Positivity of a weakly singular operator and approximation of wave scattering from the sphere

Citation for published version:
Duncan, DB 2022, 'Positivity of a weakly singular operator and approximation of wave scattering from the sphere', *Journal of Integral Equations and Applications*, vol. 34, no. 3, pp. 317-333. https://doi.org/10.1216/jie.2022.34.317

Digital Object Identifier (DOI):
10.1216/jie.2022.34.317

Published In:
Journal of Integral Equations and Applications

JOURNAL OF INTEGRAL EQUATIONS AND APPLICATIONS
Vol. , No. , YEAR
https://doi.org/jie.YEAR..PAGE

POSITIVITY OF A WEAKLY SINGULAR OPERATOR AND APPROXIMATION OF WAVE SCATTERING FROM THE SPHERE

DUGALD B DUNCAN

ABSTRACT. We investigate properties of a family of integral operators $\mathscr{B}$ with a weakly singular compactly supported zonal kernel function on the surface S of the unit 3D sphere. The support is over a spherical cap of height $h \in (0,2]$. Operators like this arise in some common types of approximations of time domain boundary integral equations (TDBIE) describing the scattering of acoustic waves from the surface of the sphere embedded in an infinite homogeneous medium where h is directly related to the time step size.

We show that the Legendre polynomials of degree $\ell \geq 0$ satisfy $\int_0^h P_\ell(1-z^2/2)\,dz > 0$ for all $h \in (0,2]$ and, using spherical harmonics and the Funk-Hecke formula for the eigenvalues of $\mathscr{B}$, that this is a key to unlocking positivity results for a subfamily of these operators. As well as positivity results we give detailed upper and lower bounds on the eigenvalues of $\mathscr{B}$ and on $\int_S u(\mathbf{x})\,(\mathscr{B}u)(\mathbf{x})\,d\mathbf{x}$. We give various examples of where these results are useful in numerical approximations of the TDBIE on the sphere and show that positivity of $\mathscr{B}$ is a necessary condition for these approximation schemes to be well-defined. We also show the connection between the results for eigenvalues and the separation of variables solution of the TDBIE on the sphere. Finally we show how this relates to scattering from an infinite flat surface and Cooke's 1937 result $\int_0^r J_0(z)\,dz > 0$ for all $r > 0$.

1. Introduction

We investigate properties, including of the eigenvalues, of a family of operators $\mathscr{B} : H^{-1/2}(S) \to H^{1/2}(S)$ with a weakly singular kernel on the surface S of the unit sphere in three space dimensions. We discuss the Hilbert spaces $H^{\pm 1/2}(S)$ later. The operator family is defined by

$$(\mathscr{B}u)(\mathbf{x}) = \frac{1}{2\pi}\int_S \frac{H(h-|\mathbf{x}-\mathbf{y}|)F(|\mathbf{x}-\mathbf{y}|)u(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y}, \quad \forall \mathbf{x} \in S,\, h \in (0,2] \tag{1.1}$$

where $F(0) > 0$, $F \in L_1(0,2)$ and H is the Heaviside function. Note that the unit sphere has diameter 2 and so $|\mathbf{x}-\mathbf{y}| \leq 2$ for all pairs of points on its surface. The Heaviside function acts to cut off the kernel function outside a spherical cap on the sphere when $h < 2$.

Operators like this arise in the approximation of time domain boundary integral equations (TDBIEs) for wave scattering from surfaces (not only from spheres) by Galerkin and other methods which use temporal basis functions with support of width $\mathscr{O}(h)$. Depending on the method used, the parameter h is the time step size or a small multiple of it, and the function $F(r)$ is related to the time discretisation basis functions. F is usually a piecewise polynomial parameterised by h, and cuts off for $r > h$. We have included the Heaviside function explicitly in the definition of the operator to make this clear,

2020 *Mathematics Subject Classification.* 65R20, 42C10.

Key words and phrases. numerical approximation of time domain boundary integral equation, weakly singular operator on sphere, positivity of eigenvalues, integral positivity, properties of Legendre polynomials.

and to simplify some of the exposition below. Integral positivity of such operators (see Definition 1.1 below) is a key part of the analysis of TDBIE approximations since it guarantees that the time stepping process is well defined. It might also be a useful tool in stability and related convergence analysis.

It is important in what follows that the kernel function in (1.1) can be written as a zonal function $G(\mathbf{x}.\mathbf{y})$ depending only on the dot product $\mathbf{x}.\mathbf{y}$. The kernel function is clearly a function of the distance $|\mathbf{x}-\mathbf{y}|$, and the dot product representation follows from the identity

$$|\mathbf{x}-\mathbf{y}|^2 = (\mathbf{x}-\mathbf{y}).(\mathbf{x}-\mathbf{y}) = \mathbf{x}.\mathbf{x}+\mathbf{y}.\mathbf{y}-2\mathbf{x}.\mathbf{y} = 2-2\mathbf{x}.\mathbf{y}$$

for points $\mathbf{x},\mathbf{y} \in S$.

In our case we have kernel function

$$\frac{1}{2\pi}\frac{H(h-|\mathbf{x}-\mathbf{y}|)F(|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|} = G_0(|\mathbf{x}-\mathbf{y}|) = G(\mathbf{x}.\mathbf{y})$$

where

$$G_0(r) = \frac{H(h-r)F(r)}{2\pi r} \quad \text{and} \quad G(t) = \frac{H(h-\sqrt{2-2t})F(\sqrt{2-2t})}{2\pi\sqrt{2-2t}}. \tag{1.2}$$

The definition (1.2) of G allows us write the operator (1.1) more neatly as

$$(\mathscr{B}u)(\mathbf{x}) = \int_S G(\mathbf{x}.\mathbf{y})u(\mathbf{y})\,d\mathbf{y}. \tag{1.3}$$

The kernel function $G(\mathbf{x}.\mathbf{y})$ is of course singular when $\mathbf{x}=\mathbf{y}$, but since $F \in L_1(0,2)$ as stated in the definition of (1.1), the function G satisfies

$$\int_{-1}^{1} |G(t)|\,d\eta = \frac{1}{2\pi}\int_0^h |F(z)|\,dz < \infty.$$

In other words, $G \in L_1(-1,1)$ when $F \in L_1(0,2)$. This is important when evaluating the eigenvalues.

We also investigate the integral positivity or otherwise of the kernel function.

Definition 1.1 (Integral positivity)**.** *For $h \in (0,2]$, the operator $\mathscr{B}$ defined by (1.1) and (1.3) is said to be integrally positive if and only if*

$$\int_S u(\mathbf{x})(\mathscr{B}u)(\mathbf{x})\,d\mathbf{x} = \int_S\int_S G(\mathbf{x}.\mathbf{y})u(\mathbf{y})u(\mathbf{x})\,d\mathbf{y}\,d\mathbf{x} \geq 0 \quad \forall\, u \in H^{-1/2}(S),$$

and integrally positive definite when strict inequality holds for all nonzero $u \in H^{-1/2}(S)$.

We show below in Sections 3 and 4 that a key to obtaining results about positivity of eigenvalues of the weakly singular operator $\mathscr{B}$ on the sphere's surface, and of the integral positivity defined above, is determining if the quantity

$$I_\ell(h) := \int_0^h P_\ell(1-z^2/2)\,dz$$

is strictly positive for all integers $\ell \geq 0$ and $h \in (0,2]$, where P_ℓ is the Legendre polynomial of degree ℓ. This is the analogue of the so-called Cooke's result or inequality (see e.g. [5] or [16, Lemma 5.1])

$$\int_0^r J_0(z)\,dz > 0, \quad \forall\, r > 0$$

which plays a similar role in determining positivity properties of operator $\mathscr{B}$ applied on an infinite flat plane instead of a sphere.

