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

T J Christiansen[1] **and M Zworski**[2]

[1] Department of Mathematics, University of Missouri, Columbia, MO 65211, USA
[2] Mathematics Department, University of California, Evans Hall, Berkeley, CA 94720, USA

E-mail: christiansent@missouri.edu and zworski@math.berkeley.edu

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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, $-H_{\text{in}}$, on X_0 with eigenvalues $-\tau_n^2$. Let $\{\varphi_\lambda\}$ be the same set for the Laplacian on ∂X_0, with $-\sigma_\lambda^2$ denoting the corresponding eigenvalues. Let us define the interaction matrix by*

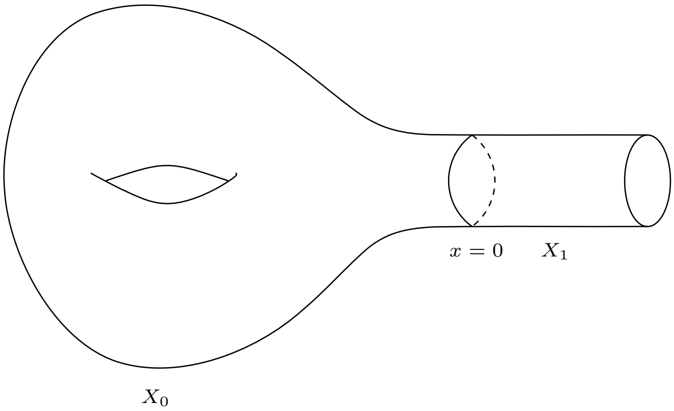

Figure 1. An example of a manifold with an infinite cylindrical end.

$$W_{N,\Lambda}(k) : L^2(\partial X_0) \longrightarrow L^2(X_0),$$
$$W_{N,\Lambda} f = \sum_{0\leqslant\tau_n\leqslant\sqrt{N}} \Psi_n \sum_{0\leqslant\sigma_\lambda\leqslant\sqrt{\Lambda}} \left(k^2 - \sigma_\lambda^2\right)^{\frac{1}{4}} \langle \Psi_n\restriction_{\partial X_0}, \varphi_\lambda\rangle\langle f, \varphi_\lambda\rangle, \tag{1.1}$$

and the effective Hamiltonian by

$$H_{N,\Lambda}(k) \stackrel{\text{def}}{=} H_{\text{in}} - \mathrm{i} W_{N,\Lambda}(k) W_{N,\Lambda}(k)^t.$$

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

$$S_{\lambda,\lambda'}(k) = -\langle (I - 2\mathrm{i} W_{N,\Lambda}(k)^t (k^2 - H_{N,\Lambda}(k))^{-1} W_{N,\Lambda}(k))\varphi_{\lambda'}, \varphi_\lambda\rangle + \mathcal{O}\big(N^{-\frac{1}{2}} + \mathrm{e}^{-\Lambda/C}\big), \tag{1.2}$$

if $\sigma_\lambda, \sigma_{\lambda'} \leqslant |k|$, and $\Lambda > k^2$. The error bound $\mathcal{O}(N^{-\frac{1}{2}})$ 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), $\sigma_\lambda, \sigma_{\lambda'} \leqslant |k|$, 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:

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

Here

$$\widetilde{H}_{\text{eff}} \stackrel{\text{def}}{=} H_{\text{in}} - \mathrm{i} W(k) W(k)^* \tag{1.4}$$

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_{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, 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 $\widetilde{S}_f(k)$ 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):

$$S_f(k) = -(I - 2\mathrm{i}W(k)^t(k^2 - H_{\mathrm{eff}})^{-1}W(k)) \tag{1.5}$$

with

$$H_{\mathrm{eff}} = H_{\mathrm{in}} - \mathrm{i}W(k)W(k)^t, \tag{1.6}$$

and, with the notation of (1.1),

$$W(k) \stackrel{\mathrm{def}}{=} W_{\infty,\infty}(k).$$

In fact, $-H_{\mathrm{eff}} = -H_{\mathrm{eff}}(k)$ 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 $(k^2 - H_{\mathrm{eff}})^{-1}$ 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 $W_a(k)^* = W_a(k)^t$. The operator $S_f(k)$, unlike $\widetilde{S}_f(k)$, 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,

$$S(k) = -\Pi_{k^2}^{\partial X_0}(I - 2\mathrm{i}W(k)^t(k^2 - H_{\mathrm{eff}})^{-1}W(k))\Pi_{k^2}^{\partial X_0} \tag{1.7}$$

where $\Pi_{k^2}^{\partial X_0}$ projects to the span of the eigenfunctions of $-\Delta_Y$, with eigenvalue at most k^2. Here Δ_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)

$$-\Pi_{k^2}^{\partial X_0}(I - 2\mathrm{i}W(k)^*(k^2 - H_{\mathrm{eff}})^{-1}W(k))\Pi_{k^2}^{\partial X_0}$$

with H_{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

$$X = X_0 \sqcup (0, \infty) \times Y, \qquad Y = \partial X_0,$$

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

$$g\restriction_U = (\mathrm{d}x)^2 + g_Y.$$

Recall that $\{\varphi_\lambda\}$ is an orthonormal set of eigenfunctions of Δ_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 $\operatorname{Im} k \geqslant 0$. We call the region with $\operatorname{Im} k \geqslant 0$ the physical region. Given $\lambda \in \mathbb{N}$, if k is in the physical region, and with $\operatorname{Im} k > 0$, there is a unique $\Phi_\lambda(p, k)$ so that

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

and

$$\Phi_\lambda\restriction_{(0,\infty)\times Y} = \mathrm{e}^{-\mathrm{i}k_\lambda x}\frac{\varphi_\lambda(y)}{\sqrt{k_\lambda}} + \sum_{\lambda'} S_{\lambda'\lambda}(k)\,\mathrm{e}^{\mathrm{i}k_{\lambda'} x}\frac{\varphi_{\lambda'}(y)}{\sqrt{k_{\lambda'}}} \tag{2.2}$$

for some $S_{\lambda'\lambda}$. 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 $\operatorname{Im} k > 0$:

$$\Phi_\lambda(p, k) = (1 - \psi)\varphi_\lambda(y)\,\mathrm{e}^{-\mathrm{i}k_\lambda x} + (-\Delta_X - k^2)^{-1}([\Delta_X, \psi](\varphi_\lambda(y)\,\mathrm{e}^{-\mathrm{i}k_\lambda x}))(p),$$
$$\psi \in C_0^\infty(X), \qquad \psi\restriction_{X_0} \equiv 1.$$

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

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

$$\Lambda_{\sigma(\Delta_{\partial X_0})} \supset \{k : \operatorname{Im} k > 0\}, \tag{2.3}$$

a Riemann surface branched at σ_λ's—see [10, section 6.7]. We remark that this Riemann surface is such that each k_λ defined above extends to be a holomorphic single-valued function. Thus, $\Phi_\lambda(p, k)$ has a meromorphic continuation to $\Lambda_{\sigma(\Delta_{\partial X_0})}$ which is regular for $\operatorname{Im} k = 0$ 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

$$S(k) = (S_{\lambda'\lambda}(k))_{\sigma_\lambda^2,\sigma_{\lambda'}^2 \leqslant k^2}.$$

We remark that if $\operatorname{Im} k > 0$, 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 $\Lambda_{\sigma(\Delta_{\partial X_0})}$ for each λ, λ'. We shall use this continuation in the proof of the theorem.

3. The formula

Let Δ_Y be the Laplacian on Y, and let $\{\sigma_\lambda^2\}$ be the eigenvalues of $-\Delta_Y$, repeated according to multiplicity, and let $\{\varphi_\lambda\}$ be an associated set of real, orthonormal eigenfunctions of the Laplacian on Y. Let $-H_{\text{in}}$ be the Laplacian with Neumann boundary conditions on X_0°, and let $\{\Psi_n\}$ 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

$$\Psi_{n,\lambda}(0) \stackrel{\text{def}}{=} \int_Y \varphi_\lambda(y)\Psi_n(0, y),$$

we follow the physics literature and define the *coupling operator* by giving its integral kernel (with integration with respect to Riemannian densities) as

$$\begin{aligned} W(p, y') &\stackrel{\text{def}}{=} \sum_{n,\lambda} \sqrt{k_\lambda}\Psi_n(p)\Psi_{n,\lambda}(0)\varphi_\lambda(y') \\ &= \sum_n \Psi_n(p) P_k \Psi_n(0, y'). \end{aligned} \tag{3.1}$$

Here $P_k = (k^2 + \Delta_Y)^{1/4}$ is defined by $P_k\varphi_\lambda = \sqrt{k_\lambda}\varphi_\lambda$. 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 $\dot{\mathcal{D}}'(X_0)$ be the space of distributions on X supported in the (closed) set X_0. We also use the following convention: for $s \geqslant 0$ the space $H^s(X_0)$ denotes restrictions of elements of $H^s(X)$ to X_0, while for $s \leqslant 0$, $H^s(X_0)$ 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

$$H^s(X_0) = \begin{cases} \bar{H}_{(s)}(X_0) & s \geqslant 0 \\ \dot{H}_{(s)}(X_0) & s \leqslant 0. \end{cases}$$

With this notation in place we can formulate

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

$$W(k)g = \delta_{\partial X_0} P_k g, \qquad g \in C^\infty(\partial X_0), \tag{3.2}$$

