

Sobolev estimates for constructive uniform-grid FFT interpolatory approximations of spherical functions

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Abstract

The fast Fourier transform (FFT) based matrix-free ansatz interpolatory approximations of periodic functions are fundamental for efficient realization in several applications. In this work we design, analyze, and implement similar constructive interpolatory approximations of spherical functions, using samples of the unknown functions at the poles and at the uniform spherical-polar grid locations $(\frac{j\pi}{N}, \frac{k\pi}{N})$, for $j = 1, \dots, N - 1$, $k = 0, \dots, 2N - 1$. The spherical matrix-free interpolation operator range space consists of a selective subspace of two dimensional trigonometric polynomials which are rich enough to contain all spherical polynomials of degree less than N . Using the $\mathcal{O}(N^2)$ data, the spherical interpolatory approximation is efficiently constructed by applying the FFT techniques (in both azimuthal and latitudinal variables) with only $\mathcal{O}(N^2 \log N)$ complexity. We describe the construction details using the FFT operators and provide complete convergence analysis of the interpolatory approximation in the Sobolev space framework that are well suited for quantification of various computer models.

We prove that the rate of spectrally accurate convergence of the interpolatory approximations in Sobolev norms (of order zero and one) are similar (up to a log term) to that of the best approximation in the finite dimensional ansatz space. Efficient interpolatory quadratures on the sphere are important for several applications including radiation transport and wave propagation computer models. We use our matrix-free interpolatory approximations to construct robust FFT-based quadrature rules for a wide class of non-, mildly-, and strongly-oscillatory integrands on the sphere. We provide numerical experiments to demonstrate fast evaluation of the algorithm and various theoretical results presented in the article.

Key words: Interpolation, Spherical functions, Sobolev norms, Cubature, Spherical integrals

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1 Introduction

Approximation of functions defined on the sphere is important for realization and understanding of various processes described in the spherical-polar coordinate system. In particular, approximation of an unknown spherical function with the requirement of exactly reproducing the function at certain locations on the sphere, namely the interpolatory approximation, plays an important role in designing efficient discrete computer models of various continuous systems.

A key tool for several large scale simulations is the FFT-based representation (in polar coordinates) of the polynomial interpolatory approximation of a function defined on the circle (and in general any periodic function). The polar-coordinate/periodic case analytical interpolatory representation facilitates fast construction of the approximation without the need to solve any matrix system of interpolation constraint equations.

For a preferred set of points on the sphere, approximations of spherical functions belong to either the non-interpolatory class or the interpolatory class for the set. Construction of each of these approximations can be further subdivided into either the matrix-free class or that require solutions of linear algebraic systems. The set of points, especially for discretizing continuous systems based on differential equations (with a known source function), can be chosen for efficiently setting up discrete computer models. For experimental data based approximations, the set of observation points are in practice predetermined and such data in general include noise.

In order to avoid data sensitivity with respect to the noise, it is efficient to choose non-interpolatory class of approximations. There is a large literature on non-interpolatory approximations, depending on whether the data observation points are scattered or can be chosen by the user, see for example [5, 10, 17, 19, 20, 22, 24, 31, 34, 35] and references therein. Among these, hyperinterpolation approximations [10, 20, 31, 34] are matrix-free and these are global spherical polynomial approximations with spherical harmonic Fourier coefficients (integrals on the sphere) further approximated by a combination of quadratures with certain degree of precision. Quadrature-free quasi-interpolatory approximations can also be constructed [17] and these are in particular suitable for a class of scattered data.

The interpolatory class approximations have the advantage of being equal to a known function at all points in the set. This is in particular ideal for setting up scientific computing models governed by differential equations with known source functions. Construction of the set of interpolation points and associated interpolatory approximations is essential to develop computer models based on the collocation method, see [2, 11] and references therein.

As described later in this section, our interest is on efficiently simulating partial differential equations with applications to wave propagation and radiation transport models. Such simulations substantially benefit from the collocation method based computer models, with a fast method to compute approximations. Matrix-free interpolatory approximations for the collocation method can be efficiently built into the computer models, without solving any algebraic system to setup the discrete collocation system. The FFT based evaluations of approximations are needed for large scale simulations and precise quantification of accuracy of approximations in Sobolev spaces is crucial in the mathematical analysis of the discrete models. The main focus of this article is on developing, analyzing, implementing such matrix-free spherical interpolatory approximations.

A general approach in approximation theory is to seek a solution (that satisfy certain modeling constraints) in the space of polynomials. Within the space of spherical polynomials, it is an open problem to construct such a powerful matrix-free representation of interpolatory approximations of spherical functions. Indeed, if a standard constraint that the spherical interpolation operator (with truncated Fourier series ansatz) should exactly reproduce polynomials

of degree, say $N \geq 3$, is imposed, then it is impossible to construct a matrix-free polynomial interpolatory approximation [32]. This important two decade old work of Sloan [32] resulted in addressing several theoretical and practical questions, including efficient design of points on the sphere, see [4, 21, 29, 33] and extensive references therein. It is still an open problem to prove the numerically observed $\mathcal{O}(N)$ Lebesgue constant growth of some of the very efficient matrix-dependent spherical polynomial interpolation operators [33].

As discussed in detail in [4, 21, 33], the quality of spherical interpolatory approximation (determined by the Lebesgue constant of the interpolation operator) is important. Further, mathematically establishing error estimates of the approximation is crucial for quantifying the validity of various computer models that use such approximations. For applications, in addition to providing a fast procedure for evaluating interpolatory spherical approximations, it is important to prove associated error estimates in the L^2 and Sobolev (energy) norms. This is because robust error estimates in various approximate computer models are usually established in such norms. Our main focus in this article is on such practical (matrix-free and FFT-based) considerations and associated robust mathematical analysis. To this end, we do not require that the interpolatory spherical approximations need to be in the space of spherical polynomials.

In [7, 11, 16] a finite dimensional space χ_N (containing the space of spherical polynomials of degree less than N) was introduced. Well-posedness of the χ_N -space based interpolation problem was established in [7], using equally spaced $2N$ azimuthal angles in $[0, 2\pi)$ and *arbitrary* $N + 1$ elevation latitudinal angles in $[0, \pi]$ so that the total number of interpolation points on the sphere (including the north and south poles) is equal to the dimension of χ_N .

For the special choice of the $N + 1$ non-uniform latitudinal angles in $[0, \pi]$ that are based on Gauss-Lobatto points, as shown in [16], the χ_N -space interpolation problem is matrix-free and Sobolev error estimates for this spherical approximation was proved in [7]. If the $N + 1$ latitudinal angles in $[0, \pi]$ are equally spaced, then the χ_N -space uniquely solvable interpolation problem was also shown to be matrix-free in [16] and the growth of the Lebesgue constant of this interpolation operator is only $\mathcal{O}(\log^2 N)$. This Lebesgue constant growth (and hence error estimates in the uniform norm) was proved in [11, 16]. As demonstrated by Sloan and Womersley in [33] for benchmark smooth and non-smooth functions, this non-polynomial interpolatory spherical approximation, with proven optimal Lebesgue constant, perform better than several matrix-dependent polynomial interpolatory approximations.

Practical construction and analysis of the matrix-free interpolation operator in this article is completely different from that in [16]. The main aim of this article is on the efficient construction of uniform-grid interpolatory spherical approximation using only the FFT operators and to provide robust mathematical analysis for quantifying the interpolatory approximations in the Sobolev norm.

This article is the final of the three part constructive approximation theory and implementation work by Ganesh et al. [16, 7] on the non-polynomial range space \mathbb{S}^2 interpolation framework introduced in [11] (for a 3D potential theory computer model). Our new FFT-based construction and Sobolev space analysis presented in this article have potential applications in various large scale computer models that require approximation of spherical functions.

In particular, in our future work, we shall focus on two important classes of specific applications of the interpolatory approximations developed in this article: (i) Deterministic and stochastic three dimensional wave propagation models, for evaluation of statistical quantities and uncertainty quantification in multiple particle configurations [12, 13, 14, 15]; and (ii) Advanced radiation transport (RT) computer models [23, 26].

The acoustic and electromagnetic wave propagation Galerkin computer models developed by Ganesh and Hawkins [12, 13, 14, 15] depend on *local* spherical-polar coordinate system based

approximations (of surface currents and integrals). These coordinate systems are imposed either on various patches on the surface of a single scatterer [13] or on individual particles in multiple particle configurations [12, 14, 15]. The future advanced algorithms and analysis for the three dimensional wave propagation models will be based on the interpolatory collocation version of deterministic and stochastic algorithms in [12, 13, 14, 15]. These algorithms will also require efficient interpolatory cubature rules for medium to highly oscillatory integrals on the sphere.

The linear RT equation (RTE) poses a significant computational challenge, even for the next generation of super computers, because of the high-dimensional phase space on which it is posed. In general, the solution of the RTE (an integro-differential equation) is a function of seven independent variables: one temporal variable, three spatial variables, one energy variable and two angular spherical-polar coordinate variables (describing the direction of radiation motion). The integral part of the RTE is an integral on the sphere and, in practice, integrands with limited smoothness properties on the sphere (similar to functions in χ_N). The industrial standard approach hitherto is to apply cubature on the sphere with certain symmetry properties, such as that in [3]. However, a recent derivation [2] demonstrates that interpolatory approximation based cubature on the sphere are efficient. As discussed in the conclusion section in [2], solutions to the RTE in practice are poorly behaved in the angular variables. Hence interpolatory approximations and associated interpolatory cubature on the sphere based on approximations in the non-polynomial space χ_N will facilitate developing future advance RT computer models.

In addition to the requirement of interpolatory approximations in both the above classes of applications, an important common tool required in this future application work is an efficient FFT evaluation based interpolatory cubature on the sphere with non-, mildly-, and strongly-oscillatory integrands and quantify the error in such cubature rules for integrands with limited smoothness properties. This article is structured as follows. After developing (i) an FFT-based interpolatory approximation in Section 2; (ii) introducing a functional framework in Section 3, based on Sobolev space decomposition [9]; and (iii) proving the quality of our spherical interpolatory approximations in Section 4, we develop an efficient FFT-based interpolatory cubature on the sphere with error estimates in Section 5. Numerical results in Section 6 (and Appendix A) demonstrate various constructive and theoretical results developed and proved in this article and efficiency over a recent matrix-free interpolatory construction [7]. We conclude this article in Appendix B with proofs of some technical results stated in Section 3. This will also be of independent interest for analysis/applications on rotationally invariant manifolds [18].

2 An interpolatory approximation of spherical functions

Let \mathbb{S}^2 be the unit sphere in \mathbb{R}^3 parameterized, for $\hat{\mathbf{x}} \in \mathbb{S}^2$, using the standard convention:

$$\hat{\mathbf{x}} = \mathbf{p}(\theta, \phi) := (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta), \quad \theta, \phi \in \mathbb{R}. \quad (1)$$

For any continuous scalar-valued function F° defined on the sphere, we denote $F := F^\circ \circ \mathbf{p}$ and observe that

$$F(\theta, \phi) = F(\theta + 2\pi, \phi) = F(\theta, \phi + 2\pi), \quad F(\theta, \phi) = F(-\theta, \phi + \pi), \quad \forall \theta, \phi \in \mathbb{R}. \quad (2)$$

Conversely, for any continuous scalar-valued function F on \mathbb{R}^2 satisfying (2), there exists a unique associated function F° on the sphere. Motivated by this observation, we define the space

$$\mathcal{C} := \{F : \mathbb{R}^2 \rightarrow \mathbb{C} : F \text{ is continuous and satisfies (2)}\} \quad (3)$$

which in view of (2) can be identified with $\mathcal{C}(\mathbb{S}^2)$, the space of complex valued continuous scalar-valued functions on the unit sphere.

In this work we will introduce a trigonometric interpolant for functions F° on $\mathcal{C}(\mathbb{S}^2)$ using the following details: For $N \in \mathbb{N}$ with $N \geq 2$, consider the equally spaced grid points

$$\theta_j = \frac{j\pi}{N}, \quad \phi_k = \frac{k\pi}{N}, \quad j, k \in \mathbb{Z}.$$

We recall that, for *any* $\phi \in \mathbb{R}$, the north and south poles are respectively $\mathbf{p}(\theta_0, \phi) = \mathbf{n}$ and $\mathbf{p}(\theta_N, \phi) = \mathbf{s}$. Using (1), the parametrized uniform grid

$$\mathcal{G}_N = \{(\theta_j, \phi_k) : j = 0, \dots, N, k = 0, \dots, 2N - 1\} \quad (4)$$

in $[0, \pi] \times [0, 2\pi)$ corresponds to a grid of $2N(N - 1) + 2$ distinct points on the sphere. We also note that, similar to (2), we have

$$\mathbf{p}(\theta_j, \phi_k) = \mathbf{p}(\theta_{j+2N}, \phi_k) = \mathbf{p}(\theta_j, \phi_{k+2N}), \quad \mathbf{p}(\theta_j, \phi_k) = \mathbf{p}(\theta_{j+N}, \phi_{k-N}). \quad (5)$$

It is convenient to introduce the space of even and odd functions

$$\mathbb{D}_N^e := \text{span} \langle \cos j\theta : j = 0, \dots, N \rangle = \text{span} \langle \cos^j \theta : j = 0, \dots, N \rangle \quad (6)$$

$$\mathbb{D}_N^o := \text{span} \langle \sin j\theta : j = 1, \dots, N + 1 \rangle = \text{span} \langle \sin \theta \cos^j \theta : j = 0, \dots, N \rangle, \quad (7)$$

and then, as in [7, 11, 16], we consider a $2N^2 - 2N + 2$ dimensional subspace of \mathcal{C} , defined as

$$\chi_N := \left\{ p_0(\theta) + \sum_{\substack{-N < m \leq N \\ \text{even } m \neq 0}} \sin^2 \theta p_m(\theta) \exp(im\phi) + \sum_{\substack{-N < m \leq N \\ \text{odd } m}} p_m(\theta) \exp(im\phi) : \right. \\ \left. p_0 \in \mathbb{D}_N^e, p_{2\ell} \in \mathbb{D}_{N-2}^e, \ell \neq 0, p_{2\ell+1} \in \mathbb{D}_{N-2}^o \right\} \quad (8)$$

$$= \left\{ \sum_{\substack{-N < m \leq N \\ \text{even } m}} p_m(\theta) \exp(im\phi) + \sum_{\substack{-N < m \leq N \\ \text{odd } m}} p_m(\theta) \exp(im\phi) : \right. \\ \left. p_{2\ell} \in \mathbb{D}_N^e, p_{2\ell}(0) = p_{2\ell}(\pi) = 0 \text{ for } \ell \neq 0, p_{2\ell+1} \in \mathbb{D}_{N-2}^o \right\}. \quad (9)$$

The equality between (8) and (9) follows from the fact that for $p \in \mathbb{D}_N^e$

$$p(0) = p(\pi) = 0 \iff p(\theta) = \sin^2 \theta q(\theta), \quad \text{with } q \in \mathbb{D}_{N-2}^e.$$

We refer to [11, Section 2] for details of arriving at the subspace χ_N of \mathcal{C} from the standard trigonometric polynomial two dimensional Fourier approximation space on $[0, 2\pi] \times [0, 2\pi]$.

It is easy to check that any function $F_N \in \chi_N$ satisfies (2). In other words, the elements of χ_N can be identified with continuous functions on the sphere. Next we consider an interpolation problem with $2N^2 - 2N + 2$ interpolatory points on the unit sphere.

The spherical χ_N -interpolatory approximation problem is defined as follows: For any $F \in \mathcal{C}$,

$$\text{find } \mathcal{Q}_N F \in \chi_N, \quad \text{such that } \mathcal{Q}_N F(\theta_j, \phi_k) = F(\theta_j, \phi_k), \quad j = 0, \dots, N, \quad k = 0, \dots, 2N - 1. \quad (10)$$

In [7, Proposition 1] we proved that the interpolation problem on χ_N , with the $2N$ uniform grid azimuthal angles ϕ_k and *arbitrary* $N + 1$ latitudinal points $\theta \in [0, \pi]$, is uniquely solvable and

hence \mathcal{Q}_N reproduces functions in χ_N . In fact the unique solution to the interpolation problem can be expressed analytically without the need to solve any linear system. That is, (10) is a matrix-free interpolation problem.

In this article, we present a constructive (FFT operators based) matrix-free proof of this result, adapted to the particular choice of uniform grid latitudinal points, for two reasons: (a) it shows, from a practical point of view, how the interpolant can be fast computed employing only the FFT techniques; (b) it will provide an indication on how the analysis of the convergence of the interpolatory approximation $\mathcal{Q}_N F$ to F could be carried out. The FFT friendly uniform grid latitudinal points provide a challenging Sobolev space analysis framework on the sphere compared to that with latitudinal points that are zeros of certain orthogonal polynomials [7]. Our analysis in this article leads to an interesting trigonometric polynomials based one dimensional inequality conjecture (that we could numerically verify for practically useful cases).