In the next section we introduce the spherical harmonic functions and function spaces on the sphere surface. In Section 3 we introduce the Funk-Hecke formula for eigenvalues of zonal operators on the sphere surface and derive lower and upper bounds for the eigenvalues of operators in the form (1.1). The proof of the key result on the eigenvalue bounds is given in Section 4. In Section 5 we give examples of the application of the results in numerical approximations of TDBIEs and of the convolution Volterra integral equation that arises in the separation of variables solution of the TDBIE. We finish with brief conclusions and discussion.

2. Functions and function spaces on the sphere surface

We first define the spherical harmonic functions which are the Fourier modes on the sphere surface, and then the Hilbert spaces $H^s(S)$ for $s \in \mathbb{R}$.

2.1. ***Spherical harmonics.*** We follow the notation of [13] here using the standard spherical surface coordinates on S with

$$\mathbf{x} = (\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)^T \in S, \quad \theta \in [0,\pi],\ \phi \in [0,2\pi]. \tag{2.1}$$

We will abuse notation sometimes to write functions with arguments $\mathbf{x} \in S$ and (θ,ϕ) interchangeably when the meaning is clear.

Consider functions or distributions u defined for $\mathbf{x}$ on S by

$$u(\mathbf{x}) \equiv u(\theta,\phi) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} u_\ell^m Y_\ell^m(\theta,\phi) \tag{2.2}$$

where the spherical harmonics

$$Y_\ell^m(\mathbf{x}) \equiv Y_\ell^m(\theta,\phi) = (-1)^\ell \sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}\, P_\ell^m(\cos\theta)\, e^{im\phi} \tag{2.3}$$

and P_ℓ^m is the associated Legendre function of degree ℓ and order m (see [14, Ch. 14]). The coefficients u_ℓ^m are given by

$$u_\ell^m = \int_0^{2\pi}\int_0^{\pi} u(\theta,\phi)\overline{Y_\ell^m(\theta,\phi)}\sin\theta\, d\theta\, d\phi \tag{2.4}$$

where the overbar denotes complex conjugation. This is a consequence of the orthonormality of the spherical harmonics:

$$\int_0^{2\pi}\int_0^{\pi} Y_k^n(\theta,\phi)\overline{Y_\ell^m(\theta,\phi)}\sin\theta\, d\theta\, d\phi = \delta_{n-m}\delta_{k-\ell}, \quad \forall\, k,\ell \geq 0,\ |n| \leq k, |m| \leq \ell$$

where δ_j is the usual discrete delta function.

2.2. *The spaces $H^{-1/2}(S)$ and $H^{1/2}(S)$*. On the surface of the sphere we define the spaces $H^s(S)$ as follows for all $s \in \mathbb{R}$, including $s = \pm 1/2$ following for example [1, Ch. 6.5] or [13, Ch. 2.5]. There are differences in detail between these two references (notation and the choice of factor $(1+\ell)$ or $(1+2\ell)$), but the resulting spaces are equivalent to the following definition.

Definition 2.1. *The function or distribution u defined on the surface of the unit sphere S is said to be in the space $H^s(S)$ if and only if the norm defined here satisfies*

$$\|u\|^2_{H^s(S)} := \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} |u_\ell^m|^2 (\ell + 1/2)^{2s} < \infty$$

where u_ℓ^m is defined by (2.4) and $s \in \mathbb{R}$.

The requirements for $u \in H^{-1/2}(S)$ are then clear, and we investigate below the properties of $\mathscr{B}u$ and which of the $H^s(S)$ spaces it is in. To do this we need to know the details of the eigenvalues of the operator.

3. Eigenvalues and eigenfunctions of operator $\mathscr{B}$

3.1. *Eigenvalues and eigenfunctions*. The Funk-Hecke formula (see e.g. [11, 15]) gives a direct means to evaluate the eigenvalues of the operator $\mathscr{B}$ from (1.1) on the surface S of the unit sphere in $\mathbb{R}^3$. The eigenfunctions are the spherical harmonics Y_ℓ^m introduced above. Note that the eigenvalues are independent of the order m and only depend on degree ℓ. This simplifies calculations greatly. It is convenient to use the notation and dot product version of the operator as given in (1.3).

Proposition 3.1 (The Funk-Hecke formula)**.** *If $G \in L_1[-1,1]$, then*

$$(\mathscr{B}Y_\ell^m)(\mathbf{x}) = \int_S G(\mathbf{x}.\mathbf{y}) Y_\ell^m(\mathbf{y})\, d\mathbf{y} = \lambda_\ell Y_\ell^m(\mathbf{x}), \quad \text{where } \lambda_\ell = 2\pi \int_{-1}^{1} G(t) P_\ell(t)\, dt$$

for all $\mathbf{x} \in S$ and all $|m| \le \ell$, $\ell \ge 0$.

As an example of this we obtain the well known formula for the eigenvalues of an operator associated with boundary integral solutions of the Laplace equation.

Example 3.2 (Single layer potential)**.** *Consider the single layer potential operator $\mathscr{S} : H^{-1/2}(S) \to H^{1/2}(S)$ defined by*

$$(\mathscr{S}u)(\mathbf{x}) = \frac{1}{4\pi} \int_S \frac{u(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}, \quad \forall \mathbf{x} \in S$$

on the sphere surface S. The kernel function is

$$\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} = \frac{1}{4\pi\sqrt{2-2\mathbf{x}.\mathbf{y}}} = G(\mathbf{x}.\mathbf{y}).$$

So in Proposition 3.1

$$G(t) = \frac{1}{4\pi\sqrt{2-2t}} \in L_1[-1,1],$$

and the eigenvalues are

$$\lambda_\ell = \frac{1}{2}\int_{-1}^{1} \frac{1}{\sqrt{2-2t}} P_n(t)\,dt = \frac{1}{2}\int_0^2 P_n\left(1-\frac{z^2}{2}\right) dz = \frac{1}{2\ell+1}, \quad \ell = 0,1,2,\dots \tag{3.1}$$

which are of course well-known. See e.g. [13, 3.2.30].

The change of variable $z = \sqrt{2-2t}$ is useful later.

3.2. ***Positivity of the eigenvalues of operator*** $\mathscr{B}$**.** Applying Proposition 3.1 to the operator $\mathscr{B}$ using the representation (1.3) with $G(t)$ defined in (1.2), we have $G \in L_1(-1,1)$ as required and so

$$\lambda_\ell = \int_{1-h^2/2}^{1} \frac{F(\sqrt{2-2t})}{\sqrt{2-2t}} P_\ell(t)\,dt = \int_0^h F(z) P_\ell\left(1-\frac{z^2}{2}\right) dz, \quad \ell = 0,1,2,\dots, \tag{3.2}$$

for $0 < h \le 2$, taking into account the compact support of the kernel function. We also use a change of variable $z = 2\sin(\eta/2)$ to obtain the alternative expression

$$\lambda_\ell = \int_0^\mu F\left(\sin(\eta/2)\right) P_\ell(\cos\eta)\cos(\eta/2)\,d\eta \tag{3.3}$$

where

$$h = 2\sin(\mu/2)$$

for $0 < \mu \le \pi$. This representation is useful because there are various identities satisfied by $P_\ell(\cos\eta)$, including a Fourier sine series used in this subsection and an integral representation used in the next.