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

$$\delta_{\partial X_0}(\varphi) = \int_{\partial X_0} \varphi\restriction_{\partial X_0} \mathrm{dvol}_Y.$$

We have

$$W(k) : H^s(Y) \to H^{\min(-1/2-, s-1)}(X_0), \qquad s \in \mathbb{R}, \tag{3.3}$$

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

$$W(k)^t f(y) = P_k(f\restriction_{\partial X_0}). \tag{3.4}$$

Proof. To prove (3.2) we need to compute, in the notation of distributions, $W(f \otimes g)$, where $f \in \bar{C}_0^\infty(X_0)$. The definition (3.1) gives

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

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

$$W_a(k)^t \stackrel{\text{def}}{=} P_k \mathbb{1}_{[0,N]}(\Delta_Y) R \mathbb{1}_{[0,\Lambda]}(H_{\text{in}}), \qquad Ru \stackrel{\text{def}}{=} u\restriction_{\partial X_0}.$$

We note that

$$W_{(\infty,\infty)}(k) = W(k),$$

and that for $N < \infty$ and $\Lambda < \infty$,

$$W_a(k) : \mathcal{D}'(Y) \longrightarrow C^\infty(X_0), \qquad W_a(k)^t : \dot{\mathcal{D}}'(X_0) \longrightarrow C^\infty(Y),$$

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

$$q(u, v) = q(k)(u, v) = \int_{X_0} \nabla u \overline{\nabla v}\, \text{dvol}_{X_0} - \mathrm{i} \int_{\partial X_0} W^t(k) u \overline{W^*(k) v}\, \text{dvol}_Y$$
$$= \int_{X_0} \nabla u \overline{\nabla v}\, \text{dvol}_{X_0} - \mathrm{i} \int_{\partial X_0} P_k R u \overline{P_k^* R v}\, \text{dvol}_Y$$

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 $H_{\text{eff}} u = w$. Moreover,

$$(w, v) = q(u, v) = -\int_{X_0} \Delta_{X_0} u \bar{v} + \int_{\partial X_0} \left(\partial_n u - \mathrm{i} P_k^2 R u\right) \bar{v},$$

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

$$0 = \partial_n u - \mathrm{i} P_k^2 R u.$$

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

$$H_{\text{eff}} u = -\Delta_{X_0} u, \qquad \partial_n u - \mathrm{i} P_k^2 R u = 0.$$

Next we investigate the relation between $(k^2 - H_{\text{eff}})^{-1}$ and the resolvent of the Laplacian on X. Denote

$$R_X(k) \stackrel{\text{def}}{=} (k^2 + \Delta_X)^{-1}, \qquad \text{for} \quad \operatorname{Im} k > 0.$$

Then, for $K \subset X$ any compact set $\mathbb{1}_K R_X(k) \mathbb{1}_K$ has a meromorphic extension to $\Lambda_{\sigma(\Delta_{\partial X_0})}$, see [10]. In lemma 4.1 we shall show that $(k^2 - H_{\text{eff}})^{-1} : L^2(X_0) \to H^2(X_0)$ exists for $k^2 \ll 0, \operatorname{Im} k > 0$, and is meromorphic on $\Lambda_{\sigma(\Delta_{\partial X_0})}$, 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 $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$, by abuse of notation we mean by k^2 the complex number which is the continuation of k^2 from the physical half-plane $\operatorname{Im} k \geqslant 0$.

Lemma 3.3. *We have the following relation between $R_X(k)$ as defined above and $(k^2 - H_{\text{eff}})^{-1} = (k^2 - H_{\text{eff}}(k))^{-1}$:*

$$(k^2 - H_{\text{eff}})^{-1} = \mathbb{1}_{X_0} R_X(k) \mathbb{1}_{X_0}$$

for $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$. 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 is 0 in a neighborhood of ∂X_0. Then

$$\big(k^2 + \Delta_{X_0}\big)\mathbb{1}_{X_0} R_X(k) g = \big(k^2 + \Delta_{X_0}\big)\mathbb{1}_{X_0} R_X(k) \mathbb{1}_{X_0} g = g \quad \text{on } X_0^\circ \tag{3.5}$$

for $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$.

Note that since $\operatorname{supp} g \subset X_0$, $(k^2 + \Delta_X) g = 0$ on X_1. Then for $\operatorname{Im} k > 0$ (that is, for k in the physical space), the requirement that $R_X(k) g \in L^2(X)$ means that

$$R_X(k) g\restriction_{X_1} = \sum a_\lambda \, \mathrm{e}^{\mathrm{i} k_\lambda x} \varphi_\lambda \tag{3.6}$$

for some constants $a_\lambda = a_\lambda(k)$. But then, using the support conditions of g there is a neighborhood $\tilde{U} \subset X_0$ of ∂X_0 so that

$$R_X(k) g\restriction_{\tilde{U}} = \sum a_\lambda \, \mathrm{e}^{\mathrm{i} k_\lambda x} \varphi_\lambda.$$

Thus,

$$\big(\partial_n - \mathrm{i} P_k^2\big)(R_X(k) g\restriction_{X_0})\restriction_{\partial X_0} = 0$$

so that $R_X(k) g\restriction_{X_0}$ 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 $\operatorname{Im} k > 0$ and all $g \in L^2(X_0)$ which are 0 in a neighborhood of ∂X_0. Since such 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 $\operatorname{Im} k > 0$ and since both sides have meromorphic continuations to $\Lambda_{\sigma(\Delta_{\partial X_0})}$ (see [10] and lemma 4.1), they must in fact agree for all $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$. □

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

$$(k^2 + \Delta_{X_0}) u = 0 \text{ on } X_0^\circ, \qquad \big(\partial_n - \mathrm{i} P_k^2\big) u\restriction_{\partial X_0} = -P_k f. \tag{3.7}$$

Proof. We first claim that there exists $F \in H^2(X_0)$ such that

$$\big(\partial_n - \mathrm{i} P_k^2\big) F\restriction_{\partial X_0} = -P_k f. \tag{3.8}$$

In fact, for $0 < h \ll 1$ define $N(h) : H^s(\partial X_0) \to H^{s-1}(\partial X_0)$ as follows:

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

Let $\chi \in C_0^\infty([0,\epsilon))$ be equal to 1 in a small neighborhood of 0, with ϵ chosen so that $X_0 \simeq (-\epsilon, 0]_x \times \partial X_0$, near the boundary. We define (note that $x < 0$)

$$[T(h)g](x,y) \stackrel{\text{def}}{=} \chi(-x)\exp\big(x\langle I - \Delta_{\partial X_0}\rangle^{\frac{1}{2}}/h\big)g(y),$$
$$T(h) : H^s(\partial X_0) \to H^{s+\frac{1}{2}}(X_0), \qquad s \geqslant 0,$$

so that

$$T(h)g\restriction_{\partial X_0} = g, \qquad \partial_n T(h)g\restriction_{\partial X_0} = N(h)g.$$

For a fixed k, $P_k^2 = \mathcal{O}(1) : H^{3/2}(\partial X_0) \to H^{1/2}(\partial X_0)$, and hence, if h is small enough, we have the following inverse:

$$\big(N(h) - \mathrm{i}P_k^2\big)^{-1} = N(h)^{-1}\big(I - \mathrm{i}P_k^2 N(h)^{-1}\big)^{-1} : H^{\frac{1}{2}}(\partial X_0) \longrightarrow H^{\frac{3}{2}}(\partial X_0).$$

Using this and the mapping properties of $T(h)$ we construct

$$F \stackrel{\text{def}}{=} -T(h)\big(N(h) - \mathrm{i}P_k^2\big)^{-1}P_k f \in H^2(X_0),$$

which satisfies (3.8).

We now set

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

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

$$\begin{aligned}((k^2 - H_{\text{eff}})^{-1}\big(k^2 + \Delta_{X_0}\big)F, h) &= \big(\big(k^2 + \Delta_{X_0}\big)F, ((k^2 - H_{\text{eff}})^{-1})^* h\big)\\
&= \int_{\partial X_0}\big(\partial_n F\overline{((k^2 - H_{\text{eff}})^{-1})^* h} - F\overline{\partial_n((k^2 - H_{\text{eff}})^{-1})^* h}\big)\\
&\quad + (F, \big(k^2 + \Delta_{X_0}\big)((k^2 - H_{\text{eff}})^{-1})^* h)\\
&= \int_{\partial X_0}\big(\partial_n F\overline{((k^2 - H_{\text{eff}})^{-1})^* h} - F\overline{\partial_n((k^2 - H_{\text{eff}})^{-1})^* h}\big)\\
&\quad + (F, h).\end{aligned}$$

Now we use that $\partial_n F\restriction_{\partial X_0} = \mathrm{i}P_k^2(F\restriction_{\partial X_0}) - P_k f$, and that

$$w \in H^2(X_0) \cap \text{Domain}((k^2 - H_{\text{eff}})^*) \quad \Longrightarrow \quad \partial_n w\restriction_{\partial X_0} + \mathrm{i}\big(P_k^2\big)^* Rw = 0.$$

Thus we have

$$\begin{aligned}&((k^2 - H_{\text{eff}})^{-1}\big(k^2 + \Delta_{X_0}\big)F, h)\\
&\quad = \int_{\partial X_0}\big(\big(\mathrm{i}P_k^2(F\restriction_{\partial X_0}) - P_k f\big)\overline{((k^2 - H_{\text{eff}})^{-1})^* h} - \mathrm{i}F\overline{\big(\big(P_k^2\big)^*(k^2 - H_{\text{eff}})^{-1}\big)^* h}\big)\\
&\quad\quad + (F, h)\\
&\quad = -\int_{\partial X_0} P_k f\overline{((k^2 - H_{\text{eff}})^{-1})^* h} + (F, h) = \int_{X_0}(-(k^2 - H_{\text{eff}})^{-1}\delta_{X_0}P_k f + F)\bar{h},\end{aligned}$$

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

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

proving the lemma. □

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*

$$S_{\lambda,\lambda'}(k) = \langle S_f(k)\varphi_\lambda, \varphi_{\lambda'}\rangle_{L^2(\partial X_0)}, \tag{3.9}$$

where

$$S_f(k) = -(I - 2\mathrm{i}W(k)^t(k^2 - H_{\text{eff}})^{-1}W(k)),$$

and H_{eff} is defined in lemma 3.2.

