A mathematical formulation of the Mahaux–Weidenmüller formula for the scattering matrix

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Abstract
This paper gives a mathematical exposition of a formula for the scattering matrix for a manifold with infinite cylindrical ends or a waveguide. This formula is well known in the physics literature and we show that a variant of this formula gives the scattering matrix of the mathematics literature. Moreover, we bound the difference between the scattering matrix and an approximation of it computed using a finite rank approximation of the interaction matrix.

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1. Introduction

The purpose of this paper is to give a mathematical explanation of a formula for the scattering matrix for a manifold with infinite cylindrical ends or a waveguide. This formula, which is well known in the physics literature, is sometimes referred to as the Mahaux–Weidenmüller formula [9]. We show that a version of this formula given in (1.7) below gives the standard scattering matrix used in the mathematics literature. We also show that the finite-rank approximation of the interaction matrix gives an approximation of the scattering matrix with errors inversely proportional to a fixed dimension-dependent power of the rank.

**Theorem 1.** Let \( X = X_0 \cup (0, \infty) \times \partial X_0 \) be a manifold with cylindrical ends—see section 2 for a precise definition and figure 1 for an illustration. Let \( \{ \Psi_n \}_{n=0}^\infty \) be an orthonormal set of real eigenfunctions of the Neumann Laplacian, \( -\Delta_{\text{Neu}}, \) on \( X_0 \) with eigenvalues \( -\tau_n^2 \). Let \( \{ \varphi_\lambda \} \) be the same set for the Laplacian on \( \partial X_0 \), with \( -\sigma_\lambda^2 \) denoting the corresponding eigenvalues. Let us define the interaction matrix by
Figure 1. An example of a manifold with an infinite cylindrical end.

\[ W_{N,\Lambda}(k) : L^2(\partial X_0) \longrightarrow L^2(X_0), \]

\[ W_{N,\Lambda} f = \sum_{0 \leq \tau \leq \sqrt{N} \Lambda_1} \sum_{0 \leq \sigma \leq \sqrt{N} / \Lambda_1 (k^2 - \sigma^2)} (\psi_n |_{\partial X_0}, \varphi_\lambda)(f, \varphi_\lambda), \tag{1.1} \]

and the effective Hamiltonian by

\[ H_{N,\Lambda}(k) \overset{\text{def}}{=} H_{\text{in}} - i W_{N,\Lambda}(k) W_{N,\Lambda}^*(k). \]

Then for \( k \in \mathbb{R} \), the entries of the scattering matrix (see section 2) are given by

\[ S_{\lambda,\lambda'}(k) = -\langle (I - 2i W_{N,\Lambda}(k)^* (k^2 - H_{N,\Lambda}(k))^{-1} W_{N,\Lambda}(k)) \phi_\lambda, \phi_{\lambda'} \rangle + O(N^{-1} + e^{-\Lambda / C}), \tag{1.2} \]

if \( \sigma_\lambda, \sigma_{\lambda'} \leq |k| \), and \( \Lambda > k^2 \). The error bound \( O(N^{-1}) \) is optimal—see section 6, and the constant can be chosen uniformly for \( k \) lying in compact sets.

Theorem 2 provides a related result, for other values of \( k \). Also, we remark that the matrix defined by the leading term in (1.2), \( \sigma_\lambda, \sigma_{\lambda'} \leq |k| \), is in fact unitary—see lemma 5.1.

The physics literature contains several versions of the Mahaux–Weidenmüller formula. One commonly found formula—see for instance \([1, 11]\) and references given there—is given as follows:

\[ \tilde{S}_f(k) = - (I - 2i W(k)^*(k^2 - \tilde{H}_{\text{eff}})^{-1}) W(k). \tag{1.3} \]

Here

\[ \tilde{H}_{\text{eff}} \overset{\text{def}}{=} H_{\text{in}} - i W(k) W(k)^* \tag{1.4} \]

where \(-H_{\text{in}}\) is the Neumann Laplacian in the ‘interaction region’ \( X_0 \), a compact piece of the waveguide or manifold with infinite cylindrical end, and \( W(k) \) is the frequency-dependent interaction matrix. When applied in numerical simulations only a finite number of modes of \( H_{\text{in}} \) are taken which results in a finite-rank approximation of \( W(k) \), as described in (1.1).

The formula, in its finite-rank version, is the basis of random matrix models in scattering theory—see \([6, \text{section III.D}]\). For some recent experimental results related to the formula see for instance \([14]\).

Formula (1.3) is not strictly speaking correct. The advantage of (1.3) is that \( \tilde{S}_f(k) \) is unitary for real \( k \) by a linear algebra argument. It is also close to the correct scattering matrix given below.
As shown in proposition 3.5, the scattering matrix [2] which is standard in the mathematical literature is recovered from an expression close to (1.3):

\[ S_f (k) = - (I - 2iW(k)(k^2 - H_{\text{eff}})^{-1}W(k)) \]  

(1.5)

with

\[ H_{\text{eff}} = H_0 - iW(k)W(k)^\dagger, \]  

(1.6)

and, with the notation of (1.1),

\[ W(k) \equiv W_{\infty, \infty}(k). \]

In fact, \(-H_{\text{eff}} = -H_{\text{eff}}(k)\) is the Laplacian on \(X_0\), with a boundary condition that depends on \(k\); see lemma 3.2. Lemma 3.3 demonstrates the relationship between \((k^2 - H_{\text{eff}})^{-1}\) and the resolvent of the Laplacian on \(X\).

This correct version (1.5) appears in [1], though again only a finite number of modes are included. We note that our sign convention, while agreeing with [1], is not consistent with many other authors. It appears that this sign is correct, and that the difference can be traced to a different normalization of the scattering matrix. The difference between (1.3) and (1.5) does not appear in many of the physics papers, where generally only an approximation \(W_a(k)\) of \(W(k)\) is used, and the approximation is such that \(W_a(k)^* = W_a(k)^\dagger\). The operator \(S_f (k)\), unlike \(\tilde{S}_f (k)\), is typically not unitary for real \(k\).

However, (1.5) gives what one might call the extended, or full, scattering matrix. To get the usual finite-dimensional unitary scattering matrix (whose dimension changes at roots of the eigenvalues of the cross section of the end), we put, for \(k\) real,

\[ S(k) = - \Pi^{X_0}_{k^2} (I - 2iW(k)(k^2 - H_{\text{eff}})^{-1}W(k)) \Pi^{X_0}_{k^2} \]  

(1.7)

where \(\Pi^{X_0}_{k^2}\) projects to the span of the eigenfunctions of \(-\Delta_Y\), with eigenvalue at most \(k^2\). Here \(\Delta_Y\) is the Laplacian on the cross section of the end. Proposition 3.5 shows that this is the unitary scattering matrix which appears in the mathematical literature. Lemma 5.1 gives an algebraic proof that the matrix given by (1.7) is unitary for \(k \in \mathbb{R}\). Note that if \(k \in \mathbb{R}\), the operator defined by (1.3) is unitary, but the finite-rank operator (corresponding to a finite-dimensional matrix)

\[ - \Pi^{X_0}_{k^2} (I - 2iW(k)^*(k^2 - H_{\text{eff}})^{-1}W(k)) \Pi^{X_0}_{k^2} \]

with \(H_{\text{eff}}\) given by (1.4), is not unitary in general, if \(W(k)\) takes into account contributions of evanescent modes. Evanescent modes correspond to the eigenvalues of \(-\Delta_Y\) larger than \(k^2\).

Let us add that the papers [1] and [11] already have a fairly mathematically careful description of the Mahaux–Weidenmüller formula. In [12] a detailed analysis of several one-dimensional models is also provided. Another related approach to scattering/transport is due to Fisher–Lee [5], see also [3].

**Remark 1.** We use the notation \((u, v)\) to denote the Hermitian inner product, and \(\langle u, v \rangle\) to denote the form which is linear in both arguments.

### 2. Scattering matrix

In this section, we recall the general assumptions for manifolds with cylindrical ends and the definition of the scattering matrix.

Our model is a manifold \(X\) with infinite cylindrical ends and smooth metric \(g\)—see figure 1. In physics language that means a waveguide with periodic boundary conditions. The same arguments apply to waveguides with Dirichlet or Robin boundary condition but
we choose to avoid mild technical complications associated with that setting. For purely notational reasons we also assume that there is only one end. Then

\[ X = X_0 \cup (0, \infty) \times Y, \quad Y = \partial X_0, \]

where \( X_0 \) is a compact manifold with a smooth boundary \( Y \). We require that \( g|_{(0, \infty) \times Y} = (dx)^2 + g_Y \), where \( g_Y \) is a metric on \( Y \). Moreover, we choose our decomposition so that there is a neighborhood \( U \subset X_0 \) of \( \partial X_0 \) on which \( g \) is also a product:

\[ g|_U = (dx)^2 + g_Y. \]

Recall that \( \{ \varphi_\lambda \} \) is an orthonormal set of eigenfunctions of \( \Delta Y \). We use the convention that the energy is \( k^2 \), and \( k_\lambda = \sqrt{k^2 - \sigma_\lambda^2} \), with the imaginary part chosen to be non-negative when \( \text{Im} k \geq 0 \). We call the region with \( \text{Im} k \geq 0 \) the physical region. Given \( \lambda \in \mathbb{N} \), if \( k \) is in the physical region, and with \( \text{Im} k > 0 \), there is a unique \( \Phi_\lambda(p, k) \) so that

\[ (-\Delta_X - k^2) \Phi_\lambda(p, k) = 0 \text{ on } X \quad (2.1) \]

and

\[ \Phi_\lambda|_{(0, \infty) \times Y} = e^{-ik_x x} \varphi_\lambda(y) + \sum_{\lambda'} S_{\lambda'}(k) e^{ik'_{\lambda'} x} \varphi_{\lambda'}(y) \quad (2.2) \]

for some \( S_{\lambda'}. \) To see this we use the resolvent \( (-\Delta_X - k^2)^{-1} \) which is a bounded operator \( L^2(X) \to H^2(X) \), for \( \text{Im} k > 0 \):

\[ \Phi_\lambda(p, k) = (1 - \psi) \varphi_\lambda(y) e^{-ik_x x} + (-\Delta_X - k^2)^{-1}([-\Delta_X, \psi](\varphi_\lambda(y) e^{-ik_x x}))(p), \]

\[ \psi \in C^\infty_0(X), \quad \psi|_{X_0} \equiv 1. \]

Since on \( X_1 \) we have \( -\Delta_X = -\partial_x^2 - \Delta_Y \), separation of variables shows that \( \Phi_\lambda \) can be written as in (2.2).