In this subsection we examine various functions F for which the operator (1.1) has positive eigenvalues. We combine two approaches to get the results: obtain a lower bound on λ_ℓ valid for small h; and obtain a bound valid for larger h by substituting the Fourier sine series for $P_\ell(\cos\eta)$ into (3.3), integrating and showing that each term is non-negative.

Small h lower bound. We note that

$$P_\ell\left(1-\frac{z^2}{2}\right) = 1 - z^2\frac{\ell(\ell+1)}{4} + z^4\frac{(\ell^2-1)\ell(\ell+2)}{64} - z^6\frac{(\ell^2-4)(\ell^2-1)\ell(\ell+3)}{2304} + \cdots,$$

where the series continues in even powers of z with alternating signs up to and including the term $z^{2\ell}$. We substitute this into (3.2) in the following examples.

Example 3.3. *Set* $F(z) = 1$ *in (3.2). Then the eigenvalues satisfy*

$$\lambda_0 = h > 0, \quad \lambda_1 = h - h^3/6 > 0, \quad \forall\, h \in (0,2]$$

and, by Taylor expansion,

$$\lambda_\ell > h - h^3\frac{\ell(\ell+1)}{12} + \mathscr{O}(h^5) > 0 \quad \text{when} \quad 0 < h^2 < \frac{12}{\ell(\ell+1)},$$

for $\ell \ge 2$ *since the* $\mathscr{O}(h^5)$ *term is positive.*

The next example arises in a stability proof for an approximation method for a time domain boundary integral equation.

Example 3.4. *Set $F(z) = (1-4z/h)(1-z/h)^2$ in (3.2) and note that*

$$\int_0^h F(z)\,dz = 0, \quad \int_0^h F(z)z^{2k}\,dz = -C_k h^{2k+1} \le 0, \quad k \ge 1$$

where constants $C_k > 0$. Then the eigenvalues satisfy

$$\lambda_0 = 0, \quad \lambda_1 = h^3/60 > 0, \quad \lambda_2 = h^3/20 - 3h^5/560 > 0, \ h \in (0,2],$$

$$\lambda_\ell > h^3\frac{\ell(\ell+1)}{120} - h^5\frac{(\ell^2-1)\ell(\ell+2)}{4480} + \mathscr{O}(h^7) > 0 \quad \text{when} \quad 0 < h^2 < \frac{112}{3(\ell-1)(\ell+2)}.$$

for $\ell \ge 3$, since the $\mathscr{O}(h^7)$ term is positive.

Notice that the range of h where positivity is assured by this approach is dependent on ℓ.

Lower bound valid for larger h. Here we use the Fourier sine expansion [14, 14.13.3]

$$P_\ell(\cos\eta) = \sum_{k=0}^{\infty} R(\ell,k)\sin((\ell+1+2k)\eta)$$

where

$$R(\ell,k) = \frac{2\Gamma(\ell+k+1)\Gamma(k+1/2)}{\pi\Gamma(l+k+3/2)\Gamma(k+1)} > 0, \quad \forall\, \ell,k \ge 0.$$

Positivity of the coefficients is a key feature here. The strategy to establish positivity of the eigenvalues is to substitute this sine expansion into (3.3) to obtain

$$\lambda_\ell = \sum_{k=0}^{\infty} R(\ell,k) S_{\ell+1+2k}(\mu) \tag{3.4}$$

where

$$S_m = \int_0^\mu F(2\sin(\eta/2))\sin(m\eta)\cos(\eta/2)\,d\eta, \quad m \ge 1$$

and to determine if each of the S_m is also positive, giving a sum of positive terms for each eigenvalue.

Example 3.5. *Set $F(z) = 1$. Then*

$$\begin{aligned}
S_m &= \int_0^\mu \sin(m\eta)\cos(\eta/2)\,d\eta \\
&= \frac{1}{4m^2-1}\left(4m - 4m\cos(\mu/2)\cos(m\mu) + 2\sin(\mu/2)\sin(m\mu)\right) \\
&= \alpha_0(m) + \alpha_c(m,\mu)\cos(m\mu) + \alpha_s(m,\mu)\sin(m\mu) \\
&\ge \alpha_0(m) - (\alpha_c(m,\mu)^2 + \alpha_s(m,\mu)^2)^{1/2} \\
&= \frac{4m - \sqrt{16m^2 - (16m^2-4)\sin^2(\mu/2)}}{4m^2-1} > 0
\end{aligned}$$

for all $m \ge 1$ and $\mu \in (0,\pi]$. Hence the eigenvalues λ_ℓ are positive for all $h \in (0,2]$.

Submitted to Journal of Integral Equations and Applications - NOT THE PUBLISHED VERSION

Example 3.6. *Set $F(z) = (1-4z/h)(1-z/h)^2$. Then*

$$\begin{aligned} S_m &= \int_0^{\mu} F(2\sin(\eta/2))\sin(m\eta)\cos(\eta/2)\,d\eta \\ &= \alpha_0(m,\mu) + \alpha_c(m,\mu)\cos(m\mu) + \alpha_s(m,\mu)\sin(m\mu) \\ &\geq \alpha_0(m,\mu) - (\alpha_c(m,\mu)^2 + \alpha_s(m,\mu)^2)^{1/2} =: L_m(\mu). \end{aligned}$$

The coefficients $\alpha_0(m,\mu), \alpha_c(m,\mu), \alpha_s(m,\mu)$ are ratios of bivariate polynomials in m and $\sin(\mu/2)$. The details are messy, but it is relatively easy to establish that $L_m(\mu) \to -\infty$ as $\mu \to 0$ and it is positive for larger values of μ. Using an algebraic manipulation package it is possible to show that $L_m'(\mu) \geq 0$, that it is positive at $\sin(\mu/2) = \sqrt{7}/m$, and hence positive for all $\mu \in [2\sin^{-1}(\sqrt{7}/m), \pi]$.

This result then implies that all the terms in the sum (3.4) for eigenvalue λ_ℓ are positive when $\mu \in [2\sin^{-1}(\sqrt{7}/(\ell+1)), \pi]$ or equivalently when $h \in [2\sqrt{7}/(\ell+1), 2]$. Combined with the small h result in Example 3.4 we have

$$\lambda_0 = 0, \quad \lambda_1 > 0, \quad \lambda_2 > 0 \quad h \in (0,2],$$

and for $\ell \geq 3$

$$\lambda_\ell > 0 \quad h \in \left(0, \sqrt{\frac{112}{3(\ell-1)(\ell+2)}}\right) \cup \left[\frac{2\sqrt{7}}{\ell+1}, 2\right] = (0,2]$$

since the ranges above intersect.

3.3. *More detailed bounds on the eigenvalues of operator $\mathscr{B}$.* In the previous subsection we were concerned with establishing positivity of the eigenvalues of operator $\mathscr{B}$. In this subsection we derive detailed upper and lower bounds on the eigenvalues for a collection of different kernel functions by using properties of the eigenvalues of the operator obtained with $F(z) = 1$ as the key to deriving more general results. The key quantity is

$$I_\ell(h) = \int_0^h P_\ell(1-z^2/2)\,dz, \quad h \in (0,2], \quad \ell \geq 0 \tag{3.5}$$

for $\ell = 0, 1, \ldots$ and these are the eigenvalues $\lambda_\ell = I_\ell(h)$ when $F(z) = 1$. We already saw in Example 3.5 that $I_\ell(h) > 0$ for all $\ell \geq 0$, $h \in (0,2]$.

