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**EXPONENTIAL CONVERGENCE OF
SPECTRAL APPROXIMATIONS AND
TIME-DOMAIN COMPUTATION OF
SCATTERING PROBLEMS**

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Abstract

This thesis consists of two parts. The first part is on rigorous error analysis of exponential convergence of orthogonal polynomial approximations under analytic assumption. The second part is on time-domain computation of scattering problems governed by wave equations and time-dependent Maxwell's equations.

The spectral method employs global orthogonal polynomials or Fourier complex exponentials as basis functions, so it enjoys high-order accuracy (with only a few basis functions), if the underlying function is smooth (and periodic in the Fourier case). The typical algebraic order of convergence (i.e., $O(n^{-r})$, where n is the number of polynomial basis functions, and r is related to the Sobolev-regularity of the underlying function), is well documented in various monographs on spectral methods. It is widely accepted that if the function under consideration is sufficiently smooth or analytic, the convergence rate is of exponential order $O(q^n)$ (for constant $0 < q < 1$). However, there appear significantly less investigation and very limited discussions of such error bounds (mostly mentioned, but not proved e.g., in [41, 113, 17]).

In the first part of the thesis, we provide error estimates for Jacobi polynomial expansions and Jacobi-Gauss-type interpolation of analytic functions (characterized by Bernstein ellipse $\mathcal{E}_\rho$ with $\rho > 1$). More precisely, we derive error bounds of the type: $C(n)M\rho^{-n}$ with $\rho > 1$, where M is the maximum value of the analytic function on the Bernstein ellipse, and where we specify the explicit dependence of $C(n)$ on n and involved parameters. Moreover, the bounds are valid for small n , and are significantly tighter than existing ones. We also discuss superconvergence

of spectral interpolation. Indeed, the study of superconvergence phenomenon for h -version methods has had a great impact on scientific computing, especially on *a posteriori* error estimates and adaptive methods. With a belief that the scientific community would also benefit from the study of superconvergence phenomenon of spectral methods, some interesting results were obtained by Zhang [123, 124, 125]. Here, we consider general Jacobi-Gauss-type interpolation and address the implication of superconvergence points identified from interpolating analytic functions, to functions with limited regularity, that is, the leading term of the interpolation error vanishes, but there is no gain in order of convergence, which is in distinctive contrast with analytic functions.

The second part of this thesis is devoted to time-domain computation of wave scattering problems. It is known that the time-domain simulations are capable of capturing wide-band signals and modeling more general material inhomogeneities and nonlinearities, compared with the frequency-domain approaches e.g., the time-harmonic Helmholtz problems. We focus on fast and accurate computation of the exact circular/spherical nonreflecting boundary conditions (NRBCs) for acoustic wave equations and Maxwell's equations, which are used to truncate the scattering problems originally set in unbounded domains. However, a longstanding issue with the NRBC is its nonlocality in both time and space, due to the involvement of the temporal convolution and Fourier/spherical harmonic (or vector spherical harmonic in the Maxwell's case) series. We derive analytic expressions for the underlying convolution kernels, which allow for a rapid and accurate evaluation of the convolution with $O(N_t)$ operations over N_t successive time steps. In particular, for the Maxwell's equations, we derive a new formulation of the NRBC, which allows for the use of an analytic method for computing the involved inverse Laplace transform as in the acoustic case. We also propose efficient spectral solvers for the truncated problems with regular scatterers to show the accuracy and efficiency of this analytic-numerical approach.

Notation

Common Notation

$\mathbb{C}$	Set of all complex numbers
$\mathbb{R}$	Set of all real numbers
$\mathbb{N}$	Set of all nonnegative integers, i.e., $\{0, 1, 2, \dots\}$
$\mathbb{P}_N$	Set of all algebraic polynomials of degree $\leq N$
i	Complex unit, i.e., $i = \sqrt{-1}$
$\delta_{k,j}$	Kronecker delta symbol
Γ	Gamma function
$[\lambda]$	The largest integer $\leq \lambda$
$\cong$	$a_n \cong b_n$ means that for $b_n \neq 0$, $a_n/b_n \rightarrow 1$ as $n \rightarrow \infty$
$\mathcal{L}$	Laplace transform
$\mathcal{L}^{-1}$	Inverse Laplace transform
I_N	Interpolation operator at a set of generic points $\{x_j\}_{j=0}^N$

Orthogonal Polynomials

P_n	Legendre polynomial of degree n
T_n	Chebyshev polynomial of degree n
U_n	Chebyshev polynomial of the second kind of degree n
$P_n^{(\alpha,\beta)}$	Jacobi polynomial of degree n with parameter (α, β)
$P_n^{(\alpha,\alpha)}$	Gegenbauer polynomial of degree n

Spaces, Inner Products and Norms

$\omega^{\alpha,\beta}$	Jacobi weight function: $\omega^{\alpha,\beta} = (1-x)^\alpha(1+x)^\beta$
$L^2_{\omega^{\alpha,\beta}}(I)$	Weighted L^2 -space on I
$L^p(I)$	L^p -space on I with $1 \leq p \leq \infty$
$(\cdot, \cdot)_{\omega^{\alpha,\beta}}$	Inner product of $L^2_{\omega^{\alpha,\beta}}(I)$
$(\cdot, \cdot)$	Inner product of $L^2(I)$
$\ \cdot\ _{\omega^{\alpha,\beta}}$	Norm of $L^2_{\omega^{\alpha,\beta}}(I)$
$\ \cdot\ $	Norm of $L^2(I)$
$\ \cdot\ _\infty$	Norm of $L^\infty(I)$

Bessel and Hankel Functions

I_ν	Modified Bessel function of the first kind of order ν
K_ν	Modified Bessel function of the second kind of order ν
k_ν	Modified spherical Bessel function of the second kind of order ν
$H_\nu^{(1)}$	Hankel function of the first kind of order ν
$h_\nu^{(1)}$	Spherical Hankel function of the first kind of order ν

Spherical Harmonics

Y_l^m	Spherical harmonics as normalized in [87]
$\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\varphi\}$	Moving (right-handed) orthonormal coordinate basis
∇_S	Tangent gradient operator on the unit spherical surface S
$\{\mathbf{T}_l^m, \mathbf{V}_l^m, \mathbf{W}_l^m\}$	Vector spherical harmonic (VSH) (see (6.8))
$\{Y_l^m \mathbf{e}_r, \nabla_S Y_l^m, \nabla_S Y_l^m \times \mathbf{e}_r\}$	VSH defined in Morse and Feshbach [86]

Chapter 1

Introduction

In this chapter, we elaborate on motivations and backgrounds of the topics to be studied in this thesis, and highlight the main contributions. For clarity of exposition, we address these issues separately for two parts of the thesis.

1.1 Exponential convergence and superconvergence

Perhaps the most significant advantage of spectral method is its high-order accuracy. The typical convergence rate of the spectral method is $O(n^{-r})$ for every r , where r is the regularity index of the underlying function [49, 42, 41, 13, 56, 113, 17, 21, 65, 102]. If the function is analytic within a sizable domain, the expected convergence rate is $O(q^n)$ with $0 < q < 1$. This is the so-called *exponential convergence*, which is well accepted among the community of spectral and high-order methods. Such convergence results have been documented in various literature. For instance, the results on Fourier or Chebyshev series can be found in [108, 36, 98, 16, 83, 114]. In the seminal work of Gottlieb and Shu on the resolution of the Gibbs phenomenon (the interested readers are referred to Gustafsson [59] for a review of this significant contribution attributed to a series

of papers [54, 51, 52, 50, 53]), the exponential convergence, in the maximum norm (termed as the regularization error), of Gegenbauer polynomial expansions was derived, when the index λ grows linearly with the degree n . Boyd [18] provided an insightful study of the “diagonal limit” (i.e., $\lambda = \beta n$ for some constant $\beta > 0$) convergence of the Gegenbauer reconstruction algorithm in [54]. The analytic assumption in [54] is largely in the sense of [36, Eq. (1.9.8)] (also see (2.1) below).

1.1.1 Jacobi polynomial expansions

The Jacobi polynomials $P_n^{(\alpha, \beta)}(x)$ ($x \in I := [-1, 1]$ with $\alpha, \beta > -1$), normalized as in Szegő [108], are orthogonal with respect to the weight function $\omega^{\alpha, \beta}(x) = (1-x)^\alpha(1+x)^\beta$, that is,

$$\int_{-1}^1 P_n^{(\alpha, \beta)}(x) P_m^{(\alpha, \beta)}(x) \omega^{\alpha, \beta}(x) dx = \gamma_n^{\alpha, \beta} \delta_{m, n}, \quad (1.1)$$

where $\delta_{m, n}$ is the Kronecker delta, and

$$\gamma_n^{\alpha, \beta} = \frac{2^{\alpha+\beta+1} \Gamma(n+\alpha+1) \Gamma(n+\beta+1)}{(2n+\alpha+\beta+1) n! \Gamma(n+\alpha+\beta+1)}. \quad (1.2)$$

Define the $L_{\omega^{\alpha, \beta}}^2$ -orthogonal projection $\pi_N^{\alpha, \beta}: L_{\omega^{\alpha, \beta}}^2(I) \rightarrow \mathbb{P}_N$ such that

$$(\pi_N^{\alpha, \beta} u)(x) = \sum_{n=0}^N \hat{u}_n^{\alpha, \beta} P_n^{(\alpha, \beta)}(x), \quad \hat{u}_n^{\alpha, \beta} = \frac{1}{\gamma_n^{\alpha, \beta}} \int_{-1}^1 u(x) P_n^{(\alpha, \beta)}(x) \omega^{\alpha, \beta}(x) dx,$$

where $L_{\omega^{\alpha, \beta}}^2(I)$ is the weighted L^2 -space on I with norm $\|\cdot\|_{\omega^{\alpha, \beta}}$, and $\mathbb{P}_N$ is the set of all algebraic polynomials of degree $\leq N$.

If $u(x)$ is smooth, some error estimates for the truncation error $u - \pi_N^{\alpha, \beta} u$ were given in e.g., [42, 7, 58, 21], but the dependent of the constant on the regularity index of u was not very clear. The new book of Shen, Tang and Wang [102] proved the improved approximation results, one case is that, if $m \geq N+1$,

$$\left\| \partial_x^l (\pi_N^{\alpha, \beta} u - u) \right\|_{\omega^{\alpha+l, \beta+l}} \leq c(2\pi N)^{-1/4} \left(\frac{\sqrt{e/2}}{N} \right)^{N-l+1} \left\| \partial_x^{N+1} u \right\|_{\omega^{\alpha+N+1, \beta+N+1}},$$

where m is the regularity index of u , and $c \cong 1$ for $N \gg 1$. We can see that if $m \sim N$, under the condition $\|\partial_x^{N+1}u\|_{\omega^{\alpha+N+1}, \beta+N+1} < \infty$, the order of convergence is $O(e^{-\beta N - \gamma \ln N})$, which is the typical convergence rate of spectral methods for sufficiently smooth functions.

If u is analytic, apart from the analytic assumption in e.g., [36, 54] (cf. (2.1) in Chapter 2), another important tool to characterize the analyticity is the so-called Bernstein ellipse. This should be traced back to the seminal work of Bernstein [15] (1912), which (also see [80]) stated that u is analytic on $[-1, 1]$, if and only if

$$\sup \lim_{n \rightarrow \infty} \sqrt[n]{E_n(u)} = \frac{1}{\rho}, \quad E_n(u) = \inf_{v \in \mathbb{P}_n} \|v - u\|_\infty.$$

Here, $\mathbb{P}_n$ is the set of all algebraic polynomials of degree at most n , and $\rho > 1$ is the sum of the semi-axes of the maximum ellipse $\mathcal{E}_\rho$ with foci ± 1 , known as the *Bernstein ellipse*, on and within which u can be analytically extended to. One immediate implication is that the best polynomial approximation in the maximum norm enjoys exponential convergence. Davis [36] stated an estimate (with proof, see [36, Page 312]) due to K. Neumann, that is, if u is analytic on and inside $\mathcal{E}_\rho$ with $\rho > 1$, then the Legendre expansion coefficient satisfies

$$\limsup_{n \rightarrow \infty} |\hat{u}_n|^{1/n} = \frac{1}{\rho}. \quad (1.3)$$

A similar result for the general Jacobi expansion was presented in [108, Theorem 9.1.1] without proof.

In fact, these results show the exponential convergence: $C(n)\rho^{-n}$ for large n . However, it is natural to ask: *How does $C(n)$ clearly depend on algebraic order of n and other parameters? Is the estimate valid for small n ?* As commented by Hale and Trefethen [62]: “the general idea of such convergence goes back to Bernstein [14] (1919), but such results do not appear in many textbooks or monographs, and there is not much uniformity in the constants in the upper bounds.”

We provide affirmative answers to the questions from precise estimate for the

Chebyshev expansion (see, e.g., [37], [98, Theorem 3.8] and [83, Theorem 5.16]):

$$|\hat{u}_n^C| \leq \frac{2M}{\rho^n}, \quad \forall n \geq 0; \quad \|u - S_N^C u\|_\infty \leq \frac{M}{(\rho - 1)\rho^N}; \quad M = \max_{z \in \mathcal{E}_\rho} |u(z)|, \quad (1.4)$$

where $\{\hat{u}_n^C\}$ are the Chebyshev expansion coefficients of u , and $S_N^C u$ is the partial sum involving the first $N + 1$ terms.

Xiang [120] provided a simple approach to obtain the bounds for Jacobi expansion coefficients of analytic functions on and within the Bernstein ellipse $\mathcal{E}_\rho$:

$$|\hat{u}_n^{\alpha,\beta}| \leq \frac{2M}{\rho^{n-1}(\rho - 1)} \sqrt{\frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}}}, \quad \hat{u}_n^{\alpha,\beta} = \frac{1}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 u(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx. \quad (1.5)$$

The key step of Xiang's approach is to insert the Chebyshev expansion $u(x) = \sum_{j=0}^\infty \hat{u}_j^C T_j(x)$ into the Jacobi expansion coefficients and rewrite

$$\hat{u}_n^{\alpha,\beta} = \frac{1}{\gamma_n^{\alpha,\beta}} \sum_{j=n}^\infty \hat{u}_j^C \int_{-1}^1 T_j(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx,$$

so (1.4) can be utilized.

The first purpose of Chapter 2 is to take a different approach to derive sharp estimates for general Jacobi expansion of analytic functions. The assertion of sharpness is in the following sense:

- (i) The bound for general Jacobi case is tighter than (1.5) (see Remark 2.3).
- (ii) Refined estimates can be obtained for Gegenbauer expansion ($\alpha = \beta > -1$), Chebyshev-type expansion ($\alpha = k - 1/2, \beta = l - 1/2$ for non-negative integers k, l), and Legendre-type expansion ($\alpha = k, \beta = l$ for non-negative integers k, l). The argument can recover the bounds known to be the sharpest (e.g., the Chebyshev case), and some obtained estimates are new and significantly improve the existing ones (see, e.g., Remark 2.5).

A second purpose along this line is to extend the argument to analyze Gegenbauer-Gauss quadrature of analytical functions. We obtain sharper estimates for more general cases (see Section 2.5 in Chapter 2).

1.1.2 Spectral interpolation and differentiation

The heart of a collocation/pseudospectral method is the spectral differentiation process, that is, given a set of Gauss-type points $\{x_j\}_{j=0}^N$, e.g., on $[-1, 1]$, the derivative values $\{u'(x_j)\}$ can be approximated by an exact differentiation of the polynomial interpolant $\{(I_N u)'(x_j)\}$. Such a direct differentiation technique is also called a differencing method in the literature (see, e.g., [109, 41, 96]). For the first time, Tadmor [109] showed the exponential accuracy of differencing analytic functions on Chebyshev-Gauss points, where the main argument was based on analyzing the (continuous) Chebyshev coefficients and the aliasing error, and where the intimate relation between Fourier and Chebyshev basis functions played an essential role in the analysis. Reddy and Weideman [96] took a different approach and improved the estimate in [109] for Chebyshev differencing of functions analytic on and within $\mathcal{E}_\rho$ with $\rho > 1$. As pointed out in [96], although the exponential convergence of spectral differentiation of analytic functions is appreciated and mentioned in the literature (see, e.g., [41, 113, 17]), the rigorous proofs (merely for the Fourier and Chebyshev methods) can only be found in [109, 96]. Indeed, to the best of our knowledge, the theoretical justification even for the Legendre method is lacking. It is worthwhile to point out that under the regularity condition (M): $\|u^{(k)}\|_{L^\infty} \leq cM^k$, the super-geometric convergence of Legendre spectral differentiation was proved by Zhang [123]. Similar estimate was nontrivially extended to the Chebyshev collocation method in [124].

This motivates us to derive sharp estimates of exponential convergence, in the maximum norm, of spectral interpolation and differentiation on general Jacobi-Gauss-type points, provided that the underlying function is analytic on and within the Bernstein ellipse. The essential argument is based on the classical Hermite's contour integral (see (3.2) below). In particular, when interpolating at Gegenbauer-Gauss-type points, we can clearly characterize the dependence of the constant on the interesting parameters, armed with a delicate estimate of lower bound of the Gegenbauer polynomial on the Bernstein ellipse. It is important

to remark that the Chebyshev polynomial takes a very simple explicit form (see, e.g., [36] or (4.32) below), but the Gegenbauer polynomial has a complicated expression. Accordingly, compared with the Chebyshev case in [96], the analysis for Gegenbauer case is much more involved. We report the results in Chapter 4.

1.1.3 Superconvergence of spectral interpolation

In numerical computation, we often observe that the convergent rate exceeds the best possible global rate at some special points. Those points are called superconvergent points, and the phenomenon is called the superconvergence phenomenon. The study of superconvergence phenomenon for h -version method has had a great impact on scientific computing, especially on *a posteriori* error estimates and adaptive methods. Here, we are interested in finding e.g., the points $\{y_j\}$ such that

$$\max_j |(I_N u - u)'(y_j)| \sim N^{-\gamma} \max_x |(I_N u - u)'(x)|, \quad (1.6)$$

for some $\gamma > 0$, where $I_N u$ is the Lagrange interpolant of u on a set of Jacobi-Gauss-type (i.e., Jacobi-Gauss, Jacobi-Gauss-Radau, or Jacobi-Gauss-Lobatto) points. We are also keen in the analysis of gain in order of N^γ .

This study is motivated by a recent work of Zhang [125], where the superconvergence points of Chebyshev interpolation of analytic functions characterized by the Bernstein ellipse, were identified and analyzed. We remark that in the Chebyshev case, a special closed form in the trigonometry function can be utilized, which offers greatly simplification of the analysis. Two issues remain open: *What happens to general Jacobi polynomials? Is the superconvergence phenomenon still valid for functions with limited regularity?*

In Chapter 3, we provide answers to these two questions. Answer to the first one is affirmative. The main effort here is devoted to identifying superconvergence points for interpolation by general Jacobi polynomials. For functions with limited regularity, the answer is partially positive in the sense that the convergence rate

remains the same at all points. Nevertheless, the numerical error is significantly smaller at those superconvergence points obtained for analytic functions. We present the estimates at the superconvergence points in Chapter 4, as this falls into the general framework presented in Section 4.1.

1.2 Time-domain wave scattering problems

Time-domain simulation, which is capable of capturing wide-band signals and modeling more general material inhomogeneities and nonlinearities, has attracted much attention [110, 76, 79]. A longstanding issue with many simulations resides in how to deal with the unbounded computational domain. Various approaches including the boundary element methods (cf. [28]), infinite element methods (cf. [46]), perfectly matched layers (PML) (cf. [12]), nonreflecting boundary condition methods (cf. [75, 60]), and among others (cf. [82, 110]), have been proposed to surmount this obstacle. We also point out the interesting works related to the use of artificial boundary conditions in other contexts [63, 8, 9, 122, 64].

Although the use of exact nonreflecting boundary conditions (NRBCs) is desirable and beneficial (cf. the review papers [47, 48] and the references therein), the practitioners are usually plagued with their complications and computational inefficiency. Some types of NRBCs based on different principles have been proposed (see, e.g., [39, 11, 112, 104, 105, 55, 60, 48]), but a critical point of time-domain computation is the efficient treatment for NRBCs that can scale and integrate well with the solver for the underlying truncated problem (cf. [111, 67]). In practice, if an accurate NRBC is imposed, the artificial boundary could be placed as close as possible to the scatterer that can significantly reduce the computational cost.

In this thesis, we restrict our attention to the exact circular/spherical NRBC. One major difficulty lies in that such an NRBC is *global* in space and time in nature, as it involves the Fourier/spherical harmonic/vector spherical harmonic

expressions in space, and history dependence in time induced by a convolution. The convolution kernel, termed as *nonreflecting boundary kernel* (NRBK) in [3], is the inverse Laplace transform of an expression that includes the logarithmic derivative of a modified Bessel function. The rapid computation of the NRBK and the involved convolution is of independent interest. Alpert, Greengard and Hagstrom [3] proposed a rational approximation of the logarithmic derivative with a least squares implementation, which allows for a reduction of the use of poles from $O(\nu)$ to $O(\log \nu \log \frac{1}{\varepsilon})$ (where $\nu \gg 1$ is the order of the modified Bessel function and ε is a given tolerance), and a recursive convolution. Jiang and Greengard [72, 73] further considered some interesting applications to Schrödinger equations in one and two dimensions. Li [77] introduced a more accurate low-order approximation of the three-dimensional NRBK at a slightly expensive cost, where the observation that the Laplace transform of the three-dimensional NRBK is exactly a rational function lies at the heart of this algorithm. However, in many cases, the expressions are *not* rational functions. For instance, the two-dimensional NRBK also contains the contributions from the branch-cut along the negative real axis (see Theorem 5.1 below). Lubich and Schädle [81] developed some fast algorithms for the temporal convolution with $O(N_t \log N_t)$ operations (over N_t successive time steps) arising from NRBCs with nonrational expressions for other equations (e.g., Schrödinger equations and damped wave equations).