The resolvent, \( (-\Delta_X - k^2)^{-1} \), continues meromorphically to

\[ \Lambda_{\sigma(\Delta X_0)} \supset \{ k : \text{Im} k > 0 \}, \quad (2.3) \]

a Riemann surface branched at \( \sigma_\lambda' \)'s—see [10, section 6.7]. We remark that this Riemann surface is such that each \( k_\lambda \) defined above extends to be a holomorphic single-valued function. Thus, \( \Phi_\lambda(p, k) \) has a meromorphic continuation to \( \Lambda_{\sigma(\Delta X_0)} \) which is regular for \( \text{Im} k = 0 \) except when \( k_{\lambda'} \)'s are 0, or when \( k^2 \in \sigma(-\Delta_X) \).

The full, or extended, scattering matrix is the infinite matrix

\[ S_f(k) = (S_{\lambda', \lambda}(k))_{\lambda, \lambda' \in \mathbb{N}}. \]

For \( k \in \mathbb{R} \), the matrix more commonly called the scattering matrix is the finite-dimensional matrix given by

\[ S(k) = (S_{\lambda', \lambda}(k))_{\lambda^2, \lambda'^2 \leq k^2}. \]

We remark that if \( \text{Im} k > 0 \), while each entry \( S_{\lambda', \lambda}(k) \) is well defined away from its poles, there is not a canonical choice for ‘the’ scattering matrix. However, in general it is \( (\sqrt{k_\lambda}/\sqrt{k_{\lambda'}})S_{\lambda', \lambda}(k) \), not \( S_{\lambda', \lambda} \), which has a meromorphic continuation to \( \Lambda_{\sigma(\Delta X_0)} \) for each \( \lambda, \lambda' \). We shall use this continuation in the proof of the theorem.
3. The formula

Let $\Delta_Y$ be the Laplacian on $Y$, and let $\{\sigma_i^2\}$ be the eigenvalues of $-\Delta_Y$, repeated according to multiplicity, and let $\{\psi_i\}$ be an associated set of real, orthonormal eigenfunctions of the Laplacian on $Y$. Let $-H_{in}$ be the Laplacian with Neumann boundary conditions on $X_0$, and let $\{\phi_n\}$ be a set of real, orthonormal eigenfunctions of $H_{in}$.

First, we define the operator $W(k)$ by explicitly giving its Schwartz kernel. Our starting point is the representation of $W(k)$ from [1] or [11]. We write $p$ to represent a point in $X_0$, and $y$ or $y'$ to represent a point in $Y$; on $U \subset X_0$ we may write $p = (x, y)$, with $\{x = 0\} = \partial X_0$.

Then, with $\Psi_{1n,\lambda}(0) \equiv \int_Y \psi_{\lambda}(y) \phi_{1n}(0, y)$, we follow the physics literature and define the coupling operator by giving its integral kernel (with integration with respect to Riemannian densities) as

$$W(p, y') \equiv \sum_{n, \lambda} \sqrt{k_{\lambda}} \psi_{1n}(p) \phi_{\lambda}(y') = \sum_n \psi_{n}(p) P_k \psi_{n}(0, y').$$

(3.1)

Here $P_k = (k^2 + \Delta_Y)^{1/4}$ is defined by $P_k \phi_\lambda = \sqrt{k_{\lambda}} \phi_\lambda$. While either choice of the square root is possible, it is crucial that this is consistent with that used to define the scattering matrix; see (2.2). The series converges in the sense of distributions. Hence, $W(p, y')$ is understood as a distribution on $X \times Y$—see lemma 3.1 below.

This definition (3.1) appears normally in the physics literature. When we take all the eigenstates then $W$ (and especially $W_t$) takes a very simple form given in the following lemma. When, as is done in the physics literature, we take only finitely many states, the formula for $W_t$ is given in the remark after the lemma.

Let $\mathcal{D}'(X_0)$ be the space of distributions on $X$ supported in the (closed) set $X_0$. We also use the following convention: for $s \geq 0$ the space $H^s(X_0)$ denotes restrictions of elements of $H^s(X)$ to $X_0$, while for $s \leq 0$, $H^s(X_0)$ denotes elements of $H^s(X)$ supported in the (closed) set $X_0$. See [7, appendix B.2] for a careful discussion: in the notation used there

$$H^s(X_0) = \begin{cases} \tilde{H}^s(X_0) & s \geq 0 \\ H^s(X_0) & s \leq 0. \end{cases}$$

With this notation in place we can formulate

**Lemma 3.1.** The operator (3.1) is equal to

$$W(k)g = \delta_{\partial X_0} P_k g, \quad g \in C^\infty(\partial X_0),$$

(3.2)

where $\delta_{\partial X_0} \in \mathcal{D}'(X_0)$ is the distribution defined by

$$\delta_{\partial X_0}(\varphi) = \int_{\partial X_0} \varphi \|_{\partial X_0} \, dy.$$

We have

$$W(k) : H^s(Y) \to H^{\min(-1/2, -s-1)}(X_0), \quad s \in \mathbb{R},$$

(3.3)

and $W(k)g|_{X_0} = 0$. The transpose, $W(k)^t : H^{1/2s}(X_0) \to H^{-1/2s}(Y), s > 0$, is given by

$$W(k)^t f(y) = P_k(f|_{\partial X_0}).$$

(3.4)
Proof. To prove (3.2) we need to compute, in the notation of distributions, $W(f \otimes g)$, where $f \in \bar{\mathcal{C}}^\infty_0(X_0)$. The definition (3.1) gives

$$W(f \otimes g) = \sum_n \left( \int_{X_0} \Psi_n f \right) \left( \int_{\partial X_0} \Psi_n |_{\partial X_0} P_k g \right)$$

$$= \int_{\partial X_0} \left( \sum_n \left( \int_{X_0} \Psi_n f \right) \Psi_n |_{\partial X_0} \right) P_k g$$

$$= \int_{\partial X_0} f|_{\partial X_0} P_k g,$$

which proves (3.2) and, by duality, (3.4). The mapping property of $W(k)t$ follows from the fact that $f \mapsto f|_{\partial X_0}$ takes $H^s + 1/2(X_0)$ for $s > 0$, and $P_k : H^s(\partial X_0) \rightarrow H^{s-1/2}(\partial X_0)$. The mapping property (3.3) follows by duality.

Remark 2. In lemma 3.1 all the structure of the basis of the eigenvectors of $H$ in and $\Delta_Y$ disappears. The question which we address in section 4 is how close the approximation based on using only finitely many basis elements gets to the actual scattering matrix. Then for $a = (N, \Lambda) \in [0, \infty)^2$ we define

$$W_a(k) \overset{\text{def}}{=} P_k \mathbb{I}_{[0,N]}(\Delta_Y) R \mathbb{I}_{[0,\Lambda]}(H_{in}), \quad Ru \overset{\text{def}}{=} u|_{\partial X_0},$$

We note that $W_{(\infty, \infty)}(k) = W(k)$, and that for $N < \infty$ and $\Lambda < \infty$,

$$W_a(k) : \mathcal{D}'(Y) \rightarrow C^\infty(X_0), \quad W_a(k)^t : \mathcal{D}'(X_0) \rightarrow C^\infty(Y),$$

where $C^\infty(X_0)$ denotes extendable smooth functions on the compact manifold $X_0$.

We make the definition (1.6) of $H_{eff}$ rigorous via the quadratic form

$$q(u, v) = q(k)(u, v) = \int_{X_0} \nabla u \nabla v \, dvol_{X_0} - i \int_{\partial X_0} W^t(k)u \overline{W(k)v} \, dvol_Y$$

$$= \int_{X_0} \nabla u \nabla v \, dvol_{X_0} - i \int_{\partial X_0} P_k Ru \overline{P_k Rv} \, dvol_Y$$

with form domain $H^1(X_0)$. If

$$q(u, v) = (w, v)$$

for some $w \in L^2(X_0)$ and all $v \in H^1(X_0)$, then $u$ is in the domain of $H_{eff}$ and $H_{eff}u = w$. Moreover,

$$(w, v) = q(u, v) = -\int_{X_0} \Delta_X u \overline{v} + \int_{\partial X_0} \left( \partial_n u - i P_k^2 Ru \right) \overline{v},$$

where $\partial_n u$ denotes the outward unit normal derivative at the boundary. Since this must hold for all $v \in H^1(X_0)$, $-\Delta_X u = w$ and

$$0 = \partial_n u - i P_k^2 Ru.$$

We note that $u \in H^2(X_0)$ where the space is defined by restricting elements of $H^2(X)$ to $X_0$—see [7, appendix B]. We summarize this in the following:

Lemma 3.2. Suppose $u \in \text{Domain}(H_{eff})$. Then $u \in H^2(X_0)$, and

$$H_{eff}u = -\Delta_X u, \quad \partial_n u - i P_k^2 Ru = 0.$$
Next we investigate the relation between \((k^2 - H_{\text{eff}})^{-1}\) and the resolvent of the Laplacian on \(X\). Denote
\[
R_X(k) \overset{\text{def}}{=} (k^2 + \Delta_X)^{-1}, \quad \text{for } \text{Im} \, k > 0.
\]
Then, for \(K \subset X\) any compact set \(\mathbb{1}_K R_X(k) \mathbb{1}_K\) has a meromorphic extension to \(\Lambda_{\sigma(\Delta_{X_0})}\), see [10]. In lemma 4.1 we shall show that \((k^2 - H_{\text{eff}})^{-1}: L^2(X_0) \rightarrow H^2(X_0)\) exists for \(k^2 < 0, \text{Im} \, k > 0\), and is meromorphic on \(\Lambda_{\sigma(\Delta_{X_0})}\), the Riemann surface (2.3). One could provide an alternate proof using the first part of the proof of lemma 3.3 and the results of [10] on the meromorphic continuation of \(R_X(k)\).

We remark that when we use \(k \in \Lambda_{\sigma(\Delta_{X_0})}\), by abuse of notation we mean by \(k^2\) the complex number which is the continuation of \(k^2\) from the physical half-plane \(\text{Im} \, k \geq 0\).

**Lemma 3.3.** We have the following relation between \(R_X(k)\) as defined above and \((k^2 - H_{\text{eff}})^{-1}\):
\[
(k^2 - H_{\text{eff}})^{-1} = \mathbb{1}_{X_0} R_X(k) \mathbb{1}_{X_0}
\]
for \(k \in \Lambda_{\sigma(\Delta_{X_0})}\). In particular, the poles of \((k^2 - H_{\text{eff}})^{-1}\) are the same as the poles of \(R_X(k)\).