The first few cases are easily calculated explicitly and give

$$I_0(h) = h, \quad I_1(h) = h - \frac{1}{6}h^3, \quad I_2(h) = h - \frac{1}{2}h^3 + \frac{3}{40}h^5. \tag{3.6}$$

We also have from (3.1) in the single layer potential Example 3.2 that $I_\ell(2) = 1/(\ell+1/2)$. However we want results valid for all integer values $\ell \geq 0$ and all $h \in (0,2]$ and not just these special cases.

The next result is the main building block here.

Lemma 3.7. *The eigenvalues of the operator $\mathscr{B}$ defined by (1.1) with $F(z) = 1$ are*

$$\lambda_\ell = I_\ell(h) = \int_0^h P_\ell(1-z^2/2)\,dz, \quad \ell \geq 0.$$

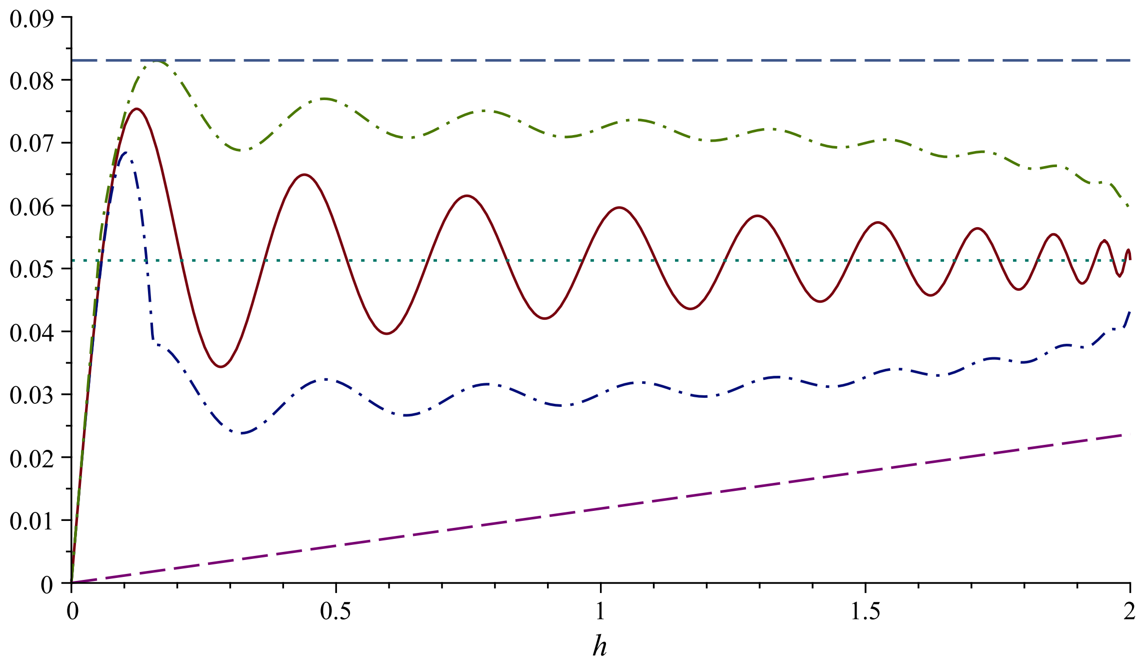

FIGURE 1. The function $I_{19}(h)$ is plotted (solid line) along with the detailed upper and lower bounds (dash-dot) and the simpler upper and lower bounds (dash) given in Lemma 3.7. The dotted line is the value $1/w_{19} = 2/39$.

They satisfy

$$\frac{C_{\mathrm{low}} h}{w_\ell} \le \max\left\{h - \frac{\ell(\ell+1)}{12}h^3, \frac{2}{\pi w_\ell}\left(\mathrm{Si}(w_\ell \mu(h)) - \ln\left(\frac{2h}{\mu(h)}\right)\right)\right\} \le \lambda_\ell$$

and

$$\lambda_\ell \le \min\left\{h, \frac{2}{\pi w_\ell}\left(\mathrm{Si}(w_\ell \mu(h)) + \ln\left(\frac{2h}{\mu(h)}\right)\right)\right\} \le \frac{C_{\mathrm{up}}}{w_\ell}$$

for all $\ell \ge 0$ *and* $h \in [0,2]$, *where*

$$w_\ell = \ell + 1/2, \tag{3.7}$$

$$\mu(h) = 2\sin^{-1}(h/2) \in [0,\pi],$$

$C_{\mathrm{low}} = (\mathrm{Si}(2\pi) - \ln(2))/\pi \approx 0.23$ *and* $C_{\mathrm{up}} = 2(\mathrm{Si}(\pi) + \ln(2))/\pi \approx 1.62$.

Proof. The proof uses an integral representation of $P_\ell(\cos\theta)$. It is lengthy and is given in detail in §4. □

The function $I_{19}(h)$ is plotted in Figure 1 along with the upper and lower bounds found in Lemma 3.7. Clearly there is scope to sharpen the bounds, particularly the lower bound, but this result captures the important details.

We now extend Lemma 3.7 to a wider subfamily of cases.

Theorem 3.8. *If function F in (1.1) satisfies*

$$F \in C^1[0,h], \quad F(0) > 0 \quad \text{and} \quad F(z) \geq 0,\ F'(z) \leq 0 \quad \text{for } z \in [0,h], \tag{3.8}$$

then the eigenvalues of the operator $\mathscr{B}$ defined by (1.1) are

$$\lambda_\ell = \int_0^h F(z) P_\ell(1 - z^2/2)\, dz, \quad \ell \geq 0$$

and satisfy

$$0 < \frac{C_{\text{low}}}{w_\ell} \int_0^h F(z)\, dz \leq \lambda_\ell \leq \frac{C_{\text{up}}}{w_\ell} F(0) \tag{3.9}$$

for all $h \in (0,2]$ and $\ell \geq 0$ where C_{low} and C_{up} are given in Lemma 3.7.

Proof. Using integration by parts we have

$$\int_0^h F(z) P_\ell\left(1 - \frac{z^2}{2}\right) dz = F(h) I_\ell(h) - \int_0^h F'(z) I_\ell(z)\, dz$$

where $I_\ell(h)$ is defined above in (3.5). Using the lower bound on $I_\ell(h)$ in Lemma 3.7:

$$\int_0^h F(z) P_\ell\left(1 - \frac{z^2}{2}\right) dz \geq \frac{C_{\text{low}} h}{w_\ell} F(h) - \frac{C_{\text{low}}}{w_\ell} \int_0^h z F'(z)\, dz = \frac{C_{\text{low}}}{w_\ell} \int_0^h F(z)\, dz$$

which is strictly positive given the assumptions on $F(z)$ above. Similarly,

$$\int_0^h F(z) P_\ell\left(1 - \frac{z^2}{2}\right) dz \leq \frac{C_{\text{up}}}{w_\ell} F(h) - \frac{C_{\text{up}}}{w_\ell} \int_0^h F'(z)\, dz = \frac{C_{\text{up}}}{w_\ell} F(0)$$

and the results follow directly. □

It is important to note that Theorem 3.8 only gives bounds for a subset of operators of the family (1.1). One case not covered by this theorem, but which also has non-negative eigenvalues was given in Example 3.6. We did not derive detailed bounds for that case. Another example with positive eigenvalues and not covered by the theorem follows. In both of these examples we have positive eigenvalues even when $F(z)$ is negative for some z and so positivity of F is not a necessary condition for positivity of the eigenvalues.

