ \right\}$$

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

$$H_{R_0} = L^2(B_{R_0} \cap O_+; c^{-2}(x)dx) \text{ so that } H = L^2(O_+; c^{-2}(x)dx).$$

Furthermore the corresponding reference operator $P_h^R$ satisfies (BB5) with $d^\xi = d$.

**Proof.** The non-semiclassically-scaled version of this lemma was proved for $c = 1$ in [42, 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 $P_h^R$ to the counting function for the problem with $c = 1$ by a similar argument to [42, Lemma B.2]/Appendix B, and then using the result for the problem with $c = 1$ proven in [42, Lemma B.1]. \hfill ■

Lemma 2.4 (Scattering by a penetrable Lipschitz obstacle fits in the black-box framework) Let $O_-, A, c, \beta$, and $R_0$ be as in Definition 1.10. Let $\nu$ be the unit normal vector field on $\partial O_-$ pointing from $O_-$ into $O_+$, and let $\partial_{\nu,A}$ the corresponding conormal derivative from either $O_-$ or $O_+$. Let

$$\mathcal{H}_{R_0} = L^2(O_-, c(x)^{-2} \beta^{-1}dx) \oplus L^2(B_{R_0} \setminus \overline{O_-}),$$

so that

$$\mathcal{H} = L^2(O_+; c(x)^{-2} \beta^{-1}dx) \oplus L^2(B_{R_0} \setminus \overline{O_-}) \oplus L^2(\mathbb{R}^d \setminus B_{R_0}).$$

Let

$$\mathcal{D} := \left\{ v = (v_1, v_2, v_3) \text{ where } v_1 \in H^1(O_-), \nabla \cdot (A_- \nabla v_1) \in L^2(O_-), \right.$$  

$$v_2 \in H^1(B_{R_0} \setminus \overline{O_-}), \nabla \cdot (A_+ \nabla v_2) \in L^2(B_{R_0} \setminus \overline{O_-}),$$  

$$v_3 \in H^1(\mathbb{R}^d \setminus \overline{B_{R_0}}), \nabla v_3 \in L^2(\mathbb{R}^d \setminus \overline{B_{R_0}}),$$  

$v_1 = v_2$ and $\partial_{\nu,A} v_1 = \beta \partial_{\nu,A} v_2$ on $\partial O_-$, and  

$v_2 = v_3$ and $\partial_{\nu} v_2 = \partial_{\nu} v_3$ on $\partial B_{R_0}$\left\}. \right.$

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

$$P_{h,v} := -\hbar^2 \left(c^2 \nabla \cdot (A_- \nabla v_1), \nabla \cdot (A_+ \nabla v_2), \Delta v_3\right),$$

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 $Q_h = -\hbar^2 \Delta$, and any $R_1 > R_0$. Furthermore, the corresponding reference operator $P_h^R$ satisfies (BB5) with $d^\xi = d$.

**Proof.** The non-semiclassically-scaled version of this lemma was proved for $c = 1$ in [42, 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 [42, Lemma B.1]; for completeness we include the proof in §B. \hfill ■

**Remark 2.5** Lemma 2.3 has the obstacle $O_-$ 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 $O_-$ 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 1.12.
2.3 A black-box functional calculus for $P_h^\sharp$

The operator $P_h^\sharp$ on the torus with domain $\mathcal{D}^\sharp$ is self-adjoint with compact resolvent [22, Lemma 4.11], hence we can describe the Borel functional calculus [61, 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): for $f$ a real-valued Borel function on $\mathbb{R}$, $f(P_h^\sharp)$ is self-adjoint with domain

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

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

$$f(P_h^\sharp)(v) := \sum a_j f(\lambda_j^\sharp) \phi_j^\sharp.$$  \hfill (2.10)

For $f$ a bounded Borel function, $f(P_h^\sharp)$ 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 $\mathcal{D}^\sharp_h^m$ as the domain of $(P_h^\sharp)^m$ equipped with the norm

$$\|v\|_{\mathcal{D}^\sharp_h^m} := \|v\|_{\mathcal{H}^\sharp} + \|(P_h^\sharp)^m v\|_{\mathcal{H}^\sharp},$$  \hfill (2.11)

and $\mathcal{D}^\sharp_h^{-m}$ as its dual. We define also the partial norms, for $k > 0$, $\|v\|_{\mathcal{D}^\sharp_h^m(B)} := \|v\|_{\mathcal{H}^\sharp(B)} + \|(P_h^\sharp)^m v\|_{\mathcal{H}^\sharp(B)}$, where $B = B_r$ or $B = B_r^c$ with $R_0 \leq r \leq R_1$. In addition, we let

$$\mathcal{D}^\sharp_h^{\infty} := \bigcup_{m \geq 0} \mathcal{D}^\sharp_h^m,$$  \hfill (2.12)

so that $v \in \mathcal{D}^\sharp_h^{\infty}$ iff $(P_h^\sharp)^m v \in \mathcal{D}^\sharp_h$ for all $m \in \mathbb{Z}^+$. The following theorem is proved in [18, Pages 23 and 24]; see also [61, Theorem VIII.5].

**Theorem 2.6** The Borel functional calculus enjoys the following properties.

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

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–Sjögren construction of the functional calculus [36], [18, §2.2] (which can also be used to prove the spectral theorem to begin with; see [17]).

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

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 $n > 0$. We define an almost-analytic extension of $f$, denoted by $\tilde{f}$, by

$$\tilde{f}(z) := \left( \sum_{m=0}^{n} \frac{1}{m!} (\partial^m f(\text{Re} \, z)) (i \text{Im} \, z)^m \right) \tau \left( \frac{\text{Im} \, z}{(\text{Re} \, z)} \right)$$

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

$$f(P_h) := -\frac{1}{\pi} \int_C \frac{\partial \tilde{f}}{\partial z} (P_h^\sharp - z)^{-1} \, dz \, dy,$$  \hfill (2.13)

where $dz \, dy$ is the Lebesgue measure on $\mathbb{C}$. The integral on the right-hand side of (2.13) converges; see, e.g., [17, Lemma 1], [18, Lemma 2.2.1]. This definition can be shown to be independent of the
choices of $n$ and $\tau$, and to agree with the operators defined by the Borel functional calculus for $f \in A$; see [17, Theorems 2-5], [18, Lemmas 2.2.4-2.2.7]. The construction immediately extends by continuity to map functions $f \in C_0(\mathbb{R})$ to elements of $\mathcal{L}(\mathcal{H}^2)$, where

\[ C_0(\mathbb{R}) = \left\{ f \in C(\mathbb{R}) : \lim_{\lambda \to \pm\infty} f(\lambda) = 0 \right\}. \]

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 [36]. Here, in the presence of a black box, it can instead be used to show that, modulo residual errors, $f(P^\hbar)$ agrees with $f(Q_h)$ on the region of the torus outside the black box, with the latter being a pseudodifferential operator. Furthermore, the operator wavefront set of $f(Q_h)$ can be seen to be included in the support of $f \circ q_h$. We now state these results, obtained originally in [66].

We say that $E \in \mathcal{L}(\mathcal{H}^2)$ is $O(h^\infty)_{P^\hbar_{\pm \infty} \to D^\infty_{\hbar^2}}$ if, for any $N > 0$ and any $m > 0$, there exists $C_{N,m} > 0$ such that

\[ \|E\|_{P^\hbar_{\pm \infty} \to D^\infty_{\hbar^2}} \leq C_{N,m} h^N \]

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

**Lemma 2.7** Suppose $f \in C_0(\mathbb{R})$ is independent of $\hbar$, and $\psi_1, \psi_2 \in C^\infty(\mathbb{T}^d_{R_1})$ are constant near $B_{R_0}$. If $\psi_1$ and $\psi_2$ have disjoint supports, then

\[ \psi_1 f(P^\hbar_{\hbar}) \psi_2 = O(h^\infty)_{D^\infty_{\hbar^2} \to D^\infty_{\hbar^2}}. \]  

(2.14)

**Proof.** This follows from combining the corresponding result about the resolvent [66, Lemma 4.1] (i.e., (2.14) with $f(w) := (w - z)^{-1}$) with (2.13) and then integrating (as discussing in a slightly different context in [66, Paragraph after proof of Lemma 4.2]).

Furthermore, we can show from [66, §4] that, modulo a negligible term, away from the blackbox 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 $\mathbb{T}^d_{R_1}$, recapped in Appendix A.

**Lemma 2.8** Suppose $f \in C(\mathbb{R})$ is compactly supported and independent of $\hbar$. If $\chi \in C^\infty(\mathbb{T}^d_{R_1})$ is equal to zero near $B_{R_0}$, then

\[ \chi f(P^\hbar_{\hbar}) \chi = \chi f(Q_h) \chi + O(h^\infty)_{D^\infty_{\hbar^2} \to D^\infty_{\hbar^2}}. \]

Furthermore, $f(Q_h) \in \Psi^\infty(\mathbb{T}^d_{R_1})$ with

\[ \text{WF}_h f(Q_h) \subset \text{supp } f \circ q_h. \]

**Proof.** By [66, Lemma 4.2 and the subsequent two paragraphs],

\[ \chi f(P^\hbar_{\hbar}) \chi \chi f(Q_h) \chi + O(h^\infty)_{D^\infty_{\hbar^2} \to D^\infty_{\hbar^2}}. \]

The results of Helffer–Robert [35] (see the account in [63]) imply that $f(Q_h)$ is a pseudodifferential operator on $\mathbb{T}^d_{R_1}$. It remains to show that $\text{WF}_h f(Q_h) \subset \text{supp } f \circ q_h$. To do so, let $K_{\epsilon}$ be defined for $\epsilon > 0$ by

\[ K_{\epsilon} := \left\{ z \in T^* \mathbb{T}^d_{R_1} : \text{dist}(q_h(z), \text{supp } f) \leq \epsilon \right\}. \]

We show that $\text{WF}_h f(Q_h) \subset K_{\epsilon}$ for any $\epsilon > 0$, from which the result follows. To do so, let $b \in C^\infty(T^* \mathbb{T}^d_{R_1})$ be such that $b = 1$ on $(K_{\epsilon/2})^c$, and supp $b \subset (K_{\epsilon/2})^c$, and let $B := \text{Op}_{\mathbb{T}^d_{R_1}}(b)$. It suffices to show that $Bf(Q_h) = O(h^\infty)_{P^\hbar_{\infty} \to \infty}$. Indeed, if this is the case, then $\text{WF}_h B f(Q_h) = 0$ by (A.7). Then, by (A.8) and (A.9), $\text{WF}_h f(Q_h) \subset \text{WF}_h (I - B) f(Q_h) \subset \text{WF}_h (I - B) \subset C_{\epsilon/2}$.

It therefore remains to prove that $Bf(Q_h) = O(h^\infty)_{P^\hbar_{\infty} \to \infty}$. Let $g \in C^\infty(\mathbb{R})$ be such that $g = 0$ on $\text{supp } f$ and $g = 1$ on $q_h((K_{\epsilon/2})^c)$; such a $g$ exists since, by the definition of $K_{\epsilon/2}$,
dist(supp $f, q_h((K_e/2)^c)) \geq \varepsilon/2 > 0$. This definition then implies that $g \circ q_h = 1$ on $(K_e/2)^c$. By Part 1 of Theorem 2.6,
\[ g(Q_h)f(Q_h) = (gf)(Q_h) = 0. \]  
(2.15)

By [63] again, $g(Q_h)$ is a pseudodifferential operator with principal symbol $g \circ q_h$, which is one on $(K_e/2)^c$ and hence on WF$_h B$. Therefore, by the microlocal elliptic parametrix, Theorem A.2, there exists a pseudodifferential operator $S$ such that $B = Sg(Q_h) + O(h^\infty)_{\Psi^{-\infty}}$. Using this and (2.15), we obtain that
\[ Bf(Q_h) = Sg(Q_h)f(Q_h) + O(h^\infty)_{\Psi^{-\infty}} \]
and the proof is complete.

3 Proof of Theorem 1.1 (the main result in the black-box framework)

The decomposition (1.7) is defined in §3.1, whereas the estimates (1.8) and (1.10)–(1.14) are essentially proved in §3.2 and 3.3 respectively.

3.1 The decomposition

Let $\varphi \in C_0^\infty(\mathbb{R}^d)$ be equal to to one in $B_R$ and supported in $B_{R_1}$. For $v \in \mathcal{H}$, we define
\[ M_\varphi v := \varphi v, \]
where the multiplication is in the sense of (2.7). Let $u \in \mathcal{D}_{\text{out}}$ be solution to
\[ (P_h - 1)u = g, \]
and let
\[ w := M_\varphi u. \]
We view $w$ as an element of $\mathcal{H}^0$ and work in the torus $\mathbb{T}_R^d$.