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

$$v_\lambda\restriction_U = \sum_{\lambda'}(a_{\lambda'}\,\mathrm{e}^{\mathrm{i}k_{\lambda'}x} + b_{\lambda'}\,\mathrm{e}^{-\mathrm{i}k_{\lambda'}x})\varphi_{\lambda'}(y).$$

The boundary conditions (3.7) applied to v_λ at ∂X_0 mean that

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

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

$$\Phi_\lambda\restriction_{(0,\infty)\times Y} = \mathrm{e}^{-\mathrm{i}k_\lambda x}\frac{\varphi_\lambda(y)}{\sqrt{k_\lambda}} + \sum_{\lambda'}S_{\lambda'\lambda}\,\mathrm{e}^{\mathrm{i}k_{\lambda'}x}\frac{\varphi_{\lambda'}(y)}{\sqrt{k_{\lambda'}}}. \tag{3.10}$$

Therefore,

$$W(k)^t v_\lambda = \sum_{\lambda'}\sqrt{k_{\lambda'}}a_{\lambda'}\varphi_{\lambda'} - \frac{\mathrm{i}}{2}\varphi_\lambda = -\frac{\mathrm{i}}{2}\left(\sum_{\lambda'}S_{\lambda'\lambda}\varphi_{\lambda'} + \varphi_\lambda\right),$$

which proves the proposition. □

Equation (3.9) is valid for all real values of k (that is, k on the boundary of the physical space) with $k^2 > \sigma_\lambda^2,\ \sigma_{\lambda'}^2$, 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

$$\Pi_\Lambda^{\partial X_0} f \stackrel{\text{def}}{=} \mathbb{1}_{[0,\Lambda]}(-\Delta_{\partial X_0})f \qquad \text{for} \quad f \in L^2(\partial X_0),$$
$$\Pi_N^{\text{in}} g \stackrel{\text{def}}{=} \mathbb{1}_{[0,N]}(H_{\text{in}})g \qquad \text{for} \quad g \in L^2(X_0).$$

In parallel with this, we introduce

$$W_{\infty,\infty}(k) \stackrel{\text{def}}{=} W(k), \qquad W_{\infty,\Lambda}(k) \stackrel{\text{def}}{=} W\Pi_\Lambda^{\partial X_0},$$
$$W_{N,\Lambda}(k) \stackrel{\text{def}}{=} \Pi_N^{\text{in}}W(k)\Pi_\Lambda^{\partial X_0} = \Pi_N^{\text{in}}W_{\infty,\Lambda}(k),$$

and

$$H_{\infty,\infty} \stackrel{\text{def}}{=} H_{\text{eff}}, \qquad H_{N,\Lambda} \stackrel{\text{def}}{=} H_{in} - iW_{N,\Lambda}W_{N,\Lambda}^t, \qquad N \in \mathbb{R} \cup \{\infty\}.$$

Although $W_{N,\Lambda}, W_{\infty,\Lambda}$ depend on k, for simplicity we generally omit this in our notation. Note that $H_{\mathrm{eff}}, H_{\infty,\Lambda}$ 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 $H_{\infty,\Lambda}$, then $\partial_n u - \mathrm{i}P_k^2\Pi_\Lambda^{\partial X_0} Ru = 0$. 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, $\partial_n u = 0$.

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

$$S_{f,N,\Lambda}(k) = -(I - 2\mathrm{i}W_{N,\Lambda}(k)^t(k^2 - H_{N,\Lambda})^{-1}W_{N,\Lambda}(k)). \tag{4.1}$$

In order to bound the error in these approximations, we shall first see how close $\Pi_{\Lambda_0}^{\partial X_0} S_{f,\infty,\Lambda}$ is to $\Pi_{\Lambda_0}^{\partial X_0} S_{f,\infty,\infty}$, and then study the difference

$$\Pi_{\Lambda_0}^{\partial X_0}(S_{f,\infty,\Lambda} - S_{f,N,\Lambda})\Pi_{\Lambda_0}^{\partial X_0}.$$

4.1. *Projection on ∂X_0*

We first analyze the approximation with a finite Λ and $N = \infty$. The spectral cut-off for the boundary Laplacian, Λ, has to be taken large enough to guarantee that $\operatorname{Im} k_\lambda > 0$ for $\sigma_\lambda^2 > \Lambda$. The errors then come from *evanescent modes* and can be estimated using exponential decay. We present the results in two lemmas.

Recall that $H_{\mathrm{eff}} = H_{\mathrm{eff}}(k)$ is defined for $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$.

Lemma 4.1. *Let $\Lambda_{\sigma(\Delta_{\partial X_0})}$ 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 $(k^2 - H_{\mathrm{eff}})^{-1}$ and $(k^2 - H_{\infty,\Lambda})^{-1}$ are meromorphic on $\Lambda_{\sigma(\Delta_{\partial X_0})}$. If $k^2 - H_{\mathrm{eff}} = k^2 - H_{\mathrm{eff}}(k)$ is invertible, so is $k^2 - H_{\infty,\Lambda}(k)$ for $\Lambda > \Lambda(k)$ sufficiently large, and*

$$\|(k^2 - H_{\mathrm{eff}})^{-1} - (k^2 - H_{\infty,\Lambda})^{-1}\|_{L^2\to L^2} \leqslant C\Lambda^{-1/2}, \qquad \Lambda > \Lambda_0(k).$$

Moreover, for k restricted to a compact set $K \subset \Lambda_{\sigma(\Delta_{\partial X_0})}$ on which $k^2 - H_{\mathrm{eff}}$ is invertible, Λ_0 and C can be chosen independently of k.

Proof. Recall that U is a neighborhood of ∂X_0 which we may identify with $(-\epsilon, 0]_x \times Y$ with $g\restriction_U = (\mathrm{d}x)^2 + g_Y$. Choose $\chi_i \in C^\infty(X)$, $i = 1, 2$, so that each χ_i has support in U, $\chi_i = 1$ in a smaller neighborhood of the boundary, and

$$\chi_1\chi_2 = \chi_1, \qquad \operatorname{supp}\chi_2' \cap \operatorname{supp}\chi_1 = \emptyset.$$

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

$$R_{\Lambda,e}(k)(x, y; x', y') \stackrel{\mathrm{def}}{=} \sum_\lambda \frac{1}{2\mathrm{i}k_\lambda}\left(\mathrm{e}^{\mathrm{i}k_\lambda|x-x'|} + \left(1 - \Pi_\Lambda^{\partial X_0}\right)\mathrm{e}^{\mathrm{i}k_\lambda|x+x'|}\right)\varphi_\lambda(y)\varphi_\lambda(y').$$

Note that $R_{\Lambda,e}(k)$ is a meromorphic function of $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$ since k_λ is holomorphic on $\Lambda_{\sigma(\Delta_{\partial X_0})}$. Let $R_{\infty,e}(k)$ be the operator with Schwartz kernel given by

$$\sum_\lambda \frac{1}{2\mathrm{i}k_\lambda}\,\mathrm{e}^{\mathrm{i}k_\lambda|x-x'|}\varphi_\lambda(y)\varphi_\lambda(y'),$$

and set

$$E_\Lambda(k) = (1 - \chi_1)(k^2 - H_{\mathrm{in}})^{-1} + \chi_2 R_{\Lambda,e}(k)\chi_1, \qquad \Lambda \in \mathbb{R} \cup \{\infty\}.$$

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

$$\left(\partial_n - \mathrm{i}P_k^2\Pi_\Lambda^{\partial X_0}\right)E_\Lambda v\restriction_{\partial X_0} = 0,$$

and is meromorphic on $\Lambda_{\sigma(\Delta_{\partial X_0})}$. Moreover,

$$\left(k^2 + \Delta_{X_0}\right)E_\Lambda(k) = I - \left[\Delta_{X_0}, \chi_1\right](k^2 - H_{\text{in}})^{-1} + [\Delta_{X_0}, \chi_2]R_{\Lambda,e}(k)\chi_1$$
$$\stackrel{\text{def}}{=} I + K_\Lambda(k)$$

where $K_\Lambda(k)$ is a compact operator. Moreover, $K_\Lambda(k)$ is a meromorphic function of k in $\Lambda_{\sigma(\Delta_{\partial X_0})}$ with finite-rank poles. When $k \in \mathrm{i}\mathbb{R}_+$, $\|K_\Lambda(k)\| \to 0$ as $k^2 \to -\infty$. Thus, $I + K_\Lambda(k)$ is invertible for $k \in \mathrm{i}\mathbb{R}_+$, $-k^2 \gg 0$, 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 $\Lambda_{\sigma(\Delta_{\partial X_0})}$.