Example 3.9. *The operator defined by (1.1) with $F(z) = 1 - z^2/2$ has eigenvalues*

$$\lambda_0 = \int_0^h \left(1 - \frac{z^2}{2}\right) dz = h - \frac{h^3}{6},$$

$$\lambda_\ell = \int_0^h \left(1 - \frac{z^2}{2}\right) P_\ell\left(1 - \frac{z^2}{2}\right) dz = \frac{\ell+1}{2\ell+1} I_{\ell+1}(h) + \frac{\ell}{2\ell+1} I_{\ell-1}(h), \quad \ell \geq 1.$$

This uses the standard Legendre polynomial recurrence relation [14, 18.9(i)]

$$(\ell+1) P_{\ell+1}(x) - (2\ell+1) x P_\ell(x) + \ell P_{\ell-1}(x) = 0, \quad \ell \geq 1$$

and the change of variable $x = 1 - z^2/2$. The kernel function in this example is negative when $F(z) = 1 - z^2/2$ is negative and this happens when $z \in (\sqrt{2}, 2]$ and so will have an impact when

Submitted to Journal of Integral Equations and Applications - NOT THE PUBLISHED VERSION

$h \in (\sqrt{2}, 2]$. However, all of the eigenvalues are strictly positive for all $h \in (0,2]$ and it is easy to show using Lemma 3.7 (and basic calculus for λ_0) that

$$\frac{C_{\rm low}}{w_\ell} h \le \lambda_\ell \le \frac{7C_{\rm up}}{5w_\ell}, \quad \forall\, \ell \ge 0, h \in [0,2]$$

where $C_{\rm low}, C_{\rm up}$ are given in Lemma 3.7.

3.4. *Integral positivity.* The bounds on the eigenvalues given above allow us to examine the regularity of $\mathscr{B}u$ and to bound the bilinear form

$$(u, \mathscr{B}u)_S = \int_S u(\mathbf{x})(\mathscr{B}u)(\mathbf{x})\, d\mathbf{x} = \int_S \int_S G(\mathbf{x}.\mathbf{y}) u(\mathbf{x}) u(\mathbf{y})\, d\mathbf{y}\, d\mathbf{x},$$

where operator $\mathscr{B}$ is defined in (1.1).

Using the expansion (2.2) of u in spherical harmonics we have

$$(\mathscr{B}u)(\mathbf{x}) = \sum_{\ell=0}^{\infty} \lambda_\ell \sum_{m=-\ell}^{\ell} u_\ell^m Y_\ell^m(\mathbf{x}).$$

Using the Definition 2.1 of the $H^s(S)$ norm, we have

$$\|\mathscr{B}u\|^2_{H^s(S)} = \sum_{\ell=0}^{\infty} (\ell+1/2)^{2s} \lambda_\ell^2 \sum_{m=-\ell}^{\ell} |u_\ell^m|^2 < \infty \tag{3.10}$$

for all s such that $(\ell+1/2)^{2s}\lambda_\ell^2 \le C(\ell+1/2)^{-1}$, since $u \in H^{-1/2}(S)$. Also, orthonormality of the spherical harmonics gives

$$(u, \mathscr{B}u)_S = \sum_{\ell=0}^{\infty} \lambda_\ell \sum_{m=-\ell}^{\ell} |u_\ell^m|^2. \tag{3.11}$$

We can then apply the bounds on the eigenvalues we found above.

Corollary 3.10. *When the function F in the definition (1.1) of operator $\mathscr{B}$ satisfies the conditions of Theorem 3.8, we have*

$$\mathscr{B}u \in H^{1/2}(S)$$

and

$$0 < C_{\rm low} \|u\|^2_{H^{-1/2}(S)} \int_0^h F(z)\, dz < (u, \mathscr{B}u)_S \le F(0) C_{\rm up} \|u\|^2_{H^{-1/2}(S)}$$

for all $u \in H^{-1/2}(S)$ and $h \in (0,2]$. Hence $\sqrt{(u,\mathscr{B}u)_S}$ is a norm equivalent to the $H^{-1/2}(S)$ norm for each fixed h.

Proof. We use the bounds (3.9) in (3.10) to get the first result, and in (3.11) for the second, along with Definition 2.1 of the $H^s(S)$ norm for all fixed $h \in (0,2]$. Note that the lower bound depends on h and $\to 0$ as $h \to 0$. □

4. Proof of Lemma 3.7

Lemma 3.7 gives upper and lower bounds on the eigenvalues $\lambda_\ell = I_\ell(h)$ for $\ell \geq 0$ of the operator $\mathscr{B}$ defined by (1.1) when $F(z) = 1$. Using the expressions for $I_\ell(h), \ell = 0,1,2$ given in (3.6), we find by elementary calculus that

$$\frac{h}{3w_\ell} \leq \lambda_\ell \leq \frac{3}{2w_\ell} \quad \text{for } \ell \in \{0,1,2\} \quad \text{where } w_\ell = \ell + \frac{1}{2}. \tag{4.1}$$

This gives an indication of the sort of bounds we might expect to obtain in the general case $\ell \geq 0$ and $0 < h \leq 2$. In particular, the lower bound depends on h. More generally we have: a positivity result from Example 3.5

$$I_\ell(h) > 0, \quad h \in (0,2], \quad \ell = 0,1,2,\ldots; \tag{4.2}$$

and a small h lower bound from Example 3.3

$$I_\ell(h) > h - h^3 \frac{\ell(\ell+1)}{12} > 0 \quad \text{when} \quad 0 < h^2 < \frac{12}{\ell(\ell+1)} \tag{4.3}$$

for $\ell \geq 2$. We also have a crude upper bound:

$$I_\ell(h) = \int_0^h P_\ell(1 - z^2/2)\,dz \leq h, \quad \ell = 0,1,2,\ldots \tag{4.4}$$

for all $h \in [0,2]$ since $|P_\ell(x)| \leq 1$ for all $x \in [-1,1]$.

To obtain more detailed results we use the identity [14, 14.12(i)]

$$P_\ell(\cos\theta) = \frac{\sqrt{2}}{\pi} \int_0^\theta \frac{\cos(w_\ell \eta)}{\sqrt{\cos\eta - \cos\theta}}\,d\eta \quad \text{where} \quad w_\ell = \ell + \frac{1}{2},\ \ell = 0,1,2,\ldots$$

to get

$$\begin{aligned}
I_\ell(h) \quad &:= \quad \int_0^h P_\ell\left(1 - \frac{z^2}{2}\right) dz = \int_0^{\mu(h)} \frac{P_\ell(\cos\theta)\sin\theta}{\sqrt{2 - 2\cos\theta}}\,d\theta \\
&= \quad \frac{\sqrt{2}}{\pi} \int_0^{\mu(h)} \frac{\sin\theta}{\sqrt{2 - 2\cos\theta}} \int_0^\theta \frac{\cos(w_\ell\eta)}{\sqrt{\cos\eta - \cos\theta}}\,d\eta\,d\theta \\
&= \quad \frac{\sqrt{2}}{\pi} \int_0^{\mu(h)} \cos(w_\ell\eta) \left(\int_\eta^{\mu(h)} \frac{\sin\theta}{\sqrt{2 - 2\cos\theta}} \frac{d\theta}{\sqrt{\cos\eta - \cos\theta}} \right) d\eta \\
&= \quad \frac{\sqrt{2}}{\pi} \int_0^{\mu(h)} \cos(w_\ell\eta) \left(\int_{z(\eta)}^h \frac{dz}{\sqrt{\cos\eta - 1 + z^2/2}} \right) d\eta \\
&= \quad \frac{2}{\pi} \int_0^{\mu(h)} \cos(w_\ell\eta) \left(\int_{z(\eta)}^h \frac{dz}{\sqrt{z^2 - z(\eta)^2}} \right) d\eta \\
&= \quad \frac{2}{\pi} \int_0^{\mu(h)} \cos(w_\ell\eta) \left(\int_1^{h/z(\eta)} \frac{ds}{\sqrt{s^2 - 1}} \right) d\eta \\
&= \quad \frac{2}{\pi} \int_0^{\mu(h)} \cos(w_\ell\eta)\, g\left(\frac{h}{z(\eta)}\right) d\eta \qquad (4.5)
\end{aligned}$$