Next we consider some FFT based operators that we use in the construction of the matrix-free interpolatory approximation. Let $\mathbf{DST}_N : \mathbb{C}^{N-1} \rightarrow \mathbb{C}^{N-1}$ and $\mathbf{DCT}_N : \mathbb{C}^{N+1} \rightarrow \mathbb{C}^{N+1}$ denote the discrete sine and cosine transform (*of type I*) defined as

$$(\mathbf{DST}_N(\mathbf{y}))_j := \sum_{k=1}^{N-1} y_k \sin\left(\frac{kj\pi}{N}\right), \quad j = 1, \dots, N-1, \quad (11)$$

$$(\mathbf{DCT}_N(\mathbf{x}))_j := \sum_{k=0}^N{}'' x_k \cos\left(\frac{kj\pi}{N}\right), \quad j = 0, \dots, N, \quad (12)$$

where \sum'' means the usual summation with only half the first and last terms included. These operators can easily be constructed using the standard FFT operator. Let \mathbf{iDST}_N and \mathbf{iDCT}_N respectively denote the inverse discrete sine and cosine transforms. We will also need the inverse of the discrete Fourier transform $\mathbf{iFFT}_M : \mathbb{C}^M \rightarrow \mathbb{C}^M$,

$$(\mathbf{iFFT}_M(\mathbf{z}))_j := \frac{1}{M} \sum_{k=0}^{M-1} z_k \exp\left(-\frac{2kj\pi i}{M}\right), \quad j = 0, \dots, M-1, \quad (13)$$

with the associated forward discrete Fourier transform denoted by \mathbf{FFT}_M . For construction of the matrix-free interpolation operator we will use only the above explicitly defined operators. Their inverses are defined in the following proposition and are used to prove the properties of the spherical interpolatory operator \mathcal{Q}_N in (10).

Proposition 2.1 *For any given data*

$$F_{j,k} = F(\theta_j, \phi_k), \quad j = 0, \dots, N, \quad k = 0, \dots, 2N-1,$$

representing a function $F \in \mathcal{C}$ at the grid locations \mathcal{G}_N in (4), the well defined interpolatory

approximation in (10) can be efficiently constructed using the FFT appropriate matrix-free ansatz

$$\begin{aligned}
(\mathcal{Q}_N F)(\theta, \phi) &= \frac{2}{N} \sum_{0 \leq m \leq N/2} \left[\sum_{\ell=0}^N \alpha_\ell^{2m} \cos \ell\theta \right] \exp(2mi\phi) \\
&+ \frac{2}{N} \sum_{-N/2 < m \leq -1} \left[\sum_{\ell=0}^N \alpha_\ell^{2m+2N} \cos \ell\theta \right] \exp(2mi\phi) \\
&+ \frac{2}{N} \sum_{1 \leq n \leq (N+1)/2} \left[\sum_{\ell=1}^{N-1} \beta_\ell^{2n-1} \sin \ell\theta \right] \exp((2n-1)i\phi), \\
&+ \frac{2}{N} \sum_{(-N+1)/2 < n \leq 0} \left[\sum_{\ell=1}^{N-1} \beta_\ell^{2n-1+2N} \sin \ell\theta \right] \exp((2n-1)i\phi),
\end{aligned} \tag{14}$$

where the coefficients $(\alpha_\ell^{2m})_{\ell=0}^N$ and $(\beta_\ell^{2n-1})_{\ell=1}^{N-1}$, for $m = 0, \dots, N-1$ and $n = 1, \dots, N$, can be computed using the data and the following fast algorithm:

1. Compute inverse transform data

$$(f_{j,m})_{m=0}^{2N-1} := \mathbf{iFFT}_{2N}((F_{j,k})_{k=0}^{2N-1}), \quad j = 0, \dots, N. \tag{15}$$

2. Then compute the coefficients in (14) using the sine and cosine transforms as

$$(\alpha_\ell^{2m})_{\ell=0}^N := \mathbf{DCT}_N((f_{j,2m})_{j=0}^N), \quad m = 0, \dots, N-1, \tag{16a}$$

$$(\beta_\ell^{2n-1})_{\ell=1}^{N-1} := \mathbf{DST}_N((f_{j,2n-1})_{j=1}^{N-1}), \quad n = 1, \dots, N. \tag{16b}$$

Proof. With coefficient vectors α and β as in (14)-(16), we first define, for $0 \leq m \leq N/2$ and $1 \leq n \leq (N+1)/2$, the even and odd functions:

$$p_{2m}(\theta) = \frac{2}{N} \sum_{\ell=0}^N \alpha_\ell^{2m} \cos \ell\theta \in \mathbb{D}_N^e, \quad p_{2n-1}(\theta) = \frac{2}{N} \sum_{\ell=1}^{N-1} \beta_\ell^{2n-1} \sin \ell\theta \in \mathbb{D}_{N-2}^o,$$

and similarly define for $-N/2 < m \leq -1$ and $(-N+1)/2 < n \leq 0$ the even and odd functions:

$$p_{2m}(\theta) = \frac{2}{N} \sum_{\ell=0}^N \alpha_\ell^{2m+2N} \cos \ell\theta \in \mathbb{D}_N^e, \quad p_{2n-1}(\theta) = \frac{2}{N} \sum_{\ell=1}^{N-1} \beta_\ell^{2n-1+2N} \sin \ell\theta \in \mathbb{D}_{N-2}^o.$$

In particular, for $0 \leq m \leq N/2$, $1 \leq n \leq (N+1)/2$, $j = 0, \dots, N$, and $k = 1, \dots, N-1$, we have

$$p_{2m}(\theta_j) = \left(\mathbf{iDCT}_N(\alpha_\ell^{2m})_{\ell=0}^N \right)_j, \quad p_{2n-1}(\theta_k) = \left(\mathbf{iDST}_N(\beta_\ell^{2n-1})_{\ell=1}^{N-1} \right)_k.$$

Using (9) and (14), to prove that $\mathcal{Q}_N F \in \chi_N$, it is sufficient to show that $p_m(0) = p_m(\pi) = 0$ for $m \neq 0$. Applying property (2), we obtain

$$F_{0,k} = F(0, \phi_k) = F(0, \cdot), \quad F_{N,k} = F(\pi, \phi_k) = F(\pi, \cdot), \quad \text{for } k = 0, \dots, 2N-1,$$

and therefore, $(f_{0,m})_{m=0}^{2N-1}$ and $(f_{N,m})_{m=0}^{2N-1}$ are the result of applying the iFFT operator to constant vectors. Thus,

$$f_{0,m} = \begin{cases} F(0, 0), & \text{if } m = 0, \\ 0, & \text{otherwise,} \end{cases} \quad f_{N,m} = \begin{cases} F(\pi, 0), & \text{if } m = 0, \\ 0, & \text{otherwise.} \end{cases} \tag{17}$$

Furthermore taking into account (17), we easily see that for $0 \leq m \leq N/2$ it holds

$$\begin{aligned} p_{2m}(\pi) &= \frac{2}{N} \sum_{\ell=0}^N \alpha_{\ell}^{2m} \cos(\ell\pi) = \left(\mathbf{iDCT}_N((\alpha_{\ell}^{2m})_{\ell=0}^N) \right)_N \\ &= \left(\mathbf{iDCT}_N(\mathbf{DCT}_N((f_{j,2m})_{j=0}^N)) \right)_N = f_{N,2m} = \begin{cases} F(\pi, 0), & \text{if } m = 0, \\ 0, & \text{otherwise.} \end{cases} \end{aligned} \quad (18)$$

For $-N/2 \leq m \leq -1$, proceeding analogously we obtain

$$p_{2m}(\pi) = \frac{2}{N} \sum_{\ell=0}^N \alpha_{\ell}^{2m+2N} \cos(\ell\pi) = \left(\mathbf{iDCT}_N(\mathbf{DCT}_N((f_{j,2m+2N})_{j=0}^N)) \right)_N = f_{N,2m+2N} = 0.$$

Similarly we derive

$$p_{2m}(0) = f_{0,2m} = \begin{cases} F(0, 0), & \text{if } m = 0, \\ 0, & \text{otherwise.} \end{cases} \quad (19)$$

Thus $\mathcal{Q}_N F \in \chi_N$ and that

$$\mathcal{Q}_N F(\theta_j, \phi_k) = F(\theta_j, \phi_k), \quad j \in \{0, N\}, \quad k = 0, \dots, 2N-1. \quad (20)$$

To check that $\mathcal{Q}_N F$ interpolates F at the rest of the grid points in \mathcal{G}_N , we can use a similar argument. For $j = 1, \dots, N-1$ and $k = 0, \dots, 2N-1$, using

$$\begin{aligned} (\mathcal{Q}_N F)(\theta_j, \phi_k) &= \sum_{-N/2 < m \leq N/2} p_{2m}(\theta_j) \exp(2mi\phi_k) + \sum_{(-N+1)/2 < n \leq (N+1)/2} p_{2n-1}(\theta_j) \exp((2n-1)i\phi_k) \\ &= \sum_{0 \leq m \leq N/2} \left(\mathbf{iDCT}_N((\alpha_{\ell}^{2m})_{\ell=0}^N) \right)_j \exp(2mi\phi_k) \\ &\quad + \sum_{1 \leq n \leq (N+1)/2} \left(\mathbf{iDST}_N((\beta_{\ell}^{2n-1})_{\ell=1}^{N-1}) \right)_j \exp((2n-1)i\phi_k) \\ &\quad + \sum_{-N/2 < m \leq -1} \left(\mathbf{iDCT}_N((\alpha_{\ell}^{2m+2N})_{\ell=0}^N) \right)_j \exp(2mi\phi_k) \\ &\quad + \sum_{(-N+1)/2 < n \leq 0} \left(\mathbf{iDST}_N((\beta_{\ell}^{2n-1+2N})_{\ell=1}^{N-1}) \right)_j \exp((2n-1)i\phi_k) \\ &= \sum_{n=0}^N f_{j,n} \exp\left(\frac{ni\pi k}{N}\right) + \sum_{n=-N+1}^{-1} f_{j,n+2N} \exp\left(\frac{ni\pi k}{N}\right) \\ &= \sum_{n=0}^N f_{j,n} \exp\left(\frac{ni\pi k}{N}\right) + \sum_{n=N+1}^{2N-1} f_{j,n} \exp\left(\frac{(n-2N)i\pi k}{N}\right) \\ &= \sum_{n=0}^{2N-1} f_{j,n} \exp\left(\frac{ni\pi k}{N}\right) = \left(\mathbf{FFT}_{2N}((f_{j,n})_{n=0}^{2N-1}) \right)_k \\ &= \left(\mathbf{FFT}_{2N} \left(\mathbf{iFFT}_{2N}((F_{j,k})_{k=0}^{2N-1}) \right) \right)_k = F_{j,k} = F(\theta_j, \phi_k), \end{aligned}$$

where in the penultimate step we have used $\exp\left(\frac{(n-2N)i\pi k}{N}\right) = \exp\left(\frac{ni\pi k}{N}\right)$. Combining this result with (20), we proved that the matrix-free representation in (14) solves the interpolation

problem (10). The uniqueness of the interpolant follows either from similar arguments or as a consequence of the existence of the solution since the underlying matrix in the interpolation problem is square. \square

Remark 2.2 It is easy to see that the matrix-free representation (14) also provides fast evaluation in the azimuthal variable ϕ , using the FFT. We note that the process described in Proposition 2.1 does not need that $F \in \mathcal{C}$: It suffices F to be a continuous function in $[0, \pi] \times [0, 2\pi]$, but if $F \notin \mathcal{C}$, the interpolant is a trigonometric polynomial which need not be in χ_N . \square

Remark 2.3 Roughly speaking the process explained in Proposition 2.1 consists in applying the FFT to the matrix F_{kj} by columns and then the DCT and DST to the even and odd rows respectively. Obviously, we can also revert the order of application of these transformations. In any case, the calculations are fast requiring only $\mathcal{O}(N^2 \log N)$ operations and are parallelizable. Moreover, the matrix-free representation can be exploited for performing fast evaluations of the interpolatory approximation for example, on dyadic grids, or by combining with appropriate piecewise polynomial interpolation. \square

We conclude this section by presenting the main result of this article, namely the convergence of the matrix-free interpolatory approximation in Sobolev norms $\|\cdot\|_{\mathcal{H}^s(\mathbb{S}^2)}$ on the sphere for $s \in [0, 1]$ with the regularity of spherical functions to be approximated also measured in Sobolev norms. We introduced these spaces, in terms of spherical harmonics, in the next section. Before presenting the result, we need the following technical hypothesis. Although we do not have a proof of the hypothesis, at least for all practical cases, we have numerically verified that the hypothesis is true: In Appendix 1 we demonstrate that the hypothesis is true for any integer $2 \leq N \leq 2^{14}$. The $N = 2^{14} = 16,384$ case correspond to the spherical interpolation problem with over 500 million data locations. Thus we have verified the hypothesis for almost all practical application of the interpolant studied in this article. In Appendix 1, we provide details of how we numerically verified the hypothesis.

Hypothesis 1 (Numerically verified in Appendix 1):

For each $j = 1, 2, 3$, there exists $c_{\mathbb{H}}^{(j)} < 1$, independent of N , so that

$$-2 \int_0^\pi |p_N(\theta)|^2 \cos(2N\theta) \sin \theta \, d\theta \leq c_{\mathbb{H}}^{(j)} \int_0^\pi |p_N(\theta)|^2 \sin \theta \, d\theta, \quad \forall p_N \in A_N^j, \quad (21)$$

where

$$A_N^1 := \mathbb{D}_{N-2}^e, \quad A_N^2 := \mathbb{D}_{N-2}^o, \quad \text{and} \quad A_N^3 := \{\sin^2(\theta)q_{N-2}(\theta) : q_{N-2} \in \mathbb{D}_{N-2}^e\} \subset \mathbb{D}_N^e. \quad (22)$$

Now we state the main theoretical spectrally accurate convergence result of the article.

Theorem 2.4 Suppose that Hypothesis 1 holds. Then, for $F \in \mathcal{H}^t$ with $t > 5/2$ there exists $C_t > 0$ so that, for $s \in [0, 1]$,

$$\|F - \mathcal{Q}_N F\|_{\mathcal{H}^s} \leq C_t N^{s-t} (\log N)^{s/2} \|F\|_{\mathcal{H}^t}. \quad (23)$$

Remark 2.5 A similar estimate in the continuous function space norm ($\|\cdot\|_\infty$) for the spherical interpolation operator (using Chebyshev polynomial basis based matrix-free representation) was proved in [16]:

$$\|\mathcal{F} - \mathcal{Q}_N F\|_\infty \leq C(\log N)^2 N^{-m} \|F \circ \mathbf{x}^{-1}\|_{\mathcal{C}^m(\mathbb{S}^2)},$$

where $\mathcal{C}^m(\mathbb{S}^2)$ denotes the space of functions on \mathbb{S}^2 with continuous derivatives up to order m , endowed with the natural norm. We recall that $\mathcal{H}^{1+\epsilon}(\mathbb{S}^2) \subset \mathcal{C}^0(\mathbb{S}^2)$, for any $\epsilon > 0$.

Convergence analysis of Galerkin computer models of partial differential equations (PDEs) are usually studied in the Hilbert space setting Sobolev (and equivalent energy) norms and hence our new result is widely applicable, for example, in analyzing fully discrete Galerkin methods for approximating PDE (and its equivalent boundary integral equation) based models. Fully discrete Galerkin methods are obtained by approximating Galerkin integrals (and also integral operators) in the model by finite sums (quadratures/cubatures). In Section 5 we demonstrate the applicability of the Sobolev norm estimate (23) for analyzing efficient interpolatory cubatures. \square

Remark 2.6 In [7] a similar interpolation process was studied with a non-uniform distribution of the nodes in the elevation angle, namely, that which makes $\cos \theta_n$ the Gauss-Lobatto points. The convergence in this non-uniform grid case was shown to be very similar to that stated in Theorem 2.4 but without the penalizing $\log N$ term. As demonstrated in Section 6, the FFT-based approximation considered in this article is computationally more efficient than that in [7]. However, the mathematical analysis for the equally spaced grid points case is challenging in the Sobolev framework as shown in the next two sections. \square

3 Functional framework and properties

In this section we describe orthogonal decompositions of some Sobolev spaces [9] that are crucial for proving Theorem 2.4. To this end, we introduce some fundamental properties of various norms that we state in this section and prove these properties in Appendix B.

3.1 Spherical harmonics and Sobolev spaces on the sphere

The Sobolev spaces on the unit sphere can be introduced in several equivalent forms. One can work, for instance, with an atlas of the surface, associated local charts and partition of unity functions and defined them in terms of $H^s(\mathbb{R}^2)$. This general approach is valid for any sufficiently smooth surface [1, 27]. We may also construct the Sobolev spaces on the sphere as a Hilbert scale using the eigenfunctions of the Laplace-Beltrami operator, namely, the spherical harmonics. We follow the spectral approach [28] for functional framework and introduce essential details that we use throughout this article.

