

DETERMINING TRANSMISSION EIGENVALUES OF ANISOTROPIC INHOMOGENEOUS MEDIA FROM FAR FIELD DATA*

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Abstract. We characterize the interior transmission eigenvalues of penetrable anisotropic acoustic scattering objects by a technique known as inside-outside duality. This method has recently been identified to be able to link interior eigenvalues of the penetrable scatterer with the behavior of the eigenvalues of the far field operator for the corresponding exterior time-harmonic scattering problem. A basic ingredient for the resulting connection is a suitable self-adjoint factorization of the far field operator based on wave number-dependent function spaces. Under certain conditions on the anisotropic material coefficients of the scatterer, inside-outside duality allows us to rigorously characterize interior transmission eigenvalues from multi-frequency far field data. This theoretical characterization moreover allows us to derive a simple numerical algorithm for the approximation of interior transmission eigenvalues. Since it is merely based on far field data, the resulting eigenvalue solver does not require knowledge of the scatterer or its material coefficient; several numerical examples show its feasibility and accuracy for noisy data.

Key words. Inside-outside duality, transmission eigenvalues, anisotropic scattering.

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1. Introduction

Interior transmission eigenvalues provide information about material properties of penetrable scattering objects that is particularly useful for the characterization of such objects from time-harmonic wave measurements. For example, it is known that unique determination of anisotropic inhomogeneous media from far field data fails for multi-static and multi-frequency far field measurements; see [12, 1]. However, as shown in [3, 7], interior transmission eigenvalues provide upper and lower bounds on the norm of the matrix-valued material parameter, thus yielding helpful structural side constraints for methods in non-destructive testing.

Establishing bounds on the material parameters of isotropic or anisotropic inhomogeneous media has recently motivated the development of numerical algorithms for the computation of transmission eigenvalues from far field data; see [3, 7, 4]. All these analytic bounds and numerical techniques were inspired by ideas from [5] where the first (lower) bounds on the index of refraction were obtained from the knowledge of the first transmission eigenvalue and the failure of the linear sampling method [2, 6] at transmission eigenvalues was used to detect these interior eigenvalues. Taking a more general viewpoint, the above-mentioned papers show the currently rising interest in the application of interior transmission eigenvalues for non-destructive testing and, more generally, in inverse scattering theory.

A technique able to compute interior transmission eigenvalues for isotropic acoustic scatterers that is completely different from the one mentioned above was introduced in [15]. The latter reference relies on ideas from the work [10] on the so-called inside-outside duality between the Dirichlet eigenvalue problem inside a bounded domain and the exterior scattering problem outside of this domain. To indicate the statement of

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this duality, recall first that for a fixed wave number $k > 0$ the eigenvalues of the far field operator $F = F_k$ lie on a circle in the complex plane and accumulate at zero from the left, that is, only a finite number of eigenvalues of F_k have positive real part. Now, inside-outside duality between the interior and the exterior problem can roughly be stated as follows. The number k_0^2 is an interior Dirichlet eigenvalue of $-\Delta$ if and only if one of the eigenvalues of F_k tends to zero from the right as the wave number $k > 0$ tends to k_0 . As is shown in [10, 19], this duality provides a full characterization of interior Dirichlet, Neumann, and Robin eigenvalues by far field data from the eigenvalues of the corresponding far field operators for a continuum of wave numbers. Moreover it allows the designing of a numerical algorithm with provable convergence, see [13].

In this paper, we establish a corresponding connection for the case of a penetrable anisotropic acoustic scattering object $D \subset \mathbb{R}^3$ which is described by the following time-harmonic wave equation at the wave number $k > 0$:

$$\operatorname{div}(A\nabla u) + k^2 u = 0 \quad \text{in } \mathbb{R}^3, \quad (1.1)$$

where the material parameter $A = \operatorname{Id} + Q$ is assumed to be real-valued, symmetric, and positive definite in \mathbb{R}^3 and the matrix-valued contrast $Q: \mathbb{R}^3 \rightarrow \mathbb{R}^{3 \times 3}$ is supported and sign-definite in the closure of the scatterer D . On the boundary ∂D , u , and its co-normal derivative are continuous. If ν and $[\cdot]_{\partial D}$ denote the exterior unit normal to D and the jump of a function across ∂D , respectively, then

$$[u]_{\partial D} = 0 \quad \text{and} \quad [\nu^\top A \nabla u]_{\partial D} = 0.$$

For the scattering model (1.1), the squared wave number $k^2 > 0$ is called a transmission eigenvalue if there exists a non-trivial pair (u, w) of functions defined in D such that

$$\operatorname{div}(A\nabla u) + k^2 u = 0 \quad \text{in } D, \quad \Delta w + k^2 w = 0 \quad \text{in } D, \quad (1.2)$$

$$u = w \quad \text{on } \partial D, \quad \nu^\top A \nabla u = \frac{\partial w}{\partial \nu} \quad \text{on } \partial D. \quad (1.3)$$

Links between this quadratic, non-self-adjoint eigenvalue problem to scattering theory are well-described (see for instance [8]). For example, if w is an incident field wave such that the resulting scattered wave vanishes outside D , then restricting both the corresponding total field u and the incident field w to D yields a transmission eigenpair for the eigenvalue k^2 .

Connecting the interior transmission eigenvalue problem (1.2) with the far field operators corresponding to (1.1) for varying $k > 0$ heavily relies on a suitable factorization $F = H^* T H$ of the far field operator F . Note that the same factorization also forms the basis of the so-called factorization method; see [14]. A crucial requirement for the proof of inside-outside duality is the density of the image space of H in the preimage space of T . For impenetrable scatterers, this condition is naturally satisfied and the corresponding trace spaces $H^{\pm 1/2}$ are independent of the wave number. For scattering from a penetrable anisotropic object $D \subset \mathbb{R}^3$, the ‘‘simplest’’ image and preimage space of H and T is $L^2(D, \mathbb{C}^3)$, and the middle space of the factorization can indeed be used, e.g., for the analysis of the factorization method. However, in our context, the range of H is not dense in $L^2(D, \mathbb{C}^3)$ and has to be replaced by the closure of this range in $L^2(D, \mathbb{C}^3)$, a k -dependent vector-valued space of gradient fields solving the Helmholtz equation.

The k -dependent middle space complicates the analysis of inside-outside duality for interior transmission eigenvalues compared to eigenvalues of impenetrable obstacles.

Under the general assumption that the contrast Q is sign-definite, it is nevertheless still possible to show that whenever an eigenvalue of the far field operator tends to zero from the “wrong” side as k tends to k_0 , then k_0^2 must be an interior transmission eigenvalue. The price to pay for the (currently necessary) k -dependent middle spaces is that the converse direction (and hence the characterization) can only be shown under assumptions on the contrast. We prove the complete characterization of the first few interior transmission eigenvalues by using the behavior of the eigenvalues of the far field operator for contrasts Q that are perturbations of a sufficiently large scalar constant times the identity matrix. Note that the corresponding conditions for the scalar, isotropic Helmholtz equation $\Delta u + k^2 n^2 u = 0$ considered in [15] required the contrast to be constant and either small or large enough. Extending the results from this paper to the Helmholtz equation, $\operatorname{div}(A\nabla u) + k^2 n^2 u = 0$, involving two material parameters is possible but is out of the scope of this paper.

Let us now briefly indicate the precise statement of inside-outside duality for transmission eigenvalues. To this end, consider incident plane waves $u^i(\mathbf{x}, \boldsymbol{\theta}) = \exp(ik\boldsymbol{\theta} \cdot \mathbf{x})$ with direction $\boldsymbol{\theta} \in \mathbb{S}^2 = \{\mathbf{x} \in \mathbb{R}^3, |\mathbf{x}| = 1\}$, and a solution $u(\cdot, \boldsymbol{\theta})$ to the anisotropic Helmholtz Equation (1.1) subject to Sommerfeld’s radiation condition for the scattered field $u^s(\cdot, \boldsymbol{\theta}) = u(\cdot, \boldsymbol{\theta}) - u^i(\cdot, \boldsymbol{\theta})$,

$$\frac{\partial u^s}{\partial r}(r\hat{\mathbf{x}}, \boldsymbol{\theta}) - ik u^s(r\hat{\mathbf{x}}, \boldsymbol{\theta}) = \mathcal{O}(r^{-2}) \quad \text{as } r \rightarrow \infty, \text{ uniformly in } \hat{\mathbf{x}} \in \mathbb{S}^2. \tag{1.4}$$

Solutions to the Helmholtz equation outside D that satisfy (1.4) are called radiating and possess a first-order expansion in terms of radiating spherical waves,

$$u^s(r\hat{\mathbf{x}}, \boldsymbol{\theta}) = \frac{e^{ikr}}{4\pi r} u^\infty(\hat{\mathbf{x}}, \boldsymbol{\theta}) + \mathcal{O}(r^{-2}), \quad r \rightarrow \infty.$$

The function $u^\infty : \mathbb{S}^2 \times \mathbb{S}^2 \rightarrow \mathbb{C}$ in the latter asymptotic expansion is called the far field pattern of the scattered fields. It gives rise to the far field operator $F : L^2(\mathbb{S}^2) \rightarrow L^2(\mathbb{S}^2)$,

$$(Fg)(\hat{\mathbf{x}}) := \int_{\mathbb{S}^2} u^\infty(\hat{\mathbf{x}}, \boldsymbol{\theta}) g(\boldsymbol{\theta}) \, dS(\boldsymbol{\theta}), \quad \hat{\mathbf{x}} \in \mathbb{S}^2,$$

which is compact and normal according to [16]. Furthermore, the eigenvalues λ_j of F lie on the circle of radius $8\pi^2/k$ with center $8\pi^2 i/k$ in the complex plane. Depending on the sign of the contrast function $Q = A - \operatorname{Id}$, the eigenvalues $\lambda_j = \lambda_j(k)$ converge to zero, either from the left or from the right, as $j \rightarrow \infty$ such that $\operatorname{Re} \lambda_j \geq 0$ for j large enough. This allows us to order the phases of the λ_j and to define a smallest or a largest phase. For instance, if $\operatorname{Re} \lambda_j < 0$ for large $j \in \mathbb{N}$, then the smallest phase $\vartheta_* = \min_{j \in \mathbb{N}} \vartheta_j$ of the eigenvalues $\lambda_j = r_j \exp(i\vartheta_j)$, $\vartheta_j \in [0, \pi)$, is well-defined. The aim of this paper is to characterize transmission eigenvalues by the behavior of the smallest and largest phase respectively. Under conditions to be stated below, we will show, e.g., that certain transmission eigenvalues $k_0^2 > 0$ are characterized by the fact that the smallest phase $\vartheta_* = \vartheta_*(k)$ of $F = F_k$ tends to 0 as k tends to k_0 in case that Q is positive definite. Additionally, if $\vartheta_*(k)$ tends to zero as k tends to k_0 , then $k_0^2 > 0$ is a transmission eigenvalue.

We finally note that the transmission eigenvalue problem (1.2) has to be understood in a weak sense: $k^2 > 0$ is an interior transmission eigenvalue if there exists a non-trivial eigenpair $(u, w) \in H^1(D) \times H^1(D)$ such that $u - w \in H_0^1(D)$ and

$$\int_D (A\nabla u \cdot \nabla \bar{\psi} - k^2 u \bar{\psi}) \, d\mathbf{x} = 0, \quad \int_D (\nabla w \cdot \nabla \bar{\psi} - k^2 w \bar{\psi}) \, d\mathbf{x} = 0 \quad \forall \psi \in H_0^1(D),$$

$$\int_D (A\nabla u \cdot \nabla \bar{\psi} - k^2 u \bar{\psi}) \, d\mathbf{x} = \int_D (\nabla w \cdot \nabla \bar{\psi} - k^2 w \bar{\psi}) \, d\mathbf{x} \quad \forall \psi \in H^1(D). \quad (1.5)$$

The remainder of the paper is organized as follows. In Section 2, we introduce a factorization of the far field operator and provide several crucial properties of the operators arising in this factorization. In Section 3, we show important properties of the eigenvalues of the far field operator and their phases. These properties will be exploited in Section 4 when considering the behavior of the smallest or largest phase when the square of the corresponding wave number is close to a transmission eigenvalue. In sections 5 and 6, we finally prove a characterization of transmission eigenvalues under the condition that a certain derivative is nonzero. This implicit condition is then transformed into an explicit condition on the contrast and the transmission eigenvalue. Relying on three computational examples, we finally show in Section 7 that inside-outside duality can be exploited for the numerical computation of interior eigenvalues.

2. A particular factorization of the far field operator

In this section, we prove a factorization for the far field operator F and examine the properties of the arising operators. The factorization will be similar to the one derived in [16]. However, we need to slightly adapt the factorization to suit the particular requirements of our later theory.

We assume throughout the paper that $D \subset \mathbb{R}^3$ is a bounded Lipschitz domain and that $Q \in L^\infty(D, \mathbb{R}^{3 \times 3})$ takes (almost everywhere) values in the space of symmetric 3×3 matrices. Moreover, denoting $\mathbf{z}^* = \bar{\mathbf{z}}^\top$, we assume for all $\mathbf{z} \in \mathbb{C}^3$ and almost all $\mathbf{x} \in D$ that either $\mathbf{z}^* Q(\mathbf{x}) \mathbf{z} \geq q_0 |\mathbf{z}|^2$ for some $q_0 > 0$, or that $\mathbf{z}^* Q(\mathbf{x}) \mathbf{z} \leq q_0 |\mathbf{z}|^2$ for $-1 < q_0 < 0$. In the first and second case, Q is positive and negative definite, respectively, and extending Q by zero to all of \mathbb{R}^3 , the material parameter $A = \text{Id} + Q$ is always positive definite.

Defining a source term $\mathbf{f} = Q \nabla u^i \in L^2(D, \mathbb{C}^3)$ allows to write the weak formulation of the differential equation (1.1) for the radiating scattered field $u^s \in H_{\text{loc}}^1(\mathbb{R}^3)$ as

$$\int_{\mathbb{R}^3} (A \nabla u^s \cdot \nabla \psi - k^2 u^s \psi) \, d\mathbf{x} = - \int_D \mathbf{f} \cdot \nabla \psi \, d\mathbf{x} \quad \forall \psi \in C_0^\infty(\mathbb{R}^3). \quad (2.1)$$

Using either a volume integral equation approach or a variational formulation on a bounded domain involving an exterior Dirichlet-to-Neumann operator [16, 22], one shows that the latter problem is of Fredholm type. More precisely, that the uniqueness of the solution implies the existence of the solution for all source terms $\mathbf{f} \in L^2(D, \mathbb{C}^3)$. We assume in the following that uniqueness of the solution to (2.1) holds. This assumption is satisfied if A is a sufficiently smooth function on \mathbb{R}^3 or if A is piecewise smooth with sufficiently regular jump discontinuities such that a unique continuation principle holds (for details see, e.g., [23]).