We now define our frequency cut-offs. By (2.1), there exists $\tilde{\mu} > 1$ and $c_{\text{cell}} > 0$ such that
\[ |\xi| \geq \tilde{\mu} \implies \langle \xi \rangle^{-2}(q_h(x, \xi) - 1) \geq c_{\text{cell}} > 0. \]
Therefore, by (2.6), there exists $\mu > 1$ such that
\[ q_h(x, \xi) \geq \mu \implies \langle \xi \rangle^{-2}(q_h(x, \xi) - 1) \geq c_{\text{cell}} > 0. \]
(3.1)

Let $\psi \in C_0^\infty(\mathbb{R})$ be such that
\[ \psi = \begin{cases} 1 \text{ in } B(0, 2), \\ 0 \text{ in } (B(0, 4))^c. \end{cases} \]
(3.2)

We now fix $\frac{1}{2} \leq \mu' \leq \frac{\mu}{2}$, and define
\[ \psi_\mu := \psi \left( \frac{\cdot}{\mu} \right), \quad \psi_{\mu'} := \psi \left( \frac{\cdot}{\mu'} \right). \]
(3.3)

These definitions imply that
\[ (1 - \psi_{\mu'})(1 - \psi_\mu) = (1 - \psi_{\mu'}) \]
(4.4)

(since $4\mu' \leq 2\mu$), and
\[ 1 \notin \text{ supp}(1 - \psi_{\mu'}) \]
(3.5)

(since $2\mu' \geq 1$). Let
\[ \Lambda := 5\mu \]
(3.6)
(note that, by (3.1), both \( \mu \) and \( \Lambda \) only depend on \( q_h \)), and observe that

\[
\text{supp } \psi_\mu \subset [-\Lambda, \Lambda].
\]

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

\[
\Pi_L := \psi_\mu(P^\sharp_h),
\]

and additionally

\[
\Pi_H := (1 - \psi_\mu)(P^\sharp_h) = \text{Id} - \Pi_L \quad \text{and} \quad \Pi'_H := (1 - \psi_\mu')(P^\sharp_h).
\]

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

\[
\Pi'_H \Pi_H = \Pi_H.
\]

By Part 3 of Theorem 2.6, the operators \( \Pi_L \), \( \Pi_H \), and \( \Pi'_H \) are bounded on \( \mathcal{H}^\sharp \), with

\[
\| \Pi_L \|_{\mathcal{L}(\mathcal{H}^\sharp)}, \quad \| \Pi_H \|_{\mathcal{L}(\mathcal{H}^\sharp)}, \quad \| \Pi'_H \|_{\mathcal{L}(\mathcal{H}^\sharp)} \leq 1,
\]

and they commute with \( P^\sharp_h \) 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 \( \varphi \) is compactly supported imply that \( w \in \mathcal{D}^\sharp \). By the definition of \( \psi_\mu \) (3.3), (2.10), and the fact that \( \text{Sp } P^\sharp_h \) is discrete, \( \Pi_L w \) projects non-trivially only on a finite number of eigenspaces of \( P^\sharp_h \), and thus \( \Pi_L w \in \mathcal{D}_{h, \infty}^\sharp \). Therefore \( \Pi_H w = w - \Pi_L w \in \mathcal{D}^\sharp \). We now define

\[
u_H := \Pi_H w \in \mathcal{D}^\sharp, \quad u_L := \Pi_L w \in \mathcal{D}_{h, \infty}^\sharp.
\]

We show that we can split \( u_L \) as

\[
u_L = u_A + u_e,
\]

where \( u_A \in \mathcal{D}^\sharp_{h, \infty} \) satisfies (1.9)–(1.13) (or (1.14) if \( \rho = 1 \)), and that \( u_H \) and \( u_e \) satisfy

\[
\| u_H \|_{\mathcal{H}^\sharp} + \| P^\sharp_h u_H \|_{\mathcal{H}^\sharp} \lesssim \| g \|_{\mathcal{H}},
\]

and

\[
\| u_e \|_{\mathcal{H}^\sharp} + \| P^\sharp_h u_e \|_{\mathcal{H}^\sharp} \lesssim \| g \|_{\mathcal{H}},
\]

and we then define

\[
u_H := u_H + u_e
\]

so that the decomposition (1.7), (1.8) and (1.9)–(1.13) (or (1.14) if \( \rho = 1 \)) holds.

In §3.2 we prove the estimate (3.12) for \( u_H \). In §3.3 we prove that the decomposition (3.11) holds, with \( u_A \) satisfying (1.9)–(1.13) (or (1.14) if \( \rho = 1 \)) and \( u_e \) satisfying (3.13) We highlight that all the arguments from now on consider \( h \in H \).

3.2 Proof of the bound (3.12) on \( u_H \) (the high-frequency component)

We proceed in three steps: we first use the abstract information we have about \( P^\sharp \) to bound \( \Pi_H w \) by \( \| g \|_{\mathcal{H}} \) modulo a commutator term living away from the black box \( B_{R_\varnothing} \). 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 \( T_{R_\varnothing}^d \). 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 \( T_{R_\varnothing}^d \).
Step 1: An abstract estimate in $\mathcal{H}^s$

Since $\Pi_H$ commutes with $P^2_h$, 
\[
(P^2_h - 1)(\Pi_H w) = \Pi_H (P^2_h - 1)(w)
\]
\[
= \Pi_H (P^2_h - 1)(w) = \Pi_H \varphi g + \Pi_H [P_h, M_\varphi] u = \Pi_H \varphi g + \Pi_H [P^2_h, M_\varphi] u,
\]
where we used the fact that we can replace $P^2_h$ by $P_h$ (and vice versa) on $\text{supp} \varphi \subset B_{R_0}$ by (BB2) and (2.5)). For $\lambda \in \mathbb{R}$, let 
\[
g(\lambda) := (\lambda - 1)^{-1}(1 - \psi_\mu)(\lambda),
\]
where $g$ 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 (3.14), we get 
\[
\Pi_H w = \Pi_H \Pi_H w = g(P^2_h)(P^2_h - 1)\Pi_H w = g(P^2_h)(\Pi_H \varphi g + \Pi_H [P^2_h, M_\varphi] u).
\]
Since $g$ is in $C_0(\mathbb{R})$, $g(P^2_h)$ is uniformly bounded from $\mathcal{H}^s \to \mathcal{H}^s$ by Part 3 of Theorem 2.6. Combining this fact with (3.15), we obtain 
\[
\|\Pi_H w\|_{\mathcal{H}^s} \lesssim \|\Pi_H \varphi g\|_{\mathcal{H}^s} + \|\Pi_H [P^2_h, M_\varphi] u\|_{\mathcal{H}^s}.
\]

Writing $P^2_h \Pi_H w = \Pi_H w + (P^2_h - 1)\Pi_H w$ and using (3.14) again, we obtain 
\[
\|\Pi_H w\|_{\mathcal{H}^s} + \|P^2_h \Pi_H w\|_{\mathcal{H}^s} \lesssim \|\Pi_H \varphi g\|_{\mathcal{H}^s} + \|\Pi_H [P^2_h, M_\varphi] u\|_{\mathcal{H}^s}.
\]

Hence, by (3.10) 
\[
\|\Pi_H w\|_{\mathcal{H}^s} + \|P^2_h \Pi_H w\|_{\mathcal{H}^s} \lesssim \|\varphi g\|_{\mathcal{H}^s} + \|\Pi_H [P^2_h, M_\varphi] u\|_{\mathcal{H}^s} 
\lesssim \|g\|_{\mathcal{H}^s} + \|\Pi_H [P^2_h, M_\varphi] u\|_{\mathcal{H}^s}.
\]

Step 2: Viewing $\Pi_H [P^2_h, M_\varphi]$ as a semiclassical pseudodifferential operator on $\mathbb{T}^d_R$

To prove (3.12) from (3.16), it therefore remains to bound the commutator term $\Pi_H [P^2_h, M_\varphi] u$. Since $[P^2_h, M_\varphi]$ lives away from $\mathcal{H}^s$, we consider the high-frequency cut-off in terms of the semiclassical pseudodifferential calculus thanks to Lemma 2.8.

Since $\varphi$ is compactly supported in $B_{R_0}$ and equal to one near $B_{R_0}$, in $\mathcal{H}^s$ we can write $[P^2_h, M_\varphi]$ as (using the notation in §2.1) 
\[
[P^2_h, M_\varphi] = (0, [Q_h, \varphi]) = (0, \phi [Q_h, \varphi] \phi) = (0, [Q_h, \varphi] \phi)
\]
where $\phi \in C^\infty_c(\mathbb{R}^d)$ is supported in $B_{R_0}$, equal to zero near $B_{R_0}$, and such that 
\[
\phi = 1 \text{ near } \text{supp } \nabla \varphi.
\]

Let $\chi \in C^\infty_c(\mathbb{R}^d)$ be supported in $B_{R_0}$, equal to zero near $B_{R_0}$, and equal to one near $\text{supp } \phi$. 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 
\[
\Pi_H [P^2_h, M_\varphi] = \chi \Pi_H \chi \varphi [P^2_h, M_\varphi] \phi + O(h^\infty)_{D^*_h \to D^*_h}
\]
\[
= \chi \Pi_H \chi [P^2_h, M_\varphi] \phi + O(h^\infty)_{D^*_h \to D^*_h},
\]
where we used the last equality in (3.17) to obtain the second line. By Lemma 2.8 with $f(P^2_h) = \psi_\mu(P^2_h) = \Pi_L$, there exists $\Pi_L^\varphi \in \Psi^\infty(T^d_{R_1})$ such that 
\[
\chi \Pi_L = \chi \Pi_L^\varphi + O(h^\infty)_{D^*_h \to D^*_h} \quad \text{and} \quad \text{WF} \Pi_L^\varphi \subset \text{supp } \psi_\mu \circ \varrho_h.
\]

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Hence, taking $\Pi^y_H := I - \Pi^y_H \in \Psi^{-1}_h(\mathbb{T}^d_{R_\mu})$, 
\[ \chi \Pi^y_H \chi = \chi \Pi^y_H \chi + O(h^\infty)_{P^d_{h,\to} \to \mathbb{T}^d_{R_\mu} \to} \quad \text{and} \quad \WF_h \Pi^y_H \subset \supp(1 - \psi_\mu) \circ q_h; \quad (3.20) \]
in other words, modulo negligible terms, $\chi \Pi^y_H \chi$ is a high-frequency cut-off defined from the semiclassical pseudodifferential calculus. We here emphasise that, since $\chi$ is supported in $B_{R_\mu}$ and vanishes near $B_{R_0}$, $\chi \Pi^y_H \chi$ can be seen both as an element of $\mathcal{L}(\mathcal{H})$ and of $\Psi^{-1}_h(\mathbb{T}^d_{R_\mu})$. By (3.19) and (3.20), for any $N$ and any $m$,  
\[ \| \Pi^y_H [P^d_{h,\circ} M_\circ] u \|_{\mathcal{H}_1} \leq \| \chi \Pi^y_H \chi [P^d_{h,\circ} M_\circ] \phi u \|_{\mathcal{H}_1} + C_{N,m} h^N \| [P^d_{h,\circ} M_\circ] \phi u \|_{\mathbb{D}^\infty_{-m} + C_{N} h^N} \| \phi^u \|_{\mathcal{H}_1} , \]
with $\phi$ compactly supported in $B_{R_\mu} \setminus B_{R_0}$ and equal to one on $\supp \phi$. Taking $m = 1$, then $N = M + 1$ and using the resolvent estimate (1.4) we get 
\[ \| \Pi^y_H [P^d_{h,\circ} M_\circ] u \|_{\mathcal{H}_1} \leq \| \chi \Pi^y_H \chi [P^d_{h,\circ} M_\circ] \phi u \|_{\mathcal{H}_1} + C_{M+1} h^{M+1} \| \phi^u \|_{\mathcal{H}_1} \]
\[ = \| \chi \Pi^y_H \chi [P^d_{h,\circ} M_\circ] \phi u \|_{\mathcal{H}_1} + C_{M+1} h^{M+1} \| \phi^u \|_{\mathcal{H}_1} \]
\[ \leq \| \Pi^y_H \chi [P^d_{h,\circ} M_\circ] \phi u \|_{\mathcal{H}_1} + \| g \|_{\mathcal{H}_1} \quad (3.21) \]
Finally, by the definition of $P^d_{h,\circ}$ (2.5) and the fact that $\phi$ equals zero near $B_{R_0}$, 
\[ \| \chi \Pi^y_H \chi [P^d_{h,\circ} M_\circ] \phi u \|_{\mathcal{H}_1} = \| \chi \Pi^y_H \chi (Q_h - 1, \varphi) \phi u \|_{L^2(\mathbb{T}^d_{R_\mu})} \]

hence by (3.21), 
\[ \| \Pi^y_H [P^d_{h,\circ} M_\circ] u \|_{\mathcal{H}_1} \leq \| \chi \Pi^y_H \chi (Q_h - 1, \varphi) \phi u \|_{L^2(\mathbb{T}^d_{R_\mu})} + \| g \|_{\mathcal{H}_1} \quad (3.22) \]

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

Combining (3.16) and (3.22), we see that to prove (1.8) we only need to bound $\chi \Pi^y_H \chi (Q_h - 1, \varphi) \phi u$ in $L^2(\mathbb{T}^d_{R_\mu})$. To do this, we use the semiclassical parametrix construction given by Theorem A.2.

**Lemma 3.1** The operator $Q_h - 1$ is semiclassically elliptic on the semiclassical wavefront set of $h^{-1} \chi \Pi^y_H \chi (Q_h - 1, \varphi)$.