It is worthwhile to point out that there has been significantly less study of the NRBC for Maxwell's equations, where one finds the existing formulations (see, e.g., [61, 26]) actually present a great challenge for evaluation. In Chapter 6, we present a new formulation of the NRBC, which allows for computing the involved temporal convolution through the algorithm for that of the acoustic wave equations in Chapter 5.

The nonlocality of the NRBC in space can be efficiently handled by Fourier/spherical harmonic/vector spherical harmonic expansions when the scatterer

is a disk or a ball. Recently, a systematic approach, based on the boundary perturbation technique (also called the *transformed field expansion* (TFE) method (cf. [89])), has been developed in [90, 40, 91] for time-harmonic Helmholtz equations in exterior domains with general bounded obstacles, under which the whole algorithm boils down to solving a sequence of Helmholtz equations in a regular domain. In Chapter 5, we highlight that this notion can be extended to time-domain computation, though it has not been investigated before as far as we know.

1.3 Main contributions and outline

The main contents and contributions of this dissertation are highlighted as follows.

- In Chapter 2, we provide a rigorous and delicate analysis for exponential decay of Jacobi polynomial expansions of analytic functions associated with the Bernstein ellipse. Using an argument that can recover the best estimate for the Chebyshev expansion, we derive various new and sharp bounds of the expansion coefficients, which are featured with explicit dependence of all related parameters and valid for degree $n \geq 1$. We demonstrate the sharpness of the estimates by comparing with existing ones, in particular, the very recent results in [120]. We also extend this argument to estimate the Gegenbauer-Gauss quadrature remainder of analytic functions, which leads to some new tight bounds for quadrature errors.
- In Chapter 3, we extend the study of superconvergence properties of Chebyshev-Gauss-type spectral interpolation in [125] to general Jacobi-Gauss-type interpolations. We follow the same principle as in [125] to identify the superconvergence points from interpolating analytic functions at the general Jacobi-Gauss-type points. We show the implications of this study to general functions with limited regularity, that is, at the superconvergence points

for analytic functions, the leading term of the interpolation error vanishes, but there is no gain in order of convergence, which is in distinctive contrast with interpolating analytic functions.

- In Chapter 4, we provide a general framework for spectral interpolation and differentiation, when the underlying function is analytic on and within the Bernstein ellipse. We obtain the error bounds for general Jacobi-Gauss-type interpolations, and explicitly characterize the dependence of the underlying parameters and constants, whenever possible. We present a rigorous analysis for spectral interpolation on Gegenbauer-Gauss-type points.
- In Chapter 5, we are concerned with fast and accurate computation of exterior wave equations truncated via exact circular and spherical NRBCs, known to be nonlocal in both time and space. We first derive analytic expressions for the underlying convolution kernels, which allow for a rapid and accurate evaluation of the convolution with $O(N_t)$ operations over N_t successive time steps. To handle the nonlocality in space, we introduce the notion of boundary perturbation, which enables us to handle general bounded scatterers by solving a sequence of wave equations in a regular domain. We propose an efficient spectral-Galerkin solver with Newmark scheme in time for the truncated wave equation in the regular domain. We also provide ample numerical results to show high-order accuracy of the NRBCs and efficiency of the proposed scheme.
- In Chapter 6, we present a fast and accurate algorithm for computing the exact spherical NRBC for time-dependent Maxwell's equations. It is essentially based on a new formulation of the NRBC, which allows for the use of an analytic method for computing the involved inverse Laplace transform. We apply the algorithm proposed in Chapter 5 to solve the interior truncated problem with a spherical scatterer, and improve the temporal accuracy to fourth order by using Richardson extrapolation. We provide

some numerical examples to show that the algorithm leads to very accurate results.

- The last chapter is for some concluding remarks and future works.

Part I

Exponential Convergence of Spectral Approximations

Chapter 2

Jacobi Polynomial Expansions of Analytic Functions[†]

As already described in Subsection 1.1.1, the main purposes of this chapter are to derive sharp error bounds for Jacobi polynomial expansions of analytic functions, and to analyze the Gegenbauer-Gauss quadrature along this line. We take a routine that can recover the best estimate for the Chebyshev case, and that allows us to derive much tighter bounds than those in e.g., the very recent paper by Xiang [120]. Moreover, we extend this argument to estimate the Gegenbauer-Gauss quadrature remainder of analytic functions, which leads to some new sharp bounds (see Theorem 2.4 and Remark 2.11 below).

This chapter is organized as follows. We review some basics of analytic functions and Bernstein ellipse in Section 2.1, and collect relevant properties of Jacobi polynomials and Gamma functions in Section 2.2. In Section 2.3, we provide the main tools to be used to derive the estimate of Jacobi expansions. In Section 2.4, we derive the sharp bounds for general Jacobi expansions of analytic functions,

[†]The main part of this chapter is based on the paper [126]: “X.D. Zhao, L.L. Wang and Z.Q. Xie. Sharp error bounds for Jacobi expansions and Gegenbauer-Gauss quadrature of analytic functions. *SIAM J. Numer. Anal.*, 51(3):1443–1469, 2013.”

followed by some refined results for Chebyshev-type and Legendre-type expansions. With the previous sharp bounds for Jacobi expansion coefficients, we can estimate the truncation error straightforwardly. In Section 2.5, we extend the argument to analyze the Gegenbauer-Gauss quadrature errors. Finally, in Section 2.6, we provide some numerical results to show the sharpness of the bounds by comparing them with existing ones.

2.1 Analytic functions and Bernstein ellipse

Suppose that $u(x)$ is analytic on $[-1, 1]$. Based on the notion of analytic continuation, there always exists a simple connected region R in the complex plane containing $[-1, 1]$ into which $u(x)$ can be continued analytically. The analyticity may be characterized by the growth of the derivatives of u . More precisely, let $\mathcal{C}$ be a simple positively oriented closed contour surrounding $[-1, 1]$ and lying in R . Then we have (see, e.g., [36]):

$$\frac{|u^{(m)}(x)|}{m!} \leq \frac{L(\mathcal{C}) \max_{z \in \mathcal{C}} |u(z)|}{2\pi\delta^{m+1}}, \quad \forall x \in [-1, 1], \quad (2.1)$$

where $L(\mathcal{C})$ is the length of $\mathcal{C}$, and δ is the distance from $\mathcal{C}$ to $[-1, 1]$ (can be viewed as the distance from $[-1, 1]$ to the nearest singularity of u in the complex plane). Mathematically, an appropriate contour to characterize the analyticity is the so-called Bernstein ellipse. It is known (see, e.g., [36]) that the Bernstein ellipse is transformed from the circle

$$\mathcal{C}_\rho = \{w = \rho e^{i\theta} : \theta \in [0, 2\pi]\}, \quad i = \sqrt{-1}, \quad \rho > 1, \quad (2.2)$$

via the Joukowski transformation $z = (w + w^{-1})/2$ (cf. [84]), that is,

$$\mathcal{E}_\rho := \left\{ z \in \mathbb{C} : z = \frac{1}{2}(w + w^{-1}), \quad w \in \mathcal{C}_\rho \right\}, \quad (2.3)$$

where $\mathbb{C}$ is the set of all complex numbers. It has the foci at ± 1 , and the major and minor semi-axes are

$$a = \frac{1}{2}(\rho + \rho^{-1}), \quad b = \frac{1}{2}(\rho - \rho^{-1}), \quad (2.4)$$

respectively, so the sum of two semi-axes is ρ . The perimeter of $\mathcal{E}_\rho$ can be approximated by (see Ramanujan [94]): $\pi(3\rho - \sqrt{4\rho^2 - \rho^{-2}})$. We also refer to the very recent result (see [117, Eq. (2.15)]):

$$L(\mathcal{E}_\rho) \leq \frac{(24 - 5\sqrt{2}\pi)\rho - (8 - (1 + \sqrt{2})\pi)(\rho^2 - \rho^{-2})/\rho - (16 - 5\pi)\sqrt{\rho^2 + \rho^{-2}}}{2(3 - 2\sqrt{2})}. \quad (2.5)$$

In Figure 2.1, we plot the circle $w = \rho e^{i\theta}$ and Bernstein ellipse $\mathcal{E}_\rho$ under the Joukowski transformation.

Figure 2.1: Circle $|w| = \rho = 1.5$ (left), and Bernstein ellipse $\mathcal{E}_\rho$ (right).

The distance from $\mathcal{E}_\rho$ to the interval $[-1, 1]$ is defined as

$$d_\rho = \frac{1}{2}(\rho + \rho^{-1}) - 1. \quad (2.6)$$

We see that d_ρ increases with respect to ρ , and $d_\rho \rightarrow 0^+$ as $\rho \rightarrow 1^+$ (so the ellipse reduces to the interval $[-1, 1]$). Thus, by the theory of analytic continuation, we have that *for any analytic function u on $[-1, 1]$, there always exists a Bernstein ellipse $\mathcal{E}_\rho$ with $\rho > 1$ such that the continuation of u is analytic on and within $\mathcal{E}_\rho$* . Hereafter, we denote by

$$\mathcal{A}_\rho := \{u : u \text{ is analytic on and within } \mathcal{E}_\rho\}, \quad 1 < \rho < \rho_{\max}, \quad (2.7)$$

where $\mathcal{E}_{\rho_{\max}}$ labels the largest ellipse within which u is analytic. In particular, if $\rho_{\max} = \infty$, u is an entire function.

2.2 Jacobi polynomials and Gamma functions

In this section, we collect some properties of Jacobi polynomials and Gamma functions of relevance to this thesis.

2.2.1 Jacobi polynomials

Let $P_n^{(\alpha, \beta)}(x)$ be the Jacobi polynomial of degree n , as normalized in Szegő [108] (cf. (1.1)-(1.2)). In particular, we denote the Legendre polynomial by $P_n(x)$ ($= P_n^{(0,0)}(x)$), and the Chebyshev polynomial by $T_n(x)$ ($= \arccos(n \cos x)$).

The Jacobi polynomials are generated by the three-term recurrence relation:

$$\begin{aligned} P_{n+1}^{(\alpha, \beta)}(x) &= (A_n^{(\alpha, \beta)}x - B_n^{(\alpha, \beta)})P_n^{(\alpha, \beta)}(x) - C_n^{(\alpha, \beta)}P_{n-1}^{(\alpha, \beta)}(x), \quad n \geq 1, \\ P_0^{(\alpha, \beta)}(x) &= 1, \quad P_1^{(\alpha, \beta)}(x) = \frac{1}{2}(\alpha + \beta + 2)x + \frac{1}{2}(\alpha - \beta), \end{aligned} \quad (2.8)$$

where

$$A_n^{(\alpha, \beta)} = \frac{(2n + \alpha + \beta + 1)(2n + \alpha + \beta + 2)}{2(n + 1)(n + \alpha + \beta + 1)}, \quad (2.9a)$$

$$B_n^{(\alpha, \beta)} = \frac{(\beta^2 - \alpha^2)(2n + \alpha + \beta + 1)}{2(n + 1)(n + \alpha + \beta + 1)(2n + \alpha + \beta)}, \quad (2.9b)$$

$$C_n^{(\alpha, \beta)} = \frac{(n + \alpha)(n + \beta)(2n + \alpha + \beta + 2)}{(n + 1)(n + \alpha + \beta + 1)(2n + \alpha + \beta)}. \quad (2.9c)$$

Another recurrence relation reads (see, e.g., [108, Eqs. (4.5.5)-(4.5.6)]):

$$(1 - x^2)\partial_x P_n^{(\alpha, \beta)}(x) = \widehat{A}_n^{(\alpha, \beta)}P_{n-1}^{(\alpha, \beta)}(x) + \widehat{B}_n^{(\alpha, \beta)}P_n^{(\alpha, \beta)}(x) + \widehat{C}_n^{(\alpha, \beta)}P_{n+1}^{(\alpha, \beta)}(x), \quad (2.10)$$

where

$$\begin{aligned} \widehat{A}_n^{(\alpha, \beta)} &= \frac{2(n + \alpha)(n + \beta)(n + \alpha + \beta + 1)}{(2n + \alpha + \beta)(2n + \alpha + \beta + 1)}, \\ \widehat{B}_n^{(\alpha, \beta)} &= (\alpha - \beta) \frac{2n(n + \alpha + \beta + 1)}{(2n + \alpha + \beta)(2n + \alpha + \beta + 2)}, \\ \widehat{C}_n^{(\alpha, \beta)} &= -\frac{2n(n + 1)(n + \alpha + \beta + 1)}{(2n + \alpha + \beta + 1)(2n + \alpha + \beta + 2)}. \end{aligned} \quad (2.11)$$

The Jacobi polynomials satisfy the Rodrigues' formula

$$(1-x)^\alpha(1+x)^\beta P_n^{(\alpha,\beta)}(x) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n} \left[(1-x)^{\alpha+n}(1+x)^{\beta+n} \right], \quad n \geq 0, \quad (2.12)$$

and the following identities:

$$\partial_x P_n^{(\alpha,\beta)}(x) = \frac{1}{2}(n+\alpha+\beta+1)P_{n-1}^{(\alpha+1,\beta+1)}(x), \quad (2.13)$$

$$P_n^{(\alpha+1,\beta)}(x) = \frac{2}{2n+\alpha+\beta+2} \frac{(n+\alpha+1)P_n^{(\alpha,\beta)}(x) - (n+1)P_{n+1}^{(\alpha,\beta)}(x)}{1-x}, \quad (2.14)$$

$$P_n^{(\alpha,\beta+1)}(x) = \frac{2}{2n+\alpha+\beta+2} \frac{(n+\beta+1)P_n^{(\alpha,\beta)}(x) + (n+1)P_{n+1}^{(\alpha,\beta)}(x)}{1+x}. \quad (2.15)$$

The Chebyshev polynomial of the second kind, denoted by $U_n(x)$, can be expressed by

$$U_n(x) = \frac{\sin((n+1)\arccos(x))}{\sqrt{1-x^2}} = \frac{T'_{n+1}(x)}{n+1} = \sqrt{\frac{\pi}{2}} \frac{P_n^{(1/2,1/2)}(x)}{\sqrt{\gamma_n^{1/2,1/2}}}, \quad (2.16)$$

where $\gamma_n^{1/2,1/2}$ is given in (1.2).

The Chebyshev polynomials enjoy the following important properties:

$$P_n^{(-1/2,-1/2)}(x) = P_n^{(-1/2,-1/2)}(1)T_n(x) = \frac{\Gamma(n+1/2)}{\sqrt{\pi}n!}T_n(x), \quad (2.17a)$$

$$T'_n(x) = 2n \sum_{\substack{k=0 \\ k+n \text{ odd}}}^{n-1} \frac{1}{c_k} T_k(x), \quad (2.17b)$$

where $c_0 = 2$ and $c_k = 1$ for $k \geq 1$.

2.2.2 Gamma functions

The Gamma function (see, e.g., [1]), defined by

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} dt, \quad \forall z \in \mathbb{C} \text{ with } \operatorname{Re} z > 0,$$

satisfies (cf. [118])

$$\Gamma(x)\Gamma(x+1/2) = 2^{1-2x} \sqrt{\pi} \Gamma(2x), \quad \forall x \geq 0, \quad (2.18)$$

and

$$\Gamma(x)\Gamma(-x) = -\frac{\pi}{x \sin(\pi x)}, \quad \forall x > 0. \quad (2.19)$$

In the analysis, we also use the following property of the Gamma function (see [1, Eq. (6.1.38)]):

$$\Gamma(x+1) = \sqrt{2\pi} x^{x+1/2} \exp\left(-x + \frac{\theta}{12x}\right), \quad \forall x > 0, \quad 0 < \theta < 1. \quad (2.20)$$

Lemma 2.1. *For any constants a, b , we have that for $n \geq 1$, $n + a > 1$, and $n + b > 1$,*

$$\exp\left(-\Upsilon_n^{b,a}\right)n^{a-b} \leq \frac{\Gamma(n+a)}{\Gamma(n+b)} \leq \exp\left(\Upsilon_n^{a,b}\right)n^{a-b}, \quad (2.21)$$

where

$$\Upsilon_n^{a,b} = \frac{a-b}{2(n+b-1)} + \frac{1}{12(n+a-1)} + \frac{(a-1)(a-b)}{n}. \quad (2.22)$$

Proof. Let θ_1, θ_2 be two constants in $(0, 1)$. We find from (2.20) that

$$\begin{aligned} \frac{\Gamma(n+a)}{\Gamma(n+b)} &= \frac{(n+a-1)^{n+a-1/2}}{(n+b-1)^{n+b-1/2}} \exp\left(b-a + \frac{\theta_1}{12(n+a-1)} - \frac{\theta_2}{12(n+b-1)}\right) \\ &\leq (n+a-1)^{a-b} \left(1 + \frac{a-b}{n+b-1}\right)^{n+b-1/2} \exp\left(b-a + \frac{1}{12(n+a-1)}\right) \\ &\leq n^{a-b} \left(1 + \frac{a-1}{n}\right)^{a-b} \exp\left(b-a + \frac{(a-b)(n+b-1/2)}{n+b-1} + \frac{1}{12(n+a-1)}\right) \\ &\leq n^{a-b} \exp\left(\frac{a-b}{2(n+b-1)} + \frac{1}{12(n+a-1)} + \frac{(a-1)(a-b)}{n}\right) \\ &:= \exp\left(\Upsilon_n^{a,b}\right)n^{a-b}, \end{aligned}$$

where we used the fact that $1+x \leq e^x$, for real x . The left side inequality can be easily obtained by changing the role of a and b above. $\square$

Remark 2.1. *Applying (2.21)-(2.22) to $\gamma_n^{\alpha,\beta}$ (cf. (1.2)) leads to that for $\alpha, \beta > -1$, $n \geq 1$, and $n + \alpha + \beta > 0$,*

$$\begin{aligned} \gamma_n^{\alpha,\beta} &= \frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)n!\Gamma(n+\alpha+\beta+1)} \\ &\leq \frac{2^{\alpha+\beta+1}}{2n+\alpha+\beta+1} \exp\left(\Upsilon_n^{\alpha+1,1} + \Upsilon_n^{\beta+1,\alpha+\beta+1}\right) = C_n \frac{2^{\alpha+\beta}}{n}, \end{aligned} \quad (2.23)$$

where

$$C_n := C_n(\alpha, \beta) = \frac{2n \exp(\Upsilon_n^{\alpha+1,1} + \Upsilon_n^{\beta+1,\alpha+\beta+1})}{2n + \alpha + \beta + 1}. \quad (2.24)$$

Note that for fixed α and β ,

$$\Upsilon_n^{\alpha,\beta} = O(n^{-1}), \quad C_n = 1 + O(n^{-1}). \quad (2.25)$$

2.3 Main analysis tools

The following important representation is crucial to our analysis.

Lemma 2.2. *Let $\{\hat{u}_n^{\alpha,\beta}\}$ be the Jacobi polynomial expansion coefficients given by*

$$\hat{u}_n^{\alpha,\beta} = \frac{1}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 u(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx, \quad \alpha, \beta > -1, \quad n \geq 0. \quad (2.26)$$

If $u \in \mathcal{A}_\rho$ (cf. (2.7)) with $\rho > 1$, we have the representation

$$\hat{u}_n^{\alpha,\beta} = \frac{1}{\pi i} \sum_{j=0}^{\infty} \sigma_{n,j}^{\alpha,\beta} \oint_{\mathcal{E}_\rho} \frac{u(z)}{w^{n+j+1}} dz, \quad n \geq 0, \quad (2.27)$$

where $z = (w + w^{-1})/2$ with $w = \rho e^{i\theta}$, $\theta \in [0, 2\pi]$, and

$$\sigma_{n,j}^{\alpha,\beta} = \frac{1}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 U_{n+j}(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx, \quad n, j \geq 0. \quad (2.28)$$

Here, $U_{n+j}(x)$ is the Chebyshev polynomial of the second kind of degree $n+j$ (cf. (2.16)).

Proof. We first show that

$$\hat{u}_n^{\alpha,\beta} = \frac{1}{\pi i} \oint_{\mathcal{E}_\rho} Q_n^{(\alpha,\beta)}(z) u(z) dz, \quad (2.29)$$

where

$$Q_n^{(\alpha,\beta)}(z) := \frac{1}{2\gamma_n^{\alpha,\beta}} \int_{-1}^1 \frac{P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x)}{z - x} dx, \quad (2.30)$$

and $\gamma_n^{\alpha,\beta}$ is given by (1.2). Recall the Cauchy's integral formula:

$$\frac{d^n}{dx^n} u(x) = \frac{n!}{2\pi i} \oint_{\mathcal{E}_\rho} \frac{u(z)}{(z - x)^{n+1}} dz. \quad (2.31)$$

Using (2.26), the Rodrigues' formula (2.12), (2.31) and integration by parts leads to

$$\begin{aligned}
\hat{u}_n^{\alpha,\beta} &= \frac{1}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 u(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\
&= \frac{1}{\gamma_n^{\alpha,\beta}} \frac{(-1)^n}{2^n n!} \int_{-1}^1 \omega^{\alpha+n,\beta+n}(x) \frac{d^n}{dx^n} u(x) dx \\
&= \frac{1}{\gamma_n^{\alpha,\beta}} \frac{1}{2^n n!} \int_{-1}^1 \left(\frac{n!}{2\pi i} \oint_{\mathcal{E}_\rho} \frac{u(z)}{(z-x)^{n+1}} dz \right) \omega^{\alpha+n,\beta+n}(x) dx \\
&= \frac{1}{2^n \gamma_n^{\alpha,\beta}} \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \left(\int_{-1}^1 \frac{\omega^{\alpha+n,\beta+n}(x)}{(z-x)^{n+1}} dx \right) u(z) dz.
\end{aligned} \tag{2.32}$$

We find from integration by parts that

$$\int_{-1}^1 \frac{\omega^{\alpha+n,\beta+n}(x)}{(z-x)^{n+1}} dx = \frac{(-1)^n}{n!} \int_{-1}^1 \frac{1}{z-x} \frac{d^n}{dx^n} \omega^{\alpha+n,\beta+n}(x) dx. \tag{2.33}$$

Inserting (2.33) into (2.32), we derive from the Rodrigues' formula (2.12) that

$$\hat{u}_n^{\alpha,\beta} = \frac{1}{2\pi i} \frac{1}{\gamma_n^{\alpha,\beta}} \oint_{\mathcal{E}_\rho} \left(\int_{-1}^1 \frac{\omega^{\alpha,\beta}(x) P_n^{(\alpha,\beta)}(x)}{z-x} dx \right) u(z) dz = \frac{1}{\pi i} \oint_{\mathcal{E}_\rho} Q_n^{(\alpha,\beta)}(z) u(z) dz,$$

where $Q_n^{(\alpha,\beta)}(z)$ is given in (2.30).