To factorize F , we define the injective Herglotz operator $H = H_k : L^2(\mathbb{S}^2) \rightarrow L^2(D, \mathbb{C}^3)$,

$$Hg = \nabla v_g, \quad v_g(\mathbf{x}) = \int_{\mathbb{S}^2} g(\boldsymbol{\theta}) e^{ik\boldsymbol{\theta} \cdot \mathbf{x}} \, dS(\boldsymbol{\theta}), \quad \mathbf{x} \in D. \quad (2.2)$$

The function v_g (extended using its defining integral to all of \mathbb{R}^3) is called a Herglotz wave function. The adjoint $H^* : L^2(D, \mathbb{C}^3) \rightarrow L^2(\mathbb{S}^2)$ of the Herglotz operator is

$$(H^* \mathbf{h})(\hat{\mathbf{x}}) = -ik\hat{\mathbf{x}} \cdot \int_D \mathbf{h}(\mathbf{y}) e^{-ik\hat{\mathbf{x}} \cdot \mathbf{y}} \, d\mathbf{y} = \int_D (\nabla_{\mathbf{y}} e^{-ik\hat{\mathbf{x}} \cdot \mathbf{y}}) \cdot \mathbf{h}(\mathbf{y}) \, d\mathbf{y}, \quad \hat{\mathbf{x}} \in \mathbb{S}^2.$$

The latter function $H^*\mathbf{h}$ is the far field of the divergence of a volume potential for the Helmholtz equation with source term $\mathbf{h} \in L^2(D, \mathbb{C}^3)$. If we denote by $\Phi(\mathbf{x}, \mathbf{y}) = \exp(ik|\mathbf{x} - \mathbf{y}|)/(4\pi|\mathbf{x} - \mathbf{y}|)$, $\mathbf{x} \neq \mathbf{y} \in \mathbb{R}^3$, the radiating fundamental solution to the Helmholtz equation is

$$H^*\mathbf{h} = \int_D (\nabla_{\mathbf{y}}\Phi(\cdot, \mathbf{y}))^\infty \cdot \mathbf{h}(\mathbf{y}) \, d\mathbf{y} = - \left(\operatorname{div} \int_D \Phi(\cdot, \mathbf{y}) \mathbf{h}(\mathbf{y}) \, d\mathbf{y} \right)^\infty = -(\operatorname{div} \mathbf{w})^\infty = -w^\infty,$$

where

$$\mathbf{w} = \int_D \Phi(\cdot, \mathbf{y}) \mathbf{h}(\mathbf{y}) \, d\mathbf{y} \in H_{\text{loc}}^2(\mathbb{R}^3, \mathbb{C}^3)$$

and

$$w = \operatorname{div} \mathbf{w} = \int_D \nabla_{\mathbf{y}}\Phi(\cdot, \mathbf{y}) \cdot \mathbf{h}(\mathbf{y}) \, d\mathbf{y} \in H_{\text{loc}}^1(\mathbb{R}^3). \tag{2.3}$$

Interchanging the divergence with the integral in the last equation can be validated, e.g., since all kernels are weakly singular. We finally define the operator $T = T_k : L^2(D, \mathbb{C}^3) \rightarrow L^2(D, \mathbb{C}^3)$ by

$$T\mathbf{f} = Q(\mathbf{f} - \nabla v), \tag{2.4}$$

where $v \in H_{\text{loc}}^1(\mathbb{R}^3)$ is the weak, radiating solution to (2.1) with \mathbf{f} replaced by $Q\mathbf{f}$ and

$$\operatorname{div}(A\nabla v) + k^2 v = \operatorname{div}(Q\mathbf{f}) \quad \text{in } \mathbb{R}^3. \tag{2.5}$$

That is, $\int_{\mathbb{R}^3} (A\nabla v \cdot \nabla \psi - k^2 v \psi) \, d\mathbf{x} = \int_D Q\mathbf{f} \cdot \nabla \psi \, d\mathbf{x}$ holds for all $\psi \in H^1(\mathbb{R}^3)$ with compact support.

LEMMA 2.1. *The far field operator F can be written as $F = -H^*TH$.*

Proof. First we define an auxiliary operator $G = G_k : L^2(D, \mathbb{C}^3) \rightarrow L^2(\mathbb{S}^2)$ by $G\mathbf{f} = v^\infty$ where $v \in H_{\text{loc}}^1(\mathbb{R}^3)$ is the weak, radiating solution to (2.5). For $g \in L^2(\mathbb{S}^2)$, it follows that $G(Hg) = v^\infty$ where v solves

$$\operatorname{div}(A\nabla v) + k^2 v = \operatorname{div}(Q\mathbf{f}) \quad \text{with } \mathbf{f}(\mathbf{x}) := \nabla_{\mathbf{x}} \int_{\mathbb{S}^2} g(\boldsymbol{\theta}) e^{ik\mathbf{x} \cdot \boldsymbol{\theta}} \, dS(\boldsymbol{\theta}), \quad \mathbf{x} \in \mathbb{R}^3.$$

By the superposition principle and the definition of F , we deduce that $F = -GH$.

Next, consider for some $\mathbf{h} \in L^2(D, \mathbb{C}^3)$ the functions w and \mathbf{w} from (2.3). Since $w^\infty = -H^*\mathbf{h}$ and since $w = \operatorname{div} \mathbf{w}$ for $\mathbf{w} \in H_{\text{loc}}^2(\mathbb{R}^3)$, that is the radiating solution to $\Delta \mathbf{w} + k^2 \mathbf{w} = \mathbf{h}$ in \mathbb{R}^3 , it follows that $w \in H_{\text{loc}}^1(\mathbb{R}^3)$ is the weak radiating solution to

$$\Delta w + k^2 w = \operatorname{div} \mathbf{h} \quad \text{in } \mathbb{R}^3. \tag{2.6}$$

Since $A = Q + \operatorname{Id}$, (2.5) can equivalently be written as

$$\Delta v + k^2 v = \operatorname{div}[Q(\mathbf{f} - \nabla v)] \stackrel{(2.4)}{=} \operatorname{div} T\mathbf{f} \quad \text{in } \mathbb{R}^3.$$

Since we defined the operator G via (2.5), setting $\mathbf{h} = T\mathbf{f}$ in (2.6) shows $G = H^*T$, and thus $F = -H^*TH$. □

The following lemma lists important properties of the operator T_k for $k > 0$ or $k = i$. To this end, we denote by $\overline{\mathcal{R}(H)}$ the closure of the range of H in $L^2(D, \mathbb{C}^3)$.

LEMMA 2.2.

- (a) For all $\mathbf{f} \in L^2(D, \mathbb{C}^3)$ and $k > 0$, it holds that $\text{Im}(T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} \leq 0$.
- (b) If $\text{Im}(T_k \mathbf{f}, \mathbf{f}) = 0$ for a non-trivial $\mathbf{f} \in \overline{\mathcal{R}(H)}$ and $k > 0$, then there is a function $w \in H^1(D)$ with $\nabla w = \mathbf{f}$ such that k^2 is a transmission eigenvalue with corresponding transmission eigenpair $(w - v, w)$ where $v \in H^1_{\text{loc}}(\mathbb{R}^3)$ is the weak solution to (2.5).
- (c) If $k^2 > 0$ is a transmission eigenvalue with corresponding transmission eigenpair (u, w) , then $(T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C})} = 0$ for $\mathbf{f} := \nabla w \in \overline{\mathcal{R}(H)}$.
- (d) If Q is positive definite and $k = i$, then T_i is coercive. There exists $c > 0$ such that

$$(T_i \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} \geq c \|\mathbf{f}\|_{L^2(D, \mathbb{C}^3)}^2 \quad \forall \mathbf{f} \in L^2(D, \mathbb{C}^3).$$

If Q is negative definite, then the operator $-T_i$ is coercive. There exists $c > 0$ such that

$$-(T_i \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} \geq c \|\mathbf{f}\|_{L^2(D, \mathbb{C}^3)}^2 \quad \forall \mathbf{f} \in L^2(D, \mathbb{C}^3).$$

(e) For $k > 0$ the difference $T_k - T_i$ is a compact operator from $L^2(D, \mathbb{C}^3)$ into $L^2(D, \mathbb{C}^3)$.

Proof.

(a) We write $T_k \mathbf{f} = Q\mathbf{g}$, where $\mathbf{g} = \mathbf{f} - \nabla v$ and $v \in H^1_{\text{loc}}(\mathbb{R}^3)$ solves (2.5); i.e.,

$$\int_{\mathbb{R}^3} [\nabla v \cdot \nabla \bar{\psi} - k^2 v \bar{\psi}] \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q(\mathbf{f} - \nabla v) \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q\mathbf{g} \, d\mathbf{x} \quad \forall \psi \in C^\infty_0(\mathbb{R}^3). \tag{2.7}$$

By the density of $C^\infty_0(\mathbb{R}^3)$ in $H^1(\mathbb{R}^3)$, the latter equation also holds for all $\psi \in H^1(D)$ with compact support. Using standard arguments (see, e.g. [16, Lemma 3.2(a)]), we compute that

$$\begin{aligned} (T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} &= (Q\mathbf{g}, \mathbf{g} + \nabla v)_{L^2(D, \mathbb{C}^3)} = (Q\mathbf{g}, \mathbf{g})_{L^2(D, \mathbb{C}^3)} + \int_D Q\mathbf{g} \cdot \nabla \bar{v} \, d\mathbf{x} \\ &= (Q\mathbf{g}, \mathbf{g})_{L^2(D, \mathbb{C}^3)} + \int_{|\mathbf{x}| < R} [|\nabla v|^2 - k^2 |v|^2] \, d\mathbf{x} - \int_{|\mathbf{x}| = R} \bar{v} \frac{\partial v}{\partial \nu} \, dS. \end{aligned} \tag{2.8}$$

Since $(Q\mathbf{g}, \mathbf{g})_{L^2(D, \mathbb{C}^3)}$ is real valued, taking the imaginary part of the last equation and letting $R \rightarrow \infty$ implies, due to the radiation condition, that

$$\text{Im}(T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} = -\frac{ik}{4\pi^2} \int_{\mathbb{S}^2} |v^\infty|^2 \, dS \leq 0. \tag{2.9}$$

(b) Let $\text{Im}(T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} = 0$ for $\mathbf{f} \in \overline{\mathcal{R}(H)}$ and define v as in the proof of (a). Equation (2.9) implies that $v^\infty = 0$. Due to Rellich’s Lemma, this implies that v vanishes in $\mathbb{R}^3 \setminus \bar{D}$. Thus, the variational formulation (2.7) for v reduces to

$$\int_D [\nabla \bar{\psi} \cdot A \nabla v - k^2 \bar{\psi} v] \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q\mathbf{f} \, d\mathbf{x} \quad \forall \psi \in H^1(D). \tag{2.10}$$

Since $\mathbf{f} \in \overline{\mathcal{R}(H)}$, there is a sequence of Herglotz wave functions

$$w_j(\mathbf{x}) = \int_{\mathbb{S}^2} \mathbf{g}_j(\boldsymbol{\theta}) e^{ik\mathbf{x} \cdot \boldsymbol{\theta}} \, dS(\boldsymbol{\theta}), \quad \mathbf{x} \in \mathbb{R}^3, \, j \in \mathbb{N},$$

such that $\mathbf{f}_j = \nabla w_j$ converges to $\mathbf{f} \in L^2(D, \mathbb{C}^3)$ as $j \rightarrow \infty$. Define v_j as the solution to (2.7) with \mathbf{f} replaced by \mathbf{f}_j . The continuity of the corresponding solution operator implies that $\|v_j - v\|_{H^1(D)} \leq C \|\mathbf{f}_j - \mathbf{f}\|_{L^2(D, \mathbb{C}^3)} \rightarrow 0$ as $j \rightarrow \infty$. Convergence of $\mathbf{f}_j = \nabla w_j$ in $L^2(D, \mathbb{C}^3)$ moreover implies that the restrictions of $w_j \in C^\infty(\mathbb{R}^3)$ to D converge in the quotient space $H^1(D)/\mathbb{C}$ to some function $w \in H^1(D)$. (The L^2 -norm of the gradient is a norm in $H^1(D)/\mathbb{C}$ by a well-known Poincaré inequality.) Since w_j satisfies the homogeneous Helmholtz equation $\Delta w_j + k^2 w_j = 0$ in D , this property carries over to w . In particular, $\nabla w = \mathbf{f}$ and $Q\mathbf{f} = Q\nabla w$. We rewrite (2.10) as

$$\int_D [\nabla \bar{\psi} \cdot A \nabla v - k^2 \bar{\psi} v] \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q \nabla w \, d\mathbf{x} \quad \forall \psi \in H^1(D).$$

Using $Q = A - \text{Id}$, the latter variational equation is equivalent to

$$\int_D [\nabla \bar{\psi} \cdot A \nabla (w - v) - k^2 \bar{\psi} (w - v)] \, d\mathbf{x} = \int_D [\nabla \bar{\psi} \cdot \nabla w - k^2 \bar{\psi} w] \, d\mathbf{x} = 0 \quad \forall \psi \in H^1(D). \tag{2.11}$$

Choosing the test function ψ in $H_0^1(D)$, the last term on the right vanishes since $w \in H^1(D)$ is a weak solution to the Helmholtz equation in D , $\int_D \nabla w \cdot \nabla \bar{\psi} \, d\mathbf{x} = \int_D k^2 w \bar{\psi} \, d\mathbf{x}$ for all $\psi \in H_0^1(D)$. Therefore, (2.11) shows that $w - v$ is a weak solution to $\text{div}(A \nabla (w - v)) + k^2 (w - v) = 0$ in D . If w vanishes, then $\mathbf{f} = \nabla w$ vanishes which is excluded by assumption. Thus, the above equations show that $(w - v, w)$ is a transmission eigenpair to the eigenvalue k^2 ; see (1.5).