**Proof.** By (A.9), (A.11), (3.20) and the support properties of $\psi_\mu$ given by (3.2), (3.3),  
\[ \WF_h (h^{-1} \chi \Pi^y_H \chi (Q_h - 1, \varphi)) \subset \WF_h \Pi^y_H \subset \supp (1 - \psi_\mu) \circ q_h \subset \{ q_h \geq \mu \} \]

But, on $\{ q_h \geq \mu \}$, by definition of $\mu$ (3.1),
\[ (\xi)^{-2} (q_h(x,\xi) - 1) \geq c_{\text{ell}} > 0, \]

and the proof is complete. \[ \square \]

Since $h^{-1} \chi \Pi^y_H \chi (Q_h - 1, \varphi) \in \Psi^{1}_{h}(\mathbb{T}^d_{R_\mu})$ by Theorem A.1, we can therefore apply the elliptic parametrix construction given by Theorem A.2 with $A = h^{-1} \chi \Pi^y_H \chi (Q_h - 1, \varphi)$, $B = Q_h - 1$, and $m = 1, k = 2$. Hence, there exists $S \in \Psi^{1}_{-1}(\mathbb{T}^d_{R_\mu})$ and $R = O(h^\infty)_{\Psi^{-\infty}}$ with 
\[ \WF_h S \subset \WF_h (h^{-1} \Pi^y_H [Q_h - 1, \varphi]), \quad (3.23) \]
and such that 
\[ \chi \Pi^y_H \chi (Q_h - 1, \varphi) \phi u = h S (Q_h - 1) \phi u + R \phi u \]

We apply both sides of this identity to $\phi u$ and then use (BB2) and the fact that $\phi$ is equal to zero near $B_{R_0}$ and supported in $B_{R_\mu}$; the result is that 
\[ \chi \Pi^y_H \chi (Q_h - 1, \varphi) \phi u = h S (Q_h - 1) \phi u + R \phi u \]
\[
\begin{align*}
&= hS(P_h - 1)\phi u + R\phi u \\
&= hS\phi(P_h - 1)u + hS[P_h - 1, \phi]u + R\phi u \\
&= hS\phi(P_h - 1)u + hS[Q_h - 1, \phi]u + R\phi u. 
\end{align*}
\] (3.24)

The following lemma combined with (A.10) shows that
\[
S[Q_h - 1, \phi] = O(h^\infty)_{\Psi^{-\infty}}. \tag{3.25}
\]

**Lemma 3.2**
\[
WF_h S \cap WF_h[Q_h - 1, \phi] = \emptyset.
\]

**Proof.** By (3.23) and the definition of \(Q_h\) (2.2),
\[
WF_h S \subset WF_h[Q_h - 1, \phi] \subset (\text{supp} \nabla \phi) \times \mathbb{R}^d
\]
Similarly,
\[
WF_h[Q_h - 1, \phi] \subset (\text{supp} \nabla \phi) \times \mathbb{R}^d,
\]
Now, by (3.18), \(\text{supp} \nabla \phi\) and \(\text{supp} \nabla \phi\) are disjoint, and the result follows. \(\blacksquare\)

Therefore, by (3.24), (3.25) and the definition of \(O(h^\infty)_{\Psi^{-\infty}}\) (A.4), for any \(N\), there exists \(C_N, C'_N > 0\) such that
\[
\sum \| \chi \Pi^\phi_H \chi[Q_h - 1, \phi] \phi u \|_{L^2(\mathbb{T}^d_{N_h})} \leq h \| S\phi(P_h - 1)u \|_{L^2(\mathbb{T}^d_{N_h})} + C_N h^N \| \phi u \|_{L^2(\mathbb{T}^d_{N_h})} + C'_N h^N \| \phi u \|_{L^2(\mathbb{T}^d_{N_h})} = h \| S\phi(P_h - 1)u \|_{L^2(\mathbb{T}^d_{N_h})} + C_N h^N \| \phi u \|_H + C'_N h^N \| \phi u \|_H,
\]
where \(\phi\) is compactly supported in \(B_{R_0} \setminus B_{R_0}\) and equal to one on \(\text{supp} \phi\). Taking \(N := M + 1\) and using the resolvent estimate (1.4), we then obtain that
\[
\sum \| \chi \Pi^\phi_H \chi[Q_h - 1, \phi] \phi u \|_{L^2(\mathbb{T}^d_{N_h})} \lesssim h \| S\phi(P_h - 1)u \|_{L^2(\mathbb{T}^d_{N_h})} + h \| g \|_H 
\]
where we used in the second line the fact that \(S \in \Psi^{-1}(\mathbb{T}^d_{N_h}) \subset \Psi^0(\mathbb{T}^d_{N_h})\) together with Part (iii) of Theorem A.1. Now, since \(\phi\) is equal to zero near \(B_{R_0}\) and supported in \(B_{R_0}\), we get
\[
\| \phi(P_h - 1)u \|_{L^2(\mathbb{T}^d_{N_h})} = \| \phi(P_h - 1)u \|_H = \| \phi g \|_H \leq \| g \|_H.
\]

Thus, (3.26) implies that
\[
\| \chi \Pi^\phi_H \chi[Q_h - 1, \phi] \phi u \|_{L^2(\mathbb{T}^d_{N_h})} \lesssim h \| g \|_H.
\]

Combining this last estimate with (3.16) and (3.22) we conclude that
\[
\| \Pi_H w \|_{H^s} + \| P^\phi_k H w \|_{H^s} \lesssim \| g \|_H;
\]

hence (3.12) holds.

### 3.3 Decomposition (3.11) of \(u_L\), and proof of the bounds (1.10)–(1.14) and (3.13) (the low-frequency component)

By Assumption 2 in Theorem 1.1, there exists \(E_0 = O(h^\infty)_{\mathcal{D}^{\infty}_{\Psi^{-\infty}} \rightarrow \mathcal{D}^{\infty}_{\Psi^{-\infty}}}\) with
\[
\mathcal{E}(P^\phi_k) = E_0 + E_0, \tag{3.27}
\]
and the low-frequency estimate (1.5) holds. By (3.7) (a consequence of the definition of $\Lambda$ (3.6)), $\mathcal{E}$ is nowhere zero on the support of $\psi_\mu$; therefore the function $\psi_\mu/\mathcal{E}$ is well-defined and in $C_0(\mathbb{R})$. The definition of $\Pi_L$ (3.8) and Part 1 of Theorem 2.6 imply that

$$
\Pi_L = \psi_\mu (P^2_h) = \mathcal{E}(P^2_h) \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) = \mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) + E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h). \tag{3.28}
$$

Then, by Part 3 of Theorem 2.6 and the fact that $E_0 = O(h^\infty)_{\mathcal{D}^\infty_{\rho}} \rightarrow \mathcal{D}^\infty_{\rho}$,

$$
E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) = O(h^\infty)_{\mathcal{D}^\infty_{\rho}} \rightarrow \mathcal{D}^\infty_{\rho}. \tag{3.29}
$$

### 3.3.1 The case $\rho = 1$

We first assume that $\rho = 1$ and we show the decomposition (3.11), together with the bound (1.14) on $u_A$ and the bound (3.13) on $u_\epsilon$. In this case, we let

$$
u_A := E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) w \quad \text{and} \quad u_\epsilon := E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) w,
$$

so that (3.11) holds by (3.27) and (3.8). Then, using the low-frequency estimate (1.5), Part 3 of Theorem 2.6, and finally the resolvent estimate (1.4), we get

$$
\|D(\alpha)_{\mathcal{A}}\|_{\mathcal{H}^1} = \left\| D(\alpha) E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) w \right\|_{\mathcal{H}^1} \leq C_{\mathcal{E}}(\alpha, h) \left\| \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) w \right\|_{\mathcal{H}^1}
$$

$$
\leq C_{\mathcal{E}}(\alpha, h) \sup_{\lambda \in \mathbb{R}} \left| \frac{1}{\mathcal{E}(\lambda)} \psi_\mu(\lambda) \right| \| w \|_{\mathcal{H}^1} = C_{\mathcal{E}}(\alpha, h) \sup_{\lambda \in \mathbb{R}} \left| \frac{1}{\mathcal{E}(\lambda)} \psi_\mu(\lambda) \right| \| w \|_{\mathcal{H}^1}
$$

$$
\lesssim C_{\mathcal{E}}(\alpha, h) \sup_{\lambda \in \mathbb{R}} \left| \frac{1}{\mathcal{E}(\lambda)} \psi_\mu(\lambda) \right| \| w \|_{\mathcal{H}^1}
$$

thus (1.14) holds. In addition, the bound (3.13) follows from (3.29) together with the resolvent estimate (1.4).

### 3.3.2 The decomposition (3.11)

We now tackle the general case. Given $R_0$ and $\tilde{R}$, let $R_1, R_{II}, R_{III}, R_{IV}$, be such that $R_0 < R_1 < R_{II} < R_{III} < R_{IV} < \tilde{R}$ and $\rho = 1$ near $B_{R_{V}}$. In addition, let $\rho_1 \in C^\infty(\mathbb{T}^d_{\tilde{R}})$ be equal to one near $B_{R_0}$ and such that supp$(1 - \rho_1) \subset (B_{R_{III}})^c$ and supp$\rho_1 \subset B_{R_{III}}$ (see Figure 3.1).

Using (3.28), we decompose $u_L = \Pi_L w$ as

$$
u_L = \Pi_L \rho_1 w + \Pi_L (1 - \rho_1) w
$$

$$
= E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) \rho_1 w + E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^2_h) \rho_1 w + \Pi_L (1 - \rho_1) w,
$$

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and we define
\[ u_R^A := \mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w \quad \text{and} \quad u_\infty := \Pi_L (1 - \rho_1) w. \] (3.30)

We further decompose \( u_\infty \) below as
\[ u_\infty = u_\infty^A + u_\varepsilon, \] (3.31)
(see (3.40) below) and define
\[ u_A := u_R^A + u_\infty^A \quad \text{and} \quad u_\varepsilon := \tilde{u}_\varepsilon + E_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w \] (3.32)
(with the first definition implying (1.9)). These definitions imply that \( u_L = u_A + u_\varepsilon \), i.e., that (3.11) holds. To complete the proof, we now need to show that (1.10)–(1.13), and (3.13) hold.

### 3.3.3 Proof of (1.10) and (1.11) for the localised term \( u_A^R \).

Using, respectively, the definition of \( u_R^A \) (3.30), the fact that \( \rho = 1 \) on \( B_{R_{111}} \), the low-frequency estimate (1.5), Part 3 of Theorem 2.6, and finally the resolvent estimate (1.4) we obtain
\[
\|D(\alpha)u_A^R\|_{H^t(B_{R_{111}})} = \|D(\alpha)\mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w\|_{H^t(B_{R_{111}})} \leq \rho D(\alpha)\mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w\|_{H^t} \\
\leq C_{E}(\alpha, h) \| \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w\|_{H^t} \leq C_{E}(\alpha, h) \sup_{\lambda \in \mathbb{R}} \left| \frac{1}{\mathcal{E}(\lambda)} \psi_\mu(\lambda) \right| \|w\|_{H^t} \\
= C_{E}(\alpha, h) \sup_{\lambda \in \mathbb{R}} \left| \frac{1}{\mathcal{E}(\lambda)} \psi_\mu(\lambda) \right| \|w\|_{H^t} \lesssim C_{E}(\alpha, h) \sup_{\lambda \in \mathbb{R}} \left| \frac{1}{\mathcal{E}(\lambda)} \psi_\mu(\lambda) \right| h^{-M-1}\|g\|_H; \]

thus (1.10) holds.

Let \( \rho_2 \in C^\infty(\mathbb{T}^d_{R_1}) \) be supported in \( B_{R_{111}} \) and such that \( \rho_2 = 1 \) on \( \text{supp} \rho_1 \) (see Figure 3.1). By (3.27), Part 1 of Theorem 2.6, and the pseudo-locality of the functional calculus (Lemma 2.7),
\[
(1 - \rho_2)\mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 = (1 - \rho_2)\mathcal{E} (P^*_K) \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 + O(h^\infty)_{D^{1,\infty}_K \rightarrow D^1_K} \\
= (1 - \rho_2)\Pi_L \rho_1 + O(h^\infty)_{D^{1,\infty}_K \rightarrow D^1_K} = O(h^\infty)_{D^{1,\infty}_K \rightarrow D^1_K}. \] (3.33)

On the other hand, since \( \rho_2 = 0 \) on \( B_{R_{111}} \),
\[
\|u_A^R\|_{D^{m,\frac{t}{1}}(B_{R_{111}})} = \|(1 - \rho_2)\mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w\|_{D^{m,\frac{t}{1}}(B_{R_{111}})} \leq \|(1 - \rho_2)\mathcal{E}_0 \left( \frac{1}{\mathcal{E}} \psi_\mu \right) (P^*_K) \rho_1 w\|_{D^{m,\frac{t}{1}}}. \]

Combining this with (3.33) and then using the resolvent estimate (1.4), we obtain (1.11).