Since $z = (w + w^{-1})/2$, we have from the generating function of the Chebyshev polynomial of the second kind (cf. [1]) that

$$\frac{1}{z-x} = \frac{2}{w} \frac{1}{w^{-2} - 2xw^{-1} + 1} = \frac{2}{w} \sum_{k=0}^{\infty} \frac{U_k(x)}{w^k}. \tag{2.34}$$

Inserting it into (2.30), we find from the orthogonality of the Jacobi polynomials (cf. (1.1)) that

$$\begin{aligned}
Q_n^{(\alpha,\beta)}(z) &= \frac{1}{\gamma_n^{\alpha,\beta}} \sum_{k=0}^{\infty} \frac{1}{w^{k+1}} \int_{-1}^1 U_k(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\
&= \frac{1}{\gamma_n^{\alpha,\beta}} \sum_{k=n}^{\infty} \frac{1}{w^{k+1}} \int_{-1}^1 U_k(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\
&= \frac{1}{\gamma_n^{\alpha,\beta}} \sum_{j=0}^{\infty} \frac{1}{w^{n+j+1}} \int_{-1}^1 U_{n+j}(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\
&= \sum_{j=0}^{\infty} \frac{\sigma_{n,j}^{\alpha,\beta}}{w^{n+j+1}},
\end{aligned} \tag{2.35}$$

where $\sigma_{n,j}^{\alpha,\beta}$ is defined in (2.28). Substituting the last identity of (2.35) into (2.29) leads to the desired formula (2.27). $\square$

Note that the contour integral expressions of $\hat{u}_n^{\alpha,\beta}$ in (2.29) and (2.30) are special cases of the general formulas in [38, Eq. (2.2) and Eq. (2.3)] (which were derived by a quite different approach).

The establishment of sharp bounds heavily relies on estimating $\sigma_{n,j}^{\alpha,\beta}$. The following explicit formulas follow from (2.28) and some properties of Jacobi polynomials in Subsection 2.2.1. We remark that the formula (2.38) can be found in various books e.g., [36, 83], while the formula (2.39) is due to Heine (see [24]). We also highlight that the formula (2.40) for the general Jacobi case seems new.

Corollary 2.1. *Let $n \geq 0$.*

(i) *For $\alpha = \beta > -1$ (Gegenbauer polynomial),*

$$\sigma_{n,j}^{\alpha,\alpha} = 0, \quad \text{for odd } j, \quad (2.36)$$

and $\sigma_{n,j}^{\alpha,\alpha}$ for even j are computed by (2.40) below.

(ii) *For $\alpha = \beta = 1/2$ (Chebyshev polynomial of the second kind),*

$$\sigma_{n,0}^{1/2,1/2} = \frac{\sqrt{\pi}}{2} \frac{\Gamma(n+2)}{\Gamma(n+3/2)}; \quad \sigma_{n,j}^{1/2,1/2} = 0, \quad \text{for } j \geq 1. \quad (2.37)$$

(iii) *For $\alpha = \beta = -1/2$ (Chebyshev polynomial),*

$$\sigma_{n,j}^{-1/2,-1/2} = \begin{cases} \frac{2\sqrt{\pi}\Gamma(n+1)}{\Gamma(n+1/2)}, & \text{for even } j, \\ 0, & \text{for odd } j. \end{cases} \quad (2.38)$$

(iv) *For $\alpha = \beta = 0$ (Legendre polynomial),*

$$\sigma_{n,j}^{0,0} = \begin{cases} \frac{2n+1}{2} \frac{\Gamma(l+1/2)}{\Gamma(l+1)} \frac{\Gamma(n+l+1)}{\Gamma(n+l+3/2)}, & \text{for even } j = 2l, \\ 0, & \text{for odd } j. \end{cases} \quad (2.39)$$

(v) For general $\alpha, \beta > -1$ (Jacobi polynomial),

$$\begin{aligned} \sigma_{n,j}^{\alpha,\beta} &= \frac{\sqrt{\pi}(2n + \alpha + \beta + 1)\Gamma(n + \alpha + \beta + 1)}{2\Gamma(n + \alpha + 1)} \\ &\times \sum_{m=0}^j \frac{(-1)^m \Gamma(2n + j + m + 2)\Gamma(n + m + \alpha + 1)}{m!(j - m)!\Gamma(n + m + 3/2)\Gamma(2n + m + \alpha + \beta + 2)}. \end{aligned} \quad (2.40)$$

Proof. (i) The property (2.36) is a direct consequence of the parity of Gegenbauer polynomials.

(ii) For $\alpha = \beta = 1/2$, we find from (2.16) and the orthogonality (1.1)-(1.2) that

$$\begin{aligned} \sigma_{n,j}^{1/2,1/2} &= \sqrt{\frac{\pi}{2}} \frac{1}{\sqrt{\gamma_{n+j}^{1/2,1/2}}} \frac{1}{\gamma_n^{1/2,1/2}} \int_{-1}^1 P_{n+j}^{(1/2,1/2)}(x) P_n^{(1/2,1/2)}(x) (1 - x^2)^{1/2} dx \\ &= \sqrt{\frac{\pi}{2}} \frac{1}{\sqrt{\gamma_{n+j}^{1/2,1/2}}} \delta_{j,0}, \end{aligned}$$

where $\delta_{j,0}$ is the Kronecker delta. Working out the constant leads to (2.37).

(iii) For $\alpha = \beta = -1/2$, if $j = 2l$, by (2.16), (2.17a) and (2.17b), we have

$$\begin{aligned} \sigma_{n,2l}^{-1/2,-1/2} &= \frac{1}{\gamma_n^{-1/2,-1/2}} \frac{1}{n + 2l + 1} \int_{-1}^1 T'_{n+2l+1}(x) P_n^{(-1/2,-1/2)}(x) (1 - x^2)^{-1/2} dx \\ &= \frac{2}{\gamma_n^{-1/2,-1/2}} \int_{-1}^1 T_n(x) P_n^{(-1/2,-1/2)}(x) (1 - x^2)^{-1/2} dx = \frac{2\sqrt{\pi} \Gamma(n + 1)}{\Gamma(n + 1/2)}, \end{aligned}$$

which, together with (2.36), implies (2.38).

(iv) For $\alpha = \beta = 0$, we derive from [108, Eq. (4.9.8)] that

$$\begin{aligned} \sigma_{n,2l}^{0,0} &= \frac{1}{\gamma_n^{0,0}} \int_{-1}^1 P_n(x) U_{n+2l}(x) dx = \frac{2n + 1}{2} \int_0^\pi P_n(\cos \theta) \sin((n + 2l + 1)\theta) d\theta \\ &= \frac{2n + 1}{2} \frac{\Gamma(l + 1/2)}{\Gamma(l + 1)} \frac{\Gamma(n + l + 1)}{\Gamma(n + l + 3/2)}, \quad l \geq 0. \end{aligned}$$

This yields (2.39).

(v) By [6, Lemma 7.1.1] (also see [102, Theorem 3.21]), we have the following

formula:

$$\begin{aligned} & \frac{1}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 P_{n+j}^{(a,b)}(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\ &= \frac{\Gamma(n+j+a+1)}{\Gamma(n+j+a+b+1)} \frac{(2n+\alpha+\beta+1)\Gamma(n+\alpha+\beta+1)}{\Gamma(n+\alpha+1)} \\ & \quad \times \sum_{m=0}^j \frac{(-1)^m \Gamma(2n+j+m+a+b+1) \Gamma(n+m+\alpha+1)}{m!(j-m)! \Gamma(n+m+a+1) \Gamma(2n+m+\alpha+\beta+2)}, \end{aligned} \quad (2.41)$$

for $a, b, \alpha, \beta > -1$ and $n, j \geq 0$. Hence, a combination of (1.2), (2.16), (2.28) and (2.41) leads to the formula (2.40). $\square$

With the aid of Lemma 2.2, we can derive the following estimate, from which our sharp bounds stem.

Lemma 2.3. *For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, we have that for $\alpha, \beta > -1$, and $n \geq 0$,*

$$|\hat{u}_n^{\alpha,\beta}| \leq \frac{M}{\rho^n} \left(|\sigma_{n,0}^{\alpha,\beta}| + \frac{1}{\rho} |\sigma_{n,1}^{\alpha,\beta}| + \frac{1}{\rho^2} \sum_{j=0}^{\infty} |\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}| \frac{1}{\rho^j} \right), \quad (2.42)$$

where $M = \max_{z \in \mathcal{E}_\rho} |u(z)|$ and $\{\sigma_{n,j}^{\alpha,\beta}\}$ are given by (2.28).

Proof. Since $z = (w + w^{-1})/2 \in \mathcal{E}_\rho$ with $w \in \mathcal{C}_\rho$ (cf. (2.2)-(2.3)), we can rewrite $\hat{u}_n^{\alpha,\beta}$ in (2.27) as

$$\begin{aligned} \hat{u}_n^{\alpha,\beta} &= \frac{1}{2\pi i} \sum_{j=0}^{\infty} \sigma_{n,j}^{\alpha,\beta} \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+j+1}} \left(1 - \frac{1}{w^2}\right) dw \\ &= \frac{1}{2\pi i} \sum_{j=0}^{\infty} \sigma_{n,j}^{\alpha,\beta} \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+j+1}} dw - \frac{1}{2\pi i} \sum_{j=0}^{\infty} \sigma_{n,j}^{\alpha,\beta} \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+j+3}} dw \\ &= \frac{1}{2\pi i} \sigma_{n,0}^{\alpha,\beta} \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+1}} dw + \frac{1}{2\pi i} \sigma_{n,1}^{\alpha,\beta} \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+2}} dw \\ & \quad + \frac{1}{2\pi i} \sum_{j=0}^{\infty} (\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}) \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+j+3}} dw. \end{aligned} \quad (2.43)$$

Hence, we arrive at

$$\begin{aligned} |\hat{u}_n^{\alpha,\beta}| &\leq \frac{M}{2\pi} \frac{2\pi\rho}{\rho^{n+1}} |\sigma_{n,0}^{\alpha,\beta}| + \frac{M}{2\pi} \frac{2\pi\rho}{\rho^{n+2}} |\sigma_{n,1}^{\alpha,\beta}| + \frac{M}{2\pi} \frac{2\pi\rho}{\rho^{n+3}} \sum_{j=0}^{\infty} |\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}| \frac{1}{\rho^j} \\ &= \frac{M}{\rho^n} |\sigma_{n,0}^{\alpha,\beta}| + \frac{M}{\rho^{n+1}} |\sigma_{n,1}^{\alpha,\beta}| + \frac{M}{\rho^{n+2}} \sum_{j=0}^{\infty} |\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}| \frac{1}{\rho^j}. \end{aligned} \quad (2.44)$$

This ends the proof. $\square$

Observe from the proof that we split the contour integral on $\mathcal{E}_\rho$ into two parts on $\mathcal{C}_\rho$, which actually allows us to take advantage of cancelation of $\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}$. Indeed, the bound (2.42) is tight, as we will see shortly that this argument can recover the best estimate for the Chebyshev case (see [98, Theorem 3.8] and (2.57)) and improve the bounds in [120] (see (1.5)).

2.4 Main results

For clarity of exposition, we first present the result on the general Jacobi polynomial expansions, followed by the refined results on the Chebyshev-type expansions ($\alpha = k - 1/2, \beta = l - 1/2$ with $k, l \in \mathbb{N} := \{0, 1, 2, \dots\}$), and Legendre-type expansions ($\alpha = k, \beta = l$ with $k, l \in \mathbb{N}$).

2.4.1 General Jacobi expansions

Theorem 2.1. *For any $u \in \mathcal{A}_\rho$ with $\rho > 1, \alpha, \beta > -1$, and $n \geq 0$, we have*

$$|\hat{u}_n^{\alpha,\beta}| \leq \frac{M}{\rho^n} \left[|\sigma_{n,0}^{\alpha,\beta}| + \frac{|\sigma_{n,1}^{\alpha,\beta}|}{\rho} + \frac{2}{\rho(\rho-1)} \sqrt{\frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}}} \right], \quad (2.45)$$

where

$$\sigma_{n,0}^{\alpha,\beta} = \frac{\sqrt{\pi}}{2} \frac{(2n+1)! \Gamma(n+\alpha+\beta+1)}{\Gamma(n+3/2) \Gamma(2n+\alpha+\beta+1)}, \quad \sigma_{n,1}^{\alpha,\beta} = \frac{(\beta-\alpha)(2n+2)}{2n+\alpha+\beta+2} \sigma_{n,0}^{\alpha,\beta}, \quad (2.46)$$

and $\gamma_n^{\alpha,\beta}$ is defined in (1.2).

In particular, if $\alpha = \beta$, we have

$$|\hat{u}_n^{\alpha,\alpha}| \leq \frac{M}{\rho^n} \left[|\sigma_{n,0}^{\alpha,\alpha}| + \frac{2}{\rho^2-1} \sqrt{\frac{\gamma_0^{\alpha,\alpha}}{\gamma_n^{\alpha,\alpha}}} \right]. \quad (2.47)$$

Proof. By (2.42),

$$|\hat{u}_n^{\alpha,\beta}| \leq \frac{M}{\rho^n} |\sigma_{n,0}^{\alpha,\beta}| + \frac{M}{\rho^{n+1}} |\sigma_{n,1}^{\alpha,\beta}| + \frac{M}{\rho^{n+2}} \sum_{j=0}^{\infty} |\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}| \frac{1}{\rho^j}. \quad (2.48)$$

The factors $\sigma_{n,0}^{\alpha,\beta}$ and $\sigma_{n,1}^{\alpha,\beta}$ in (2.46) are computed from (2.40) directly, so it suffices to estimate the infinite sum in (2.48). Recall the identity (cf. [83]):

$$U_k(x) - U_{k-2}(x) = 2T_k(x), \quad k \geq 2. \quad (2.49)$$

Then we infer from (2.28) that

$$\begin{aligned} \sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta} &= \frac{1}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 (U_{n+j+2}(x) - U_{n+j}(x)) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\ &= \frac{2}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 T_{n+j+2}(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx, \quad n, j \geq 0. \end{aligned} \quad (2.50)$$

Thus, using the Cauchy-Schwartz inequality, the orthogonality (1.1), and the fact $|T_k(x)| \leq 1$, leads to

$$|\sigma_{n,j+2}^{\alpha,\beta} - \sigma_{n,j}^{\alpha,\beta}| \leq \frac{2}{\sqrt{\gamma_n^{\alpha,\beta}}} \left(\int_{-1}^1 T_{n+j+2}^2(x) \omega^{\alpha,\beta}(x) dx \right)^{1/2} \leq 2 \sqrt{\frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}}}. \quad (2.51)$$

Therefore, the bound (2.45) follows from $\sum_{j=0}^{\infty} \rho^{-j} = 1/(1 - \rho^{-1})$, as $\rho > 1$.

For $\alpha = \beta$, since $|\sigma_{n,2l+1}^{\alpha,\alpha}| = 0$, for all $l \geq 0$ (cf. Corollary 2.1 (i)), we have

$$\sum_{j=0}^{\infty} |\sigma_{n,j+2}^{\alpha,\alpha} - \sigma_{n,j}^{\alpha,\alpha}| \frac{1}{\rho^j} = \sum_{l=0}^{\infty} |\sigma_{n,2l+2}^{\alpha,\alpha} - \sigma_{n,2l}^{\alpha,\alpha}| \frac{1}{\rho^{2l}} \leq 2 \sqrt{\frac{\gamma_0^{\alpha,\alpha}}{\gamma_n^{\alpha,\alpha}}} \frac{1}{1 - \rho^{-2}}.$$

This yields the refined bound in (2.47). $\square$

Remark 2.2. Using (2.21)-(2.22), we can characterize the explicit dependence of the upper bounds in (2.45) and (2.47) on n, α and β . Indeed, we derive from (2.46) and (2.21) that for $\alpha, \beta > -1, n \geq 1$, and $n + \alpha + \beta > 0$,

$$\begin{aligned} \sigma_{n,0}^{\alpha,\beta} &= \frac{\sqrt{\pi}}{2} \frac{\Gamma(n + \alpha + \beta + 1)}{\Gamma(n + 3/2)} \frac{\Gamma(2n + 2)}{\Gamma(2n + \alpha + \beta + 1)} \\ &\leq \frac{\sqrt{\pi}}{2} \left(\exp(\Upsilon_n^{\alpha+\beta+1,3/2}) n^{\alpha+\beta+1-3/2} \right) \left(\exp(\Upsilon_{2n}^{2,\alpha+\beta+1}) (2n)^{2-(\alpha+\beta+1)} \right) \\ &= \frac{\sqrt{\pi n}}{2^{\alpha+\beta}} \exp(\Upsilon_n^{\alpha+\beta+1,3/2} + \Upsilon_{2n}^{2,\alpha+\beta+1}), \end{aligned}$$

which implies

$$\begin{aligned} |\sigma_{n,1}^{\alpha,\beta}| &= \frac{|\alpha - \beta|(2n + 2)}{2n + \alpha + \beta + 2} \sigma_{n,0}^{\alpha,\beta} \\ &\leq \frac{|\alpha - \beta|(2n + 2)}{2n + \alpha + \beta + 2} \frac{\sqrt{\pi n}}{2^{\alpha+\beta}} \exp(\Upsilon_n^{\alpha+\beta+1,3/2} + \Upsilon_{2n}^{2,\alpha+\beta+1}). \end{aligned}$$

Similarly, by (1.2) and (2.21),

$$\begin{aligned} \frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}} &= (2n + \alpha + \beta + 1) \frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)} \frac{\Gamma(n + 1)\Gamma(n + \alpha + \beta + 1)}{\Gamma(n + \alpha + 1)\Gamma(n + \beta + 1)} \\ &\leq (2n + \alpha + \beta + 1) \frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)} \exp(\Upsilon_n^{1,\alpha+1} + \Upsilon_n^{\alpha+\beta+1,\beta+1}). \end{aligned}$$

Consequently, we infer from (2.45) that for $\alpha, \beta > -1, n \geq 1$, and $n + \alpha + \beta > 0$,

$$\begin{aligned} |\hat{u}_n^{\alpha,\beta}| &\leq \frac{M}{\rho^n} \left[\left(1 + \frac{1}{\rho} \frac{|\alpha - \beta|(2n + 2)}{2n + \alpha + \beta + 2} \right) \frac{\sqrt{\pi n}}{2^{\alpha+\beta}} \exp(\Upsilon_n^{\alpha+\beta+1,3/2} + \Upsilon_n^{2,\alpha+\beta+1}) \right. \\ &\quad \left. + \frac{2\sqrt{2n + \alpha + \beta + 1}}{\rho(\rho - 1)} \sqrt{\frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)}} \sqrt{\exp(\Upsilon_n^{1,\alpha+1} + \Upsilon_n^{\alpha+\beta+1,\beta+1})} \right] \\ &\leq \widehat{C}_n M \left(\frac{\sqrt{\pi}}{2^{\alpha+\beta}} \left(1 + \frac{|\alpha - \beta|}{\rho} \right) + \sqrt{\frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)}} \frac{2\sqrt{2}}{\rho(\rho - 1)} \right) \frac{\sqrt{n}}{\rho^n}, \end{aligned}$$

where we used the fact $2n + \alpha + \beta + 2 > 2n$, and denote

$$\begin{aligned} \widehat{C}_n &= \max \left\{ \frac{n + 1}{n} \exp(\Upsilon_n^{\alpha+\beta+1,3/2} + \Upsilon_n^{2,\alpha+\beta+1}), \right. \\ &\quad \left. \sqrt{\frac{2n + \alpha + \beta + 1}{2n}} \sqrt{\exp(\Upsilon_n^{1,\alpha+1} + \Upsilon_n^{\alpha+\beta+1,\beta+1})} \right\}. \end{aligned} \quad (2.52)$$

Similarly, we find from (2.47) that for $\alpha > -1, n \geq 1$, and $n + 2\alpha > 0$,

$$|\hat{u}_n^{\alpha,\alpha}| \leq \overline{C}_n M \left(\frac{\sqrt{\pi}}{2^{2\alpha}} + \frac{\Gamma(\alpha + 1)}{\sqrt{\Gamma(2\alpha + 2)}} \frac{2\sqrt{2}}{\rho^2 - 1} \right) \frac{\sqrt{n}}{\rho^n},$$

where

$$\begin{aligned} \overline{C}_n &= \max \left\{ \exp(\Upsilon_n^{2\alpha+1,3/2} + \Upsilon_n^{2,2\alpha+1}), \right. \\ &\quad \left. \sqrt{\frac{2n + 2\alpha + 1}{2n}} \exp(\Upsilon_n^{1,\alpha+1} + \Upsilon_n^{2\alpha+1,\alpha+1}) \right\}. \end{aligned} \quad (2.53)$$

By (2.25), we know that $\widehat{C}_n = 1 + O(n^{-1})$ and $\overline{C}_n = 1 + O(n^{-1})$. $\square$

Remark 2.3. It is worthwhile to show that the bound obtained from this way is tighter than (1.5) in [120]. Indeed, it follows from (1.1), (2.16) and (2.17b) that

for $n \geq 1$ and $j = 0, 1$,

$$\begin{aligned}\sigma_{n,j}^{\alpha,\beta} &= \frac{1}{\gamma_n^{\alpha,\beta}} \frac{1}{n+j+1} \int_{-1}^1 T'_{n+j+1}(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\ &= \frac{2}{\gamma_n^{\alpha,\beta}} \sum_{\substack{k=0 \\ k+n+j+1 \text{ odd}}}^{n+j} \frac{1}{c_k} \int_{-1}^1 T_k(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx \\ &= \frac{2}{\gamma_n^{\alpha,\beta}} \int_{-1}^1 T_{n+j}(x) P_n^{(\alpha,\beta)}(x) \omega^{\alpha,\beta}(x) dx,\end{aligned}$$

where $c_0 = 2$ and $c_k = 1$ for $k \geq 1$. Following (2.50)-(2.51), we have

$$|\sigma_{n,j}^{\alpha,\beta}| \leq 2 \sqrt{\frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}}}, \quad n \geq 1, \quad j = 0, 1.$$

Finally, a straightforward calculation leads to

$$\frac{M}{\rho^n} \left[|\sigma_{n,0}^{\alpha,\beta}| + \frac{|\sigma_{n,1}^{\alpha,\beta}|}{\rho} + \frac{2}{\rho(\rho-1)} \sqrt{\frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}}} \right] \leq \frac{2M}{\rho^{n-1}(\rho-1)} \sqrt{\frac{\gamma_0^{\alpha,\beta}}{\gamma_n^{\alpha,\beta}}}. \quad (2.54)$$

Moreover, we claim from (2.47) that the strict inequality holds, when $\alpha = \beta > -1$.