(c) Let $k^2 > 0$ be a transmission eigenvalue with eigenpair $(u, w) \in H^1(D) \times H^1(D)$. Setting $\mathbf{f} = \nabla w$, we will show that $(T_k \mathbf{f}, \mathbf{f}) = 0$. To this end, recall that the set of Herglotz wave functions of the form (2.2) for densities $g \in L^2(\mathbb{S}^2)$ is dense in the set of H^1 -solutions to the Helmholtz equation in D . Thus, there exists a sequence $g_j \in L^2(\mathbb{S}^2)$ such that the corresponding Herglotz wave functions w_j converge to w in $H^1(D)$. Therefore, $\mathbf{f} = \nabla w \in \overline{\mathcal{R}(H)}$.

Since k^2 is a transmission eigenvalue, (1.5) implies that $v = u - w \in H_0^1(D)$ satisfies

$$\int_D [\nabla v \cdot \nabla \bar{\psi} - k^2 v \bar{\psi}] \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q(\nabla w - \nabla v) \, d\mathbf{x} \quad \forall \psi \in H^1(D).$$

Setting $\psi = w$ yields

$$\int_D [\nabla v \cdot \bar{\mathbf{f}} - k^2 v \bar{w}] \, d\mathbf{x} = \int_D Q(\mathbf{f} - \nabla v) \cdot \bar{\mathbf{f}} \, d\mathbf{x} = (T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)}.$$

Since $\mathbf{f} \in \overline{\mathcal{R}(H)}$, there is a sequence $(w_j)_{j \in \mathbb{N}}$ of Herglotz wave functions such that $\nabla w_j \rightarrow \mathbf{f}$ as $j \rightarrow \infty$. By definition, $\mathbf{f} = \nabla w$ which implies that $\|\nabla(w - w_j)\|_{L^2(D, \mathbb{C}^3)} \rightarrow 0$ as $j \rightarrow \infty$. Using Poincaré’s inequality as in part (b), we deduce that by adding suitable constants $c_j \in \mathbb{C}$ to w_j , the sequence $w_j + c_j$ converges to w in $H^1(D)$. Exploiting the fact that $v = u - w$ has mean value zero due to the third equation of (1.5) with constant ψ yields

$$\begin{aligned} \int_D [\nabla v \cdot \bar{\mathbf{f}} - k^2 v \bar{w}] \, d\mathbf{x} &= \lim_{j \rightarrow \infty} \int_D [\nabla v \cdot \nabla \bar{w}_j - k^2 v (\overline{w_j + c_j})] \, d\mathbf{x} \\ &= \lim_{j \rightarrow \infty} \int_D [\nabla v \cdot \nabla \bar{w}_j - k^2 v \bar{w}_j] \, d\mathbf{x} \\ &= \lim_{j \rightarrow \infty} \int_D [\nabla v \cdot \nabla \bar{w}_j + v \text{div} \nabla \bar{w}_j] \, d\mathbf{x} = 0 \end{aligned}$$

by Green’s first identity. Therefore, $(T_k \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} = 0$.

(d) We first consider the case of positive definite Q . Relying on (2.8) for $k=i$ and $\mathbf{f} \in L^2(D, \mathbb{C}^3)$, we exploit the ellipticity of the sesquilinear form in (2.7) for $k=i$ to conclude that $(T_i \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} \geq \|v\|_{H^1(\mathbb{R}^3)}^2 \geq \|v\|_{H^1(D)}^2$ with v solving (2.7) for $k=i$. According to Lemma A.1, the solution operator to (2.7) is closed from $L^2(D, \mathbb{C}^3)$ into $H^1(D)$ which implies that $\|v\|_{H^1(D)} \geq C\|\mathbf{f}\|_{L^2(D, \mathbb{C}^3)}$. If Q is negative definite, the same arguments allow us to estimate

$$\begin{aligned} (T_i \mathbf{f}, \mathbf{f})_{L^2(D, \mathbb{C}^3)} &= (Q\mathbf{f}, \mathbf{f}) - \int_D Q\mathbf{f} \cdot \nabla v \, d\mathbf{x} = (Q\mathbf{f}, \mathbf{f}) - \int_D \nabla \bar{v} \cdot A \nabla v \, d\mathbf{x} - \|v\|_{L^2(D, \mathbb{C}^3)} \\ &\leq -\min\{c_0, 1\} \|v\|_{H^1(\mathbb{R}^3)}^2 \leq -C\|\mathbf{f}\|_{L^2(D, \mathbb{C}^3)}^2. \end{aligned}$$

(e) This assertion follows from standard embedding arguments (e.g. [16, Lemma 3.2(d)]). □

The eigenvalues λ_j of the far field operator F lie on a circle with radius $8\pi^2/k$ and center at $8\pi^2i/k$ in the complex plane. Since F is compact, these eigenvalues converge to zero as $j \rightarrow \infty$. If the contrast Q is sign-definite, they either approach the origin from the left or from the right. Using the results of Lemma 2.2, this can be shown as in [15, Lemma 4.1].

LEMMA 2.3. *Assume that $k^2 > 0$ is not a transmission eigenvalue. If Q is positive definite or negative definite, then $\operatorname{Re} \lambda_j < 0$ and $\operatorname{Re} \lambda_j > 0$ for j large enough, respectively.*

3. Spectrum of the far field operator at transmission eigenvalues

Next we take a closer look at the behavior of the eigenvalues of F . As already mentioned above, the eigenvalues λ_j of F lie on a circle in the complex plane with center $8\pi^2i/k$ and radius $8\pi^2/k$ and tend to zero from the left or right, depending on the sign of Q . Let us assume for a moment that $k^2 > 0$ is not a transmissions eigenvalue such that none of the eigenvalues λ_j of F can vanish. This allows us to write the eigenvalues λ_j in polar coordinates,

$$\lambda_j = r_j e^{i\vartheta_j} \quad r_j > 0, \vartheta_j \in (0, \pi).$$

If Q is positive definite, Lemma 2.3 states that there is $N = N(k) \in \mathbb{N}$ such that $\operatorname{Re}(\lambda_j) < 0$ for $j \geq N$. In particular, there is a well-defined and unique smallest phase among all phases ϑ_j of eigenvalues of F ,

$$\vartheta_* = \min_{j \in \mathbb{N}} \vartheta_j.$$

We denote the corresponding eigenvalue as λ_* . If Q is negative definite, there is $N = N(k) \in \mathbb{N}$ such that $\operatorname{Re}(\lambda_j) > 0$ for $j \geq N$. In this case the unique largest phase

$$\vartheta^* = \max_{j \in \mathbb{N}} \vartheta_j$$

is well-defined, and we denote the corresponding eigenvalue as λ^* . The next lemma characterizes these maximal phases (see [19, Theorem 3] for a proof).

THEOREM 3.1. *Assume that $k^2 > 0$ is not a transmission eigenvalue. If Q is positive or negative definite, then*

$$\cot \vartheta_* = \max_{g \in L^2(\mathbb{S}^2)} \frac{\operatorname{Re}(Fg, g)_{L^2(\mathbb{S}^2)}}{\operatorname{Im}(Fg, g)_{L^2(\mathbb{S}^2)}} \quad \text{and} \quad \cot \vartheta^* = \min_{g \in L^2(\mathbb{S}^2)} \frac{\operatorname{Re}(Fg, g)_{L^2(\mathbb{S}^2)}}{\operatorname{Im}(Fg, g)_{L^2(\mathbb{S}^2)}}, \quad (3.1)$$

respectively. The maximum or minimum is attained at any eigenvalue to λ_* and λ^* , respectively.

Since $F = -H^*TH$, we note that

$$(Fg, g)_{L^2(S^2)} = -(T_kHg, Hg)_{L^2(D, \mathbb{C}^3)} = -(T_k\mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}$$

with $\mathbf{w} := Hg \in L^2(D, \mathbb{C}^3)$. Let us define

$$X = X_k := \overline{\mathcal{R}(H)} \subset L^2(D)$$

such that (3.1) can equivalently be written as

$$\cot \vartheta_* = \max_{\mathbf{w} \in X} \frac{\operatorname{Re}(T_k\mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}}{\operatorname{Im}(T_k\mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}} \quad \text{and} \quad \cot \vartheta^* = \min_{\mathbf{w} \in X} \frac{\operatorname{Re}(T_k\mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}}{\operatorname{Im}(T_k\mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}}. \quad (3.2)$$

REMARK 3.2. We know from Lemma 2.2 that the denominator $\operatorname{Im}(T_k\mathbf{w}, \mathbf{w})$ can only vanish if k^2 is a transmission eigenvalue. Thus, (3.2) indicates the particular behavior of the phases ϑ_* and ϑ^* close to transmission eigenvalues.

ASSUMPTION 3.3. From now on, we assume that the Lipschitz domain $D = \cup_{i=1}^I D_i$ can be decomposed into $I \in \mathbb{N}$ connected components D_i such that each D_i is a simply connected Lipschitz subdomain with connected boundary and $\overline{D_i} \cap \overline{D_j} = \emptyset$ if $1 \leq i \neq j \leq I$. To further characterize X , we recall Theorem 3.37 from [21].

THEOREM 3.4 ([21, Theorem 3.37]). If $\mathbf{w} \in L^2(D, \mathbb{C}^3)$ satisfies $\operatorname{curl}(\mathbf{u}) = 0$ in the distributional sense, i.e.

$$\int_D \mathbf{w} \cdot \nabla \times \overline{\psi} \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D, \mathbb{C}^3),$$

then there is a scalar potential $\phi_{\mathbf{w}} \in H^1(D)$ such that $\mathbf{w} = \nabla \phi_{\mathbf{w}}$. The potential $\phi_{\mathbf{w}}$ is unique up to adding functions that are constant on each connected component D_i , $i = 1, \dots, I$, of D .

To exclude additive constants, we use the space

$$H_\diamond^1(D) := \left\{ w \in H^1(D), \int_{D_i} w \, d\mathbf{x} = 0 \text{ for all connected components } D_i \subset D, i = 1, \dots, I \right\}.$$

This space is a Hilbert space for the inner product $(\phi, \psi) \mapsto \int_D \nabla \phi \cdot \nabla \overline{\psi} \, d\mathbf{x}$, again due to a Poincaré inequality. Defining $L^2(D, \mathbb{C}^3, \operatorname{curl} 0) := \{\mathbf{u} \in L^2(D, \mathbb{C}^3), \operatorname{curl}(\mathbf{u}) = 0\}$ as the space of curl-free functions in $L^2(D, \mathbb{C}^3)$, we can thus define an operator

$$E: L^2(D, \mathbb{C}^3, \operatorname{curl} 0) \rightarrow H_\diamond^1(D), \quad \mathbf{w} \mapsto E(\mathbf{w}) = \phi_{\mathbf{w}},$$

mapping a curl-free vector field \mathbf{w} to its unique scalar potential $\phi_{\mathbf{w}}$ in $H_\diamond^1(D)$, such that $\nabla E(\mathbf{w}) = \mathbf{w}$ in $L^2(D, \mathbb{C}^3)$. Obviously, E is continuous,

$$C \|\phi_{\mathbf{w}}\|_{H^1(D)} \leq \|\phi_{\mathbf{w}}\|_{H_\diamond^1(D)} = \|\nabla \phi_{\mathbf{w}}\|_{L^2(D, \mathbb{C}^3)} = \|\mathbf{w}\|_{L^2(D, \mathbb{C}^3)} \quad \forall \mathbf{w} \in L^2(D, \mathbb{C}^3, \operatorname{curl} 0).$$

LEMMA 3.5. *It holds that*

$$\begin{aligned}
 X = \overline{\mathcal{R}(H)} = & \left\{ \mathbf{w} \in L^2(D, \mathbb{C}^3), \int_D \mathbf{w} \cdot \nabla \times \phi \, d\mathbf{x} = 0 \quad \forall \phi \in C_0^\infty(D, \mathbb{C}^3), \right. \\
 & \left. \exists d \in \mathbb{C}^I : \sum_{i=1}^I \int_{D_i} [\nabla E(\mathbf{w}) \cdot \nabla \psi - k^2(E(\mathbf{w}) + d_i)\psi] \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D) \right\}.
 \end{aligned}
 \tag{3.3}$$

Proof. Recall from the definition of the Herglotz wave function v_g in (2.2) that $Hg = \nabla v_g$. First we show that $\overline{\mathcal{R}(H)} \subset X$. Let $\mathbf{w} \in \mathcal{R}(H)$ be such that $\mathbf{w} = \nabla v_g$ for a function $g \in L^2(\mathbb{S}^2)$. Since \mathbf{w} is a gradient field, it follows immediately that \mathbf{w} is curl-free, i.e., $\int_D \mathbf{w} \cdot \nabla \times \phi \, d\mathbf{x} = 0$ for all $\phi \in C_0^\infty(D, \mathbb{C}^3)$. Moreover, $\nabla v_g = \nabla E(\mathbf{w}) = \mathbf{w}$ which implies that for each connected component D_i , for $i = 1, \dots, I$, of D there exists $d_i \in \mathbb{C}$ such that $v_g = E(\mathbf{w}) + d_i$ on D_i . Since v_g solves the Helmholtz equation,

$$0 = \sum_{i=1}^I \int_{D_i} [\nabla(E(\mathbf{w}) + d_i) \cdot \nabla \psi - k^2(E(\mathbf{w}) + d_i)\psi] \, d\mathbf{x} \quad \forall \psi \in C_0^\infty(D).$$