where

$$z(\eta) = \sqrt{2-2\cos\eta} = 2\sin(\eta/2), \quad \mu(h) = \cos^{-1}\left(1-\frac{h^2}{2}\right),$$

for $\eta \in [0,\pi]$, $h \in (0,2]$, and

$$g(w) = \int_1^w \frac{ds}{\sqrt{s^2-1}} = \ln\left(w+\sqrt{w^2-1}\right),\ w \geq 1.$$

Note that $g(1)=0$ and $g(w)\geq 0$ is an increasing function of $w \geq 1$. For small η

$$g\left(\frac{h}{z(\eta)}\right) = -\ln\eta + \ln(2h) - \frac{6-h^2}{24h^2}\eta^2 + \mathscr{O}(\eta^4)$$

has a logarithmic singularity in η. We split g into two pieces and define the function $g_1(\eta,h)$ such that

$$g\left(\frac{h}{z(\eta)}\right) = g_1(\eta,h) + \ln\left(\frac{\mu(h)}{\eta}\right) \quad \text{for } 0 \leq \eta \leq \mu(h) \leq \pi. \tag{4.6}$$

We have

$$g_1(\eta,h)\geq 0, \quad \partial_\eta g_1(\eta,h) \leq 0, \quad \partial_\eta^2 g_1(\eta,h) \leq 0 \quad \text{for } 0 \leq \eta \leq \mu(h) \leq \pi$$

with

$$g_1(0,h) = \ln\left(\frac{2h}{\mu(h)}\right) \quad \text{and} \quad g_1(\mu(h),h) = 0.$$

So $g_1(\eta,h)$ is a continuous, decreasing function of η.

We use (4.6) to split the integral in (4.5) into two parts. The first part is

$$I_\ell^{(a)}(h) = \frac{2}{\pi}\int_0^{\mu(h)} \cos(w_\ell\eta)\ln\left(\frac{\mu(h)}{\eta}\right)d\eta = \frac{2}{\pi w_\ell}\mathrm{Si}(w_\ell\mu(h)) \tag{4.7}$$

where Si is the sine integral function [14, 6.2.9]. The second part is

$$I_\ell^{(b)}(h) = \frac{2}{\pi}\int_0^{\mu(h)} \cos(w_\ell\eta) g_1(\eta,h)\, d\eta \tag{4.8}$$

and does not evaluate to a closed form expression.

We are interested in both an upper and a lower bound on $I_\ell(h)$.

Upper bound. The upper bound is relatively straightforward to obtain using integration by parts in (4.8):

$$\begin{aligned} I_\ell^{(b)}(h) &= \frac{-2}{w_\ell\pi}\int_0^{\mu(h)} \sin(w_\ell\eta)\partial_\eta g_1(\eta,h)\, d\eta \\ &\leq \frac{-2}{w_\ell\pi}\int_0^{\mu(h)} \partial_\eta g_1(\eta,h)\, d\eta = \frac{2g_1(0,h)}{w_\ell\pi} \\ &= \frac{2}{w_\ell\pi}\ln\left(\frac{2h}{\mu(h)}\right). \end{aligned}$$

Combining the results from (4.4) and (4.7) with that for $I_\ell^{(b)}$ above we get

$$I_\ell(h) \leq \min\left\{h, \frac{2}{\pi w_\ell}\left(\mathrm{Si}(w_\ell\mu(h)) + \ln\left(\frac{2h}{\mu(h)}\right)\right)\right\} \leq \frac{C_{\mathrm{up}}}{w_\ell} \tag{4.9}$$

using standard properties of the functions involved, where $C_{\rm up} = 2(\mathrm{Si}(\pi) + \ln(2))/\pi \approx 1.62$. This bound is consistent with the upper bounds found directly for $\ell = 0,1,2$ in (4.1).

Lower bound. Using the integration by parts result above again we have

$$I_\ell^{(b)}(h) \geq -\frac{2}{w_\ell \pi} \ln\left(\frac{2h}{\mu(h)}\right)$$

and hence

$$I_\ell(h) \geq \frac{2}{w_\ell \pi}\left(\mathrm{Si}(w_\ell \mu(h)) - \ln\left(\frac{2h}{\mu(h)}\right)\right). \tag{4.10}$$

This lower bound is negative as $h \to 0$ and so is not sharp in that range since we already have the non-negative lower bounds (4.2) and (4.3).

Nevertheless (4.10) is useful for larger h, and we show here that it is positive when $h \in (h_0, 2]$ with $h_0 = \mathscr{O}(w_\ell^{-1})$. First note that

$$\ln 2 \geq \ln\left(\frac{2h}{\mu(h)}\right) \geq \ln\left(\frac{4}{\pi}\right)$$

and it is a decreasing function of h. Then using a standard property

$$\mathrm{Si}(x) \geq \mathrm{Si}(1) \approx 0.946 \quad \forall\, x \geq 1,$$

we have

$$\mathrm{Si}(w_\ell \mu(h)) - \ln\left(\frac{2h}{\mu(h)}\right) \geq \mathrm{Si}(1) - \ln 2 \approx 0.253 > 0$$

for all $w_\ell \mu(h) \geq 1$ or equivalently $h \geq 2\sin(1/(2w_\ell)) = h_0$. Note that

$$h_0 = 2\sin\left(\frac{1}{2w_\ell}\right) < \frac{12}{\ell(\ell+1)} \quad \ell = 0,1,2,\ldots$$

and so the ranges where the small h lower bound (4.3) and the bound (4.10) are positive overlap.

Finally, we combine the bounds (4.3) and (4.10), and incorporate the $I_0(h), I_1(h)$ results from (3.6) to get

$$I_\ell(h) \geq \max\left\{h - h^3\frac{\ell(\ell+1)}{12}, \frac{2}{w_\ell \pi}\left(\mathrm{Si}(w_\ell \mu(h)) - \ln\left(\frac{2h}{\mu(h)}\right)\right)\right\} \geq \frac{C_{\rm low} h}{w_\ell}$$

where

$$C_{\rm low} = \frac{1}{\pi}(\mathrm{Si}(2\pi) - \ln 2) \approx 0.231$$

and the result is valid for all $h \in [0,2]$ and $\ell \geq 0$.