One may refer to Section 2.6 for numerical evidence. $\square$

2.4.2 Chebyshev-type expansions

In view of (2.38), it follows from (2.43) that the Chebyshev coefficient takes the simplest form:

$$\hat{u}_n^{-1/2, -1/2} = \frac{\sigma_{n,0}^{-1/2, -1/2}}{2\pi i} \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+1}} dw. \quad (2.55)$$

Thus, using (2.38) and (2.42) leads to

$$|\hat{u}_n^{-1/2, -1/2}| \leq \frac{2\sqrt{\pi} \Gamma(n+1)}{\Gamma(n+1/2)} \frac{M}{\rho^n}. \quad (2.56)$$

This leads to the estimate for the expansion coefficients, denoted by $\{\hat{u}_n^C\}$ as before, in terms of $\{T_n(x)\}$,

$$|\hat{u}_n^C| \leq \frac{2M}{\rho^n}, \quad n \geq 0, \quad (2.57)$$

as documented in, e.g., [98].

For the Chebyshev polynomial of the second kind, we find from (2.27) the closed-form formula like (2.55),

$$\hat{u}_n^{1/2,1/2} = \frac{\sigma_{n,0}^{1/2,1/2}}{\pi i} \oint_{\mathcal{E}_\rho} \frac{u(z)}{w^{n+1}} dz, \quad (2.58)$$

but the contour integration is on $\mathcal{E}_\rho$. It follows from (2.37) and (2.43) that

$$\begin{aligned} |\hat{u}_n^{1/2,1/2}| &\leq \frac{\sigma_{n,0}^{1/2,1/2}}{\pi} \left| \oint_{\mathcal{E}_\rho} \frac{u(z)}{w^{n+1}} dz \right| \\ &= \frac{1}{4\sqrt{\pi}} \frac{(n+1)!}{\Gamma(n+3/2)} \left| \oint_{\mathcal{C}_\rho} \frac{u(z)}{w^{n+1}} \left(1 - \frac{1}{w^2}\right) dw \right| \\ &\leq \frac{\sqrt{\pi}}{2} \frac{(n+1)!}{\Gamma(n+3/2)} \frac{M}{\rho^n} \left(1 + \frac{1}{\rho^2}\right). \end{aligned} \quad (2.59)$$

Like (2.57), if we rescale the expansion in terms of $\{U_n\}$, i.e.,

$$\hat{u}_n^U = \frac{2}{\pi} \int_{-1}^1 u(x) U_n(x) \sqrt{1-x^2} dx,$$

then we find from (2.16) and (2.59) that

$$|\hat{u}_n^U| = \frac{2}{\sqrt{\pi}} \frac{\Gamma(n+3/2)}{\Gamma(n+2)} |\hat{u}_n^{1/2,1/2}| \leq \frac{M}{\rho^n} \left(1 + \frac{1}{\rho^2}\right). \quad (2.60)$$

Remark 2.4. *It is seen from (2.58) that the coefficient of the Chebyshev polynomial of second kind takes the simplest form on the contour $\mathcal{E}_\rho$. This motivates us to estimate the contour integral directly by*

$$\left| \oint_{\mathcal{E}_\rho} \frac{u(z)}{w^{n+1}} dz \right| \leq \frac{M}{\rho^{n+1}} \oint_{\mathcal{E}_\rho} |dz| = \frac{M}{\rho^{n+1}} L(\mathcal{E}_\rho),$$

which implies

$$|\hat{u}_n^U| \leq \frac{M}{\rho^{n+1}} \frac{L(\mathcal{E}_\rho)}{\pi}. \quad (2.61)$$

Using the upper bound $\pi\sqrt{\rho^2 + \rho^{-2}}$ of $L(\mathcal{E}_\rho)$ (cf. [96]) (note that it is larger than the upper bound in (2.5), see [117, Remark 3.5]), we derive

$$\frac{L(\mathcal{E}_\rho)}{\pi\rho} < \sqrt{1 + \frac{1}{\rho^4}} < 1 + \frac{1}{\rho^2}.$$

This shows the estimate (2.61) is sharper than (2.60). $\square$

Before presenting the refined results for $\alpha = k + 1/2, \beta = l + 1/2$ with $k, l \in \mathbb{N}$, a direct consequence of (2.14)-(2.15) yields that for any $k, l \in \mathbb{N} = \{0, 1, \dots\}$,

$$(1-x)^k(1+x)^l P_n^{(\alpha+k, \beta+l)}(x) = \sum_{i=n}^{n+k+l} d_i^{\alpha+k, \beta+l} P_i^{(\alpha, \beta)}(x), \quad (2.62)$$

where $\{d_i^{\alpha+k, \beta+l}\}_{i=n}^{n+k+l}$ is a unique set of constants (with $d_n^{\alpha, \beta} = 1$), computed from (2.14)-(2.15) recursively.

Proof of (2.62): To this end, let $\{c_j\}$ be a set of generic constants. Using (2.14) and (2.15) repeatedly leads to

$$\begin{aligned} & (1-x)^k(1+x)^l P_n^{(\alpha+k, \beta+l)}(x) \\ &= (1-x)^{k-1}(1+x)^l (c_1 P_n^{(\alpha+k-1, \beta+l)}(x) + c_2 P_{n+1}^{(\alpha+k-1, \beta+l)}(x)) \\ &= \dots = (1+x)^l \sum_{m=n}^{n+k} c_m P_m^{(\alpha, \beta+l)}(x) = \dots = \sum_{m=n}^{n+k+l} c_m P_m^{(\alpha, \beta)}(x). \end{aligned}$$

This ends the proof. $\square$

We point out that for $\alpha = \beta = 0$, $\{(1-x)^k(1+x)^l P_n^{(k, l)}(x)\}$ (up to a certain constant factor) are defined as generalized Jacobi polynomials in [57].

With the property in (2.62), we can derive the refined results for $\alpha = k + 1/2, \beta = l + 1/2$ with $k, l \in \mathbb{N}$. Indeed, we find that $\{\sigma_{n,j}^{k+1/2, l+1/2}\}$ can be computed explicitly by the following formula.

Proposition 2.1. *For any $k, l, n, j \in \mathbb{N}$,*

$$\sigma_{n,j}^{k+1/2, l+1/2} = \sqrt{\frac{\pi}{2}} \frac{1}{\gamma_n^{k+1/2, l+1/2}} \sum_{m=n}^{n+k+l} d_m^{k+1/2, l+1/2} \sqrt{\gamma_m^{1/2, 1/2}} \delta_{m, n+j}, \quad (2.63)$$

where $\{d_m^{k+1/2, l+1/2}\}_{m=n}^{n+k+l}$ are given in (2.62) and $\delta_{m, n+j}$ is the Kronecker delta.

Proof. Using (2.62) (with $\alpha = \beta = 1/2$), (2.28), and the properties of Jacobi polynomials (cf. (1.1) and (2.16)) leads to

$$\begin{aligned} \sigma_{n,j}^{k+1/2, l+1/2} &= \frac{1}{\gamma_n^{k+1/2, l+1/2}} \sum_{m=n}^{n+k+l} d_m^{k+1/2, l+1/2} \int_{-1}^1 U_{n+j}(x) P_m^{(1/2, 1/2)}(x) (1-x^2)^{1/2} dx \\ &= \frac{1}{\gamma_n^{k+1/2, l+1/2}} \sqrt{\frac{\pi}{2}} \sum_{m=n}^{n+k+l} d_m^{k+1/2, l+1/2} \sqrt{\gamma_m^{1/2, 1/2}} \delta_{m, n+j}, \end{aligned}$$

This completes the proof. $\square$

Equipped with (2.63), we can obtain the bound for Chebyshev-type expansion coefficients by computing $\{d_m^{k+1/2, l+1/2}\}$ explicitly. To fix the idea, we just consider the case $k = 1$ and $l = 0$. One finds

$$d_n^{3/2, 1/2} = 1, \quad d_{n+1}^{3/2, 1/2} = -\frac{2n+2}{2n+3},$$

and

$$\sigma_{n,0}^{3/2, 1/2} = \frac{\sqrt{\pi}}{4} \frac{n!(n+2)}{\Gamma(n+3/2)}, \quad \sigma_{n,1}^{3/2, 1/2} = -\frac{\sqrt{\pi}}{4} \frac{(n+1)!}{\Gamma(n+3/2)}, \quad \sigma_{n,j}^{3/2, 1/2} = 0, \quad j \geq 2.$$

The estimate (2.42) reduces to

$$\begin{aligned} \hat{u}_n^{3/2, 1/2} &\leq \frac{M}{\rho^n} \left[\sigma_{n,0}^{3/2, 1/2} + \frac{\sigma_{n,1}^{3/2, 1/2}}{\rho} + \frac{\sigma_{n,0}^{3/2, 1/2}}{\rho^2} + \frac{\sigma_{n,1}^{3/2, 1/2}}{\rho^3} \right] \\ &= \frac{M}{\rho^n} \left(1 + \frac{1}{\rho^2} \right) \left[\sigma_{n,0}^{3/2, 1/2} + \frac{\sigma_{n,1}^{3/2, 1/2}}{\rho} \right]. \end{aligned}$$

Thus, we have

$$|\hat{u}_n^{3/2, 1/2}| \leq \frac{\sqrt{\pi}}{4} \frac{(n+1)!}{\Gamma(n+3/2)} \frac{M}{\rho^n} \left(1 + \frac{1}{\rho^2} \right) \left(\frac{n+2}{n+1} + \frac{1}{\rho} \right), \quad (2.64)$$

and by (2.21), we have for $n \geq 0$,

$$\frac{(n+1)!}{\Gamma(n+3/2)} \leq \sqrt{n} \exp(\Upsilon_n^{2, 3/2}). \quad (2.65)$$

Actually, the infinite sum in (2.42) does not appear for the Chebyshev-type expansions, which allows us to derive very tight bounds. However, for the Legendre-type expansions, some care has to be taken to handle this sum.

2.4.3 Legendre-type expansions

We first consider the Legendre case. By (1.2) and (2.46),

$$\gamma_n^{0,0} = \frac{2}{2n+1}, \quad \frac{\gamma_0^{0,0}}{\gamma_n^{0,0}} = 2n+1, \quad \sigma_{n,0}^{0,0} = \frac{\sqrt{\pi} \Gamma(n+1)}{\Gamma(n+1/2)},$$

so the estimate (2.47) reduces to

$$|\hat{u}_n^{0,0}| \leq \frac{M}{\rho^n} \left[\frac{\sqrt{\pi} \Gamma(n+1)}{\Gamma(n+1/2)} + \frac{2\sqrt{2n+1}}{\rho^2 - 1} \right]. \quad (2.66)$$

In fact, we can improve this estimate, as highlighted in the following theorem, by using the explicit information of $\sigma_{n,2l}^{0,0}$.

Theorem 2.2. *Let $\{\hat{u}_n^{0,0}\}$ be the Legendre expansion coefficients of any $u \in \mathcal{A}_\rho$ with $\rho > 1$. Then for any $n \geq 1$,*

$$|\hat{u}_n^{0,0}| \leq \frac{M\sqrt{\pi n}}{\rho^n} \left(1 + \frac{n+2}{2n+3} \frac{1}{\rho^2-1}\right) \exp\left(\frac{8n-1}{12n(2n-1)}\right). \quad (2.67)$$

Proof. A straightforward calculation from (2.39) yields

$$\sigma_{n,2l+2}^{0,0} - \sigma_{n,2l}^{0,0} = -\frac{n+2l+2}{2(l+1)(n+l+3/2)} \sigma_{n,2l}^{0,0}, \quad l \geq 0, \quad (2.68)$$

which implies $\{\sigma_{n,2l}^{0,0}\}$ is strictly descending with respect to l . Hence, we have

$$|\sigma_{n,2l+2}^{0,0} - \sigma_{n,2l}^{0,0}| = \frac{n+2l+2}{2(l+1)(n+l+3/2)} \sigma_{n,2l}^{0,0} \leq \frac{n+2}{2n+3} \sigma_{n,0}^{0,0}, \quad (2.69)$$

where we used the fact that $n+2l+2/((l+1)(n+l+3/2))$ is strictly descending with respect to l . Then, we obtain the improved bound from (2.42):

$$\begin{aligned} |\hat{u}_n^{0,0}| &\leq \frac{M}{\rho^n} \sigma_{n,0}^{0,0} \left(1 + \frac{n+2}{2n+3} \sum_{l=0}^{\infty} \frac{1}{\rho^{2l+2}}\right) \\ &= \frac{\sqrt{\pi} M}{\rho^n} \frac{\Gamma(n+1)}{\Gamma(n+1/2)} \left(1 + \frac{n+2}{2n+3} \frac{1}{\rho^2-1}\right), \end{aligned} \quad (2.70)$$

and by (2.21),

$$\frac{\Gamma(n+1)}{\Gamma(n+1/2)} \leq \sqrt{n} \exp\left(\frac{8n-1}{12n(2n-1)}\right), \quad n \geq 1. \quad (2.71)$$

This completes the proof. $\square$

Remark 2.5. *We compare the bound in (2.67) with the existing ones. Davis [36, Page 313] stated the bound*

$$|\hat{u}_n^{0,0}| \leq \frac{2n+1}{2} \frac{ML(\mathcal{E}_\rho)}{\rho^n(\rho-1)},$$

where clearly the algebraic order of n in the numerator is not optimal. The following asymptotic bound can be obtained from [74, Eq. (32) and Eq. (38)] and [36, Eq. (12.4.25)]:

$$|\hat{u}_n^{0,0}| \leq \frac{M\sqrt{\pi n}}{\rho^n} \frac{\sqrt{\rho^4+1}}{\rho^2-1}, \quad n \gg 1,$$

while the asymptotic estimate derived from (2.67) is

$$|\hat{u}_n^{0,0}| \leq \frac{M\sqrt{\pi n}}{\rho^n} \frac{\rho^2 - 1/2}{\rho^2 - 1}, \quad n \gg 1, \quad (2.72)$$

which is sharper. Another bound for comparison is obtained in the recent paper [120]:

$$|\hat{u}_n^{0,0}| \leq \frac{2\sqrt{n}M}{\rho^n} \left(1 + \frac{1}{\rho^2 - 1}\right), \quad n \geq 1, \quad (2.73)$$

which is also inferior to our estimate (2.67). Some comparisons in numerical perspective are given in Section 2.6. $\square$

Like the Chebyshev case, we can derive similar refined estimates for the Legendre-type expansions with $\alpha = k, \beta = l$ and $k, l \in \mathbb{N}$. The counterpart of Proposition 2.1 is stated as follows, which can be obtained by using (2.62) (with $\alpha = \beta = 0$), (2.28), and the properties of Jacobi polynomials (e.g., (1.1)) as before.

Proposition 2.2. *For any $k, l, n, j \in \mathbb{N}$,*

$$\sigma_{n,j}^{k,l} = \frac{1}{\gamma_n^{k,l}} \sum_{m=n}^{n+k+l} d_m^{k,l} \gamma_m^{0,0} \sigma_{m,n+j-m}^{0,0}, \quad (2.74)$$

where $\{d_m^{k,l}\}_{m=n}^{n+k+l}$ are the same as in (2.62) and $\{\sigma_{m,n+j-m}^{0,0}\}$ are computed by (2.39).

Once again, to fix the idea, we just consider the case $k = 1$ and $l = 0$. One finds $d_n^{1,0} = 1, d_{n+1}^{1,0} = -1$, and

$$\sigma_{n,j}^{1,0} = \frac{1}{\gamma_n^{1,0}} (\gamma_n^{0,0} \sigma_{n,j}^{0,0} - \gamma_{n+1}^{0,0} \sigma_{n+1,j-1}^{0,0}) = \frac{n+1}{2n+1} \sigma_{n,j}^{0,0} - \frac{n+1}{2n+3} \sigma_{n+1,j-1}^{0,0}.$$

By (2.39),

$$\sigma_{n,2l}^{1,0} = \frac{n+1}{2n+1} \sigma_{n,2l}^{0,0}, \quad \sigma_{n,2l+1}^{1,0} = -\frac{n+1}{2n+3} \sigma_{n+1,2l}^{0,0}, \quad l \geq 0.$$

Therefore, with (2.68) and (2.69), the estimate (2.42) reduces to

$$\begin{aligned}
|\hat{u}_n^{1,0}| &\leq \frac{M}{\rho^n} |\sigma_{n,0}^{1,0}| + \frac{M}{\rho^{n+1}} |\sigma_{n,1}^{1,0}| + \frac{M}{\rho^{n+2}} \sum_{j=0}^{\infty} |\sigma_{n,j+2}^{1,0} - \sigma_{n,j}^{1,0}| \frac{1}{\rho^j} \\
&= \frac{M}{\rho^n} \frac{n+1}{2n+1} \left(\sigma_{n,0}^{0,0} + \frac{1}{\rho^2} \sum_{l=0}^{\infty} |\sigma_{n,2l+2}^{0,0} - \sigma_{n,2l}^{0,0}| \frac{1}{\rho^{2l}} \right) \\
&\quad + \frac{M}{\rho^{n+1}} \frac{n+1}{2n+3} \left(\sigma_{n+1,0}^{0,0} + \frac{1}{\rho^2} \sum_{l=0}^{\infty} |\sigma_{n+1,2l+2}^{0,0} - \sigma_{n+1,2l}^{0,0}| \frac{1}{\rho^{2l}} \right) \\
&\leq \sigma_{n,0}^{0,0} \frac{n+1}{2n+1} \frac{M}{\rho^n} \left(1 + \frac{n+2}{2n+3} \frac{1}{\rho^2 - 1} \right) \\
&\quad + \sigma_{n+1,0}^{0,0} \frac{n+1}{2n+3} \frac{M}{\rho^{n+1}} \left(1 + \frac{n+3}{2n+5} \frac{1}{\rho^2 - 1} \right).
\end{aligned}$$

Working out the expressions of $\sigma_{n,0}^{0,0}$ and $\sigma_{n+1,0}^{0,0}$ by (2.46), we have

$$\begin{aligned}
|\hat{u}_n^{1,0}| &\leq \frac{M}{\rho^n} \frac{\sqrt{\pi} \Gamma(n+2)}{\Gamma(n+3/2)} \left\{ \frac{1}{2} + \frac{n+2}{2(2n+3)} \frac{1}{\rho^2 - 1} \right. \\
&\quad \left. + \frac{1}{\rho} \frac{n+1}{2n+3} \left(1 + \frac{n+3}{2n+5} \frac{1}{\rho^2 - 1} \right) \right\}. \tag{2.75}
\end{aligned}$$

Note that the ratio of the Gamma functions can be bounded as in (2.65).

The same process applies to other $k, l \in \mathbb{N}$, but the derivation seems tedious.

2.4.4 Estimate for truncated Jacobi expansions

Given a cut-off number $N \geq 1$ and $N \in \mathbb{N}$, we define the partial sum

$$(\pi_N^{\alpha,\beta} u)(x) = \sum_{n=0}^{N-1} \hat{u}_n^{\alpha,\beta} P_n^{(\alpha,\beta)}(x), \tag{2.76}$$

where $\{\hat{u}_n^{\alpha,\beta}\}$ are the Jacobi expansion coefficients defined in (2.26). To this end, let $L_{\omega^{\alpha,\beta}}^2(I)$ be the weighted L^2 -space on $I = (-1, 1)$, and its norm is denoted by $\|\cdot\|_{\omega^{\alpha,\beta}}$, where we drop the weight function, if $\alpha = \beta = 0$.