Thus, $\mathbf{w} \in X$. If we additionally show that X is closed in the topology of $L^2(D, \mathbb{C}^3)$, it follows that $\overline{\mathcal{R}(H)} \subset X$. To this end, assume that $X \ni \mathbf{w}_j \rightarrow \mathbf{w}$ in $L^2(D, \mathbb{C}^3)$ as $j \rightarrow \infty$ and that $E(\mathbf{w}_j) + \sum_{i=1}^I d_i^{(j)} \mathbf{1}_{D_i}$ solves the Helmholtz equation. It is clear that the first condition in (3.3) for \mathbf{w}_j implies that $\int_D \mathbf{w}_j \cdot \nabla \times \phi \, d\mathbf{x} = 0$ for all $\phi \in C_0^\infty(D, \mathbb{C}^3)$. Rewriting (3.4) as

$$\sum_{i=1}^I \int_{D_i} [\mathbf{w}_j \cdot \nabla \psi - k^2(E(\mathbf{w}_j) + d_i^{(j)})\psi] \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D),$$

the continuity of E from $L^2(D, \mathbb{C}^3)$ into $H_\diamond^1(D)$ shows that merely the convergence of the vectors $d^{(j)} \in \mathbb{C}^I$ needs to be shown. This follows from the observation that, for arbitrary $\psi \in C_0^\infty(D)$,

$$\sum_{i=1}^I (d_i^{(j)} - d_i^{(\ell)}) \int_{D_i} \psi \, d\mathbf{x} = \int_D [(\mathbf{w}_j - \mathbf{w}_\ell) \cdot \nabla \psi - k^2 E(\mathbf{w}_j - \mathbf{w}_\ell)\psi] \, d\mathbf{x} \rightarrow 0 \quad (j, \ell \rightarrow \infty).$$

Now we consider the orthogonal decomposition $X = \overline{\mathcal{R}(H)} \oplus \overline{\mathcal{R}(H)}^\perp$ and show that the orthogonal complement of $\overline{\mathcal{R}(H)}$ is trivial. Assume that $\mathbf{w}_0 \in \overline{\mathcal{R}(H)}^\perp \subset X$. Since $\mathbf{w}_0 \in X$, condition (3.4) shows that there is $d \in \mathbb{C}^I$ such that $E(\mathbf{w}_0) + \sum_{i=1}^I d_i \mathbf{1}_{D_i}$ solves

$$\sum_{i=1}^I \int_{D_i} [\nabla E(\mathbf{w}_0) \cdot \nabla \psi - k^2(E(\mathbf{w}_0) + d_i)\psi] \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D).$$

According to [14, Theorem 7.3], the space of Herglotz wave functions v_g is dense in the H^1 -solutions of the Helmholtz equation. Therefore, there is a sequence $(g_j)_{j \in \mathbb{N}} \subset L^2(\mathbb{S}^2)$ such that $v_{g_j} \rightarrow E(\mathbf{w}_0) + \sum_{i=1}^I d_i \mathbf{1}_{D_i}$ in $H^1(D)$ as $j \rightarrow \infty$. In particular,

$$\left| \int_D (\nabla E(\mathbf{w}_0) - \nabla v_{g_j}) \cdot \nabla \overline{v_{g_j}} \, d\mathbf{x} \right| \leq \|\nabla E(\mathbf{w}_0) - \nabla v_{g_j}\|_{L^2(D, \mathbb{C}^3)} \|\nabla v_{g_j}\|_{L^2(D, \mathbb{C}^3)} \rightarrow 0,$$

since $\|\nabla v_{g_j}\|_{L^2(D, \mathbb{C}^3)}$ is bounded. Therefore,

$$\int_D |\nabla v_{g_j}|^2 \, d\mathbf{x} - \int_D \nabla E(\mathbf{w}_0) \cdot \nabla \overline{v_{g_j}} \, d\mathbf{x} \rightarrow 0 \quad (j \rightarrow \infty).$$

Since $\mathbf{w}_0 = \nabla E(\mathbf{w}_0) \in \overline{\mathcal{R}(H)}^\perp$, the second term on the left vanishes for all $j \in \mathbb{N}$. It follows that $\mathbf{w}_0 = \lim_{j \rightarrow \infty} \nabla v_{g_j} = 0$, which concludes the proof. \square

Note that we needed to include constants $d \in \mathbb{C}^I$ in the definition of the space X since the operator E merely extracts the potential $\phi_{\mathbf{w}}$ of a function $\mathbf{w} \in X_k$ that has vanishing means but does not take the Helmholtz equation into consideration. To avoid the need to deal with these constants, we next define $E_k : L^2(D, \mathbb{C}^3, \text{curl}0) \rightarrow H^1(D)$ that again maps \mathbf{w} to a scalar potential $\phi_{\mathbf{w}} \in H^1(D)$. Moreover, if $\mathbf{w} \in X_k$, then the potential $\phi_{\mathbf{w}}$ solves the Helmholtz equation. To this end, we define functions $\chi_i \in C_0^\infty(D)$, $i = 1, \dots, I$, such that χ_i has support in D_i and $\int_{D_i} \chi_i \, d\mathbf{x} = 1$. Plugging in χ_i into (3.4) and solving for d_i shows that $d_i = -\int_{D_i} (k^{-2} \nabla E(\mathbf{w}) \cdot \nabla \chi_i - E(\mathbf{w}) \chi_i) \, d\mathbf{x}$.

LEMMA 3.6. *Define $E_k : L^2(D, \mathbb{C}^3, \text{curl}0) \rightarrow H^1(D)$ for $k > 0$ by*

$$E_k : \mathbf{w} \mapsto \phi_{\mathbf{w}} = E(\mathbf{w}) + \sum_{j=1}^I \mathbf{1}_{D_j} \int_D \left[E(\mathbf{w}) \chi_j - \frac{1}{k^2} \nabla E(\mathbf{w}) \cdot \nabla \chi_j \right] \, d\mathbf{x}. \quad (3.5)$$

Then E_k is well-defined and bounded, and for fixed \mathbf{w} , the function $k \mapsto E_k(\mathbf{w})$ is continuously differentiable taking values in $H^1(D)$. The derivative $k \mapsto dE_k(\mathbf{w})/dk$ is constant on each connected component of D . If $\mathbf{w} \in X_k$, then $\phi_{\mathbf{w}} = E_k(\mathbf{w})$ solves the Helmholtz equation,

$$\int_D [\nabla \phi_{\mathbf{w}} \cdot \nabla \overline{\psi} - k^2 \phi_{\mathbf{w}} \overline{\psi}] \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D).$$

Proof. It remains to compute the derivative of $k \mapsto E_k(\mathbf{w})$. Considering (3.5), E_k is clearly differentiable and the derivative equals $dE_k(\mathbf{w})/dk = 2k^{-3} \sum_{j=1}^I \mathbf{1}_{D_j} \int_D \mathbf{w} \cdot \nabla \chi_j \, d\mathbf{x}$. \square

4. Phase behavior at transmission eigenvalues

Since we will now investigate the behavior of the largest or the smallest phase of the wave number $k > 0$, the dependency of all introduced quantities on k becomes relevant. Therefore, we denote this dependence whenever necessary, e.g., as $X_k, T_k, \vartheta_*(k)$, and $\vartheta^*(k)$. Tackling the dependency of X_k on k requires us to introduce a projection operator P_k from $L^2(D, \mathbb{C}^3)$ onto X_k . This is, roughly speaking, due to (3.2) which plays a crucial role for inside-outside duality. Indeed, using such a projection, one can rewrite (3.2) using the k -independent space $L^2(D, \mathbb{C}^3)$ instead of X_k ,

$$\cot \vartheta_*(k) = \max_{\mathbf{w} \in L^2(D, \mathbb{C}^3)} \frac{\text{Re}(T_k P_k \mathbf{w}, P_k \mathbf{w})}{\text{Im}(T_k P_k \mathbf{w}, P_k \mathbf{w})}$$

and

$$\cot \vartheta^*(k) = \min_{\mathbf{w} \in L^2(D, \mathbb{C}^3)} \frac{\text{Re}(T_k P_k \mathbf{w}, P_k \mathbf{w})}{\text{Im}(T_k P_k \mathbf{w}, P_k \mathbf{w})}.$$

THEOREM 4.1. *Let $k_0 > 0$ and $\mathbf{w}_0 \in X_{k_0}$ such that $(T_{k_0} \mathbf{w}_0, \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} = 0$. If $P_k : L^2(D, \mathbb{C}^3) \rightarrow X_k$ is a projection onto X_k that is continuously differentiable with respect to $k > 0$ and if*

$$\alpha(k_0) := \left[\frac{d}{dk} (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} \right] \Big|_{k=k_0} \in \mathbb{R} \setminus \{0\},$$

then the following statement holds: if Q is positive definite, then

$$\lim_{k \nearrow k_0} \vartheta_* = 0 \quad \text{if } \alpha(k_0) > 0 \quad \text{and} \quad \lim_{k \searrow k_0} \vartheta_* = 0 \quad \text{if } \alpha(k_0) < 0.$$

If Q is negative definite, then

$$\lim_{k \searrow k_0} \vartheta^* = \pi \quad \text{if } \alpha(k_0) > 0 \quad \text{and} \quad \lim_{k \nearrow k_0} \vartheta^* = \pi \quad \text{if } \alpha(k_0) < 0.$$

Proof. The proof exploits the differentiability of P_k with respect to k to set up a Taylor expansion of order one of $k \mapsto (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)$ together with the fact that k_0^2 is a transmission eigenvalue to deduce the stated result. We refer to [15, Lemma 5.1] for a full proof; the latter proof is indeed valid for general projections, despite the fact that the claim merely considers the orthogonal projection onto X_k . \square

We will first compute the derivative of $k \mapsto (T_k \mathbf{w}_0, \mathbf{w}_0)$.

LEMMA 4.2. *Let $0 \neq \mathbf{w}_0 \in L^2(D, \mathbb{C}^3)$ so that $(T_{k_0} \mathbf{w}_0, \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} = 0$. Then the weak radiating solution v_{k_0} to $\operatorname{div}(A \nabla v_{k_0}) + k_0^2 v_{k_0} = \operatorname{div}(Q \mathbf{w}_0)$ in \mathbb{R}^3 (see (2.5) for a weak formulation) belongs to $H_0^1(D)$ and*

$$\frac{d}{dk} (T_k \mathbf{w}_0, \mathbf{w}_0) \Big|_{k=k_0} = -2k_0 \int_D |v_{k_0}|^2 \, d\mathbf{x}.$$

Proof. Since $(T_{k_0} \mathbf{w}_0, \mathbf{w}_0) = 0$, it follows that the far field $v_{k_0}^\infty = 0$ and v_{k_0} vanishes in $\mathbb{R}^3 \setminus D$ (see the proof of Theorem 2.2(a) and (b)). Thus, $v_{k_0} \in H_0^1(D)$. By definition, we have $T_{k_0} \mathbf{w}_0 = Q(\mathbf{w}_0 - \nabla v_{k_0})$. For arbitrary $k > 0$, we define $v_k \in H_{\text{loc}}^1(\mathbb{R}^3)$ as the radiating solution to

$$\int_{\mathbb{R}^3} (A \nabla v_k \cdot \nabla \bar{\psi} - k^2 v_k \bar{\psi}) \, d\mathbf{x} = \int_D (Q \mathbf{w}_0) \cdot \nabla \bar{\psi} \, d\mathbf{x} \quad \forall \psi \in C_0^\infty(\mathbb{R}^3). \tag{4.1}$$

The map $k \mapsto v_k$ is Fréchet-differentiable, and $v'_{k_0} := [dv/dk]|_{k=k_0} \in H_{\text{loc}}^1(\mathbb{R}^3)$ solves

$$\int_{\mathbb{R}^3} (A \nabla v'_{k_0} \cdot \nabla \bar{\psi} - 2k_0 v_{k_0} \bar{\psi} - k_0^2 v'_{k_0} \bar{\psi}) \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(\mathbb{R}^3). \tag{4.2}$$

By a density argument, both (4.1) and (4.2) also hold for all $\psi \in H^1(\mathbb{R}^3)$ with compact support. Moreover, for $k = k_0$ the solution $v_{k_0} \in H_0^1(D)$ has compact support and hence (4.1) holds in this case even for all $\psi \in H_{\text{loc}}^1(\mathbb{R}^3)$. Thus,

$$\begin{aligned} \frac{d}{dk} (T_k \mathbf{w}_0, \mathbf{w}_0) \Big|_{k=k_0} &= - \int_D Q \nabla v'_{k_0} \cdot \overline{\mathbf{w}_0} \, d\mathbf{x} = - \int_D (Q \overline{\mathbf{w}_0}) \cdot \nabla v'_{k_0} \, d\mathbf{x} \\ &\stackrel{(4.1)}{=} - \int_D (A \nabla \overline{v_{k_0}} \cdot \nabla v'_{k_0} - k_0^2 \overline{v_{k_0}} v'_{k_0}) \, d\mathbf{x}. \end{aligned}$$

Exploiting Green’s identity, (4.2), and the symmetry of A yields

$$\int_D A \nabla \overline{v_{k_0}} \cdot \nabla v'_{k_0} \, d\mathbf{x} = \int_D \nabla \overline{v_{k_0}} \cdot A \nabla v'_{k_0} \, d\mathbf{x} = \int_D (2k_0 v_{k_0} \overline{v_{k_0}} + k_0^2 v'_{k_0} \overline{v_{k_0}}) \, d\mathbf{x},$$

that is, $(d/dk)(T_k \mathbf{w}_0, \mathbf{w}_0)|_{k=k_0} = -2k_0 \int_D |v_{k_0}|^2 \, d\mathbf{x}$. □

Recall now the operator E_k from (3.5) that maps curl-free vector fields to a scalar potential.