Using the associated Legendre polynomial

$$P_n^m(x) := \frac{(-1)^m}{2^n n!} (1-x^2)^{m/2} \frac{d^{m+n}}{dx^{m+n}} (x^2-1)^n, \quad (24)$$

we define

$$Q_n^m(\theta) := \left(\frac{2n+1}{2} \frac{(n-m)!}{(n+m)!} \right)^{1/2} P_n^{|m|}(\cos \theta), \quad Q_n^{-m} := Q_n^m, \quad 0 \leq m \leq n, \quad n = 0, 1, \dots \quad (25)$$

Denoting

$$e_m(\phi) := \frac{1}{\sqrt{2\pi}} \exp(im\phi), \quad m \in \mathbb{Z}, \quad (26)$$

we introduce the spherical harmonics [4, 28], a polynomial of degree n on the \mathbb{S}^2 , as

$$Y_n^m(\theta, \phi) := (-1)^{(m+|m|)/2} Q_n^m(\theta) e_m(\phi), \quad m = -n, \dots, n, \quad n = 0, 1, \dots \quad (27)$$

It is well known that $\{Y_n^m : n = 0, 1, 2, \dots, |m| \leq n\}$ is an orthonormal basis of

$$\mathcal{H}^0 := \left\{ F : \mathbb{R}^2 \rightarrow \mathbb{R} : F \text{ satisfies (2), } \int_0^\pi \int_0^{2\pi} |F(\theta, \phi)|^2 \sin \theta \, d\phi \, d\theta < \infty \right\},$$

endowed with the natural inner product and the induced norm $\|F\|_{\mathcal{H}^0}$. That is, if we define for any $F \in \mathcal{H}^0$,

$$\widehat{F}_{n,m} := \int_0^\pi \int_0^{2\pi} F(\theta, \phi) \overline{Y_n^m(\theta, \phi)} \sin \theta \, d\phi \, d\theta \quad (28)$$

then

$$F = \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} \widehat{F}_{n,m} Y_n^m, \quad \|F\|_{\mathcal{H}^0}^2 = \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} |\widehat{F}_{n,m}|^2.$$

We recall that for any $F^\circ : \mathbb{S}^2 \rightarrow \mathbb{C}$, we have denoted $F = F^\circ \circ \mathbf{p}$. We follow the standard convention to identify $[Y_n^m]^\circ$ with Y_n^m , using the identity $[Y_n^m]^\circ = Y_n^m \circ \mathbf{p}$. Clearly, if $\mathcal{L}^2(\mathbb{S}^2)$ denotes the space of all square integrable functions on \mathbb{S}^2 , we have

$$\mathcal{H}^0 = \{F : F^\circ \in \mathcal{L}^2(\mathbb{S}^2)\}, \quad \text{with } \|F\|_{\mathcal{H}^0} = \|F^\circ\|_{\mathcal{L}^2(\mathbb{S}^2)}.$$

The Sobolev spaces \mathcal{H}^s for $s \in \mathbb{R}$, and their counterparts $\mathcal{H}^s(\mathbb{S}^2)$, can be defined proceeding analogously. Hence, the Sobolev norm of order s is given by

$$\|F\|_{\mathcal{H}^s}^2 := \sum_{m=-\infty}^{\infty} \sum_{n=|m|}^{\infty} \left(n + \frac{1}{2}\right)^s |\widehat{F}_{n,m}|^2,$$

which is well defined for instance if $F \in \mathbb{T} := \text{span} \langle Y_n^m : n = 0, 1, \dots, |m| \leq n \rangle$. We may also define \mathcal{H}^s as the completion of \mathbb{T} in $\|\cdot\|_{\mathcal{H}^s}$. Finally, the Sobolev space on \mathbb{S}^2 can be defined as

$$\mathcal{H}^s(\mathbb{S}^2) := \{F^\circ : F \in \mathcal{H}^s\}.$$

3.2 Sobolev-like spaces for the Fourier modes and properties

We will introduce now an orthogonal decomposition of the Sobolev spaces \mathcal{H}^s which will play an essential role in the analysis of the convergence of our interpolator. This decomposition, first introduced in [9], consists essentially in periodic one variable functions in θ which are Fourier coefficients, in ϕ , of functions on the sphere.

Given $f \in L_{\text{loc}}^1(\mathbb{R})$ we denote

$$(f \otimes e_m)(\theta, \phi) := f(\theta) e_m(\phi), \quad m \in \mathbb{Z}.$$

For $s \geq 0$, we can define the spaces

$$W_m^s := \{f \in L_{\text{loc}}^1(\mathbb{R}) : f \otimes e_m \in \mathcal{H}^s\},$$

endowed with the image norm

$$\|f\|_{W_m^s} := \|f \otimes e_m\|_{\mathcal{H}^s}.$$

Then

$$f = \sum_{n=|m|}^{\infty} \widehat{f}_m(n) Q_n^m, \quad \|f\|_{W_m^s} = \left(\sum_{n=|m|}^{\infty} (n + \frac{1}{2})^{2s} |\widehat{f}_m(n)|^2 \right)^{1/2} \quad (29)$$

with convergence in W_m^s , where

$$\widehat{f}_m(n) := \int_0^\pi f(\theta) Q_n^m(\theta) \sin \theta \, d\theta = \int_0^\pi \int_0^{2\pi} (f \otimes e_m)(\theta, \phi) \overline{Y_n^m(\theta, \phi)} \sin \theta \, d\phi \, d\theta = (\widehat{f \otimes e_m})_{n,m}.$$

Clearly, $W_m^s = W_{-m}^s$ and for $r > s$ the injection $W_m^r \subset W_m^s$ is compact. Moreover, using (29),

$$\|f\|_{W_m^s} \leq (|m| + \frac{1}{2})^{s-r} \|f\|_{W_m^r}, \quad \forall r \geq s. \quad (30)$$

We note that (2) imposes periodicity and parity conditions on the elements of W_m^s , namely

$$f \in W_m^s \implies f(\cdot + 2\pi) = f, \quad f(-\cdot) = (-1)^m f. \quad (31)$$

If we define the mapping

$$(\mathcal{F}_m F)(\theta) := \sum_{n=|m|}^{\infty} \widehat{F}_{n,m} Q_n^m(\theta) = \int_0^{2\pi} F(\theta, \phi) e_{-m}(\phi) \, d\phi,$$

it is easy to prove that $\mathcal{F}_m : \mathcal{H}^s \rightarrow W_m^s$ is just a right inverse of $f \mapsto f \otimes e_m$ and that

$$\|\mathcal{F}_m F\|_{W_m^s} \leq \|F\|_{\mathcal{H}^s}.$$

In particular, we have

$$\|F\|_{\mathcal{H}^s}^2 = \sum_{m=-\infty}^{\infty} \|\mathcal{F}_m F\|_{W_m^s}^2. \quad (32)$$

In other words, $\{W_m^s\}_m$ gives rise to an orthogonal sum decomposition of \mathcal{H}^s in its Fourier modes in the azimuthal angle ϕ . Clearly,

$$\|f\|_{W_m^0}^2 = \|f\|_{L_{\sin}^2}^2 := \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta,$$

and therefore the space for $s = 0$ is independent of m , provided that one ignores how f is extended outside of $[0, \pi]$ (see (31)). For $m = 1, 2$ it is possible to derive integral expressions for these norms, as we show in the proof (in Appendix B.1) of the following technical result.

Theorem 3.1 *Let*

$$\|f\|_{Z_0^1}^2 := \frac{1}{4} \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta + \int_0^\pi |f'(\theta)|^2 \sin \theta \, d\theta, \quad (33)$$

$$\|f\|_{Z_m^1}^2 := m^2 \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f'(\theta)|^2 \sin \theta \, d\theta, \quad (34)$$

$$\|f\|_{Z_m^2}^2 := m^4 \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin^3 \theta} + m^2 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f''(\theta)|^2 \sin \theta \, d\theta. \quad (35)$$

Then, for all $m \in \mathbb{Z}$ with $|m| \geq 1$,

$$\|f\|_{W_0^1} = \|f\|_{Z_0^1} \leq \|f\|_{W_m^1} \leq \frac{\sqrt{5}}{2} \|f\|_{Z_m^1} \leq \frac{\sqrt{5}}{2} \|f\|_{W_m^1}. \quad (36)$$

Moreover, for all $m \in \mathbb{Z}$ with $|m| \geq 2$,

$$\frac{1}{\sqrt{3}} \|f\|_{W_m^2} \leq \|f\|_{Z_m^2} \leq \sqrt{3} \|f\|_{W_m^2}. \quad (37)$$

Proof. See Appendix B.1. □

From this result, one can deduce that, for $m \neq 0$, $W_m^1 \subset C(\mathbb{R})$. Hence, assume for simplicity that f is a real valued function in $W_m^1 = Z_m^1$, then it is easy to verify that $f^2, (f^2)' \in L_{\text{loc}}^1(\mathbb{R})$. From the Sobolev embedding theorem one concludes that f^2 , and therefore f , is a continuous function. It can be seen next that necessarily, $f(0) = f(\pi) = 0$, since otherwise the first integral in the right hand side of (34) could not be finite. This is no longer true for $m = 0$ as it can easily be seen by considering the counterexample $|\log |\sin \theta||^{1/2} \in W_0^1$.

On the other hand, from Theorem 3.1 we obtain

$$\|f\|_{W_m^1} \leq \frac{\sqrt{5}}{2} \|f\|_{W_{m+2n}^1}, \quad \forall n \in \mathbb{N}, \quad (38)$$

and

$$\|f\|_{W_m^2} \leq 3 \|f\|_{W_{m+2n}^2}, \quad \forall n \in \mathbb{N}, \quad |m| \geq 2. \quad (39)$$

We finish analyzing the regularity of W_m^s from a classical Sobolev point of view. To this end, we introduce the 2π -periodic Sobolev spaces

$$H_{\#}^r := \left\{ f \in H_{\text{loc}}^r(\mathbb{R}) : f = f(\cdot + 2\pi) \right\} \quad (40)$$

endowed with the norm

$$\|f\|_{H_{\#}^r}^2 := |\widehat{f}(0)|^2 + \sum_{m \neq 0} |m|^{2r} |\widehat{f}(m)|^2, \quad \widehat{f}(m) = \frac{1}{2\pi} \int_0^{2\pi} f(\theta) \exp(-im\theta) d\theta. \quad (41)$$

For $r = 0$, $\|\cdot\|_{H_{\#}^0}$ is, up to the factor $\sqrt{2\pi}$, the $L^2(0, 2\pi)$ norm. For non-negative integer values of r , an equivalent norm is given by

$$\left[\int_0^{2\pi} |f(\theta)|^2 d\theta + \int_0^{2\pi} |f^{(r)}(\theta)|^2 d\theta \right]^{1/2}. \quad (42)$$

Proposition 3.2 *For all $r > 0$ there exists $C_r > 0$ independent of m and f such that*

$$\|f\|_{H_{\#}^r} \leq C_r \|f\|_{W_m^{r+1/2}}, \quad \forall f \in W_m^{r+1/2}. \quad (43)$$

Further,

$$\|f\|_{W_m^0} \leq \|f\|_{H_{\#}^0}, \quad \|f\|_{W_m^1} \leq C(1 + |m|) \|f\|_{H_{\#}^1}, \quad (44)$$

with C independent of f and m .

Proof. See Appendix B.2. □

4 Error estimates for spherical interpolatory approximations

In this section we prove Theorem 2.4 after deriving several associated one dimensional interpolant properties.

4.1 Fourier analysis

We consider the following even and odd one dimensional interpolation problem, for the data $f(\theta_j)$, $j = 0, \dots, N$:

$$\text{Find } q_N^e f \in \mathbb{D}_N^e f, \quad \text{such that } q_N^e f(\theta_j) = f(\theta_j), \quad j = 0, \dots, N,$$

$$\text{Find } q_N^o f \in \mathbb{D}_{N-2}^o, \quad \text{such that } q_N^o f(\theta_j) = f(\theta_j), \quad j = 1, \dots, N-1.$$

For notational convenience, we introduce

$$q_N^m := \begin{cases} q_N^e, & \text{if } m \text{ is even,} \\ q_N^o, & \text{if } m \text{ is odd.} \end{cases}$$

Then, as proved in [7, Section 4.1, Lemma 3], we have the following Fourier expression connecting the matrix-free interpolant on the sphere, defined in (10), and the even and odd interpolants, as a result of an aliasing process in ϕ : for all $F \in \mathcal{H}^r$ with $r > 1$

$$(\mathcal{Q}_N F)(\theta, \phi) = \sum_{-N+1 \leq m \leq N} (q_N^m \rho_N^m F)(\theta) e_m(\phi), \quad \text{with } \rho_N^m F := \sum_{\ell=-\infty}^{\infty} \mathcal{F}_{m+2\ell N} F. \quad (45)$$

Then, error in the spherical interpolatory approximation can be estimated as

$$\begin{aligned} \|\mathcal{Q}_N F - F\|_{\mathcal{H}^s}^2 &= \sum_{-N+1 \leq m \leq N} \|q_N^m \rho_N^m F - \mathcal{F}_m F\|_{W_m^s}^2 + \left[\sum_{m \geq N+1} + \sum_{m \leq -N} \right] \|\mathcal{F}_m F\|_{W_m^s}^2 \\ &\leq \sum_{-N+1 \leq m \leq N} \|q_N^m \mathcal{F}_m F - \mathcal{F}_m F\|_{W_m^s}^2 + \sum_{-N+1 \leq m \leq N} \|q_N^m (\rho_N^m F - \mathcal{F}_m F)\|_{W_m^s}^2 \\ &\quad + \left[\sum_{m \geq N+1} + \sum_{m \leq -N} \right] \|\mathcal{F}_m F\|_{W_m^s}^2 \end{aligned} \quad (46)$$

Thus, for proving Theorem 2.4, we have to bound three terms which depend on the approximation properties of q_N^m , the stability of this interpolant and the error introduced by ignoring the tail of the Fourier series (in θ). The two first properties concerning for the one-dimensional interpolant q_N^m will be explored in the next subsection.

4.2 Error estimates for one dimensional interpolants

Let I_N be the trigonometric interpolant for 2π -periodic functions defined by

$$I_N f \in \text{span}\langle e_m : -N < m \leq N \rangle, \quad \text{such that } I_N g(\theta_j) = g(\theta_j), \quad j = -N+1, \dots, N. \quad (47)$$

Then, if we denote $g_- = g(-\cdot)$, it is easy to show that the average function

$$q_N g := \frac{1}{2} [I_N g + (I_N g_-)_-] \in \text{span}\langle e_m : -N \leq m \leq N \rangle$$

solves also (47) and preserves the parity of the integrand, i.e., if g is even/odd then so is $q_N g$. Further,

$$q_N g \in \mathbb{D}_N^e \oplus \mathbb{D}_{N-2}^o.$$

It is now straightforward to check that for f_e and f_o 2π -periodic even and odd respectively functions, we have

$$q_N^e f_e = q_N f_e, \quad q_N^o f_o = q_N f_o.$$

These relations and the well known Sobolev convergence estimates for I_N (cf. [30, Ch. 8]), yield

$$\|q_N^m f - f\|_{H_{\#}^s} \leq CN^{s-t} \|f\|_{H_{\#}^t}, \quad \text{for any } f \in H_{\#}^t \cap W_m^1, \quad 0 \leq s \leq t, \quad t > 1/2. \quad (48)$$

In the above inequality and in the remainder of this section, it is convenient to use C to represent a generic positive constant that is independent of the truncation parameter N .

In this subsection we will derive convergence estimates for q_N^m very similar to (48) but with the norms $\|\cdot\|_{W_m^s}$ instead. We prove such results for the interpolant q_N^m in Theorem 4.11, after developing ten auxiliary results in this subsection. To this end, we first start with inverse estimate:

Lemma 4.1 *For any $s \geq 0$, there exists $C > 0$ such that, for any $r_N \in \mathbb{D}_N^e$, $s_N \in \mathbb{D}_{N-2}^o$, the following estimate holds*

$$\|r_N\|_{W_0^s} \leq CN^s \|r_N\|_{W_0^0}, \quad \|s_N\|_{W_1^s} \leq CN^s \|s_N\|_{W_1^0}. \quad (49)$$

Proof. The above inverse inequality for the case $s = 1$ was established in [7, Lemma 6] and the proof is similar for $s \geq 0$. \square

Proposition 4.2 *For all $m \in \mathbb{Z}$ and $N \geq 2$, there exist projections p_N^m on \mathbb{D}_N^e for even m and on \mathbb{D}_{N-2}^o for odd m which satisfy the following convergence estimate*

$$\|p_N^m f - f\|_{W_m^s} \leq C_{s,t} N^{s-t} \|f\|_{W_m^t}, \quad (50)$$

where $0 \leq s \leq t$ with $t > 1$ and $C_{s,t}$ independent of f . Moreover,

$$p_N^m f(0) = f(0), \quad \text{and} \quad p_N^m f(\pi) = f(\pi).$$

Proof. For $m \neq 0$ we can choose p_N^m to be the truncated partial sum

$$T_N^m f := \sum_{0 \leq n \leq N-1} \widehat{f}_m(n) Q_n^m \in \text{span}\langle Q_n^m : n \leq N-1 \rangle \subset \begin{cases} \mathbb{D}_{N-1}^e, & \text{if } m \text{ is even,} \\ \mathbb{D}_{N-2}^o, & \text{if } m \text{ is odd,} \end{cases}$$

with the choice of $Q_n^m = 0$ for $n < |m|$ in (29) so that the sum above is void for $n < |m|$. The definition of the norms of W_m^s implies

$$\|T_N^m f - f\|_{W_m^s}^2 = \sum_{n \geq N} |n + \frac{1}{2}|^{2s} |\widehat{f}_m(n)|^2 \leq (N + \frac{1}{2})^{2s-2t} \|f\|_{W_m^t}^2. \quad (51)$$

We observe that (50) holds actually for any $t \geq s$ and also that for $m \neq 0$, $p_N^m f(0) = p_N^m f(\pi) = 0$ and $f \in W_m^1$ vanishes at $\{0, \pi\}$.

