VECTORIAL BALL PROLATE SPHEROIDAL WAVE FUNCTIONS
WITH THE DIVERGENCE FREE CONSTRAINT

JING ZHANG\(^1\), GUIDOUM IKRAM\(^1\) HUIYUAN LI\(^2\)

Abstract. In this paper, we introduce one family of vectorial prolate spheroidal wave functions of real order \(\alpha > -1\) on the unit ball in \(\mathbb{R}^3\), which satisfy the divergence free constraint, thus are termed as divergence free vectorial ball PSWFs. They are vectorial eigenfunctions of an integral operator related to the finite Fourier transform, and solve the divergence free constrained maximum concentration problem in three dimensions, i.e., to what extent can the total energy of a band-limited divergence free vectorial function be concentrated on the unit ball? Interestingly, any optimally concentrated divergence free vectorial functions, when represented in series in vector spherical harmonics, shall be also concentrated in one of the three vectorial spherical harmonics modes. Moreover, divergence free ball PSWFs are exactly the vectorial eigenfunctions of the second order Sturm-Liouville differential operator which defines the scalar ball PSWFs. Indeed, the divergence free vectorial ball PSWFs possess a simple and close relation with the scalar ball PSWFs such that they share the same merits. Simultaneously, it turns out that the divergence free ball PSWFs solve another second order Sturm-Liouville eigen equation defined through the curl operator \(\nabla \times\) instead of the gradient operator \(\nabla\).

1. Introduction

In the early 1960s, Slepian, Landau and Pollak answered an open question: to what extent are functions, which are confined to a finite bandwidth, also concentrated in the time domain? (cf. [16, 20]). Any square integrable function \(f(\xi)\) is bandlimited, if its Fourier transform \(\psi(t)\) has a finite support \([-c, c]\) such that

\[
f(\xi) = \int_{-1}^{1} \psi(t) e^{i\xi t} \, dt, \quad \xi \in (-\infty, \infty).
\]

(1.1)

The related issue is to what extent that the energy of such \(f(\xi)\) can be maximally concentrated on finite interval \(I = (-1, 1)\), that is,

\[
\max \left\{ \int_{I} |f(\xi)|^2 d\xi \bigg/ \int_{\mathbb{R}} |f(\xi)|^2 d\xi \right\}.
\]

The above problem is equivalent to

\[
\max_{\psi} \left\{ \int_{I} \int_{I} \frac{\sin c(x - t)}{\pi(x - t)} \psi(x) \cdot \overline{\psi(t)} dx dt \bigg/ \int_{I} |\psi(t)|^2 dt \right\}.
\]

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\(^1\)School of Mathematics and Statistics & Hubei Key Laboratory of Mathematical Sciences, Central China Normal University, Wuhan 430079, China. The work of the first and the second authors is partially supported by the National Natural Science Foundation of China (NSFC 11671166) and the Fundamental Research Funds for the Central Universities (CCNU19TS033, CCNU19TD010).

\(^2\)State Key Laboratory of Computer Science/Laboratory of Parallel Computing, Institute of Software, Chinese Academy of Sciences, Beijing 100190, China. Email: huiyuan@iscas.ac.cn. The research of the third author is partially supported by the National Natural Science Foundation of China (NSFC 11871455 and NSFC 11971016).
It actually comes down to the study of the following integral equation:

$$\lambda_n(c)\psi_n(x;c) = \int_{-1}^{1} e^{icxt} \psi(t; c) dt, \quad c > 0, \quad x \in I. \quad (1.3)$$

Eigenfunctions, $\psi_n(x;c)$, $n = 1, 2, \ldots$, of the integral equation $(1.2)$, therein referred to as prolate spheroidal wave functions (PSWFs), are discovered coincidentally to be the eigenfunctions of an integral operator related to the finite Fourier transform:

$$\lambda_n(c)\psi_n(x;c) = \int_{-1}^{1} e^{icxt} \psi(t; c) dt, \quad c > 0, \quad x \in I. \quad (1.3)$$

From this perspective, PSWFs are initially defined as the bandlimited functions most concentrated on the finite interval $I$. On the other hand, the PSWFs are exactly eigenfunctions of the second-order singular Sturm-Liouville differential equation:

$$\partial_x \left( (1 - x^2) \partial_x \psi_n(x;c) \right) + \left( \lambda_n(c) - c^2 x^2 \right) \psi_n(x;c) = 0, \quad c > 0, \quad x \in I, \quad (1.4)$$

which naturally form an orthogonal basis of the $L^2$ space.

There has been abundant literature addressing this research topic in more than 50 years past. Indeed, PSWFs of order zero and multidimensional extensions (cf. [11, 19, 23]) have enjoyed applications in a wide range of science and engineering (cf. [10, 15, 21]). Notably, they are also well suited to approximate bandlimited functions, and have been proven to be a useful basis for spectral method, which enjoy a much higher resolution for highly oscillatory waves over the Legendre polynomial based methods (cf. [4, 7, 24]). These attractive properties have motivated us to use PSWFs as basis functions in the study of the acoustic wave equation and of the Maxwell system with large wave number, the two most common wave equations encountered in physics or in engineering. It is well known that a physically realizable time-harmonic electromagnetic field in a linear, isotropic, homogeneous medium must be divergence free (cf. [8, 14, 6]). One may ask whether there are some kinds of vectorial PSWFs that can be optimally concentrated within a given finite domain and satisfy the divergence free constraint, i.e., $\nabla \cdot \psi(x) = 0$.

To answer this question, we shall consider in this paper the concentration problem on the unit ball $B := \{x \in \mathbb{R}^3 : \|x\| \leq 1\}$. By extending the finite Fourier transform $(1.1)$ to the one for vectorial functions on the unit ball $B$,

$$\int_{B} e^{-i\langle x, \tau \rangle} \psi(\tau; c)(1 - |	au|^2)^{\alpha} d\tau = \lambda \psi(x; c), \quad x \in B, \quad c > 0, \quad \alpha > -1, \quad (1.5)$$

we aim at finding some kinds of divergence free vectorial eigenfunctions of the above equation. For this purpose, we first show that any divergence free vectorial function takes the form

$$\psi(x) = x \times \nabla \phi(x) + \nabla \times (x \times \nabla) \theta(x).$$

Further we identify that all divergence free eigenfunctions of $(1.5)$ are constituted only by vectorial functions of the form $x \times \nabla \phi(x)$. In the sequel, with the help of spherical harmonics $Y_l^m(\hat{x})$ in the spherical-polar coordinates $x = r\hat{x}$ with $r \geq 0$ and $\hat{x} \in S^2$, we define the divergence free ball PSWFs as the band-limited vectorial functions

$$\psi_{k,\ell}^{m,n}(x; c) = x \times \nabla[\phi_k^m(r; c) Y_l^m(\hat{x})] = \phi_k^m(r; c) x \times \nabla Y_l^m(\hat{x}), \quad 1 \leq \ell \leq 2n+1, \quad k, n \geq 0,$n which satisfy the integral equation $(1.5)$ and are optimally concentrated on the ball.

Recalling that vectorial spherical harmonics fall into three types of modes, $x Y_l^m(\hat{x})$, $r \nabla Y_l^m(\hat{x})$ and $x \times \nabla Y_l^m(\hat{x})$, we discover the interesting phenomenon that any optimally concentrated band limited and divergence free functions will certainly concentrate on the one of the three mode types. Simultaneously, it turns out that the divergence free ball PSWFs are exactly the eigenfunctions of the second order Sturm-Liouville differential operator,

$$[-(1 - \|x\|^2)^{-\alpha} \nabla \cdot ((1 - \|x\|^2)^{\alpha+1} \nabla) - \Delta_0 + c^2\|x\|^2] \psi(x; c) = \lambda \psi(x; c), \quad x \in B, \quad \alpha > -1, \quad (1.6)$$
where $\Delta_0 = (\mathbf{x} \times \nabla) \cdot (\mathbf{x} \times \nabla)$ is the Laplace-Beltrami operator. This eigen-equation extends the differential property of the one dimensional PSWFs defined by Slepian. More astonishingly, we find the divergence free ball PSWFs solve the following eigen-equation composed by the curl operator $\nabla \times$ instead of the gradient operator $\nabla$,

$$
\left[(1-\|\mathbf{x}\|^2)^{-\alpha} \nabla \times \left((1-\|\mathbf{x}\|^2)^{\alpha+1} \nabla \times \right) - \Delta_0 + c^2 \|\mathbf{x}\|^2\right] \psi(x; c) = (\chi + 2\alpha + 2) \psi(x; c), \quad x \in \mathbb{B}, \; \alpha > -1.
$$

Moreover, we explore their connections with scalar ball PSWFs. The scalar ball PSWFs, denoted by $\psi_{k,\ell}^{\alpha,n}(x; c)$, $1 \leq \ell \leq 2n+1$, $k, n \geq 0$, are bandlimited functions share the same merit of divergence free vectorial ball PSWFs such that they are scalar eigenfunctions of the integral equation (1.5) and the differential equation (1.6) (cf. [23]). As a result, in the spherical-polar coordinates, divergence free vectorial ball PSWFs have the simple representation by the scalar ball PSWFs,

$$
\psi_{k,\ell}^{\alpha,n}(x; c) = (\mathbf{x} \times \nabla)\psi_{k,\ell}^{\alpha,n}(x; c), \quad 1 \leq \ell \leq 2n+1, \; k \in \mathbb{N}_0, \; n \in \mathbb{N}.
$$

We organise the remainder of the paper as follows. In Section 2, we collect some relevant properties of the Jacobi Polynomials, spherical harmonics and ball polynomials to facilitate the discussions in the forthcoming sections (cf. [9, 18]).