Now

$$\|E_\Lambda(k) - E_\infty(k)\|_{L^2\to L^2} \leqslant C \max_{\sigma_\lambda^2>\Lambda} |k_\lambda|^{-1}.$$

For k in a compact set of $\Lambda_{\sigma(\Delta_{\partial X_0})}$ and $\sigma_\lambda > \Lambda \geqslant \Lambda_0(k)$, sufficiently large, we have $\operatorname{Im} k_\lambda > 0$, and since

$$x \in \operatorname{supp} \chi_2', \qquad x' \in \operatorname{supp} \chi_1 \quad \Longrightarrow \quad |x - x'|, |x + x'| > \epsilon_0 > 0,$$

we have

$$\|K_\Lambda(k) - K_\infty(k)\|_{L^2\to L^2} \leqslant C \max_{\sigma_\lambda^2>\Lambda} \frac{|k_\lambda| + 1}{|k_\lambda|} \mathrm{e}^{-\epsilon_0 \operatorname{Im} k_\lambda/2}.$$

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

$$\|(k^2 - H_{\text{eff}})^{-1} - (k^2 - H_{\infty,\Lambda})^{-1}\| \leqslant C\Lambda^{-1/2}$$

for Λ sufficiently large (depending on k or K, ϵ_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 $\Lambda \in \mathbb{R}_+ \cup \{\infty\}$,

$$P_k^{-1} S_{f,\infty,\Lambda}(k) P_k = -\left(I - 2\mathrm{i} P_k^{-1} W_{\infty,\Lambda}(k)^t (k^2 - H_{\infty,\Lambda})^{-1} W_{\infty,\Lambda}(k) P_k\right) \tag{4.2}$$

has a meromorphic continuation to $\Lambda_{\sigma(\Delta_{\partial X_0})}$. The conjugation by P_k is necessary because while P_k^2 is a well-defined operator for $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$, P_k is not. Thus the operators $W_{\infty,\Lambda}(k)P_k$ and $P_k^{-1}W_{\infty,\Lambda}(k)^t$ are well defined on $\Lambda_{\sigma(\Delta_{\partial X_0})}$, while in general $W_{\infty,\Lambda}(k)$ and $W_{\infty,\Lambda}^t(k)$ are not. The existence of the meromorphic continuation of (4.2) means that $(\sqrt{k_{\lambda'}}/\sqrt{k_\lambda})\langle S_{f,\infty,\Lambda}(k)\varphi_{\lambda'}, \varphi_\lambda\rangle$ has a meromorphic continuation to $\Lambda_{\sigma(\Delta_{\partial X_0})}$.

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

$$\left\| P_k^{-1}\Pi_{\Lambda_0}^{\partial X_0}(S_f(k) - S_{f,\infty,\Lambda}(k))P_k f\right\|_{L^2(\partial X_0)} \leqslant C \max_{\sigma_\lambda^2>\Lambda}(|k_\lambda| \exp(-\epsilon' \operatorname{Im} k_\lambda))\|f\|_{L^2(\partial X_0)}.$$

In particular, by lemma 4.1 this holds for all Λ sufficiently large depending on k. We note that the constants C and ϵ' 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 $\operatorname{Im} k_\lambda > 0$ when $\sigma_\lambda^2 > \Lambda_0$.

We note that since $\Pi_\Lambda^{\partial X_0} f = f$, the $H^{3/2}$ norm of f is bounded by a Λ-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_Λ satisfies

$$\big(k^2 + \Delta_{X_0}\big)u_\Lambda = 0 \text{ on } X_0^\circ, \qquad \big(\partial_n u_\Lambda - \mathrm{i} P_k^2 \Pi_\Lambda^{\partial X_0} R u_\Lambda\big) = -P_k^2 f.$$

Choose $\chi \in C_c^\infty((-\epsilon/2, 0])$ to be one in a neighborhood of 0. Since $U \subset X_0$ is a neighborhood of ∂X_0 which can be identified with $(-\epsilon, 0]_x \times Y_y$, 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 $\Pi_\Lambda^{\partial X_0} \chi g \in L^2(U) \subset L^2(X_0)$ via

$$\big(\Pi_\Lambda^{\partial X_0} \chi g\big)(x, y) = \sum_{\sigma_\lambda^2 \leqslant \Lambda} \varphi_\lambda(y) \int_{y' \in \partial X_0} (\chi(x) g(x, y') \varphi_\lambda(y'))\, \mathrm{dvol}_Y.$$

Then

$$u_\Lambda = (1 - \chi) u_\infty + \Pi_\Lambda^{\partial X_0} \chi u_\infty + (k^2 - H_{\infty,\Lambda})^{-1} \big(k^2 + \Delta_{X_0}\big)\big(1 - \Pi_\Lambda^{\partial X_0}\big) \chi u_\infty \tag{4.3}$$

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

Note that by using $\Pi_{\Lambda_0}^{\partial X_0} f = f$

$$u_\infty\restriction_U = \sum_{\sigma_\lambda^2 \leqslant \Lambda} (a_\lambda \mathrm{e}^{-\mathrm{i}k_\lambda x} + b_\lambda \mathrm{e}^{\mathrm{i}k_\lambda x}) \varphi_\lambda + \sum_{\sigma_\lambda^2 > \Lambda} b_\lambda \mathrm{e}^{\mathrm{i}k_\lambda x} \varphi_\lambda \tag{4.4}$$

for some constants a_λ, b_λ, so that, using orthonormality of φ_λ's,

$$\|u_\infty\|_{L^2}^2 \geqslant \|u_\infty\restriction_U\|_{L^2}^2 \geqslant \int_{-\epsilon}^0 \sum_{\sigma_\lambda^2 > \Lambda} |b_\lambda \mathrm{e}^{\mathrm{i}k_\lambda x}|^2 \,\mathrm{d}x$$

$$= \int_{-\epsilon}^0 \sum_{\sigma_\lambda^2 > \Lambda} |b_\lambda \mathrm{e}^{\mathrm{i}k_\lambda x}|^2 \,\mathrm{d}x = \sum_{\sigma_\lambda^2 > \Lambda} |b_\lambda|^2 \frac{\mathrm{e}^{2\epsilon \operatorname{Im} k_\lambda} - 1}{2 \operatorname{Im} k_\lambda}. \tag{4.5}$$

Also,

$$\big(k^2 + \Delta_{X_0}\big)\big(1 - \Pi_\Lambda^{\partial X_0}\big) \chi u_\infty = \big[\partial_x^2, \chi\big]\big(1 - \Pi_\Lambda^{\partial X_0}\big) \tilde{\chi} u_\infty,$$

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

$$\big\|\big(k^2 + \Delta_{X_0}\big)\big(1 - \Pi_\Lambda^{\partial X_0}\big) \chi u_\infty\big\|^2 = \big\|\big[\partial_x^2, \chi\big]\big(1 - \Pi_\Lambda^{\partial X_0}\big) \tilde{\chi} u_\infty\big\|^2$$

$$\leqslant C\langle \epsilon^{-4}\rangle \int_{-\epsilon/2}^0 \sum_{\sigma_\lambda^2 > \Lambda} \langle k_\lambda\rangle^2 |b_\lambda \mathrm{e}^{\mathrm{i}k_\lambda x}|^2 \,\mathrm{d}x$$

$$\leqslant C\langle \epsilon^{-4}\rangle \sum_{\sigma_\lambda^2 > \Lambda} \langle k_\lambda\rangle^2 |b_\lambda|^2 \frac{\mathrm{e}^{\epsilon \operatorname{Im} k_\lambda} - 1}{2 \operatorname{Im} k_\lambda}$$

$$= C\langle \epsilon^{-4}\rangle \sum_{\sigma_\lambda^2 > \Lambda} \langle k_\lambda\rangle^2 |b_\lambda|^2 \frac{\mathrm{e}^{\epsilon 2 \operatorname{Im} k_\lambda} - 1}{2 \operatorname{Im} k_\lambda} \left(\frac{1}{\mathrm{e}^{\epsilon \operatorname{Im} k_\lambda} + 1}\right).$$

Thus (4.5) gives

$$\big\|\big(k^2 + \Delta_{X_0}\big)\big(1 - \Pi_\Lambda^{\partial X_0}\big) \chi u_\infty\big\| \leqslant C\langle \epsilon^{-2}\rangle \|u_\infty\|_{L^2} \max_{\sigma_\lambda^2 > \Lambda} (|k_\lambda| \,\mathrm{e}^{-\epsilon \operatorname{Im} k_\lambda/2}).$$

Using (4.3), the estimate

$$\|(k^2 - H_{\infty,\Lambda})^{-1} g\|_{H^1} \leqslant (1 + |k|) \|(k^2 - H_{\infty,\Lambda})^{-1} g\|_{L^2},$$

and the previous lemma, we obtain

$$\left\| \Pi_{\Lambda_0}^{\partial X_0} R(u_\infty - u_\Lambda) \right\|_{L^2(\partial X)} \leqslant C\langle \epsilon^{-2} + |k|\rangle \|(k^2 - H_{\infty,\Lambda})^{-1}\| \|u_\infty\|_{L^2} \max_{\sigma_\lambda^2 > \Lambda} (|k_\lambda| \, \mathrm{e}^{-\epsilon \operatorname{Im} k_\lambda/2}).$$

Thus far each constant C can be chosen independent of k, though of course $\|u_\infty\|$ depends on k in a continuous fashion on compact sets on which $k^2 - H_{\text{eff}}$ is invertible. Note that $P_k^{-1} P_k \Pi_\Lambda^{\partial X_0} = \Pi_\Lambda^{\partial X_0}$ is a bounded operator. Thus, using the expression for S_f, $S_{f,\infty,\Lambda}$ and the previous lemma finishes the proof. □

4.2. The cut-off in the interior

We now turn our attention to the error introduced by using Π_N^{in}. Throughout this section we assume that $\Lambda < \infty$.