THEOREM 4.3. *If $k_0 > 0$ and $0 \neq \mathbf{w}_0 \in X_{k_0}$ satisfy $(T_{k_0} \mathbf{w}_0, \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} = 0$, we set $\phi_{\mathbf{w}_0} = E_{k_0} \mathbf{w}_0 \in H^1(D)$. Assume that $P_k : L^2(D, \mathbb{C}^3) \rightarrow X_k$ is a projection that is continuously differentiable in $k > 0$. Then*

$$\left. \frac{d}{dk} (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} \right|_{k=k_0} = -2k_0 \int_D |v_{k_0}|^2 \, d\mathbf{x} + 4k_0 \operatorname{Re} \int_D v_{k_0} \overline{\phi_{\mathbf{w}_0}} \, d\mathbf{x}.$$

Proof. By definition of P_k , it holds that $P_k \mathbf{w}_0 \in X_k$. That is, up to additive constants, $P_k \mathbf{w}_0$ is a gradient field of a scalar potential solving the Helmholtz equation. More precisely, lemmas 3.5 and 3.6 state that $P_k \mathbf{w}_0 = \nabla \phi_{\mathbf{w}_0}(k)$ where $\phi_{\mathbf{w}_0}(k) = E_k(P_k \mathbf{w}_0) \in H^1(D)$ is the unique scalar potential to $P_k \mathbf{w}_0$ solving $\Delta \phi_{\mathbf{w}_0}(k) + k^2 \phi_{\mathbf{w}_0}(k) = 0$ weakly in D . That is,

$$\int_D (\nabla \phi_{\mathbf{w}_0}(k) \cdot \nabla \overline{\psi} - k^2 \phi_{\mathbf{w}_0}(k) \overline{\psi}) \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D). \tag{4.3}$$

In particular, the operator that maps \mathbf{w}_0 to $\phi_{\mathbf{w}_0}(k) = E_k(P_k \mathbf{w}_0)$ is well-defined and continuous from $L^2(D, \mathbb{C}^3)$ into $H^1(D)$. By our assumption of the differentiability of P_k and Lemma 3.6, the function $k \mapsto \phi_{\mathbf{w}_0}(k) = E_k(P_k \mathbf{w}_0)$ is also differentiable as a map from $L^2(D, \mathbb{C}^3)$ into $H^1(D)$. Thus, differentiating (4.3) with respect to k shows that $\phi'_{\mathbf{w}_0}(k) = d\phi_{\mathbf{w}_0}(k)/dk \in H^1(D)$ is a weak solution to $\Delta \phi'_{\mathbf{w}_0}(k) + k^2 \phi'_{\mathbf{w}_0}(k) = -2k \phi_{\mathbf{w}_0}(k)$. In particular,

$$\int_D (\nabla \phi'_{\mathbf{w}_0}(k) \cdot \nabla \overline{\psi} - k^2 \phi'_{\mathbf{w}_0}(k) \overline{\psi}) \, d\mathbf{x} = 2k \int_D \overline{\psi} \phi_{\mathbf{w}_0}(k) \, d\mathbf{x} \quad \forall \psi \in H_0^1(D). \tag{4.4}$$

Applying the chain rule to $k \mapsto (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)$, one obtains

$$\begin{aligned} \frac{d}{dk} (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} &= (T'_k P_k \mathbf{w}_0, P_k \mathbf{w}_0) + (T_k P'_k \mathbf{w}_0, P_k \mathbf{w}_0) + (T_k P_k \mathbf{w}_0, P'_k \mathbf{w}_0) \\ &= (T'_k P_k \mathbf{w}_0, P_k \mathbf{w}_0) + \overline{(T_k^* P_k \mathbf{w}_0, P'_k \mathbf{w}_0)} + (T_k P_k \mathbf{w}_0, P'_k \mathbf{w}_0). \end{aligned}$$

Next, we show that $T_{k_0} \mathbf{w}_0 = T_{k_0}^* \mathbf{w}_0$. Recall from the proof of Lemma 4.2 that $T_{k_0} \mathbf{w}_0 = Q(\mathbf{w}_0 - \nabla v_{k_0})$ where $v_{k_0} \in H_{\text{loc}}^1(\mathbb{R}^3) \cap H_0^2(D)$ solves $\operatorname{div}(A \nabla v_{k_0}) + k_0^2 v_{k_0} = \operatorname{div}(Q \mathbf{w}_0)$ in \mathbb{R}^3 ; i.e.,

$$\int_D (A \nabla v_{k_0} \cdot \nabla \overline{\psi} - k_0^2 v_{k_0} \overline{\psi}) \, d\mathbf{x} = \int_D Q(\mathbf{w}_0 - \nabla v_{k_0}) \cdot \nabla \overline{\psi} \, d\mathbf{x} \quad \forall \psi \in H^1(D). \tag{4.5}$$

The symmetry of Q together with (4.5) implies that

$$\begin{aligned}
 (T_{k_0} \mathbf{w}_0, \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} &= (Q \mathbf{w}_0, \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} - \int_D \nabla v_{k_0} \cdot (Q \overline{\mathbf{w}_0}) \, d\mathbf{x} \\
 &= (\mathbf{w}_0, Q \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} - \int_D (A \nabla v_{k_0} \cdot \nabla \overline{v_{k_0}} - k_0^2 v_{k_0} \overline{v_{k_0}}) \, d\mathbf{x} \\
 &= (\mathbf{w}_0, Q \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} - \int_D Q \nabla \overline{v_{k_0}} \cdot \mathbf{w}_0 \, d\mathbf{x} \\
 &= (\mathbf{w}_0, Q[\mathbf{w}_0 - \nabla v_{k_0}])_{L^2(D, \mathbb{C}^3)} = (\mathbf{w}_0, T_{k_0} \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)}.
 \end{aligned}$$

In particular, $T_{k_0}^* \mathbf{w}_0 = T_{k_0} \mathbf{w}_0$, and Lemma 4.2 shows that

$$\frac{d}{dk} (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} \Big|_{k=k_0} = -2k_0 \int_D |v_{k_0}|^2 \, d\mathbf{x} + 2\operatorname{Re} (T_{k_0} \mathbf{w}_0, P_{k_0}' \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)}.$$

Since $Q = A - \operatorname{Id}$, we exploit (4.5) to finally obtain

$$\begin{aligned}
 2\operatorname{Re} (T_{k_0} \mathbf{w}_0, P_{k_0}' \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} &= 2\operatorname{Re} \int_D (Q \mathbf{w}_0 - Q \nabla v_{k_0}) \cdot P_{k_0}' \overline{\mathbf{w}_0} \, d\mathbf{x} \\
 &= 2\operatorname{Re} \int_D (Q \mathbf{w}_0 - Q \nabla v_{k_0}) \cdot \nabla \overline{\phi_{\mathbf{w}_0}'(k_0)} \, d\mathbf{x} \\
 &\stackrel{(4.5)}{=} 2\operatorname{Re} \int_D (\nabla v_{k_0} \cdot \nabla \overline{\phi_{\mathbf{w}_0}'(k_0)} - k_0^2 v_{k_0} \overline{\phi_{\mathbf{w}_0}'(k_0)}) \, d\mathbf{x} \\
 &\stackrel{(4.4)}{=} 4k_0 \operatorname{Re} \int_D v_{k_0} \overline{\phi_{\mathbf{w}_0}} \, d\mathbf{x}.
 \end{aligned}$$

□

Since Theorem 4.3 computes the derivative of $k \mapsto (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)$ for arbitrary differentiable projections P_k , it remains to show the existence of such projections. The following lemma will be helpful.

LEMMA 4.4. *For $\mathbf{w} \in L^2(D, \mathbb{C}^3)$ and $k > 0$, there exists a unique vector potential $\mathbf{A} = \mathbf{A}_{\mathbf{w}} \in H_0(\operatorname{curl}, D) \cap H(\operatorname{div} 0, D)$ such that*

$$\mathbf{w} = \nabla \phi_{\mathbf{w}} + \nabla \times \mathbf{A}_{\mathbf{w}} \quad \text{where } \phi_{\mathbf{w}} := E_k(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}}) \in H^1(D).$$

If $\mathbf{w} \in X_k$, then $\mathbf{A}_{\mathbf{w}} = 0$ and $\phi_{\mathbf{w}}$ is a weak solution to the Helmholtz equation,

$$\int_D (\nabla \phi_{\mathbf{w}} \cdot \nabla \overline{\psi} - k^2 \phi_{\mathbf{w}} \overline{\psi}) \, d\mathbf{x} = 0 \quad \forall \psi \in C_0^\infty(D).$$

Proof. Due to [21, Theorem 3.45, Remark 3.46], a function \mathbf{w} in $L^2(D, \mathbb{C}^3)$ can be decomposed as

$$\mathbf{w} = \nabla \phi_{\mathbf{w}} + \nabla \times \mathbf{A}_{\mathbf{w}}$$

with a scalar potential $\phi_{\mathbf{w}} \in H^1(D)$ and a vector potential $\mathbf{A}_{\mathbf{w}} \in H_0(\operatorname{curl}, D) \cap H(\operatorname{div} 0, D)$; i.e., $\operatorname{div} \mathbf{A}_{\mathbf{w}} = 0$ in D . The potential $\mathbf{A}_{\mathbf{w}}$ is unique since the difference $\mathbf{A} = \mathbf{A}_{\mathbf{w}}^1 - \mathbf{A}_{\mathbf{w}}^2 \in H_0(\operatorname{curl}, D)$ of two vector potentials $\mathbf{A}_{\mathbf{w}}^{1,2}$ solves $\nabla \times \nabla \times \mathbf{A} = 0$. Thus, $\|\nabla \times \mathbf{A}_{\mathbf{w}}\|_{L^2(D, \mathbb{C}^3)} = 0$, and Friedrich's inequality (see, e.g., [21, Corollary 3.51]) implies that $\mathbf{A}_{\mathbf{w}}$ vanishes. Moreover, $\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}} \in L^2(D, \mathbb{C}^3, \operatorname{curl} 0)$ is curl-free, so $\phi_{\mathbf{w}} := E_k(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}}) \in H^1(D)$ is well-defined. If $\mathbf{w} \in X_k$, then \mathbf{w} is a gradient field and

$\nabla \times \mathbf{w} = \nabla \times \nabla \times \mathbf{A}_{\mathbf{w}} = 0$ in D . Thus, $\mathbf{A}_{\mathbf{w}}$ vanishes due to the same arguments as above, and $\phi_{\mathbf{w}} = E_k(\mathbf{w})$ solves the Helmholtz equation due to Theorem 3.6. \square

To define a first projection operator P_k , we exploit, as in the last lemma, the relation $\phi_{\mathbf{w}} = E_k(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}})$ for arbitrary $\mathbf{w} \in L^2(D, \mathbb{C}^3)$. Assuming that $k^2 > 0$ is not a Dirichlet eigenvalue of $-\Delta$ in D , we additionally define $\hat{w} = \hat{w}_{\mathbf{w},k} \in H_0^1(D)$ to be the unique weak solution to the boundary value problem $\Delta \hat{w} + k^2 \hat{w} = \Delta \phi_{\mathbf{w}} + k^2 \phi_{\mathbf{w}}$ in D and $\hat{w} = 0$ on ∂D . More precisely,

$$\int_D [\nabla \hat{w} \cdot \nabla \bar{\psi} - k^2 \hat{w} \bar{\psi}] \, d\mathbf{x} = \int_D [\nabla \phi_{\mathbf{w}} \cdot \nabla \bar{\psi} - k^2 \phi_{\mathbf{w}} \bar{\psi}] \, d\mathbf{x} \quad \forall \psi \in H_0^1(D). \tag{4.6}$$

The latter problem is of Fredholm type. By the assumption that k^2 is not a Dirichlet eigenvalue of $-\Delta$ in D , a unique solution $\hat{w} \in H_0^1(D)$ exists and depends continuously on $\phi_{\mathbf{w}}$.

LEMMA 4.5. *If $k_0^2 > 0$ is not a Dirichlet eigenvalue of $-\Delta$ in D , then $P_{k_0} : L^2(D, \mathbb{C}^3) \rightarrow X_{k_0}$,*

$$P_{k_0} \mathbf{w} = \nabla \phi_{\mathbf{w}} - \nabla \hat{w} \quad \text{for } \mathbf{w} \in L^2(D, \mathbb{C}^3),$$

where $\phi_{\mathbf{w}} = E_{k_0}(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}})$ and $\hat{w} = \hat{w}_{\mathbf{w},k_0} \in H_0^1(D)$ solves (4.6), is a continuous projection onto X_{k_0} . There exists $\varepsilon = \varepsilon(k_0) > 0$ such that for each $\mathbf{w} \in L^2(D, \mathbb{C}^3)$ the function $(k_0 - \varepsilon, k_0 + \varepsilon) \ni k \mapsto P_k \mathbf{w}$ is continuously differentiable in k with values in $L^2(D, \mathbb{C}^3)$.

Proof. To check that P_{k_0} maps into X_{k_0} , we note that $\nabla(\phi_{\mathbf{w}} - \hat{w})$ is a vector field that possesses a scalar potential solving the Helmholtz equation weakly in D . Thus, (3.3) and (3.4) imply that $P_{k_0} \mathbf{w} \in X_{k_0}$. Continuity of P_{k_0} from $L^2(D, \mathbb{C}^3)$ into $X_{k_0} \subset L^2(D, \mathbb{C}^3)$ with respect to the norm in $L^2(D, \mathbb{C}^3)$ is clear. To check that P_{k_0} is indeed a projection onto X_{k_0} , choose $\mathbf{w} \in X_{k_0}$ and consider $\phi_{\mathbf{w}} = E_{k_0}(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}})$. Lemma 4.4 states that $\mathbf{A}_{\mathbf{w}} = 0$, i.e., $\phi_{\mathbf{w}} = E_{k_0}(\mathbf{w}) \in H^1(D)$ and $\phi_{\mathbf{w}}$ solves the Helmholtz equation. That is, the right-hand side in (4.6) vanishes. The latter is, by assumption, uniquely solvable which shows that $\hat{w} = 0$ and $P_{k_0} \mathbf{w} = \nabla \phi_{\mathbf{w}} = \mathbf{w}$.

Concerning differentiability, recall from Lemma 3.6 that $k \mapsto \phi_{\mathbf{w}} = E_k(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}})$ is differentiable with values in $L^2(D, \mathbb{C}^3)$ and, moreover, that the derivative $k \mapsto \phi'_{\mathbf{w}}$ is constant on each connected component of D . Thus, $k \mapsto \nabla \phi'_{\mathbf{w}} = 0$. That is, $k \mapsto \nabla \phi_{\mathbf{w}}$ is constant. Differentiability of $k \mapsto \nabla \hat{w}$ follows from differentiating (4.6) with respect to k as in the proof of Theorem 4.3. \square

If the boundary ∂D is sufficiently regular, i.e. $\partial D \in C^4$, then we can avoid excluding Dirichlet eigenvalues using a different projection, again based on the decomposition $\phi_{\mathbf{w}} = E_k(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}})$ for $\mathbf{w} \in L^2(D, \mathbb{C}^3)$. Define $\hat{w} = \hat{w}_{\mathbf{w},k} \in H_0^2(D)$ as a weak solution to $[\Delta + k^2] \hat{w} = -[\Delta + k^2] \phi_{\mathbf{w}}$; i.e.,

$$\int_D [\Delta + k^2] \hat{w} [\Delta + k^2] \bar{\psi} \, d\mathbf{x} = \int_D \phi_{\mathbf{w}} [\Delta + k^2] \bar{\psi} \, d\mathbf{x} \quad \forall \psi \in H_0^2(D). \tag{4.7}$$

Relying on Holmgren’s Theorem, it is not difficult to show that the sesquilinear form in the latter formulation is elliptic on $H_0^2(D)$. That is, $\hat{w} \in H_0^2(D)$ is well-defined for $k > 0$ and $\mathbf{w} \in L^2(D, \mathbb{C}^3)$.