### 3.3.4 The term away from the black-box \( u_\infty^A \).

**Step 1: the decomposition (3.31), and bound (3.13) on \( u_\varepsilon \).** Let \( \gamma_1 \in C^\infty(\mathbb{T}^d_{R_1}) \) be equal to zero near \( B_{R_0} \), and such that \( \gamma_1 = 1 \) near \( (B_{R_1})^c \). Since \( \text{supp}(1 - \gamma_1) \) and \( \text{supp}(1 - \rho_1) \) are disjoint (see Figure 3.1), by the pseudo-locality of the functional calculus given by Lemma 2.7,
\[
\Pi_L (1 - \rho_1) = \gamma_1 \Pi_L (1 - \rho_1) + O(h^\infty)_{D^{1,\infty}_K \rightarrow D^1_K} \\
= \gamma_1 \Pi_L \gamma_1 (1 - \rho_1) + O(h^\infty)_{D^{1,\infty}_K \rightarrow D^1_K}. \]

Therefore, by Lemma 2.8,
\[
\Pi_L (1 - \rho_1) = \gamma_1 \Pi_L \gamma_1 (1 - \rho_1) + O(h^\infty)_{D^{1,\infty}_K \rightarrow D^1_K}, \] (3.34)
where \( \Pi_L^\Psi \in \Psi^\infty(\mathbb{T}^d_{R_1}) \) and
\[
\text{WF} \Pi_L^\Psi \subset \text{supp} \psi_\mu \circ q_h. \] (3.35)
By (2.6), since $\psi_\mu$ is compactly supported, there exists $\lambda > 1$ such that
\[
\text{supp } \psi_\mu \circ q_h \subset \mathbb{T}^d_h \times B \left(0, \frac{\lambda}{2}\right).
\] (3.36)

Now, let $\tilde{\varphi} \in C_\infty^\infty$ be compactly supported in $B(0, \lambda^2)$ and equal to one on $B(0, \lambda^2/4)$. By (3.36) and (3.35) together with (A.11), $\text{WF}_h \left(1 - \text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right)\right) \cap \text{WF}_h \left(\Pi_L^\varphi\right) = \emptyset$. Therefore, by (A.10), as operators on the torus,
\[
\Pi_L^\varphi = \text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right) \Pi_L^\varphi + E_1,
\] (3.37)
where $E_1 = O(\hbar^\infty)_{\psi, -\infty}$. Since $\gamma_1 = 0$ near $B_{R_\infty}$, by the definitions of $\mathcal{P}^d$ (2.5), $\| \cdot \|_{\mathcal{P}_h^d} = (2.11)$, and $\| \cdot \|_{H^{\infty}(\mathcal{T}^d_h)} = (2.12)$,
\[
\| \gamma_1 w \|_{\mathcal{P}_h^d} \lesssim m \| \gamma_1 w \|_{H^{\infty}(\mathcal{T}^d_h)} \lesssim m \| \gamma_1 w \|_{\mathcal{P}_h^d} \quad \text{for all } w \in \mathcal{P}_h^d,
\] (3.38)
and thus $\gamma_1 E_1 \gamma_1 = O(\hbar^\infty)_{\mathcal{P}_h^d} \to \mathcal{P}_h^d$. Therefore, combining this with (3.37) and (3.34), we obtain that
\[
\Pi_L(1 - \rho_1) = \gamma_1 \text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right) \Pi_L^\varphi \gamma_1(1 - \rho_1) + E_2,
\] (3.39)
where $E_2 = O(\hbar^\infty)_{\mathcal{P}_h^d} \to \mathcal{P}_h^d$. We let
\[
u_\infty := \gamma_1 \text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right) \Pi_L^\varphi \gamma_1(1 - \rho_1) w \quad \text{and} \quad \tilde{u}_r := E_2 w;
\] (3.40)
then (3.11) holds by (3.39) and (3.30). The bound (3.13) on $u_\infty$ follows directly from the definition of $\nu_\infty$ (3.32), together with (3.29), the fact that $E_2 = O(\hbar^\infty)_{\mathcal{P}_h^d} \to \mathcal{P}_h^d$, and the resolvent estimate (1.4).

**Step 2: $u_\infty$ is regular in $(B_{R_\infty})^c$ (i.e., proving the bound (1.12)).** By the definition of $u_\infty^\infty$ (3.40) and the fact that $\gamma_1 = 1$ on $(B_{R_\infty})^c$,
\[
\|\partial^\alpha u_\infty^\infty\|_{H^0((B_{R_\infty})^c)} = \left\|\partial^\alpha \text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right) \Pi_L^\varphi \gamma_1(1 - \rho_1) w\right\|_{H^0((B_{R_\infty})^c)}
\leq \left\|\partial^\alpha \text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right) \Pi_L^\varphi \gamma_1(1 - \rho_1) w\right\|_{L^2(\mathcal{T}_h^d)}.
\] (3.41)

We now bound the right-hand side of (3.41). By Lemma A.3, $\text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right)$ is given as a Fourier multiplier on the torus (defined by (A.12)), i.e.,
\[
\text{Op}_h \rho^{\sharp} \left(\tilde{\varphi}(\xi^2)\right) = \tilde{\varphi}(-h^2\Delta).
\] (3.42)

Let $v \in L^2(\mathbb{T}^d_h)$ be arbitrary, and let $\hat{v}(j)$ be the Fourier coefficients of $v$. By (A.12),
\[
\tilde{\varphi}(-h^2\Delta)v = \sum_{j \in \mathbb{Z}^d} \hat{v}(j)\tilde{\varphi}(h^2|j|^2\pi^2/R_h^2)e_j,
\]
where the normalised eigenvectors $e_j$ are defined by (A.1). Hence, for any multi-index $\alpha$,
\[
\partial^\alpha \tilde{\varphi}(-h^2\Delta)v = \sum_{j \in \mathbb{Z}^d} \hat{v}(j)\tilde{\varphi}(h^2|j|^2\pi^2/R_h^2) \left(\frac{\imath \pi j}{R_h}\right)^\alpha e_j
\]

\[
= \sum_{j \in \mathbb{Z}^d, |j| \leq \frac{R_h}{\hbar}} \hat{v}(j)\tilde{\varphi}(h^2|j|^2\pi^2/R_h^2) \left(\frac{\imath \pi j}{R_h}\right)^\alpha e_j,
\]

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

\[
\|\partial^\alpha \tilde{\varphi}(-h^2 \Delta) v\|_{L^2(\mathbb{T}^d)}^2 = \sum_{j \in \mathbb{Z}^d, |j| \leq \frac{1}{4} \lambda} |\hat{\tilde{\varphi}}(h^2 |j|^2 / R^2_\xi)\left(\frac{1}{R_\xi}\right)^\alpha|^2 \\
\leq \lambda^{2|\alpha|} h^{-2|\alpha|} \sum_{j \in \mathbb{Z}^d} |\hat{\tilde{\varphi}}(j)|^2 \\
= \lambda^{2|\alpha|} h^{-2|\alpha|} \|v\|_{L^2(\mathbb{T}^d)}^2.
\]

We now use (3.43) with $\tilde{\varphi}$ and combine the resulting estimate with (3.41) and (3.42). Using the fact that $\Pi^\Psi_4$ from an elliptic-regularity estimate.

Theorem 1.16 is proved by directly verifying the assumptions of Theorem 1.1. Theorems 1.6 and 1.12 are proved using the following two corollaries of Theorem 1.1. In the first corollary (Corollary 4.1), the low-frequency estimate (1.5) comes from a heat-flow estimate, and in the second (Corollary 4.2) from an elliptic-regularity estimate.
Corollary 4.1 Let $P_h$ be a semiclassical black-box operator on $\mathcal{H}$ satisfying the polynomial resolvent estimate (1.4) in $H \subset (0, h_0]$. Assume further that (i) $P_h^* \geq a(h) > 0$ for some $a(h) > 0$, and (ii) for some $\alpha$-family of black-box differentiation operators $(D(\alpha))_{\alpha \in \mathfrak{A}}$ (Definition 2.2), there exists $\rho \in C^\infty(\mathbb{T}_{R_1})$ equal to one near $B_{R_0}$ such that the following localised heat-flow estimate holds,

$$
\| \rho D(\alpha)e^{-\mathbb{H} t} P_h^\alpha \|_{\mathcal{H}^1 \to \mathcal{H}^2} \leq C(\alpha) t^{\alpha/2} \quad \text{for all } \alpha \in \mathfrak{A}, \; 0 < t < 1, \; h \in H. \tag{4.1}
$$

Then, if $R > 0$ is such that $R_0 < R < R_2$, $g \in \mathcal{H}$ is compactly supported in $B_R$, and $u(h) \in D_{\text{out}}$ satisfies (1.6), there exists $u_A \in D_{\mathcal{H}}^{2,\infty}$ and $u_{H^2} \in D_{\mathcal{H}}^2$ such that $u$ decomposes as (1.7). Furthermore, $u_{H^2}$ satisfies (1.8) and there exists $R_1, R_{H^1}, R_{H^1}, R_{H^1}$, and $R_2$, with $R_0 < R_1 < R_{H^1} < R_{H^1} < R_{H^1} < R_{H^2} < R_2$, such that $u_A$ decomposes as $u_A = u_A^{R_1} + u_A^\infty$ with, for some $\lambda > 1$,

$$
\| D(\alpha)u_A^{R_1} \|_{\mathcal{H}^1(B_{R_1})} \lesssim C(\alpha) h^{-\alpha - M - 1} \| g \|_{\mathcal{H}} \quad \text{for all } h \in H \quad \text{and } \alpha \in \mathfrak{A}, \tag{4.2}
$$

$$
\| D^{\alpha} u_A^\infty \|_{\mathcal{H}^1(B_{R_1})} \lesssim \lambda^{\alpha/2} h^{-\alpha - M - 1} \| g \|_{\mathcal{H}} \quad \text{for all } h \in H \quad \text{and } \alpha \in \mathfrak{A}, \tag{4.3}
$$

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

$$
\| u_A^\infty \|_{\mathcal{H}^{2+m}(B_{R_1})} + \| D^{\alpha} u_A^\infty \|_{\mathcal{H}^{2+m}(P_{H^1}R_1)} \leq C_{N,m} h^N \| g \|_{\mathcal{H}} \quad \text{for all } h \in H \quad \text{and } \alpha \in \mathfrak{A}. \tag{4.4}
$$

In addition, if $\rho = 1$, the decomposition (1.7) can be constructed in such a way that instead of (4.2)–(4.4), $u_A$ satisfies the global regularity estimate

$$
\| D(\alpha)u_A \|_{\mathcal{H}^2} \lesssim C(\alpha) h^{-\alpha - M - 1} \| g \|_{\mathcal{H}} \quad \text{for all } h \in H \quad \text{and } \alpha \in \mathfrak{A}. \tag{4.5}
$$

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

Proof. Since $P_h^\alpha \geq a(h) > 0$, $\text{Sp} P_h^\alpha \subset [a(h), \infty)$. Therefore, by Parts 4 and 3 of Theorem 2.6, $e^{-P_h^\alpha} = E(P_h^\alpha)$, where $E(\lambda) = E_0(\lambda) := e^{-|\lambda|}$. Such an $E$ is in $C_0(\mathbb{R})$, never vanishes, and satisfies (1.5) with $C_E(\alpha, h) := C(\alpha) h^{-\alpha}$ by (4.1) with $t := h^2$. The result therefore follows from Theorem 1.1.

Corollary 4.2 Let $P_h$ be a semiclassical black-box operator on $\mathcal{H}$ satisfying the polynomial resolvent estimate (1.4) in $H \subset (0, h_0]$. Assume further that, for some $\alpha$-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,

$$
\| D(\alpha)w \|_{\mathcal{H}^2} \leq \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha, h) \| (P_h^\ell)^{\frac{1}{2}} w \|_{\mathcal{H}^2} \quad \text{for all } \alpha \in \mathfrak{A}, \; w \in D_h^{2,\infty}, \; \text{and } h \in H, \tag{4.6}
$$

for some $C_\ell(\alpha, h) > 0$, $\ell = 0, \ldots, L(\alpha)$. Then, if $R_0 < R < R_1$, $g \in \mathcal{H}$ is compactly supported in $B_R$, and $u(h) \in D_{\text{out}}$ satisfies (1.6), there exists $u_A \in D_{\mathcal{H}}^{2,\infty}$, $u_{H^2} \in D_{\mathcal{H}}^2$ such that $u$ can be written as (1.7), $u_{H^2}$ satisfies (1.8), and $u_A$ satisfies

$$
\| D(\alpha)u_A \|_{\mathcal{H}^2} \lesssim \left( \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha, h) \right) h^{-M-1} \| g \|_{\mathcal{H}} \quad \text{for all } \alpha \in \mathfrak{A} \quad \text{and } h \in H, \tag{4.7}
$$

where the omitted constant is independent of $h$ and $\alpha$.

Proof. Let $\rho := 1$, $E(\lambda) := (\lambda)^{-L}$ and $C_\alpha(\alpha, h) := \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha, h)$. We now need to show that the bound (4.6) implies that the bound (1.5) holds with these choices of $E$ and $C_E$. Given $v \in D_h^{2,\infty}$, let $w := (P_h^\ell)^{-L} v \in D_h^{1,\infty}$. The bound (4.6) implies that

$$
\| \rho D(\alpha) (P_h^\ell)^{-L} v \|_{\mathcal{H}^2} \leq \sum_{\ell=0}^{L(\alpha)} C_\ell(\alpha, h) \| (P_h^\ell)^{\frac{1}{2}} (P_h^\ell)^{-L} v \|_{\mathcal{H}^2} \quad \text{for all } \alpha \in \mathfrak{A} \quad \text{and } h \in H. \tag{4.8}
$$

Since $(\lambda)^{-L} \lambda^\ell \leq 1$, by Part 3 of Theorem 2.6, the term in brackets on the right-hand side of (4.8) is bounded by $C_E(\alpha, h) \| v \|_{\mathcal{H}^1}$, and then (1.5) follows. The result (4.7) then follows from the bound (1.14) in Theorem 1.1.
4.1 Proof of Theorem 1.6

The plan is to apply Corollary 4.1. Let \( h := k^{-1} \), \( g := h^2 f \), and define \( H \) and \( P_h \) as in Lemma 2.3. By Lemma 2.3, \( P_h \) is a semiclassical black-box operator on \( \mathcal{H} \).

The assumption that \( C_{so(k)}(k) \) is polynomially bounded means that (1.4) holds with

\[
H := \{ h : h = k^{-1} \text{ with } k \in K \},
\]

(4.9)

and thus we only need to show that the heat-flow estimate (4.1) is satisfied. As in Corollary 4.1, we choose \( \rho \) to be equal to one near \( B_{R_0} \), and further assume that \( \rho \) is supported in \( B_{(R_0 + c)/2} \) (i.e., in a region where \( A \) and \( c \) are known to be analytic). Since \( \mathcal{O}_- \) is analytic, and \( A \) and \( c \) are analytic on a domain including the support of \( \rho \), by the results of Escauriaza–Montaner–Zhang [25, 24], the heat-flow estimate (4.1) is satisfied with \( D(\alpha) := \partial^\alpha \) and

\[
C(\alpha) = \nu^{-1-|\alpha|/2}|\alpha|!,
\]

for some \( \nu > 0 \) that is also, without loss of generality, \( < 1 \) (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., [61, Theorem VIII.7]).