**Proof.** Suppose \(g \in L^2(X_0) \subset L^2(X)\) and \(g = 0\) in a neighborhood of \(\partial X_0\). Then
\[
(k^2 + \Delta_X) |_{X_0} R_X(k) g = (k^2 + \Delta_X) |_{X_0} R_X(k) g |_{X_0} = g \quad \text{on } X_0^0
\]
for \(k \in \Lambda_{\sigma(\Delta_{X_0})}\).

Note that since \(\text{supp} \, g \subset X_0\), \((k^2 + \Delta_X) g = 0\) on \(X_1\). Then for \(\text{Im} \, k > 0\) (that is, for \(k\) in the physical space), the requirement that \(R_X(k) g \in L^2(X)\) means that
\[
R_X(k) g |_{X_1} = \sum a_{\lambda} e^{i k \cdot \lambda} \varphi_{\lambda}
\]
for some constants \(a_{\lambda} = a_{\lambda}(k)\). But then, using the support conditions of \(g\) there is a neighborhood \(\bar{U} \subset X_0\) of \(\partial X_0\) so that
\[
R_X(k) g |_{\bar{U}} = \sum a_{\lambda} e^{i k \cdot \lambda} \varphi_{\lambda}.
\]
Thus,
\[
(\partial_n - i P^2_k)(R_X(k) g |_{\partial X_0}) = 0
\]
so that \(R_X(k) g |_{\partial X_0}\) is in the domain of \(H_{\text{eff}} = H_{\text{eff}}(k)\). Together with (3.5), this means that
\[
(k^2 - H_{\text{eff}})^{-1} g = \mathbb{1}_{X_0} R_X(k) g
\]
for all \(k\) with \(\text{Im} \, k > 0\) and all \(g \in L^2(X_0)\) which are 0 in a neighborhood of \(\partial X_0\). Since \(g\) are dense in \(L^2(X_0)\), this must in fact hold for all \(g \in L^2(X_0)\).

Since \((k^2 - H_{\text{eff}})^{-1} = \mathbb{1}_{X_0} R_X(k) \mathbb{1}_{X_0}\) for all \(k\) with \(\text{Im} \, k > 0\) and since both sides have meromorphic continuations to \(\Lambda_{\sigma(\Delta_{X_0})}\) (see [10] and lemma 4.1), they must in fact agree for all \(k \in \Lambda_{\sigma(\Delta_{X_0})}\).

**Lemma 3.4.** Suppose \((k^2 - H_{\text{eff}})^{-1}\) exists. For \(f \in H^1(\partial X_0)\), let
\[
u = (k^2 - H_{\text{eff}})^{-1} W(k) f.
\]
Then
\[
(k^2 + \Delta_{X_0}) \nu = 0 \quad \text{on } X_0^0, \quad \partial_n - i P^2_k \nu |_{\partial X_0} = -P_k f.
\]

**Proof.** We first claim that there exists \(F \in H^2(X_0)\) such that
\[
(\partial_n - i P^2_k) F |_{\partial X_0} = -P_k f.
\]
In fact, for $0 < h \ll 1$ define $N(h) : H^s(\partial X_0) \to H^{s-1}(\partial X_0)$ as follows:

$$N(h) = \frac{1}{h} (I - \Delta_{\partial X_0})^\frac{1}{2}, \quad N(h)^{-1} = \mathcal{O}(h) : H^{s-1}(\partial X_0) \to H^s(\partial X_0).$$

Let $\chi \in C_c^\infty(\{0, \epsilon\})$ be equal to 1 in a small neighborhood of 0, with $\epsilon$ chosen so that $X_0 \subset (-\epsilon, 0] \times \partial X_0$, near the boundary. We define (note that $x < 0$)

$$[T(h)g](x, y) \overset{\text{def}}{=} \chi(-x) \exp \left( x \frac{(I - \Delta_{\partial X_0})^\frac{1}{2}}{h} \right) g(y),$$

so that

$$T(h) : H^s(\partial X_0) \to H^{s+\frac{1}{2}}(X_0), \quad s \geq 0,$$

which satisfies (3.8).

We now set

$$v = F - (k^2 - H_{\text{eff}})^{-1}(k^2 + \Delta_{X_0})F,$$

and observe that $v$ satisfies equations (3.7). It remains to show that $v = u$.

To see that we let $h \in C^\infty(X_0)$, and apply Green’s formula to compute

$$((k^2 - H_{\text{eff}})^{-1}(k^2 + \Delta_{X_0})F, h) = \int_{\partial X_0} (\partial_n F((k^2 - H_{\text{eff}})^{-1})^* h - F \partial_n((k^2 - H_{\text{eff}})^{-1})^* h)$$

$$+ (F, (k^2 + \Delta_{X_0})((k^2 - H_{\text{eff}})^{-1})^* h)$$

$$= \int_{\partial X_0} (\partial_n F((k^2 - H_{\text{eff}})^{-1})^* h - F \partial_n((k^2 - H_{\text{eff}})^{-1})^* h)$$

$$+ (F, h).$$

Now we use that $\partial_n F|_{\partial X_0} = i P_k^2 F|_{\partial X_0} - P_k f$, and that

$$u \in H^2(X_0) \cap \text{Domain}(k^2 - H_{\text{eff}})^* \implies \partial_n u|_{\partial X_0} + i(P_k^2)^* R w = 0.$$ 

Thus we have

$$((k^2 - H_{\text{eff}})^{-1}(k^2 + \Delta_{X_0})F, h)$$

$$= \int_{\partial X_0} ((i P_k^2 F|_{\partial X_0} - P_k f)((k^2 - H_{\text{eff}})^{-1})^* h - i F((P_k^2)^* (k^2 - H_{\text{eff}})^{-1})^* h)$$

$$+ (F, h)$$

$$= -\int_{\partial X_0} P_k f((k^2 - H_{\text{eff}})^{-1})^* h + (F, h) = \int_{X_0} (- (k^2 - H_{\text{eff}})^{-1} \delta_{X_0} P_k f + F) h,$$

where the last expression follows from the definition of $\delta_{X_0}$. Since this holds for all $h \in C^\infty(X_0)$,

$$v = F - (k^2 - H_{\text{eff}})^{-1}(k^2 + \Delta_{X_0})F = (k^2 - H_{\text{eff}})^{-1} \delta_{X_0} P_k f = u,$$

proving the lemma. \qed

8
We can now state and prove the main result of this section. It provides a justification of (1.5) and (1.7).

**Proposition 3.5.** Let $W$ be given by (3.1). Then the $\lambda\lambda'$ entry of the scattering matrix defined in section 2 is given by

$$S_{\lambda,\lambda'}(k) = \langle S_f(k) \varphi_{\lambda}, \varphi_{\lambda'} \rangle_{L^2(\partial X_0)},$$

where

$$S_f(k) = -(I - 2iW(k)'(k^2 - H_{\text{eff}})^{-1}W(k)),$$

and $H_{\text{eff}}$ is defined in lemma 3.2.

**Proof.** We use lemma 3.4 to express the action of $(k^2 - H_{\text{eff}})^{-1}W(k)\psi_{\lambda}$. Suppose $v_\lambda = (k^2 - H_{\text{eff}})^{-1}W(k)\psi_{\lambda}$. Let $U \subset X_0$ be a neighborhood of $\partial X_0$. On $U$ we may use coordinates $(x, y)$, with $y \in Y$. Since $v_\lambda$ lies in the null space of $-\Delta_{X_0} - k^2$, we have that

$$v_\lambda\big|_U = \sum_{\lambda'}(a_{\lambda'} e^{ik_{\lambda'} x} + b_{\lambda'} e^{-ik_{\lambda'} x})\varphi_{\lambda'}(y).$$

The boundary conditions (3.7) applied to $v_\lambda$ at $\partial X_0$ mean that

$$\sum_{\lambda'} ik_{\lambda'}(a_{\lambda'} - b_{\lambda'})\varphi_{\lambda'} - i \sum_{\lambda'} k_{\lambda'}(a_{\lambda'} + b_{\lambda'})\varphi_{\lambda'} = -P_k \varphi_{\lambda}.$$

Then $b_{\lambda'} = 1/(2i\sqrt{k_{\lambda'}})$ and $b_{\lambda'} = 0$ if $\lambda' \neq \lambda$. Thus $v_\lambda$ is the restriction to $X_0$ of $-i\Phi_{\lambda}/2$, where $\Phi_{\lambda}$ is determined by (2.1) and (2.2):

$$\Phi_{\lambda}|_{(0,\infty) \times Y} = e^{-ik_{\lambda} x} \frac{\varphi_{\lambda}(y)}{\sqrt{k_{\lambda}}} + \sum_{\lambda'} S_{\lambda,\lambda'}(x) e^{ik_{\lambda'} x} \frac{\varphi_{\lambda'}(y)}{\sqrt{k_{\lambda'}}}.$$

Therefore,

$$W(k)'v_\lambda = \sum_{\lambda'} \sqrt{k_{\lambda}} a_{\lambda'} \varphi_{\lambda'} - \frac{i}{2} \varphi_\lambda = -\frac{i}{2} \left( \sum_{\lambda'} S_{\lambda,\lambda'} \varphi_{\lambda'} + \varphi_\lambda \right),$$

which proves the proposition. \qed

Equation (3.9) is valid for all real values of $k$ (that is, $k$ on the boundary of the physical space) with $k^2 > \sigma^2_{\lambda}$, $\sigma^2_{\lambda'}$, since the matrix coming from the right-hand side is unitary and hence the singularities of $\langle S_f(k) \varphi_{\lambda}, \varphi_{\lambda'} \rangle_{L^2(\partial X_0)}$ resulting from poles of $(H_{\text{eff}} - k^2)^{-1}$ are removable.

4. Accuracy of approximations

Here we investigate the accuracy of the approximations made to use (1.5) in numerical computations. Set

$$\Pi^A_{\lambda} f \equiv \mathbb{1}_{[0,\Lambda)}(-\Delta_{X_0}) f \quad \text{for} \quad f \in L^2(\partial X_0),$$

$$\Pi^N_{\lambda} g \equiv \mathbb{1}_{[0,\Lambda)}(H_{\text{in}}) g \quad \text{for} \quad g \in L^2(X_0).$$

In parallel with this, we introduce

$$W_{\infty,\Lambda}(k) \equiv W(k), \quad W_{\infty}(k) \equiv W \Pi^A_{\Lambda},$$

$$W_{N,\Lambda}(k) \equiv \Pi^N_{\Lambda} W(k) \Pi^A_{\Lambda} = \Pi^N_{\Lambda} W_{\infty}(k),$$

and

$$H_{\infty} \equiv H_{\text{eff}}, \quad H_{N,\Lambda} \equiv H_{\text{in}} - i W_{N,\Lambda} W_{N,\Lambda}^*, \quad N \in \mathbb{R} \cup \{\infty\}. $$
Although $W_{N,\Lambda}, W_{\infty,\Lambda}$ depend on $k$, for simplicity we generally omit this in our notation. Note that $H_{\text{eff}}, H_{\Sigma,\Lambda}$ and $H_{N,\Lambda}$ also depend on $k$.