Notice that $\pi_N^{\alpha,\beta} u$ is the $L_{\omega^{\alpha,\beta}}^2$ -projection of u upon $\mathbb{P}_{N-1}$ (denoting the set of all algebraic polynomials of degree at most $N-1$), that is, $\pi_N^{\alpha,\beta} u$ is the best approximation to u in the norm $\|\cdot\|_{\omega^{\alpha,\beta}}$. With the previous bounds for the expansion coefficients, we can estimate the truncation error straightforwardly.

Theorem 2.3. For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, $\alpha, \beta > -1$, $N \geq 1$, and $N + \alpha + \beta > 0$, we have

$$\left\| \pi_N^{\alpha, \beta} u - u \right\|_{\omega^{\alpha, \beta}} \leq \left(\sqrt{\frac{\pi}{2^{\alpha+\beta}}} \left(1 + \frac{|\alpha - \beta|}{\rho} \right) + \frac{2\sqrt{\gamma_0^{\alpha, \beta}}}{\rho(\rho - 1)} \right) \frac{\tilde{C}_N M}{\rho^{N-1} \sqrt{\rho^2 - 1}}, \quad (2.77)$$

where $\gamma_0^{\alpha, \beta}$ is given in (1.2) and

$$\tilde{C}_N = \max \left\{ 1, \widehat{C}_N \sqrt{C_N} \right\},$$

with C_N and $\widehat{C}_N$ being defined in (2.24) and (2.52), respectively.

Proof. By the orthogonality (cf (1.1)-(1.2)) of Jacobi polynomials, we have

$$\left\| \pi_N^{\alpha, \beta} u - u \right\|_{\omega^{\alpha, \beta}}^2 = \sum_{n=N}^{\infty} |\hat{u}_n^{\alpha, \beta}|^2 \gamma_n^{\alpha, \beta}.$$

By (2.23) and (2.2), we have that for $n \geq N \geq 1$ and $N + \alpha + \beta > 0$,

$$\begin{aligned} |\hat{u}_n^{\alpha, \beta}| \sqrt{\gamma_n^{\alpha, \beta}} &\leq \widehat{C}_n M \frac{\sqrt{n}}{\rho^n} \sqrt{C_n \frac{2^{\alpha+\beta}}{n}} \\ &\quad \times \left(\frac{\sqrt{\pi}}{2^{\alpha+\beta}} \left(1 + \frac{|\alpha - \beta|}{\rho} \right) + \sqrt{\frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)} \frac{2\sqrt{2}}{\rho(\rho - 1)}} \right) \\ &= M \widehat{C}_n \sqrt{C_n} \left(\sqrt{\frac{\pi}{2^{\alpha+\beta}}} \left(1 + \frac{|\alpha - \beta|}{\rho} \right) + \sqrt{\frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{\Gamma(\alpha + \beta + 2)} \frac{2\sqrt{2^{\alpha+\beta+1}}}{\rho(\rho - 1)}} \right) \frac{1}{\rho^n}. \end{aligned}$$

Therefore, by (1.2) and Remark 2.2, we have

$$\begin{aligned} \left\| \pi_N^{\alpha, \beta} u - u \right\|_{\omega^{\alpha, \beta}} &\leq \tilde{C}_N M \left(\sqrt{\frac{\pi}{2^{\alpha+\beta}}} \left(1 + \frac{|\alpha - \beta|}{\rho} \right) + \frac{2\sqrt{\gamma_0^{\alpha, \beta}}}{\rho(\rho - 1)} \right) \left(\sum_{n=N}^{\infty} \frac{1}{\rho^{2n}} \right)^{1/2} \\ &= \left(\sqrt{\frac{\pi}{2^{\alpha+\beta}}} \left(1 + \frac{|\alpha - \beta|}{\rho} \right) + \frac{2\sqrt{\gamma_0^{\alpha, \beta}}}{\rho(\rho - 1)} \right) \frac{\tilde{C}_N M}{\rho^{N-1} \sqrt{\rho^2 - 1}}. \end{aligned}$$

This ends the proof. $\square$

Remark 2.6. Note that $\left\{ \frac{d^l}{dx^l} P_n^{(\alpha, \beta)}(x) \right\}_{n \geq l}$ are mutually orthogonal with respect to $\omega^{\alpha+l, \beta+l}$, so we can estimate $\left\| (\pi_N^{\alpha, \beta} u - u)^{(l)} \right\|_{\omega^{\alpha+l, \beta+l}}$ in a similar fashion. $\square$

Remark 2.7. *Some refined estimates can be obtained from the refined bounds for special cases, e.g., $\alpha = \beta$ or $\alpha = \beta = 0, -1/2$. Here, we just state the result for the Legendre case:*

$$\|\pi_N^{0,0}u - u\| \leq \left(1 + \frac{N+2}{2N+3} \frac{1}{\rho^2-1}\right) \frac{\tilde{C}_N M \sqrt{\pi}}{\rho^{N-1} \sqrt{\rho^2-1}}, \quad (2.78)$$

where $\tilde{C}_N = \exp\left(\frac{8N-1}{12N(2N-1)}\right)$. It follows from Theorem 2.2 and the above process. Note that Xiang [120] derived the following estimate for the Legendre expansion:

$$\|\pi_N^{0,0}u - u\| \leq \frac{2\sqrt{2}M}{\rho^{N-2}(\rho-1)^2}. \quad (2.79)$$

The estimate (2.78) is tighter. □

2.5 Extension to Gegenbauer-Gauss quadrature

Recall that the remainder of Gauss-quadrature with the nodes $\{x_j\}_{j=1}^n$ and weights $\{\omega_j\}_{j=1}^n$, takes the form (see, e.g., [37]):

$$E_n[u] = \int_{-1}^1 u(x)\omega(x) dx - \sum_{j=1}^n u(x_j)\omega_j = \frac{1}{\pi i} \oint_{\mathcal{E}_\rho} \frac{q_n(z)}{p_n(z)} u(z) dz, \quad (2.80)$$

where $\{x_j\}_{j=1}^n$ are the zeros of $p_n(x)$, orthogonal with respect to the weight function $\omega(x)$, and

$$q_n(z) = \frac{1}{2} \int_{-1}^1 \frac{p_n(x)\omega(x)}{z-x} dx. \quad (2.81)$$

The Gegenbauer-Gauss quadrature remainder (2.80)-(2.81) with the nodes being zeros of the Gegenbauer polynomial $P_n^{(\alpha,\alpha)}(x)$, takes the form

$$E_n^{GG}[u] = \frac{\gamma_n^{\alpha,\alpha}}{\pi i} \oint_{\mathcal{E}_\rho} \frac{Q_n^{(\alpha,\alpha)}(z)}{P_n^{(\alpha,\alpha)}(z)} u(z) dz, \quad \forall u \in \mathcal{A}_\rho, \quad (2.82)$$

where $Q_n^{(\alpha,\alpha)}(z)$ is defined as in (2.30). By (2.35) and (2.36), we have

$$Q_n^{(\alpha,\alpha)}(z) = \frac{1}{2\gamma_n^{\alpha,\alpha}} \int_{-1}^1 \frac{P_n^{(\alpha,\alpha)}(x)\omega^{\alpha,\alpha}(x)}{z-x} dx = \sum_{j=0}^{\infty} \frac{\sigma_{n,j}^{\alpha,\alpha}}{w^{n+j+1}} = \sum_{l=0}^{\infty} \frac{\sigma_{n,2l}^{\alpha,\alpha}}{w^{n+2l+1}}. \quad (2.83)$$

Remark 2.8. We point out that (2.82)-(2.83) are also valid for general Jacobi-Gauss quadrature. However, the error estimates heavily rely on the explicit formula of $P_n^{(\alpha,\beta)}(z)$ with $z \in \mathcal{E}_\rho$, which is only available for $\alpha = \beta$ (see Lemma 2.4 below). Hence, we merely consider the Gegenbauer-Gauss case. $\square$

The analysis of quadrature errors (even for the Chebyshev case) has attracted much attention (see, e.g., [24, 23, 10, 45, 37, 44, 68, 69]). Just to mention that Chawla and Jain [24, Theorem 5] obtained the estimate:

$$|E_n^{CG}[u]| \leq \frac{2\pi M}{\rho^{2n} - 1}, \quad \forall u \in \mathcal{A}_\rho, \quad \forall n \geq 1. \quad (2.84)$$

Hunter [68] derived the general bound

$$|E_n^{GG}[u]| \leq \frac{4 \int_{-1}^1 (1-x^2)^\alpha dx}{\rho^{2n-2}(\rho^2 - 1)}, \quad n \geq 1, \quad (2.85)$$

and some refined results for $\alpha = \pm 1/2$ and $\beta = \pm 1/2$ by expanding $Q_n^{(\alpha,\alpha)}/P_n^{(\alpha,\alpha)}$ into the Laurent series of w in the disk enclosed by $\mathcal{C}_\rho$ (defined in (2.2)) and manipulating the series. It is worthwhile to note that Gautschi and Varga [45] estimated the Jacobi-Gauss quadrature (with $P_n^{(\alpha,\beta)}$ and $Q_n^{(\alpha,\beta)}$ in place of $P_n^{(\alpha,\alpha)}$ and $Q_n^{(\alpha,\alpha)}$ in (2.82), respectively) by

$$|E_n^{JG}[u]| \leq \pi^{-1} \gamma_n^{\alpha,\beta} M L(\mathcal{E}_\rho) \max_{z \in \mathcal{E}_\rho} |Q_n^{(\alpha,\beta)}(z)/P_n^{(\alpha,\beta)}(z)|, \quad (2.86)$$

and attempted to find the exact maximum value on the Bernstein ellipse, which was feasible for $\alpha = \pm 1/2$ and $\beta = \pm 1/2$ again. Some conjectures and empirical results were explored in [45] for the general Jacobi case.

Using the explicit expression of Legendre polynomials on the Bernstein ellipse (see, e.g., [36, Lemma 12.4.1]), Kambo [74] obtained the bound for the Legendre-Gauss quadrature:

$$|E_n^{LG}[u]| \leq \pi^{-1} \gamma_n^{0,0} M L(\mathcal{E}_\rho) \frac{\max_{z \in \mathcal{E}_\rho} |Q_n^{(0,0)}(z)|}{\min_{z \in \mathcal{E}_\rho} |P_n(z)|} \leq \frac{d_n M}{\rho^{2n}} \frac{\rho^2 + 1}{\rho^2 - 2}, \quad \rho > \sqrt{2}, \quad (2.87)$$

where $0 < d_n \leq \pi$. While this bound is only valid for $\rho > \sqrt{2}$, it holds for all n , when compared with the asymptotic estimate (with $n \gg 1$) for the Legendre-Gauss quadrature in [22].

In what follows, we aim to extend our analysis to estimate $E_n^{GG}[u]$ in (2.82). The essential tools include the explicit formula for the Gegenbauer polynomial $P_n^{(\alpha, \alpha)}(z)$ on $\mathcal{E}_\rho$ derived in Lemma 2.4 (also see [121]), and the previous argument for estimating $Q_n^{(\alpha, \alpha)}(z)$.

Lemma 2.4. *Let $z = \frac{1}{2}(w + w^{-1}) \in \mathcal{E}_\rho$ and $w \in \mathcal{C}_\rho$. Then we have*

$$P_n^{(\alpha, \alpha)}(z) = A_n^\alpha \sum_{k=0}^n g_k^\alpha g_{n-k}^\alpha w^{n-2k}, \quad n \geq 0, \quad \alpha > -1, \quad \alpha \neq -1/2, \quad (2.88)$$

where

$$\begin{aligned} g_0^\alpha &= 1, \quad g_k^\alpha = \frac{\Gamma(k + \alpha + 1/2)}{k! \Gamma(\alpha + 1/2)}, \quad 1 \leq k \leq n, \\ \text{and} \quad A_n^\alpha &= \frac{\Gamma(2\alpha + 1) \Gamma(n + \alpha + 1)}{\Gamma(\alpha + 1) \Gamma(n + 2\alpha + 1)}. \end{aligned} \quad (2.89)$$

Proof. We carry out the proof by induction. Apparently, by (2.8), $P_0^{(\alpha, \alpha)}(z) = 1$, so (2.88)-(2.89) hold for $n = 0$. Similarly, we can verify the case with $n = 1$.

Assume that the formula holds for $P_{n-2}^{(\alpha, \alpha)}(z)$ and $P_{n-1}^{(\alpha, \alpha)}(z)$ with $n \geq 2$. It follows from the three-term recurrence relation (2.8) and (2.88)-(2.89) that

$$\begin{aligned} P_n^{(\alpha, \alpha)}(z) &= \frac{n + \alpha}{n(n + 2\alpha)} \left[(2n + 2\alpha - 1) z P_{n-1}^{(\alpha, \alpha)}(z) - (n + \alpha - 1) P_{n-2}^{(\alpha, \alpha)}(z) \right] \\ &= \frac{n + \alpha}{n(n + 2\alpha)} \left[(n + \alpha - 1/2) A_{n-1}^\alpha \sum_{k=0}^{n-1} g_k^\alpha g_{n-1-k}^\alpha (w^{n-2k} + w^{n-2k-2}) \right. \\ &\quad \left. - (n + \alpha - 1) A_{n-2}^\alpha \sum_{k=0}^{n-2} g_k^\alpha g_{n-2-k}^\alpha w^{n-2k-2} \right] \\ &= \frac{\Gamma(2\alpha + 1) \Gamma(n + \alpha + 1)}{n \Gamma(\alpha + 1) \Gamma(n + 2\alpha + 1)} \left[(n + \alpha - 1/2) \sum_{k=0}^{n-1} g_k^\alpha g_{n-1-k}^\alpha w^{n-2k} \right. \\ &\quad \left. + (n + \alpha - 1/2) \sum_{k=0}^{n-1} g_k^\alpha g_{n-1-k}^\alpha w^{n-2k-2} \right. \\ &\quad \left. - (n + 2\alpha - 1) \sum_{k=0}^{n-2} g_k^\alpha g_{n-2-k}^\alpha w^{n-2k-2} \right] \\ &= \frac{A_n^\alpha}{n} \left[(n + \alpha - 1/2) g_{n-1}^\alpha (w^n + w^{-n}) + \sum_{k=1}^{n-1} D_{n,k}^\alpha g_k^\alpha g_{n-k}^\alpha w^{n-2k} \right], \end{aligned}$$

where

$$D_{n,k}^\alpha = (n + \alpha - 1/2) \left(\frac{g_{n-k-1}^\alpha}{g_{n-k}^\alpha} + \frac{g_{k-1}^\alpha}{g_k^\alpha} \right) - (n + 2\alpha - 1) \frac{g_{n-k-1}^\alpha}{g_{n-k}^\alpha} \frac{g_{k-1}^\alpha}{g_k^\alpha}.$$

One verifies from (2.89) that

$$g_n^\alpha = \frac{n + \alpha - 1/2}{n} g_{n-1}^\alpha, \quad D_{n,k}^\alpha = n. \quad (2.90)$$

This completes the induction. $\square$

Remark 2.9. *This formula excludes the Chebyshev case. For $\alpha = -1/2$, we define*

$$g_0^{-1/2} = g_n^{-1/2} = 1, \quad g_k^{-1/2} = 0, \quad 1 \leq k \leq n-1, \quad \text{and} \quad A_n^{-1/2} = \frac{\Gamma(n+1/2)}{2\sqrt{\pi}n!}, \quad (2.91)$$

since (see, e.g., [36])

$$T_n(z) = \frac{1}{2}(w^n + w^{-n}) = \frac{1}{2A_n^{-1/2}} P_n^{(-1/2, -1/2)}(z). \quad (2.92)$$

Hence, we understand that (2.88) holds for $\alpha = -1/2$ with the constants given by (2.91). $\square$

We expand $Q_n^{(\alpha, \alpha)} / P_n^{(\alpha, \alpha)}$ in Laurent series of $w \in \mathcal{C}_\rho$, and then we use an argument as for Lemma 2.3 to obtain the tight error bound. However, this situation is reminiscent of that in Gautschi and Varga [45], that is, computable bounds can be derived for general α . We highlight that the computational part (see (2.93)) is independent of ρ and u .

The main estimate is stated as follows.

Theorem 2.4. *For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, we have that for $\alpha > -1$ and $n \geq 1$,*

$$\left| E_n^{GG}[u] \right| \leq \gamma_n^{\alpha, \alpha} \left[\left| \mu_{n,0}^{\alpha, \alpha} \right| + \max_{l \geq 0} \left| \mu_{n,2l+2}^{\alpha, \alpha} - \mu_{n,2l}^{\alpha, \alpha} \right| \frac{1}{\rho^2 - 1} \right] \frac{M}{\rho^{2n}}, \quad (2.93)$$

where $\{\mu_{n,2l}^{\alpha, \alpha}\}_{l \geq 0}$ are computed by the recursive formula:

$$\mu_{n,2l}^{\alpha, \alpha} = \frac{1}{g_n^\alpha} \left(\frac{\sigma_{n,2l}^{\alpha, \alpha}}{A_n^\alpha} - \sum_{k=1}^{\min\{n, l\}} g_k^\alpha g_{n-k}^\alpha \mu_{n,2l-2k}^{\alpha, \alpha} \right), \quad l \geq 1, \quad \mu_{n,0}^{\alpha, \alpha} = \frac{\sigma_{n,0}^{\alpha, \alpha}}{A_n^\alpha g_n^\alpha}. \quad (2.94)$$

Proof. A straightforward calculation from (2.83) (note that $\sigma_{n,2l+1}^{\alpha,\alpha} = 0$ for all $l \geq 0$) and (2.88) leads to

$$\frac{Q_n^{(\alpha,\alpha)}(z)}{P_n^{(\alpha,\alpha)}(z)} = \sum_{l=0}^{\infty} \frac{\mu_{n,2l}^{\alpha,\alpha}}{w^{2n+2l+1}} \quad \text{with} \quad \sigma_{n,2l}^{\alpha,\alpha} = A_n^\alpha \sum_{k=0}^{\min\{n,l\}} g_k^\alpha g_{n-k}^\alpha \mu_{n,2l-2k}^{\alpha,\alpha}, \quad (2.95)$$

so solving out $\mu_{n,2l}^{\alpha,\alpha}$ yields (2.94).

Next, following the same lines as the derivation of (2.43), we infer from (2.82) and (2.95),

$$\begin{aligned} |E_n^{GG}[u]| &\leq \gamma_n^{\alpha,\alpha} \frac{M}{2\pi} \left| \sum_{l=0}^{\infty} \mu_{n,2l}^{\alpha,\alpha} \oint_{\mathcal{C}_\rho} \frac{1}{w^{2n+2l+1}} \left(1 - \frac{1}{w^2}\right) dw \right| \\ &\leq \gamma_n^{\alpha,\alpha} \frac{M}{2\pi} \left[\frac{2\pi\rho}{\rho^{2n+1}} |\mu_{n,0}^{\alpha,\alpha}| + \frac{2\pi\rho}{\rho^{2n+3}} \sum_{l=0}^{\infty} |\mu_{n,2l+2}^{\alpha,\alpha} - \mu_{n,2l}^{\alpha,\alpha}| \frac{1}{\rho^{2l}} \right] \\ &\leq \gamma_n^{\alpha,\alpha} \frac{M}{\rho^{2n}} \left[|\mu_{n,0}^{\alpha,\alpha}| + \max_{l \geq 0} |\mu_{n,2l+2}^{\alpha,\alpha} - \mu_{n,2l}^{\alpha,\alpha}| \sum_{l=0}^{\infty} \frac{1}{\rho^{2l+2}} \right] \\ &= \gamma_n^{\alpha,\alpha} \frac{M}{\rho^{2n}} \left[|\mu_{n,0}^{\alpha,\alpha}| + \max_{l \geq 0} |\mu_{n,2l+2}^{\alpha,\alpha} - \mu_{n,2l}^{\alpha,\alpha}| \frac{1}{\rho^2 - 1} \right]. \end{aligned} \quad (2.96)$$

This completes the proof. $\square$

Remark 2.10. We find from (2.94) that for $\alpha = -1/2$,

$$\mu_{n,0}^{-1/2,-1/2} = \frac{2\pi}{\gamma_n^{-1/2,-1/2}}, \quad \left| \mu_{n,2l+2}^{-1/2,-1/2} - \mu_{n,2l}^{-1/2,-1/2} \right| = \frac{2\pi\delta_{\kappa,0}}{\gamma_n^{-1/2,-1/2}},$$

where $\kappa := \text{mod}(l+1, n)$ and $\delta_{\kappa,0}$ is the Kronecker delta. Hence, it follows from (2.96) that

$$|E_n^{CG}[u]| \leq \frac{2\pi M}{\rho^{2n}} \left[1 + \frac{1}{\rho^2} \sum_{j=1}^{\infty} \frac{1}{\rho^{2(jn-1)}} \right] = \frac{2\pi M}{\rho^{2n} - 1}, \quad n \geq 1, \quad (2.97)$$

which is the same as (2.84) derived in [24]. $\square$

Remark 2.11. We find from (2.94) that for $\alpha = 1/2$,

$$\mu_{n,2l}^{1/2,1/2} = \begin{cases} (-1)^\kappa \frac{\pi}{2} \frac{1}{\gamma_n^{1/2,1/2}}, & \text{if } \kappa := \text{mod}(l, n+1) = 0, 1, \\ 0, & \text{otherwise,} \end{cases} \quad (2.98)$$

which implies

$$\begin{aligned}
& \sum_{l=0}^{\infty} \left| \mu_{n,2l+2}^{1/2,1/2} - \mu_{n,2l}^{1/2,1/2} \right| \frac{1}{\rho^{2l}} = \left| \mu_{n,2}^{1/2,1/2} - \mu_{n,0}^{1/2,1/2} \right| + \sum_{j=1}^{\infty} \left| \mu_{n,2j(n+1)}^{1/2,1/2} \right| \frac{1}{\rho^{2j(n+1)-2}} \\
& + \sum_{j=1}^{\infty} \left(\left| \mu_{n,2j(n+1)+2}^{1/2,1/2} - \mu_{n,2j(n+1)}^{1/2,1/2} \right| \frac{1}{\rho^{2j(n+1)}} + \left| \mu_{n,2j(n+1)+2}^{1/2,1/2} \right| \frac{1}{\rho^{2j(n+1)+2}} \right) \\
& = \frac{\pi}{2} \frac{1}{\gamma_n^{1/2,1/2}} \left(2 + (\rho + \rho^{-1})^2 \sum_{j=1}^{\infty} \frac{1}{\rho^{2j(n+1)}} \right) \\
& = \frac{\pi}{2} \frac{1}{\gamma_n^{1/2,1/2}} \left(2 + \frac{(\rho + \rho^{-1})^2}{\rho^{2n+2} - 1} \right).
\end{aligned}$$

Hence, it follows from (2.96) that for the Chebyshev-Gauss quadrature of the second kind,

$$|E_n^{GG}[u]| \leq \frac{\pi M}{2\rho^{2n}} \left(1 + \frac{1}{\rho^2} \left(2 + \frac{(\rho + \rho^{-1})^2}{\rho^{2n+2} - 1} \right) \right) = \frac{\pi M(\rho^2 + 2 + \rho^{-2n-4})}{2(\rho^{2n+2} - 1)}. \quad (2.99)$$

Note that by a delicate technique, Hunter [68, Eq. (4.8)] obtained the following estimate:

$$|E_n^{GG}[u]| \leq \frac{\pi M(\rho^2 + 2 + \rho^{-2})}{2(\rho^{2n+2} - 1)}. \quad (2.100)$$

We see that (2.99) is sharper. $\square$

For general $\alpha > -1$, the derivation of an explicit bound for

$$\Theta_n^\alpha := \max_{l \geq 0} \theta_{n,l}^\alpha, \quad \theta_{n,l}^\alpha := \gamma_n^{\alpha,\alpha} \left| \mu_{n,2l+2}^{\alpha,\alpha} - \mu_{n,2l}^{\alpha,\alpha} \right|, \quad n \geq 1, \quad (2.101)$$

seems nontrivial. We have only empirical results bases on computation. Some indications are listed as follows.