### 2. Mathematical Preliminary

In this section, we review the Jacobi Polynomials, and introduce the spherical harmonics and ball polynomials to introduce the spherical harmonics and ball polynomials to facilitate the discussions in the forthcoming sections (cf. [9, 18]).

#### 2.1. Notations and Vector Calculus

We begin by introducing some conventions and notations. Denote by $\mathbb{N}_0$ and $\mathbb{N}$ the collection of nonnegative integers and positive integers, respectively. Let $\mathbb{R}^d$ ($d \in \mathbb{N}$) be the $d$-dimensional Euclidean space. Throughout this paper, we shall always use bold letters such as $\mathbf{x}$ and $\mathbf{y}$ to denote column vectors. For instance, we write $\mathbf{x} = (x_1, x_2, \ldots, x_d)^t \in \mathbb{R}^d$ as a column vector, where $(\cdot)^t$ denotes matrix or vector transpose. The inner product of $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$ is denoted by $\mathbf{x} \cdot \mathbf{y}$ or $(\mathbf{x}, \mathbf{y}) := x_1 y_1 + \cdots + x_d y_d$, and the norm of $\mathbf{x}$ is denoted by $\|\mathbf{x}\| := \sqrt{(\mathbf{x}, \mathbf{x})} = \sqrt{\mathbf{x}^t \mathbf{x}}$. The unit sphere $\mathbb{S}^2$ and the unit ball $\mathbb{B}$ of $\mathbb{R}^3$ are respectively defined by

$$
\mathbb{S}^2 := \{ \hat{x} \in \mathbb{R}^3 : \|\hat{x}\| = 1 \}, \quad \mathbb{B} := \{ x \in \mathbb{R}^3 : r = \|x\| \leq 1 \}.
$$

For each $x \in \mathbb{R}^3$, we introduce its polar-spherical coordinates $(r, \hat{x})$ such that $r = \|x\|$ and $x = r \hat{x} := r(\hat{x}_1, \hat{x}_2, \hat{x}_3) \in \mathbb{S}^2$. Define the inner product of $L^2(\mathbb{S}^2)$ as

$$
(f,g)_{\mathbb{S}^2} := \int_{\mathbb{S}^2} f(\hat{x})g(\hat{x})d\sigma(\hat{x}),
$$

where $d\sigma$ is the surface measure.

Define the spherical gradient operator $\nabla_0$ and the Laplace-Beltrami operator $\Delta_0$,

$$
\nabla_0 = \|x\| (\mathbf{\nabla} - \hat{x}(\hat{x} \cdot \mathbf{\nabla})) = r \mathbf{\nabla} - x \partial_r, \quad (2.1)
$$

$$
\Delta_0 = \nabla_0 \cdot \nabla_0 = \|x\|^2 \Delta - (x \cdot \nabla)(x \cdot \nabla + 1). \quad (2.2)
$$

Indeed, $\nabla_0$ and $\Delta_0$ represent the spherical components of $\nabla$ and $\Delta$, respectively. Hence,

$$
\hat{x} \cdot \nabla_0 = 0. \quad (2.3)
$$
Further, denote by \( \mathbf{a} \times \mathbf{b} \) the cross product of two vectors \( \mathbf{a}, \mathbf{b} \in \mathbb{R}^3 \). We introduce the curl operator \( \text{curl} = \nabla \times \) and the divergence operator \( \text{div} = \nabla \cdot \) for vectorial functions in \( \mathbb{R}^3 \). We are interested in the vector calculus involving

\[
\mathbf{x} \times \nabla = (x_2 \partial_{x_3} - x_3 \partial_{x_2}, x_3 \partial_{x_1}, x_1 \partial_{x_2} - x_2 \partial_{x_1}),
\]

which is closely related to \( \nabla_0 \) and \( \Delta_0 \). The following two lemmas on \( \mathbf{x} \times \nabla \) will be used frequently in the paper. Their proofs will be postponed to Appendix A.

**Lemma 2.1.** It holds that

\[
\begin{align*}
\mathbf{x} \times \nabla &= -\nabla \times \mathbf{x} = \hat{\mathbf{x}} \times \nabla_0, \\
\nabla \cdot (\mathbf{x} \times \nabla) &= \mathbf{x} \cdot (\mathbf{x} \times \nabla) = 0, \\
(\mathbf{x} \times \nabla) \cdot (\mathbf{x} \times \nabla) &= \Delta_0, \\
\Delta_0 (\mathbf{x} \times \nabla) &= (\mathbf{x} \times \nabla) \Delta_0.
\end{align*}
\]

**Lemma 2.2.** It holds that

\[
\begin{align*}
\mathbf{x} \times (\mathbf{x} \times \nabla) &= \mathbf{x} (\mathbf{x} \cdot \nabla) - ||\mathbf{x}||^2 \nabla = -||\mathbf{x}|| \nabla_0, \\
\nabla \cdot (\mathbf{x} \times (\mathbf{x} \times \nabla)) &= -\Delta_0, \\
\nabla \times (\mathbf{x} \times (\mathbf{x} \times \nabla)) &= \mathbf{x} \Delta - (\mathbf{x} \cdot \nabla + 2) \nabla, \\
\nabla \cdot (\nabla \times (\mathbf{x} \times \nabla)) &= 0, \\
\mathbf{x} \cdot (\nabla \times (\mathbf{x} \times \nabla)) &= \Delta_0.
\end{align*}
\]

The following lemma is a direct consequence of Proposition 1.8.4 in [9].

**Lemma 2.3.** For \( f, g \in C^1(\mathbb{S}^{d-1}) \) and \( 1 \leq i \neq j \leq d \),

\[
\int_{\mathbb{S}^{d-1}} f(\hat{\mathbf{x}})[\hat{\mathbf{x}} \times \nabla_0 g(\hat{\mathbf{x}})]d\sigma(\hat{\mathbf{x}}) = -\int_{\mathbb{S}^{d-1}} [\hat{\mathbf{x}} \times \nabla_0 f(\hat{\mathbf{x}})]g(\hat{\mathbf{x}})d\sigma(\hat{\mathbf{x}}).
\]

2.2. Jacobi Polynomials. We now briefly review some relevant properties of Jacobi Polynomials. For real \( \alpha, \beta > -1 \), the normalized Jacobi polynomials, denoted by \( \{J_k^{(\alpha,\beta)}(\eta)\}_{k \geq 0} \), are orthonormal with respect to the Jacobi weight function \( \omega^{\alpha,\beta}(\eta) = (1-\eta)^{\alpha}(1+\eta)^{\beta} \) over \( I := (-1, 1) \),

\[
\int_{-1}^{1} J_k^{(\alpha,\beta)}(\eta)J_l^{(\alpha,\beta)}(\eta)\omega_{\alpha,\beta}(\eta)d\eta = 2^{\alpha+\beta+2}\delta_{kl}.
\]

They satisfy the three-term recurrence relation:

\[
\begin{align*}
\eta J_k^{(\alpha,\beta)}(\eta) &= a_k^{(\alpha,\beta)}J_{k+1}^{(\alpha,\beta)}(\eta) + b_k^{(\alpha,\beta)}J_k^{(\alpha,\beta)}(\eta) + a_{k-1}^{(\alpha,\beta)}J_{k-1}^{(\alpha,\beta)}(\eta), \\
J_0^{(\alpha,\beta)}(\eta) &= \frac{1}{h_0^{(\alpha,\beta)}}, \\
J_1^{(\alpha,\beta)}(\eta) &= \frac{1}{2h_1^{(\alpha,\beta)}}((\alpha + \beta + 2)\eta + (\alpha - \beta)),
\end{align*}
\]

where \( \eta \in I \), and

\[
\begin{align*}
a_k^{(\alpha,\beta)} &= \sqrt{\frac{4(k+1)(k+\alpha+1)(k+\beta+1)(k+\alpha+\beta+1)}{(2k+\alpha+\beta+1)(2k+\alpha+\beta+2)(2k+\alpha+\beta+3)}}, \\
b_k^{(\alpha,\beta)} &= \sqrt{\frac{\beta^2 - \alpha^2}{(2k+\alpha+\beta)(2k+\alpha+\beta+2)}}, \\
h_k^{(\alpha,\beta)} &= \sqrt{\frac{\Gamma(k+\alpha+1)\Gamma(k+\beta+1)}{2(2k+\alpha+\beta+1)\Gamma(k+1)\Gamma(k+\alpha+\beta+1)}}.
\end{align*}
\]

The Jacobi polynomials are the eigenfunctions of the Sturm-Liouville problem

\[
\mathcal{L}_{\eta}^{(\alpha,\beta)}J_k^{(\alpha,\beta)}(\eta) := -\frac{1}{\omega_{\alpha,\beta}(\eta)}\partial_\eta(\omega_{\alpha+1,\beta+1}(\eta)\partial_\eta J_k^{(\alpha,\beta)}(\eta)) = \lambda_k^{(\alpha,\beta)}J_k^{(\alpha,\beta)}(\eta), \quad \eta \in I,
\]
and the corresponding eigenvalues are $\lambda^{(\alpha,\beta)}_k = k(\alpha + \beta + 1)$.