A quadratic form argument (see lemmas 3.2 and 4.4), using the form domain $H^1(X_0)$, shows that if $u$ is in the domain of $H_{\Sigma,\Lambda}$, then $\partial_u u - iP_{\Delta}^{\Lambda} Ru = 0$. However, for $N < \infty$ the domain of $H_{N,\Lambda}$ is the set of elements of $H^2(X_0)$ which satisfy the Neumann boundary condition, $\partial_u u = 0$.

Likewise, we define the approximations of the (full) scattering matrix obtained by using the approximation $H_{N,\Lambda} = H_{\text{eff}}$ by $S_{f, N, \Lambda}$:

$$S_{f, N, \Lambda}(k) = -(I - 2iW_{N,\Lambda}(k) (k^2 - H_{N,\Lambda})^{-1} W_{N,\Lambda}(k)).$$

In order to bound the error in these approximations, we shall first see how close $\Pi^\Lambda_{\Lambda} S_{f, N, \Lambda}$ is to $\Pi^\Lambda_{\Lambda_0} S_{f, N, \Lambda}$ and then study the difference

$$\Pi^\Lambda_{\Lambda_0} (S_{f, N, \Lambda} - S_{f, N, \Lambda}) \Pi^\Lambda_{\Lambda_0}.$$

### 4.1. Projection on $\partial X_0$

We first analyze the approximation with a finite $\Lambda$ and $N = \infty$. The spectral cut-off for the boundary Laplacian, $\Lambda$, has to be taken large enough to guarantee that $\Im \lambda > 0$ for $\sigma^2 > \Lambda$. The errors then come from evanescent modes and can be estimated using exponential decay.

We present the results in two lemmas.

**Lemma 4.1.** Let $\Lambda_{\sigma(\Delta x_0)}$ be the Riemann surface, given in (2.3), to which the resolvent of $-\Delta X = (-\Delta x - k^2)^{-1}$, has a meromorphic continuation (see [10, section 6.7]). Then the operators $(k^2 - H_{\text{eff}})^{-1}$ and $(k^2 - H_{\Sigma,\Lambda})^{-1}$ are meromorphic on $\Lambda_{\sigma(\Delta x_0)}$. If $k^2 - H_{\text{eff}} = k^2 - H_{\Sigma,\Lambda}(k)$ is invertible, so is $k^2 - H_{\Sigma,\Lambda}(k)$ for $\Lambda > \Lambda_0$ sufficiently large, and

$$\| (k^2 - H_{\text{eff}})^{-1} - (k^2 - H_{\Sigma,\Lambda})^{-1} \|_{L^2 \to L^2} \leq C\Lambda^{-1/2}, \quad \Lambda > \Lambda_0(k).$$

Moreover, for $k$ restricted to a compact set $K \subset \Lambda_{\sigma(\Delta x_0)}$ on which $k^2 - H_{\text{eff}}$ is invertible, $\Lambda_0$ and $C$ can be chosen independently of $k$.

**Proof.** Recall that $U$ is a neighborhood of $\partial X_0$ which we may identify with $(-\epsilon, 0] \times Y$ with $g_{\Lambda} = (dx)^2 + g_Y$. Choose $\chi \in C^\infty(X), i = 1, 2$, so that each $\chi_i$ has support in $U, \chi_i = 1$ in a smaller neighborhood of the boundary, and

$$\chi_1 \chi_2 = \chi_1, \quad \text{supp } \chi_2 \cap \text{supp } \chi_1 = \emptyset.$$

Set $R_{\Lambda, e}(k)$ to be the operator on $L^2((-\infty, 0] \times Y)$ defined by the Schwartz kernel

$$R_{\Lambda, e}(k)(x, y; x', y') \overset{\text{def}}{=} \sum_\lambda \frac{1}{2ik_\lambda} \left( e^{ik_\lambda |x-x'|} + (1 - \Pi^\Lambda_{\Lambda_0}) e^{ik_\lambda |x-x'|} \right) \varphi_k(y) \varphi_k(y').$$

Note that $R_{\Lambda, e}(k)$ is a meromorphic function of $k \in \Lambda_{\sigma(\Delta x_0)},$ since $k_\lambda$ is holomorphic on $\Lambda_{\sigma(\Delta x_0)}.$ Let $R_{\Lambda, e}(k)$ be the operator with Schwartz kernel given by

$$\sum_\lambda \frac{1}{2ik_\lambda} e^{ik_\lambda |x-x'|} \varphi_k(y) \varphi_k(y'),$$

and set

$$E_{\Lambda}(k) = (1 - \chi_1)(k^2 - H_{\text{eff}})^{-1} + \chi_1 R_{\Lambda, e}(k) \chi_1, \quad \Lambda \in \mathbb{R} \cup \{\infty\}.$$

Then, for the same values of $\Lambda$, $E_{\Lambda} v$ satisfies the boundary conditions of $H_{\Sigma,\Lambda}$, that is

$$\left( \partial_n - iP_{\Delta}^{\Lambda} \Pi^\Lambda_{\Lambda_0} \right) E_{\Lambda} v \big|_{\partial X_0} = 0,$$
and is meromorphic on $\Lambda_{\sigma(\Delta_{\lambda}k)}$. Moreover,

$$(k^2 + \Delta_{\lambda}k)E_\lambda(k) = I - \left[\Delta_{\lambda}k, \chi_1\right](k^2 - H_{\text{lim}})^{-1} + \left[\Delta_{\lambda}k, \chi_1\right]R_{\lambda,\epsilon}(k)\chi_1$$

\[\def \equiv \equiv I + K_\lambda(k)\]

where $K_\lambda(k)$ is a compact operator. Moreover, $K_\lambda(k)$ is a meromorphic function of $k$ in $\Lambda_{\sigma(\Delta_{\lambda}k)}$ with finite-rank poles. When $k \in \mathbb{iR}_+, \|K_\lambda(k)\| \to 0$ as $k^2 \to -\infty$. Thus, $I + K_\lambda(k)$ is invertible for $k \in \mathbb{iR}_+, -k^2 \gg 0$, and by analytic Fredholm theory (see for instance [13, section 2.4]) we have that

$$(k^2 - H_{\infty,\lambda}(k))^{-1} = E_\lambda(k)(I + K_\lambda(k))^{-1}$$

for $k$ in the physical space, and it has a meromorphic continuation to $\Lambda_{\sigma(\Delta_{\lambda}k)}$.

Now

$$\|E_\lambda(k) - E_{\infty}(k)\|_{L^2 \to L^2} \leq C \max_{\sigma_k^2 > \lambda}\frac{|k_\lambda|}{|k_\lambda|}^{-1}.$$

For $k$ in a compact set of $\Lambda_{\sigma(\Delta_{\lambda}k)}$ and $\sigma_k > \lambda \geq \lambda_0(k)$, sufficiently large, we have $\text{Im} k_\lambda > 0$, and since

$$x \in \text{supp} \chi_2, \quad x' \in \text{supp} \chi_1 \implies |x - x'|, |x + x'| > \epsilon_0 > 0,$$

we have

$$\|K_\lambda(k) - K_{\infty}(k)\|_{L^2 \to L^2} \leq C \max_{\sigma_k^2 > \lambda}\frac{|k_\lambda| + 1}{|k_\lambda|} e^{-\epsilon_0 \text{Im} k_\lambda/2}.$$

This constant is independent of $k$. Thus, if $\Lambda$ is big enough, $I + K_\lambda(k) = K_{\infty}(k)$ is invertible with small norm, and

$$\|(k^2 - H_{\text{eff}})^{-1} - (k^2 - H_{\infty,\lambda})^{-1}\| \leq CA^{-1/2}$$

for $\Lambda$ sufficiently large (depending on $k$ or $K$, $\epsilon_0$ and $\|(k^2 - H_{\text{eff}})^{-1}\|$). The constant can be chosen independently of $k$ on a fixed compact set $K$ where $k^2 - H_{\text{eff}}$ is invertible.

**Remark 3.** Using this lemma and definition (4.1) of $S_{f,\infty,\lambda}$, we can see that for $\Lambda \in \mathbb{R}_+ \cup \{\infty\}$, $P_{k}^{-1}S_{f,\infty,\lambda}(x)P_{k} = -(I - 2iP_{k}^{-1}W_{\infty,\lambda}(k)\dot{f}(k^2 - H_{\infty,\lambda})^{-1}W_{\infty,\lambda}(k)P_{k})$ (4.2) has a meromorphic continuation to $\Lambda_{\sigma(\Delta_{\lambda}k)}$. The conjugation by $P_{k}$ is necessary because while $P_{k}^2$ is a well-defined operator for $k \in \Lambda_{\sigma(\Delta_{\lambda}k)}$, $P_{k}$ is not. Thus the operators $W_{\infty,\lambda}(k)P_{k}$ and $P_{k}^{-1}W_{\infty,\lambda}(k)\dot{f}$ are well defined on $\Lambda_{\sigma(\Delta_{\lambda}k)}$, while in general $W_{\infty,\lambda}(k)$ and $W_{\infty,\lambda}(k)\dot{f}$ are not. The existence of the meromorphic continuation of (4.2) means that $(\sqrt{k_\lambda^2 / \lambda_0^2})S_{f,\infty,\lambda}(x)\psi, \psi \psi_\lambda)$ has a meromorphic continuation to $\Lambda_{\sigma(\Delta_{\lambda}k)}$.

**Lemma 4.2.** Fix $\lambda_0 < \infty$ and $k$ so that $k^2 - H_{\text{eff}}$ is invertible and $\text{Im} k_\lambda > 0$ if $\sigma_k^2 > \lambda_0$. Suppose $f \in L^2(\partial X_0)$ satisfies $\Pi_{\lambda}X_0 f = f$ for $\Lambda \geq \lambda_0$. Then, for $\Lambda \geq \Lambda_0$ such that $k^2 - H_{\infty,\lambda}$ is invertible, we have for some $\epsilon' > 0$

$$\|P_{k}^{-1}\Pi_{\lambda}^X X_0 (S_{f,\infty,\lambda}(k) - S_{f,\infty,\lambda}(k))P_{k} f \|_{L^2(\partial X_0)} \leq C \max_{\sigma_k^2 > \lambda}(|k_\lambda| \exp(-\epsilon' \text{Im} k_\lambda)) \|f\|_{L^2(\partial X_0)}.$$

In particular, by lemma 4.1 this holds for all $\Lambda$ sufficiently large depending on $k$. We note that the constants $C$ and $\epsilon'$ can be chosen independently of $k$ if $k$ is restricted to a fixed compact set $K$ on which both $k^2 - H_{\text{eff}}$ and $k^2 - H_{\infty,\lambda}$ are invertible and for which $\text{Im} k_\lambda > 0$ when $\sigma_k^2 > \lambda_0$.