For $m = 0$, we cannot ensure that $\mathbf{T}_N^0 f(\{0, \pi\}) = f(\{0, \pi\})$ which prompts us to consider a different projection. In this case, we choose \mathbf{p}_N^0 to be the interpolant

$$\mathbf{p}_N^0 \in \mathbb{D}_N^e, \quad \text{such that} \quad \mathbf{p}_N^0(\eta_j) = f(\eta_j), \quad j = 0, \dots, N$$

where $\{\cos \eta_j\}_j$ are the Gauss-Lobatto quadrature points, which includes the endpoints, that is, $\eta_0 = 0$, and $\eta_N = \pi$. In [7, Appendix A, Proposition 6] we proved that for all $t > 1$ there exists $C_t > 0$ such that

$$\|\mathbf{p}_N^0 f - f\|_{W_0^0} \leq C_t N^{-t} \|f\|_{W_0^t}, \quad \forall f \in W_0^t. \quad (52)$$

Using (49) and (51), we first obtain

$$\begin{aligned} \|\mathbf{p}_N^0 f - f\|_{W_0^s} &\leq \|\mathbf{p}_N^0(f - \mathbf{T}_N^0 f)\|_{W_0^s} + \|\mathbf{T}_N^0 f - f\|_{W_0^s} \\ &\leq CN^s \|\mathbf{p}_N^0(f - \mathbf{T}_N^0 f)\|_{W_0^0} + (N + \frac{1}{2})^{s-t} \|f\|_{W_0^t} \\ &\leq CN^s [\|\mathbf{p}_N^0 f - f\|_{W_0^0} + \|\mathbf{T}_N^0 f - f\|_{W_0^0}] + (N + \frac{1}{2})^{s-t} \|f\|_{W_0^t} \\ &\leq C \left[(N + \frac{1}{2})^s \|\mathbf{p}_N^0 f - f\|_{W_0^0} + 2(N + \frac{1}{2})^{s-t} \|f\|_{W_0^t} \right] \end{aligned}$$

and hence the desired result (50) follows by applying (52) □

Lemma 4.3 ([7, Proposition 4]) *For $f \in Z_0^1$, there exists $C > 0$ such that*

$$\|f\|_{H_{\#}^0} \leq C [\|f\|_{L_{\sin}^2} + \|f\|_{L_{\sin}^2}^{1/2} \|f'\|_{L_{\sin}^2}^{1/2}]$$

For the next result, we introduce $s_N, \tilde{s}_N \in \mathbb{D}_N^e$, the orthogonal and interpolating approximations of the $\sin(\cdot)$ function on $[0, \pi]$. That is,

$$s_N \in \mathbb{D}_N^e \quad \text{such that} \quad s_N(\theta_j) = \sin \theta_j, \quad j = 0, \dots, N, \quad (53a)$$

$$\tilde{s}_N \in \mathbb{D}_N^e \quad \text{such that} \quad \int_0^\pi (\tilde{s}_N(\theta) - \sin \theta) p_N(\theta) d\theta = 0, \quad \forall p_N \in \mathbb{D}_N^e. \quad (53b)$$

Lemma 4.4 *For all $N \geq 1$*

$$\|\tilde{s}_N - \sin(\cdot)\|_{L^\infty(0, \pi)} \leq \frac{2}{\pi N}, \quad \|s_N - \tilde{s}_N\|_{L^\infty(0, \pi)} \leq \frac{2}{\pi N}.$$

Proof. We prove the result for even N . The odd N case follows similarly. Straightforward calculations show that for $\theta \in [0, \pi]$

$$\sin \theta = \frac{2}{\pi} - \frac{4}{\pi} \sum_{j=1}^{\infty} \frac{\cos 2j\theta}{4j^2 - 1}.$$

On the other hand, we have the aliasing effect

$$\mathbf{q}_N^e(\cos((2j + 2\ell N) \cdot)) = \cos(2j \cdot) = \mathbf{q}_N^e(\cos((-2j + 2\ell N) \cdot)), \quad 0 \leq j \leq N, \quad \forall \ell \in \mathbb{Z}.$$

These properties imply that

$$\begin{aligned}
\tilde{s}_N(\theta) &= \frac{2}{\pi} - \frac{4}{\pi} \sum_{j=1}^{N/2} \frac{\cos 2j\theta}{4j^2 - 1} \\
s_N(\theta) &= \frac{2}{\pi} \left[1 - \sum_{\ell=1}^{\infty} \frac{2}{(2\ell N)^2 - 1} \right] \\
&\quad - \frac{4}{\pi} \sum_{j=1}^{N/2-1} \left[\frac{1}{4j^2 - 1} + \sum_{\ell=1}^{\infty} \left(\frac{1}{(2j + 2\ell N)^2 - 1} + \frac{1}{(-2j + 2\ell N)^2 - 1} \right) \right] \cos 2j\theta \\
&\quad - \frac{4}{\pi} \left[\frac{1}{N^2 - 1} + \sum_{\ell=1}^{\infty} \frac{1}{(N + 2\ell N)^2 - 1} \right] \cos N\theta.
\end{aligned}$$

Then, for any $\theta \in [0, \pi]$,

$$|\tilde{s}_N(\theta) - \sin \theta| \leq \frac{4}{\pi} \sum_{j=N/2+1}^{\infty} \frac{1}{4j^2 - 1} = \frac{2}{\pi(N+1)} \leq \frac{2}{\pi N}. \quad (54)$$

On the other hand,

$$\begin{aligned}
|\tilde{s}_N(\theta) - s_N(\theta)| &\leq \frac{4}{\pi} \left[\sum_{\ell=2}^{\infty} \frac{1}{(\ell N)^2 - 1} \right. \\
&\quad \left. + \sum_{j=1}^{N/2-1} \sum_{\ell=1}^{\infty} \left(\frac{1}{(2j + 2\ell N)^2 - 1} + \frac{1}{((N - 2j) + (2\ell - 1)N)^2 - 1} \right) \right] \\
&= \frac{4}{\pi} \left[\sum_{\ell=1}^{\infty} \frac{1}{(N + \ell N)^2 - 1} + \sum_{j=1}^{N/2-1} \sum_{\ell=1}^{\infty} \frac{1}{(2j + \ell N)^2 - 1} \right] \\
&= \frac{4}{\pi} \sum_{j=1}^{N/2} \sum_{\ell=1}^{\infty} \frac{1}{(2j + \ell N)^2 - 1} \leq \frac{2}{\pi} \sum_{j=1}^N \sum_{\ell=1}^{\infty} \frac{1}{(j + \ell N)^2 - 1} \\
&= \frac{2}{\pi} \sum_{j=N+1}^{\infty} \frac{1}{j^2 - 1} = \frac{2}{\pi N}.
\end{aligned}$$

□

In order to prove the next result, it is convenient to consider the quadrature rules

$$\mathcal{L}_N^1 g := \frac{\pi}{N} \sum_{k=0}^N g\left(\frac{k\pi}{N}\right), \quad \mathcal{L}_N^2 g := \frac{\pi}{N} \sum_{j=1}^N g\left(\frac{(j-1/2)\pi}{N}\right).$$

Since

$$\mathcal{L}_N^1 \cos(m \cdot) = \begin{cases} \pi, & \text{if } m = 2\ell N, \\ 0, & \text{otherwise,} \end{cases} \quad \mathcal{L}_N^2 \cos(m \cdot) = \begin{cases} (-1)^\ell \pi, & \text{if } m = 2\ell N, \\ 0, & \text{otherwise,} \end{cases}$$

we easily deduce the equalities

$$\mathcal{L}_N^1 g_N = \mathcal{L}_N^2 g_N = \int_0^\pi g_N(\theta) d\theta, \quad \forall g_N \in \mathbb{D}_{2N-1}^e,$$

and therefore

$$\mathcal{L}_N^1(|g_N|^2) = \mathcal{L}_N^2(|g_N|^2) = \|g_N\|_{H_{\#}^0}^2, \quad \forall g_N \in \mathbb{D}_{N-1}^e \cup \mathbb{D}_{N-1}^o. \quad (55)$$

Moreover,

$$\mathcal{L}_N^1(|g_N|^2) \leq 2\|g_N\|_{H_{\#}^0}^2, \quad \mathcal{L}_N^2(|g_N|^2) \leq \|g_N\|_{H_{\#}^0}^2, \quad \forall g_N \in \mathbb{D}_N^e. \quad (56)$$

Besides, for g sufficiently smooth

$$\mathcal{L}_N^2 g - \mathcal{L}_N^1 g = -4 \sum_{\ell=0}^{\infty} \int_0^{\pi} g(\theta) \cos(2N(1+2\ell)\theta) d\theta. \quad (57)$$

That is, the difference in the quadrature rules is four times the sum of the Fourier coefficients in the cosine series of order $2(1+2\ell)N$.

The well known estimate for the error of the composite rectangular rule

$$\left| \mathcal{L}_N^1 g - \int_0^{\pi} g(\theta) d\theta \right| \leq \pi N^{-1} \int_0^{\pi} |g'(\theta)| d\theta \quad (58)$$

will be used repeatedly in this section. Further it is useful to note the relation

$$\mathcal{L}_{2N}^1 = \frac{1}{2}(\mathcal{L}_N^1 + \mathcal{L}_N^2). \quad (59)$$

In the proofs below we use the fact that if $f \in W_m^1$, with $m \neq 0$, then f is continuous with $f(0) = f(\pi) = 0$.

Proposition 4.5 *Suppose that Hypothesis 1 holds. Let $f \in W_m^1$ with $m \neq 0$. Then*

$$\|q_N^m f\|_{L_{\sin}^2} \leq C[\|f\|_{L_{\sin}^2} + N^{-1}\|f'\|_{L_{\sin}^2} + N^{-1/2}\|q_N^m f\|_{H_{\#}^0}] \quad (60)$$

with C independent of f and m .

Proof. Since

$$\|q_N^m f\|_{L_{\sin}^2}^2 = \int_0^{\pi} |q_N^m f(\theta)|^2 s_N(\theta) d\theta + \int_0^{\pi} |q_N^m f(\theta)|^2 (\sin \theta - s_N(\theta)) d\theta, \quad (61)$$

using Lemma 4.4,

$$\|q_N^m f\|_{L_{\sin}^2}^2 \leq \int_0^{\pi} g_N(\theta) d\theta + CN^{-1}\|q_N^m f\|_{H_{\#}^0}^2 = \mathcal{L}_{2N}^1 g_N + CN^{-1}\|q_N^m f\|_{H_{\#}^0}^2$$

where $g_N := |q_N^m f|^2 s_N \in \mathbb{D}_{3N}^e$. Applying (59) we deduce the bound

$$\|q_N^m f\|_{L_{\sin}^2}^2 \leq \mathcal{L}_N^1 g_N + \frac{1}{2}(\mathcal{L}_N^2 g_N - \mathcal{L}_N^1 g_N) + CN^{-1}\|q_N^m f\|_{H_{\#}^0}^2. \quad (62)$$

Since $f(0) = f(\pi) = 0$ and $q_N^m f(\theta_j) = f(\theta_j)$, for all $j = 0, \dots, N$, using Lemma 4.4 we easily deduce the following bound:

$$\begin{aligned} \mathcal{L}_N^1 g_N &= \frac{\pi}{N} \sum_{j=1}^{N-1} |f(\theta_j)|^2 \sin \theta_j + \frac{\pi}{N} \sum_{j=1}^{N-1} |q_N^m f(\theta_j)|^2 (s_N(\theta_j) - \sin \theta_j) \\ &\leq \frac{1}{N} \sum_{j=1}^{N-1} |f(\theta_j)|^2 \sin \theta_j + CN^{-1} \mathcal{L}_N^1(|q_N^m f|^2) =: E_1 + CN^{-1} \mathcal{L}_N^1(|q_N^m f|^2). \end{aligned} \quad (63)$$

Also, using (56),

$$\mathcal{L}_N^1(|q_N^m f|^2) \leq 2\|q_N^m f\|_{H_\#^0}^2. \quad (64)$$

On the other hand, E_1 in (63) can be bounded using the error of the rectangular rule (58):

$$\begin{aligned} E_1 &= \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta + \left[\mathcal{L}_N^1(|f|^2 \sin(\cdot)) - \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta \right] \\ &\leq \|f\|_{L_{\sin}^2}^2 + \frac{\pi}{N} \int_0^\pi |(|f(\theta)|^2 \sin \theta)'| \, d\theta \\ &\leq \|f\|_{L_{\sin}^2}^2 + \frac{\pi}{N} \int_0^\pi |f(\theta)|^2 \, d\theta + \frac{\pi}{N} \int_0^\pi |2f(\theta)f'(\theta)| \sin \theta \, d\theta \\ &\leq \|f\|_{L_{\sin}^2}^2 + CN^{-1} \left[\|f\|_{L_{\sin}^2}^2 + \|f\|_{L_{\sin}^2} \|f'\|_{L_{\sin}^2} + \int_0^\pi |f(\theta)f'(\theta)| \sin \theta \, d\theta \right] \\ &\leq \|f\|_{L_{\sin}^2}^2 + CN^{-2} \|f'\|_{L_{\sin}^2}^2. \end{aligned} \quad (65)$$

We stress that in (65) we have used Lemma 4.3 and, in the last step, the inequality

$$\|f\|_{L_{\sin}^2} \|f'\|_{L_{\sin}^2} + \int_0^\pi |f(\theta)f'(\theta)| \sin \theta \leq N\|f\|_{L_{\sin}^2} + N^{-1}\|f'\|_{L_{\sin}^2}.$$

Finally, using the fact that $|q_N^m f|^2 s_N \in \mathbb{D}_{3N}^e$ and applying (57) and Hypothesis 1, we deduce the bound

$$\begin{aligned} \frac{1}{2}(\mathcal{L}_N^2 g_N - \mathcal{L}_N^1 g_N) &= -2 \int_0^\pi |q_N^m f|^2(\theta) s_N(\theta) \cos(2N\theta) \, d\theta \\ &= -2 \int_0^\pi |q_N^m f|^2(\theta) \sin \theta \cos(2N\theta) \, d\theta \\ &\quad -2 \int_0^\pi |q_N^m f|^2(\theta) (\sin \theta - s_N(\theta)) \cos(2N\theta) \, d\theta \\ &\leq \max\{c_H^{(2)}, c_H^{(3)}\} \int_0^\pi |q_N^m f|^2(\theta) \sin \theta \, d\theta + CN^{-1} \|q_N^m f\|_{H_\#^0}^2, \end{aligned} \quad (66)$$

where we have used again Lemma 4.4. Collecting (63)-(66) in (62) (with $c_H := \max\{c_H^{(2)}, c_H^{(3)}\}$) we conclude

$$(1 - c_H) \|q_N^m f\|_{L_{\sin}^2}^2 \leq C [\|f\|_{L_{\sin}^2}^2 + N^{-2} \|f'\|_{L_{\sin}^2}^2 + N^{-1} \|q_N^m f\|_{H_\#^0}^2].$$

Hence the desired result (60) follows. \square

Corollary 4.6 *Suppose that Hypothesis 1 holds. For all $r > 1$ there exists $C_r > 0$ so that for all $f \in W_m^r$ [with $f(0) = f(\pi) = 0$ for $m = 0$]*

$$\|q_N^m f\|_{W_m^0} \leq C [\|f\|_{W_m^0} + N^{-1} \|f\|_{W_m^1} + N^{-r} \|f\|_{W_m^r}], \quad (67)$$

with C_r independent of N , m and f .

Proof. In light of Proposition 4.5, we just have to bound

$$N^{-1/2} \|q_N^m f\|_{H_\#^0} \leq N^{-1/2} \|q_N^m f - f\|_{H_\#^0} + N^{-1/2} \|f\|_{H_\#^0}. \quad (68)$$

For the second term we can apply Lemma 4.3 and the inequality $2ab \leq N^{1/2}a + N^{-1/2}b$, to show that

$$N^{-1/2}\|f\|_{H_{\#}^0} \leq CN^{-1/2}(\|f\|_{L_{\sin}^2} + \|f\|_{L_{\sin}^2}^{1/2}\|f'\|_{L_{\sin}^2}^{1/2}) \leq C[\|f\|_{L_{\sin}^2} + N^{-1}\|f'\|_{L_{\sin}^2}]. \quad (69)$$

On the other hand, (48) implies that for all $r > 1$ there exists C_r so that

$$N^{-1/2}\|q_N^m f - f\|_{H_{\#}^0} \leq C_r N^{-r}\|f\|_{H_{\#}^{r-1/2}} \leq C'_r N^{-r}\|f\|_{W_m^r}, \quad (70)$$

where we have applied in the last step Proposition 3.2. We note that C_r is again independent of m . Applying (69) and (70) in (68) we deduce the bound

$$N^{-1/2}\|q_N^m f\|_{H_{\#}^0} \leq C_r[\|f\|_{H_{\#}^0} + N^{-1}\|f\|_{W_m^1} + N^{-r}\|f\|_{W_m^r}]$$

and hence the desired results (67) follows. \square

To prove stability estimates in W_m^1 , it is convenient to introduce the notation

$$\|f\|_{L_{\sin^r}^2}^2 := \int_0^\pi |f(\theta)|^2 \sin^r \theta \, d\theta,$$

(in particular with $r = 1, -1, -2$ or -3) and use the equivalence of norms described in Theorem 3.1 involving the two terms

$$|m|\|q_N^m f\|_{L_{\sin^{-1}}^2} \quad \text{and} \quad \|(q_N^m f)'\|_{L_{\sin}^2}. \quad (71)$$

The second term is easily controlled by using inverse inequality and the results developed so far.

Lemma 4.7 *Suppose that Hypothesis 1 holds. There exists $C > 0$ independent of m , f and N such that*

$$\|(q_N^m f)'\|_{L_{\sin}^2} \leq CN^{-1}[\|f\|_{W_m^0} + N^{-1}\|f\|_{W_m^1} + N^{-r}\|f\|_{W_m^r}]. \quad (72)$$

Proof. Lemma 4.1 and the equivalent norms presented in Theorem 3.1 allow us to conclude, as a byproduct, the inverse inequality

$$\|(q_N^m f)'\|_{L_{\sin}^2} \leq CN\|q_N^m f\|_{L_{\sin}^2}. \quad (73)$$

Hence applying Corollary 4.6 will lead to the derivation of the bound (72). \square

The analysis of the first term in (71) is rather more delicate. Thus, before entering in the analysis we need to prove some technical results.