We can therefore apply Corollary 4.1 with an arbitrary \( R_1 > R \), and we obtain \( u_{H^2} \in \mathcal{D}^i \) and \( u_A \in \mathcal{D}^\infty \) with \( u_A = u_{R_0} + u_{R_1}^{c} \) satisfying (1.7), (1.8), (1.9), and the bounds (4.2)–(4.4). Observe that \( u_{H^2} \) and \( u_A \) satisfy the Dirichlet boundary condition (1.17) since they are in \( \mathcal{D}^i \) (2.4). Furthermore, the low-frequency bounds (4.2)–(4.4) give directly the bounds (1.22)–(1.24).

The bound (1.8) implies that

\[
\|u_{H^2}\|_{L^2(\mathcal{T}_{R_1}^d \cap \mathcal{O}_-)} + k^{-2}\|\nabla \cdot (A\nabla u_{H^2})\|_{L^2(\mathcal{T}_{R_1}^d \cap \mathcal{O}_-)} \lesssim k^{-2}\|f\|_{L^2(B_{R_0} \cap \mathcal{O}_+)},
\]

(4.10)

and then Green’s first identity (see, e.g., [47, Lemma 4.3]) and the fact that \( A \) satisfies (1.15) imply that

\[
\|u_{H^2}\|_{L^2(\mathcal{T}_{R_1}^d \cap \mathcal{O}_-)} + k^{-1}\|\nabla u_{H^2}\|_{L^2(\mathcal{T}_{R_1}^d \cap \mathcal{O}_-)} + k^{-2}\|\nabla \cdot (A\nabla u_{H^2})\|_{L^2(\mathcal{T}_{R_1}^d \cap \mathcal{O}_-)} \lesssim k^{-2}\|f\|_{L^2(B_{R_0} \cap \mathcal{O}_+)};
\]

see, e.g., [33, Lemma 3.10]. That is, (1.21) holds for \( |\alpha| = 0 \) and 1. To obtain (1.21) for \( |\alpha| = 2 \), we combine (4.10) with the \( H^2 \) regularity result of, e.g., [47, Part (i) of Theorem 4.18, pages 137-138], applied with \( \Omega_1 = B_R \cap \mathcal{O}_+ \) and \( \Omega_2 = B_{(R + R_1)/2} \cap \mathcal{O}_+ \). Finally, the proof that \( u_{R_0}^c \) is analytic in \( B_{R_0} \) and \( u_{R_1}^c \) is analytic in \( (B_{R_1})^c \) follows from Appendix C and the bounds (1.22) and (1.23), respectively.

4.2 Proof of Theorem 1.12

The plan is to apply Corollary 4.2. Let \( h := k^{-1} \), \( g := h^2 f \), and define \( H \) and \( P_h \) as in Lemma 2.3.

By Lemma 2.3, \( P_h \) is a semiclassical black-box operator on \( \mathcal{H} \).

The assumption that \( C_{so(k)}(k) \) is polynomially bounded means that (1.4) holds with \( H \) given by (4.9) and thus we only need to show that the regularity estimate (4.6) is satisfied for appropriate \( D(\alpha), C(\alpha, h) \), and \( L(\alpha) \).

We claim that for \( n \) even with \( n \leq 2m \)

\[
\|w\|_{H^i(\mathcal{O}_-)} \leq \frac{n/2}{\sum_{t=0}^{\infty} \tilde{C}_t(n) \left( |(\nabla \cdot (A\nabla)^t w)|_{L^2(\mathcal{T}_{R_1}^d \cap \mathcal{O}_+)} \right)} \quad \text{for all } w \in \mathcal{D}^\infty,
\]

(4.11)

where \( \tilde{C}_t(n) \) also depends on \( \mathcal{O}_-, A \), and \( c \). If (4.11) holds, then the regularity estimate (4.6) is satisfied with (i) \( D(\alpha) := |\partial^{\alpha}\mathcal{O}_-| \), (ii) \( \mathcal{A} \) consisting of multi-indices \( \alpha \) such that \( |\alpha| \) is even and \( |\alpha| \leq 2m \), (iii) \( L(\alpha) := |\alpha|/2 \), and (iv)

\[
C_t(\alpha, h) := h^{-2t}\tilde{C}_t(|\alpha|).
\]

(4.12)

We assume that (4.11) holds, and show how the result of the theorem follows from Corollary 4.2. Applying this corollary, we obtain \( u_{H^2}, u_A \) satisfying (1.7), (1.8), and (4.7). Observe that \( u_{H^2} \),...
and \(u_A\) satisfy the transmission conditions (1.35) since they are in \(D^4\). By (4.12), there exists \(C_2 = C_2(m) > 0\) such that, for \(|\alpha| \leq 2m,
\[
L(\alpha) \sum_{\ell=0}^{L(\alpha)} C_2(\alpha, h) \leq C_2(m) h^{-|\alpha|}.
\]

The low-frequency bound (4.7) therefore gives (1.38) for all \(\alpha \in \mathfrak{a}\), i.e., for all \(\alpha\) with \(|\alpha|\) even and \(\leq 2m\). The bound (1.38) then holds for all \(\alpha\) with \(|\alpha| \leq 2m\) by interpolation (see, e.g., [47, Theorem B.8], [12, §4.2]). Finally, (1.37) follows from the high-frequency estimate (1.8), together with Green’s identity and (4.11) applied with \(n = 2\) (similar to the end of the proof of Theorem 1.6).

We therefore only need to prove (4.11). The two ingredients to do this are the regularity result

\[
\|v\|_{H^{\alpha+2}(\Omega) \oplus H^{\alpha+2}(\mathbb{T}^d_{R^\beta} \cap O_\beta)} \lesssim \|\nabla \cdot (A \nabla v)\|_{H^{\alpha}(\Omega) \oplus H^\alpha(\mathbb{T}^d_{R^\beta} \cap O_\beta)} + \|v\|_{H^1(\Omega) \oplus H^1(\mathbb{T}^d_{R^\beta} \cap O_\beta)},
\]

(4.13) for all integers \(n \leq 2m - 2\), and the bound

\[
\|v\|_{H^{\alpha+2}(\Omega) \oplus H^{\alpha+2}(\mathbb{T}^d_{R^\beta} \cap O_\beta)} \lesssim \|\nabla \cdot (A \nabla v)\|_{L^2(\Omega) \oplus L^2(\mathbb{T}^d_{R^\beta} \cap O_\beta)} + \|v\|_{L^2(\Omega) \oplus L^2(\mathbb{T}^d_{R^\beta} \cap O_\beta)},
\]

(4.14) where both bounds are valid for all \(v \in D^d\), and the omitted constants in both depend on \(A, c, \beta\).

The bound (4.14) is proved using Green’s first identity (see, e.g., [47, Lemma 4.3]), the fact that \(v\) satisfies the transmission conditions in (2.9), and the fact that \(A\) satisfies (1.15); see, e.g., [33, Lemma 3.10] for an analogous bound in \(\mathbb{R}^d\) for the case \(\beta = 1\).

Regarding (4.13): standard elliptic regularity results imply that, given \(\Omega_1, \Omega_2\) with \(O_\beta \subset \Omega_1 \subset \Omega_2 \subset B_{R_1}\),

\[
\|v\|_{H^{\alpha+2}(\Omega) \oplus H^{\alpha+2}(\Omega_1 \cap O_\beta)} \lesssim \|\nabla \cdot (A \nabla v)\|_{H^{\alpha}(\Omega) \oplus H^\alpha(\Omega_1 \cap O_\beta)} + \|v\|_{H^1(\Omega) \oplus H^1(\Omega_1 \cap O_\beta)} \quad \text{for all } \Omega, v \in D^d;
\]

(4.15) and (4.13) follows.

We now use (4.13) and (4.14) to prove (4.11) by induction. The bound (4.11) with \(n = 2\) follows from combining (4.13) with \(n = 0\) and \(v = w\) and (4.14) with \(v = w\) (observe that choosing \(v = w\) in both is allowed since \(w \in D^d\)). We now assume that we have proved (4.11) for \(n\) even and \(n - 2q\) for some \(0 \leq q \leq m - 1\); i.e.,

\[
\|w\|_{H^{2q}} \lesssim \sum_{\ell=0}^{q} \|\nabla \cdot (A \nabla)^\ell w\|_{L^2} \quad \text{for all } w \in D^d_{H^\infty},
\]

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

Applying (4.13) with \(n = 2q\) and \(v = w\), we have

\[
\|w\|_{H^{2q+2}} \lesssim \|\nabla \cdot (A \nabla w)\|_{H^{2q}} + \|w\|_{H^1},
\]

(4.17) (again omitting the domains of the norms for brevity). The desired bound (4.11) with \(n = 2q + 2\) then follows by using in (4.17) the inequality (4.16) with \(w\) replaced by \(\nabla \cdot (A \nabla w)\) (which is allowed since \(w \in D^d_{H^\infty}\) implies that \(P_h w \in D^d_{H^\infty}\) by (2.12)), and then using (4.14) with \(v = w\).

4.3 Proof of Theorem 1.16

Let \(h := h^{-1}\), \(g := h^2 f\), and define \(H\) and \(P_h\) as in Lemma 2.3 with \(O_- = \emptyset\). By Lemma 2.3, \(P_h\) is a semiclassical black-box operator on \(H\). The reference operator is given by \(P_h = -h^2 c^2 \nabla \cdot (A \nabla)\), acting on the torus \(\mathbb{T}^d_{R^\beta}\).
The assumption that $C_{\text{pol}}(k)$ is polynomially bounded means that the bound (1.4) holds with $H$ given by (4.9); i.e., the assumption in Point 1 of Theorem 1.1 is satisfied.

We now construct $\mathcal{E}$ and $\mathcal{E}_0$ satisfying the assumptions in Point 2 of Theorem 1.1. Let $\Lambda > 0$ be as in Theorem 1.1, and let $\mathcal{E} \in C^\infty_c(\mathbb{R})$ be such that $\mathcal{E} = 1$ in $[-\Lambda, \Lambda]$, and $\mathcal{E} = 0$ outside $[-2\Lambda, 2\Lambda]$. The results of Helffer-Robert [35] (see the account in [63]) imply that $\mathcal{E}(P^2_h) = \mathcal{E}(-h^2c^2\nabla \cdot (A\nabla))$ is a pseudo-differential operator on the torus $T^d_R$. Then, the same argument as in the proof of Lemma 2.8 shows that

$$\text{WF}_h \mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) \subset \text{supp} \mathcal{E} \circ q,$$

where $q(x, \xi) = c(x)^2(A(x)\xi, \xi)$ is the semi-classical principal symbol of $-h^2c^2\nabla \cdot (A\nabla)$. Hence, since $\mathcal{E}$ is compactly supported and $A$ satisfies (1.15), there exists $\Lambda_0 > 0$ such that

$$\text{WF}_h \mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) \subset T^d_R \times B \left(0, \frac{\Lambda_0}{2}\right).$$

(4.18)

Let $\tilde{\varphi} \in C^\infty_c$ be compactly supported in $B(0, \Lambda_0^2)$ and equal to one on $B(0, \Lambda_0^2/4)$. By (4.18) and (A.11), $\text{WF}_h \left(1 - \text{Op}_h(\tilde{\varphi}([\xi]^2))\right) \cap \text{WF}_h \mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) = \emptyset$, therefore

$$\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) = \text{Op}_h(\tilde{\varphi}([\xi]^2))\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) + O(h^\infty)_{\Psi^{-\infty}}.$$  

Then, by Lemma A.3,

$$\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) = \tilde{\varphi}(-h^2\Delta)\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) + O(h^\infty)_{\Psi^{-\infty}}.$$  

(4.19)

We now define

$$\mathcal{E}_0 := \tilde{\varphi}(-h^2\Delta)\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)),$$

(4.20)

and thus (4.19) implies that

$$\mathcal{E}(P^2_h) = \mathcal{E}_0 + O(h^\infty)_{D^{-\infty}h \rightarrow D^{\infty}h}.$$  

We now need to show that a low-frequency estimate of the form (1.5) is satisfied. Since $\tilde{\varphi}$ is compactly supported in $B(0, \Lambda_0^2)$, the definition of $\mathcal{E}_0$ (4.20) and the same argument used to show the bound (3.43) imply that

$$\|\partial^\alpha \mathcal{E}_0 v\|_{L^2(T^d_R)} \leq \Lambda_0^{[\alpha]}h^{-[\alpha]}\|\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) v\|_{L^2(T^d_R)}$$

for all $v \in L^2(T^d_R)$ and multi-indices $\alpha$.

Then, since $\mathcal{E}(-h^2c^2\nabla \cdot (A\nabla)) \in \Psi^{-\infty}(T^d_R)$, there exists $C > 0$ such that

$$\|\partial^\alpha \mathcal{E}_0 v\|_{L^2(T^d_R)} \leq C\Lambda_0^{[\alpha]}h^{-[\alpha]}\|v\|_{L^2(T^d_R)}$$

for all $v \in L^2(T^d_R)$ and multi-indices $\alpha$.

Therefore, the assumption in Point 2 of Theorem 1.1 is satisfied with $D(\alpha) := \partial^\alpha$, $C_{\mathcal{E}}(\alpha, h) := CA_0^{[\alpha]}h^{-[\alpha]}$ and $\rho = 1$. The result then follows from Theorem 1.1; indeed, the bound (1.41) follows immediately from (1.14), and (1.40) follows from (1.8) after using Green’s identity and elliptic regularity in the same way as at the end of the proof of Theorem 1.6 — see (4.10) and the surrounding text.

5 Proofs of Theorems 1.7 and 1.14 and Corollary 1.9 (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 1.7 and 1.14 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 1.6 and 1.12.