### 2.3. Spherical harmonics and ball polynomials.

We first define the trivariate harmonic polynomials of total degree $n \in \mathbb{N}_0$ through the spherical coordinates $x = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)^t$,

\[
Y_n^1(x) = \frac{\sqrt{n}}{2^n} P^{(0,0)}_n(\cos \theta), \quad Y_n^2(x) = \frac{\sqrt{n}}{2^{n+1}} P^{(2,0)}_n(\cos \theta) \cos \phi, \quad 1 \leq \ell \leq n,
\]

\[
Y_{2\ell+1}^n(x) = \frac{\sqrt{n}}{2^{\ell+1} \pi} P^{(2\ell,0)}_n(\cos \theta) \sin \phi, \quad 1 \leq \ell \leq n.
\]

Thus, the spherical harmonics are eigenfunctions of the Laplace-Beltrami operator, with respect to the weight function $\varpi$.

Lemma 2.4 (9, Theorem 11.1.5). The ball orthogonal polynomials are the eigenfunctions of the differential operator:

\[
\mathcal{L}_x^{(\alpha)} P_{k,\ell}^{\alpha,n}(x) := (-\Delta + \nabla \cdot x(2\alpha + x \cdot \nabla) - 6\alpha) P_{k,\ell}^{\alpha,n}(x) = \gamma_{n+2k}^{(\alpha)} P_{k,\ell}^{\alpha,n}(x),
\]

where $\gamma_{nm}^{(\alpha)} := m(m + 2\alpha + 3)$.

The Sturm-Liouville operator $\mathcal{L}_x^{(\alpha)}$ takes different forms, which serve as preparations for the study of vectorial ball polynomials in the forthcoming sections.
Theorem 2.1 ([9] Theorem 2.2). For \( \alpha > -1 \), it holds that
\[
\mathcal{L}_x^{(\alpha)} = -(1 - \|x\|^2)\alpha - \nabla \cdot (1 - \|x\|^2)(1 - \|x\|^2)\alpha \nabla
= -(1 - \|x\|^2)\alpha - \nabla \cdot (1 - \|x\|^2)\alpha + 1 \nabla - \Delta_0
= -(1 - r^2)\partial^2 - \frac{d - 1}{r} \partial r + (2\alpha + 4) r \partial r - \frac{1}{r^2} \Delta_0,
\]
where \( \Delta_0 \) is the spherical part of \( \Delta \) and involves only derivatives in \( \hat{x} \).

2.4. Vector spherical harmonics. Now, we introduce the definition of vectorial spherical harmonics (cf. [1]),
\[
Y^{n,1}_\ell(\hat{x}) = \hat{x} Y^n_\ell(\hat{x}),
\]
\[
Y^{n,2}_\ell(\hat{x}) = r \nabla Y^n_\ell(\hat{x}) = \nabla_0 Y^n_\ell(\hat{x}),
\]
\[
Y^{n,3}_\ell(\hat{x}) = \hat{x} \times \nabla Y^n_\ell(\hat{x}) = \hat{x} \times \nabla_0 Y^n_\ell(\hat{x}).
\]
and the relations among scalar and vector spherical harmonics (cf. [1]):
\[
\nabla \cdot (f(r) Y^{n,1}_\ell(\hat{x})) = (\partial_r + \frac{2}{r}) f(r) Y^n_\ell(\hat{x}),
\]
\[
\nabla \cdot (f(r) Y^{n,2}_\ell(\hat{x})) = -\frac{n(n + 1)}{r} f(r) Y^n_\ell(\hat{x}),
\]
\[
\nabla \cdot (f(r) Y^{n,3}_\ell(\hat{x})) = 0,
\]
and
\[
\nabla \times (f(r) Y^{n,1}_\ell(\hat{x})) = -\frac{1}{r} f(r) Y^{n,3}_\ell(\hat{x}),
\]
\[
\nabla \times (f(r) Y^{n,2}_\ell(\hat{x})) = (\partial_r + \frac{1}{r}) f(r) Y^{n,3}_\ell(\hat{x}),
\]
\[
\nabla \times (f(r) Y^{n,3}_\ell(\hat{x})) = -\frac{n(n + 1)}{r} f(r) Y^{n,1}_\ell(\hat{x}) - (\partial_r + \frac{1}{r}) f(r) Y^{n,2}_\ell(\hat{x}).
\]

Moreover, it can be checked that the vector spherical harmonics are orthogonal in the same sense as the spherical harmonics,
\[
Y^{n,1}_\ell(\hat{x}) \cdot Y^{n,2}_\ell(\hat{x}) = 0, \quad Y^{n,1}_\ell(\hat{x}) \cdot Y^{n,3}_\ell(\hat{x}) = 0, \quad Y^{n,2}_\ell(\hat{x}) \cdot Y^{n,3}_\ell(\hat{x}) = 0.
\]
Moreover, the following orthogonality holds for \((\ell, n), (i, m) \in \mathcal{Y}_0\) and \(1 \leq i, j \leq 3\),
\[
\int_{S^2} Y^{n,1}_\ell(\hat{x}) \cdot Y^{m, j}_\ell(\hat{x}) d\sigma(\hat{x}) = [\delta_{i,1} + n(n + 1)(1 - \delta_{i,1})] \delta_{j, \ell} \delta_{nm}.
\]

Thanks to the above lemma, it is then straightforward to prove the following result.

Theorem 2.2. The vector spherical harmonics \( Y^{n,3}_\ell(\hat{x}) \) are eigenfunctions of \( \Delta_0 \),
\[
\Delta_0 Y^{n,3}_\ell(\hat{x}) = -n(n + 1) Y^{n,3}_\ell(\hat{x}), \quad \forall \hat{x} \in S^2.
\]

Proof. Thanks to (2.4d), we have
\[
\Delta_0 Y^{n,3}_\ell(\hat{x}) \overset{2.11c}{=} \Delta_0 (x \times \nabla) Y^n_\ell(\hat{x}) \overset{2.4d}{=} (x \times \nabla) \Delta_0 Y^n_\ell(\hat{x}) \overset{2.10}{=} -n(n + 1)(x \times \nabla) Y^n_\ell(\hat{x}) \overset{2.11a}{=} -n(n + 1) Y^{n,3}_\ell(\hat{x}).
\]
This gives the proof. \( \square \)
3. Divergence free ball PSWFs as vectorial eigenfunctions of finite Fourier transform

In this section, one may answer this question: whether there are some kinds of band-limited vectorial functions that can be optimally spatially-concentrated within a given spatial domain and satisfy the divergence free constraint.

3.1. Scalar ball PSWFs. Let us first review briefly the scalar version of this question in arbitrary dimensions. The optimal concentration problem for scalar functions is shown to be closely related to prolate spheroidal wave functions (PSWFs) of real order $\alpha > -1$ on the unit ball (cf. [23]), which are the eigenfunctions of a compact (finite) Fourier integral operator $\mathcal{F}_c^{(\alpha)} : L^2_{\varpi_{\alpha}}(\mathbb{B}) \to L^2_{\varpi_{\alpha}}(\mathbb{B})$, defined by

$$
\mathcal{F}_c^{(\alpha)}[\phi](x) = \int_{\mathbb{B}} e^{-ic|x|}\phi(\tau)\varpi_\alpha(\tau)d\tau, \quad x \in \mathbb{B}, \quad c > 0, \quad \alpha > -1.
$$

(3.1)

**Definition 3.1. (Ball PSWFs).** For real $\alpha > -1$ and real $c \geq 0$, the prolate spheroidal wave functions on a $d$-dimensional unit ball $\mathbb{B}^d$, denoted by $\{\psi_{k,\ell}^{(\alpha,n)}(x; c)\}_{k,n \in \mathbb{N}_0}$, are eigenfunctions of the integral operator $\mathcal{F}_c^{(\alpha)}$ defined in (3.1),

$$
\mathcal{F}_c^{(\alpha)}[\psi_{k,\ell}^{(\alpha,n)}](x; c) = (-i)^{n+2k}\lambda^{(\alpha)}_{n,k}(c)\psi_{k,\ell}^{(\alpha,n)}(x; c), \quad x \in \mathbb{B},
$$

(3.2)

where $c$ is the bandwidth parameter and the modulus of eigenvalues $\{\lambda^{(\alpha)}_{n,k}(c)\}_{k,n \in \mathbb{N}_0}$ are arranged for fixed $n$ as

$$
\lambda^{(\alpha)}_{n,0}(c) > \lambda^{(\alpha)}_{n,1}(c) > \cdots > \lambda^{(\alpha)}_{n,k}(c) > \cdots > 0.
$$

Note that for $\alpha = 0$, $\mathcal{F}_c^{(0)}$ is reduced to the finite Fourier transform on the ball. And $\psi_{k,\ell}^{0,n}(x; c)$ are the band-limited functions most concentrated on the unit ball.