Our results will use the following standard:

Lemma 4.3. *Suppose $\widetilde{X}$ is a compact Riemannian manifold without boundary and $\chi \in C_0^\infty(\mathbb{R})$ is equal to 1 in a neighborhood of 0. Suppose that $Y \subset \widetilde{X}$ is a smooth embedded submanifold of codimension 1. Then*

$$\|(1 - \chi(-h^2 \Delta_{\widetilde{X}}))u\restriction_Y\|_{L^2(Y)} \leqslant C\sqrt{h}\|u\|_{H^1(\widetilde{X})}.$$

If $v \in H^2(\widetilde{X}\backslash Y) \cap H^1(\widetilde{X})$, then

$$\|(1 - \chi(-h^2 \Delta_{\widetilde{X}}))v\restriction_Y\|_{L^2(Y)} \leqslant Ch\|v\|_{H^2(\widetilde{X}\backslash Y)}.$$

Proof. Both statements in the lemma are local. In fact, if P is another elliptic second-order operator on $\widetilde{X}$, then for some constant C_P the calculus of semiclassical pseudodifferential operators (see for instance [4, appendix E]) shows that

$$(1 - \chi(-h^2 \Delta))(1 - \chi(-h^2 C_P (P + C_P))) = (1 - \chi(-h^2 \Delta)) + \mathcal{O}_{H^{-k} \to H^k}(h^N),$$

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 $\widetilde{X} = \mathbb{R}^n$ 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

$$\mathcal{F}_{x' \mapsto \xi'} \left((1 - \chi(-h^2 \Delta_{\widetilde{X}}))u\restriction_Y \right)(\xi') = \int_{\mathbb{R}} (1 - \chi(h^2 |\xi|^2)) \hat{u}(\xi_1, \xi') \, \mathrm{d}\xi_1. \tag{4.6}$$

Hence, by the Cauchy–Schwartz inequality,

$$\|(1 - \chi(-h^2 \Delta_{\widetilde{X}}))u\restriction_Y\|_{L^2(Y)}^2 \leqslant C \int_{\mathbb{R}^n} F(\xi', h)(1 - \chi(h^2 |\xi|^2))|\hat{u}(\xi)|^2 (1 + |\xi|^2) \, \mathrm{d}\xi,$$

where

$$\begin{aligned} F(\xi', h) &\stackrel{\text{def}}{=} \int_{\mathbb{R}} (1 - \chi(h^2 |\xi|^2))(1 + |\xi|^2)^{-1} \, \mathrm{d}\xi_1 \\ &\leqslant \int_{|\xi_1| > c/h} (1 + |\xi_1|^2)^{-1} \, \mathrm{d}\xi_1 + \mathbb{1}_{|\xi'| > c/h}(\xi') \int_{\mathbb{R}} (|\xi'|^2 + |\xi_1|^2)^{-1} \, \mathrm{d}\xi_1 \\ &\leqslant Ch. \end{aligned}$$

This proves the first part of the lemma.

For the second part, we can assume that supp$v \subset \{x \in \mathbb{R}^n : |x| \leqslant R\}$ as we can localize to a compact set. We then write

$$\hat{v}(\xi) = \int_0^R (\mathrm{e}^{-\mathrm{i}x_1\xi_1}\mathcal{F}_{x'\mapsto\xi'}v(x_1,\xi') + \mathrm{e}^{\mathrm{i}x_1\xi_1}\mathcal{F}_{x'\mapsto\xi'}v(-x_1,\xi'))\,\mathrm{d}x_1. \tag{4.7}$$

Since $v \in H^1(\mathbb{R}^n)$, $\mathcal{F}_{x'\mapsto\xi'}v(0,\xi') \in L^2(\mathbb{R}^{n-1})$ is well defined and hence we can integrate by parts to obtain

$$\hat{v}(\xi) = \frac{1}{\xi_1^2}\sum_{\pm}\left(\mp\mathcal{F}_{x'\mapsto\xi'}\partial_{x_1}v(0\pm,\xi') - \int_0^R \mathrm{e}^{\mp\mathrm{i}x_1\xi_1}\mathcal{F}_{x'\mapsto\xi'}\partial_{x_1}^2 v(\pm x_1,\xi')\,\mathrm{d}x_1\right).$$

Since $v \in H^2(\mathbb{R}^n_{\pm})$, $\partial_{x_1}v(0\pm,\xi')$ is well defined in $L^2(\mathbb{R}^{n-1})$. We now use the following decomposition:

$$(1-\chi(h^2\xi^2))\hat{v} = \hat{v}_1 + \hat{v}_2, \qquad \hat{v}_1(\xi) \stackrel{\text{def}}{=} 1\!\!1_{|\xi_1|>c/h}(\xi)(1-\chi(h^2\xi^2))\hat{v}(\xi),$$

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:

$$\begin{aligned}\|v_2\restriction_Y\|^2_{L^2(Y)} &\leqslant C\int_{\mathbb{R}^n} G(\xi',h)|\hat{v}(\xi)|^2(1+|\xi'|^2)^2\,\mathrm{d}\xi \\ &\leqslant \max_{\xi'\in\mathbb{R}^{n-1}} G(\xi',h)\|v\|^2_{H^2(\widetilde{X}\setminus Y)},\end{aligned}$$

where

$$\begin{aligned}G(\xi',h) &\stackrel{\text{def}}{=} \int_{|\xi_1|<c/h}(1-\chi(h^2|\xi|^2))(1+|\xi'|^2)^{-2}\,\mathrm{d}\xi_1 \\ &\leqslant 1\!\!1_{|\xi'|>c/h}(\xi')\int_0^{2c/h}(1+|\xi'|^2)^{-2}\,\mathrm{d}\xi_1 \\ &\leqslant Ch^3,\end{aligned}$$

which is a better estimate than needed.

To estimate the contribution of v_1 we use (4.7):

$$\|v_1\restriction_Y\|^2_{L^2(Y)} \leqslant C_R\|v\|^2_{H^2(\widetilde{X}\setminus Y)}\left(\int_{|\xi_1|>1/h}\frac{1}{\xi_1^2}\,\mathrm{d}\xi_1\right)^2 \leqslant C_R h^2\|v\|^2_{H^2(\widetilde{X}\setminus Y)},$$

which completes the proof. □

Like H_{eff}, $H_{N,\Lambda} = H_{N,\Lambda}(k)$ is a well-defined operator for $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$.

Lemma 4.4. *Fix $\Lambda < \infty$, and suppose that $k^2 - H_{\infty,\Lambda}$ is invertible, $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$. Then, for N sufficiently large, $k^2 - H_{N,\Lambda}$ is invertible, and*

$$\|(k^2 - H_{\infty,\Lambda})^{-1} - (k^2 - H_{N,\Lambda})^{-1}\|_{H^{-1}(X_0)\to H^1(X_0)} \leqslant CN^{-1/4}.$$

The constant C can be chosen uniformly for k in a compact set $K \subset \Lambda_{\sigma(\Delta_{\partial X_0})}$ on which $k^2 - H_{\infty,\Lambda}$ 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

$$\begin{aligned}q_{\infty,\Lambda}(k,E)(u,v) &= \int_{X_0}\nabla u\overline{\nabla v} - \mathrm{i}\int_{\partial X_0} W^t_{\infty,\Lambda}u\overline{W^*_{\infty,\Lambda}v} - E\int_{X_0}u\bar{v} \\ &= \int_{X_0}\nabla u\overline{\nabla v} - \mathrm{i}\int_{\partial X_0} P_k\Pi_\Lambda^{\partial X_0}Ru\overline{P_k^*\Pi_\Lambda^{\partial X_0}Rv} - E\int_{X_0}u\bar{v}\end{aligned}$$

and

$$q_{N,\Lambda}(k,E)(u,v) = \int_{X_0} \nabla u \overline{\nabla v} - \mathrm{i}\int_{\partial X_0} W^t_{N,\Lambda} u \overline{W^*_{N,\Lambda} v} - E\int_{X_0} u\overline{v}$$
$$= \int_{X_0} \nabla u \overline{\nabla v} - \mathrm{i}\int_{\partial X_0} P_k \Pi^{\partial X_0}_\Lambda R \Pi^{\mathrm{in}}_N u \overline{P^*_k \Pi^{\partial X_0}_\Lambda R \Pi^{\mathrm{in}}_N v} - E\int_{X_0} u\overline{v}.$$