Lemma 4.8 *There exists $C > 0$ so that for all $r_N \in \mathbb{D}_{N-2}^e$ with $N \geq 2$,*

$$|r_N(0)|^2 + |r_N(\pi)|^2 \leq CN^2 \log N \mathcal{L}_N^1(|r_N|^2 \sin(\cdot)). \quad (74)$$

Proof. For each $j = 1, \dots, N-1$ define

$$L_j^N := (-1)^{j+1} \sin^2 \theta_j \frac{\sin N\theta}{N \sin \theta (\cos \theta - \cos \theta_j)} \in \mathbb{D}_{N-2}^e.$$

It is a simple exercise to verify that

$$L_j^N(\theta_i) = \begin{cases} 1, & i = j, \\ 0, & \text{otherwise.} \end{cases}$$

Thus, $\{L_j^N\}$ is the Lagrange basis for the interpolation problem on \mathbb{D}_{N-2}^e with grid points $\{\theta_j\}_{j=1}^{N-1}$. Consequently,

$$r_N = \sum_{j=1}^{N-1} r_N(\theta_j) L_j^N.$$

Since

$$L_j^N(0) = (-1)^{j+1} 2 \cos^2(\theta_j/2),$$

we obtain

$$|r_N(0)|^2 \leq \left[\sum_{j=1}^{N-1} 2|r_N(\theta_j)| \right]^2 \leq \frac{2N}{\pi} \left[\sum_{j=1}^{N-1} \sin^{-1} \theta_j \right] \left[\frac{\pi}{N} \sum_{j=1}^{N-1} |r_N(\theta_j)|^2 \sin \theta_j \right] \quad (75)$$

$$\leq \frac{4N^2}{\pi} \left[\sum_{1 \leq j \leq N/2} \frac{1}{j} \right] \mathcal{L}_N^1(|r_N|^2 \sin(\cdot)), \quad (76)$$

where we have used the inequality

$$\sin \theta_{N-j} = \sin \theta_j \geq \frac{2\theta_j}{\pi} = \frac{2j}{N}, \quad \forall j = 0, \dots, \lfloor N/2 \rfloor.$$

Hence, for $N \geq 2$, the desired result (74) for $r_N(0)$ follows from the inequality

$$\sum_{1 \leq j \leq N/2} \frac{1}{j} \leq 2 \log N.$$

The bound for $r_N(\pi)$ in (74) can be established analogously. \square

Next we establish bounds for q_N^m , by investigating separately the cases for even m (i.e., operator q_N^e) and for odd m (i.e., operator q_N^o).

Proposition 4.9 *Suppose that Hypothesis 1 holds. There exists $C > 0$ such that for any integer $m \neq 0$ and $f \in W_{2m}^2$,*

$$|2m| \|q_N^e f\|_{L_{\sin^{-1}}^2} \leq C [\|f\|_{W_{2m}^1} + N^{-1} \|f\|_{W_{2m}^2}]. \quad (77)$$

Proof. We assume throughout this proof that f is a real valued function. We consider the function $g_{2N}(\theta) := |(q_N^e f(\theta))|^2 / \sin^2(\theta) s_{2N}(\theta) \in \mathbb{D}_{4N-4}^e$. Using the definition of \tilde{s}_{2N} in (53) and Lemma 4.4,

$$\begin{aligned} \|q_N^e f\|_{L_{\sin^{-1}}^2}^2 &= \int_0^\pi \left| \frac{q_N^e f}{\sin \theta} \right|^2 \tilde{s}_{2N}(\theta) d\theta = \int_0^\pi g_{2N}(\theta) d\theta + \int_0^\pi \left| \frac{q_N^e f}{\sin \theta} \right|^2 (\tilde{s}_{2N}(\theta) - s_{2N}(\theta)) d\theta \\ &\leq \mathcal{L}_{2N}^1 g_{2N} + \frac{1}{\pi N} \|q_N^e f\|_{L_{\sin^{-2}}^2}^2 \\ &= \mathcal{L}_N^1 g_{2N} + \frac{1}{2} (\mathcal{L}_{2N}^2 g_{2N} - \mathcal{L}_N^1 g_{2N}) + \frac{1}{\pi N} \|q_N^e f\|_{L_{\sin^{-2}}^2}^2. \end{aligned} \quad (78)$$

Proceeding similarly as in (66), using Hypothesis 1 (for $q_N^e f(\theta)/\sin \theta \in \mathbb{D}_{N-2}^o$) and again Lemma 4.4, we obtain

$$\begin{aligned}
\frac{1}{2}(\mathcal{L}_N^2 g_{2N} - \mathcal{L}_N^1 g_{2N}) &= -2 \int_0^\pi g_N(\theta) \cos(2N\theta) d\theta \\
&= -2 \int_0^\pi \left| \frac{q_N^e f(\theta)}{\sin \theta} \right|^2 \sin \theta \cos 2N\theta d\theta - 2 \int_0^\pi \left| \frac{q_N^e f(\theta)}{\sin \theta} \right|^2 (\tilde{s}_{2N}(\theta) - \sin \theta) \cos(2N\theta) d\theta \\
&\leq c_H^{(2)} \int_0^\pi \left| \frac{q_N^e f(\theta)}{\sin \theta} \right|^2 \sin \theta d\theta + \frac{2}{\pi N} \|q_N^e f\|_{L^2_{\sin^{-2}}}^2
\end{aligned} \tag{79}$$

Using (79) in (78) and the identity

$$\mathcal{L}_N^1(|q_N^e f / \sin(\cdot)|^2) = \|q_N^e f\|_{L^2_{\sin^{-2}}}^2,$$

we easily derive the bound

$$\|q_N^e f\|_{L^2_{\sin^{-1}}}^2 \leq \frac{1}{1 - c_H^{(2)}} \left[\mathcal{L}_N^1 g_{2N} + \frac{3}{\pi N} \mathcal{L}_N^1(|q_N^e f / \sin(\cdot)|^2) \right]. \tag{80}$$

The first term in the above bound can be estimated as follows. Using the definition of s_{2N} , (58) and the Cauchy-Schwarz inequality (combined with the inequality $2ab \leq Na^2 + N^{-1}b^2$), we obtain

$$\begin{aligned}
\mathcal{L}_N^1 g_{2N} &= \frac{\pi}{N} \sum_{j=1}^{N-1} \frac{|q_N^e f(\theta_j)|^2}{\sin^2 \theta_j} s_{2N}(\theta_j) = \frac{\pi}{N} \sum_{j=1}^{N-1} \frac{|q_N^e f(\theta_j)|^2}{\sin \theta_j} = \frac{\pi}{N} \sum_{j=1}^{N-1} \frac{|f(\theta_j)|^2}{\sin \theta_j} \\
&\leq \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin \theta} + \frac{\pi}{N} \left[\int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin^2 \theta} + \int_0^\pi 2|f(\theta)f'(\theta)| \frac{d\theta}{\sin \theta} \right] \\
&\leq \left(1 + \frac{3\pi}{2}\right) \|f\|_{L^2_{\sin^{-1}}}^2 + \frac{\pi}{2N^2} (\|f\|_{L^2_{\sin^{-3}}}^2 + 2\|f'\|_{L^2_{\sin^{-1}}}^2).
\end{aligned} \tag{81}$$

On the other hand since $(q_N^e f)(0) = f(0) = 0 = f(\pi) = (q_N^e f)(\pi)$ and using the fact that $q_N^e f \in \mathbb{D}_N^e$, we obtain

$$(q_N^e f / \sin)(0) = (q_N^e f / \sin)(\pi) = 0.$$

Hence

$$\begin{aligned}
\mathcal{L}_N^1(q_N^e f / \sin(\cdot))^2 &= \frac{\pi}{N} \sum_{j=1}^{N-1} \left| \frac{q_N^e f(\theta_j)}{\sin \theta_j} \right|^2 = \frac{\pi}{N} \sum_{j=1}^{N-1} \left| \frac{f(\theta_j)}{\sin \theta_j} \right|^2 \\
&\leq \int_0^\pi \frac{|f(\theta)|^2}{\sin^2 \theta} d\theta + \frac{\pi}{N} \left[2 \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin^3 \theta} + \int_0^\pi 2f(\theta)f'(\theta) \frac{d\theta}{\sin^2 \theta} \right] \\
&\leq N \left[\left(\pi + \frac{1}{2}\right) \|f\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \left\{ (3\pi + \frac{1}{2}) \|f\|_{L^2_{\sin^{-3}}}^2 + \pi \|f'\|_{L^2_{\sin^{-1}}}^2 \right\} \right].
\end{aligned}$$

In other words,

$$N^{-1} \mathcal{L}_N^1(|q_N^e f / \sin(\cdot)|^2) \leq C \left[\|f\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \left(\|f'\|_{L^2_{\sin^{-1}}}^2 + \|f\|_{L^2_{\sin^{-3}}}^2 \right) \right]. \tag{82}$$

Plugging (81) and (82) in (80), and taking into account the definitions of the equivalent norms $\|\cdot\|_{Z_m^1}$ and $\|\cdot\|_{Z_m^2}$ (see Theorem 3.1), we obtain the desired result (77). \square

For the next result, we recall that the equivalence norms relation in (37) is valid only for $|m| \geq 2$.

Proposition 4.10 *Suppose that Hypothesis 1 holds. There exists $C > 0$ such that for any $f \in W_{2m+1}^2$ with $m \neq -1, 0$,*

$$|2m+1| \|q_N^0 f\|_{L^2_{\sin^{-1}}} \leq (C + C' \sqrt{\log N}) [\|f\|_{W_{2m+1}^1} + N^{-1} \|f\|_{W_{2m+1}^2}]. \quad (83)$$

Proof. Following the same steps as in the proof of Proposition 4.9, using Hypothesis 1 again with $j = 1$ (because $q_N^0 f(\theta)/\sin(\theta) \in \mathbb{D}_{N-2}^e$), we obtain

$$\|q_N^0 f\|_{L^2_{\sin^{-1}}}^2 \leq \frac{1}{1 - c_H^{(1)}} \left[\mathcal{L}_N^1 g_{2N} + \frac{3}{\pi N} \mathcal{L}_N^1 \left(q_N^0 f / \sin(\cdot) \right)^2 \right]. \quad (84)$$

First term can be treated as in (81) to get

$$\mathcal{L}_N^1 g_{2N} \leq C \left[\|f\|_{L^2_{\sin^{-1}}}^2 + N^{-2} (\|f\|_{L^2_{\sin^{-3}}}^2 + \|f'\|_{L^2_{\sin^{-1}}}^2) \right]. \quad (85)$$

The main difference compared with the even $2m$ case dealt in the previous Proposition arises in the second term, since we now have

$$\begin{aligned} \mathcal{L}_N^1 \left(q_N^0 f / \sin(\cdot) \right)^2 &= \frac{\pi}{2N} \left[\left| \left(\frac{q_N^0 f}{\sin} \right)(0) \right|^2 + \left| \left(\frac{q_N^0 f}{\sin} \right)(\pi) \right|^2 \right] + \frac{\pi}{N} \sum_{j=1}^{N-1} \frac{|f(\theta_j)|^2}{\sin^2 \theta_j} \\ &=: S_1 + S_2. \end{aligned}$$

The first term S_1 did not appear in the proof of Proposition 4.9, since $q_N^0 f \in \mathbb{D}_{N-2}^o$, or, equivalently, $q_N^0 f / \sin \in \mathbb{D}_{N-2}^e$. Thus, we can expect $(q_N^0 f / \sin)(0), (q_N^0 f / \sin)(\pi) \neq 0$.

Clearly, the second term can be bounded as in (82):

$$N^{-1} S_2 \leq C \left[\|f\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \left(\|f'\|_{L^2_{\sin^{-1}}}^2 + \|f\|_{L^2_{\sin^{-3}}}^2 \right) \right]. \quad (86)$$

For S_1 we apply Lemma 4.8 and we follow arguments similar to the derivation of (81) to obtain

$$\begin{aligned} N^{-1} S_1 &\leq C \log N \mathcal{L}_N^1 (|q_N^0 f|^2 / \sin(\cdot)) = C \log N \left[\frac{\pi}{N} \sum_{j=1}^{N-1} \frac{|f(\theta_j)|^2}{\sin \theta_j} \right] \\ &\leq C' \log N \left[\|f\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \|f'\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \|f\|_{L^2_{\sin^{-3}}}^2 \right]. \end{aligned} \quad (87)$$

Thus we have proved the inequality

$$\|q_N^0 f\|_{L^2_{\sin^{-1}}}^2 \leq (C_1 + C_2 \log N) \left[\|f\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \|f'\|_{L^2_{\sin^{-1}}}^2 + N^{-2} \|f\|_{L^2_{\sin^{-3}}}^2 \right].$$

The desired result (83) now follows from Theorem 3.1. \square

Now we are ready to establish convergence estimates for q_N^m similar to (48) in $\|\cdot\|_{W_m^s}$ norms.

Theorem 4.11 *Suppose that Hypothesis 1 holds. There exists $C > 0$ so that for any $f \in W_m^2$,*

$$\|q_N^m f\|_{W_m^0} \leq C \left[\|f\|_{W_m^0} + N^{-1} \|f\|_{W_m^1} + N^{-2} \|f\|_{W_m^2} \right], \quad (88a)$$

$$\|q_N^{2m} f\|_{W_{2m}^1} \leq C \left[N \|f\|_{W_{2m}^0} + \|f\|_{W_{2m}^1} + N^{-1} \|f\|_{W_{2m}^2} \right], \quad (88b)$$

$$\|q_N^{2m+1} f\|_{W_{2m+1}^1} \leq C(1 + \sqrt{\log N}) \left[N \|f\|_{W_{2m+1}^0} + \|f\|_{W_{2m+1}^1} + N^{-1} \|f\|_{W_{2m+1}^2} \right]. \quad (88c)$$

Moreover, for all $r \geq 2$ there exists $C_r > 0$ so that for all m

$$\|q_N^m f - f\|_{W_m^0} \leq C_r N^{-r} \|f\|_{W_m^r}, \quad (89a)$$

$$\|q_N^{2m} f - f\|_{W_{2m}^1} \leq C_r N^{1-r} \|f\|_{W_{2m}^r}, \quad (89b)$$

$$\|q_N^{2m+1} f - f\|_{W_{2m+1}^1} \leq C_r (1 + \sqrt{\log N}) N^{1-r} \|f\|_{W_{2m+1}^r}. \quad (89c)$$

Proof. We recall that for $m \neq 0$, if $f \in W_m^2$, then f vanishes at $0, \pi$. We first consider the case $m \neq 0$: Corollary 4.6 yields the bounds (88a); the bound (88b) follows from Lemma 4.7 and Proposition 4.9; and (88c) is a consequence of Lemma 4.7 and Proposition 4.10. The latter conclusion applies also for the case $m \neq -1$. For $m = 0, -1$, (88c) can be deduced similarly, via the inverse inequalities applied to estimate (88a). For $m = 0$, and under the additional assumption that $f(0) = f(\pi) = 0$, the bound (88a) was also established in Corollary 4.6. The estimate (88b) follows from combining (88a) and the inverse inequalities stated in Lemma 4.1.

With p_N^m being the projection introduced in Proposition 4.2, we observe that

$$\|q_N^m f - f\|_{L_{\sin}^2} \leq \|q_N^m (f - p_N^m f)\|_{L_{\sin}^2} + \|p_N^m f - f\|_{L_{\sin}^2}.$$

Further, $(f - p_N^m f)(0) = (f - p_N^m f)(\pi) = 0$ even for $m = 0$. Thus Corollary 4.6 (or (88) in the cases proven up to now) can be applied to derive the bound

$$\|q_N^m f - f\|_{L_{\sin}^2} \leq C [\|f - p_N^m f\|_{L_{\sin}^2} + N^{-1} \|f - p_N^m f\|_{W_m^1} + N^{-2} \|f - p_N^m f\|_{W_m^2}],$$

where C is independent of m and f . Now (89a) follows from Proposition 4.2.

To prove (89b), we proceed as before, using Lemma 4.7 and Proposition 4.9, to obtain the inequality

$$\|q_N^{2m} f - f\|_{W_{2m}^1} \leq C [N \|f - p_N^{2m} f\|_{W_{2m}^0} + \|f - p_N^{2m} f\|_{W_{2m}^1} + N^{-1} \|f - p_N^{2m} f\|_{W_m^2}].$$

Hence Proposition 4.2 yields the estimate (89b).

The procedure for proving estimate (89c) is completely analogous. We note that (88a)-(88b) for $m = 0$ in the general case (i.e., for functions not vanishing at $\{0, \pi\}$) can be now deduced from (89a)-(89b). \square

Next we are ready to conclude Section 4 by proving the main spectrally accurate convergence result of this article, namely, Theorem 2.4.

4.3 Proof of Theorem 2.4

The proof starts from (46) where we have derived

$$\|\mathcal{Q}_N F - F\|_{\mathcal{H}^s}^2 \leq E_1 + E_2 + E_3$$

with

$$E_1 := \sum_{-N+1 \leq m \leq N} \|q_N^m \mathcal{F}_m F - \mathcal{F}_m F\|_{W_m^s}^2 \quad (90)$$

$$E_2 := \sum_{-N+1 \leq m \leq N} \|q_N^m (\rho_N^m F - \mathcal{F}_m F)\|_{W_m^s}^2 \quad (91)$$

$$E_3 = \left[\sum_{m \geq N+1} + \sum_{m \leq -N} \right] \|\mathcal{F}_m F\|_{W_m^s}^2 \quad (92)$$

For the sake of simplicity we can restrict ourselves to consider only $F \in \text{span}\{Y_n^m\}$ which makes the sums above to be finite. The general case can be deduced by a density argument. Moreover, we can take $s \in \{0, 1\}$ since the result for intermediate values of s follows from the theory of interpolation of Sobolev spaces [27].