We then define the associated integral operator $Q_c^{(\alpha)} : L^2_{\varpi_{\alpha}}(\mathbb{B}) \to L^2_{\varpi_{\alpha}}(\mathbb{B})$, defined by

$$
Q_c^{(\alpha)} = (\mathcal{F}_c^{(\alpha)})^* \circ \mathcal{F}_c^{(\alpha)}, \quad c > 0, \quad \alpha > -1.
$$

One verifies that

**Lemma 3.1 (23 Theorem 4.1)].** Let $c > 0, \alpha > -1$ and $\phi \in L^2_{\varpi_{\alpha}}(\mathbb{B})$. Then we have

$$
Q_c^{(\alpha)}[\phi](x) = \int_{\mathbb{B}} K_c^{(\alpha)}(x, \tau)\phi(\tau)\varpi_\alpha(\tau)d\tau, \quad x \in \mathbb{B},
$$

where

$$
K_c^{(\alpha)}(x, \tau) := \frac{(2\pi)^{\frac{d}{2}}}{(c\|\tau - x\|)^{\frac{d}{2}}} \int_0^1 s^{\frac{d}{2}}(1 - s^2)^\alpha J_{\frac{d}{2}}(cs\|\tau - x\|)ds.
$$

The following theorem indicates that the ball PSWFs are eigenfunctions of $\mathcal{F}_c^{(\alpha)}$ and $Q_c^{(\alpha)}$ simultaneously.

**Lemma 3.2 (23 Theorem 4.1)].** For $\alpha > -1$ and $c > 0$, the ball PSWFs $\{\psi_{k,\ell}^{(\alpha,n)}(x; c)\}_{k,n \in \mathbb{N}_0}$ are also the eigenfunctions of $Q_c^{(\alpha)}$ :

$$
Q_c^{(\alpha)}[\psi_{k,\ell}^{(\alpha,n)}](x; c) = \mu^{(\alpha)}_{n,k}(c)\psi_{k,\ell}^{(\alpha,n)}(x; c),
$$

and the eigenvalues satisfy

$$
\mu^{(\alpha)}_{n,k}(c) = |\lambda^{(\alpha)}_{n,k}(c)|^2.
$$
3.2. Divergence of the finite Fourier transform of a divergence free field. To solve the optimal concentration problem for band-limited and divergence free vector fields, it is crucial to choose fields \( E(x; c) \) such that:

- They are vectorial eigenfunctions of the (finite) Fourier integral operator, i.e.,
  \[ \hat{F}^{(a)}[E](x; c) = \lambda E(x; c). \]  
  \[ (3.3) \]

- They satisfy the divergence free constraint, i.e., \( \nabla \cdot E(x; c) = 0 \).

To this end, we first represent a vector field \( E \in L^2(\mathbb{R}^3) \) as a series in vector spherical harmonics under spherical coordinates,

\[
E(x) = \sum_{n=0}^{\infty} \sum_{\ell=1}^{2n+1} \left[ E_{\ell}^{n,1}(r) Y_{\ell}^{n,1}(\hat{x}) + E_{\ell}^{n,2}(r) Y_{\ell}^{n,2}(\hat{x}) + E_{\ell}^{n,3}(r) Y_{\ell}^{n,3}(\hat{x}) \right]. 
\]  
\[ (3.4) \]

The divergence of \( E \) can be directly obtained from \( (2.12a)-(2.12c) \),

\[
\nabla \cdot E = \sum_{n=0}^{\infty} \sum_{\ell=1}^{2n+1} \left[ (\partial_r + \frac{2}{r})E_{\ell}^{n,1}(r) - \frac{n(n+1)}{r} E_{\ell}^{n,2}(r) \right] Y_{\ell}^{n}(\hat{x}). 
\]

Hence, the divergence free constraint \( \nabla \cdot E = 0 \) is equivalent to

\[
E_{\ell}^{n,1}(r) = \frac{C}{r^2}, \quad \text{and} \quad E_{\ell}^{n,2}(r) = \frac{1}{n(n+1)} (\partial_r - \frac{1}{r}) [rE_{\ell}^{n,1}(r)], \quad (\ell, n) \in \mathbb{Y}. 
\]  
\[ (3.5) \]

Then \( (3.4), (3.5) \) and \( (2.13c) \) state that a divergence free field \( E \in L^2(\mathbb{R}^3) \) or \( E \in L^2(\mathbb{B}^3) \) is necessarily taking the form,

\[
E = \sum_{n=1}^{\infty} \sum_{\ell=1}^{2n+1} \left[ E_{\ell}^{n,3}(r) Y_{\ell}^{n,3}(\hat{x}) - \frac{1}{n(n+1)} \nabla \times (rE_{\ell}^{n,1}(r) Y_{\ell}^{n,3}(\hat{x})) \right] \]

\[ (3.6) \]

\[
\begin{align*}
2.11a & \sum_{n=1}^{\infty} \sum_{\ell=1}^{2n+1} \left[ (x \times \nabla) (E_{\ell}^{n,3}(r) Y_{\ell}^{n}(\hat{x})) - \frac{1}{n(n+1)} \nabla \times (x \times \nabla) (rE_{\ell}^{n,1}(r) Y_{\ell}^{n}(\hat{x})) \right] \\
& := \sum_{n=1}^{\infty} \sum_{\ell=1}^{2n+1} \left[ E_{\ell}^{n,3}(x) + E_{\ell}^{n,1}(x) \right].
\end{align*}
\]

In the forthcoming discussion, we shall visit the divergence of the finite Fourier transform of a divergence free vectorial field. By resorting to the spherical-polar coordinates \( x = r\hat{x} \) and \( \tau = \tau \hat{\tau} \) with \( r, \tau \geq 0 \) and \( \hat{x}, \hat{\tau} \in \mathbb{S}^2 \), we deduce that

\[
[F^{(a)} E_{\ell}^{n,3}](x) = \int_{\mathbb{B}} e^{-ic(x,\tau)} E_{\ell}^{n,3}(\tau) \omega_{\alpha}(\tau) d\tau
\]

\[ (3.4) \]

\[
\begin{align*}
2.11a & \int_{\mathbb{B}} (1 - \tau^2) \alpha^2 E_{\ell}^{n,3}(\tau) d\tau \int_{\mathbb{S}^2} e^{-icr(\hat{x},\hat{\tau})} (\hat{\tau} \times \nabla) Y_{\ell}^{n}(\hat{\tau}) d\sigma(\hat{\tau}) \\
& - \int_{\mathbb{B}} (1 - \tau^2) \alpha^2 E_{\ell}^{n,3}(\tau) d\tau \int_{\mathbb{S}^2} [(\hat{\tau} \times \nabla) e^{-icr(\hat{x},\hat{\tau})} Y_{\ell}^{n}(\hat{\tau}) d\sigma(\hat{\tau}) \\
& = - \int_{\mathbb{B}} [(x \times \nabla) e^{-ic(x,\tau)} E_{\ell}^{n,3}(\tau) Y_{\ell}^{n}(\hat{\tau}) \omega_{\alpha}(\tau) d\tau \\
& = \int_{\mathbb{B}} [(x \times \nabla) e^{-ic(x,\tau)} E_{\ell}^{n,3}(\tau) Y_{\ell}^{n}(\hat{\tau}) \omega_{\alpha}(\tau) d\tau \\
& = (x \times \nabla) \int_{\mathbb{B}} e^{-ic(x,\tau) E_{\ell}^{n,3}(\tau) Y_{\ell}^{n}(\hat{\tau}) \omega_{\alpha}(\tau) d\tau,
\end{align*}
\]
where \( \nabla_x \) (resp. \( \nabla_x \)) is understood as the gradient operator with respect to the variable \( x \). In view of (2.4b), the finite Fourier transform of \( E^{n,3}_\ell(x) \) is always divergence free,

\[
[\nabla \cdot \mathcal{F}_c^{(a)} E^{n,3}_\ell(x)] = 0. \tag{3.7}
\]

Meanwhile,

\[
[\nabla \cdot \mathcal{F}_c^{(a)} E^{n,1}_\ell(x)] = -\frac{1}{n(n+1)} \nabla \cdot \int_B \nabla \times (\nabla \times \nabla \tau) \left[ \tau E^{n,1}_\ell(\tau) Y^n(\tau) \right] e^{-ic(x,\tau)\omega_n(\tau)} d\tau \\
= -\frac{1}{n(n+1)} \int_B \nabla \times (\nabla \times \nabla \tau) \left[ \tau E^{n,1}_\ell(\tau) Y^n(\tau) \right] \cdot (-ic) e^{-ic(x,\tau)\omega_n(\tau)} d\tau \\
= \mathcal{F}_c^{(a)} E^{n,1}_\ell(x) = \tau E^{n,1}_\ell(\tau) Y^n(\tau) e^{-ic(x,\tau)\omega_n(\tau)} d\tau.
\]

Owing to the compactness of the finite Fourier transform operator \( \mathcal{F}_c^{(a)} \),

\[
[\nabla \cdot \mathcal{F}_c^{(a)} E^{n,1}_\ell(x)] = 0 \quad \text{is equivalent to} \quad E^{n,1}_\ell(r) = 0 = E^{n,2}_\ell(r). \tag{3.8}
\]

Since the finite Fourier transform of any divergence free vectorial eigenfunction of (3.3) is necessarily divergence free, the equations (3.7) and (3.8) reveal that a divergence free eigenfunction of (3.3) can only be expressed as

\[
E(x; c) = \sum_{n=1}^{\infty} \sum_{\ell=1}^{2n+1} E^{n,3}_\ell(r; c) Y^n_\ell(x) = x \times \nabla \sum_{n=1}^{\infty} \sum_{\ell=1}^{2n+1} E^{n,3}_\ell(r; c) Y^n_\ell(x) \\
:= x \times \nabla \sum_{n=1}^{\infty} \sum_{\ell=1}^{2n+1} \phi^n_\ell(x, c).
\]

Thus the eigenvalue problem (3.3) can be reduced to the scalar eigenvalue problem

\[
\mathcal{F}_c^{(a)} \phi(x; c) = \lambda^{(a)} \phi(x; c),
\]

which link up the definition 3.1 of scalar ball PSWFs.