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:

$$q_{\infty,\Lambda}(k,E)(u,u) - q_{N,\Lambda}(k,E)(u,u)$$
$$= \int_{\partial X_0} \left(\left|P_k \Pi^{\partial X_0}_\Lambda R u\right|^2 - \left|P_k \Pi^{\partial X_0}_\Lambda R \Pi^{\mathrm{in}}_N u\right|^2 \right)$$
$$= \int_{\partial X_0} \left(\left(P_k \Pi^{\partial X_0}_\Lambda R u\right) \overline{P_k \Pi^{\partial X_0}_\Lambda R\left(I - \Pi^{\mathrm{in}}_N\right) u} + P_k \Pi^{\partial X_0}_\Lambda R\left(I - \Pi^{\mathrm{in}}_N\right) u \overline{P_k \Pi^{\partial X_0}_\Lambda R \Pi^{\mathrm{in}}_N u} \right).$$

We have the following estimates:

$$\begin{aligned} &\left\| \Pi^{\partial X_0}_\Lambda R\left(I - \Pi^{\mathrm{in}}_N\right) u \right\|_{H^\ell(\partial X_0)} \leqslant C_{\ell,\Lambda} \left\| R\left(I - \Pi^{\mathrm{in}}_N\right) u \right\|_{L^2(\partial X_0)} \leqslant C_{\ell,\Lambda} N^{-1/4} \|u\|_{H^1(X_0)} \\ &\left\| \Pi^{\partial X_0}_\Lambda R u \right\|_{H^\ell(\partial X_0)} \leqslant C_{\ell,\Lambda} \|Ru\|_{L^2(\partial X_0)} \leqslant C_{\ell,\Lambda} \|u\|_{H^1(X_0)}. \end{aligned} \tag{4.8}$$

To obtain the first, we apply lemma 4.3 to $\widetilde{X} \stackrel{\mathrm{def}}{=} X_0 \sqcup X_0^\circ$ 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

$$H^1(X_0) \simeq H^1_{\mathrm{ev}}(\widetilde{X})$$

(here ev refers to even functions) and the action of the Neumann Laplacian on X_0 is the same as the action of $\Delta_{\tilde{X}}$ 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 $E \ll 0$,

$$|q_{\infty,\Lambda}(k,E)(u,u) - q_{N,\Lambda}(k,E)(u,u)| \leqslant C_\Lambda(k) N^{-1/4} \|u\|^2_{H_1}$$
$$\leqslant C_\Lambda(k) N^{-1/4}\, \mathrm{Re}(q_{\infty,\Lambda}(k,E)(u,u)).$$

The constant depends continuously on k. Here we use the fact that $\mathrm{Im}\, k_\lambda > 0$ for all but finitely many λ, ensuring that $\mathrm{Re}\, q_{\infty,\Lambda}(k,E)(u,u)$ bounds $\|u\|^2_{H^1(X_0)}$ from above for $E \ll 0$. Thus, by [8, theorem 3.4],

$$\|(H_{\infty,\Lambda} - E)^{-1} - (H_{N,\Lambda} - E)^{-1}\|_{L^2(X_0)\to L^2(X_0)} \leqslant C N^{-1/4}$$

for N sufficiently large depending on E, k and Λ. 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

$$\begin{aligned} (A - z)^{-1} = &\{I - (I + (z - z_0)(B - z)^{-1})(z - z_0)((A - z_0)^{-1} - (B - z_0)^{-1})\}^{-1} \\ &\times (I + (z - z_0)(B - z)^{-1})(A - z_0)^{-1}. \end{aligned} \tag{4.9}$$

Consequently, if $k^2 - H_{\infty,\Lambda}$ is invertible, so is $k^2 - H_{N,\Lambda}$ for sufficiently large N, with

$$\|(k^2 - H_{\infty,\Lambda})^{-1} - (k^2 - H_{N,\Lambda})^{-1}\|_{L^2(X_0)\to L^2(X_0)} \leqslant C N^{-1/4}.$$

Here the constant will depend on k and Λ, as will the lower bound on the N for which this holds. These can be chosen uniformly if k is restricted to lie in 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 $\mathrm{Re}(q_{\infty,\Lambda}(k,E)(u,u)) \geqslant c_0\|u\|^2_{H^1(X_0)}$ for some $c_0 > 0$ and all $u \in H^1(X_0)$. Suppose $w \in L^2(X_0)$ and set $u = (H_{\infty,\Lambda} - E)^{-1}w$, $u_N = (H_{N,\Lambda} - E)^{-1}w$. Then

$$c_0\|u\|^2_{H^1} \leqslant \mathrm{Re}(q_{\infty,\Lambda}(k,E)(u,u)) = \mathrm{Re}(w,u)$$

so that

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

This shows that we can (uniquely) continuously extend $(H_{\infty,\Lambda} - E)^{-1}$ 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,

$$\begin{aligned} c_0\|u-u_N\|^2_{H^1} &\leqslant \mathrm{Re}(q_{\infty,\Lambda}(k,E)(u-u_N,u-u_N)) \\ &= \mathrm{Re}(q_{\infty,\Lambda}(k,E)(u,u-u_N) - q_{\infty,\Lambda}(k,E)(u_N,u-u_N)) \\ &= \mathrm{Re}((w,u-u_N) - (w,u-u_N) \\ &\quad + q_{N,\Lambda}(k,E)(u_N,u-u_N) - q_{\infty,\Lambda}(k,E)(u_N,u-u_N)) \\ &\leqslant CN^{-1/4}\|u_N\|_{H^1}\|u-u_N\|_{H^1} \\ &\leqslant CN^{-1/4}(\|u\|_{H^1} + \|u-u_N\|_{H^1})\|u-u_N\|_{H^1}. \end{aligned}$$

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

$$\|u-u_N\|_{H^1} \leqslant CN^{-1/4}(\|u\|_{H^1} + \|u-u_N\|_{H^1}),$$

which then means that for sufficiently large N

$$\|u-u_N\|_{H^1} \leqslant CN^{-1/4}\|u\|_{H^1}.$$

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

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

$$\left\|\Pi_\Lambda^{\partial X_0} P_k^{-1}(S_{f,\infty,\Lambda}(k) - S_{f,N,\Lambda}(k))P_k f\right\| \leqslant CN^{-1/2}\|f\|_{L^2(\partial X_0)}.$$

The constant C can be chosen independently of k, if k is restricted to a compact set $K \subset \Lambda_{\sigma(\Delta_{\partial X_0})}$ on which $k^2 - H_{\infty,\Lambda}$ and $k^2 - H_{N,\Lambda}$ are invertible.

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

$$u_\infty = (k^2 - H_{\infty,\Lambda})^{-1}W_{\infty,\Lambda}P_k f \qquad \text{and} \qquad u_N = (k^2 - H_{N,\Lambda})^{-1}W_{N,\Lambda}P_k f.$$

That is, u_∞ satisfies

$$\begin{aligned} &\left(k^2 + \Delta_{X_0}\right)u_\infty = 0 \quad \text{on } X_0^\circ \\ &\partial_n u_\infty - \mathrm{i}P_k^2\Pi_\Lambda^{\partial X_0}Ru_\infty = -P_k^2 f \end{aligned}$$

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

$$\begin{aligned} &\left(k^2 + \Delta_{X_0} + \mathrm{i}W_{N,\Lambda}W_{N,\Lambda}^t\right)u_N = W_{N,\Lambda}P_k f \quad \text{on } X_0^\circ \\ &\partial_n u_N\restriction_{\partial X_0} = 0. \end{aligned}$$

Note that our assumptions on f mean that the $H^{3/2}$ norm of f is bounded by a Λ-dependent constant times the L^2 norm of f.

We wish to understand $\Pi_N^{\mathrm{in}} u_\infty$. Let Ψ_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

$$\begin{aligned}\left(\tau_n^2 - k^2\right)(u_\infty, \Psi_n)_{L^2(X_0)} &= -\int_{X_0} (\Delta_{X_0}\Psi_n u_\infty - \Psi_n \Delta_{X_0} u_\infty)\, \mathrm{dvol}_{X_0} \\ &= \int_{\partial X_0} \Psi_n \partial_n u_\infty \, \mathrm{dvol}_Y \\ &= \int_{\partial X_0} \Psi_n \left(\mathrm{i} P_k^2 \Pi_\Lambda^{\partial X_0} R u_\infty - P_k^2 f\right) \mathrm{dvol}_Y .\end{aligned}$$

That is,

$$\left(-\Delta_{X_0} - k^2\right)\Pi_N^{\mathrm{in}} u_\infty = \mathrm{i} W_{N,\Lambda} W_{\infty,\Lambda}^t u_\infty - W_{N,\Lambda} P_k f.$$

Thus,

$$\begin{aligned} u_N &= \Pi_N^{\mathrm{in}} u_\infty - (k^2 - H_{N,\Lambda})^{-1}\left((k^2 - H_{N,\Lambda})\Pi_N^{\mathrm{in}} u_\infty - W_{N,\Lambda} P_k f\right) \\ &= \Pi_N^{\mathrm{in}} u_\infty + \mathrm{i}(k^2 - H_{N,\Lambda})^{-1} W_{N,\Lambda}\left(W_{\infty,\Lambda}^t - W_{N,\Lambda}^t\right) u_\infty \\ &= \Pi_N^{\mathrm{in}} u_\infty + \mathrm{i}(k^2 - H_{N,\Lambda})^{-1} W_{N,\Lambda} P_k \Pi_\Lambda^{\partial X_0} R\left(I - \Pi_N^{\mathrm{in}}\right) u_\infty . \end{aligned} \tag{4.10}$$

The second part of lemma 4.3 gives the following estimate:

$$\left\| R\left(1 - \Pi_N^{\mathrm{in}}\right) u_\infty \right\|_{L^2(\partial X)} \leqslant C N^{-1/2} \|u_\infty\|_{H^2(X_0)},$$

and consequently,

$$\left\| P_k \Pi_\Lambda^{\partial X_0} R\left(I - \Pi_N^{\mathrm{in}}\right) u_\infty \right\| \leqslant C N^{-1/2} \|u_\infty\|_{H^2(X_0)}$$

with constant C depending continuously on k.