- (i) Observe from (2.98) that for fixed n , $\{\theta_{n,l}^{1/2}\}_{l \geq 0}$ are $(n+1)$ -periodic (see Figure 2.2 (a)), and the maximum is attained at $l = j(n+1), j = 0, 1, \dots$. We compute ample samples of n, l and α , and find very similar “periodic” behaviors (see Figure 2.2 (b)-(c) for $\alpha = 0, 1$).
- (ii) Another interesting empirical observation is that for fixed α , the maximum value Θ_n^α converges to a constant value, and it decreases as α increases (see Figure 2.2 (d)). Note that for the Legendre case, $\Theta_n^0 \approx 4$.

Figure 2.2: (a)-(c): Profiles of $\theta_{n,l}^\alpha$ with $n = 36, \alpha = 1/2, 0, 1$ and $0 \leq l \leq 250$. We mark by “ $\square$ ” the location of the maximum value Θ_n^α is attached. (d): The maximum value Θ_n^α with $\alpha = 0, 3/2, 5, 10$ and $10 \leq n \leq 100$, where we compute $\{\theta_{n,l}^\alpha\}$ for l up to 1000.

2.6 Numerical results

In this section, we present various numerical results to show the tightness of the bounds derived in this chapter, and to compare them to other existing ones mentioned in the previous part.

In the first example, we purposely choose the Chebyshev and Legendre expansions with known expansion coefficients:

$$u_1(x) = \frac{3}{5-4x} = T_0(x) + \sum_{n=1}^{\infty} \frac{T_n(x)}{2^{n-1}}, \quad u_2(x) = \frac{2}{\sqrt{5-4x}} = \sum_{n=0}^{\infty} \frac{P_n(x)}{2^n}, \quad (2.102)$$

which follow from generating functions of Chebyshev and Legendre polynomials (cf. [108]).

Note that the function u_1 has a simple pole at $z = 5/4$, so the semi-major axis (cf. (2.4)) should satisfy

$$1 < a = (\rho + \rho^{-1})/2 < 5/4 \implies 1 < \rho < 2.$$

One also verifies that

$$M = \max_{z \in \mathcal{E}_\rho} |u_1(z)| = \frac{3\rho}{(2\rho - 1)(2 - \rho)}.$$

Then the estimate (2.57) reduces to

$$\hat{u}_n^C = \frac{1}{2^{n-1}} \leq \frac{6}{(2\rho - 1)(2 - \rho)\rho^{n-1}} := B_n^C(\rho), \quad 1 < \rho < 2, \quad n \geq 1.$$

Similarly, for the Legendre expansion of u_2 , the result (2.67) becomes

$$\begin{aligned} \hat{u}_n^{0,0} &= \frac{1}{2^n} \leq \frac{\sqrt{\pi n}}{\rho^n} \left(1 + \frac{n+2}{2n+3} \frac{1}{\rho^2 - 1} \right) \exp\left(\frac{8n-1}{12n(2n-1)}\right) \sqrt{\frac{4\rho}{(2\rho-1)(2-\rho)}} \\ &:= B_n^L(\rho), \quad 1 < \rho < 2, \quad n \geq 1. \end{aligned}$$

We take $\rho = 1.98$, and plot the exact coefficients $\hat{u}_n^C$ and $\hat{u}_n^{0,0}$, and the bounds B_n^C and B_n^L in Figure 2.3 (a) and (b), respectively. Actually, the bound for the Chebyshev case (see (2.57)) can be considered as one benchmark for illustrating tightness of the upper bound. Indeed, the result for the Legendre case stated in Theorem 2.2 seems as sharp as that for the Chebyshev case.

Next, we compare the bounds for the Legendre expansion coefficients in Theorem 2.2 and (2.73) (obtained by [120]). For clarity, we drop the common part $M\sqrt{n}/\rho^n$, and denote the remaining factors in the upper bounds (2.67) and (2.73) by

$$b_n(\rho) = \sqrt{\pi} \left(1 + \frac{n+2}{2n+3} \frac{1}{\rho^2 - 1} \right) \exp\left(\frac{8n-1}{12n(2n-1)}\right), \quad \tilde{b}(\rho) = 2 \left(1 + \frac{1}{\rho^2 - 1} \right).$$

(a) Chebyshev case

(b) Legendre case

Figure 2.3: Expansion coefficients of u_1, u_2 in (2.102) against their error bounds. (a) $e_n(\rho)$ (b) $e_n(\rho)$ with ρ near 1Figure 2.4: (a): Comparison of error bounds for Legendre expansions in (2.67) and (2.73). (b): Samples of $e_n(\rho)$ for ρ close to 1.

In Figure 2.4 (a), we plot the difference $e_n(\rho) := \tilde{b}(\rho) - b_n(\rho)$ for various ρ and $1 \leq n \leq 80$. We see that $e_n(\rho) > 0$ and the difference is of magnitude around 6, when ρ is close to 1. Moreover, for fixed ρ , the difference is roughly a constant for slightly large n . In Figure 2.4 (b), we plot some sample $e_n(\rho)$ for ρ close to 1, we see that our bound is much sharper.

We next make a similar comparison of bounds for Jacobi and Gegenbauer

(a) $\alpha = 1, \beta = 0$ (b) $\alpha = \beta = 2$

Figure 2.5: (a): Comparison of error bounds for Jacobi expansion with $\alpha = 1, \beta = 0$ in (1.5) and (2.75). (b): Comparison of error bounds for Gegenbauer expansion with $\alpha = \beta = 2$ in (1.5) and (2.47).

(a) $\alpha = 1/2$ (b) $\alpha = 2$

Figure 2.6: (a): Comparison of error bounds for the Gegenbauer-Gauss quadrature with $\alpha = 1/2$ in (2.99) and (2.100). (b): Comparison of error bounds for the Gegenbauer-Gauss quadrature with $\alpha = 2$ in (2.85) and (2.93).

expansions. For example, for $\alpha = 1$ and $\beta = 0$, we extract the factors in (1.5) and (2.75) by dropping $M\sqrt{n}/\rho^n$. We plot in Figure 2.5 (a) the difference of two remaining parts (i.e., that of (1.5) subtracts that of (2.75)). Once again, our bound is much tighter. Likewise, we depict in Figure 2.5 (b) the extracted bounds

from (1.5) and (2.47) with $\alpha = \beta = 2$. The situation is akin to the Legendre case, where the bounds obtained in this chapter are sharper.

Finally, we turn to the comparison of error bounds for the Gegenbauer-Gauss quadrature remainder. For $\alpha = 1/2$, we extract the factors in (2.99) and (2.100) by dropping M/ρ^{2n} as before. We plot in Figure 2.6 (a) the difference of two remaining parts in (2.100) and in (2.99)). Once again, our bound is much tighter. Likewise, we depict in Figure 2.6 (b) the extracted bounds from (2.85) and (2.93) with $\alpha = 2$, and observe similar behaviors.

Superconvergence of Spectral Interpolation[†]

As addressed in Subsection 1.1.3, we aim to extend the study of superconvergence properties of Chebyshev-Gauss-type spectral interpolation in [125] to general Jacobi-Gauss-type interpolation, and to discuss the implication of this study to functions with limited regularity. Following the same principle as in [125], we are able to locate the superconvergence points for Jacobi-Gauss-type interpolation (see Subsection 3.1.2). For the indication of superconvergence points (identified from interpolating analytic functions) to functions which are not analytic, we examine it from two perspectives, and illustrate that the leading term of the interpolation error of functions with finite regularity vanishes at superconvergence points, but there is no gain in order of convergence, as opposite to the analytic case. Nevertheless, the numerical error is significantly smaller at those superconvergence points (see Section 3.2). We will conduct the superconvergence analysis in Chapter 4, as this can be analyzed in the same manner as for exponential convergence of spectral interpolation.

[†]The main part of this chapter is based on the paper [116]: “L.L. Wang, X.D. Zhao and Z. Zhang. Superconvergence of Jacobi-Gauss-type spectral interpolation. *J. Sci. Comput.*, DOI: 10.1007/s10915-013-9777-x, 2013.”

This chapter is organized as follow. We identify in Section 3.1 superconvergence points from interpolating analytic functions, and in Section 3.2, we address the implication to functions with limited regularity. We provide some numerical results in the last section to show the superconvergence phenomenon, although the theoretical estimates are given in Chapter 4.

3.1 Superconvergence points

In this section, we identify superconvergence points for derivatives of general Jacobi-Gauss-type interpolants under analytic assumption.

3.1.1 Jacobi-Gauss-type points and Hermite's contour integral

Let $\{x_j\}_{j=0}^N$ be a set of generic distinct interpolation points on $[-1, 1]$, and let $I_N : C([-1, 1]) \rightarrow \mathbb{P}_N$ be the Lagrange interpolation operator such that $\{(I_N u)(x_j) = u(x_j)\}_{j=0}^N$ for any $u \in C([-1, 1])$, where $\mathbb{P}_N$ is the set of all real polynomials of degree at most N .

Let $P_N^{(\alpha, \beta)}(x)$ be the Jacobi polynomial of degree N (cf. (1.1)-(1.2)), and some relevant properties of Jacobi polynomials are given in Subsection 2.2.1. Recall that Jacobi-Gauss-type interpolation is on one of the following sets of points:

- The Jacobi-Gauss (JG) points $\{x_j = \xi_{G,j}^{\alpha, \beta}\}_{j=0}^N$ are zeros of the Jacobi polynomial $P_{N+1}^{(\alpha, \beta)}(x)$.
- The (left) Jacobi-Gauss-Radau (JGR) points $\{x_j = \xi_{R,j}^{\alpha, \beta}\}_{j=0}^N$ (with fixed left endpoint $x_0 = -1$) are zeros of $(1+x)P_N^{(\alpha, \beta+1)}(x)$. With a change of variable $x \rightarrow -x$, JGR interpolation with fixed right endpoint $x_N = 1$, can be obtained.
- The Jacobi-Gauss-Lobatto (JGL) points $\{x_j = \xi_{L,j}^{\alpha, \beta}\}_{j=0}^N$ (with $x_0 = -1, x_N = 1$) are zeros of $(1-x^2)\partial_x P_N^{(\alpha, \beta)}(x)$.

It is known from the seminal work of Bernstein [15] that any analytic function $u(x)$ on $[-1, 1]$ can be continued analytically to an elliptic domain enclosed by the so-called *Bernstein ellipse* $\mathcal{E}_\rho$, with foci ± 1 and ρ being the sum of semi-axes (see Section 2.1 in Chapter 2 for some properties of the Bernstein ellipse).

We now introduce the major analysis tool – *Hermite's contour integral* (see, e.g., [36, Eqs. (3.6.5)-(3.6.6)]), that is, for any $u \in \mathcal{A}_\rho$ (cf. (2.7)),

$$(I_N u)(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \frac{Q_{N+1}(z) - Q_{N+1}(x)}{z - x} \frac{u(z)}{Q_{N+1}(z)} dz, \quad \forall x \in [-1, 1], \quad (3.1)$$

and

$$(u - I_N u)(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \frac{Q_{N+1}(x)}{z - x} \frac{u(z)}{Q_{N+1}(z)} dz, \quad \forall x \in [-1, 1]. \quad (3.2)$$

In particular, for Jacobi-Gauss-type interpolation, we have

$$Q_{N+1}(x) = c_N \left\{ P_{N+1}^{(\alpha, \beta)}(x), (1+x)P_N^{(\alpha, \beta+1)}(x) \text{ or } (1-x^2)\partial_x P_N^{(\alpha, \beta)}(x) \right\}, \quad (3.3)$$

where c_N is any nonzero factor.

Thus, by (3.2),

$$(u - I_N u)'(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \left(\frac{Q'_{N+1}(x)}{z - x} + \frac{Q_{N+1}(x)}{(z - x)^2} \right) \frac{u(z)}{Q_{N+1}(z)} dz, \quad (3.4)$$

and

$$(u - I_N u)''(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \left(\frac{Q''_{N+1}(x)}{z - x} + \frac{2Q'_{N+1}(x)}{(z - x)^2} + \frac{2Q_{N+1}(x)}{(z - x)^3} \right) \frac{u(z)}{Q_{N+1}(z)} dz. \quad (3.5)$$

Likewise, we can compute higher order derivatives by direct differentiation.

3.1.2 Superconvergence points for derivatives

As observed in [125] for the Chebyshev case, a differentiation of Q_{N+1} magnifies a factor of N or N^2 , so the highest derivative of Q_{N+1} dominates the error, and superconvergence can be attained at zeros of the highest derivative of $Q_{N+1}(x)$. Following the same principle, we have the following claim.

Proposition 3.1. *If we interpolate a function $u \in \mathcal{A}_\rho$ at the zeros of $Q_{N+1}(x)$ (e.g., (3.3)), then the superconvergence points for the first (resp. second) derivative are the zeros of $Q'_{N+1}(x)$ (resp. $Q''_{N+1}(x)$), and likewise for higher order derivatives.*

Remark 3.1. *Extreme points of $Q_{N+1}(x)$ are superconvergence points of the first derivative.* $\square$

Applying the above rule, we can locate superconvergence points for Jacobi-Gauss-type interpolation as follows.

Proposition 3.2 (Jacobi-Gauss interpolation). *For Jacobi-Gauss interpolation at zeros of $Q_{N+1}(x) = P_{N+1}^{(\alpha, \beta)}(x)$, the first derivative superconverges at N interior Jacobi-Gauss-Lobatto points, i.e., zeros of $\partial_x P_{N+1}^{(\alpha, \beta)}(x)$; the second derivative superconverges at $N - 1$ Jacobi-Gauss points with the parameter $(\alpha + 2, \beta + 2)$, i.e., zeros of $P_{N-1}^{(\alpha+2, \beta+2)}(x) (= \zeta_N^{\alpha, \beta} \partial_x^2 P_{N+1}^{(\alpha, \beta)}(x)$ by (2.13)).*

Proposition 3.3 ((left) Jacobi-Gauss-Radau interpolation). *For (left) Jacobi-Gauss-Radau interpolation at zeros of $(1+x)P_N^{(\alpha, \beta+1)}(x)$, the first derivative superconverges at zeros of*

$$Q'_{N+1}(x) = \partial_x P_{N+1}^{(\alpha, \beta)}(x) + \frac{N + \beta + 1}{N + 1} \partial_x P_N^{(\alpha, \beta)}(x); \quad (3.6)$$

the second derivative superconverges at zeros of $Q''_{N+1}(x)$.

Remark 3.2. *Note that the identity (3.6) (up to a constant multiple) follows from (2.15).* $\square$

Proposition 3.4 (Jacobi-Gauss-Lobatto interpolation). *For Jacobi-Gauss-Lobatto interpolation at zeros of $(1-x^2)\partial_x P_N^{(\alpha, \beta)}(x)$, the first derivative superconverges at zeros of*

$$\begin{aligned} Q'_{N+1}(x) = & \partial_x P_{N+1}^{(\alpha, \beta)}(x) + (\beta - \alpha) \frac{2N + \alpha + \beta + 1}{(N + 1)(2N + \alpha + \beta)} \partial_x P_N^{(\alpha, \beta)}(x) \\ & - \frac{(N + \alpha)(N + \beta)(2N + \alpha + \beta + 2)}{N(N + 1)(2N + \alpha + \beta)} \partial_x P_{N-1}^{(\alpha, \beta)}(x); \end{aligned} \quad (3.7)$$

the second derivative superconverges at zeros of $Q''_{N+1}(x)$.

Remark 3.3. For Legendre-Gauss-Lobatto (LGL) case, (3.7) reduces to

$$Q'_{N+1}(x) = P'_{N+1}(x) - P'_{N-1}(x) = (2N+1)P_N(x),$$

where the last identity can be found in e.g., [108]. Therefore, superconvergence points of first derivative for LGL interpolation are Legendre-Gauss points (involving only N points); while superconvergence points for second derivative are $N-1$ interior LGL points. In fact, only the Legendre case enjoys this property. $\square$

3.1.3 Computation of superconvergence points

It is known that Jacobi-Gauss-type points $\{x_j\}$ can be computed by the eigenmethod (see, e.g., [43, 102]). It is known that between every two consecutive zeros of $Q_{N+1}(x)$, there exists exactly one extreme point of $Q_{N+1}(x)$, so we can set $\{y_j^0 = (x_{j-1} + x_j)/2\}_{j=1}^N$ as initial guesses, and then use the Newton's iterative method to locate the superconvergence points $\{y_j\}_{j=1}^N$ for first derivative. Similarly, we can compute those for second derivative by using $\{(y_{j-1} + y_j)/2\}$ as initial guesses. In Figure 3.1, we plot zeros of $Q'_{N+1}(x)$ with $Q_{N+1}(x) = (1-x^2)\partial_x P_N^{(\alpha,\beta)}(x)$ for some α, β and N .

Figure 3.1: Zeros (marked by “*”) and extreme points (marked by “o”) of $Q_{N+1}(x)$.

3.2 Implication to general non-analytic function-

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We reiterate that the superconvergence points are at which *the leading term of the error remainder vanishes* (see (3.4)-(3.5) and Propositions 3.2-3.4). It is also based on this principal that Zhang [125] locates the superconvergence points for the function values, when one interpolates the first derivative values.

A natural question to ask is *what would be the indication of superconvergence points (identified from interpolating analytic functions) to functions which are not analytic?* We will examine this from two perspectives, and illustrate that *the leading term of the interpolation error of functions with finite regularity vanishes at superconvergence points, but there is no gain in order of convergence, as opposite to the analytic case.*

The first perspective is from the remainder of the interpolation error for $u \in C^{k+1}[-1, 1]$ with finite integer k (see [93]):

$$R_N(x) = (u - I_N u)(x) = \frac{(-1)^k}{k!} \sum_{j=0}^N h_j(x) \int_{x_j}^x (t - x_j)^k u^{(k+1)}(t) dt, \quad (3.8)$$

where $\{h_j\}$ are the Lagrange basis polynomials given by

$$h_j(x) = \frac{Q_{N+1}(x)}{(x - x_j)Q'_{N+1}(x_j)}, \quad 0 \leq j \leq N.$$

A direct calculation leads to

$$R'_N(x) := \frac{(-1)^k}{k!} (R_1(x) + R_2(x)),$$

where

$$\begin{aligned} R_1(x) &= \sum_{j=0}^N \frac{Q'_{N+1}(x)}{(x - x_j)Q'_{N+1}(x_j)} \int_{x_j}^x (t - x_j)^k u^{(k+1)}(t) dt; \\ R_2(x) &= \sum_{j=0}^N \frac{Q_{N+1}(x)(x - x_j)^{k-1}}{Q'_{N+1}(x_j)} u^{(k+1)}(x) \\ &\quad - \sum_{j=0}^N \frac{Q_{N+1}(x)}{(x - x_j)^2 Q'_{N+1}(x_j)} \int_{x_j}^x (t - x_j)^k u^{(k+1)}(t) dt. \end{aligned}$$

Observe that at interpolation points $\{x_i\}_{i=0}^N$, we have $R'_N(x_i) = (-1)^k R_1(x_i)/k!$, while at superconvergence points $\{y_i\}_{i=1}^N$, we have $R'_N(y_i) = (-1)^k R_2(y_i)/k!$. In fact, $R_1(x)$ dominates the error. For example, we consider the function:

$$u(x) = x^a \exp\left(\frac{1}{2} \sin(x/3)\right), \quad x \in (-1, 1), \quad (3.9)$$

where $a > 1$ is a non-integer number with integer part $[a]$. It is clear that $u \in C^{[a]}[-1, 1]$, but $u \notin C^{[a]+1}[-1, 1]$. Denote

$$\begin{aligned} e_N &= \max_{|x| \leq 1} |R_N(x)|, \quad E_N = \max_{|x| \leq 1} |R'_N(x)|, \\ E_N^x &= \max_{0 \leq j \leq N} |R'_N(x_j)|, \quad E_N^y = \max_{1 \leq i \leq N} |R'_N(y_i)|. \end{aligned} \quad (3.10)$$

We compute e_N and E_N by a dense sampling of uniform points on $[-1, 1]$, and evaluate the derivatives and integrals in $R_1(x)$ and $R_2(x)$ exactly.