### 3.3. Divergence free ball PSWFs

Based on the previous discussions in this section, we give the following definition.

**Definition 3.2. (Divergence free ball PSWFs).** For real \( \alpha > -1 \) and real \( c \geq 0 \), the divergence free ball prolate spheroidal wave functions on a unit ball \( \mathbb{B} \), denoted by \( \{ \psi^{\alpha,n}_{k,\ell}(x; c) \}_{k \in \mathbb{N}_0} \), are eigenfunctions of the integral operator \( \mathcal{F}_c^{(a)} \) defined in (3.2), that is,

\[
\mathcal{F}_c^{(a)} \psi^{\alpha,n}_{k,\ell}(x; c) = (-1)^n + 2k \lambda^{(a)}_{n,k}(c) \psi^{\alpha,n}_{k,\ell}(x; c), \quad x \in \mathbb{B}, \tag{3.9}
\]

where \( \{ \lambda^{(a)}_{n,k}(c) \}_{k,n \in \mathbb{N}} \) are modulus of the corresponding eigenvalues defined in (3.2), and \( c \) is the bandwidth parameter.

Two main issues of the divergence free vectorial ball PSWFs on \( \mathbb{B} \) need to be addressed:

- In the spherical-polar coordinates, divergence free vectorial ball PSWFs \( \psi^{\alpha,n}_{k,\ell}(x; c) \) have the simple representation by the scalar ball PSWFs \( \psi^{\alpha,n}_{k,\ell}(x; c) \), i.e.,

\[
\psi^{\alpha,n}_{k,\ell}(x; c) = (x \times \nabla) \psi^{\alpha,n}_{k,\ell}(x; c), \quad (\ell, n) \in \mathbb{Y}, \quad k \in \mathbb{N}_0. \tag{3.10}
\]

- With the aid of Lemma 3.2 and (3.9), we can derive that \( \{ \psi^{\alpha,n}_{k,\ell}(x; c) \}_{k \in \mathbb{N}_0} \) are also the eigenfunctions of \( Q_c^{(a)} \) :

\[
Q_c^{(a)} \psi^{\alpha,n}_{k,\ell}(x; c) = \mu^{(a)}_{n,k}(c) \psi^{\alpha,n}_{k,\ell}(x; c),
\]
and the eigenvalues are the same as those defined in (3.2) such that have the relation:
\[ \mu_{n,k}^{(\alpha)}(c) = |\lambda_{n,k}^{(\alpha)}(c)|^2. \]

It is straightforward to prove the following orthogonality result.

**Theorem 3.1.** For any \( c > 0 \) and \( \alpha > -1 \), divergence free vectorial ball PSWFs \( \{\psi_{k,\ell}^{(\alpha)}(x; c)\}_{\ell \in \mathbb{N}_0} \) are all real, smooth, and orthogonal in \( L^2_B(\mathbb{R})^3 \).

\[
\int_B \psi_{k,\ell}^{(\alpha)}(x; c) \cdot \psi_{j,\ell}^{(\alpha)}(x; c) \varphi_\alpha(x) dx = n(n+1)\delta_{k,j}\delta_{\ell,\ell}, \delta_{n,m} \quad (\ell, n, m) \in \mathbb{T}, k, j \in \mathbb{N}_0.
\]

**Proof.** In view of (2.9), we have
\[
(\psi_{k,\ell}^{(\alpha)}, \psi_{j,\ell}^{(\alpha)})_{\omega_\alpha} = (x \times \nabla \psi_{k,\ell}^{(\alpha)}, x \times \nabla \psi_{j,\ell}^{(\alpha)})_{\omega_\alpha}
= (x \times \nabla_0 \psi_{k,\ell}^{(\alpha)}, x \times \nabla_0 \psi_{j,\ell}^{(\alpha)})_{\omega_\alpha}
= - (\Delta_0 \psi_{k,\ell}^{(\alpha), n}(2r^2 - 1; c) \Delta_0 \psi_{j,\ell}^{(\alpha), m}(2r^2 - 1; c))_{\omega_\alpha}
= n(n+1)(r^n \phi_{k,\ell}^{(\alpha), n}(2r^2 - 1; c) Y_{\ell}^{(\alpha), m}(x) \psi_{j,\ell}^{(\alpha), m})_{\omega_\alpha}
= n(n+1)(\psi_{k,\ell}^{(\alpha), n} \psi_{j,\ell}^{(\alpha), m})_{\omega_\alpha} = n(n+1)\delta_{mn}\delta_{\ell,\ell}, \delta_{j,k}.
\]

This gives the proof. \( \Box \)

### 4. Divergence free ball PSWFs as vectorial eigenfunctions of Sturm-Liouville operators

In this section, we show that the divergence free vectorial ball PSWFs are eigenfunctions of two differential operators.

#### 4.1. Sturm-Liouville equations of the first kind

For \( \alpha > -1 \), we define the second-order Sturm-Liouville differential operator \( \mathcal{L}_{c,x}^{(\alpha)} \) with a parameter \( c \geq 0 \),
\[
\mathcal{L}_{c,x}^{(\alpha)} := \mathcal{L}_{c,x}^{(\alpha)}(x) + c^2 \|x\|^2 = -(1 - \|x\|^2)^{-\alpha} \nabla \cdot (I - xx^t)(1 - \|x\|^2)^\alpha \nabla + c^2 \|x\|^2,
\]
for \( x \in \mathbb{B} \). Throughout this paper, composite differential operators are understood in the convention of right associativity, for instance,
\[
\nabla \cdot (I - xx^t)(1 - \|x\|^2)\alpha \nabla = \nabla \cdot [(I - xx^t)(1 - \|x\|^2)\alpha \nabla].
\]

Obviously, \( \mathcal{L}_{c,x}^{(\alpha)} \) extends the definition of \( \mathcal{L}_{c,x}^{(\alpha)} \) such that \( \mathcal{L}_{c,x}^{(\alpha)} = \mathcal{L}_{0,x}^{(\alpha)}(x) \) and \( \mathcal{L}_{c,x}^{(\alpha)} = \mathcal{L}_{c,x}^{(\alpha)} + c^2 \|x\|^2. \)

In the forthcoming discussion, we shall demonstrate that the second-order Sturm-Liouville differential operator \( \mathcal{L}_{c,x}^{(\alpha)} \) only have one kind of divergence free vectorial eigenfunctions, which are divergence free vectorial ball PSWFs. For this purpose, we first prove the following result.

**Lemma 4.1.** It holds that
\[
(x \times \nabla) \mathcal{L}_{c,x}^{(\alpha)} = \mathcal{L}_{c,x}^{(\alpha)} (x \times \nabla),
\]
\[
\nabla \times \mathcal{L}_{c,x}^{(\alpha)} = [\mathcal{L}_{c,x}^{(\alpha)} + 2\alpha + 4] \nabla \times + 2c^2 x \times,
\]
\[
\mathcal{L}_{c,x}^{(\alpha)} \nabla \times x \times \nabla = \nabla \times x \times \nabla [\mathcal{L}_{c,x}^{(\alpha)} - (2\alpha + 2)] + 2c^2 \|x\|^2 \nabla_0.
\]

**Proof.** We obtain from a technical reduction together with (2.2) that
\[
\mathcal{L}_{c,x}^{(\alpha)} = -(1 - \|x\|^2)^{-\alpha} \nabla \cdot (1 - \|x\|^2)^{\alpha+1} \nabla - \Delta_0 + c^2 \|x\|^2
= -[(1 - \|x\|^2)\Delta - 2(\alpha + 1)(x \cdot \nabla)] - \|x\|^2 \Delta - (x \cdot \nabla)(x \cdot \nabla + 1) + c^2 \|x\|^2
= -\Delta_0 + (x \cdot \nabla)(x \cdot \nabla + 2\alpha + 3) + c^2 \|x\|^2.
\]

Then the identity \( \mathcal{L}_{c,x}^{(\alpha)} (x \times \nabla) = (x \times \nabla) \mathcal{L}_{c,x}^{(\alpha)} \) is an immediate consequence of (A.1) - (A.3).