Let $g \in L^2(\partial X_0)$, $h \in H^{1/2+}(X_0)$. Then $Rh \in L^2(\partial X_0)$, and

$$|(W_{N,\Lambda} g, h)_{X_0}| = \left|\left(g, P_k^* \Pi_\Lambda^{\partial X_0} R \Pi_N^{\mathrm{in}} h\right)_{\partial X_0}\right| \leqslant \|g\|_{L^2(\partial X_0)} \|h\|_{H^{1/2+}(X_0)}.$$

That is,

$$\|W_{N,\Lambda} g\|_{H^{-1}(X_0)} \leqslant \|W_{N,\Lambda} g\|_{H^{-1/2-}(X_0)} \leqslant C \|g\|_{L^2(X_0)}$$

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

$$\|(k^2 - H_{N,\Lambda})^{-1}\|_{H^{-1}(X_0)\to H^1(X_0)} \leqslant C.$$

Using these estimates in (4.10), we find that

$$\|u_\infty - u_N\|_{H^1} \leqslant C N^{-1/2},$$

implying the desired bound by restricting to ∂X_0 and using again the fact that $P_k^{-1} P_k \Pi_\Lambda^{\partial X_0} = \Pi_\Lambda^{\partial X_0}$ is a bounded operator. □

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 Π_N^{in} and $\Pi_\Lambda^{\partial X_0}$.

Lemma 5.1. *Let $k \in \mathbb{R}$. Then $S(k)$ defined by (1.7) and $\Pi_{k^2}^{\partial X_0} S_{f,N,\Lambda}(k) \Pi_{k^2}^{\partial X_0}$, for $\Lambda, N \in \mathbb{R}_+ \cup \{\infty\}$, are unitary.*

Proof. That $S(k)$ is unitary for k real is well known. It can be seen as follows. Recall that $S(k) = \Pi_{k^2}^{\partial X_0} S_{f,\infty,\infty}(k) \Pi_{k^2}^{\partial X_0}$.

We note that $\left(P_k^2\right)^* \varphi_\lambda = \overline{k_\lambda} \varphi_\lambda$ and k_λ is real for $\sigma_\lambda^2 \leqslant k^2$ and pure imaginary for $\sigma_\lambda^2 > k^2$. Therefore,

$$\Pi_{k^2}^{\partial X_0} W^t(k) = \Pi_{k^2}^{\partial X_0} W^*(k) \qquad \text{and} \qquad \left(I - \Pi_{k^2}^{\partial X_0}\right) W^t(k) = -\left(I - \Pi_{k^2}^{\partial X_0}\right) W^*(k). \tag{5.1}$$

Thus, we have

$$W(k)^{t*} \Pi_\Lambda^{\partial X_0} W^*(k) + W(k) \Pi_\Lambda^{\partial X_0} W^t(k) = 2 W(k) \Pi_\Lambda^{\partial X_0} \Pi_{k^2}^{\partial X_0} W^t(k). \tag{5.2}$$

Using this and the resolvent identity gives

$$\begin{aligned}
&(k^2 - H_{N,\Lambda})^{-1} - (k^2 - H_{N,\Lambda}^*)^{-1} \\
&\quad = \mathrm{i}(k^2 - H_{N,\Lambda})^{-1}\left(-\Pi_N^{\mathrm{in}} W^{t*} \Pi_\Lambda^{\partial X_0} W^* \Pi_N^{\mathrm{in}} - \Pi_N^{\mathrm{in}} W \Pi_\Lambda^{\partial X_0} W^t \Pi_N^{\mathrm{in}}\right)(k^2 - H_{N,\Lambda}^*)^{-1} \\
&\quad = -2\mathrm{i}(k^2 - H_{N,\Lambda})^{-1} \Pi_N^{\mathrm{in}} W \Pi_{k^2}^{\partial X_0} \Pi_\Lambda^{\partial X_0} W^t \Pi_N^{\mathrm{in}} (k^2 - H_{N,\Lambda}^*)^{-1}.
\end{aligned} \tag{5.3}$$

Therefore,

$$\begin{aligned}
&\Pi_{k^2}^{\partial X_0} S_{f,N,\Lambda}(k) \Pi_{k^2}^{\partial X_0} \left(\Pi_{k^2}^{\partial X_0} S_{f,N,\Lambda}(k) \Pi_{k^2}^{\partial X_0}\right)^* \\
&\quad = \Pi_{k^2}^{\partial X_0}\left(I - 2\mathrm{i} W_{N,\Lambda}^t(k)(k^2 - H_{N,\Lambda})^{-1} W_{N,\Lambda}(k)\right) \\
&\qquad \times \Pi_{k^2}^{\partial X_0}\left(I + 2\mathrm{i} W_{N,\Lambda}^*(k)((k^2 - H_{N,\Lambda})^{-1})^* \left(W_{N\lambda}^t(k)\right)^*\right) \Pi_{k^2}^{\partial X_0} \\
&\quad = \Pi_{k^2}^{\partial X_0}\left(I - 2\mathrm{i} W_{N,\Lambda}^t(k)\left[(k^2 - H_{N,\Lambda})^{-1} - (k^2 - H_{N,\Lambda}^*)^{-1}\right] W_{N,\Lambda}(k)\right. \\
&\qquad \left. + 4 W_{N,\Lambda}^t (k^2 - H_{N,\Lambda})^{-1} W_{N,\Lambda} \Pi_{k^2}^{\partial X_0} W_{N,\Lambda}^t(k)(k^2 - H_{N,\Lambda}^*)^{-1} W_{N,\Lambda}(k)\right) \Pi_{k^2}^{\partial X_0}
\end{aligned} \tag{5.4}$$

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

$$\Pi_{k^2}^{\partial X_0} S_{f,N,\Lambda}(k) \Pi_{k^2}^{\partial X_0} \left(\Pi_{k^2}^{\partial X_0} S_{f,N,\Lambda}(k) \Pi_{k^2}^{\partial X_0}\right)^* = I \tag{5.5}$$

as desired. □

Theorem 2. *Let X be a manifold with infinite cylindrical ends, and $S_{\lambda\lambda'}(k)$, $S_{f,N,\Lambda}(k)$ be as defined via (2.1), (2.2) and (4.1). Suppose $k \in \Lambda_{\sigma(\Delta_{\partial X_0})}$ and $\Lambda_0 \in \mathbb{R}$ are such that $k^2 - H_{\mathrm{eff}} = k^2 - H_{\mathrm{eff}}(k)$ is invertible, and $\operatorname{Im} k_\lambda > 0$ if $\sigma_\lambda^2 > \Lambda_0$. Then, for σ_λ^2, $\sigma_{\lambda'}^2 \leqslant \Lambda_0$ and $\Lambda \geqslant \Lambda_0$,*

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

We recall that $k^2 - H_{\mathrm{eff}}$ is invertible if k is in the physical space with $\operatorname{Im} k > 0$, $\operatorname{Im} k_\lambda > 0$ for all λ, and that $(k^2 - H_{\mathrm{eff}})^{-1}$ is meromorphic on $\Lambda_{\sigma(\Delta_{\partial X_0})}$.

Proof. The proof follows from writing

$$\begin{aligned}
\frac{\sqrt{k_{\lambda'}}}{\sqrt{k_\lambda}} S_{\lambda\lambda'}(k) &= \left\langle P_k^{-1} S_f(k) P_k \varphi_{\lambda'}, \varphi_\lambda \right\rangle \\
&= \left\langle P_k^{-1} S_{f,N,\Lambda}(k) P_k \varphi_{\lambda'}, \varphi_\lambda \right\rangle + \left\langle P_k^{-1}(S_f(k) - S_{f,\infty,\Lambda}(k)) P_k \varphi_{\lambda'}, \varphi_\lambda \right\rangle \\
&\quad + \left\langle P_k^{-1}(S_{f,\infty,\Lambda}(k) - S_{f,N,\Lambda}(k)) P_k \varphi_{\lambda'}, \varphi_\lambda \right\rangle,
\end{aligned} \tag{5.6}$$

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

We now prove theorem 1.

Proof. If $k^2 - H_{\rm eff}$ 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 $k^2 - H_{\rm eff}$ is not invertible.