Regarding Lemma 5.4: this argument came out of ideas introduced in [65], was then formalised in
[64], and has been used extensively in the analysis of the Helmholtz FEM; see, e.g., [1, 39, 48, 64,
52, 53, 75, 73, 20, 14, 45, 15, 30, 34, 29, 43].

Before stating Lemma 5.4 we need to introduce some notation. Let $C_{\text{cont}} = C_{\text{cont}}(A, c^{-2}, R, k_0)$
be the \textit{continuity constant} of the sesquilinear form $a(\cdot, \cdot)$ (defined in (1.26)) in the norm
$\| \cdot \|_{H^1_k(B_R \cap \mathcal{O}_+)}$; i.e.

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

By the Cauchy-Schwarz inequality and (1.27),

$$C_{\text{cont}} \leq \max \{A_{\max}, c_{\min}^{-2}\} + C_{\text{DtN}}. \quad (5.1)$$

The following definitions are stated for the sesquilinear form of the Dirichlet problem (1.26). 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 (1.26) is given by

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

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

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

Green’s second identity applied to solutions of the Helmholtz equation satisfying the Sommerfeld radiation condition (1.2) implies that $\langle \text{DtN}_k \psi, \varphi \rangle_{\partial B_R} = \langle \text{DtN}_k \phi, \psi \rangle_{\partial B_R}$ for all $\phi, \psi \in H^{1/2}(\partial B_R)$ (see, e.g., [68, Lemma 6.13]); thus $a(\varphi, u) = a(\varphi, v)$ and so the definition (5.2) implies that

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

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

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

**Lemma 5.4 (Conditions for quasioptimality) If

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

then the Galerkin equations (1.29) have a unique solution which satisfies

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

References for the proof. See, e.g., [43, 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 $O_-, A, c, R, R_i$, and $R_{iv}$ are as in Theorem 1.6. Let $(V_N)^\infty_{N=0}$ be the piecewise-polynomial approximation spaces described in [52, §5], [53, §5.1.1]; assume further that the triangulations fit $B_{R_i}$ and $B_{R_{iv}}$ exactly.

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

- $C_1, C_2, \sigma > 0$, 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

$$k \eta(V_N) \leq C_1 \frac{hk}{p} \left(1 + \frac{hk}{p}\right) + C_2 k^{1+M} \left(\frac{hk}{\sigma}\right)^p + C_N k^{1-N} \quad \text{for all } k \geq k_0. \quad (5.5)$$

Lemma 5.6 (Bound on $\eta(V_N)$ for the transmission problem) Let $d = 2$ or 3 and let $\beta = 1$. Suppose that $A, c, \text{ and } O_-$ are as in Definition 1.10 and, given an integer $p$, satisfy the regularity assumptions in Theorem 1.14. Let $(V_N)^\infty_{N=0}$ be a sequence of piecewise-polynomial approximation spaces of degree $p$ satisfying Assumption 1.13.

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

$$k \eta(V_N) \leq (1 + hk) \left(\tilde{C}_1 hk + \tilde{C}_2 k^{M+1}(hk)^p\right) \quad \text{for all } k \geq k_0. \quad (5.6)$$

Proof of Theorems 1.7/1.14 assuming Lemmas 5.5/5.6. Theorem 1.14 follows immediately by combining Lemmas 5.4 and 5.6 and the inequality (5.1).

Theorem 1.7 follows in a similar way, except that we first choose $N > 1$, and then let $k_1 > 0$ be such that

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

Theorem 1.7 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 $f \in L^2(B_R \cap O_+), \text{ let } v = \mathcal{S}^* f$. By (5.3) and Theorem 1.6, $v = v_{H^2} + v_A$, where $v_{H^2}$ and $v_A$ satisfy the bounds (1.21)–(1.24) with $u$ replaced by $v$.

The proof of Lemma 5.5 is very similar to the proofs of [52, Theorem 5.5] and [53, Proposition 5.3] (covering the constant-coefficient Helmholtz equation in, respectively, $\mathbb{R}^d$ and the exterior of an analytic Dirichlet obstacle). There are two differences.

1. In [52], [53] the function $v_A$ is analytic on the whole of $B_R \cap O_+$, whereas here $v_A = v_A^R + v_A^\infty$ with $v_A^R$ and $v_A^\infty$ analytic in subsets of the domain and $O(k^{-\infty})$ in the complements of these subsets; see (1.22)–(1.24) and Figure 1.1.

2. The results in [52], [53] are proved under the assumption that

$$\|\partial^\alpha v_A\|_{L^2(B_R \cap O_+)} \leq C_1(C_2)|\alpha| \max \{|\alpha|, k\}^{1+M} \|f\|_{L^2(B_R \cap O_+)} \quad \text{(5.7)}$$

for some $C_1, C_2 > 0$ independent of $k$ and $\alpha^2$. In our case, $v_A^\infty$ satisfies a bound of this form, namely (1.23), but $v_A^R$ satisfies (1.22), i.e., the max $\{|\alpha|, k\}^{1+M}$ in (5.7) is replaced by $|\alpha|! k^{1+M}$.

The consequence of Point 1 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 [52, Theorem 5.5] and [53, Proposition 5.3]. Since this term can be made arbitrarily-small for $k$ sufficiently large, the only

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2Strictly speaking, [52, Theorem 5.5] covers (5.7) with $M = 0$, but the modifications to the proof in the case $M > 0$ are straightforward; see [43, Proof of Lemma 6.5].
consequence is that Lemma 5.5 and Theorem 1.7 are valid for \( k \) sufficiently large (as opposed to for all \( k \geq k_0 \) with \( k_0 \) arbitrary).

The consequence of Point 2 is that \( k(hk/\sigma)^p \) appears on the right-hand side of (5.5), instead of the stronger \( k(hk/(\sigma p))^{p} \) on the right-hand sides of the corresponding bounds in [52, Theorem 5.5] and [53, Proposition 5.3] (see also [43, Equation 6.5]). This difference is the reason that we prove quasioptimality of the \( h p \)-FEM under the conditions (1.30) instead of (1.33).

We now go through the proof of [52, Theorem 5.5], outlining the necessary changes to prove the bound (5.5) on \( k \eta(V_N) \).

Exactly as in the proof of [52, Theorem 5.5], there exists \( C_3 > 0 \) (dependent only on the constants in [52, Assumption 5.2] defining the element maps from the reference element) such that

\[
\min_{w_N \in V_N} \| v - w_N \|_{H^1_k(B_R \cap \Omega^+)} \leq C_3 \left( \frac{h k}{p} \right)^p \| f \|_{L^2(B_R \cap \Omega^+)} ,
\]  

(5.8)

for all \( v \in H^2(B_R \cap \Omega^+) \); recall that this result follows from the polynomial-approximation result of [52, Theorem B.4] and the definition (1.18) of the norm \( \| \cdot \|_{H^1_k} \). Applying the bound (5.8) to \( v_{H^2} \) and using (1.21) with \( |\alpha| = 2 \), we obtain

\[
\min_{w_N \in V_N} \| v_{H^2} - w_N \|_{H^1_k(B_R \cap \Omega^+)} \leq C_3 C_1 \left( \frac{h k}{p} \right)^p \| f \|_{L^2(B_R \cap \Omega^+)} ;
\]

we then let \( C_1 := C_1 C_3 \).

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

\[
\min_{w_N \in V_N} \| v_{A} - w_N \|_{H^1_k(B_R \cap \Omega^+)} \leq \left( C_2 k^M \left( \frac{hk}{\sigma} \right)^p + C_3 k^{-N} \right) \| f \|_{L^2(B_R \cap \Omega^+)} ,
\]  

(5.9)

for some \( C_2 > 0 \) independent of \( k, h, p, \) and \( N \) and some \( C_3 > 0 \) independent of \( k, h, \) and \( p \). Furthermore, taking into account the regions where \( v_{A}^R \) and \( v_{A}^\infty \) are analytic (see Figure 1.1) and using (1.24), we find that

\[
\min_{w_N \in V_N} \| v_{A}^R - w_N \|_{H^1_k(B_R \cap \Omega^+)} \leq \min_{w_N \in V_N} \| v_{A}^R - w_N \|_{H^1_k(B_R \cap \epsilon \Omega^+)} + \| v_{A}^R \|_{H^1_k(B_R \cap (B_R \cap \epsilon \Omega^+)^c)}
\]

\[
\leq \min_{w_N \in V_N} \| v_{A}^R - w_N \|_{H^1_k(B_R \cap \epsilon \Omega^+)} + C_N' k^{-N} \| f \|_{L^2(B_R \cap \Omega^+)}
\]

for some \( C'_N > 0 \) independent of \( k, h, \) and \( p \), and similarly,

\[
\min_{w_N \in V_N} \| v_{A}^\infty - w_N \|_{H^1_k(B_R \cap \Omega^+)} \leq \min_{w_N \in V_N} \| v_{A}^\infty - w_N \|_{H^1_k(B_R \cap (B_R \cap \epsilon \Omega^+)^c)} + C_N'' k^{-N} \| f \|_{L^2(B_R \cap \Omega^+)}
\]

for some \( C''_N > 0 \), independent of \( k, h, \) and \( p \). To prove (5.9), therefore, we only need to show that

\[
\min_{w_N \in V_N} \| v_{A}^R - w_N \|_{H^1_k(B_R \cap \epsilon \Omega^+)} \leq C_2 \left( \frac{hk}{\sigma} \right)^p \| f \|_{L^2(B_R \cap \Omega^+)}
\]  

(5.10)

and

\[
\min_{w_N \in V_N} \| v_{A}^\infty - w_N \|_{H^1_k(B_R \cap (B_R \cap \epsilon \Omega^+)^c)} \leq C_2 \left( \frac{hk}{\sigma} \right)^p \| f \|_{L^2(B_R \cap \Omega^+)} ,
\]  

(5.11)

for some \( C_2 > 0 \), independent of \( k, h, p, \) and \( N \).

Let

\[
|\nabla^n v(x)|^2 := \sum_{|\alpha|=n} \frac{n!}{\alpha!} |\partial^\alpha v(x)|^2 .
\]

Since

\[
\sum_{|\alpha|=n} \frac{n!}{\alpha!} = d^n ,
\]

(5.12)

the bound (1.22) implies that \( v_{A}^R \) satisfies

\[
\| \nabla^n v_{A}^R \|_{L^2(B_{R_{1\epsilon}} \cap \Omega^+)} \leq C_2 (C_3 \sqrt{d})^p k^{p-1+M} \| f \|_{L^2(B_R \cap \Omega^+)} \text{ for all } k \in K \text{ and for all } p \in \mathbb{Z}^+ ,
\]  

(5.13)
and the bound (1.23) implies that $v_\gamma$ satisfies

$$\|\nabla^p v_\gamma\|_{L^2((BR_0)^\tau \cap \partial_0)} \leq C_4(C_5 \sqrt{d})^p k^{p-1+M} \|f\|_{L^2(BR_0 \cap \partial_0)}$$

for all $k \in K$ and for all $p \in \mathbb{Z}^+$. 

(5.14)

We now focus on proving (5.10) using the bound (5.13). Since the bound (5.14) is stronger than (5.13), the proof of (5.11) from (5.14) follows analogously (in fact, since (5.14) is stronger than (5.7), the approximation results in [52, Theorem 5.5]/[43, Lemma 6.5], relying on (5.7), apply directly to $v_\gamma$).

The analogue of [52, Lemma C.1] follows immediately from the reasoning in the proof of [52, Lemma C.2]; see [49, Equation 4.3.38] for the analogous bound in that paper. This result is replaced byLemma 5.7 below. Once this is established, the proof of (5.10) using (5.13) now proceeds as in the proof of [52, Theorem 5.5], but with

- [52, Equation 5.8] holding with $(kM)^2$ on the right-hand side,
- the bounds on $\|\nabla^p v\|_{L^2(\tilde{K})}$ and $\|\nabla^p \hat{v}\|_{L^2(\tilde{K})}$ holding with max$\{p, k\}$ replaced by $pl_k^p$, and
- the last equation on [52, Page 1896] holding with $kM$ on the right-hand side.

The rest of the proof of [52, Theorem 5.5] consists of applying three lemmas: [52, Lemmas C.1, C.2, and C.3]. We now discuss the necessary modifications to each of these.

The analogue of [52, Lemma C.1] holds with max$\{p, k\}$ replaced by $pl_k^p$ in both bounds in the statement of the lemma. The proof of this modified result is very similar to the proof of [52, Lemma C.1]; indeed, both follow from the arguments in [49, Lemma 4.3.1], however the proof is easier in our case since there is no parameter $\epsilon$, and so [49, Equation 4.3.38] holds with the right-hand side equal to $C$ instead of $Ce^{\epsilon k}$/2. Furthermore, in the calculations at the top of [49, Page 166] we only need to consider the second of the two terms.

The result [52, Lemma C.2] is replaced by Lemma 5.7 below. Once this is established, the natural analogue of [52, Lemma C.3] follows immediately from the reasoning in the proof of [52, Lemma C.3]. We highlight that [52, Lemma C.2] contains an arbitrary parameter $R > 0$; however, the choice $R = 1$ is made in the proof of [52, Theorem 5.5]. Therefore, for simplicity, we make the choice $R = 1$ from the outset here.