The third term can be estimated with the help of (30) and (32), as follows: For $t \geq s$,

$$E_3 \leq \sum_{|m| \geq N} (|m| + \frac{1}{2})^{2s-2t} \|\mathcal{F}_m F\|_{W_m^t}^2 \leq \sum_{|m| \geq N} N^{2s-2t} \|\mathcal{F}_m F\|_{W_m^t}^2 \leq N^{2(s-t)} \|F\|_{\mathcal{H}^t}^2. \quad (93)$$

For E_1 , we apply (89) to obtain

$$E_1 \leq C(1 + \sqrt{\log N})^s N^{2s-2t} \sum_{-N+1 \leq m \leq N} \|\mathcal{F}_m F\|_{W_m^t}^2 \leq C(1 + \sqrt{\log N})^s N^{2s-2t} \|F\|_{\mathcal{H}^t}^2. \quad (94)$$

Regarding E_2 , we apply the definition of ρ_N^m in (45) and estimates (88) of Theorem 4.11 to obtain first

$$\begin{aligned} E_2 &\leq \sum_{-N+1 \leq m \leq N} \left[\sum_{\ell \neq 0} \|\rho_N^m \mathcal{F}_{m+2\ell N} F\|_{W_m^s} \right]^2 \\ &\leq C(1 + \log N)^s N^{2s} \sum_{-N+1 \leq m \leq N} \sum_{j=0}^2 N^{-2j} \left[\sum_{\ell \neq 0} \|\mathcal{F}_{m+2\ell N} F\|_{W_m^j} \right]^2. \end{aligned} \quad (95)$$

Let us study now the three terms in the last sum above. Cauchy-Schwarz inequality and (38)-(39) leads to

$$\left[\sum_{\ell \neq 0} \|\mathcal{F}_{m+2\ell N} F\|_{W_m^j} \right]^2 \leq 9 \left[\sum_{\ell \neq 0} \frac{1}{|m + 2\ell N|^{2t-2j}} \right] \left[\sum_{\ell \neq 0} |m + 2\ell N|^{2t-2j} \|\mathcal{F}_{m+2\ell N} F\|_{W_{m+2\ell N}^j}^2 \right] \quad (96)$$

for $j = 0, 1, 2$. Since

$$\sum_{\ell \neq 0} \frac{1}{|x + \ell|^r} \leq C_r, \quad \forall x \in [-1/2, 1/2]$$

with C_r depending only $r > 1$, we can bound (96) (recall that we have assumed that $t > 5/2$) as follows

$$\begin{aligned} \left[\sum_{\ell \neq 0} \|\mathcal{F}_{m+2\ell N} F\|_{W_m^j} \right]^2 &\leq C_t N^{2j-2t} \left[\sum_{\ell \neq 0} |m + 2\ell N|^{2t-2j} \|\mathcal{F}_{m+2\ell N} F\|_{W_{m+2\ell N}^j}^2 \right] \\ &\leq C_t N^{2j-2t} \left[\sum_{\ell \neq 0} \|\mathcal{F}_{m+2\ell N} F\|_{W_{m+2\ell N}^t}^2 \right] \end{aligned} \quad (97)$$

where in the last step we have applied inequality (30). Plugging (97) in (95), and using (32), we deduce finally

$$E_2 \leq C(1 + \log N)^s N^{2s-2t} \sum_{-N+1 \leq m \leq N} \sum_{\ell \neq 0} \|\mathcal{F}_{m+2\ell N} F\|_{W_{m+2\ell N}^t}^2 \leq C(1 + \log N)^s N^{2s-2t} \|F\|_{\mathcal{H}^t}^2. \quad (98)$$

Gathering bounds (93), (94) and (98), we obtain the spectrally accurate convergence estimate (23) in Theorem 2.4.

5 A FFT-based interpolatory cubature on the sphere

As described in the introduction, interpolatory cubature rules on the sphere are important in several applications, including the radiative transfer and wave propagation models. Using the FFT-based spherical interpolatory operator, for a (wavenumber) parameter κ , we develop a cubature rule to approximate the following (non-, mild-, and highly-oscillatory) integral on the sphere:

$$\mathcal{I}_\kappa F := \int_0^\pi \int_0^{2\pi} F(\theta, \phi) \exp(i\kappa \cos \theta) \sin \theta \, d\phi \, d\theta = \iint_{\mathbb{S}^2} F^\circ(\mathbf{x}) \exp(i\kappa \mathbf{x} \cdot [0, 0, 1]) \, dS(\mathbf{x}). \quad (99)$$

In the integral above the parameter κ is a real number. Therefore, (99) includes standard integrals as well as a class of highly-oscillatory integrals for large values of κ . In wave propagation applications, the $[0, 0, 1]$ corresponds to the direction of the incident wave. The rotationally invariant property of the sphere facilitates fixing such an incident direction. The above integral occurs, for example, in developing efficient computer models to simulate scattered wave (and its far-field) from an acoustically/electromagnetically small, medium, and large closed obstacles [12, 13, 14, 15] with compact simply connected surface, leading to surface integral reformulations of the model on the sphere. The integral for the $\kappa = 0$ case occurs in potential theory and radiative transport models.

For the FFT-based efficient cubature approximation of the integral, we first consider a Filon-type product integration interpolatory approximation

$$\mathcal{I}_{N,\kappa} F := \int_0^\pi \int_0^{2\pi} (\mathcal{Q}_N F)(\theta, \phi) \exp(i\kappa \cos \theta) \sin \theta \, d\phi \, d\theta. \quad (100)$$

Using the representation

$$(\mathcal{Q}_N F)(\theta, \phi) = p_0(\theta) + \sum_{\substack{-N/2 < m \leq N/2 \\ \text{odd } m \neq 0}} \sin \theta p_m(\theta) \exp(im\phi) + \sum_{\substack{-N/2 < m \leq N/2 \\ \text{even } m \neq 0}} \sin^2 \theta p_m(\theta) \exp(im\phi)$$

($p_m \in \mathbb{D}_{N-2}^e$ if $m \neq 0$), we obtain

$$\mathcal{I}_{N,\kappa} F = 2\pi \int_0^\pi p_0(\theta) \exp(i\kappa \cos \theta) \sin \theta \, d\theta = \sqrt{2\pi} \int_0^\pi (\mathcal{F}_0 \mathcal{Q}_N F)(\theta) \exp(i\kappa \cos \theta) \sin \theta \, d\theta.$$

From this property and Proposition 2.1 we see how this cubature rule can efficiently implemented:

- Compute

$$f_{j,0} := \frac{1}{2N} \sum_{k=0}^{2N-1} F(\theta_j, \phi_k)$$

- Construct

$$(\alpha_\ell^0)_{\ell=0}^N := \mathbf{DCT}_N((f_{j,0})_{j=0,\dots,N}),$$

- Return

$$\mathcal{I}_{N,\kappa} F = 2\pi \sum_{\ell=0}^N \alpha_\ell \omega_\ell(\kappa)$$

where

$$\omega_\ell(\kappa) := 2\pi \int_0^\pi \cos \ell \theta \exp(i\kappa \cos \theta) \sin \theta \, d\theta = 2\pi \int_{-1}^1 T_\ell(x) \exp(i\kappa x) \, dx. \quad (101)$$

The cost of computing $(\alpha_\ell)_{\ell=0}^N$ is about $\mathcal{O}(N^2)$, and is dominated by the first step of the algorithm. The weights (101) (T_ℓ denotes the Chebyshev polynomial of degree ℓ) can be computed in a stable and fast way in $\mathcal{O}(N)$ operations [8].

For the error analysis of the rule, based on (45)-(46), we first arrive at the following formula:

$$\mathcal{I}_{N,\kappa}F - \mathcal{I}_\kappa F = \sqrt{2\pi} \int_0^\pi [(\mathcal{F}_0 \mathcal{Q}_N F)(\theta) - (\mathcal{F}_0 F)(\theta)] \sin \theta \, d\theta \quad (102)$$

$$= \sqrt{2\pi} \int_0^\pi [(\mathfrak{q}_N^e \rho_N^0 F)(\theta) - (\mathcal{F}_0 F)(\theta)] \sin \theta \, d\theta. \quad (103)$$

Thus, with $e_N := \mathfrak{q}_N^e \rho_N^0 F - \mathcal{F}_0 F$, the cubature approximation error is bounded by $\sqrt{2\pi} \|e_N\|_{L_{\sin}^2}$, so that we first ensure the convergence should be independent of κ . Actually this estimate can be improved by performing integration by parts, to obtain high-order decay in the error for large values of κ . Using $e_N(0) = e_N(\pi) = 0$, we obtain

$$\mathcal{I}_{N,\kappa}F - \mathcal{I}_\kappa F = -\frac{\sqrt{2\pi} i}{\kappa} \int_0^\pi e'_N(\theta) \exp(i\kappa \cos \theta) \, d\theta \quad (104)$$

$$= \frac{\sqrt{2\pi}}{\kappa^2} \left[\frac{1}{\sin \theta} e'_N(\theta) \exp(i\kappa \cos \theta) \Big|_{\theta=0}^{\theta=\pi} - \int_0^\pi \left(\frac{1}{\sin \theta} e'_N(\theta) \right)' \exp(i\kappa \cos \theta) \, d\theta \right]. \quad (105)$$

We observe that for sufficiently smooth F , $e'_N(0) = e'_N(\pi) = 0$ and therefore the pointwise value of $\frac{1}{\sin(\cdot)} e'_N(\cdot)$ at these points as well as the last integral are well defined.

Below we present the error estimate and convergence result for the cubature rule. We omit a detailed analysis of the estimate since it can be proved using arguments similar to that we developed (for a similar rule) and analyzed in [7, Section 5].

Theorem 5.1 *Let $F \in \mathcal{H}^r$. For $\ell = 0, 1$ and $r > 3/2$ or $\ell = 2$ and $r > 4$*

$$|I_\kappa(F) - I_{\kappa,N}(F)| \leq C_r \kappa^{-\ell} N^{\eta(\ell)-r} \|F\|_{\mathcal{H}^r}, \quad (106)$$

where C_r independent of N and

$$\eta(\ell) := \begin{cases} 0, & \text{if } \ell = 0, \\ 3/2, & \text{if } \ell = 1, \\ 4, & \text{if } \ell = 2. \end{cases}$$

6 Numerical experiments

In this section we demonstrate the main interpolatory spectrally accurate approximation result (23) and the high-order cubature approximation result (106) for functions with various order of smoothness. We also demonstrate that the construction of full FFT-based interpolatory approximation developed in this article using the uniform-grid and the \mathcal{Q}_N operator is faster, even for small to medium sized data locations, than another efficient similarly accurate interpolation operator $\mathcal{Q}_N^{\text{gl}}$. We developed the operator $\mathcal{Q}_N^{\text{gl}}$ in [7], using Gauss-Lobatto points in latitudinal angle, that facilitates the use of the standard FFT only in the azimuthal variable.

For calculation of the \mathcal{H}^t norms, for $t = 0, 1$, used in (23), we apply the following integral based formulas:

$$\|F\|_{\mathcal{H}^0}^2 := \int_0^\pi \int_0^{2\pi} |F(\theta, \phi)|^2 \sin \theta \, d\phi \, d\theta \quad (107)$$

$$\|F\|_{\mathcal{H}^1}^2 := \frac{1}{4} \|F\|_{\mathcal{H}^0}^2 + \int_0^\pi \int_0^{2\pi} \left| \frac{\partial F}{\partial \phi}(\theta, \phi) \right|^2 \frac{1}{\sin \theta} \, d\phi \, d\theta + \int_0^\pi \int_0^{2\pi} \left| \frac{\partial F}{\partial \theta}(\theta, \phi) \right|^2 \sin \theta \, d\phi \, d\theta. \quad (108)$$

Except for some trivial cases, the above norms cannot be evaluated exactly. We computed the above norms for tabulated results in this section using over 150,000 quadrature points on the sphere, taking into account that some of the functions considered in this section have only limited smoothness properties and hence require fine grids to compute with sufficiently high accuracy.

Experiment #1 (Approximation of smooth and limited smooth functions)

For the first set of experiments we consider interpolatory approximation of test functions:

$$F_1^\circ(x, y, z) := \frac{1}{4 + x + y + z}, \quad F_j^\circ(x, y, z) := (1 - x^2)^{5/2-j} yz, \quad \text{for } j = 2, 3 \quad \text{and } (x, y, z) \in \mathbb{S}^2.$$

Recalling (1)-(2), the corresponding equivalent functions are

$$F_1(\theta, \phi) := \frac{1}{4 + \sin \theta \cos \phi + \sin \theta \sin \phi + \cos \theta}$$

$$F_j(\theta, \phi) := (1 - \sin^2 \theta \cos^2 \phi)^{5/2-j} \sin \theta \sin \phi \cos \theta, \quad j = 2, 3.$$

Clearly F_1° is a smooth function, and hence our theoretical result (23) suggests superalgebraic convergence $\mathcal{Q}_N F_1^\circ$ to F_1° in both the \mathcal{H}^0 and \mathcal{H}^1 norms. Computational results in Table 1 validate the theoretical result and demonstrate the power of obtaining machine precision accurate approximation of the smooth function with $N = 32$.

N	$\ \mathcal{Q}_N F_1 - F_1\ _{\mathcal{H}^0}$	EoC	$\ \mathcal{Q}_N F_1 - F_1\ _{\mathcal{H}^1}$	EoC
008	4.86E-06		4.40E-05	
016	2.02E-11	17.9	3.37E-10	17.0
032	5.78E-15	11.8	7.82E-15	15.4

Table 1: Approximation of F_1 by $\mathcal{Q}_N F_1$: Errors and estimate order of convergence (EoC)

The functions F_2° and F_3° have only limited regularity. It can be shown that, for any $\varepsilon > 0$, $F_2^\circ \in \mathcal{H}^{4-\varepsilon}$ and $F_3^\circ \in \mathcal{H}^{2-\varepsilon}$. Indeed, using an atlas with local charts around the singularities [points $(\pm 1, 0, 0) \in \mathbb{S}^2$] one can easily see that the Sobolev regularity of F_j° are the same as the functions $\tilde{F}_j^\circ(y, z) := (y^2 + z^2)^{5/2-j} y$. Hence according to our theoretical result (23), the estimated order of convergence (EoC) in approximating F_2 by $\mathcal{Q}_N F_2$ in the $\mathcal{H}^0, \mathcal{H}^1$ norms are respectively *almost* 4 and 3 and that for F_3 by $\mathcal{Q}_N F_3$ are respectively *almost* 2 and 1. Computational results in Table 2 validate the theoretical result (23).

Experiment #2 (Accuracy and fast evaluation comparison with a recent work)

For this experiment we compare the performance in construction, in terms of error and computation time, of the FFT-based interpolant developed in this article with the interpolant considered

N	$\ \mathcal{Q}_N F_2 - F_2\ _{\mathcal{H}^0}$	EoC	$\ \mathcal{Q}_N F_2 - F_2\ _{\mathcal{H}^1}$	EoC
008	1.43E-03		1.41E-02	
016	8.14E-05	4.14	1.55E-03	3.18
032	5.01E-06	4.02	1.90E-04	3.03
064	3.12E-07	4.01	2.36E-05	3.00
128	1.87E-08	4.06	3.07E-06	2.95

N	$\ \mathcal{Q}_N F_3 - F_3\ _{\mathcal{H}^0}$	EoC	$\ \mathcal{Q}_N F_3 - F_3\ _{\mathcal{H}^1}$	EoC
008	2.76E-02		3.21E-01	
016	6.92E-03	2.00	1.58E-01	1.02
032	1.73E-03	2.00	7.93E-02	1.00
064	4.33E-04	2.00	3.97E-02	1.00
128	1.08E-04	2.00	1.99E-02	0.99

Table 2: Approximation of F_2 and F_3 by $\mathcal{Q}_N F_2$ and $\mathcal{Q}_N F_3$: Errors and EoC

in [7] (and first proposed, not analyzed, in [16]). This interpolant shares the same discrete space, χ_N , and the nodes in the azimuthal angle $\{\phi_j\}$. The difference is on the nodes in the latitudinal angle which were chosen in [7] to be the non-uniform grid points $\{\theta_i = \arccos \eta_i\}_{i=0}^N$ where $\{\eta_i\}_{i=0}^N$ are the Gauss-Lobatto points of the quadrature rule for approximating integrals in $[-1, 1]$. In other words, $\eta_0 = -1$, $\eta_N = 1$ and η_i for $i = 1, \dots, N-1$ are the roots of $P'_N(x)$ where P_N is the Lagrange polynomial of degree N . We recall that this non-uniform Gauss-Lobatto points based interpolant is denoted as $\mathcal{Q}_N^{\text{gl}}$.