We note that since $\Pi_{\lambda}X_0 f = f$, the $H^3/2$ norm of $f$ is bounded by a $\Lambda$-dependent multiple of the $L^2$ norm of $f$.
Proof. For \( \Lambda \in [\Lambda_0, \infty) \cup \{ \infty \} \), set \( u_{\Lambda} = (k^2 - H_{\infty, \Lambda})^{-1} W_{\infty, \Lambda} P_k f \). That means that \( u_{\Lambda} \) satisfies

\[
(k^2 + \Delta_{X_0}) u_{\Lambda} = 0 \quad \text{on } X_0, \quad \left( \partial_n u_{\Lambda} - i P_k^2 \tilde{\Pi}_X^0 R u_{\Lambda} \right) = - P_k^2 f.
\]

Choose \( \chi \in C^\infty_0((-\epsilon/2, 0]) \) to be one in a neighborhood of 0. Since \( U \subset X_0 \) is a neighborhood of \( \partial X_0 \) which can be identified with \( (-\epsilon, 0] \times Y_0 \), we can consider \( \chi = \chi(x) \) to be defined on \( X_0 \) by extending it to be 0 outside of \( U \). For \( g \in L^2(X) \), define \( \tilde{\Pi}_X^0 \chi g \in L^2(U) \subset L^2(X_0) \) via

\[
(\tilde{\Pi}_X^0 \chi g)(x, y) = \sum_{\sigma_+ \leq \Lambda} \psi_k(y) \int_{y \in \partial X_0} \left( \chi(x) g(x, y') \psi_k(y') \right) \text{dvol}_y.
\]

Then

\[
u_{\Lambda} \big|_U = (1 - \chi) u_{\infty} + \tilde{\Pi}_X^0 \chi u_{\infty} + (k^2 - H_{\infty, \Lambda})^{-1} (k^2 + \Delta_{X_0})(1 - \tilde{\Pi}_X^0) \chi u_{\infty}
\]

(4.3)

since the function on the right-hand side satisfies the same boundary conditions as \( u_{\Lambda} \) and is in the null space of \( k^2 + \Delta_{X_0} \).

Note that by using \( \tilde{\Pi}_X^0 \chi f = f \)

\[
u_{\Lambda} \big|_U = (1 - \chi) u_{\infty} + \sum_{\sigma_+ \leq \Lambda} (a_j e^{-ik_j x} + b_j e^{ik_j x}) \psi_k + \sum_{\sigma_+ > \Lambda} b_j e^{ik_j x} \psi_k
\]

(4.4)

for some constants \( a_j, b_j \), so that, using orthonormality of \( \psi_k \)'s,

\[
\|u_{\infty}\|_{L^2}^2 \geq \|u_{\infty}\|_{L^2}^2 \geq \int_{-\epsilon}^0 \sum_{\sigma_+ > \Lambda} |b_j|^2 e^{2\text{Im} k_j} - \frac{1}{2 \text{Im } k_j}.
\]

(4.5)

Also,

\[
(k^2 + \Delta_{X_0})(1 - \tilde{\Pi}_X^0) \chi u_{\infty} = \left[ \hat{\alpha}^2, \chi \right] (1 - \tilde{\Pi}_X^0) \tilde{\chi} u_{\infty},
\]

where \( \tilde{\chi} \) has the same properties as \( \chi \) and \( \tilde{\chi} \chi = \chi \). Our argument below takes advantage of the fact that the support of \( [\hat{\alpha}^2, \chi] \) is contained in \([-\epsilon/2, 0]\), while the expansion (4.4) is valid for \( x \in (-\epsilon, 0) \). Hence,

\[
\| (k^2 + \Delta_{X_0})(1 - \tilde{\Pi}_X^0) \chi u_{\infty} \|^2 \leq C (\epsilon^{-4}) \int_{-\epsilon/2}^0 \sum_{\sigma_+ > \Lambda} (k_j)^2 |b_j e^{ik_j x}|^2 \text{d}x
\]

\[
\leq C (\epsilon^{-4}) \sum_{\sigma_+ > \Lambda} (k_j)^2 |b_j|^2 e^{2\text{Im} k_j} - \frac{1}{2 \text{Im } k_j}
\]

\[
= C (\epsilon^{-4}) \sum_{\sigma_+ > \Lambda} (k_j)^2 |b_j|^2 e^{2\text{Im} k_j} - \frac{1}{2 \text{Im } k_j} \left( \frac{1}{e^{2\text{Im} k_j}} + 1 \right).
\]

Thus (4.5) gives

\[
\| (k^2 + \Delta_{X_0})(1 - \tilde{\Pi}_X^0) \chi u_{\infty} \| \leq C (\epsilon^{-2}) \| u_{\infty} \|_{L^2} \max_{\sigma_+ > \Lambda} (|k_j| e^{-\text{Im} k_j/2}).
\]

Using (4.3), the estimate

\[
\|(k^2 - H_{\infty, \Lambda})^{-1} g\|_{L^2} \leq (1 + |k|) \|(k^2 - H_{\infty, \Lambda})^{-1} g\|_{L^2}.
\]
and the previous lemma, we obtain
\[
\|\Pi_{X_0}^\Lambda R(u - u_\Lambda)\|_{L^2(\partial X)} \leq C (\epsilon^{-2} + |k|) \|(k^2 - H_{\infty, \Lambda})^{-1}\|\|u_\Lambda\|_{L^2} \max_{\sigma^2 > \Lambda} \|k_\sigma| e^{-\epsilon \Im k_\sigma/2}\).
\]
Thus far each constant C can be chosen independent of k, though of course \(\|u_\Lambda\|\) depends on k in a continuous fashion on compact sets on which \(k^2 - H_{\text{eff}}\) is invertible. Note that \(P^{-1}_k \Pi_{X_0}^\Lambda = \Pi_{X_0}^\Lambda\) is a bounded operator. Thus, using the expression for \(S_f, S_{f, \infty, \Lambda}\) and the previous lemma finishes the proof. \(\square\)

4.2. The cut-off in the interior

We now turn our attention to the error introduced by using \(\Pi_{X_0}^\Lambda\). Throughout this section we assume that \(\Lambda < \infty\).

Our results will use the following standard:

Lemma 4.3. Suppose \(\tilde{X}\) is a compact Riemannian manifold without boundary and \(\chi \in C^\infty_0(\mathbb{R})\) is equal to 1 in a neighborhood of 0. Suppose that \(Y \subset \tilde{X}\) is a smooth embedded submanifold of codimension 1. Then
\[
\|(1 - \chi(-h^2 \Delta_{\tilde{X}}))u\|_{L^2(Y)} \leq C \sqrt{h}\|u\|_{H^1(\tilde{X})},
\]
If \(v \in H^2(\tilde{X}\setminus Y) \cap H^1(\tilde{X})\), then
\[
\|(1 - \chi(-h^2 \Delta_{\tilde{X}}))v\|_{L^2(Y)} \leq C h\|v\|_{H^1(\tilde{X}\setminus Y)}.
\]

Proof. Both statements in the lemma are local. In fact, if \(P\) is another elliptic second-order operator on \(\tilde{X}\), then for some constant \(C_P\) the calculus of semiclassical pseudodifferential operators (see for instance [4, appendix E]) shows that
\[(1 - \chi(-h^2 \Delta))(1 - \chi(-h^2 C_P (P + C_P))) = (1 - \chi(-h^2 \Delta)) + O_{H^{-k}\to H^k}(h^N),\]
for all \(N\) and \(k\). Hence, we can use any other second-order elliptic operator and that property is invariant under changes of coordinates.

It follows that we can assume that \(\tilde{X} = \mathbb{R}^n\) and \(Y = \{x_1 = 0\}, \mathbb{R}^n \ni x = (x_1, x')\) (the compactness is irrelevant for the local statement).

Denoting the Fourier transform by \(\mathcal{F}\) we write
\[
\mathcal{F}_{x' \to x'} ((1 - \chi(-h^2 \Delta_{\tilde{X}}))u\|_{L^2(Y)} = \int_{\mathbb{R}^n} (1 - \chi(h^2 |\xi|^2))\hat{u}(\xi_1, \xi) \, d\xi_1. \quad (4.6)
\]

Hence, by the Cauchy–Schwartz inequality,
\[
\|(1 - \chi(-h^2 \Delta_{\tilde{X}}))u\|_{L^2(Y)} \leq C \int_{\mathbb{R}^n} F(\xi', h)(1 - \chi(h^2 |\xi|^2))\hat{u}(\xi)^2(1 + |\xi|^2) \, d\xi,
\]
where
\[
F(\xi', h) \overset{\text{def}}{=} \int_{\mathbb{R}} (1 - \chi(h^2 |\xi|^2))(1 + |\xi|^2)^{-1} \, d\xi_1
\]
\[
\leq \int_{|\xi'| > c/h} (1 + |\xi|^2)^{-1} \, d\xi_1 + 1_{|\xi'| > c/h}(\xi') \int_{\mathbb{R}} (|\xi|^2 + |\xi|^2)^{-1} \, d\xi_1
\]
\[
\leq Ch.
\]
This proves the first part of the lemma.
For the second part, we can assume that supp\(v \subset \{ x \in \mathbb{R}^n : |x| \leq R \}\) as we can localize to a compact set. We then write
\[
\hat{v}(\xi) = \int_0^R \left( e^{-i\xi \cdot x} F_{\mathcal{X} x \to \mathcal{X}} v(x_1, \xi) + e^{i\xi \cdot x} F_{\mathcal{X} x \to \mathcal{X}} v(-x_1, \xi) \right) \, dx_1.
\]
Since \(v \in H^1(\mathbb{R}^n), F_{\mathcal{X} x \to \mathcal{X}} v(0, \xi') \in L^2(\mathbb{R}^n)\) is well defined and hence we can integrate by parts to obtain
\[
\hat{v}(\xi) = \frac{1}{\xi_1} \sum_{\pm} \left( \pm F_{\mathcal{X} x \to \mathcal{X}} \partial_{x_1} v(0\pm, \xi') - \int_0^R e^{i\xi_1 \cdot \xi} F_{\mathcal{X} x \to \mathcal{X}} \partial_{x_1} v(\pm x_1, \xi) \, dx_1 \right).
\]
Since \(v \in H^2(\mathbb{R}^n), \partial_{x_1} v(0\pm, \xi')\) is well defined in \(L^2(\mathbb{R}^n)\). We now use the following decomposition:
\[
(1 - \chi(h^2 |\xi|^2)) \hat{v} = \hat{v}_1 + \hat{v}_2, \quad \hat{v}_1(\xi) \overset{\text{def}}{=} \mathbb{1}_{|\xi| > c/h} (1 - \chi(h^2 |\xi|^2)) \hat{v}(\xi),
\]
noting that \(|\xi'| > c/h\) on the support of \(\hat{v}_2(\xi)\). We first estimate the contribution of \(v_2\) as in the proof of the first part of the lemma:
\[
\|v_2\|_{L^2(Y)}^2 \leq C \int_{\mathbb{R}^n} G(\xi', h) |\hat{v}(\xi)|^2 (1 + |\xi|)^2 \, d\xi
\]
\[
\leq \max_{\xi \in \mathbb{R}^n} G(\xi', h) \|v\|_{H^2(\mathcal{X})}^2,
\]
where
\[
G(\xi', h) \overset{\text{def}}{=} \int_{|\xi'| < c/h} (1 - \chi(h^2 |\xi'|^2))(1 + |\xi'|)^2 \, d\xi_1
\]
\[
\leq \mathbb{1}_{|\xi'| > c/h}(\xi') \int_0^{2c/h} (1 + |\xi'|)^2 \, d\xi_1
\]
\[
\leq C h^3,
\]
which is a better estimate than needed.