**Lemma 5.7 (Analogue of Lemma C.2 in [52])** Let $d \in \{1, 2, 3\}$, and let $\tilde{K} \subset \mathbb{R}^d$ be the reference simplex. Let $\gamma, \tilde{C} > 0$ be given. Then there exist constants $C, \sigma > 0$ that depend solely on $\gamma$ and $\tilde{C}$ such that the following is true: For any function $u$ that satisfies for some $C_u, h, \kappa \geq 1$ the conditions

$$\|\nabla^nu\|_{L^2(\tilde{K})} \leq C_u(\gamma h)^n n! \kappa^n, \quad \text{for } n = 2, 3, \ldots,$$

if

$$\kappa h \leq \tilde{C}$$

and $p \in \mathbb{N}$ then

$$\inf_{\pi \in \mathcal{P}_p} \|u - \pi\|_{W^{2, \infty}(\tilde{K})} \leq CC_u \left(\frac{\kappa h}{\sigma}\right)^{p+1}$$

(5.15)

where $\mathcal{P}_p$ denotes the space of polynomials on $\tilde{K}$ of degree $\leq p$.

We make the following remarks:

- Both [52, Lemma C.2] and Lemma 5.7 are applied with $\kappa = k$, but we keep the $\kappa$ notation here for consistency with [52].

- The analogues of (5.15) and (5.16) in [52, Lemma C.2] are, respectively,

$$h + \frac{\kappa h}{p} \leq \tilde{C} \quad \text{and} \quad \inf_{\pi \in \mathcal{P}_p} \|u - \pi\|_{W^{2, \infty}(\tilde{K})} \leq CC_u \left[\left(\frac{h}{\sigma + h}\right)^{p+1} + \left(\frac{\kappa h}{\sigma p}\right)^{p+1}\right].$$

The fact that Lemma 5.7 has replaced $hk/p$ by $hk$ is the reason why we do not quite obtain the optimal conditions for quasioptimality.

- As $h \to 0$ with $\kappa$ fixed, the approximation error in (5.16) is $O(h^{p+1})$, as expected.
It therefore remains to prove Lemma 5.7.

**Proof of Lemma 5.7.** We proceed as in the proof of [52, Lemma C.2], replacing \( \max\{n, \kappa\} \) by \( n \kappa^p \) in the third and fourth displayed equations in this proof. The analogue of [52, Equation C.6] is now
\[
\|\nabla^n \tilde{u}\|_{L^\infty(\overline{\hat{K}})} \leq C C_u p^3 (\sqrt{\gamma})^n (n + 2)! \kappa^{n+2}, \quad \text{for } n = 0, 1, 2, \ldots,
\]
and the analogue of [52, Equation C.7] is now
\[
\mu := \gamma \sqrt{\overline{\hat{d}}}.
\]
The Taylor series of \( \tilde{u} \) then converges in the \( L^\infty \) norm in a ball of radius \( 1/(\mu h) \). As in [52, Lemma C.2], let \( r_0 := \text{diam}(\hat{K}) \) and consider two cases: \( \mu_h > 1/(2r_0) \) and \( \mu_h \geq (1/(2r_0). \) (We note that in [52, Lemma C.2] the ball has radius \( 1/(\mu h) \) and the two cases are \( \mu_h \leq (1/(2r_0) \) and \( \mu_h > 1/(2r_0) \).)

For the case \( \mu_h \leq (1/(2r_0) \) we approximate \( \tilde{u} \) by its truncated Taylor series \( T_p u \). With \( b_\hat{K} \) the barycenter of \( \hat{K} \),
\[
\|\tilde{u} - T_p u\|_{L^\infty(B_{r_0}(b_\hat{K}))} \leq S,
\]
where
\[
S := CC_u p^3 \sum_{n=p+1}^\infty (n + 2)(n + 1)((\mu h r_0)^n). \quad (5.17)
\]
To compare with [52, Lemma C.2]: because of the presence of the max in (5.7), there are two sums in [52, Lemma C.2], denoted by \( S_1 \) and \( S_2 \). We deal with \( S (5.17) \) in a similar way to how the sum \( S_2 \) is dealt with in [52, Lemma C.3].

The series in (5.17) converges if \( \mu h r_0 < 1 \), and this is the case because we’re in the situation that \( \mu h \leq (1/(2r_0) \). If \( 0 < a \leq a_0 < 1 \), then
\[
\sum_{n=p+1}^\infty (n + 2)(n + 1)a^n = \frac{\partial^2}{\partial a^2} \left( \frac{a^{p+3}}{1-a} \right) \leq C' a^{p+1} p^2
\]
where \( C' \) depends on \( a_0 \) but is independent of \( p \). Choose \( \tilde{\mu} > \mu \) such that \( \tilde{\mu} h r_0 < 1 \) (this is possible since \( \mu h r_0 < 1/2) \). Then
\[
S \leq CC_u C' p^5 (h \kappa r_0)^{p+1} \leq CC_u C' C'' (h \kappa \tilde{\mu} r_0)^{p+1},
\]
for some \( C'' > 0 \) (depending on \( \tilde{\mu} \) and \( \mu \), but independent of \( h, p, \) and \( \kappa \)), where we have used the exponential decay of \( (\tilde{\mu}/\mu)^{p+1} \) as \( p \to \infty \) to absorb the \( p^5 \) term.

We now let \( \sigma = 1/(\tilde{\mu} r_0) \) and proceed exactly as in [52, Lemma C.3] (i.e., using the Cauchy integral formula) to obtain
\[
\|\tilde{u} - T_p u\|_{W^{2,\infty}(\overline{\hat{K}})} \leq CC_u C' C'' \left( \frac{h \kappa}{\sigma} \right)^{p+1},
\]
which concludes the proof in the case \( \mu h \leq (1/(2r_0) \).

For the case \( \mu h > (1/(2r_0) \), we proceed as in [52, Lemma C.2], observing that (5.15) implies that \( 1/(\mu h) \geq (1/(C_\mu)) : 2 r_1. \) Then, exactly as in [52, Lemma C.2], \( \tilde{u} \) is analytic on \( \hat{U}_{2r_1} := \cup_{x \in \hat{K}} B_{2r_1}(x) \subset C^d. \) The analogue of the fifth displayed equation on [52, Page 1910] is then
\[
\|\tilde{u}\|_{L^\infty(\hat{U}_{r_1})} \leq CC_u p^3 (\theta h)^2,
\]
for some \( \theta > 0 \), independent of \( p, \kappa, \) and \( h, \) and where \( \hat{U}_{r_1} := \cup_{x \in \hat{K}} B_{2r_1}(x) \). We proceed as in [52, Lemma C.2], using approximation results for analytic functions on triangles/tetrahedra from [49, Prop. 3.2.16] and [23, Theorem 1]. We use the fact that given \( r_0, \mu, \) and \( b, \) there exists \( \sigma, C'' > 0 \) (dependent on \( r_0, \mu, \) and \( b \)) such that
\[
p^b e^{-bp} \leq CC'' \left( \frac{1}{2 r_0} \right)^{p+1} \text{ for all } p \geq 0,
\]
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and then obtain, using that $1/(2r_0\mu) < \kappa h$ in this case, that

$$\inf_{\pi \in p} \|u - \pi\|_{W^{2,\infty}(\mathcal{K})} \leq C C'' \left( \frac{hk}{\sigma} \right)^{p+1},$$

which completes the proof in this case.

\section{5.3 Proof of Lemma 5.6}

Given $f \in L^2(B_R)$, let $v = S^* f$. By (5.3) and Theorem 1.12, $v = v_{H^z} + v_A$, where $v_{H^z}$ and $v_A$ satisfy the bounds (1.37) and (1.38) with $u$ replaced by $v$.

By the definition of the $H^k$ norm (1.18) and the bound (1.39), there exists $C_{\text{int}} = C_{\text{int}}(\ell, d) > 0$ such that

$$\min_{w_N \in V_N} \|w - w_N\|_{H^k(B_R)} \leq C_{\text{int}}(\ell, d) (1 + h\kappa) h^\ell \left( \|w\|_{H^{\ell+1}(B_R \cap \mathcal{O}_+)} + \|w\|_{H^{\ell+1}(B_R \cap \mathcal{O}_-)} \right)$$

(5.18)

for all $w = (w_+, w_-) \in H^{\ell+1}(B_R \cap \mathcal{O}_+) \times H^{\ell+1}(B_R \cap \mathcal{O}_-)$. Applying (5.18) with $\ell = 1$ to $v_{H^z}$ and using (1.37) with $|\alpha| = 2$, we obtain that

$$\min_{w_N \in V_N} \|v_{H^z} - w_N\|_{H^1(B_R)} \leq C_{\text{int}}(1, d) (1 + h\kappa) h C \|f\|_{L^2(B_R)}.$$  (5.19)

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

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

i.e., $C_{\text{Sob}}$ 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., [47, Theorem 4.20], [16, Theorem 5.2.1, Part (i)] imply that $u_{\pm,A} \in H^{p+1}$ for $p$ odd and $H^{p+2}$ for $p$ even. For $p$ odd we apply Theorem 1.12 with $m = (p + 1)/2$ and for $p$ even with $m = (p + 2)/2$. In both cases, we apply (5.18) with $\ell = p$ to $v_A = (v_{A,}, v_{A,-})$ and use (1.38) with $|\alpha| = p + 1$ to obtain that

$$\min_{w_N \in V_N} \|v_A - w_N\|_{H^1(B_R)} \leq C_{\text{int}}(p) (1 + h\kappa) h^p C_{\text{Sob}}(p, d) C_2(p) k^{p+M} \|f\|_{L^2(B_R)}.$$  (5.20)

The bound on $\eta(V_N)$ in (5.6) then follows from combining (5.19) and (5.20), with $\tilde{C}_1 := C_{\text{int}}(1, d) C_1$ and $\tilde{C}_2 := C_{\text{int}}(p, d) C_{\text{Sob}}(p, d) C_2$.

\section{5.4 Proof of Corollary 1.9}

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

$$|u|_{H^2(B_R)} \leq C_{\text{osc}} k \|u\|_{H^1(B_R)}$$

(5.21)

by [41, Theorem 9.1 and Remark 9.10], where $C_{\text{osc}}$ depends on $A, c, d,$ and $R$, but is independent of $k$. The combination of (5.21) and (5.8) then imply that

$$\min_{w_N \in V_N} \|u - w_N\|_{H^1(B_R)} \leq C_3 C_{\text{osc}} h k \left( 1 + \frac{h\kappa}{p} \right) \|u\|_{H^1(B_R)}.$$  (5.22)

Combining (1.31), (5.22), and (1.30), we obtain the result (1.34) with $C_6 := C_3 C_{\text{osc}}$.

\section{A Semiclassical pseudodifferential operators on the torus}

Recall that for $R_0 > 0$ we defined the torus

$$\mathbb{T}^d_{R_0} := \mathbb{R}^d/(2R_0\mathbb{Z})^d.$$  

This appendix reviews the material about semiclassical pseudodifferential operators on $\mathbb{T}^d_{R_0}$ used in §3.2, and appearing in Lemma 2.8, with our default references being [76] and [22, Appendix E].
**Semiclassical Sobolev spaces.** We consider functions or distributions on the torus as periodic functions or distributions on $\mathbb{R}^d$. To eliminate confusion between Fourier series and integrals, for $f \in L^2(T^*_R)$ we define the Fourier coefficients

$$\hat{f}(j) := \int_{T^*_R} f(x) e^{-i j \cdot x} \, dx,$$

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

$$e_j(x) = (2R_d)^{-d/2} \exp \left( i \pi j \cdot x / R_d \right)$$

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

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

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

$$(hD)^\alpha f = \sum_{j \in \mathbb{Z}^d} (hj)^\alpha \hat{f}(j) e_j.$$

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

$$H^m_h(T^*_R) := \left\{ u \in L^2(T^*_R), \langle j \rangle^m \hat{f}(j) \in L^2(\mathbb{Z}^d) \right\},$$

and use the norm

$$\|u\|^2_{H^m_h(T^*_R)} := \sum_{j \in \mathbb{Z}^d} |\hat{f}(j)|^2 (hj)^{2m};$$

see [76, §8.3], [22, §E.1.8]. In this appendix, we abbreviate $H^m_h(T^*_R)$ to $H^m_h$ and $L^2(T^*_R)$ 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 $\mathcal{F}_h$ (see [76, §3.3]) on the torus be defined for $h > 0$ by

$$\mathcal{F}_h \phi(\xi) := \int_{T^*_R} \exp \left( -i x \cdot \xi / h \right) \phi(x) \, dx,$$

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

$$\|u\|^2_{H^m_h(\mathbb{R}^d)} := (2\pi h)^{-d} \int_{\mathbb{R}^d} |\xi|^m |\mathcal{F}_h u(\xi)|^2 \, d\xi.$$ 

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

**Phase space.** The set of all possible positions $x$ and momenta (i.e. Fourier variables) $\xi$ is denoted by $T^* \mathbb{R}^d_R$; this is known informally as “phase space”. Strictly, $T^* \mathbb{R}^d_R := \mathbb{R}^d_R \times (\mathbb{R}^d)^*$, but for our purposes, we can consider $T^* \mathbb{R}^d_R$ as $\{(x, \xi) : x \in \mathbb{R}^d_R, \xi \in \mathbb{R}^d\}$. 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,

$$T^*_R := \mathbb{R}^d \times B^d,$$

where $B^d$ denotes the closed unit ball, considered as the closure of the image of $\mathbb{R}^d$ under the radial compactification map

$$RC : \xi \mapsto \xi / (1 + |\xi|);$$

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

$$\|u\|^2_{L_h^2(\mathbb{R}^d)} := (2\pi h)^{-d} \int_{\mathbb{R}^d} |\xi|^m |\mathcal{F}_h u(\xi)|^2 \, d\xi.$$
see [22, §E.1.3]. Near the boundary of the ball, $|\xi|^{-1} \circ \text{RC}^{-1}$ is a smooth function, vanishing to first order at the boundary, with $((|\xi|^{-1} \circ \text{RC}^{-1}, \xi \circ \text{RC}^{-1}))$ 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 $\xi$ only), we abuse notation by dropping the composition with $\text{RC}$ 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 $h$, and thus can be considered as an $h$-dependent family of functions. Such a family $\alpha = (a_h)_{0 < \hbar \leq h_0}$, with $a_h \in C^\infty(\mathbb{R}^d)$, 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 $\alpha, \beta$

$$|\partial_\alpha^\alpha \partial^\beta a(x, \xi)| \leq C_{\alpha, \beta} (\xi)^{m-|\beta|}$$

for all $(x, \xi) \in T^*\mathbb{R}^d$ and for all $0 < h \leq h_0$,

where $C_{\alpha, \beta}$ does not depend on $h$; see [76, p. 207], [22, §E.1.2].