Figure 3.2: Errors for $a = 7/2$ (left) and $a = 11/2$ (right) with $\alpha = \beta = 0$.

In Figure 3.2, we plot e_N, E_N, E_N^x, E_N^y and the reference lines N^{-a}, N^{1-a} in log-log scale with $a = 7/2, 11/2$. We find that (i) the errors E_N, E_N^x, E_N^y decay at the same rate as N^{1-a} (expected order for E_N , see, e.g., [102]); (ii) the convergence rate in the first derivative is one order lower than e_N ; and (iii) E_N^x dominates the error E_N . We also see that it is more accurate at superconvergence points, but there is no gain in convergence order. This should be in contrast

with interpolating analytic functions, where an order of N^2 can be gained at the superconvergence points (see Theorem 4.2).

We next take a different viewpoint from the spectral expansion of a function with finite regularity. Let us consider the JGL case (see Proposition 3.4). Define

$$\phi_0(x) = 1, \quad \phi_1(x) = x, \quad \phi_k(x) = (1 - x^2)\partial_x P_{k-1}^{(\alpha, \beta)}(x), \quad k \geq 2. \quad (3.11)$$

The so-defined $\{\phi_k\}_{k \geq 2}$ are mutually orthogonal in $L_{\omega^{\alpha-1, \beta-1}}^2(-1, 1)$ (where $\omega^{\alpha-1, \beta-1} = (1-x)^{\alpha-1}(1+x)^{\beta-1}$), which follows from (2.13) and the orthogonality of Jacobi polynomials. Moreover, $\{\phi_k\}_{k \geq 0}$ form a complete basis of $X := \mathbb{P}_1 \cup L_{\omega^{\alpha-1, \beta-1}}^2(-1, 1)$ (which reduces to $L_{\omega^{\alpha-1, \beta-1}}^2(-1, 1)$, if $\alpha, \beta > 0$). For any $u \in X$, we expand it as $u(x) = \sum_{k=0}^{\infty} \hat{u}_k \phi_k(x)$, where $\{\hat{u}_k\}$ can be uniquely determined. Then we have

$$(u - I_N u)(x) = \hat{u}_{N+1}(\phi_{N+1} - I_N \phi_{N+1})(x) + \sum_{k=N+2}^{\infty} \hat{u}_k(\phi_k - I_N \phi_k)(x). \quad (3.12)$$

We have $I_N \phi_{N+1} \equiv 0$ (which is actually aliased). Indeed, from the expansion: $(I_N \phi_{N+1})(x) = \sum_{k=0}^N \tilde{u}_k P_k^{(\alpha, \beta)}(x)$, we find that the pseudospectral coefficients $\{\tilde{u}_k\}$ vanish, as

$$\tilde{u}_k = \frac{1}{\gamma_k} \sum_{j=0}^N \phi_{N+1}(x_j) P_k^{(\alpha, \beta)}(x_j) \omega_j = 0, \quad 0 \leq k \leq N,$$

where $\{\gamma_k\}$ are constants, $\{\omega_j\}$ are the JGL quadrature weights and we have used the fact $\phi_{N+1}(x_j) = 0$ for $0 \leq j \leq N$. This implies

$$(u - I_N u)'(x) = \hat{u}_{N+1} \phi'_{N+1}(x) + \sum_{k=N+2}^{\infty} \hat{u}_k (\phi_k - I_N \phi_k)'(x). \quad (3.13)$$

Consequently, at the zeros of ϕ'_{N+1} (i.e., the superconvergence points $\{y_j\}_{j=1}^N$ in Proposition 3.4), the leading term of the error remainder in (3.13) vanishes.

In summary, we infer from the previous discussions that at the superconvergence points, the leading term of the interpolation error remainder for functions with limited regularity, vanishes. This leads to better accuracy, but there is no gain in order of convergence, which should be in contrast with interpolating analytic functions.

3.3 Numerical results

We present in this section some numerical examples to illustrate the superconvergence phenomenon by comparing the convergence behavior between the superconvergence points and the interpolation points, and the theoretical superconvergence estimates are given in Chapter 4.

(a) LGL interpolation error curve

(b) ρ^N multiple of the errors (LGL) (c) JGL interpolation error curve ($\alpha = \beta = 1$) (d) ρ^N multiple of the errors (JGL $\alpha = \beta = 1$)

Figure 3.3: Superconvergence of Gauss-Lobatto interpolation.

We first consider the function:

$$u(x) = \frac{1}{1 + 25x^2}, \quad (3.14)$$

which has two simple poles at $\pm i/5$ in the complex plane. Hence, it is analytic within the Bernstein ellipse satisfying $(\rho - \rho^{-1})/2 < 1/5$, so we have $1 < \rho < (1 + \sqrt{5^2 + 1})/5 \approx 1.2198$.

Let us look at the Legendre-Gauss-Lobatto case. We know from Remark 3.3 that the superconvergence points for the first derivative are the N Legendre-Gauss points $\{y_j\}_{j=1}^N$. Let $r_N(x) = (u - I_N u)(x)$. In Figure 3.3 (a), we plot the error curve $r'_N(x)$ and the samples $\{r'_N(x_j)\}_{j=0}^N$ and $\{r'_N(y_j)\}_{j=1}^N$ with $N = 55$. Observe that the interior LGL points are the extreme points of $r'_N(x)$, while the magnitude of the errors at the superconvergence points is significantly smaller. We now numerically verify the claims in Corollary 4.1:

$$\max_{1 \leq j \leq N} |r'_N(y_j)| \sim \max_{|x| \leq 1} |r_N(x)| \sim N^{-2} \max_{0 \leq j \leq N} |r'_N(x_j)|.$$

For this purpose, we eliminate the exponential order ρ^{-N} with $\rho = 1.2198$, and plot them with various N in Figure 3.3 (b). The numerical results agree well with what we have claimed. Very similar behavior is observed from Figure 3.3 (c)-(d) for the Jacobi-Gauss-Lobatto interpolation with $\alpha = \beta = 1$.

Figure 3.4: Superconvergence of GGR interpolation: $\alpha = 0$ (left) and $\alpha = 1$ (right).

Next, we consider the interpolation of $u(x) = \frac{1}{x-2}$, which has a simple pole $x = 2$ on the x -axis. It is analytic on and within the Bernstein ellipse with $1 < \rho < 2 + \sqrt{3}$. In Figure 3.4, we plot the maximum interpolation error and the error at the superconvergence points for the first derivative of the Gauss-Radau interpolation. Once again, we observe the same convergence behavior as claimed in Corollary 4.1.

Chapter 4

Exponential Convergence of Spectral Interpolation[†]

In this chapter, we derive a general framework for error estimates of spectral interpolation and differentiation at general Jacobi-Gauss-type points, provided that the underlying function is analytic on and within the Bernstein ellipse. Then the error estimates at the corresponding superconvergence points identified in Chapter 3 can be obtained straightforwardly.

As described in Subsection 1.1.2, we mainly focus on the analysis of sharp estimates for the exponential convergence of spectral interpolation and differentiation on Gegenbauer-Gauss (GG) and Gegenbauer-Gauss-Lobatto (GGL) points. The essential argument is based on a delicate lower bound estimate of the Gegenbauer polynomial on the Bernstein ellipse (see Subsection 4.3.1). Compared with the Chebyshev case in [96], the analysis in this case is much more involved.

This chapter is organized as follows. We present a general framework for the error estimates in Section 4.1, which, together with the properties of Jacobi polynomials, leads to the exponential estimates for general Jacobi-Gauss-type

[†]The main part of this chapter is based on the paper [121]: “Z.Q. Xie, L.L. Wang and X.D. Zhao. On exponential convergence of Gegenbauer interpolation and spectral differentiation. *Math. Comp.*, 82(282):1017–1036, 2013.”

interpolation in Section 4.2. In Section 4.3, we obtain the refined lower bound of the Gegenbauer polynomials on the Bernstein ellipse with a delicate analysis, which allows us to obtain error estimates for Gegenbauer-Gauss-type interpolation, and clearly characterize the dependence of the constant on the interesting parameters. In the final section, we provide some numerical results to show the sharpness of our error bounds.

4.1 Error estimates: a general framework

Recall the reminders in (3.2) and (3.4)-(3.5): for any $u \in \mathcal{A}_\rho$ with $\rho > 1$ (cf. (2.7)),

$$(u - I_N u)(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \frac{Q_{N+1}(x)}{z - x} \frac{u(z)}{Q_{N+1}(z)} dz, \quad \forall x \in [-1, 1], \quad (4.1)$$

$$(u - I_N u)'(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \left(\frac{Q'_{N+1}(x)}{z - x} + \frac{Q_{N+1}(x)}{(z - x)^2} \right) \frac{u(z)}{Q_{N+1}(z)} dz, \quad (4.2)$$

$$(u - I_N u)''(x) = \frac{1}{2\pi i} \oint_{\mathcal{E}_\rho} \left(\frac{Q''_{N+1}(x)}{z - x} + \frac{2Q'_{N+1}(x)}{(z - x)^2} + \frac{2Q_{N+1}(x)}{(z - x)^3} \right) \frac{u(z)}{Q_{N+1}(z)} dz, \quad (4.3)$$

where $\mathcal{E}_\rho$ is the Bernstein ellipse defined in (2.3), $\{x_j\}_{j=0}^N$ are Jacobi-Gauss-type points, that is, zeros of

$$Q_{N+1}(x) = c_N \left\{ P_{N+1}^{(\alpha, \beta)}(x), (1+x)P_N^{(\alpha, \beta+1)}(x) \text{ or } (1-x^2)P_{N-1}^{(\alpha+1, \beta+1)}(x) \right\}, \quad (4.4)$$

$c_N \neq 0$, and I_N is the Lagrange interpolation operator on $\{x_j\}_{j=0}^N$.

In this section, we analyze interpolation errors of analytical functions, and intend to estimate

$$\max_j \left| (u - I_N u)^{(k)}(x_j) \right|, \quad \max_i \left| (u - I_N u)^{(k)}(y_i) \right|, \quad k = 1, 2, \quad (4.5)$$

where $\{y_i\}$ are the corresponding superconvergence points in Proposition 3.1.

From the remainders in (4.1)-(4.3), we derive the following general results. Note that at this stage, the estimates depend on several constants involving N , which will be estimated in Sections 4.2-4.3 for specific sets of interpolation points.

Theorem 4.1. *Let $\{x_j\}_{j=0}^N$ be the zeros of $Q_{N+1}(x)$ defined in (4.4), and let $I_N u$ be the associated Lagrange interpolant. Denote*

$$m_Q = \min_{z \in \mathcal{E}_\rho} |Q_{N+1}(z)|, \quad M_Q = \max_{|x| \leq 1} |Q_{N+1}(x)|, \quad M_{Q'} = \max_{|x| \leq 1} |Q'_{N+1}(x)|, \quad (4.6)$$

and likewise $M_{Q''}$. For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, define $M = \max_{z \in \mathcal{E}_\rho} |u(z)|$. Then

(i) for the interpolation error, we have

$$\max_{|x| \leq 1} |(u - I_N u)(x)| \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho} \frac{M_Q}{m_Q}, \quad (4.7)$$

(ii) for the first derivative, we have

$$\max_{0 \leq j \leq N} |(u - I_N u)'(x_j)| \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho} \frac{M_{Q'}}{m_Q}, \quad (4.8)$$

and at the corresponding superconvergence points $\{y_j\}_{j=1}^N$ (i.e., zeros of $Q'_{N+1}(x)$), we have

$$\max_{1 \leq j \leq N} |(u - I_N u)'(y_j)| \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho^2} \frac{M_Q}{m_Q}, \quad (4.9)$$

(iii) for the second derivative, we have

$$\max_{0 \leq j \leq N} |(u - I_N u)''(x_j)| \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho} \left(\frac{M_{Q''}}{m_Q} + \frac{2}{d_\rho} \frac{M_{Q'}}{m_Q} \right), \quad (4.10)$$

and at the corresponding superconvergence points $\{z_j\}_{j=1}^{N-1}$ (i.e., zeros of $Q''_{N+1}(x)$), we have

$$\max_{1 \leq j \leq N-1} |(u - I_N u)''(z_j)| \leq \frac{ML(\mathcal{E}_\rho)}{\pi d_\rho^2} \left(\frac{M_{Q'}}{m_Q} + \frac{1}{d_\rho} \frac{M_Q}{m_Q} \right). \quad (4.11)$$

Here, the constants $L(\mathcal{E}_\rho)$ and d_ρ are defined in (2.5) and (2.6), respectively.

Proof. By (4.1), we have the bound of the point-wise error:

$$|(u - I_N u)(x)| \leq \frac{M|Q_{N+1}(x)|}{2\pi m_Q} \oint_{\mathcal{E}_\rho} \frac{|dz|}{|z - x|} \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho} \frac{M_Q}{m_Q}, \quad x \in [-1, 1],$$

which implies (4.7).

As $Q_{N+1}(x_j) = 0$, we derive from (4.2) that

$$\max_{0 \leq j \leq N} |(u - I_N u)'(x_j)| \leq \frac{M_{Q'} M}{2\pi m_Q} \max_{0 \leq j \leq N} \oint_{\mathcal{E}_\rho} \frac{|dz|}{|z - x_j|} \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho} \frac{M_{Q'}}{m_Q}, \quad (4.12)$$

which leads to (4.8). Analogously, (4.10) follows from (4.3).

Using the fact $Q'_{N+1}(y_j) = 0$ (resp. $Q''_{N+1}(z_j) = 0$, see Proposition 3.1), we can obtain (4.9) (resp. (4.11)) in a fashion very similar to (4.12). $\square$

The following property is a direct consequence of Theorem 4.1.

Corollary 4.1. *At superconvergence points, the maximum of the first derivative of the interpolation error converges at the same rate as the maximum interpolation error. Similarly, the maximum of the second derivative of the interpolation error at superconvergence points enjoys the same convergence rate as that of the first derivative.*

Proof. We claim the first statement from (4.7) and (4.9). Similarly, by (4.2),

$$\max_{|x| \leq 1} |(u - I_N u)'(x)| \leq \frac{ML(\mathcal{E}_\rho)}{2\pi d_\rho} \left(\frac{M_{Q'}}{m_Q} + \frac{1}{d_\rho} \frac{M_Q}{m_Q} \right). \quad (4.13)$$

Thus, the second claim follows from (4.11) and (4.13). $\square$

Remark 4.1. *Since the above error bounds share the common factor $1/m_Q$, it suffices to show that $M_{Q'} \sim N^\gamma M_Q$ and $M_{Q''} \sim N^\delta M_{Q'}$ (for $\gamma, \delta > 0$) to obtain the gain in order of N at superconvergence points.* $\square$

4.2 Error estimates of Jacobi-Gauss-type interpolation

To derive the error bounds, it remains to estimate the constants $M_Q, M_{Q'}, M_{Q''}$ and m_Q . For a specific set of interpolation points, the former three constants are not difficult to obtain from the relevant properties of orthogonal polynomials (which only contribute to some powers of N), but much care has to be taken to estimate m_Q (which actually leads to the exponential convergence). Note that for the Chebyshev case, $Q_{N+1}(z)$ with $z \in \mathcal{E}_\rho$ has a simple closed form, so the estimation of m_Q becomes straightforward (see, e.g., [36, 83, 96, 125]).

In the following, we first consider the general Jacobi-Gauss and Jacobi-Gauss-Lobatto interpolations, and then refine the results for Gegenbauer-Gauss-type interpolation in the next section.

4.2.1 Jacobi-Gauss interpolation

In this case, we have $Q_{N+1}(x) = P_{N+1}^{(\alpha, \beta)}(x)$, and need to estimate the corresponding $M_Q, M_{Q'}, M_{Q''}$ and m_Q in Theorem 4.1.

Let $q := \max(\alpha, \beta)$ with $\alpha, \beta > -1$. Then we obtain from Szegő [108, Theorem 7.32.1] and (2.21)-(2.22) that

$$\begin{aligned} M_Q &= \max_{|x| \leq 1} |P_{N+1}^{(\alpha, \beta)}(x)| \\ &= \begin{cases} |P_{N+1}^{(\alpha, \beta)}(x')| \leq c_N(\alpha, \beta)N^{-1/2}, & q < -1/2; \\ \frac{\Gamma(N+q+2)}{\Gamma(N+2)\Gamma(q+1)} \leq \frac{\exp(\Upsilon_N^{q+2,2})}{\Gamma(q+1)}N^q, & q \geq -1/2, \end{cases} \end{aligned} \quad (4.14)$$

where x' is one of two maximum points nearest $(\beta - \alpha)/(\alpha + \beta + 1)$, and $c_N(\alpha, \beta) \cong 1$ for large N . Hence, by (2.13) and (4.14),

$$\begin{aligned} M_{Q'} &= \max_{|x| \leq 1} |\partial_x P_{N+1}^{(\alpha, \beta)}(x)| = \frac{1}{2}(N + \alpha + \beta + 2) \max_{|x| \leq 1} |P_N^{(\alpha+1, \beta+1)}(x)| \\ &\leq \frac{1}{2}(N + \alpha + \beta + 2) \frac{\exp(\Upsilon_N^{q+2,1})}{\Gamma(q+2)} N^{q+1}; \\ M_{Q''} &\leq \frac{1}{4}(N + \alpha + \beta + 2)(N + \alpha + \beta + 3) \frac{\exp(\Upsilon_N^{q+2,0})}{\Gamma(q+3)} N^{q+2}. \end{aligned} \quad (4.15)$$

To estimate m_Q , we resort to the asymptotic representation (see Szegő [108, Theorem 8.21.9]):

$$P_N^{(\alpha, \beta)}(z) = \phi_0(w; \alpha, \beta) N^{-1/2} w^N + O(N^{-1}), \quad \forall z = \frac{1}{2}(w + w^{-1}) \in \mathcal{E}_\rho, \quad (4.16)$$

where $\phi_0(w; \alpha, \beta)$ is regular for $|w| = \rho > 1$, and $|w| = 1$ but $w \neq \pm 1$. Thus, we have

$$m_Q = \min_{z \in \mathcal{E}_\rho} |P_{N+1}^{(\alpha, \beta)}(z)| \geq C(\rho; \alpha, \beta) N^{-\frac{1}{2}} \rho^{N+1} (1 + O(N^{-1})), \quad (4.17)$$

where $C(\rho; \alpha, \beta) = \min_{|w|=\rho} |\phi_0(w; \alpha, \beta)|$, independent of N .

With a little abuse of notation, we use $c_N(\alpha, \beta)$ to denote the generic positive constant such that $c_N(\alpha, \beta) \cong 1$ for large N . For example, for $q = \max(\alpha, \beta) \geq -1/2$, we denote

$$c_N := c_N(\alpha, \beta) = \frac{\exp(\Upsilon_N^{q+2,1})}{1 + O(N^{-1})},$$

which is extracted from the ratio $M_{Q'}/m_Q$, and likewise for M_Q/m_Q and $M_{Q''}/m_Q$. Then the error bounds for Jacobi-Gauss interpolation follow from Theorem 4.1.