5. Applications in numerical approximation

Consider the scattering of acoustic waves from a unit sphere embedded in an infinite homogeneous medium with sound speed 1. This is described by the PDE

$$\frac{\partial^2 v}{\partial t^2} = \Delta v \quad \forall\, |\mathbf{x}| > 1, t > 0$$

with initial and (sound soft) boundary data

$$v(\mathbf{x},0) = 0 = \frac{\partial v}{\partial t}(\mathbf{x},0) \quad \forall\, |\mathbf{x}| > 1 \quad \text{and} \quad v(\mathbf{x},t) = a(\mathbf{x},t) \quad \forall\, \mathbf{x} \in S, t \geq 0.$$

where $-a(\mathbf{x},t)$ is the known incident field on the sphere surface. One way to find the solution of this problem is to use the single layer time domain boundary integral equation (TDBIE) (see e.g. [2, 12])

$$\text{(5.1)} \qquad \frac{1}{4\pi}\int_S \frac{u(\mathbf{y},t-|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} = a(\mathbf{x},t) \quad \forall\, \mathbf{x} \in S, t > 0$$

to obtain the surface potential $u(\mathbf{x},t)$ given the incident field data $a(\mathbf{x},t)$ on the surface of the sphere. We assume that both u and a are 0 for all $t \leq 0$ and have appropriate regularity. Then the scattered field $v(\mathbf{x},t)$ can be obtained everywhere outside the sphere using

$$v(\mathbf{x},t) = \frac{1}{4\pi}\int_S \frac{u(\mathbf{y},t-|\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y} \quad \forall\, |\mathbf{x}| > 1, t > 0.$$

To illustrate the application of the results we have derived in the previous sections we give some basic ideas below about the approximation of TDBIEs. We note that different TDBIE formulations are also used, see e.g. [3, 10, 12], and that TDBIEs may also be used for scattering from general surfaces with appropriate changes of domains for the independent variables.

5.1. ***Separation of variables.*** The surface potential u and the incident field a on the sphere can be written using (2.2) in terms of the spherical harmonics (2.3) and the surface angle variables as

$$u(\mathbf{x},t) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} u_\ell^m(t) Y_\ell^m(\theta,\phi), \quad a(\mathbf{x},t) = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} a_\ell^m(t) Y_\ell^m(\theta,\phi).$$

It can be shown [10] that the amplitude functions $u_\ell^m(t)$ satisfy the convolution Voltera integral equation (VIE) of the 1st kind

$$\text{(5.2)} \qquad \int_0^t H(2-z)P_\ell(1-z^2/2)v(t-z)\,dz = 2b(t), \quad t > 0$$

where $(v,b) = (u_\ell^m, a_\ell^m)$ for each $\ell \geq 0$ and $|m| \leq \ell$ and $(v(t),b(t)) = (0,0)$ for all $t \leq 0$.

There are many approximation methods for 1st kind convolution VIEs (see e.g. [4]), but for illustration here we first consider a simple collocation approximation based on a piecewise constant approximation of $v(t)$ on a uniform time grid with step size Δt. The approximation is

$$v(t) \approx \sum_{m=1}^{M} v^m \psi_m(t), \quad \psi_m(t) = \begin{cases} 1, & t \in (t_{m-1},t_m) \\ 0, & \text{otherwise} \end{cases}.$$

Substituting this into (5.2) and collocating (forcing it to hold) at time levels $t_n = n\Delta t, n = 1,2,\ldots,M$ we get

$$q^0 v^n + q^1 v^{n-1} + \cdots + q^{n-1} v^1 = 2b(t^n), \quad n = 1,2,\ldots,M$$

where

$$q^m = \int_{t_m}^{t_{m+1}} H(2-z)P_\ell(1-z^2/2)\,dz, \quad m = 0,1,\ldots,M-1$$

and so the approximation is advanced in time by

$$v^n = \frac{1}{q^0}\left(2b(t^n) - \sum_{m=1}^{n-1} q^{n-m} v^m\right), \quad n = 1,2,\ldots,M. \tag{5.3}$$

Clearly we need $q^0 \neq 0$ for this to make sense and this is guaranteed for all $\ell \geq 0$ by Lemma 3.7 setting $h = \Delta t$ there (provided $\Delta t \leq 2$).

Collocation methods with different basis functions also give approximations similar to (5.3) with the same requirement that $q^0 \neq 0$. Two examples follow.

Example 5.1. *The collocation scheme based on the continuous piecewise linear approximation gives*

$$q^0 = \int_0^{\Delta t} P_\ell(1 - z^2/2)(1 - z/\Delta t)\,dz > 0 \qquad (\Delta t \leq 2)$$

using Theorem 3.8 with $h = \Delta t$ and $F(z) = 1 - z/\Delta t$.

Example 5.2. *The 4th order accurate backward time approximation [9] based on cubic B-splines has*

$$q^0 = \int_0^{2\Delta t} P_\ell(1 - z^2/2)(3B_3(1 + z/\Delta t) + B_3(z/\Delta t))\,dz > 0 \qquad (\Delta t \leq 1)$$

where the cubic B-spline shape function is

$$B_3(r) = \frac{1}{6}\begin{cases} 4 - 6r^2 + 3|r|^3, & |r| \leq 1 \\ (2 - |r|)^3, & 1 \leq |r| \leq 2 \\ 0, & |r| \geq 2. \end{cases}$$

This again uses Theorem 3.8, but with $h = 2\Delta t$ and $F(z) = 3B_3(1 + z/\Delta t) + B_3(z/\Delta t)$. Properties of B_3 guarantee that this $F(z)$ satisfies the hypotheses of the Theorem.

Further examples of schemes for VIEs similar to (5.3) based on polynomial splines of various degrees in [8] and on more complicated C^∞ functions in [7] also satisfy the conditions in Theorem 3.8 required to guarantee positivity of q^0.

5.2. *Finite element approximation.* One approach to the approximation of TDBIEs on more general surfaces is to approximate the surface potential by piecewise polynomial finite element basis functions in both time and space (see e.g. [2, 12]), and we consider that here for the sphere surface. We have

$$u(\mathbf{x},t) \approx u_h(\mathbf{x},t) = \sum_{m=0}^{M}\sum_{j=1}^{N} u_j^m \psi_m(t)\phi_j(\mathbf{x}) \quad t \in [0,T],\ \mathbf{x} \in S$$

where the space basis functions ϕ_j are locally supported on curved elements on the surface, and the time basis functions ψ_m have support on intervals of length $\mathscr{O}(\Delta t)$ where Δt is the uniform time step size. Applying the Galerkin approach in space and, for ease of illustration only, simple collocation in time where the time basis functions are translates of a basic shape, we have

$$\frac{1}{4\pi}\int_S\int_S \phi_k(\mathbf{x})\frac{u_h(y, t_n - |\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\,d\mathbf{y}\,d\mathbf{x} = \int_S \phi_k(\mathbf{x})a(\mathbf{x},t_n)\,d\mathbf{x}$$

for $n = 1, \ldots, M$ and each $k = 1, \ldots, N$. Rearranging, we have the marching on in time process

$$\mathbf{u}^n = (Q^0)^{-1} \left(4\pi \mathbf{a}^n - \sum_{m=1}^{n-1} Q^{n-m} \mathbf{u}^m \right) \quad n = 1, \ldots, M \tag{5.4}$$

analogous to (5.3), where unknowns $\mathbf{u}^n$ and incident field data $\mathbf{a}^n$ are

$$\mathbf{u}^n = (u_1^n, u_2^n, \ldots, u_N^n)^T, \; \{\mathbf{a}^n\}_k = \int_S \phi_k(\mathbf{x}) a(\mathbf{x}, t_n)\, d\mathbf{x}.$$

The matrices Q are

$$\{Q^{n-m}\}_{k,j} = \int_S \int_S \phi_k(\mathbf{x}) \phi_j(\mathbf{y}) \frac{\psi_m(t_n - |\mathbf{x}-\mathbf{y}|)}{|\mathbf{x}-\mathbf{y}|}\, d\mathbf{y}\, d\mathbf{x}.$$

Clearly to obtain $\mathbf{u}^n$ at each step in (5.4) we need Q^0 to be non-singular.