LEMMA 4.6. *Assume that $\partial D \in C^4$. Then the map $R_k : L^2(D, \mathbb{C}^3) \rightarrow X_k$,*

$$R_k \mathbf{w} = \nabla \phi_{\mathbf{w}} - \nabla [\Delta + k^2] \hat{w}_{\mathbf{w}}, \quad \mathbf{w} \in L^2(D, \mathbb{C}^3),$$

where $\phi_{\mathbf{w}} = E_k(\mathbf{w} - \nabla \times \mathbf{A}_{\mathbf{w}}) \in H^1(D)$ and $\hat{w}_{\mathbf{w}} \in H_0^2(D) \cap H^3(D)$ is as defined in (4.7), defines a projection onto X_k . For $\mathbf{w} \in L^2(D, \mathbb{C}^3)$, the function $k \mapsto R_k \mathbf{w}$ is continuously differentiable in k with values in $L^2(D, \mathbb{C}^3)$.

Proof. It is clear that the solution \hat{w} to (4.7) belongs to $H_0^2(D)$ by ellipticity and since $\|\hat{w}\|_{H^2(D)} \leq C\|\phi_{\mathbf{w}}\|$. Due to the regularity assumptions for ∂D , [11, Theorem 2.20] states that $\hat{w} \in H^4(D)$ if $\phi_{\mathbf{w}} \in H^2(D)$ such that $[\Delta + k^2]\phi_{\mathbf{w}} \in L^2(D)$. Moreover, $\|\hat{w}\|_{H^4(D)} \leq C\|\phi_{\mathbf{w}}\|_{H^2(D)}$. Interpolation estimates for Sobolev spaces (see, Appendix B of [20]) then imply that $\hat{w} \in H^3(D)$ if $\phi_{\mathbf{w}} \in H^1(D)$ and $\|\hat{w}\|_{H^3(D)} \leq C\|\phi_{\mathbf{w}}\|_{H^1(D)}$. The latter bound applies in our setting and shows firstly that $\nabla[\Delta + k^2]\hat{w} \in L^2(D)$ and secondly that R_k is well-defined and bounded.

The variational formulation (4.7) is tailored such that $\phi_{\mathbf{w}} - [(\Delta + k^2)\hat{w}] \in H^1(D)$ is a weak solution to the Helmholtz equation. Thus, $\nabla\phi_{\mathbf{w}} - \nabla[(\Delta + k^2)\hat{w}]$ satisfies both (3.3) and (3.4), and we conclude that $R_k \mathbf{w} \in X_k$. Moreover, if $\mathbf{w} \in X_k$, then $\phi_{\mathbf{w}}$ satisfies the Helmholtz equation, the right-hand side in (4.7) vanishes, and thus $\hat{w} = 0$. This shows that $R_k \mathbf{w} = \mathbf{w}$ if $\mathbf{w} \in X_k$. Continuous differentiability of $k \mapsto \nabla\hat{w}$ for $k > 0$ follows from differentiating (4.7) with respect to k as in the proof of Theorem 4.3. \square

5. Conditional characterization of transmission eigenvalues

In the next theorem, we complete inside-outside duality under the condition that the derivative

$$\alpha(k_0) := \left. \frac{d}{dk} (T_k P_k \mathbf{w}_0, P_k \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} \right|_{k=k_0}$$

that we computed in Theorem 4.3 does not vanish for a transmission eigenvalue $k_0^2 > 0$. One direction of this (conditional) characterization has already been shown in Theorem 4.1.

THEOREM 5.1 (Inside-outside duality). *Assume that $k_0 > 0$ and that $(k_0 - \varepsilon, k_0 + \varepsilon) \setminus \{k_0\}$ does not contain interior transmission eigenvalues.*

(a) *If Q is positive definite and $\lim_{k_0 - \varepsilon < k \nearrow k_0} \vartheta_*(k) = 0$ or $\lim_{k_0 + \varepsilon > k \searrow k_0} \vartheta_*(k) = 0$, then k_0^2 is a transmission eigenvalue. Further, if Q is negative definite and $\lim_{k_0 + \varepsilon > k \searrow k_0} \vartheta^*(k) = \pi$ or $\lim_{k_0 - \varepsilon < k \nearrow k_0} \vartheta^*(k) = \pi$, then k_0^2 is a transmission eigenvalue, too.*

(b) *If k_0^2 is either not a Dirichlet eigenvalue of $-\Delta$ in D or if $\partial D \in C^4$ the following holds. If k_0^2 is a transmission eigenvalue and if Q is positive definite, then $\lim_{k \nearrow k_0} \vartheta_* = 0$ or $\lim_{k \searrow k_0} \vartheta_* = 0$ if $\alpha(k_0) > 0$ or $\alpha(k_0) < 0$, respectively. If Q is negative definite and if k_0^2 is a transmission eigenvalue, then $\lim_{k \searrow k_0} \vartheta^* = \pi$ or $\lim_{k \nearrow k_0} \vartheta^* = \pi$ if $\alpha(k_0) > 0$ or $\alpha(k_0) < 0$, respectively.*

Proof.

(a) Assume that Q is positive definite and that $\lim_{k_0 - \varepsilon < k \nearrow k_0} \vartheta_*(k) = 0$. Due to Theorem 3.1,

$$\max_{\mathbf{w} \in X_k} \frac{\operatorname{Re}(T_k \mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}}{\operatorname{Im}(T_k \mathbf{w}, \mathbf{w})_{L^2(D, \mathbb{C}^3)}} \rightarrow \infty \quad \text{for } k \nearrow k_0.$$

Thus, there is a sequence $\{k_j\}_{j \in \mathbb{N}} \subset (k_0 - \varepsilon, k_0)$ such that $k_j \nearrow k_0$ and $\mathbf{w}_j \in X_{k_j}$ with $\|\mathbf{w}_j\|_{L^2(D, \mathbb{C}^3)} = 1$ such that $0 > \operatorname{Im}(T_{k_j} \mathbf{w}_j, \mathbf{w}_j)_{L^2(D, \mathbb{C}^3)} \rightarrow 0$ as $j \rightarrow \infty$ and $\operatorname{Re}(T_{k_j} \mathbf{w}_j, \mathbf{w}_j)_{L^2(D, \mathbb{C}^3)} \leq 0$ for j large enough. Let $v_j \in H_{\text{loc}}^1(\mathbb{R}^3)$ be the corresponding weak radiating solution to

$$\operatorname{div}(A \nabla v_j) + k^2 v_j = \operatorname{div}(Q \mathbf{w}_j) \quad \text{in } \mathbb{R}^3. \tag{5.1}$$

Since the sequence \mathbf{w}_j is bounded in $L^2(D, \mathbb{C}^3)$, there exists a weakly convergent subsequence $\mathbf{w}_j \rightharpoonup \mathbf{w}_0$ in $L^2(D, \mathbb{C}^3)$ as $j \rightarrow \infty$. In particular, $\mathbf{w}_0 \in X_{k_0}$, and $v_j \rightharpoonup v_{k_0}$ weakly in $H^1(B(0, R))$ for all radii $R > 0$ where $v_{k_0} \in H^1_{\text{loc}}(\mathbb{R}^3)$ is the corresponding weak radiating solution to (5.1) with right-hand side $\text{div}(Q\mathbf{w}_0)$. In the proof of Lemma 2.2, we have already shown that

$$\text{Im}(T_{k_j} \mathbf{w}_j, \mathbf{w}_j)_{L^2(D, \mathbb{C}^3)} = \frac{k}{4\pi^2} \|v_j^\infty\|_{L^2(\mathbb{S}^2)}^2.$$

The left hand side converges to zero and the right hand side to $k_0/(4\pi^2) \|v_{k_0}\|_{L^2(\mathbb{S}^2)}^\infty$. We conclude that $v_{k_0}^\infty = 0$ and v_{k_0} vanish in the exterior of D by Rellich’s Lemma.

Assume now that $k_0^2 > 0$ is not a transmission eigenvalue. Then it follows that \mathbf{w}_0 and v_{k_0} vanish everywhere such that \mathbf{w}_j and v_j converge weakly to zero as $j \rightarrow \infty$. As in the proof of Lemma 2.2, we define $\mathbf{g}_j = (\mathbf{w}_j - \nabla v_j)$ and find

$$(T_{k_j} \mathbf{w}_j, \mathbf{w}_j)_{L^2(D, \mathbb{C}^3)} = (Q\mathbf{g}_j, \mathbf{g}_j)_{L^2(D, \mathbb{C}^3)} + \int_D [|\nabla v_j|^2 - k_j^2 |v_j|^2] \, d\mathbf{x} - \int_{|x|=R} \frac{\partial v_j}{\partial \nu} \overline{v_j} \, dS.$$

Considering the real part of this equation shows that

$$\int_D |\nabla v_j|^2 \, d\mathbf{x} \leq \int_D k_j^2 |v_j|^2 \, d\mathbf{x} + \int_{|x|=R} \frac{\partial v_j}{\partial \nu} \overline{v_j} \, dS.$$

Since v_j converges weakly to zero in $H^1(B(0, R))$ for arbitrary large $R > 0$, the v_j converge strongly in $L^2(D)$ to zero. The integrals $\int_{|x|=R} (\partial v_j / \partial \nu) \overline{v_j} \, dS$ also tend to zero as $j \rightarrow \infty$ since the far field v^∞ of v_{k_0} vanishes. Thus, the right hand side tends to zero. That is, $\int_D |\nabla v_j|^2 \, d\mathbf{x} \rightarrow 0$ as $j \rightarrow \infty$. Therefore, $v_j \rightarrow 0$ strongly in $H^1(D)$. The closedness of the solution operator to (5.1) (see Lemma A.1) implies that $\mathbf{w}_j \rightarrow 0$ in $L^2(D, \mathbb{C}^3)$ as $j \rightarrow \infty$, which contradicts the assumption $\|\mathbf{w}_j\|_{L^2(D, \mathbb{C}^3)} = 1$. This proves the assertion for positive definite Q . The case where $\lim_{k_0+\varepsilon > k \searrow k_0} \vartheta_*(k) = 0$ or $Q \leq 0$ can be treated using analogous arguments. Part (b) directly follows from Lemma 4.1. \square

6. Explicit conditions for the contrast

In this section, we show that if Q is positive definite there exist transmission eigenvalues k_0^2 with positive derivative $\alpha(k_0) > 0$ under certain assumptions on the contrast Q stated below. To outline the subsequent estimates, we will first set up conditions for constant and isotropic contrast $Q = q \text{Id}$ and in a second step derive conditions for perturbations of such contrasts. To simplify notation, we abbreviate the L^2 -norm by $\|u\| := \|u\|_{L^2(D)}$ or $\|\mathbf{u}\| := \|\mathbf{u}\|_{L^2(D, \mathbb{C}^3)}$.

Assume for a moment that k_0^2 is an interior transmission eigenvalue with eigenpair $(u_0, w_0) \in L^2(D) \times L^2(D)$ for contrast Q , and recall that $v_{k_0} = v_0 := u_0 - w_0 \in H^1_0$ satisfies

$$\int_D (A \nabla v_{k_0} \cdot \nabla \overline{\psi} - k_0^2 v_{k_0} \overline{\psi}) \, d\mathbf{x} = \int_D (Q \nabla w_0 \cdot \nabla \overline{\psi} \, d\mathbf{x} \quad \forall \psi \in H^1(D). \tag{6.1}$$

The choice $\psi = 1$ shows that $v_{k_0} \in \tilde{H}^1_0(D)$ where

$$\tilde{H}^1_0(D) := \left\{ \varphi \in H^1_0(D), \int_D \varphi \, d\mathbf{x} = 0 \right\}.$$

Before setting up conditions for Q , we further note by the min-max principle that the smallest eigenvalue ρ_0 of the eigenvalue problem to find $(\rho, \varphi) \in \mathbb{R} \times \tilde{H}^1_0(D)$ such that

$$\int_D \nabla \varphi \cdot \nabla \overline{\psi} \, d\mathbf{x} = \rho \int_D \varphi \overline{\psi} \, d\mathbf{x} \quad \forall \psi \in \tilde{H}^1_0(D) \tag{6.2}$$

is larger than the first Dirichlet eigenvalue of $-\Delta$ in D and given by $\rho_0 = \inf_{\varphi \in \tilde{H}_0^1(D)} \|\nabla \varphi\|^2 / \|\varphi\|^2$. Moreover, we denote by $1/\mu_0$ the smallest nontrivial Neumann eigenvalue of $-\Delta$ in D .

THEOREM 6.1. *Choose $0 < k^2 < 2\rho_0$ and $q_0 > 0$ such that*

$$q_0 > \max \left\{ \frac{k^2 - \rho_0}{\rho_0 - k^2/2}, 0 \right\} \quad \text{and} \quad \frac{(q_0 + 2)((q_0 - 1)^2 - 5)}{(q_0 + 1)^2} > 8\rho_0\mu_0. \quad (6.3)$$

Setting $Q = q_0 \text{Id}$ guarantees the existence of at least one transmission eigenvalue $k_0^2 < k^2$, and for all transmission eigenvalues $k_0^2 \leq k^2$, the derivative $\alpha(k_0^2) > 0$ is positive.