It can be readily checked that
\[
\partial_x (x \cdot \nabla) = (x \cdot \nabla + 1) \partial_x, \quad \partial_x \|x\|^2 = \|x\|^2 \partial_x + 2x.
\]
As a result,

$${\partial}_x \mathcal{L}_{c,x}^{(a)} = \frac{4}{3} \partial_z [-\Delta + (x \cdot \nabla) (x \cdot \nabla + 2\alpha + 3) + c^2 ||x||^2]$$

$$= [-\Delta + (x \cdot \nabla + 1)(x \cdot \nabla + 2\alpha + 4) + c^2 ||x||^2] \partial_x + 2c^2 x_i$$

$$= [-\Delta + (x \cdot \nabla)(x \cdot \nabla + 2\alpha + 5) + c^2 ||x||^2] \partial_x + (2\alpha + 4) \partial_x + 2c^2 x_i$$

which implies

$$\nabla \times \mathcal{L}_{c,x}^{(a)} = \left[ \mathcal{L}_{c,x}^{(a+1)} + 2\alpha + 4 \right] \nabla \times + 2c^2 x \times .$$

In the sequel,

$$\mathcal{L}_{c,x}^{(a)} \nabla \times \nabla \frac{\partial}{\partial_x} \left[ \nabla \times \mathcal{L}_{c,x}^{(a-1)} - (2\alpha + 2) \nabla \times - 2c^2 x \nabla \nabla \right] \nabla \times$$

$$= \nabla \times x \nabla \left[ \mathcal{L}_{c,x}^{(a-1)} - (2\alpha + 2) - 2c^2 x \nabla \nabla \right] \nabla \times \nabla ,$$

which together with (2.5a) gives the desired result (4.4). The proof is completed.

The following Lemma recall the scalar ball PSWFs as eigenfunctions of the second-order differential operator \(\mathcal{L}_{c,x}^{(a)}\).

**Lemma 4.2.** [23, Theorem 4.1] For real \(\alpha > -1\) and real \(c \geq 0\), the ball prolate spheroidal wave functions, denoted by \(\{\psi_{k,\ell}^{(a)}(x;c)\}_{(\ell,n) \in \mathcal{Y}}\), are eigenfunctions of the differential operator defined in \(\mathcal{L}_{c,x}^{(a)}\) defined in (4.1), that is,

$$\mathcal{L}_{c,x}^{(a)} \psi_{k,\ell}^{(a)}(x;c) = \chi_{n,k}^{(a)}(c) \psi_{k,\ell}^{(a)}(x;c), \quad x \in \mathbb{B},$$

(4.6)

where \(c\) is the bandwidth parameter, and \(\{\chi_{n,k}^{(a)}(c)\}_{k,n \in \mathbb{N}_0}\) are real, positive eigenvalues ordered for fixed \(n\) as follows

$$0 < \chi_{n,0}^{(a)}(c) < \chi_{n,1}^{(a)}(c) < \cdots < \chi_{n,k}^{(a)}(c) < \cdots .$$

(4.7)

With the aid of Lemma 4.1, Lemma 3.1 and the relation (3.10), we can derive the following result,

$$\mathcal{L}_{c,x}^{(a)} \psi_{k,\ell}^{(a)}(x;c) = \mathcal{L}_{c,x}^{(a)} \nabla \psi_{k,\ell}^{(a)}(x;c) \quad \text{and} \quad \mathcal{L}_{c,x}^{(a)} \psi_{k,\ell}^{(a)}(x;c)$$

(4.8)

which means that any \(\{\chi_{n,k}^{(a)}(c)\}, \psi_{k,\ell}^{(a)}(x;c)\) with \((\ell,n) \in \mathcal{Y}, k \in \mathbb{N}_0\) is a divergence free vectorial pair of \(\mathcal{L}_{c,x}^{(a)}\).

**Remark 4.1.** We would like to point out that Lemma 4.1 provides us an approach for solving the vectorial eigen problem (4.8) with the divergence free constraint via the scalar eigen problem. More precisely, (4.2) states that, \((\chi, x \times \nabla \phi)\) is a divergence free vectorial eigen pair of \(\mathcal{L}_{c,x}^{(a)}\) if \((\chi, \phi)\) is an eigen pair of \(\mathcal{L}_{c,x}^{(a)}\) with \(x \times \nabla \phi \neq 0\); conversely, \((\chi, \phi)\) is an eigen pair of \(\mathcal{L}_{c,x}^{(a)}\) if \((\chi, x \times \nabla \phi)\) is a vectorial eigen pair of \(\mathcal{L}_{c,x}^{(a)}\).

Next, we shall demonstrate that the Strum-Liouville operator \(\mathcal{L}_{c,x}^{(a)}\) can not have other divergence free vectorial eigenfunctions in \(L^2_\mathbb{B}(\mathbb{R}^3)\). Thanks to the form of (3.6), it suffices to show that any \(E(x) = \nabla \times x \times \nabla E(x)\) can not be a divergence free vectorial eigenfunctions of \(\mathcal{L}_{c,x}^{(a)}\). Indeed,

$$\mathcal{L}_{c,x}^{(a)} E(x) = \mathcal{L}_{c,x}^{(a)} \nabla \times x \times \nabla E(x)$$

(4.9)
Thus by (2.5b), (2.5d), and (2.9), the following equality holds
\[ 0 = \nabla \cdot \mathcal{L}^{(a)}_{c,x} E(x)(x) = 2c^2 \Delta_0 E(x), \]
if and only if \( E(x) = \theta(r) Y^0_1(\hat{x}) \). In return, the spherical component of \( E \) is constant and \( \nabla \times x \times \nabla E(x) = \nabla \times \hat{x} \times [\nabla_0 E(x)] = 0 \). This fact indicates that the vectorial functions \( \nabla \times \hat{x} \times \nabla E(x) \) are not eigenfunctions of the Strum-Liouville operator \( \mathcal{L}^{(a)}_{c,x} \).

Finally, a combination of the previous discussions leads to the following result.

**Theorem 4.1.** For real \( \alpha > -1 \) and real \( c \geq 0 \), the divergence free ball PSWFs \( \psi^{a,n}_{k,\ell}(x;c) \), \((\ell,n) \in \mathcal{Y}, k \in \mathbb{N}_0, \) are eigenfunctions of the differential operator \( \mathcal{L}^{(a)}_{c,x} \),
\[
\mathcal{L}^{(a)}_{c,x} \psi^{a,n}_{k,\ell}(x;c) = \chi^{(a)}_{n,k}(c) \psi^{a,n}_{k,\ell}(x;c), \quad x \in \mathbb{B}, \tag{4.10}
\]
where the eigenvalues \( \{\chi^{(a)}_{n,k}(c)\}_{k,n \in \mathbb{N}} \) are defined as in Lemma 4.2.

**Remark 4.2.** If \( c = 0 \), we find readily from the previous discussions that
\[
\psi^{a,n}_{k,\ell}(x;0) = (x \times \nabla) P^{a,n}_{k,\ell}(x), \quad \chi^{(a)}_{n,k}(0) = \gamma^{(a)}_{n+2,k}. \tag{4.11}
\]

### 4.2. Sturm-Liouville equations of the second kind.

For \( \alpha > -1 \), we define the second-order Sturm-Liouville operators of the second kind,
\[
\mathcal{G}^{(a)}_{c,x} := (1 - |x|^2)^{-\alpha} \nabla \times (1 - |x|^2)^{\alpha+1} \nabla \times -\Delta_0 + c^2 |x|^2, \tag{4.12}
\]
for \( x \in \mathbb{B} \), and real \( c \geq 0 \). We are able to show that the divergence free ball PSWFs \( \psi^{a,n}_{k,\ell}(x;c) \) are the eigenfunctions of the second-order Sturm-Liouville operators \( \mathcal{G}^{(a)}_{c,x} \). As a preparation, we first obtain the following result.

**Lemma 4.3.** It holds that
\[
(x \times \nabla) \mathcal{G}^{(a)}_{c,x} = (x \times \nabla) [\mathcal{L}^{(a)}_{c,x} + 2(\alpha+1)], \tag{4.13}
\]
\[
\mathcal{G}^{(a)}_{c,x} \nabla \times x \times \nabla = \nabla \times x \times \nabla \mathcal{L}^{(a-1)}_{c,x} + 2c^2 |x| \nabla_0 - 2(\alpha + 1) \nabla \Delta_0. \tag{4.14}
\]

**Proof.** Firstly, it can be readily shown that
\[
(\nabla \times)^2 = \nabla \nabla \cdot -\Delta, \tag{4.15}
\]
\[
x \times \nabla x = \nabla x - (x \cdot \nabla + 1). \tag{4.16}
\]