To estimate the contribution of \(v_1\) we use (4.7):
\[
\|v_1\|_{L^2(Y)}^2 \leq C \int_{\mathbb{R}^n} \left( \int_{|\xi| > c/h} \frac{1}{\xi_1} \, d\xi_1 \right)^2 \leq C R^4 \|v\|_{H^2(\mathcal{X})}^2,
\]
which completes the proof.

Like \(H_{\text{eff}}, H_{N, \Lambda} = H_{N, \Lambda}(k)\) is a well-defined operator for \(k \in \Lambda_{\sigma(\Delta x_0)}\).

**Lemma 4.4.** Fix \(\Lambda < \infty, \text{ and suppose that } k^2 - H_{\infty, \Lambda} \text{ is invertible, } k \in \Lambda_{\sigma(\Delta x_0)}\). Then, for \(N\) sufficiently large, \(k^2 - H_{N, \Lambda} \text{ is invertible, and }\)
\[
\| (k^2 - H_{\infty, \Lambda})^{-1} - (k^2 - H_{N, \Lambda})^{-1} \|_{H^{-1}(X_0) \to H^1(X_0)} \leq C N^{-1/4}.
\]
The constant \(C\) can be chosen uniformly for \(k\) in a compact set \(K \subset \Lambda_{\sigma(\Delta x_0)}\), on which
\(k^2 - H_{\infty, \Lambda} \text{ is invertible.}\)

**Proof.** As in section 3 we will use quadratic forms to reinterpret our operators. Thus, for \(N \in \mathbb{R}^+, \ E \in \mathbb{C}, \) set
\[
q_{\infty, \Lambda}(k, E)(u, v) = \int_{X_0} \nabla u \nabla v - i \int_{iX_0} W_{\infty, \Lambda} u \overline{W_{\infty, \Lambda} v} - E \int_{X_0} u \overline{v}
\]
\[
= \int_{X_0} \nabla u \nabla v - i \int_{iX_0} P_{\Lambda} \Pi_{\Lambda} X_0 R u \overline{\Pi_{\Lambda} X_0 R v} - E \int_{X_0} u \overline{v}
\]
and
\[ q_{N,\Lambda}(k, E)(u, v) = \int_{X_0} \nabla u \overline{\nabla v} - i \int_{\partial X_0} W_{N,\Lambda}^u W_{N,\Lambda} \overline{v} - E \int_{X_0} u \overline{v} \]
\[ = \int_{X_0} \nabla u \overline{\nabla v} - i \int_{\partial X_0} P_{\Lambda} \Pi^\Lambda X_0 R \Pi^\Lambda u \Pi^\Lambda X_0 R \Pi^\Lambda \overline{v} - E \int_{X_0} u \overline{v}. \]

Here we take both form domains to be \( H^1(X_0) \). The quadratic forms \( q_{\infty,\Lambda}(k, E) \) and \( q_{N,\Lambda}(k, E) \) are associated with operators \( H_{\infty,\Lambda} - E \) and \( H_{N,\Lambda} - E \) respectively. We expand the difference of the quadratic forms as follows:

\[ q_{\infty,\Lambda}(k, E)(u, u) = q_{N,\Lambda}(k, E)(u, u) \]
\[ = \int_{\partial X_0} \left( \left| P_{\Lambda} \Pi^\Lambda X_0 R u \right|^2 - \left| P_{\Lambda} \Pi^\Lambda X_0 R \Pi^\Lambda u \right|^2 \right) \]
\[ = \int_{\partial X_0} \left( \left( P_{\Lambda} \Pi^\Lambda X_0 R u \right) P_{\Lambda} \Pi^\Lambda X_0 R (I - \Pi^\Lambda) u + P_{\Lambda} \Pi^\Lambda X_0 R (I - \Pi^\Lambda) u \right) \left( P_{\Lambda} \Pi^\Lambda X_0 R \Pi^\Lambda u \right). \]

We have the following estimates:
\[ \left\| \Pi^\Lambda X_0 R (I - \Pi^\Lambda) u \right\|_{H^1(\partial X_0)} \leq C_{\Lambda} \left\| R (I - \Pi^\Lambda) u \right\|_{L^2(\partial X_0)} \leq C_{\Lambda} N^{-1/4} \left\| u \right\|_{H^1(X_0)} \]
\[ \left\| \Pi^\Lambda X_0 R u \right\|_{H^1(\partial X_0)} \leq C_{\Lambda} \left\| Ru \right\|_{L^2(\partial X_0)} \leq C_{\Lambda} \left\| u \right\|_{H^1(X_0)}. \]

(4.8)

To obtain the first, we apply lemma 4.3 to \( \tilde{X} \overset{\text{def}}{=} X_0 \cup X_0^\circ \) where the metric on \( \tilde{X} \) is obtained by reflecting the metric on \( X_0 \) through \( Y = \partial X_0 \). Since the metric has product structure near \( Y \) this means that
\[ H^1(X_0) \simeq H^1_{\text{ev}}(\tilde{X}) \]
(here ev refers to even functions) and the action of the Neumann Laplacian on \( X_0 \) is the same as the action of \( \Delta_\Phi \) on even functions. Applying lemma 4.3 with \( h = 1/\sqrt{N} \) gives (4.8).

Applying (4.8) to estimate the difference of the quadratic forms we obtain, for \( E \ll 0 \),
\[ \left| q_{\infty,\Lambda}(k, E)(u, u) - q_{N,\Lambda}(k, E)(u, u) \right| \leq C_{\Lambda} N^{-1/4} \left\| u \right\|_{H^1(\partial X_0)}^2 \]
\[ \leq C_{\Lambda} (k) N^{-1/4} \text{Re} (q_{\infty,\Lambda}(k, E)(u, u)). \]

The constant depends continuously on \( k \). Here we use the fact that \( \text{Im} k_\lambda > 0 \) for all but finitely many \( \lambda \), ensuring that \( \text{Re} q_{\infty,\Lambda}(k, E)(u, u) \) bounds \( \left\| u \right\|_{H^1(\partial X_0)}^2 \) from above for \( E \ll 0 \). Thus, by [8, theorem 3.4],
\[ \left\| (H_{\infty,\Lambda} - E)^{-1} - (H_{N,\Lambda} - E)^{-1} \right\|_{L^2(X_0) \to L^2(X_0)} \leq C N^{-1/4} \]
for \( N \) sufficiently large depending on \( E, k \) and \( \Lambda \). This dependence on \( k \) is continuous on regions where \( k^2 - H_{\infty,\Lambda} \) is invertible. To extend this to other values of \( E \) (in particular, \( E = k^2 \)), we use
\[ (A - z)^{-1} = \frac{1}{(I - (A - z)(B - z)^{-1})(z - z_0)((A - z_0)^{-1} - (B - z_0)^{-1})} \]
\[ \times (I - (z - z_0)(B - z)^{-1}(A - z_0)^{-1}). \]

(4.9)

Consequently, if \( k^2 - H_{\infty,\Lambda} \) is invertible, so is \( k^2 - H_{N,\Lambda} \) for sufficiently large \( N \), with
\[ \left\| (k^2 - H_{\infty,\Lambda})^{-1} - (k^2 - H_{N,\Lambda})^{-1} \right\|_{L^2(X_0) \to L^2(X_0)} \leq C N^{-1/4}. \]

Here the constant will depend on \( k \) and \( \Lambda \), as will the lower bound on the \( N \) for which this holds. These can be chosen uniformly if \( k \) is restricted to lie in \( \mathbb{K} \).
Now we show that there is a similar bound from $H^{-1}(X_0)$ to $H^1(X_0)$. We choose $E$ so that $\text{Re}(q_{\sigma,\lambda}(k, E)(u, u)) \geq c_0 ||u||_{H^1(X_0)}^2$ for some $c_0 > 0$ and all $u \in H^1(X_0)$. Suppose $w \in L^2(X_0)$ and set $u = (H_{\sigma,\lambda} - E)^{-1} w, u_N = (H_{N,\lambda} - E)^{-1} w$. Then 

$$c_0 ||u||_{H^1}^2 \leq \text{Re}(q_{\sigma,\lambda}(k, E)(u, u)) = \text{Re}(w, u)$$

so that 

$$c_0 ||u||_{H^1} \leq ||w||_{H^{-1}}.$$

This shows that we can (uniquely) continuously extend $(H_{\sigma,\lambda} - E)^{-1}$ to be a bounded operator from $H^{-1}(X_0)$ to $H^1(X_0)$ when $E \ll 0$ (the duality argument shows that we can extend the operator to the dual of $H^1(X_0)$ and $H^{-1}(X_0)$ is contained in that dual as the space of elements of $H^1(X)$ supported in $X_0$). The resolvent equation extends this to other values of $E$. Likewise, 

$$c_0 ||u - u_N||_{H^1}^2 \leq \text{Re}(q_{\sigma,\lambda}(k, E)(u - u_N, u - u_N)) = \text{Re}(q_{\sigma,\lambda}(k, E)(u, u - u_N) - q_{\sigma,\lambda}(k, E)(u_N, u - u_N))$$

$$= \text{Re}(w, u - u_N) - q_{\sigma,\lambda}(k, E)(u_N, u - u_N)$$

$$+ q_{\sigma,\lambda}(k, E)(u_N, u - u_N) - q_{\sigma,\lambda}(k, E)(u_N, u - u_N)$$

$$\leq C N^{-1/4} ||u_N||_{H^1} ||w||_{H^1} + ||u - u_N||_{H^1}^2$$

$$\leq C N^{-1/4} (||u||_{H^1} + ||u - u_N||_{H^1}) ||u - u_N||_{H^1}.$$

We allow the constant $C$ to change from line to line. This implies that 

$$||u - u_N||_{H^1} \leq C N^{-1/4} (||u||_{H^1} + ||u - u_N||_{H^1}),$$

which then means that for sufficiently large $N$ 

$$||u - u_N||_{H^1} \leq C N^{-1/4} ||u||_{H^1}.$$ 

Using (4.9) this can be extended to other values of $E$. Again, these constants can be chosen uniformly for $k \in K$. \hfill \Box