Using the unitarity proved in lemma 5.1, along with the fact that $\sigma_{\lambda'}^2 \leqslant k^2, \sigma_\lambda^2 \leqslant k^2$, 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 $N,\ \Lambda \in \mathbb{R}_+ \cup \{\infty\}$ $(\sqrt{k_{\lambda'}}/\sqrt{k_\lambda})\langle S_{f,N,\Lambda}(k)\varphi_\lambda, \varphi_{\lambda'}\rangle$ has a meromorphic extension to $\Lambda_{\sigma(\Delta_{\partial X_0})}$, as can be seen from formula (4.1) and the fact that $(k^2 - H_{N,\Lambda})^{-1}$ continues meromorphically to $\Lambda_{\sigma(\Delta_{\partial X_0})}$. Hence

$$k \in (-\sigma_\lambda, \sigma_\lambda) \cap (-\sigma_{\lambda'}, \sigma_{\lambda'})$$

has a neighborhood in $\Lambda_{\sigma(\Delta_{\partial X_0})}$ on which $\langle S_{f,N,\Lambda}\varphi_{\lambda'}, \varphi_\lambda\rangle$ is holomorphic, $N, \Lambda \in \mathbb{R}_+ \sqcup \{\infty\}$.

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

$$S_{\lambda\lambda'} - \langle S_{f,N,\Lambda}\varphi_{\lambda'}, \varphi_\lambda\rangle$$

is bounded by $C(N^{-\frac{1}{2}} + \mathrm{e}^{-\Lambda/C})$ on the boundary of the neighborhood chosen above, since $(k^2 - H_{\rm eff})^{-1}$ 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 $(k^2 - H_{\rm eff})^{-1}$, as long as $k^2 \neq \sigma_\lambda^2, \sigma_{\lambda'}^2$.

To finish the proof, consider what happens at a point $k_0 \in \mathbb{R}, k_0^2 = \sigma_\lambda^2 \geqslant \sigma_{\lambda'}^2$. (The case $\sigma_\lambda^2 < \sigma_{\lambda'}^2$ follows by symmetry.) If $\sigma_\lambda^2 = \sigma_{\lambda'}^2$, then since $\sqrt{k_{\lambda'}}/\sqrt{k_\lambda} = 1$ (except for the removeable singularity at $k_\lambda = 0$), $\langle S_{f,N,\Lambda}(k)\varphi_{\lambda'}, \varphi_\lambda\rangle$ has a meromorphic extension to a neighborhood of k_0 in $\Lambda_{\sigma(\Delta_{\partial X_0})}$. The boundedness at k_0, again obtained from unitarity, ensures that there exists a neighborhood of k_0 on which $\langle S_{f,N,\Lambda}\varphi_{\lambda'}, \varphi_\lambda\rangle$ is holomorphic. Thus the previous argument using the maximum principle holds here as well.

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

$$|T_{\lambda\lambda'}(k)|^2 \leqslant |k_{\lambda'}||k_\lambda|^{-1} \quad \text{for } k^2 \geqslant \sigma_{\lambda^2}, \qquad k \in \mathbb{R}.$$

Thus, $\sqrt{k_\lambda}T_{\lambda\lambda'}(k)$ 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_λ. 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

$$\langle S_{f,N,\Lambda}(k)\varphi_{\lambda'}, \varphi_\lambda\rangle\restriction_{k=k_0} = 0 \qquad \text{for} \quad \sigma_{\lambda'}^2 < \sigma_\lambda^2 = k_0^2, \qquad N, \Lambda \in \mathbb{R}_+ \cup \{\infty\}.$$

Thus the approximation is exact in this special case. □

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 $\Pi_N^{\rm in}$ 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 ($\overline{X}$ has a boundary, $\{-\pi\}$), it is easy to see the arguments of the previous sections follow-through, with ∂X_0 replaced by $Y = \{0\}$. Because Y is a point, the full scattering matrix is a scalar, and is easily computed to be $S(k) = \mathrm{e}^{2\pi \mathrm{i}k}$.

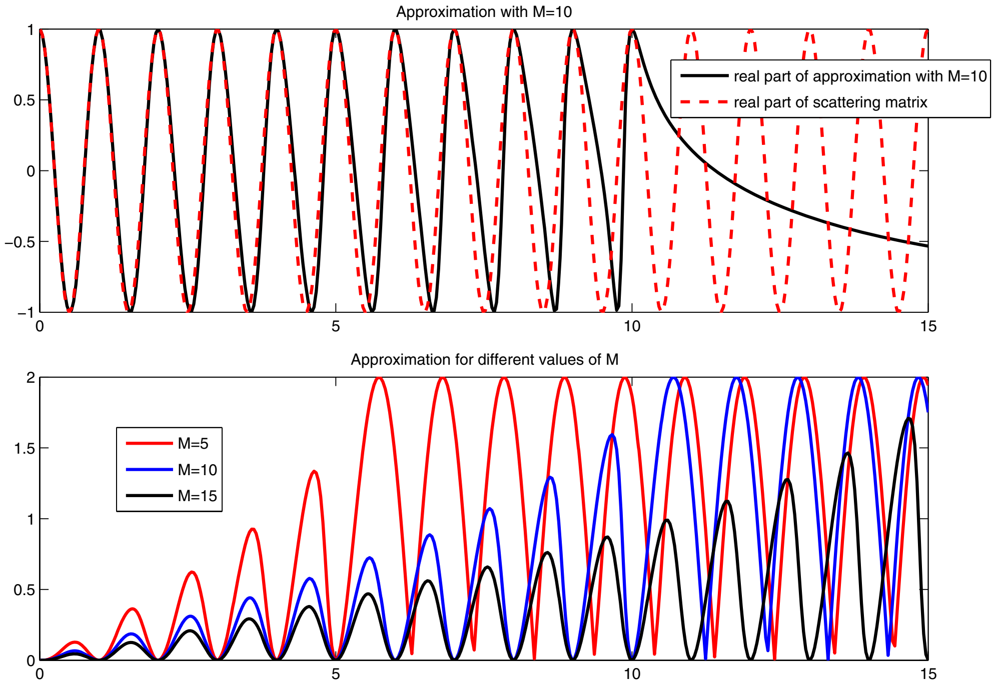

Figure 2. An illustration of the example in section 6: the top figure shows the real parts of the approximation and of the scattering matrix, and the lower one, the graphs of $|S_{M^2}(k) - S(k)|$ for different values of M.

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

For this example,

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

Since there is no sense in the cut-off $\Pi_\Lambda^{\partial X_0}$ for this problem, we use only one subscript on our approximations of W:

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

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 $\widetilde{W}_{M^2} = \widetilde{W}_{M^2}(k)$ the $M+1$ vector $\pi^{-1/2}(1, \sqrt{2}, \ldots, \sqrt{2})^t$.

Note that if $\mathrm{i}a^t a \neq -1$,

$$(I + \mathrm{i}aa^t)^{-1} = I - \mathrm{i}(1 + \mathrm{i}a^t a)^{-1}aa^t.$$

Set $D_{M^2} = D_{M^2}(k)$ to be the $M+1 \times M+1$ matrix given by $((k^2 - n^2)\delta_{nm})$. We see that when $k \notin \mathbb{Z}$ so that $D_{M^2}(k)$ is invertible, the approximation $S_{M^2}(k)$ is given by

$$\begin{aligned} S_{M^2}(k) &= -1 + 2\mathrm{i}\widetilde{W}_{M^2}^t\left(D_{M^2} + \mathrm{i}\widetilde{W}_{M^2}\widetilde{W}_{M^2}^t\right)^{-1}\widetilde{W}_{M^2} \\ &= -1 + 2\mathrm{i}\left(D_{M^2}^{-1/2}\widetilde{W}_{M^2}\right)^t\left(I + \mathrm{i}D_{M^2}^{-1/2}\widetilde{W}_{M^2}\left(D_{M^2}^{-1/2}\widetilde{W}_{M^2}\right)^t\right)^{-1}D_{M^2}^{-1/2}\widetilde{W}_{M^2}. \end{aligned}$$

Set $B_{M^2} = D_{M^2}^{-1/2}\widetilde{W}_{M^2}$ and $\beta_{M^2} = B_{M^2}^t B_{M^2}$. Then, for $k \notin \mathbb{Z}$,

$$S_{M^2}(k) = -1 + 2\mathrm{i}B_{M^2}^t\left(I - \mathrm{i}(1+\mathrm{i}\beta_{M^2})^{-1}B_{M^2}B_{M^2}^t\right)B_{M^2}$$
$$= -1 + 2\mathrm{i}\left(\beta_{M^2} - \mathrm{i}\frac{\beta_{M^2}^2}{1+i\beta_{M^2}}\right). \tag{6.1}$$

Now

$$\beta_{M^2} = \frac{1}{\pi}\left(\frac{1}{k} + \sum_{n=1}^{M}\frac{2k}{k^2-n^2}\right). \tag{6.2}$$

We note that

$$\lim_{M\to\infty}\beta_{M^2} = \cot\pi k;$$

one can use this and (6.1) to see that

$$\lim_{M\to\infty}S_{M^2}(k) = \mathrm{e}^{2\pi\mathrm{i}k} = S(k)$$

when $k^2 \notin \mathbb{N}_0$. Using (6.1) and (6.2), we see that for $k \in \mathbb{R}\backslash\mathbb{Z}$ and $M > |k|$,

$$C_1/M \leqslant |S_{M^2}(k) - S(k)| \leqslant C_2/M$$

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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