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

$$(\text{Op}_h(a)v)(x) := (2\pi \hbar)^{\frac{d}{2}} \int_{\xi \in \mathbb{R}^d} \int_{y \in \mathbb{R}^d} \exp \left(i (x - y) \cdot \xi / \hbar \right) a(x, \xi) v(y) dy d\xi; \quad (A.3)$$

[76, §4.1] [22, Page 543]. The integral in (A.3) need not converge, and can be understood either as an oscillatory integral in the sense of [76, §3.6], [37, §7.8], or as an iterated integral, with the $y$ integration performed first; see [22, Page 543]. It can be shown that for any symbol $\alpha$, $\text{Op}_h(a)$ preserves Schwartz functions, and extends by duality to act on tempered distributions [76, §4.4].

We use below that if $a = a(\xi)$ depends only on $\xi$, then

$$\text{Op}_h(a) = F^{-1}_h M_a F_h,$$

where $M_a$ denotes multiplication by $a$; i.e., in this case $\text{Op}_h(a)$ 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

$$(\text{Op}_h(a)^T v) = (\text{Op}_h(a)v),$$

since the right side is again periodic [76, §5.3.1]. We thus blur the notational distinction, and mainly omit the superscript $T$ in this appendix.

If $A$ can be written in the form above, i.e. $A = \text{Op}_h(a)$ with $a \in S^m$, we say that $A$ is a semiclassical pseudodifferential operator of order $m$ on the torus and we write $A \in \Psi^m_h(T^*_R)$; furthermore that we often abbreviate $\Psi^m_h(T^*_R)$ to $\Psi^m$ in this Appendix. We use the notation $a \in h^s S^m$ if $h^{-1}a \in S^m$; similarly $A \in h^s \Psi^m$ if $h^{-1}A \in \Psi^m$.

Theorem A.1 (Composition and mapping properties of semiclassical pseudodifferential operators [76, Theorem 8.10], [22, Proposition E.17 and Proposition E.19]) If $A \in \Psi^{m_1}_h$ and $B \in \Psi^{m_2}_h$, then

(i) $AB \in \Psi^{m_1 + m_2}_h$,

(ii) $[A, B] \in h^{\Psi^{m_1 + m_2 - 1}_h}$.

(iii) For any $s \in \mathbb{R}$, $A$ is bounded uniformly in $h$ as an operator from $H^s_h$ to $H^{-s-1}_h$.

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

$$\|A\|_{H^{-s-1}_h \rightarrow H^s_h} \leq C_{s,N} h^N; \quad (A.4)$$

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

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Principal symbol $\sigma_h$. Let the quotient space $S^m/hS^{m-1}$ be defined by identifying elements of $S^m$ that differ only by an element of $hS^{m-1}$. For any $m$, there is a linear, surjective map

$$\sigma_h^m : \Psi^m_h \to S^m/hS^{m-1},$$

called the principal symbol map, such that, for $a \in S^m$,

$$\sigma_h^m(\text{Op}_h(a)) = a \mod hS^{m-1};$$

(A.5)

see [76, Page 213], [22, Proposition E.14] (observe that (A.5) implies that $\ker(\sigma_h^m) = h\Psi^m_h$).

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

Operator wavefront set $\text{WF}_h$. We say that $(x_0, \zeta_0) \in T^*\mathbb{T}^d_R$ is not in the semiclassical operator wavefront set of $A = \text{Op}_h(a) \in \Psi^m_h$, denoted by $\text{WF}_h A$, if there exists a neighbourhood $U$ of $(x_0, \zeta_0)$ such that for all multi-indices $\alpha, \beta$ and all $N \geq 1$ there exists $C_{\alpha, \beta, U, N} > 0$ (independent of $h$) such that, for all $0 < h \leq h_0$,

$$|\partial_\zeta^\alpha \partial_x^\beta a(x, \xi)| \leq C_{\alpha, \beta, U, N} h^N |\xi|^{-N} \text{ for all } (x, \text{RC}(\xi)) \in U.$$  

(A.6)

For $\zeta_0 = \text{RC}(\zeta_0)$ in the interior of $B^d$, the factor $|\xi|^{-N}$ 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 $h$; see [76, Page 194], [22, Definition E.27]. For $\zeta_0 \in \partial B^d = S^{d-1}$, by contrast, the definition says that the symbol decays rapidly in a conic neighborhood of the direction $\zeta_0$, in addition to decaying in $h$.

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

$$\text{WF}_h A = \emptyset \text{ if and only if } A = O(h^\infty)_{\Psi^{-\infty}},$$

(see [22, E.2.2]),

$$\text{WF}_h(A + B) \subseteq \text{WF}_h A \cup \text{WF}_h B,$$

(see [22, E.2.4]),

$$\text{WF}_h(AB) \subseteq \text{WF}_h A \cap \text{WF}_h B,$$

(see [76, §8.4], [22, E.2.5]),

$$\text{WF}_h (A) \cap \text{WF}_h (B) = \emptyset \text{ implies that } AB = O(h^\infty)_{\Psi^{-\infty}},$$

(by, e.g., (A.9) together with [22, E.2.3]), and

$$\text{WF}_h (\text{Op}_h(a)) \subseteq \text{supp} a$$

(A.11)

(since $(\text{supp} a)^c \subset (\text{WF}_h(\text{Op}_h(a)))^c$ by (A.6)).

Ellipticity. We say that $B \in \Psi^m_h$ is elliptic at $(x_0, \zeta_0) \in T^*\mathbb{T}^d_R$ if there exists a neighborhood $U$ of $(x_0, \zeta_0)$ and $c > 0$, independent of $h$, such that

$$|\langle \xi \rangle^{-m} |\sigma_h(B)(x, \xi)| \geq c \text{ for all } (x, \text{RC}(\xi)) \in U \text{ and for all } 0 < h \leq h_0.$$  

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

**Theorem A.2 (Elliptic parametrix [22, Proposition E.32])**  

Let $A \in \Psi^m_h(T^*_R)$ and $B \in \Psi^m_h(T^*_R)$ be such that $B$ is elliptic on $\text{WF}_h(A)$. Then there exist $S, S' \in \Psi^m_h(T^*_R)$ such that

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

with

$$\text{WF}_h S \subset \text{WF}_h A, \quad \text{WF}_h S' \subset \text{WF}_h A.$$
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 $f(-h^2\Delta)$ 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

$$f(-h^2\Delta)v = \sum_{j \in \mathbb{Z}^d} \hat{v}(j)f(h^2|j|^2/R_t^2)e_j.$$ (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 $f \in S^m(\mathbb{R}^1)$, \[ f(-h^2\Delta) = \text{Op}_h f(|\xi|^2). \]

Proof. First note that for $v \in C^{\infty}(\mathbb{T}^d_{R_t})$, \[ v = \sum_{j} \hat{v}(j)e_j \]

$$= (2R_t)^{-d/2} \int_{\mathbb{R}^d} \sum_{j} \hat{v}(j)\delta(\xi - h\pi j/R_t) \exp(i\xi x/h) \, d\xi \]

$$= (2\pi h)^d (2R_t)^{-d/2} \mathcal{F}_h^{-1} \sum_{j} \hat{v}(j)\delta(\xi - h\pi j/R_t).$$ (A.13)

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

$$\mathcal{F}_h v(\xi) = (2\pi h)^d (2R_t)^{-d/2} \sum_{j} \hat{v}(j)\delta(\xi - h\pi j/R_t).$$

Consequently,

$$\mathcal{F}_h [f(-h^2\Delta)v](\xi) = (2\pi h)^d (2R_t)^{-d/2} \sum_{j} f(h^2|j|^2/R_t^2)\hat{v}(j)\delta(\xi - h\pi j/R_t)$$

$$= (2\pi h)^d (2R_t)^{-d/2} \sum_{j} f(|\xi|^2)\hat{v}(j)\delta(\xi - h\pi j/R_t)$$

$$= f(|\xi|^2)\mathcal{F}_h[v](\xi),$$

by (A.13), from which \[ f(-h^2\Delta)v = \text{Op}_h f(|\xi|^2)(v). \]

\[ \square \]

B Proof of (BB5) for the transmission problem

By the min-max principle for self-adjoint operators with compact resolvent (see, e.g., [62, Page 76, Theorem 13.1])

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

where $(\lambda_n)_{n \geq 1}$ denotes the ordered eigenvalues of $P^#$, $\mathcal{D}^c$ is the domain of $P^#$ defined by (2.4) (with $\mathcal{D}$ given by (2.9)), $\Phi_n(\mathcal{D}^c)$ the set of all $n$-dimensional subspaces of $\mathcal{D}^c$, 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 $\mathcal{D}^c$,

$$\langle P^# u, u \rangle_{\beta,c} = h^2\langle A_+ \nabla u_+, \nabla u_+ \rangle_{L^2(\mathcal{T}^d_{R_t}\setminus \Omega_-)} + \beta^{-1}h^2\langle A_- \nabla u_-, \nabla u_- \rangle_{L^2(\Omega_-)}.$$ (B.2)
Furthermore, \[
\frac{\langle A_+ \nabla u_+, \nabla u_+ \rangle_{L^2(T^d_R)} + \beta^{-1} \langle A_- \nabla u_-, \nabla u_- \rangle_{L^2(\Omega_-)}}{\|u_+\|^2_{L^2(T^d_R) \setminus \Omega_-} + \beta^{-1} \|u_-/c\|^2_{L^2(\Omega_-)}} \geq \frac{\min ((A_+)_\text{min}, \beta^{-1}(A_-)_\text{min})}{\max (1, \beta^{-1}(c)_\text{min}^{-2})} \|\nabla u\|^2_{L^2(T^d_R)}.
\]
(B.3)

The definition of \(D^\sharp\) implies that
\[
D^\sharp \subset \{(u_1, u_2) \in H^1(T^d_R) \setminus \Omega_-) \oplus H^1(\Omega_-) \text{ such that } u_1 = u_2 \text{ on } \partial \Omega_- = H^1(T^d_R) \}. \tag{B.4}
\]

Using (B.2), (B.3), and (B.4) in (B.1), we have
\[
\lambda_n \geq \min \left( \frac{(A_+)_\text{min}, \beta^{-1}(A_-)_\text{min}}{\max (1, \beta^{-1}(c)_\text{min}^{-2})} \right) \sup_{x \in \Phi_n, (T^d_R)} \left( \frac{\inf_{1} \sup_{u \in X} h^2 \|\nabla u\|^2_{L^2(T^d_R)}}{\|u\|^2_{L^2(T^d_R)}} \right).
\]

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

\section{Real analyticity from derivative bounds of the form (1.22)}

\begin{lemma}
If \(u \in C^\infty(D)\) with
\[
\|\partial^\alpha u\|_{L^2(D)} \leq C_u(\tilde{C}_1)^{|\alpha|} |\alpha|! \text{ for all } \alpha,
\]
then \(u\) is real analytic in \(D\).
\end{lemma}

\begin{proof}
We claim that it is sufficient to prove that there exists \(n_0 \in \mathbb{Z}^+\) such that
\[
\|\partial^\alpha u\|_{L^\infty(D)} \leq \tilde{C}_u(\tilde{C}_1)^{|\alpha|}(|\alpha| + n_0)!. \tag{C.2}
\]

Indeed, the Lagrange form of the remainder in the Taylor-series up to \(n - 1\) terms then satisfies, by (C.2) and (5.12), for some \(c \in (0, 1)\),
\[
\left| \sum_{|\alpha| = n} \frac{(x - x')^\alpha}{\alpha!}(\partial^\alpha u(x' + c(x - x'))) \right| \leq \sum_{|\alpha| = n} \frac{n!}{\alpha!}(n + 1) \ldots (n + n_0) \tilde{C}_u(\tilde{C}_1)^n|x - x'|^n,
\]
\[
= \tilde{C}_u(n + 1) \ldots (n + n_0)(d\tilde{C}_1)|x - x'|^n,
\]
which \(\to 0\) as \(n \to \infty\) if \(|x - x'| < (d\tilde{C}_1)^{-1}\).

We therefore only need to prove (C.2). Let \(n_0 := [(d + 1)/2]\). Then, by the Sobolev embedding theorem (see, e.g., [47, Theorem 3.26]), (C.1), and the fact that \(|\alpha + \beta| = |\alpha| + |\beta|\), there exists \(C > 0\) such that
\[
\|\partial^\alpha u\|_{L^\infty(D)} \leq C \sum_{|\beta| \leq n_0} \|\partial^\alpha + \beta u\|_{L^2(D)} \leq C C_u C_1^{|\alpha|} \left( \sum_{|\beta| \leq n_0} C_1^{|\beta|}(|\alpha| + |\beta|)! \right),
\]
\[
\leq C C_u C_1^{|\alpha|}(|\alpha| + n_0)! \left( \sum_{|\beta| \leq n_0} C_1^{|\beta|} \right),
\]
so that (C.2) holds with \(\tilde{C}_1 := C_1\) and \(\tilde{C}_u := C C_u \left( \sum_{|\beta| \leq n_0} C_1^{|\beta|} \right)\).
\end{proof}

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