From (2.2), (4.15), (4.16) and (4.15), we observe that
\[
\mathcal{G}^{(a)}_{c,x} = (1 - |x|^2)^{-\alpha} \nabla \times (1 - |x|^2)^{\alpha+1} \nabla \times -\Delta_0 + c^2 |x|^2
\]
\[
= [(1 - |x|^2)^{-\alpha}(1 - |x|^2)^{\alpha+1} \nabla \times -2(\alpha + 1)(1 - |x|^2)^{\alpha} x] \nabla \times
\]
\[
- [(|x|^2 \Delta - x \cdot \nabla (x \cdot \nabla + 1)) + c^2 |x|^2]
\]
\[
= (1 - |x|^2)[\nabla \nabla \cdot -\Delta - 2(\alpha + 1) \nabla x \cdot -(x \cdot \nabla + 1)]
\]
\[
- |x|^2 \Delta + x \cdot \nabla (x \cdot \nabla + 1) + c^2 |x|^2
\]
\[
= [(x \cdot \nabla + 2\alpha + 2)(x \cdot \nabla + 1) - \Delta + c^2 |x|^2] + [(1 - |x|^2) \nabla \nabla \cdot -2(\alpha + 1) \nabla x \cdot ]
\]
\[
= \mathcal{G}^{(a)}_{c,x} + 2(\alpha + 1) + [(1 - |x|^2) \nabla \nabla \cdot -2(\alpha + 1) \nabla x \cdot ].
\]

Then, we have
\[
\mathcal{G}^{(a)}_{c,x} (x \times \nabla) \overset{\text{1.16}}{=} [\mathcal{L}^{(a)}_{c,x} + 2(\alpha+1)](x \times \nabla) + [(1 - |x|^2) \nabla \nabla \cdot -2(\alpha + 1) \nabla x \cdot ](x \times \nabla)
\]
\[
\overset{2.30}{=} (x \times \nabla) [\mathcal{L}^{(a)}_{c,x} + 2(\alpha+1)],
\]
which yields the identity (4.13).
Now, it remains to establish (4.14). Since $\nabla \cdot \nabla \times = 0$, we find from (4.11), (4.4) and (2.5e) that
\[
\mathcal{P}_{c,x}^{(\alpha)} \nabla \times \nabla = [\mathcal{P}_{c,x}^{(\alpha)} + 2(\alpha + 1)] \nabla \times \nabla = 2(\alpha + 1) \nabla \cdot \nabla \times \nabla \nabla,
\]
which gives the desired result (4.14). \hfill \Box

Obviously, using the formula (4.13), we deduce from (4.6) that
\[
\nabla \cdot \nabla \times (x \times \nabla) = 0, \quad \nabla \cdot \nabla \times (x \times \nabla) = 0, \quad \nabla \cdot \nabla \times (x \times \nabla) = 0.
\]

**Remark 4.3.** The above argument states that, $(\chi + 2\alpha + 2, x \times \nabla \dot{\phi})$ is a divergence free vectorial eigen pair of $\mathcal{P}_{c,x}^{(\alpha)}$ if $(\chi, \dot{\phi})$ is an eigen pair of $\mathcal{L}_{c,x}^{(\alpha)}$ with $x \times \nabla \dot{\phi} \neq 0$; conversely, $(\chi, \dot{\phi})$ is an eigen pair of $\mathcal{L}_{c,x}^{(\alpha)}$ if $(\chi + 2\alpha + 2, x \times \nabla \dot{\phi})$ is a vectorial eigen pair of $\mathcal{P}_{c,x}^{(\alpha)}$.

Next, we intend to show that $\mathcal{P}_{c,x}^{(\alpha)}$ does not possess any divergence free vectorial eigenfunction of form
\[
E(x) = \nabla \times (x \times \nabla) E(x), \quad E(x) = \theta(r) Y^n_{\ell}(\hat{x}), \quad n \in \mathbb{N}.
\]
Otherwise, we observe from (4.14) that
\[
\nabla \cdot \mathcal{P}_{c,x}^{(\alpha)} \nabla \times (x \times \nabla) = 2c^2 \nabla \cdot (\|x\| \nabla_0) - 2(\alpha + 1) \nabla \cdot \nabla \Delta_0
\]
\[
\nabla \cdot \mathcal{P}_{c,x}^{(\alpha)} \nabla \times (x \times \nabla) = 2c^2 \nabla \cdot (\|x\| \nabla_0) - 2(\alpha + 1) \nabla \cdot \nabla \Delta_0
\]
and
\[
0 = \chi \nabla \cdot E(x) = \nabla \cdot \mathcal{P}_{c,x}^{(\alpha)} E(x) = \nabla \cdot \mathcal{P}_{c,x}^{(\alpha)} \nabla \times (x \times \nabla) \theta(r) Y^n_{\ell}(\hat{x})
\]
\[
- 2n(n + 1) \left[ c^2 - (\alpha + 1) \left( \partial_r^2 + \frac{2}{r} \partial_r - \frac{n(n + 1)}{r^2} \right) \right] \theta(r) Y^n_{\ell}(\hat{x}).
\]
Equivalently,
\[
[c^2 - (\alpha + 1) \left( \partial_r^2 + \frac{2}{r} \partial_r - \frac{n(n + 1)}{r^2} \right) ] \theta(r) = 0 \quad (4.18)
\]

Meanwhile, we deduce that
\[
\chi x \cdot \nabla \times \nabla \times \nabla E = x \cdot \nabla \times \nabla \times \nabla E
\]
\[
\chi x \cdot \nabla \times \nabla \times \nabla E = x \cdot \nabla \times \nabla \times \nabla E
\]
and,
\[
- n(n + 1) \chi \theta(r) Y^n_{\ell}(\hat{x}) \quad (2.9) \chi x \cdot \nabla \times \nabla \times \nabla E(x) = x \cdot \nabla \times \nabla \times \nabla E(x)
\]
\[
- n(n + 1) \left[ (r^2 - 1) \left( \partial_r^2 + \frac{2}{r} \partial_r - \frac{n(n + 1)}{r^2} \right) \right] \theta(r) Y^n_{\ell}(\hat{x})
\]
\[
- n(n + 1) \left[ (r^2 - 1) \frac{c^2}{\alpha + 1} - 2r \partial_r + n(n + 1) \right] \theta(r) Y^n_{\ell}(\hat{x}).
\]
As a result,
\[
[(r^2 - 1) \frac{c^2}{\alpha + 1} - 2r\partial_r + n(n + 1)] \theta(r) = \chi \theta(r). \tag{4.19}
\]
This, in return, gives
\[
0 \frac{r}{2} \partial_r \left[ \frac{c^2(r^2 - 1)}{\alpha + 1} + n(n + 1) - \chi + 2 \right] \theta(r) - \left[ n(n + 1) + \frac{c^2r^2}{\alpha + 1} \right] \theta(r)
\]
\[
= \frac{r}{2} \frac{c^2(r^2 - 1)}{\alpha + 1} + n(n + 1) - \chi + 2 \partial_r \theta(r) - n(n + 1) \theta(r)
\]
\[
= \frac{1}{4} \frac{c^2(r^2 - 1)}{\alpha + 1} + n(n + 1) - \chi \left( \frac{c^2(r^2 - 1)}{\alpha + 1} + (n + 2)(n + 1) - \chi \right) \theta(r),
\]
which states that \( \theta(r) = 0 \) for \( \alpha > -1 \) and \( c > 0 \), thus \( E \) is not an eigenfunction.

With the aid of the above discussion, we can obtain the following result.

**Theorem 4.2.** For real \( \alpha > -1 \) and real \( c \geq 0 \), the divergence free ball PSWFs \( \psi_{k,\ell}^{\alpha,n}(x; c) \), \((\ell, n) \in \Upsilon, k \in \mathbb{N}_0\), are eigenfunctions of the differential operator \( \mathcal{D}_{c,\alpha} \),
\[
\mathcal{D}_{c,\alpha} \psi_{k,\ell}^{\alpha,n}(x; c) = \left[ \chi_{\alpha, k}^{(\alpha)}(c) + 2\alpha + 2 \right] \psi_{k,\ell}^{\alpha,n}(x; c), \quad x \in \mathbb{B}. \tag{4.20}
\]

5. **Numerical evaluation of the divergence free ball PSWFs**

In this section, we present an efficient algorithm to evaluate the divergence free vectorial ball PSWFs and their associated eigenvalues.

5.1. **Spectrally accurate Bouwkamp algorithm.**

**Definition 5.1.** With the polynomials \( P_{k,\ell}^{\alpha,n}(x) \) on a ball \( \mathbb{B} \) in \( \mathbb{R}^3 \), we define one kind of vectorial ball polynomials \( P_{k,\ell}^{\alpha,n}(x) \),
\[
P_{k,\ell}^{\alpha,n}(x) = (x \times \nabla) P_{k,\ell}^{\alpha,n}(x), \quad x \in \mathbb{B}, \quad (\ell, n) \in \Upsilon, \quad k \in \mathbb{N}_0.
\]
Next, we introduce below some basic properties of the vector ball polynomials \( P_{k,\ell}^{\alpha,n}(x) \), which be used for the computation of divergence free vectorial ball PSWFs.

**Lemma 5.1.** \( P_{k,\ell}^{\alpha,n}(x) \) satisfies the divergence free constraint, i.e.,
\[
\nabla \cdot P_{k,\ell}^{\alpha,n}(x) = 0, \quad x \in \mathbb{B}, \quad (\ell, n) \in \Upsilon, \quad k \in \mathbb{N}_0. \tag{5.1}
\]

**Proof.** A direct calculation leads to
\[
\nabla \cdot P_{k,\ell}^{\alpha,n}(x) = \nabla \cdot (x \times \nabla P_{k,\ell}^{\alpha,n}(x)) = -\nabla \cdot (\nabla \times x P_{k,\ell}^{\alpha,n}(x)) = 0.
\]
The proof is now completed.