Proof. If we assume that $(u_0, w_0) \in L^2(D) \times L^2(D)$ is a transmission eigenpair for the eigenvalue $k_0^2 > 0$ and contrast $Q = q_0 \text{Id}$, Theorem 2.2 implies that $\nabla w_0 =: \mathbf{w}_0 \in X_{k_0}$. Thus, $\phi_{\mathbf{w}_0} = E_{k_0}(\mathbf{w}_0) \in H^1(D)$ solves the Helmholtz equation, and

$$4k_0 \text{Re} \int_D \overline{\phi_{\mathbf{w}_0}} v_{k_0} \, d\mathbf{x} = 4k_0 \text{Re} \int_D \frac{1}{k_0^2} \nabla \overline{\phi_{\mathbf{w}_0}} \cdot \nabla v_{k_0} \, d\mathbf{x} = \frac{4}{k_0} \text{Re} \int_D \overline{\mathbf{w}_0} \cdot \nabla v_{k_0} \, d\mathbf{x}.$$

Assume that Q can be written as $Q = q_0 \text{Id}$ for a constant $q_0 > 0$. Then $A = (1 + q_0) \cdot \text{Id}$, and by substituting $\psi = v_{k_0}$ in the variational formulation (6.1), we obtain

$$\frac{4}{k_0} \int_D \overline{\mathbf{w}_0} \cdot \nabla v_{k_0} \, d\mathbf{x} = \frac{4(q_0 + 1)}{q_0 k_0} \|\nabla v_{k_0}\|^2 - \frac{4k_0}{q_0} \|v_{k_0}\|^2.$$

Thus, $\alpha(k_0)$ is given by

$$\alpha(k_0) = -2k_0 \|v_{k_0}\|^2 + \frac{4}{k} \text{Re} \int_D \overline{\mathbf{w}_0} \cdot \nabla v_{k_0} \, d\mathbf{x} = \frac{4(q_0 + 1)}{q_0 k_0} \|\nabla v_{k_0}\|^2 - 2k_0 \left(\frac{2}{q_0} + 1 \right) \|v_{k_0}\|^2. \quad (6.4)$$

Furthermore, the definition of ρ_0 from (6.2) implies that $\rho_0 \|v\|^2 \leq \|\nabla v\|^2$ for all $v \in \tilde{H}_0^1(D)$; i.e.,

$$\alpha(k_0) \geq \left(\frac{4(q_0 + 1)}{q_0 k_0} \rho_0 - 2k_0 \left(\frac{2}{q_0} + 1 \right) \right) \|v_{k_0}\|^2 > 0 \quad \text{if} \quad 4(q_0 + 1)\rho_0 - 2(q_0 + 2)k_0^2 > 0.$$

The derivative $\alpha(k_0)$ is hence positive whenever

$$k_0^2 < \frac{2(q_0 + 1)\rho_0}{q_0 + 2} =: C(q_0) \quad \text{or, equivalently,} \quad q_0 > \max \left\{ \frac{k_0^2 - \rho_0}{\rho_0 - k_0^2/2}, 0 \right\}. \quad (6.5)$$

The left inequality, in particular, implies that for transmission eigenvalues $k_0^2 < C(q_0) < 2\rho_0$, the derivative $\alpha(k_0)$ is positive. To show the existence of transmission eigenvalues k_0^2 satisfying the latter bound, we use a result from [17]: there exists at least one transmission eigenvalue less than $C(q_0)$ if $(q_0 + 2)\rho_0 + 2C(q_0)^2\mu_0 < C(q_0)q_0$. (We exploited the equation before (3.23) in [17]; note that the definitions of ρ_0 and $\mu = \mu_0$ are exchanged.) Since $C(q_0) > \rho_0$, we write this condition equivalently as

$$q_0 > \frac{2\rho_0 + 2C(q_0)^2\mu_0}{C(q_0) - \rho_0}, \quad \text{i.e.,} \quad 8\rho_0\mu_0 < \frac{(q_0 + 2)((q_0 - 1)^2 - 5)}{(q_0 + 1)^2} =: \gamma(q_0). \quad (6.6)$$

□

REMARK 6.2. When the function γ from (6.6) is restricted to $(1 + \sqrt{5}, \infty)$, then it is monotonously increasing and thus invertible. The area in the (k_0, q_0) -plane where we showed that $\alpha(k_0)$ is positive is sketched in Figure 6.1.

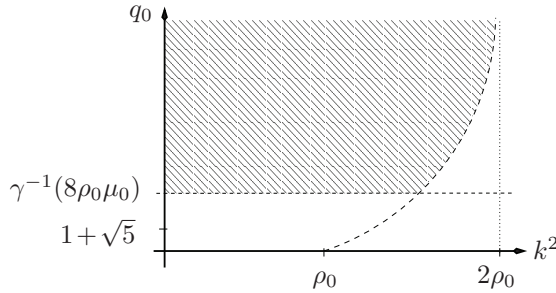


FIG. 6.1. If k_0^2 is a transmission eigenvalue for contrast $Q = q_0 \text{Id}$ and if (k_0, q_0) is inside the dashed area in the (k^2, q_0) -plane, then $\alpha(k_0) > 0$. Moreover, for each $q_0 > \gamma^{-1}(8\rho_0\mu_0)$, there exists a transmission eigenvalue k_0^2 such that (k_0, q_0) lies inside the dashed area.

Finally, we derive conditions for non-constant contrast by a perturbation argument. We assume $Q = q_0 \text{Id} + Q'$, or equivalently, $A = (1 + q_0) \text{Id} + Q'$ where $Q' \in L^\infty(D, \mathbb{R}^{3 \times 3})$ is a function taking values in the symmetric matrices such that for $c_0 > 0$ constant,

$$z^* Q(x) z = z^* [q_0 \text{Id} + Q'(x)] z \geq c_0 |z|^2 \quad \text{for almost all } x \in D \text{ and } z \in \mathbb{C}^3. \tag{6.7}$$

THEOREM 6.3. *Let $Q = q_0 \text{Id} + Q'$, for a $q_0 > 0$ and $Q' \in L^\infty(D, \mathbb{R}^{3 \times 3})$, be symmetric such that (6.7) holds and, additionally, $\|Q'\| [q_0 + \|Q'\|] < c_0(1 + c_0)$. Choose $0 < k < 2\rho_0$ such that*

$$k^2 < \frac{2\rho_0}{q_0 + 2} \left[1 + c_0 - \frac{\|Q'\|_\infty}{c_0} [1 + \|Q'\|_\infty] \right].$$

If $\|Q'\|_\infty$ is small enough (see the explicit k -independent bound (6.8)), then there exists at least one transmission eigenvalue less than k^2 , and for all such transmission eigenvalues it holds that $\alpha(k_0) > 0$.

Proof. Assume that $(u_0, w_0) \in L^2(D) \times L^2(D)$ is a transmission eigenpair for the eigenvalue $k_0^2 > 0$ and contrast Q . Choosing $\psi = v_{k_0} = u_0 - w_0$ in (4.1) and substituting the representations for Q and A , we obtain that

$$(1 + q_0) \|\nabla v_{k_0}\|^2 + \int_D Q' \nabla v_{k_0} \cdot \nabla \overline{v_{k_0}} \, dx - k_0^2 \|v_{k_0}\|^2 = \int_D (q_0 \mathbf{w}_0 \cdot \nabla \overline{v_{k_0}} + Q' \mathbf{w}_0 \cdot \nabla \overline{v_{k_0}}) \, dx.$$

Starting again as in (6.4), the derivative $\alpha(k_0)$ can hence be estimated by

$$\begin{aligned} \alpha(k_0) &= -2k_0 \|v_{k_0}\|^2 + \frac{4}{k_0} \text{Re} \int_D \overline{\mathbf{w}_0} \cdot \nabla v_{k_0} \, dx \\ &= -2k_0 \|v_{k_0}\|^2 + \frac{4}{k_0} \left[\frac{1 + q_0}{q_0} \|\nabla v_{k_0}\|^2 - \frac{k_0^2}{q_0} \|v_{k_0}\|^2 + \frac{1}{q_0} \int_D Q' (\nabla v_{k_0} - \mathbf{w}_0) \cdot \nabla \overline{v_{k_0}} \, dx \right] \\ &\geq \frac{4}{k_0 q_0} (1 + c_0) \|\nabla v_{k_0}\|^2 - 2k_0 \left(1 + \frac{2}{q_0} \right) \|v_{k_0}\|^2 - \frac{4}{k_0 q_0} \|Q'\|_\infty \|\mathbf{w}_0\| \|\nabla v_{k_0}\|. \end{aligned}$$

To substitute \mathbf{w}_0 in the last expression, we exploit that $(T_{k_0} \mathbf{w}_0, \mathbf{w}_0)_{L^2(D, \mathbb{C}^3)} = 0$ due to Theorem 2.2 and estimate

$$c_0 \|\mathbf{w}_0\|^2 \leq \int_D Q \mathbf{w}_0 \cdot \overline{\mathbf{w}_0} \, dx = (T_{k_0} \mathbf{w}_0, \mathbf{w}_0) - \int_D Q \nabla v_{k_0} \cdot \overline{\mathbf{w}_0} \, dx \leq \|Q\|_\infty \|\nabla v_{k_0}\| \|\mathbf{w}_0\|.$$

Thus, $\|\mathbf{w}_0\| \leq (q_0 + \|Q'\|_\infty)/c_0 \|\nabla v_{k_0}\|$, and

$$\alpha(k_0) \geq \frac{4}{k_0 q_0} [1 + c_0 - \|Q'\|_\infty (q_0 + \|Q'\|_\infty)/c_0] \|\nabla v_{k_0}\|^2 - 2k_0 \left(1 + \frac{2}{q_0}\right) \|v_{k_0}\|^2.$$

Recall from the last proof that $\rho_0 \|v\|^2 \leq \|\nabla v\|^2$ for all $v \in \tilde{H}_0^1(D)$. Therefore, we have the estimate

$$\alpha(k_0) \geq \frac{4}{k_0 q_0} \left[1 + c_0 - \frac{\|Q'\|_\infty}{c_0} [q_0 + \|Q'\|_\infty] - \frac{k_0^2 q_0}{2\rho_0} \left(1 + \frac{2}{q_0}\right)\right] \|\nabla v_{k_0}\|^2.$$

Since $v_{k_0} \in H_0^1(D)$ cannot be constant, multiplication with $2\rho_0/(q_0 + 2)$ yields the two conditions

$$k_0^2 < \frac{2\rho_0}{q_0 + 2} \left[1 + c_0 - \frac{\|Q'\|_\infty}{c_0} [q_0 + \|Q'\|_\infty]\right] := C(q_0, Q')$$

and

$$\|Q'\|_\infty [q_0 + \|Q'\|_\infty] < c_0(1 + c_0).$$

We proceed as in the case of constant contrast. (Recall that $1/\mu_0^2$ is the smallest non-trivial Neumann eigenvalues of $-\Delta$ in D .) Exploiting the bound from [17] for the existence of transmission eigenvalues as in the proof of Theorem 6.1 shows that there exists at least one transmission eigenvalue less than $C(q_0, Q')$ if $(c_0 + 2)\rho_0 + 2C(q_0, Q')^2 \mu_0 < C(q_0, Q')c_0$. Plugging $C(q_0, Q')$ into the last inequality explicitly shows that it can be rewritten as

$$\begin{aligned} \frac{(c_0 + 2)(q_0 + 2)}{2c_0} &< \left[1 + c_0 - \frac{\|Q'\|_\infty}{c_0} [q_0 + \|Q'\|_\infty]\right] \\ &\times \left[1 - \frac{4\rho_0 \mu_0}{(q_0 + 2)c_0} \left[1 + c_0 - \frac{\|Q'\|_\infty}{c_0} [q_0 + \|Q'\|_\infty]\right]\right]. \end{aligned} \tag{6.8}$$

For a given $q_0 > 0$, this inequality holds true if the perturbation $\|Q'\|_\infty$ is small enough. □

7. On the numerical detection of transmission eigenvalues

In this section, we present a method to numerically compute transmission eigenvalues from far field data using the theoretical results from the previous sections. The setting we choose involves a contrast function of the form $Q = q_0 \text{Id}$ for a constant $q_0 > 0$. We furthermore present numerical results both for positive and negative definite contrast and also for three different scatterers: the unit ball, the unit cube, and a non-convex object consisting of a cylinder attached to a cube.

To numerically solve the corresponding scattering problems, we rewrite the Helmholtz equation (1.1) for the total field as

$$\Delta u + k_{\text{int}}^2 u = 0 \quad \text{in } D, \quad \Delta u + k_{\text{ext}}^2 u = 0 \quad \text{in } \mathbb{R}^3 \setminus \bar{D},$$

where $k_{\text{ext}}^2 = k^2$ and $k_{\text{int}}^2 = 1/(q_0 + 1)k^2$. Writing $[\cdot]^+$ and $[\cdot]^-$ for the exterior and interior trace operators, respectively, the jump conditions for u on ∂D are

$$u|^+ = u|^- \quad \text{and} \quad (q_0 + 1) \frac{\partial u}{\partial \nu} \Big|^- = \frac{\partial u}{\partial \nu} \Big|^+ \quad \text{on } \partial D.$$

Recall that the total field $u = u^i + u^s$ decomposes into an incident plane wave u^i and the corresponding radiating scattered field u^s . To compute numerical approximations of the scattered and far field, we use a boundary integral equation due to Kleinman and Martin, see [18, 24],

$$\begin{bmatrix} N_{k_{\text{ext}}} + (1+q)N_{k_{\text{int}}} & K'_{k_{\text{ext}}} + K'_{k_{\text{int}}} \\ K_{k_{\text{ext}}} + K_{k_{\text{int}}} & -S_{k_{\text{ext}}} - 1/(q+1)S_{k_{\text{int}}} \end{bmatrix} \begin{bmatrix} u|^{+} \\ \frac{\partial u}{\partial \nu}|^{+} \end{bmatrix} = \begin{bmatrix} \frac{\partial u^i}{\partial \nu}|^{+} \\ -u^i|^{+} \end{bmatrix} \tag{7.1}$$

where S_k, K_k, K'_k and N_k are the single-layer potential, double-layer potential, adjoint double-layer potential, and hypersingular boundary operators for wave number k . Using the software package BEM++ (see [24]), we approximate the solution to this system of boundary integral equations using a Galerkin method. For a fixed set of 120 uniformly distributed directions $\{\theta_j\}_{j=1}^{120} \subset \mathbb{S}^2$ on the sphere, we approximate the far field $u^\infty(\theta_j, \theta_\ell)$, $1 \leq j, \ell \leq 120$, to the scattered field for an incident plane wave with direction θ_ℓ using well-known integral representation formulas for u^∞ . This yields approximate scattering data $(u_{\text{appr}}^\infty(\theta_j, \theta_\ell))_{j, \ell=1}^{120}$ that can be interpreted as an interpolation discretization F_{appr} of the far field operator; see [13]. Without going into details, such interpolation discretizations converge to F if, roughly speaking, the number of directions θ_j tends to infinity and the computed far fields u_{appr}^∞ converge to the exact values.