**Lemma 4.5.** Fix $\Lambda < \infty$ and $k$ so that $k^2 - H_{\sigma,\lambda}$ is invertible and $\text{Im} k \lambda > 0$ if $\sigma^2 > \Lambda$. Suppose $f \in L^2(\partial X_0)$ satisfies $\Pi_{\sigma,\lambda}^X f = f$. Then, for $N$ so that $k^2 - H_{N,\lambda}$ is invertible, there is a constant $C$ depending on $\Lambda$ and $k$ so that 

$$||\Pi_{\sigma,\lambda}^X P_k^{-1} (S_{f,\sigma,\lambda}(k) - S_{f,N,\lambda}(k)) P_k f ||_{L^2(\partial X_0)} \leq C N^{-1/2} ||f||_{L^2(\partial X_0)}.$$ 

The constant $C$ can be chosen independently of $k$, if $k$ is restricted to a compact set $K \subset \Lambda_{\sigma(\Lambda,\lambda)}$ on which $k^2 - H_{\sigma,\lambda}$ and $k^2 - H_{N,\lambda}$ are invertible.

**Proof.** Choosing $N$ so that $k^2 - H_{N,\lambda}$ is invertible, set 

$u_\infty = (k^2 - H_{\sigma,\lambda})^{-1} W_{\sigma,\lambda} P_k f$ \hspace{1cm} and \hspace{1cm} $u_N = (k^2 - H_{N,\lambda})^{-1} W_{N,\lambda} P_k f$.

That is, $u_\infty$ satisfies 

$$(k^2 + \Delta_{X_0}) u_\infty = 0 \text{ on } X_0^0$$

$$\partial_n u_\infty - i P_k^2 \Pi_{\sigma,\lambda}^X R u_\infty = -P_k^2 f$$

and $u_N$ satisfies, for $N < \infty$, 

$$(k^2 + \Delta_{X_0} + i W_{N,\lambda} W_{N,\lambda}') u_N = W_{N,\lambda} P_k f \text{ on } X_0^0$$

$$\partial_n u_N |_{\partial X_0} = 0.$$ 

Note that our assumptions on $f$ mean that the $H^{3/2}$ norm of $f$ is bounded by a $\Lambda$-dependent constant times the $L^2$ norm of $f$.\hfill 16
We wish to understand $\Pi^0_N u_\infty$. Let $\Psi_n$ be a real eigenfunction of the Neumann Laplacian on $X_0$, with $-\Delta_{X_0} \Psi_n = \tau_n^2 \Psi_n$. Suppose in addition that $\|\Psi_n\|_{L^2(X_0)} = 1$. Then
\[
(\tau_n^2 - k^2)(u_\infty, \Psi_n)_{L^2(X_0)} = -\int_{X_0} (\Delta_{X_0} \Psi_n u_\infty - \Psi_n \Delta_{X_0} u_\infty) \, dv_{X_0} \\
= \int_{\partial X_0} \Psi_n \partial_n u_\infty \, dv_Y \\
= \int_{\partial X_0} \Psi_n \left( i P_k^2 \Pi^X_\Lambda R u_\infty - P_k^2 f \right) \, dv_Y.
\]
That is,
\[
(-\Delta_{X_0} - k^2) \Pi^0_N u_\infty = iW_N, A W^\prime_X, A u_\infty - W_N, A P_k f.
\]

Thus,
\[
u_N = \Pi^0_N u_\infty - (k^2 - H_{N, A})^{-1} ((k^2 - H_{N, A}) \Pi^0_N u_\infty - W_N, A P_k f) \\
= \Pi^0_N u_\infty + i(k^2 - H_{N, A})^{-1} W_N, A (W^\prime_{N, A} - W^0_{N, A}) u_\infty \\
= \Pi^0_N u_\infty + i(k^2 - H_{N, A})^{-1} W_N, A P_k \Pi^X_\Lambda R (I - \Pi^0_N) u_\infty.
\]
(4.10)

The second part of lemma 4.3 gives the following estimate:
\[
\| R (1 - \Pi^0_N) u_\infty \|_{L^2(\partial X_0)} \leq \| u_\infty \|_{H^2(X_0)},
\]
and consequently,
\[
\| P_k \Pi^X_\Lambda R (I - \Pi^0_N) u_\infty \| \leq \| u_\infty \|_{H^2(X_0)}
\]
with constant $C$ depending continuously on $k$.

Let $g \in L^2(\partial X_0)$, $h \in H^{1/2}\ast (X_0)$. Then $Rh \in L^2(\partial X_0)$, and
\[
|(W_{N, A} g, h)_{X_0}| = \| (g, P_k^* \Pi^X_\Lambda R \Pi^0_N h)_{\partial X_0} \| \leq \| g \|_{L^2(\partial X_0)} \| h \|_{H^{1/2}(X_0)}.
\]

That is,
\[
\| W_{N, A} g \|_{H^{-1}(X_0)} \leq \| W_{N, A} g \|_{H^{-1/2}(X_0)} \leq C \| g \|_{L^2(X_0)}
\]
and the constant is independent of $N$ and depends continuously on $k$. On the other hand, lemma 4.4 shows that for $N$ sufficiently large
\[
\|(k^2 - H_{N, A})^{-1} \|_{H^{-1}(X_0) \rightarrow H^1(X_0)} \leq C.
\]

Using these estimates in (4.10), we find that
\[
\|u_\infty - u_N\|_{H^1} \leq C N^{-1/2},
\]
implying the desired bound by restricting to $\partial X_0$ and using again the fact that $P_k^{-1} P_k \Pi^X_\Lambda = \Pi^X_\Lambda$ is a bounded operator. \hfill \Box

5. Proofs of theorems

Our proof of the theorem in section 1 will use the unitarity for $k$ real not only of the finite-dimensional scattering matrix defined by (1.7), but also of the approximations of the scattering matrix obtained by introducing the projections $\Pi^0_N$ and $\Pi^X_\Lambda$.

Lemma 5.1. Let $k \in \mathbb{R}$. Then $S(k)$ defined by (1.7) and $\Pi^X_\Lambda S_{f, N, A}(k) \Pi^0_N$, for $A, N \in \mathbb{R} \cup \{ \infty \}$, are unitary.
Proof. That $S(k)$ is unitary for $k$ real is well known. It can be seen as follows. Recall that $S(k) = \prod_{k_1}^\infty S_{f,\infty,\Lambda}(k) \prod_{k_2}^\Lambda X_0$.

We note that $(P_{k_2}^\Lambda)^* \varphi_\lambda = \overline{\kappa(k_2)\varphi_\lambda}$ and $k_3$ is real for $\sigma_0^2 < k^2$.

Therefore,

$$\prod_{k_3}^\Lambda X_0 W'(k) = \prod_{k_2}^\Lambda X_0 W^*(k) \quad \text{and} \quad \left( I - \prod_{k_3}^\Lambda X_0 \right) W'(k) = -\left( I - \prod_{k_2}^\Lambda X_0 \right) W^*(k). \quad (5.1)$$

Thus, we have

$$W(k)^* \prod_{\Lambda}^\Lambda X_0 W^*(k) + W(k) \prod_{\Lambda}^\Lambda X_0 W'(k) = 2 W(k) \prod_{\Lambda}^\Lambda X_0 \prod_{k_2}^\Lambda X_0 W'(k). \quad (5.2)$$

Using this and the resolvent identity gives

$$(k^2 - H_{N,0})^{-1} - (k^2 - H_{N,0})^{-1} = i(k^2 - H_{N,0})^{-1} \left( -\prod_{\Lambda}^\Lambda W^* \prod_{\Lambda}^\Lambda X_0 W^* \prod_{\Lambda}^\Lambda W \prod_{\Lambda}^\Lambda \prod_{k_2}^\Lambda X_0 W^* \prod_{k_2}^\Lambda (k^2 - H_{N,0})^{-1} \right)$$

$$= -2i(k^2 - H_{N,0})^{-1} \prod_{\Lambda}^\Lambda W \prod_{k_2}^\Lambda X_0 W^* \prod_{k_2}^\Lambda (k^2 - H_{N,0})^{-1}. \quad (5.3)$$

Therefore,

$$\prod_{k_2}^\Lambda X_0 S_{f,N,\Lambda}(k) \prod_{k_2}^\Lambda X_0 (\prod_{k_2}^\Lambda X_0 S_{f,N,\Lambda}(k) \prod_{k_2}^\Lambda X_0)^* = \prod_{k_2}^\Lambda X_0 S_{f,N,\Lambda}(k) \prod_{k_2}^\Lambda X_0 \prod_{\Lambda}^\Lambda X_0 W^* \prod_{\Lambda}^\Lambda W \prod_{\Lambda}^\Lambda (k^2 - H_{N,0})^{-1} \prod_{k_2}^\Lambda X_0$$

where we have used (5.1). Applying identity (5.3) we find that

$$\prod_{k_2}^\Lambda X_0 S_{f,N,\Lambda}(k) \prod_{k_2}^\Lambda X_0 (\prod_{k_2}^\Lambda X_0 S_{f,N,\Lambda}(k) \prod_{k_2}^\Lambda X_0)^* = I \quad (5.5)$$

as desired. \qed

Theorem 2. Let $X$ be a manifold with infinite cylindrical ends, and $S_{f,\lambda}(k), S_{f,N,\Lambda}(k)$ be as defined via (2.1), (2.2) and (4.1). Suppose $k \in \Lambda_{\sigma/(\Lambda,0)}$ and $\Lambda_0 \in \mathbb{R}$ are such that $k^2 - H_{eff} = k^2 - H_{eff}(k)$ is invertible, and $\text{Im} k_\lambda > 0$ if $\sigma_0^2 > \Lambda_0$. Then, for $\sigma_0^2, \sigma_0^2 \leq \Lambda_0$ and $\Lambda \geq \Lambda_0$,

$$\sqrt{k_{\Lambda}} S_{f,\lambda}(k) = \left\langle P_k^{-1} S_{f,N,\Lambda}(k) P_k \varphi_\lambda, \varphi_\lambda \right\rangle + O(N^{-\frac{1}{2}} + e^{-\Lambda/C}).$$

We recall that $k^2 - H_{eff}$ is invertible if $k$ is in the physical space with $\text{Im} k > 0$, $\text{Im} k_\lambda > 0$ for all $\lambda$, and that $(k^2 - H_{eff})^{-1}$ is meromorphic on $\Lambda_{\sigma/(\Lambda,0)}$.