When we use standard piecewise linear time basis functions the matrix Q^0 is

$$\begin{aligned} \{Q^0\}_{k,j} &= \int_S \phi_k(\mathbf{x}) \int_S \frac{H(\Delta t - |\mathbf{x}-\mathbf{y}|)(1 - |\mathbf{x}-\mathbf{y}|/\Delta t)}{|\mathbf{x}-\mathbf{y}|} \phi_j(\mathbf{y})\, d\mathbf{y}\, d\mathbf{x} \\ &= \int_S \phi_k(\mathbf{x}) (\mathscr{B}\phi_j)(\mathbf{x})\, d\mathbf{x} \end{aligned}$$

where operator $\mathscr{B}$ is of the type (1.1) considered in the previous sections with $h = \Delta t$ and $F(z) = 1 - z/\Delta t$. Defining

$$v_h(\mathbf{x}) = \sum_{j=1}^{N} v_j \phi_j(\mathbf{x}) \quad \text{and} \quad \mathbf{v} = (v_1, v_2, \ldots, v_N)^T$$

then Q^0 is positive definite and non-singular if $\mathbf{v}^T Q^0 \mathbf{v} > 0$ for all $\mathbf{v} \neq 0$. This is indeed the case since

$$\mathbf{v}^T Q^0 \mathbf{v} = \int_S v_h(\mathbf{x}) (\mathscr{B} v_h)(\mathbf{x})\, d\mathbf{x} > 0$$

for any choice of space basis functions such that $v_h \in H^{-1/2}(S) \neq 0$ using Corollary 3.10.

It is important to note that this piecewise linear basis collocation in time approximation is generally not a good way to approximate TDBIEs and we have used it only to simplify the presentation in the example here. Other collocation in time schemes that generate a time marching processes like (5.4) do appear to work well and they do also satisfy the conditions of Corollary 3.10 guaranteeing non-singularity of the Q^0 matrix. Examples are the schemes based on globally C^∞ time basis functions in [7] and on cubic spline basis functions in [8].

6. Discussion and conclusions

We derived positivity results on the eigenvalues of a collection of operators in the form (1.1) on the surface of the unit sphere, as well as more detailed upper and lower bounds on the eigenvalues and an integral positivity result. We also gave examples of where these bounds are useful in establishing that the time stepping process in the numerical approximations like (5.3) and (5.4) of single layer TDBIEs on the sphere are well-defined. This is necessary, but not sufficient, for the schemes to be useful since we also need to investigate stability and convergence.

We do not consider stability and convergence in this paper, but note that they are generally hard to establish in theory and to achieve in practice for single layer TDBIE approximations based on piecewise polynomials in time and space. The combined field integral equation, a blend of single and double layer potential representations, is a promising alternative studied in [10] for the sphere and [3] for more general surfaces. These studies show complicated dependence of stability on the choice of boundary integral formulation and the geometry of the scatterer.

Scattering from spheres is of interest in its own right as well as often being used as a benchmark test for new methods and codes. For general surfaces, direct calculation of the eigenvalues of operators analogous to (1.1) is not possible, and so positivity cannot be established that way. Nevertheless, detailed results like this for spheres (and planes) may provide insights for more general studies.

Finally we return to our comment in the Introduction that positivity of $\int_0^h P_\ell(1-z^2/2)\,dz$ is the analogue of Cooke's result (see e.g. [5] or [16, Lemma 5.1]) on the positivity of $\int_0^r J_0(z)\,dz$. To explore this further consider the TDBIE (5.1) applied on an infinite 2D plane instead of the surface of the sphere. Separation of variables in this case involves applying the Fourier transform of the TDBIE over the plane and gives the convolution Volterra integral equation [6]

$$\int_0^t J_0(|\omega|z)\hat{u}(\omega,t-z)\,dz = 2\hat{a}(\omega,t), \quad t>0$$

for the time evolution of the amplitude of the Fourier component of u with spatial frequency vector ω where $\hat{u}$ and $\hat{a}$ are the 2D Fourier transforms of functions u and a over the infinite plane. Using the same approximations in time on the plane as we did for the analogous VIE (5.2) for separation of variables on the sphere, we require Cooke's result to hold where we needed positivity of $\int_0^h P_\ell(1-z^2/2)\,dz$ on the sphere. Straightforward adaptations of Theorem 3.8 and Corollary 3.10 give the necessary results for this infinite flat surface.

References

[1] K E Atkinson and W Han. *Theoretical Numerical Analysis: A Functional Analysis Framework*. Springer, 2001.

[2] A Bamberger and T Ha Duong. Formulation variationnelle espace–temps pour le calcul par potentiel retardé de la diffraction d'une onde acoustique (I). *Math. Meth. Appl. Sci.*, 8:405–435, 1986.

[3] A Barnett, L Greengard, and T Hagstrom. High-order discretization of a stable time-domain integral equation for 3d acoustic scattering. *Journal of Computational Physics*, 402:109047, 2020.

[4] H Brunner. *Collocation Methods for Volterra Integral and Related Functional Equations*. Cambridge University Press, Cambridge, 2004.

[5] R G Cooke. A monotonic property of Bessel functions. *Journal of the London Mathematical Society*, 12:180–185, 1937.

[6] P J Davies and D B Duncan. Stability and convergence of collocation schemes for retarded potential integral equations. *SIAM J. Numer. Anal.*, 42:1167–1188, 2004.

[7] P J Davies and D B Duncan. Convolution–in–time approximations of time domain boundary integral equations. *SIAM J. Sci. Comput.*, 35:B43–B61, 2013.

[8] P J Davies and D B Duncan. Convolution spline approximations for time domain boundary integral equations. *Journal of Integral Equations and Applications*, 26(3):369–412, FAL 2014.

[9] P J Davies and D B Duncan. Numerical approximation of first kind Volterra convolution integral equations with discontinuous kernels. *Journal of Integral Equations and Applications*, 29(1):41–73, 2017.

[10] C L Epstein, L Greengard, and T Hagstrom. On the stability of time-domain integral equations for acoustic wave propagation. *Discrete and Continuous Dynamical Systems - Series A*, 36:4367–4382, 2016.

[11] W Freeden and M Schreiner. *Spherical Functions of Mathematical Geosciences*. Springer-Verlag, 2009.

[12] T Ha-Duong. On retarded potential boundary integral equations and their discretisation. In M Ainsworth, P J Davies, D B Duncan, P A Martin, and B P Rynne, editors, *Topics in Computational Wave Propagation: Direct and Inverse Problems*, pages 301–336. Springer-Verlag, 2003.

[13] J-C Nedelec. *Acoustic and Electromagnetic Equations: Integral Representations for Harmonic Problems*. Springer, 2001.

[14] F W J Olver, D W Lozier, R E Boisvert, and C W Clark. *NIST Handbook of Mathematical Functions*. Cambridge University Press, 2010.

[15] R T Seeley. Spherical harmonics. *The American Mathematical Monthly*, 73:115–121, 1966.

[16] H Wendland. *Scattered Data Approximation*. Cambridge University Press, 2010.

MAXWELL INSTITUTE FOR MATHEMATICAL SCIENCES, DEPARTMENT OF MATHEMATICS, HERIOT–WATT UNIVERSITY, EDINBURGH, EH14 4AS, UK

Email address: D.B.Duncan@hw.ac.uk