To verify that our numerical approximation of $F = F_k$ is sufficiently accurate, we exploit that if the scatterer D is the unit ball with positive contrast $q_0 = 10$, one can compute the eigenvalues of the far field operator F analytically in terms of Bessel functions, relying on a series representation of the scattered field; see [9]. In Figure 7.1(a), we plot the eigenvalues λ_j and $\lambda_{j,\text{appr}}$ of the far field operator F and its approximation F_{appr} for a single wave number $k = 5$. Since analytic expressions for cubic scatterers are not available, we plot in Figure 7.1(b) the corresponding computed eigenvalues $\lambda_{j,\text{appr}}$ for the unit cube with contrast $q_0 = -0.9$ and wave number $k = 2.0$ together with the circle on which the exact eigenvalues lie.

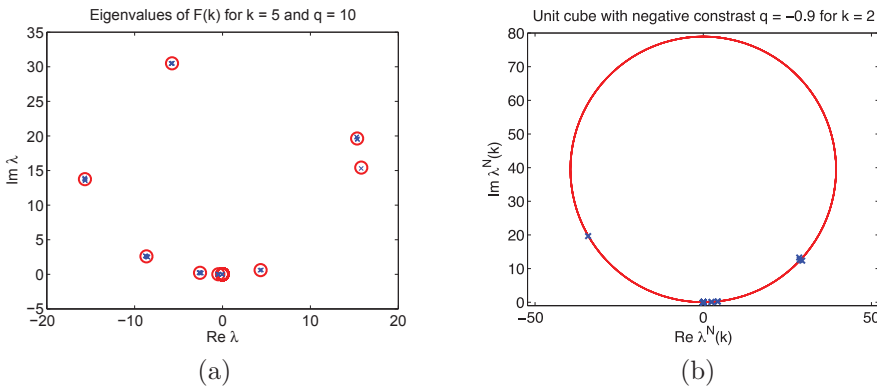


FIG. 7.1. (a) $D = B(0,1)$, $q_0 = 10$, $k = 5$. Red circles mark analytical eigenvalues of F and blue crosses mark numerically computed eigenvalues of F_{appr} . (b) $D = [-1,1]^3$, $q_0 = -0.9$, $k = 2.0$. Blue crosses mark numerically computed eigenvalues of F_{appr} ; the exact eigenvalues of D lie on the red circle.

Next we compute the eigenvalues $\lambda_{j,\text{appr}}, j = 1, \dots, 120$ of $F_{\text{appr}}(k)$ for a grid of wave numbers and examine how their phases behave close to transmission eigenvalues k_0^2 . Due to Theorem 5.1 we expect the eigenvalue λ^* with the largest phase ϑ^* or the eigenvalue λ_* with the smallest phase ϑ_* to converge to zero from either the left or the right

side, implying that either the largest phase ϑ^* converges to π or the smallest phase ϑ_* converges to zero. Due to the polar coordinate representation of the eigenvalues, small errors in the approximated eigenvalues close to zero lead to large errors in the corresponding phases. Thus, we need to stabilize the computation of the phases of the approximate eigenvalues $\lambda_{j,\text{appr}}$ and proceed as in [19]. Assuming that the noise level of $F_{\text{appr}}(k)$ is $\varepsilon(k) = \|F_{\text{appr}}(k) - F(k)\|$, we omit all eigenvalues in the circle $\{|z| \leq \varepsilon(k)\}$ around zero. To further stabilize the phase computations, we afterwards exploit the a priori knowledge that the exact eigenvalues $\lambda_j(k)$ lie on the circle $\{z \in \mathbb{C}, |z - 8\pi^2 i/k| = 8\pi^2/k\}$ in the complex plane and project the eigenvalues $\lambda_{j,\text{appr}}(k)$ orthogonally onto this circle using the map

$$\mathcal{P}: \lambda \mapsto \frac{8\pi^2 i}{k} + \frac{8\pi^2}{k} \frac{\lambda - 8\pi^2 i/k}{|\lambda - 8\pi^2 i/k|}. \quad (7.2)$$

Then, we finally compute the phases of the projected eigenvalues $\mathcal{P}[\lambda_{j,\text{appr}}(k)]$. Figure 7.2 shows the dependence of these numerically computed phases on the wave number k , both for a unit ball with positive contrast and the unit cube with negative contrast as scattering objects. To indicate the stability of these phase curves under random noise, we have perturbed the numerically computed data $(u_{\text{appr}}^\infty(\theta_j, \theta_\ell))_{j,\ell=1}^{120}$ by adding a random matrix of size 120×120 containing normally distributed entries with mean zero such that the relative noise level in the spectral matrix norm equals 5% before computing $\mathcal{P}[\lambda_{j,\text{appr}}(k)]$. Due to this artificial noise and unavoidable numerical inaccuracies, the phase of eigenvalues with multiplicity $m > 1$ appears as a vertical cluster of m dots above the corresponding wave number k in figures 7.2(a) and (b).

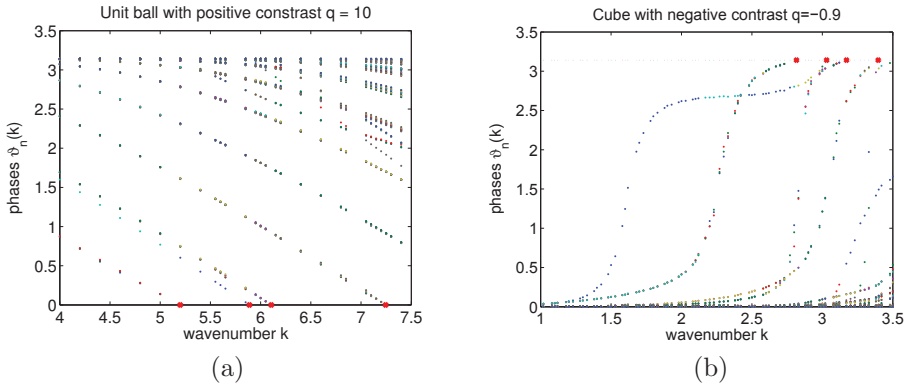


FIG. 7.2. Dots mark the phases of the projected numerical eigenvalues $\mathcal{P}[\lambda_{j,\text{appr}}]$ of $F_{\text{appr}}(k)$. (a) $D = B(0,1)$, $q_0 = 10$. (b) $D = [-1,1]^3$, $q_0 = -0.9$.

Finally, to obtain numerical approximations to interior transmission eigenvalues, we suggest the following method: In a first step, we neglect all those phases stemming from far field operator approximations $F_{\text{appr}}(k)$ with normality error $\|F_{\text{appr}}(k)F_{\text{appr}}^*(k) - F_{\text{appr}}^*(k)F_{\text{appr}}(k)\|/\|F_{\text{appr}}(k)F_{\text{appr}}^*(k)\|$ above a threshold that we consider as too high to provide accurate phase information errors. From the remaining phases, we compute those wave numbers where the discrete derivative of the smallest or largest phase changes sign, i.e., wave numbers where the extremal phase jumps. Depending on whether the extremal phase approaches the eigenvalues from the left or the right, we use the last two smallest or largest phases before the jump to linearly extrapolate the wave numbers

where the phase curve intersects the lines $\{\vartheta=0\}$ or $\{\vartheta=\pi\}$. The squares of these wave numbers are approximations of transmission eigenvalues. Table 7.1 indicates the round-about two-digit accuracy of these eigenvalue approximation schemes when the scatterer is a ball; the computed eigenvalues are marked in Figure 7.2 as red dots on $\{\vartheta=0\}$ in (a) and $\{\vartheta=\pi\}$ in (b).

		$k_{0,1}$	$k_{0,2}$	$k_{0,3}$	$k_{0,4}$
$D = B(0, 1), q_0 = 10$	computed ITE	5.199	5.888	6.106	7.245
	exact ITE	5.204	5.886	6.104	7.244
$D = [-1, 1]^3, q_0 = -0.9$	computed ITE	2.863	3.029	3.164	3.397

TABLE 7.1. Numerical approximations to the square roots $k_{0,j}, j=1, \dots, 4$, of four interior transmission eigenvalues $k_{0,j}^2$ for the two settings introduced above.

To show that the numerical scheme also works for non-convex scattering objects, we repeat this procedure for a scatterer consisting of a cylinder placed on a cube with contrast $q_0 = 10$. Figure 7.3(a) shows the geometry of this object, called *boxnose* in the sequel. Precisely the same computational technique as indicated above yields the phase curves shown in Figure 7.3(b). Finally, the above extrapolation algorithm leads to the approximations $k_{0,1} = 8.54, k_{0,2} = 8.823$, and $k_{0,3} = 9.259$ for three transmission eigenvalues $k_{0,j}^2, j = 1, 2, 3$.

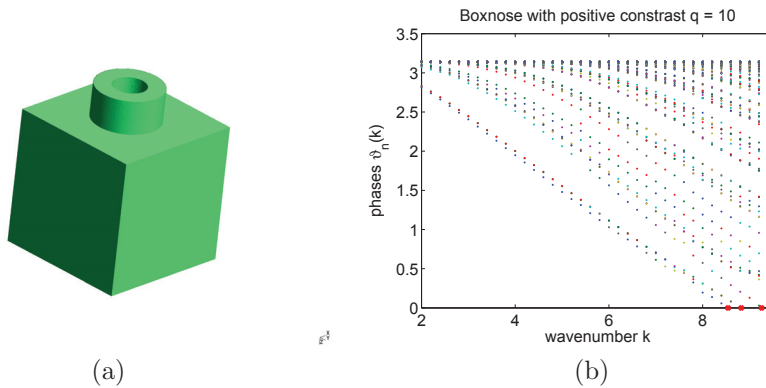


FIG. 7.3. (a) The *boxnose*. (b) Dots mark the phases of the projected numerical eigenvalues $\mathcal{P}[\lambda_{j,\text{appr}}(k)]$ of $F_{\text{appr}}(k)$. Red crosses on the k -axis mark the positions of the estimated square roots of three interior transmission eigenvalues.

Appendix A. A technical lemma.

LEMMA A.1. For $k > 0$ or $k = i$, the composition of the solution operator $L: L^2(D, \mathbb{C}^3) \rightarrow H^1_{\text{loc}}(\mathbb{R}^3)$ to the variational problem (2.7) with the restriction operator from \mathbb{R}^3 to D is closed from $L^2(D, \mathbb{C}^3)$ into $H^1(D)$.

Proof. We will merely provide the proof for $k = i$ and leave it to the reader to adapt the proof to positive wave numbers. Choose a sequence $v_j := Lf_j$ in the range of L with $\lim_{j \rightarrow \infty} v_j = v$ in $H^1(D)$. We have to show that there exists a function $f \in L^2(D, \mathbb{C}^3)$ such that $Lf = v$ and abbreviate the variational problem (2.7) as $a(v_j, \psi) = F_j(\psi)$ for all $\psi \in H^1(\mathbb{R}^3)$ with the continuous linear functional

$$F_j(\psi) := \int_D \nabla \bar{\psi} \cdot Q f_j \, d\mathbf{x}, \quad \psi \in H^1(\mathbb{R}^3),$$

as the right-hand side. The sequence v_j converges in $H^1(\mathbb{R}^3)$ and defines $F \in H^1(\mathbb{R}^3)^*$ by $F(\psi) := a(v, \psi)$ for $\psi \in H^1(\mathbb{R}^3)$. Continuity of a implies that $\|F_j - F\|_{H^1(\mathbb{R}^3)^*} \rightarrow 0$ as $j \rightarrow \infty$. Thus, it suffices to show that there is $f \in L^2(D, \mathbb{C}^3)$ such that $F(\psi) = \int_D \nabla \bar{\psi} \cdot Q \mathbf{f} \, d\mathbf{x}$. To this end, we consider the Hilbert space

$$H^\bullet_\bullet(D) = \left\{ u \in H^1(D), \int_D u \, d\mathbf{x} = 0 \right\} \quad \text{with inner product} \quad (\phi, \psi) \mapsto \int_D \nabla \phi \cdot \nabla \bar{\psi} \, d\mathbf{x}.$$

Due to Poincaré’s inequality, the resulting norm is equivalent to the standard norm in $H^1(D)$. Next, we set $\psi_\bullet = \psi - \int_D \psi \, d\mathbf{x} \in H^\bullet_\bullet(D)$ for any $\psi \in H^1(\mathbb{R}^3)$. Defining another functional $F_{\bullet,j} \in H^\bullet_\bullet(D)^*$,

$$F_{\bullet,j}(\psi_\bullet) = \int_D \nabla \psi_\bullet \cdot Q \mathbf{f}_j \, d\mathbf{x} \quad \forall \psi_\bullet \in H^\bullet_\bullet(D),$$

it follows that $F_j(\psi) = F_{j,\bullet}(\psi_\bullet)$ for all $\psi \in H^1(\mathbb{R}^3)$. Convergence of $\{F_j\}_{j \in \mathbb{N}}$ implies the existence of $F_\bullet \in H^\bullet_\bullet(D)^*$ such that $F_\bullet(\psi_\bullet) = F(\psi)$ for all $\psi \in H^1(\mathbb{R}^3)$. Recall that $(\psi_\bullet, \phi_\bullet)_{H^\bullet_\bullet(D)} = \int_D \nabla \psi_\bullet \cdot \nabla \bar{\phi}_\bullet \, d\mathbf{x}$, is an inner product in $H^\bullet_\bullet(D)$ and use Riesz’s representation theorem to obtain the existence of $v_\bullet \in H^\bullet_\bullet(D)$ such that

$$F_\bullet(\psi_\bullet) = \int_D \nabla v_\bullet \cdot \nabla \bar{\psi} \, d\mathbf{x} \quad \forall \psi_\bullet \in H^\bullet_\bullet(D).$$

Setting $\mathbf{f} := Q^{-1} \nabla v_\bullet \in L^2(D, \mathbb{C}^3)$ finally yields

$$F(\psi) = F_\bullet(\psi_\bullet) = \int_D \nabla v_\bullet \cdot \nabla \bar{\psi} \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q \mathbf{f} \, d\mathbf{x} = \int_D \nabla \bar{\psi} \cdot Q \mathbf{f} \, d\mathbf{x} \quad \forall \psi \in H^1(\mathbb{R}^3).$$

□

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