Proof. The proof follows from writing

$$\sqrt{k_{\Lambda}} S_{f,\lambda}(k) = \left\langle P_k^{-1} S_{f}(k) P_k \varphi_\lambda, \varphi_\lambda \right\rangle + \left\langle P_k^{-1} (S_{f,N,\Lambda}(k) - S_{f,\infty,\Lambda}(k)) P_k \varphi_\lambda, \varphi_\lambda \right\rangle$$

$$+ \left\langle P_k^{-1} (S_{f,N,\Lambda}(k) - S_{f,\infty,\Lambda}(k)) P_k \varphi_\lambda, \varphi_\lambda \right\rangle, \quad (5.6)$$

where we note that the first equality follows from proposition 3.5. Applying lemmas 4.2 and 4.5, we obtain the theorem. \qed

18
We now prove theorem 1.

**Proof.** If \( k^2 - H_{\text{eff}} \) is invertible this is just theorem 2, and hence it remains to prove that the estimate is valid for all \( k \in \mathbb{R} \), even if \( k^2 - H_{\text{eff}} \) is not invertible.

Using the unitarity proved in lemma 5.1, along with the fact that \( \sigma_\lambda^2 \leq k^2 \), \( \sigma_\lambda^2 \leq k^2 \), we see that each of the terms on the right-hand side of (5.6) is bounded for all \( k \in \mathbb{R} \). Also, for \( N, \Lambda \in \mathbb{R}_+ \cup \{ \infty \} \), \((\sqrt{K_+}/\sqrt{K_-})(S_{f,N,\Lambda}(k)\psi_+,\psi_-)\) has a meromorphic extension to \( \Lambda_{\sigma(\Delta_{\lambda\lambda})} \), as can be seen from formula (4.1) and the fact that \((k^2 - H_{N,\Lambda})^{-1}\) continues meromorphically to \( \Lambda_{\sigma(\Delta_{\lambda\lambda})} \). Hence

\[
k \in (-\sigma_\lambda, \sigma_\lambda) \cap (-\sigma_\lambda^*, \sigma_\lambda^*)\]

has a neighborhood in \( \Lambda_{\sigma(\Delta_{\lambda\lambda})} \) on which \((S_{f,N,\Lambda}\psi_+,\psi_-)\) is holomorphic, \( N, \Lambda \in \mathbb{R}_+ \cup \{ \infty \} \).

We will now apply the maximum principle: (5.6) and lemmas 4.2 and 4.5 show that

\[
S_{\lambda\lambda'} = (S_{f,N,\Lambda}\psi_+,-\psi_-)\]

is bounded by \( C(N^{-1} + e^{-|\lambda|^C}) \) on the boundary of the neighborhood chosen above, since \((k^2 - H_{\text{eff}})^{-1}\) is bounded there. The theorem follows as the difference is holomorphic.

In other words, we have shown that the theorem holds when \( k \in \mathbb{R} \) is on the boundary of the physical space even if \( k \) is a pole of \((k^2 - H_{\text{eff}})^{-1}\), as long as \( k^2 \neq \sigma_\lambda^2, \sigma_\lambda^* \).

To finish the proof, consider what happens at a point \( k_0 \in \mathbb{R}, k_0^2 = \sigma_\lambda^2 \geq \sigma_\lambda^* \). (The case \( \sigma_\lambda^2 < \sigma_\lambda^* \) follows by symmetry.) If \( \sigma_\lambda^2 = \sigma_\lambda^* \), then since \( \sqrt{K_+}/\sqrt{K_-} = 1 \) (except for the removable singularity at \( k_2 = 0 \)), \((S_{f,N,\Lambda}(k)\psi_+,\psi_-)\) has a meromorphic extension to a neighborhood of \( k_0 \) in \( \Lambda_{\sigma(\Delta_{\lambda\lambda})} \). The boundedness at \( k_0 \), again obtained from unitarity, ensures that there exists a neighborhood of \( k_0 \) on which \((S_{f,N,\Lambda}\psi_+,-\psi_-)\) is holomorphic. Thus the previous argument using the maximum principle holds here as well.

Now suppose \( \sigma_\lambda^2 < \sigma_\lambda^* = k_0^2 \), and set \( T_{\lambda\lambda'}(k) = (\sqrt{K_+}/\sqrt{K_-})S_{\lambda\lambda'}(k) \). Then \( T_{\lambda\lambda'} \) is meromorphic in a neighborhood of \( k_0 \). Using the unitarity of \( S(k) \) for \( k \) real,

\[
|T_{\lambda\lambda'}(k)|^2 \leq |k_{\lambda\lambda'}||k_{\lambda\lambda'}|^{-1} \text{ for } k^2 \geq \sigma_\lambda^2, \quad k \in \mathbb{R}.
\]

Thus, \( \sqrt{k_{\lambda\lambda'}}T_{\lambda\lambda'}(k) \) is bounded at \( k_0 \), and \( T_{\lambda\lambda'} \) must then also be bounded at \( k_0 \), since near \( k_0 \) it is a meromorphic function of \( k_1 \). Therefore, \( S_{\lambda\lambda'}(k_0) = 0 \). Since we have in fact only used the unitarity of \( S(k) \) for \( k \in \mathbb{R} \) and the existence of a meromorphic extension, the same argument gives

\[
|S_{f,N,\Lambda}(k)\psi_+,\psi_-)|_{k=k_0} = 0 \quad \text{for } \sigma_\lambda^2 < \sigma_\lambda^* = k_0^2, \quad N, \Lambda \in \mathbb{R}_+ \cup \{ \infty \}.
\]

Thus the approximation is exact in this special case. \( \square \)

**6. An example**

In this section, we consider the simplest one-dimensional example where things are explicitly computable and we are able to see the effects of the approximation \( \Pi_{W}^{N,\lambda} \) explicitly. Figure 2 illustrates the example that we analyze in this section.

Let \( X = (-\pi, \infty) \), with \( X_0 = (-\pi, 0] \) and \( X_1 = [0, \infty) \). We consider the operator \(-\partial_x^2\) on \( X \), with Neumann boundary conditions. Although strictly speaking this example does not fall in the class considered in the first part of the note (\( X \) has a boundary, \( \{ -\pi \} \)), it is easy to see the arguments of the previous sections follow-through, with \( \partial X_0 \) replaced by \( Y = [0] \). Because \( Y \) is a point, the full scattering matrix is a scalar, and is easily computed to be

\[
S(k) = e^{2i\pi k}\]
Figure 2. An illustration of the example in section 6: the top figure shows the real parts of the approximation and of the scattering matrix, and the lower one, the graphs of $|S_{M^2}(k) - S(k)|$ for different values of $M$.

(This figure is in colour only in the electronic version)

For this example,

$$
\Psi_n(x) = \begin{cases} 
\pi^{-1/2} & \text{if } n = 0 \\
(2/\pi)^{1/2} \cos(nx) & \text{if } n > 0.
\end{cases}
$$

Since there is no sense in the cut-off $\Pi_{\lambda}^{\beta_X_0}$ for this problem, we use only one subscript on our approximations of $W$:

$$W_{M^2}(k) \overset{\text{def}}{=} \sqrt{k} \sum_{n=0}^{M} \Psi_n(0) \Psi_n(x).$$

Similarly, we denote the approximation of $S(k)$ thus obtained by $S_{M^2}(k)$. In the notation of the paper $M = \sqrt{N}$. We denote by $\tilde{W}_{M^2} = \tilde{W}_{M^2}(k)$ the $M + 1$ vector $\pi^{-1/2}(1, \sqrt{2}, \ldots, \sqrt{2})^t$.

Note that if $ia' a \neq -1$,

$$(I + ia a')^{-1} = I - i(1 + ia'a)^{-1}aa'.$$

Set $D_M \equiv D_{M^2}(k)$ to be the $M + 1 \times M + 1$ matrix given by $((k^2 - n^2)\delta_{nm})$. We see that when $k \not\in \mathbb{Z}$ so that $D_M(k)$ is invertible, the approximation $S_{M^2}(k)$ is given by

$$S_{M^2}(k) = -1 + 2i\tilde{W}_{M^2}(D_M^{-1} + i\tilde{W}_{M^2}\tilde{W}_{M^2}^{-1})^{-1}\tilde{W}_{M^2}
= -1 + 2i(D_{M^2}^{-1/2}\tilde{W}_{M^2})^t(I + iD_{M^2}^{-1/2}\tilde{W}_{M^2}(D_{M^2}^{-1/2}\tilde{W}_{M^2})^t)^{-1}D_{M^2}^{-1/2}\tilde{W}_{M^2}.$$
Set $B_M = D^{-1/2} \tilde{W}_M$ and $\beta_M = B_M' B_M$. Then, for $k \notin \mathbb{Z}$,
\[
S_M(k) = -1 + 2i B_M' (I - i(1 + i\beta_M)^{-1} B_M' B_M^2) B_M^2
\]
\[
= -1 + 2i \left( \beta_M - \frac{i \beta_M^2}{1 + i\beta_M} \right).
\]
(6.1)

Now
\[
\beta_M = \frac{1}{\pi} \left( \frac{1}{k} + \sum_{n=1}^{M} \frac{2k}{k^2 - n^2} \right).
\]
(6.2)

We note that
\[
\lim_{M \to \infty} \beta_M = \cot \pi k;
\]
once can use this and (6.1) to see that
\[
\lim_{M \to \infty} S_M(k) = e^{2\pi i k} = S(k)
\]
when $k^2 \notin \mathbb{N}$. Using (6.1) and (6.2), we see that for $k \in \mathbb{R} \setminus \mathbb{Z}$ and $M > |k|$,\[
C_1/M \leq |S_M(k) - S(k)| \leq C_2/M
\]
for some positive constants $C_1, C_2$ depending on $k$. Since $M = \sqrt{N}$, this shows that the estimates obtained in lemma 4.5 and in the main theorem are optimal.

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