In [7] we proved that for $F \in \mathcal{H}^t$ and $s = 0, 1$,

$$\|\mathcal{Q}_N^{\text{gl}} F - F\|_{\mathcal{H}^s} \leq CN^{s-t} \|F\|_{\mathcal{H}^t},$$

which is, up to the $(\log N)^{s/2}$ term, identical to the error estimate in (23) that we proved for the FFT-based operator \mathcal{Q}_N . For our comparison testing purpose, we have chosen the function

$$F_4(\theta, \phi) = \left[\left(\frac{1}{\sqrt{3}} - \sin \theta \cos \phi \right)^2 + \left(\frac{1}{\sqrt{3}} - \sin \theta \sin \phi \right)^2 + \left(\frac{1}{\sqrt{3}} - \cos \theta \right)^2 \right]^{3/2} \in \mathcal{H}^{4-\varepsilon}$$

which corresponds to the function $F_4^\circ(\hat{\mathbf{x}}) = |\hat{\mathbf{x}} - \mathbf{x}^*|^3$, $\hat{\mathbf{x}} \in \mathbb{S}^2$ with $\mathbf{x}^* = [1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3}]$. The error in \mathcal{H}^0 and \mathcal{H}^1 norms and associated EoC are depicted in Table 3 for \mathcal{Q}_N and $\mathcal{Q}_N^{\text{gl}}$. Similar to our established theoretical results, we observe from Table 3 that although $\mathcal{Q}_N^{\text{gl}}$ performs slightly better, the difference is not significant and the estimated orders of convergence are roughly the same.

It is important to observe the difference between the *construction* and *evaluation* of the interpolation operators in the current article and that in [7]. After construction of these two interpolation operators (see Figure 1 for construction CPU time), computing our two interpolatory approximations at various observation points on \mathbb{S}^2 requires same basis function evaluations at the points, as they share the same approximation space χ_N . Unlike standard spherical harmonics based polynomial approximations, construction and evaluation of our interpolation operators do not involve Legendre polynomials. Hence we do not require use of techniques such as fast Legendre transforms for our non-polynomial approximations. Our basis functions are trigonometric polynomials and hence for evaluation of both the interpolation operators, standard FFT or NFFT [25] techniques can be used, depending on whether the observation points are equally spaced or not.

N	$\ \mathcal{Q}_N F_4 - F_4\ _{\mathcal{H}^0}$	EoC	$\ \mathcal{Q}_N^{\text{gl}} F_4 - F_4\ _{\mathcal{H}^0}$	EoC
008	1.48e-03		1.41e-03	
016	1.00e-04	3.89	9.03e-05	3.97
032	6.16e-06	4.02	5.68e-06	3.99
064	3.66e-07	4.07	3.61e-07	3.98
128	2.63e-08	3.80	2.47e-08	3.87

N	$\ \mathcal{Q}_N F_4 - F_4\ _{\mathcal{H}^1}$	EoC	$\ \mathcal{Q}_N^{\text{gl}} F_4 - F_4\ _{\mathcal{H}^1}$	EoC
008	1.43e-02		1.50e-02	
016	1.88e-03	2.93	1.90e-03	2.99
032	2.27e-04	3.05	2.20e-04	3.11
064	2.69e-05	3.08	2.83e-05	2.96
128	3.82e-06	2.82	4.26e-06	2.73

Table 3: Approximation of F_4 by $\mathcal{Q}_N F_4$ and $\mathcal{Q}_N^{\text{gl}} F_4$: \mathcal{H}^0 case (top) and \mathcal{H}^1 case (bottom).

The computational effort required for construction of both the interpolants are however important. In Figure 1, we show the low computational cost of the spherical interpolant constructed in this article compared to even the efficient matrix-free interpolant developed in [7]. The difference in the performance and computational complexity for construction of the interpolants can be easily explained just by examining both interpolants. For construction of the \mathcal{Q}_N based approximation, we proceed as follows (see Proposition 4.5): first, we apply $N - 1$ FFT transforms of $2N$ elements, corresponding to odd node indices and next, for even cases, apply $N + 1$ DCT/DST (discrete sine/cosine transform). Thus the overall computational complexity for the \mathcal{Q}_N operator approximation is $\mathcal{O}(N^2 \log N)$ operations. For construction of the $\mathcal{Q}_N^{\text{gl}}$ based approximation, the first step is similar, with $N - 1$ FFT transforms of $2N$ elements, but the second step (in the non-uniform grid latitudinal angle) is different: two different (polynomial) interpolation problems of $N + 1$ (p_N^{2m}) and $N - 1$ (p_N^{2m-1}) have to be solved N times which amounts about $\mathcal{O}(N^3)$ operations. Moreover, the interpolant \mathcal{Q}_N developed in this article can be used in a natural way with nested grids which can be easily exploited to construct error estimates almost for free, or, if the data node points are doubled, previous function evaluations can be reused to construct the associated updated interpolatory approximation.

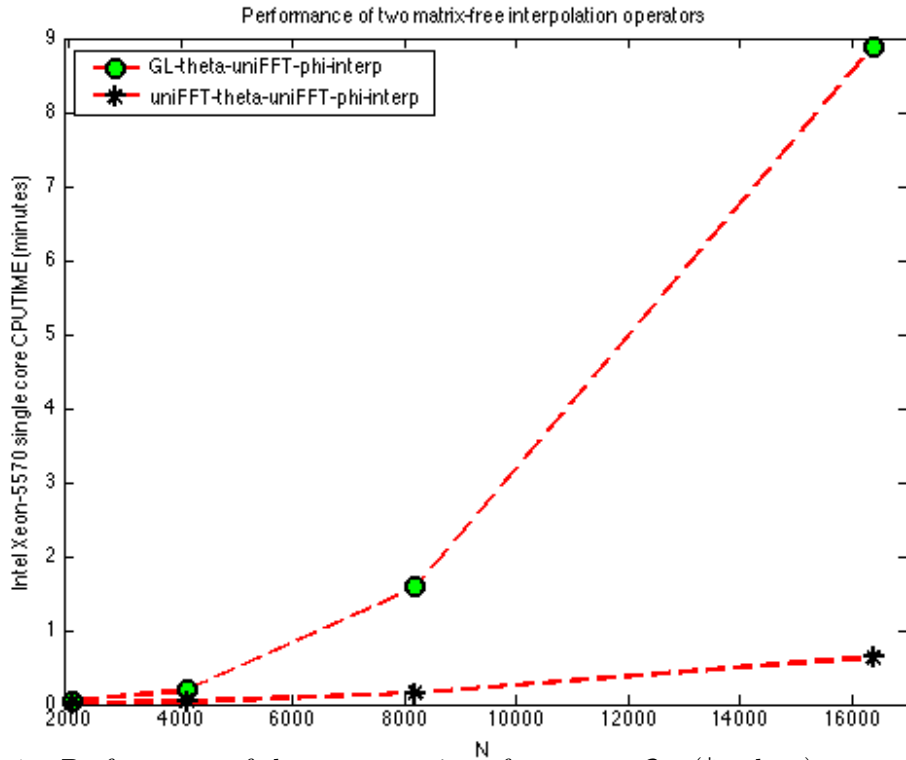
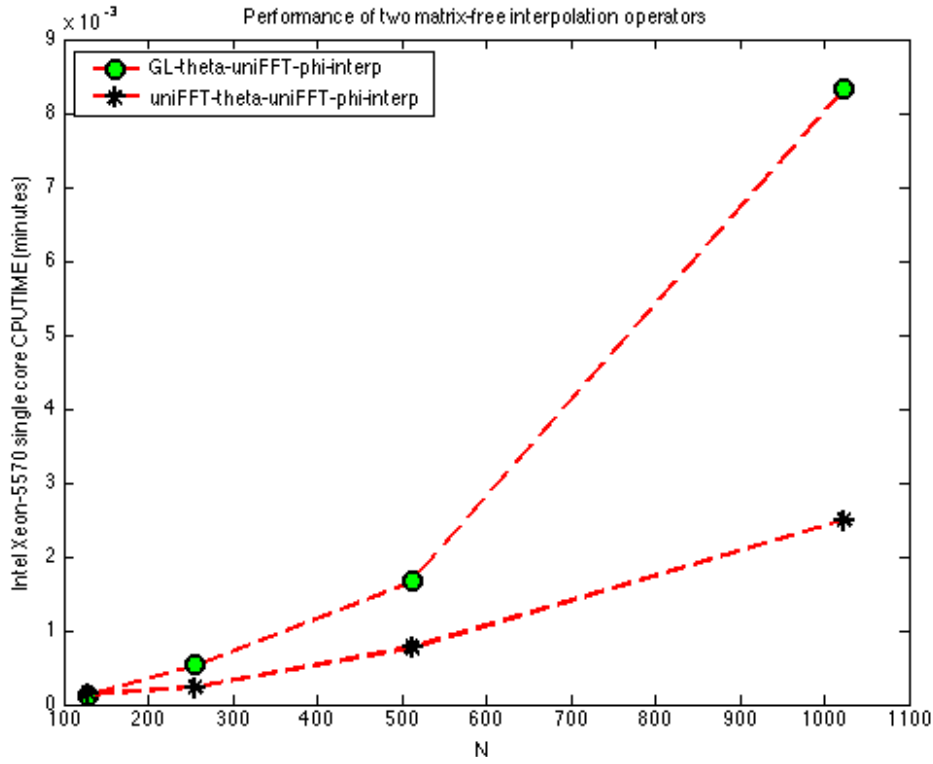


Figure 1: Performance of the construction of operator \mathcal{Q}_N (*-values) compared to that of $\mathcal{Q}_N^{\text{gl}}$ (o-values) for various data parameter $N = 2^j$, [top: $j = 7, 8, 9, 10$ and bottom: $j = 11, 12, 13, 14$] applied to the data obtained using the function F_4 . The ordinate values are the CPU TIME (in minutes) obtained using a single core of a Intel Xeon-5570 2.93GHz processor. The \mathcal{Q}_N operator facilitates application of the standard FFT in both the azimuthal and latitudinal angles while the $\mathcal{Q}_N^{\text{gl}}$ with non-uniform Gauss-Lobatto based points in the latitudinal angles provides the standard FFT evaluation only in the azimuthal variable.

Experiment #3 (Performance of the FFT-based cubature)

Using the smooth integrand function F_2 and for the limited smooth integrand F_4 , we have tested the convergence of the cubature rule developed in Section 5 to approximate the integral (99), for $\kappa = 0, 10, 10^2, \dots, 10^6$, corresponding to the total non-, mildly-, and highly-oscillatory integrands. The results for all these cases are given in Tables 4 and 5.

Each row of Tables 4 and 5 corresponds to a fixed N . We clearly observe the κ^{-2} decay of the error, for fixed N . Reading along the columns corresponds to varying values of N . For the smooth function F_1 , based on the column results in Table 4, we see the superalgebraic convergence in N , as proved in Section 1. For a fixed κ , for the case of the integrand function F_4 with limited regularity, we observe from Table 5 the convergence in general is better than the estimated theoretical result, suggesting that our estimated error result and analysis could be improved in some cases.

$N \setminus \kappa$	0	1	10	100	10^3	10^4	10^5	10^6
004	5.36E-05	1.03E-04	5.01E-05	6.77E-07	4.55E-09	6.93E-11	7.22E-13	6.83E-15
008	1.17E-08	1.28E-08	9.14E-07	4.28E-09	5.04E-11	4.35E-13	4.24E-15	4.38E-17
016	4.44E-16	1.28E-14	2.15E-13	9.89E-14	7.01E-16	2.23E-18	1.79E-19	6.07E-20

Table 4: $|\mathcal{I}_\kappa(F_1) - \mathcal{I}_{\kappa,N}(F_1)|$ for various parameters κ and N

$N \setminus \kappa$	0	1	10	100	10^3	10^4	10^5	10^6
004	1.04E-04	2.67E-03	1.72E-03	2.40E-05	1.64E-07	2.48E-09	2.58E-11	2.44E-13
008	7.92E-05	8.62E-05	5.75E-04	3.15E-06	2.95E-08	3.08E-10	3.10E-12	3.08E-14
016	4.14E-06	4.20E-06	9.47E-06	1.31E-07	1.02E-09	2.01E-11	2.11E-13	1.99E-15
032	2.22E-08	2.33E-08	8.44E-08	2.26E-08	3.67E-11	1.00E-12	1.07E-14	1.01E-16
064	2.51E-09	2.51E-09	2.73E-09	1.83E-08	4.98E-12	3.78E-14	4.02E-16	3.93E-18
128	1.54E-10	1.54E-10	1.56E-10	4.20E-10	2.21E-12	5.97E-15	1.03E-16	9.62E-19
256	3.33E-12	3.31E-12	3.34E-12	4.93E-12	4.26E-13	7.06E-16	1.11E-17	2.58E-19

Table 5: $|\mathcal{I}_\kappa(F_4) - \mathcal{I}_{\kappa,N}(F_4)|$ for various parameters κ and N

A Discussion on and verification of Hypothesis 1

In this section, we present details required to computationally verify the inequalities (21) in Hypothesis 1 and demonstrate that the hypothesis holds for almost all practical values of N . To this end, we first rewrite Hypothesis 1 in a computationally convenient form. Using the cosine change of variables $x = \cos \theta$ and the Chebyshev polynomial T_{2N} , we rewrite inequality (21) as

$$-2 \int_{-1}^1 |p_{N-2}(x)|^2 (1-x^2)^\alpha T_{2N}(x) dx \leq c_H^\alpha \int_{-1}^1 |p_{N-2}(x)|^2 (1-x^2)^\alpha dx, \quad \forall p_{N-2} \in \mathbb{P}_{N-2}, \quad (109)$$

for $\alpha = 0, 1, 2$ where $c_H^\alpha < 1$.

Next we consider a polynomial of degree $N - 2$ represented using the Chebyshev basis:

$$p_{N-2} = \sum_{j=0}^{N-2} \beta_{j+1} T_j.$$

Then (109) is equivalent to the coefficient based inequality

$$-2 \sum_{i,j=1}^{N-1} \beta_i \beta_j b_{ij}(\alpha, N) \leq c_H^\alpha \sum_{i,j=1}^{N-1} \beta_i \beta_j a_{ij}(\alpha) \quad (110)$$

where

$$a_{ij}(\alpha) := \int_{-1}^1 T_{i-1}(x) T_{j-1}(x) (1-x^2)^\alpha dx,$$

$$b_{ij}(\alpha, N) := \int_{-1}^1 T_{i-1}(x) T_{j-1}(x) T_{2N}(x) (1-x^2)^\alpha dx.$$

Observe that these quantities are easily computable using the identities

$$T_i T_j = \frac{1}{2} (T_{i+j} + T_{|i-j|}) \quad (111a)$$

$$T_{2N} = 2T_N^2 - 1 \quad (111b)$$

$$(1-x^2) = -\frac{1}{2} T_2(x) + \frac{1}{2}, \quad (1-x^2)^2 = \frac{1}{4} T_2^2(x) - \frac{1}{2} T_2(x) + \frac{1}{4} \quad (111c)$$

$$\int_{-1}^1 T_i(x) dx = \begin{cases} -\frac{2}{i^2-1}, & \text{for even } i, \\ 0, & \text{otherwise.} \end{cases} \quad (111d)$$

Thus, for numerical verification of the Hypothesis 1, we used the follow algorithm:

- Construct an auxiliary matrix C sufficiently large with $C_{i+1,j+1} = \int_{-1}^1 T_i T_j$ using (111a) and (111d).
- From C , construct $A(\alpha, N) := (a_{ij}(\alpha))_{i,j=1}^{N-1}$ and $B(\alpha, N) := (b_{ij}(\alpha, N))_{i,j=1}^{N-1}$ by applying (111a)–(111d). Hence

$$\begin{aligned} a_{ij}(0) &= c_{ij} \\ a_{ij}(1) &= -\frac{1}{4} [c_{i+2,j} + c_{|i-2|+1,j}] + \frac{1}{2} c_{ij} \\ a_{ij}(2) &= \frac{1}{16} [c_{i+2,j+2} + c_{|i-2|+1,j+2} + c_{i+2,|j-2|+1} + c_{|i-2|+1,|j-2|+1}] \\ &\quad - \frac{1}{4} [c_{i+2,j} + c_{|i-2|+1,j}] + \frac{1}{4} c_{ij} \\ b_{ij}(\alpha, N) &= \frac{1}{2} [a_{i+N,j+N}(\alpha) + a_{|i-N|+1,j}(\alpha) + a_{i,|j-N|+1}(\alpha) + a_{|i-N|+1,|j-N|+1}(\alpha)] - a_{i,j}(\alpha). \end{aligned}$$

- Compute the minimum of the generalized Rayleigh quotient for A and B

$$c_H(N; \alpha) := -2 \min_{\mathbf{b} \in \mathbb{R}^{N-1}} \frac{\mathbf{b}^\top B(\alpha, N) \mathbf{b}}{\mathbf{b}^\top A(\alpha, N) \mathbf{b}} \quad (112)$$

Both $A(\alpha, N)$ and $B(\alpha, N)$ are symmetric. Moreover, $A(\alpha, N)$ is positive definite. Thus, we can compute the Cholesky factorization $A = R^\top R$ so that (112) is equivalent to compute the smallest algebraic eigenvalue of the matrix $R^{-\top} B(\alpha, N) R^{-1}$.

We have implemented the above algorithm by precomputing C that facilitates acceleration of the algorithm for several values of N . The graphs of $c_H(\cdot; \alpha)$ for $2 \leq N \leq 2^{14}$ are depicted in Figure 2 demonstrating the validity of the hypothesis for most practically useful values of N .