**Theorem 5.1.** The corresponding eigenvalue equation based on the curl-operator for \( P_{k,\ell}^{\alpha,n}(x) \) reads
\[
\mathcal{D}_{\alpha}^{(\alpha)} P_{k,\ell}^{\alpha,n}(x) : = \left( - \frac{1}{1 - |x|^2} - \alpha \nabla \cdot (1 - |x|^2)^{\alpha + 1} \nabla - \Delta_0 \right) P_{k,\ell}^{\alpha,n}(x)
\]
\[
= (n + 2k)(n + 2k + 2\alpha + 3) P_{k,\ell}^{\alpha,n}(x).
\tag{5.2}
\]
\[
\mathcal{D}_{\alpha}^{(\alpha)} P_{k,\ell}^{\alpha,n}(x) : = \left( (1 - |x|^2)^{-\alpha} \nabla \times (1 - |x|^2)^{\alpha + 1} \nabla \times \Delta_0 \right) P_{k,\ell}^{\alpha,n}(x)
\]
\[
= (n + 2k + 1)(n + 2k + 2\alpha + 2) P_{k,\ell}^{\alpha,n}(x).
\tag{5.3}
\]
Proof. Using Lemma 2.4 and Lemma 4.1, we obtain
\[ L_0^{(a)} P^\alpha_{k,\ell}(x) = L_0^{(a)} (x \times \nabla) P^\alpha_{k,\ell}(x) = (x \times \nabla) L_0^{(a)} P^\alpha_{k,\ell}(x), \]
\[ = (x \times \nabla) (n + 2k)(n + 2k + 2\alpha + 3) P^\alpha_{k,\ell}(x). \]
We now prove (5.3). From Lemma 2.4, Lemma 4.1 and Lemma 4.3, we have
\[ \nabla \cdot \nabla \cdot \psi_{k,\ell}(x) = \psi_{k,\ell}(x) \]
\[ = \psi_{k,\ell}(x) \]

This ends the proof. □

We now use the Bouwkamp-type algorithm to evaluate \( \{ \psi_{k,\ell}^{\alpha,n} \} \) with \( 2k+n \leq N \). Following the truncation rule in [42], we set \( M = 2N + 2\alpha + 30 \) and suppose \( \{ \psi_{k,\ell}^{\alpha,n}(x; c), \chi_{n,k}^{(a)} \} \) to be the approximation of \( \{ \psi_{k,\ell}^{\alpha,n}(x; c), \chi_{n,k}^{(a)} \} \) with
\[ \psi_{k,\ell}^{\alpha,n} = \sum_{j=0}^{M+n} \beta_{n,k}^{j} P_{j,\ell}^{\alpha,n}(x), \quad 2k+n \leq N. \]
Denote \( K = [M+n] \). Thanks to the Theorem 4.1 and the three-term recurrence relation (2.8) of the normalized Jacobi polynomials. The coefficient \( \beta_{n,k}^{j} \) can be equivalently deduced from evaluating the radial component \( \phi_{k,\ell}^{\alpha,n} \) of \( \psi_{k,\ell}^{\alpha,n}(x) = \phi_{k,\ell}^{\alpha,n}(2||x||^2 - 1)Y_{\ell}^\alpha(x) \) in terms of Jacobi polynomials with the unknown coefficients \( \{ \beta_{n,k}^{j} \} \):
\[ \phi_{k,\ell}^{\alpha,n}(x; c) = \sum_{j=0}^{\infty} \beta_{n,k}^{j} J_{j}^{(\alpha,\beta_n)}(\eta). \]

Then the Bouwkamp-type algorithm gives the following finite algebraic eigen-system for \( \beta_{n,k}^{j} \) and \( \chi_{n,k}^{(a)} \) (cf. [23]),
\[ (A - \chi_{n,k}^{(a)} \cdot I) \beta_{n,k}^{j} = 0, \]
where \( \beta_{n,k}^{j} = (\beta_{n,k}^{j}, \beta_{n,k}^{j+1}, \ldots, \beta_{n,k}^{j+n}) \) and \( A \) is the \( (K+1) \times (K+1) \) symmetric tridiagonal matrix whose nonzero entries are given by
\[ A_{j,j} = j_{j}^{(\alpha,\beta_n)} + (h_{j}^{(\alpha,\beta_n)} + 1) \cdot \frac{c^2}{2}; \quad A_{j,j+1} = A_{j+1,j} = a_{j}^{(\alpha,\beta_n)} \cdot \frac{c^2}{2}, \quad 0 \leq j \leq K. \]

5.2. Numerical results. We plot some samples of the \( \psi_{k,\ell}^{\alpha,n}(x; c) \) obtained from the previously described algorithms. Figure 5.2 5.2 visualize of \( \psi_{k,\ell}^{\alpha,n}(x; c) \) with different \( k, \ell, n, \alpha \) and \( c \).

APPENDIX A. PROOFS OF LEMMA 2.1 AND LEMMA 2.2

Proof of Lemma 2.1. Since \( r \) and \( \nabla_{0} \) commute, one has
\[ \nabla_{0} x^i = \frac{1}{r} \nabla_{0} x^i \leftrightarrow \nabla x^i = \frac{1}{r} \nabla_{0} x^i \leftrightarrow \nabla x^i = \frac{1}{r} \nabla_{0} x^i, \]
and
\[ x \times \nabla_{0} = x \times \frac{1}{r} \nabla_{0} \leftrightarrow (\nabla - \nabla x^i \partial_i) = x \times \nabla = -\nabla \times x, \]
which verifies (2.4a).

In analogy to \( a \cdot (a \times b) = b \cdot (a \times b) = 0 \), one readily finds
\[ \nabla \cdot (x \times \nabla) = x \cdot (x \times \nabla) = 0, \]
which proves (2.4b).
By a technical reduction, one gets
\[
(x \times \nabla) \cdot (x \times \nabla) = \sum_{1 \leq i < j \leq 3} (x_i \partial_{x_j} - x_j \partial_{x_i})^2 = \|x\|^2 \Delta - (x \cdot \nabla)^2 - x \cdot \nabla \Delta_0,
\]
which shows (2.4c).

It is obvious that
\[
(x \cdot \nabla)(x \times \nabla) = \rho r (x \times \nabla_0) = (x \times \nabla_0) \rho \partial_r = (x \times \nabla) \times (x \cdot \nabla),
\]
(A.1)
\[
\|x\|^2 (x \times \nabla)^2 = \rho^2 (x \times \nabla_0)^2 = (x \times \nabla_0)^2 \rho^2 \Delta 0,
\]
(A.2)

 Meanwhile, it is straightforward that
\[
\Delta (x \partial_{x_j} - x_j \partial_{x_i}) = [(x \partial_{x_j}) \Delta + \partial_{x_i} \partial_{x_j}] - [(x \partial_{x_j}) \Delta + \partial_{x_j} \partial_{x_i}] = (x_i \partial_{x_j} - x_j \partial_{x_i}) \Delta,
\]
which shows
\[
\Delta (x \times \nabla) = (x \times \nabla) \Delta.
\]

As a result,
\[
\Delta_0 (x \cdot \nabla) \|x\|^2 \Delta - (x \cdot \nabla)(x \cdot \nabla + 1)(x \times \nabla)
= (x \times \nabla)\|x\|^2 \Delta - (x \cdot \nabla)(x \cdot \nabla + 1) \Delta_0.
\]
which reveals (2.4d).

The proof is now completed. □

Proof of Lemma 2.2 The well-known identity on the cross products $a \times b \times c = b(a \cdot c) - c(a \cdot b)$ yields
\[ x \times (x \times \nabla) = x(x \cdot \nabla) - ||x||^2 \nabla \left( \frac{1}{r} \right) - r \nabla_0, \]
which gives (2.5a). In return,
\[ \nabla \cdot [x \times (x \times \nabla)] = \nabla \cdot (x \cdot \nabla_0) - \left( \frac{1}{r} \nabla_0 + \hat{x} \partial_r \right) \cdot r \nabla_0 \]
which is exactly (2.5b).

Applying the identity on the double curl operator $\nabla \times \nabla \times f = \nabla(\nabla \cdot f) - \Delta f$, one obtains
\[ \nabla \times (x \times \nabla) = -\nabla \times \nabla \times x = \Delta x - \nabla \nabla \cdot x \]
\[ = x \Delta + 2 \nabla - (x \cdot \nabla + 4) \nabla = x \Delta - (x \cdot \nabla + 2) \nabla, \]
which states (2.5c). In the sequel,
\[ \nabla \cdot \nabla \times x \times \nabla = \nabla \cdot x \Delta - \nabla \cdot (x \cdot \nabla + 2) \nabla = (x \cdot \nabla + 3 \Delta) \Delta - (x \cdot \nabla + 3) \Delta = 0, \]
and
\[ x \cdot \nabla \times x \times \nabla = x \cdot x \Delta - x \cdot (x \cdot \nabla + 2) \nabla = \|x\|^2 \Delta - x \cdot \nabla (x \cdot \nabla + 1) \Delta_0, \]
which gives (2.5d) and (2.5e), respectively.
This ends the proof. □

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