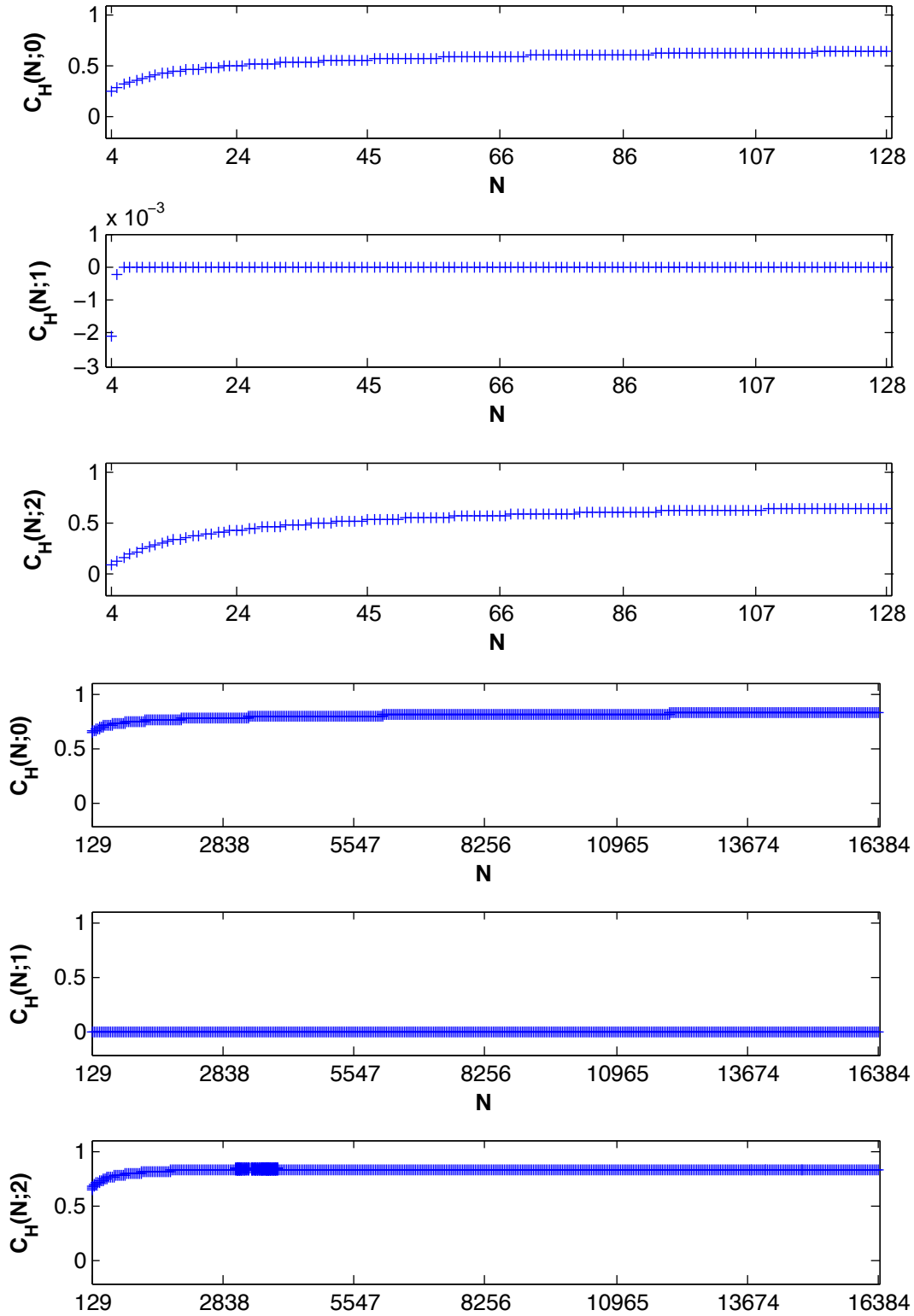


Figure 2: Plots of computed values of $c_H(N; \alpha)$ defined in (112) for $\alpha = 0, 1, 2$, respectively in the first three subplots, for $2 \leq N \leq 2^7$; and in the last three subplots for $2^7 < N \leq 2^{14}$. These plots, demonstrating $c_H(N; \alpha) < 1$, numerically validate (for almost all practical cases) that in (21), we have $c_H^{(j)} < 1$, for $j = 1, 2, 3$.

B Proofs results in Section 3

In this section we provide proofs of Theorem 3.1 and Proposition 3.2.

B.1 Proof of Theorem 3.1

Proof. First we recall that the space

$$\mathcal{H}^1 = \{F : \mathbb{R}^2 \rightarrow \mathbb{C} : F \in \mathcal{H}^0, \nabla_{\mathbb{S}^2} F \in \mathcal{H}^0 \times \mathcal{H}^0\}$$

is equipped with the norm

$$\begin{aligned} \|F\|_{\mathcal{H}^1}^2 &:= \frac{1}{4} \|F\|_{\mathcal{H}^0}^2 + \|\nabla_{\mathbb{S}^2} F\|_{\mathcal{H}^0 \times \mathcal{H}^0}^2 \\ &= \frac{1}{4} \int_0^\pi \int_0^{2\pi} |F(\theta, \phi)|^2 \sin \theta \, d\theta \\ &\quad + \int_0^\pi \int_0^{2\pi} \left| \frac{\partial F}{\partial \phi}(\theta, \phi) \right|^2 \frac{1}{\sin \theta} \, d\theta \, d\phi + \int_0^\pi \int_0^{2\pi} \left| \frac{\partial F}{\partial \theta}(\theta, \phi) \right|^2 \sin \theta \, d\theta \, d\phi. \end{aligned} \quad (113)$$

Since,

$$|\nabla_{\mathbb{S}^2}(f \otimes e_m)(\theta, \phi)|^2 = \frac{1}{2\pi} \left[\frac{m^2}{\sin^2 \theta} |f(\theta)|^2 + |f'(\theta)|^2 \right],$$

we obtain for all $m \in \mathbb{Z}$,

$$\|f\|_{W_m^1}^2 = \frac{1}{4} \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta + m^2 \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f'(\theta)|^2 \sin \theta \, d\theta. \quad (114)$$

For $|m| \geq 1$, (36) follows from (114).

Next we prove that if $|m| \geq 2$,

$$\begin{aligned} \|f\|_{W_m^2}^2 &= \frac{1}{16} \int_0^\pi |f(\theta)|^2 \sin \theta \, d\theta + \frac{9m^2}{4} \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin \theta} + (m^4 - 4m^2) \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin^3 \theta} \\ &\quad + \frac{1}{4} \int_0^\pi |f'(\theta)|^2 \sin \theta \, d\theta + (1 + 2m^2) \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f''(\theta)|^2 \sin \theta \, d\theta. \end{aligned} \quad (115)$$

It is convenient to recall that

$$\|F\|_{\mathcal{H}^2}^2 := \|\Delta_{\mathbb{S}^2} F\|_{\mathcal{H}^0}^2 + \frac{1}{2} \|\nabla_{\mathbb{S}^2} F\|_{\mathcal{H}^0 \times \mathcal{H}^0}^2 + \frac{1}{16} \|F\|_{\mathcal{H}^0}^2,$$

Where $\Delta_{\mathbb{S}^2}$ is the Laplace-Beltrami operator on the sphere [28].

Without loss of generality, we assume f to be a real valued function. The proof of (115) requires more calculations and application of integration by parts several times to take care of some cross products appearing in the integral form of the norm. Without loss of generality, for a fixed $m \in \mathbb{Z}$, we can assume $f \in \text{span} \{Q_n^m : n \geq |m|\}$ because this subspace is dense in W_m^2 . Observe that

$$f(0) = f'(0) = f(\pi) = f'(\pi) = 0. \quad (116)$$

Since

$$\begin{aligned} \frac{1}{4} \|\nabla_{\mathbb{S}^2} f \otimes e_m\|_{\mathcal{H}^0 \times \mathcal{H}^0}^2 + \frac{1}{16} \|f \otimes e_m\|_{\mathcal{H}^0}^2 &= \frac{m^2}{4} \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + \frac{1}{4} \int_0^\pi |f'(\theta)|^2 \sin \theta \, d\theta \\ &\quad + \frac{1}{16} \int_0^\pi f^2(\theta) \sin \theta \, d\theta, \end{aligned}$$

it is sufficient to analyze the term containing the Laplace-Beltrami operator:

$$\begin{aligned}
\|\Delta_{\mathbb{S}^2}(f \otimes e_m)\|_{\mathcal{H}^0}^2 &= \int_0^\pi \int_0^{2\pi} |\Delta_{\mathbb{S}^2}(f \otimes e_m)(\theta, \phi)|^2 \sin \theta \, d\theta \, d\phi \\
&= \int_0^\pi \left| -\frac{m^2}{\sin^2 \theta} f(\theta) + \frac{1}{\sin \theta} |(\sin \theta f'(\theta))'|^2 \right|^2 \sin \theta \, d\theta \\
&= m^4 \int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta} + \int_0^\pi \frac{1}{\sin \theta} |(\sin \theta f'(\theta))'|^2 d\theta \\
&\quad - 2m^2 \int_0^\pi f(\theta) (\sin \theta f'(\theta))' \frac{d\theta}{\sin^2 \theta} =: m^4 I_1 + I_2 - 2m^2 I_3. \tag{117}
\end{aligned}$$

Using (116) and integration by parts, cubature

$$\begin{aligned}
I_2 &= \int_0^\pi \left[\frac{\cos^2 \theta}{\sin \theta} |f'(\theta)|^2 + \sin \theta |f''(\theta)|^2 + \cos \theta (|f'(\theta)|^2)' \right] d\theta \\
&= \int_0^\pi \frac{\cos^2 \theta}{\sin \theta} |f'(\theta)|^2 d\theta + \int_0^\pi \sin \theta |f''(\theta)|^2 d\theta + \int_0^\pi |f'(\theta)|^2 \sin \theta d\theta \\
&= \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi \sin \theta |f''(\theta)|^2 d\theta. \tag{118}
\end{aligned}$$

Proceeding similarly, we derive

$$\begin{aligned}
I_3 &= - \int_0^\pi \left(\frac{1}{\sin^2 \theta} f(\theta) \right)' f'(\theta) \sin \theta \, d\theta \\
&= - \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi (f^2(\theta))' \frac{\cos \theta}{\sin^2 \theta} d\theta \\
&= - \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi f^2(\theta) \left(\frac{2 \cos^2 \theta}{\sin^3 \theta} + \frac{1}{\sin \theta} \right) d\theta \\
&= - \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} - \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + 2 \int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta}. \tag{119}
\end{aligned}$$

Inserting (118)-(119) in (117), we obtain (115).

The inequalities

$$\frac{1}{16} + \frac{9m^2}{4} + (m^4 - 4m^2) \leq m^4 < 3m^4, \quad \frac{1}{4} + (1 + 2m^2) \leq 3m^2, \quad \forall |m| \geq 2$$

with (115) imply the first inequality of (37). For $|m| \geq 3$ the second inequality of (37) is simply a consequence of the inequalities

$$m^4 - 4m^2 > m^4/2 > \frac{m^4}{6}, \quad 1 + 2m^2 > m^2 \geq \frac{m^2}{6}.$$

The case $|m| = 2$, has to be analyzed separately since one of the crucial terms, the third term in (115), vanishes: Using (115), we obtain

$$\|f\|_{W_m^2}^2 \geq 9 \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin \theta} + 9 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f''(\theta)|^2 \sin \theta \, d\theta. \tag{120}$$

As before it suffices to consider f to be real valued and that $f \in \text{span} \{Q_n^2 : n \geq 2\}$. Note that

$$\int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta} = \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + \int_0^\pi f^2(\theta) \frac{\cos^2 \theta}{\sin^3 \theta} d\theta. \tag{121}$$

Applying integration by parts to the second term and using (116) we obtain

$$\int_0^\pi f^2(\theta) \frac{\cos^2 \theta}{\sin^3 \theta} d\theta = \int_0^\pi (f(\theta)f'(\theta)) \left(\log(\tan(\theta/2)) + \frac{\cos \theta}{\sin^2 \theta} \right) d\theta. \quad (122)$$

Notice that for $\theta \in (0, \pi/2]$,

$$\sin \theta |\log \tan(\theta/2)| \leq 2 \tan(\theta/2) |\log \tan(\theta/2)| \leq 2e^{-1} \leq 1. \quad (123)$$

By symmetry, we can extend this bound for any $\theta \in (0, \pi)$. With the help of (123) and the inequality $2ab \leq a^2 + b^2$, from (122) we obtain

$$\begin{aligned} \int_0^\pi f^2(\theta) \frac{\cos^2 \theta}{\sin^3 \theta} d\theta &\leq \int_0^\pi |f(\theta)f'(\theta)| \frac{d\theta}{\sin \theta} + \int_0^\pi |f(\theta)f'(\theta)| \frac{d\theta}{\sin^2 \theta} \\ &\leq \frac{1}{2} \left[\int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + 2 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} \right] + \frac{1}{2} \int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta}. \end{aligned} \quad (124)$$

Inserting (124) in (121) we easily derive

$$\int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta} \leq \frac{3}{2} \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \frac{1}{2} \int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta}$$

and therefore

$$\int_0^\pi f^2(\theta) \frac{d\theta}{\sin^3 \theta} \leq 3 \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + 2 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta}. \quad (125)$$

From (120) and (125), we obtain

$$\begin{aligned} 6\|f\|_{W_m^2}^2 &\geq 54 \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + 54 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + 6 \int_0^\pi |f''(\theta)|^2 \sin \theta d\theta \\ &\geq 16 \left(3 \int_0^\pi f^2(\theta) \frac{d\theta}{\sin \theta} + 2 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} \right) \\ &\quad + 4 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f''(\theta)|^2 \sin \theta d\theta \\ &\geq 16 \int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin^3 \theta} + 4 \int_0^\pi |f'(\theta)|^2 \frac{d\theta}{\sin \theta} + \int_0^\pi |f''(\theta)|^2 \sin \theta d\theta. \end{aligned}$$

Hence the inequalities in (37) hold. \square

B.2 Proof of Proposition 3.2

Proof. Denote by Γ the maximum circle in \mathbb{S}^2 , parametrized by

$$\mathbf{q}(\theta) := (\sin \theta, 0, \cos \theta). \quad (126)$$

Given $f^\circ : \Gamma \rightarrow \mathbb{C}$ we denote $f = f^\circ \circ \mathbf{q} : \mathbb{R} \rightarrow \mathbb{C}$. The norm in the Sobolev space $H^r(\Gamma)$ can be then defined with the help of \mathbf{q} and (41):

$$\|f^\circ\|_{H^r(\Gamma)} := \|f\|_{H_r^\#}.$$

The second ingredient we will use in this proof is the trace operator γ_Γ which can be shown to be continuous from $\mathcal{H}^{r+1/2}(\mathbb{S}^2)$ onto $H^r(\Gamma)$ for all $r > 0$ (see [6, 27] for a proof of this result in \mathbb{R}^n ; the proof can be easily extended by using local charts of the unit sphere and the equivalent definitions of the Sobolev spaces involved).

Given $f \in W_m^r$, consider the mapping

$$\mathcal{P}_m f := \sqrt{2\pi}(\gamma_\Gamma F^\circ) \circ \mathbf{q}, \quad F^\circ := (f \otimes e_m) \circ \mathbf{p}^{-1}.$$

Observe that $F^\circ \in \mathcal{H}^r(\mathbb{S}^2)$ and that actually $f = \mathcal{P}_m f$, that is \mathcal{P}_m is simply the identity operator. Moreover,

$$\|\mathcal{P}_m f\|_{H_{\#}^r} \leq \sqrt{2\pi} \|\gamma_\Gamma\|_{\mathcal{H}^{r+1/2}(\mathbb{S}^2) \rightarrow H^r(\Gamma)} \|F^\circ\|_{\mathcal{H}^{r+1/2}(\mathbb{S}^2)} = \sqrt{2\pi} \|\gamma_\Gamma\|_{\mathcal{H}^{r+1/2}(\mathbb{S}^2) \rightarrow H^r(\Gamma)} \|f\|_{W_m^{r+1/2}},$$

where $\|\gamma_\Gamma\|_{\mathcal{H}^{r+1/2}(\mathbb{S}^2) \rightarrow H^r(\Gamma)}$ is the continuity constant of γ_Γ as a linear operator from $\mathcal{H}^{r+1/2}(\mathbb{S}^2)$ onto $H^r(\Gamma)$. Hence we obtain (43).

Since $W_m^0 \cong L_{\sin}^2$, the first equation in (44) is clear whereas the second equation in (44) for $m = 0$ follows directly from (114) and (42). Finally, if $m \neq 0$ using $f(0) = 0$ we observe that

$$\begin{aligned} \int_0^{\pi/2} |f(\theta)|^2 \frac{d\theta}{\sin \theta} &= \int_0^{\pi/2} \frac{1}{\sin \theta} \left| \int_0^\theta f'(\xi) d\xi \right|^2 d\theta \leq \int_0^{\pi/2} \frac{\sqrt{\theta}}{\sin \theta} \left[\int_0^\theta |f'(\xi)|^2 d\xi \right] d\theta \\ &\leq C \int_0^{\pi/2} |f'(\xi)|^2 d\xi. \end{aligned}$$

Proceeding similarly, but using now that $f(\pi) = 0$, we can bound the integral in $(\pi/2, \pi)$ and hence conclude that

$$\int_0^\pi |f(\theta)|^2 \frac{d\theta}{\sin \theta} \leq C \int_0^\pi |f'(\xi)|^2 d\xi.$$

Equation (36) now yields that

$$\|f\|_{W_m^1} \leq \frac{\sqrt{5}}{2} \|f\|_{Z_m^1} \leq C(1 + |m|) \|f\|_{H_{\#}^1}.$$

□

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