Theorem 4.2. *For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, let $(I_N u)(x)$ be the interpolant of $u(x)$ at the Jacobi-Gauss points $\{x_j\}_{j=0}^N$, and let $q = \max(\alpha, \beta)$ for $\alpha, \beta > -1$. Then*

(i) *for the interpolation error, we have*

$$\max_{|x| \leq 1} |(u - I_N u)(x)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{2\pi d_\rho C(\rho; \alpha, \beta)} \frac{1}{\rho^{N+1}} \begin{cases} 1, & q < -1/2, \\ N^{q+1/2} / \Gamma(q+1), & q \geq -1/2; \end{cases} \quad (4.18)$$

(ii) *for the first derivative, we have*

$$\max_{0 \leq j \leq N} |(u - I_N u)'(x_j)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{4\pi d_\rho C(\rho; \alpha, \beta) \Gamma(q+2)} \frac{N^{q+5/2}}{\rho^{N+1}}, \quad (4.19)$$

and at the corresponding superconvergence points $\{y_j\}_{j=1}^N$, we have

$$\begin{aligned} \max_{1 \leq j \leq N} |(u - I_N u)'(y_j)| &\leq \frac{c_N M L(\mathcal{E}_\rho)}{2\pi d_\rho^2 C(\rho; \alpha, \beta)} \frac{1}{\rho^{N+1}} \\ &\quad \times \begin{cases} 1, & q < -1/2, \\ N^{q+1/2} / \Gamma(q+1), & q \geq -1/2; \end{cases} \end{aligned} \quad (4.20)$$

(iii) *for the second derivative, we have*

$$\max_{0 \leq j \leq N} |(u - I_N u)''(x_j)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{8\pi d_\rho C(\rho; \alpha, \beta) \Gamma(q+3)} \frac{N^{q+9/2}}{\rho^{N+1}}, \quad (4.21)$$

and at the corresponding superconvergence points $\{z_j\}_{j=1}^{N-1}$, we have

$$\max_{1 \leq j \leq N-1} |(u - I_N u)''(z_j)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{2\pi d_\rho^2 C(\rho; \alpha, \beta) \Gamma(q+2)} \frac{N^{q+5/2}}{\rho^{N+1}}. \quad (4.22)$$

Remark 4.2. We see that we gain a factor of N^2 at superconvergence points. $\square$

4.2.2 Jacobi-Gauss-Lobatto interpolation

In this case, we have $Q_{N+1}(x) = (1 - x^2)P_{N-1}^{(\alpha+1, \beta+1)}(x)$. The estimates of M_Q , $M_{Q'}$ and $M_{Q''}$ follow from (4.14), (2.13) and (2.21)-(2.22),

$$M_Q = \max_{|x| \leq 1} |(1 - x^2)P_{N-1}^{(\alpha+1, \beta+1)}(x)| \leq \frac{\Gamma(N+q+1)}{\Gamma(N)\Gamma(q+2)} \leq \frac{\exp(\Upsilon_N^{q+1,0})}{\Gamma(q+2)} N^{q+1}, \quad (4.23)$$

$$\begin{aligned} M_{Q'} &= \max_{|x| \leq 1} \left| [(1 - x^2)P_{N-1}^{(\alpha+1, \beta+1)}(x)]' \right| \\ &\leq 2 \max_{|x| \leq 1} |P_{N-1}^{(\alpha+1, \beta+1)}(x)| + \frac{1}{2}(N + \alpha + \beta + 2) \max_{|x| \leq 1} |P_{N-2}^{(\alpha+2, \beta+2)}(x)| \\ &\leq \frac{2 \exp(\Upsilon_N^{q+1,0})}{\Gamma(q+2)} N^{q+1} + \frac{\exp(\Upsilon_N^{q+1,-1})}{2\Gamma(q+3)} (N + \alpha + \beta + 2) N^{q+2}, \end{aligned} \quad (4.24)$$

$$\begin{aligned} M_{Q''} &= \max_{|x| \leq 1} \left| [(1 - x^2)P_{N-1}^{(\alpha+1, \beta+1)}(x)]'' \right| \\ &\leq \frac{2 \exp(\Upsilon_N^{q+1,0})}{\Gamma(q+2)} N^{q+1} + 2(N + \alpha + \beta + 2) \frac{\exp(\Upsilon_N^{q+1,-1})}{\Gamma(q+3)} N^{q+2} \\ &\quad + \frac{\exp(\Upsilon_N^{q+1,-2})}{4\Gamma(q+4)} (N + \alpha + \beta + 2)(N + \alpha + \beta + 3) N^{q+3}, \end{aligned} \quad (4.25)$$

where $q = \max(\alpha, \beta)$.

For any $z \in \mathcal{E}_\rho$, one verifies that

$$\frac{1}{4}(\rho - \rho^{-1})^2 \leq |z^2 - 1| \leq \frac{1}{4}(\rho + \rho^{-1})^2,$$

which, together with the asymptotic representation in (4.16), implies that

$$\begin{aligned} m_Q &= \min_{z \in \mathcal{E}_\rho} |(1 - z^2)P_{N-1}^{(\alpha+1, \beta+1)}(z)| \\ &\geq \frac{1}{4}(1 - \rho^{-2})^2 C(\rho; \alpha + 1, \beta + 1) N^{-\frac{1}{2}} \rho^{N+1} (1 + O(N^{-1})), \end{aligned} \quad (4.26)$$

where $C(\rho; \alpha + 1, \beta + 1) = \min_{|w|=\rho} |\phi_0(w; \alpha + 1, \beta + 1)|$ is independent of N , and $\phi_0(w; \alpha + 1, \beta + 1)$ is given in (4.16).

With the above estimates, the error bounds for Jacobi-Gauss-Lobatto interpolation follow from Theorem 4.1.

Theorem 4.3. *For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, let $(I_N u)(x)$ be the interpolant of $u(x)$ at the Jacobi-Gauss-Lobatto points $\{x_j\}_{j=0}^N$, and let $q = \max(\alpha, \beta)$ for $\alpha, \beta > -1$.*

(i) *For the interpolation error, we have*

$$\max_{|x| \leq 1} |(u - I_N u)(x)| \leq \frac{2c_N ML(\mathcal{E}_\rho)(1 - \rho^{-2})^{-2}}{\pi d_\rho C(\rho; \alpha + 1, \beta + 1) \Gamma(q + 2)} \frac{N^{q+3/2}}{\rho^{N+1}}; \quad (4.27)$$

(ii) *For the first derivative, we have*

$$\max_{0 \leq j \leq N} |(u - I_N u)'(x_j)| \leq \frac{c_N ML(\mathcal{E}_\rho)(1 - \rho^{-2})^{-2}}{\pi d_\rho C(\rho; \alpha + 1, \beta + 1) \Gamma(q + 3)} \frac{N^{q+7/2}}{\rho^{N+1}}, \quad (4.28)$$

and at the corresponding superconvergence points $\{y_j\}_{j=1}^N$, we have

$$\max_{1 \leq j \leq N} |(u - I_N u)'(y_j)| \leq \frac{2c_N ML(\mathcal{E}_\rho)(1 - \rho^{-2})^{-2}}{\pi d_\rho^2 C(\rho; \alpha + 1, \beta + 1) \Gamma(q + 2)} \frac{N^{q+3/2}}{\rho^{N+1}}; \quad (4.29)$$

(iii) *For the second derivative, we have*

$$\max_{0 \leq j \leq N} |(u - I_N u)''(x_j)| \leq \frac{c_N ML(\mathcal{E}_\rho)(1 - \rho^{-2})^{-2}}{2\pi d_\rho C(\rho; \alpha + 1, \beta + 1) \Gamma(q + 4)} \frac{N^{q+11/2}}{\rho^{N+1}}, \quad (4.30)$$

and at the corresponding superconvergence points $\{z_j\}_{j=1}^{N-1}$, we have

$$\max_{1 \leq j \leq N-1} |(u - I_N u)''(z_j)| \leq \frac{2c_N ML(\mathcal{E}_\rho)(1 - \rho^{-2})^{-2}}{\pi d_\rho^2 C(\rho; \alpha + 1, \beta + 1) \Gamma(q + 3)} \frac{N^{q+7/2}}{\rho^{N+1}}. \quad (4.31)$$

Remark 4.3. *In the Jacobi-Gauss-Radau case, $Q_{N+1}(x)$ is a linear combination of $\{P_{N+k}^{(\alpha, \beta)}(x) : k = 0, 1\}$ (see (2.15)), so we can estimate the interpolation errors in a very similar fashion. $\square$*

It is seen from (4.17) and (4.26) that the dependence of $C(\rho, \alpha, \beta)$ and $C(\rho, \alpha + 1, \beta + 1)$ in the asymptotic on ρ is implicit. However, for the Chebyshev polynomial, we can explicitly characterize this, and also the estimate of m_Q is valid for all $N \geq 1$. Indeed, we have the closed form (see, e.g., [36]):

$$T_{N+1}(z) = \frac{1}{2}(w^{N+1} + w^{-(N+1)}), \quad z \in \mathcal{E}_\rho, \quad |w| = \rho, \quad (4.32)$$

which implies

$$\min_{z \in \mathcal{E}_\rho} |T_{N+1}(z)| \geq \frac{1}{2}(\rho^{N+1} - \rho^{-N-1}). \quad (4.33)$$

With a re-normalization of T_{N+1} , we find from (2.21) that

$$\begin{aligned} m_Q &= \min_{z \in \mathcal{E}_\rho} |P_{N+1}^{(-1/2, -1/2)}(z)| = \frac{\Gamma(N + 3/2)}{\sqrt{\pi}(N + 1)!} \min_{z \in \mathcal{E}_\rho} |T_{N+1}(z)| \\ &\geq \frac{\exp(-\Upsilon_{N+1}^{1,1/2})}{2\sqrt{\pi}} \left(1 - \frac{1}{\rho^{2N+2}}\right) N^{-1/2} \rho^{N+1}, \quad N \geq 1. \end{aligned} \quad (4.34)$$

In fact, such an estimate is also available for the Gegenbauer polynomial (i.e., $\alpha = \beta > -1$), which is derived in the next section, but the analysis is much more involved.

4.3 Refined estimates for Gegenbauer-Gauss-type interpolation

In this section, we assume $\alpha \neq -1/2$, since the estimate of m_Q in this case is already given in (4.34).

4.3.1 Lower bound for Gegenbauer polynomials on $\mathcal{E}_\rho$

Much of our analysis relies on the representation of the Gegenbauer polynomial on the Bernstein ellipse (cf. Lemma 2.4):

$$P_N^{(\alpha, \alpha)}(z) = A_N^\alpha \sum_{k=0}^N g_k^\alpha g_{N-k}^\alpha w^{N-2k}, \quad N \geq 0, \quad \alpha > -1, \quad \alpha \neq -1/2, \quad (4.35)$$

where

$$\begin{aligned} g_0^\alpha &= 1, \quad g_k^\alpha = \frac{\Gamma(k + \alpha + 1/2)}{k! \Gamma(\alpha + 1/2)}, \quad 1 \leq k \leq N, \\ \text{and } A_N^\alpha &= \frac{\Gamma(2\alpha + 1) \Gamma(N + \alpha + 1)}{\Gamma(\alpha + 1) \Gamma(N + 2\alpha + 1)}. \end{aligned} \quad (4.36)$$

In fact, the coefficients $\{g_k^\alpha\}$ relate to the following Laurent series expansion.

Lemma 4.1. *We have*

$$F_\alpha(w) := (1 - w^{-2})^{-\alpha-1/2} = \sum_{k=0}^{\infty} \frac{g_k^\alpha}{w^{2k}}, \quad (4.37)$$

which converges uniformly for all complex-valued w such that $|w| > 1$.

Proof. Recall the binomial expansion:

$$(1 - w^{-2})^{-\alpha-1/2} = \sum_{k=0}^{\infty} \frac{g_k^\alpha}{w^{2k}}, \quad \forall |w| > 1. \quad (4.38)$$

This implies (4.37). $\square$

Observe that if $\alpha = 1/2$, then $g_k^\alpha \equiv 1$ for $0 \leq k \leq N$. Therefore, the Chebyshev polynomial of the second kind has the representation

$$U_N(z) = \frac{w^{N+1} - w^{-(N+1)}}{w - w^{-1}} = w^N \sum_{k=0}^N w^{-2k} = \frac{P_N^{(1/2, 1/2)}(z)}{A_N^{1/2}}, \quad N \geq 0, \quad (4.39)$$

which can be found in [83].

In what follows, we show a similar property holds for general $\alpha > -1$ and $\alpha \neq -1/2$. More precisely, we estimate the upper bound of remainder:

$$\begin{aligned} \left| F_\alpha(w) - \frac{P_N^{(\alpha, \alpha)}(z)}{A_N^\alpha g_N^\alpha w^N} \right| &\leq \sum_{k=1}^N |d_{N,k}^{(\alpha)}| |g_k^\alpha| \rho^{-2k} + \sum_{k=N+1}^{\infty} |g_k^\alpha| \rho^{-2k} \\ &:= R_N(\rho, \alpha), \end{aligned} \quad (4.40)$$

where $z \in \mathcal{E}_\rho$ with $|w| = \rho > 1$, and

$$d_{N,k}^{(\alpha)} = 1 - \frac{g_{N-k}^\alpha}{g_N^\alpha}, \quad 1 \leq k \leq N. \quad (4.41)$$

To obtain a sharp estimate of $R_N(\rho, \alpha)$, it is necessary to understand the behavior of the coefficients $\{g_k^\alpha\}_{k=1}^N$ and $\{d_{N,k}^{(\alpha)}\}_{k=1}^N$.

Lemma 4.2. *Let $\{g_k^\alpha\}_{k=1}^N$ and $\{d_{N,k}^{(\alpha)}\}_{k=1}^N$ be the sequences as defined in (4.36) and (4.41), respectively.*

(i) *If $\alpha > 1/2$, then there holds*

$$0 < d_{N,1}^{(\alpha)} < d_{N,2}^{(\alpha)} < \cdots < d_{N,N}^{(\alpha)} < 1. \quad (4.42)$$

(ii) *If $-1 < \alpha < 1/2$ and $\alpha \neq -1/2$, then*

$$\cdots < |g_{k+1}^\alpha| < |g_k^\alpha| < \cdots < |g_1^\alpha| < g_0^\alpha = 1, \quad (4.43)$$

and we have

$$0 < -d_{N,1}^{(\alpha)} < -d_{N,2}^{(\alpha)} < \cdots < -d_{N,N-1}^{(\alpha)}, \quad (4.44)$$

and

$$|d_{N,k}^{(\alpha)} g_k^\alpha| < 1 \quad \text{for } 1 \leq k \leq N-1, \quad N \geq 3. \quad (4.45)$$

Proof. By (4.36),

$$\frac{g_{k+1}^\alpha}{g_k^\alpha} = \frac{k + \alpha + 1/2}{k + 1} \quad \text{for } \alpha \neq -1/2. \quad (4.46)$$

Thus for $\alpha > 1/2$, $\{g_k^\alpha\}$ is strictly increasing with respect to k , which, together with the fact $g_k^\alpha > 0$, implies

$$0 < d_{N,k}^{(\alpha)} = 1 - \frac{g_{N-k}^\alpha}{g_N^\alpha} < 1, \quad \text{and} \quad d_{N,k+1}^{(\alpha)} - d_{N,k}^{(\alpha)} = \frac{g_{N-k}^\alpha - g_{N-k-1}^\alpha}{g_N^\alpha} > 0.$$

This completes the proof of (i).

The property (4.43) is a direct consequence of (4.46), and (4.44) can be proved in a fashion similar to (4.42). It remains to verify (4.45). If $k = 1$, a direct calculation by using (4.36) yields

$$|d_{N,1}^{(\alpha)} g_1^\alpha| = |\alpha + 1/2| \frac{1/2 - \alpha}{N - (1/2 - \alpha)} < 1, \quad \forall N \geq 3.$$

For $2 \leq k \leq N-1$, it follows from (4.36) and (4.44) that

$$|d_{N,k}^{(\alpha)} g_k^\alpha| = \left(\frac{g_{N-k}^\alpha}{g_N^\alpha} - 1 \right) |g_k^\alpha| < \frac{g_{N-k}^\alpha}{g_N^\alpha} |g_k^\alpha| = \left(\prod_{j=0}^{k-2} \frac{1 - \frac{1/2 - \alpha}{k-j}}{1 - \frac{1/2 - \alpha}{N-j}} \right) \frac{|\alpha + 1/2|}{1 - \frac{1/2 - \alpha}{N-k+1}} < 1.$$

This ends the proof. $\square$

Lemma 4.3. For $\alpha > 1/2, \rho > 1$ and $m + 1 \geq \frac{\alpha-1/2}{2 \ln \rho}$, we have

$$\sum_{k=m+1}^{\infty} g_k^{\alpha} \rho^{-2k} \leq \frac{1}{\Gamma(\alpha + 1/2)} \exp(\Upsilon_{m+1}^{\alpha+1/2,1}) \frac{[\alpha + 1/2]!}{(2 \ln \rho)^{\alpha+1/2}} \frac{m^{[\alpha+1/2]}}{\rho^{2(m-1)}}, \quad (4.47)$$

where $\Upsilon_{m+1}^{\alpha+1/2,1}$ is given in (2.22), and $[\alpha + 1/2]$ is the largest integer not more than $\alpha + 1/2$.

Proof. By (4.36) and (2.21)-(2.22), we have for $\alpha > 1/2$,

$$\begin{aligned} \sum_{k=m+1}^{\infty} g_k^{\alpha} \rho^{-2k} &= \frac{1}{\Gamma(\alpha + 1/2)} \sum_{k=m+1}^{\infty} \frac{\Gamma(k + \alpha + 1/2)}{\Gamma(k + 1)} \rho^{-2k} \\ &\leq \frac{1}{\Gamma(\alpha + 1/2)} \sum_{k=m+1}^{\infty} \exp(\Upsilon_k^{\alpha+1/2,1}) \frac{k^{\alpha-1/2}}{\rho^{2k}} \\ &\leq \frac{1}{\Gamma(\alpha + 1/2)} \exp(\Upsilon_{m+1}^{\alpha+1/2,1}) \sum_{k=m+1}^{\infty} \frac{k^{\alpha-1/2}}{\rho^{2k}}, \end{aligned}$$

where we used the fact that $\Upsilon_k^{\alpha+1/2,1} = \frac{\alpha-1/2}{2k} + \frac{1}{12(k+\alpha-1/2)} + \frac{(\alpha-1/2)^2}{k}$ is strictly decreasing with respect to k .

Recall that the incomplete Gamma function, which is defined by $\Gamma(\alpha, x) = \int_x^{\infty} t^{\alpha-1} e^{-t} dt, \alpha > 0, x \geq 0$, satisfies (see [71, Page 899])

$$\Gamma(n+1, x) = n! e^{-x} \sum_{k=0}^n \frac{x^k}{k!}, \quad n = 0, 1, \dots$$

One verifies that under the condition $m + 1 \geq \frac{\alpha-1/2}{2 \ln \rho}$, $k^{\alpha-1/2}/\rho^{2k}$ is decreasing with respect to k . Therefore,

$$\begin{aligned} \sum_{k=m+1}^{\infty} \frac{k^{\alpha-1/2}}{\rho^{2k}} &\leq \int_m^{\infty} x^{\alpha-1/2} \rho^{-2x} dx = \frac{1}{(2 \ln \rho)^{\alpha+1/2}} \int_{2m \ln \rho}^{\infty} x^{\alpha-1/2} e^{-x} dx \\ &= \frac{1}{(2 \ln \rho)^{\alpha+1/2}} \Gamma(\alpha + 1/2, 2m \ln \rho) \\ &\leq \frac{1}{(2 \ln \rho)^{\alpha+1/2}} \Gamma([\alpha + 1/2] + 1, 2m \ln \rho) \\ &= \frac{[\alpha + 1/2]! e^{-2m \ln \rho}}{(2 \ln \rho)^{\alpha+1/2}} \sum_{k=0}^{[\alpha+1/2]} \frac{m^k (2 \ln \rho)^k}{k!} \\ &\leq \frac{[\alpha + 1/2]!}{(2 \ln \rho)^{\alpha+1/2}} \frac{m^{[\alpha+1/2]}}{\rho^{2m}} \sum_{k=0}^{\infty} \frac{(2 \ln \rho)^k}{k!} \\ &= \frac{[\alpha + 1/2]!}{(2 \ln \rho)^{\alpha+1/2}} \frac{m^{[\alpha+1/2]}}{\rho^{2(m-1)}}. \end{aligned}$$

This ends the proof of Lemma 4.3. $\square$

With the above preparations, we are ready to present the main result on the upper bound of $R_N(\rho, \alpha)$ in (4.40).

Lemma 4.4. *Let $R_N(\rho, \alpha)$ with $\rho > 1$ be the remainder as defined in (4.40).*

(i) *If $\alpha > 1/2$, then for all $N \geq m \geq 1$ and $m + 1 \geq \frac{\alpha-1/2}{2 \ln \rho}$, we have*

$$R_N(\rho, \alpha) \leq d_{N,m}^{(\alpha)} \left((1 - \rho^{-2})^{-\alpha-1/2} - 1 \right) + \frac{\exp(\Upsilon_{m+1}^{\alpha+1/2,1})}{\Gamma(\alpha+1/2)} \frac{[\alpha+1/2]!}{(2 \ln \rho)^{\alpha+1/2}} \frac{m^{[\alpha+1/2]}}{\rho^{2(m-1)}}, \quad (4.48)$$

where $[\alpha+1/2]$ is the largest integer $\leq \alpha+1/2$, and $\Upsilon_{m+1}^{\alpha+1/2,1}$ is given in (2.22).

(ii) *If $-1 < \alpha < 1/2$ and $\alpha \neq -1/2$, then for all $N \geq m \geq 1$ and $N \geq 3$,*

$$R_N(\rho, \alpha) \leq |d_{N,m}^{(\alpha)}| \left| (1 - \rho^{-2})^{-\alpha-1/2} - 1 \right| + \frac{\rho^{-2m}}{\rho^2 - 1} + \rho^{-2N}. \quad (4.49)$$

Here, the factor $d_{N,m}^{(\alpha)}$ is given by (4.41).

Proof. (i) For $\alpha > 1/2$, we obtain from (4.42) and the fact $g_k^\alpha > 0$ that

$$\begin{aligned} R_N(\rho, \alpha) &= \sum_{k=1}^m d_{N,k}^{(\alpha)} g_k^\alpha \rho^{-2k} + \sum_{k=m+1}^N d_{N,k}^{(\alpha)} g_k^\alpha \rho^{-2k} + \sum_{k=N+1}^{\infty} g_k^\alpha \rho^{-2k} \\ &\leq d_{N,m}^{(\alpha)} \sum_{k=1}^m g_k^\alpha \rho^{-2k} + \sum_{k=m+1}^N g_k^\alpha \rho^{-2k} + \sum_{k=N+1}^{\infty} g_k^\alpha \rho^{-2k} \\ &\leq d_{N,m}^{(\alpha)} \left((1 - \rho^{-2})^{-\alpha-1/2} - 1 \right) + \sum_{k=m+1}^{\infty} g_k^\alpha \rho^{-2k}, \end{aligned} \quad (4.50)$$

which, together with Lemma 4.3, leads to the estimate in (4.48).

(ii) Now, we turn to the proof of the second case: $-1 < \alpha < 1/2$ and $\alpha \neq$

$-1/2$. By (4.43), (4.44) and (4.45) in Lemma 4.2,

$$\begin{aligned} R_N(\rho, \alpha) &= \sum_{k=1}^m |d_{N,k}^{(\alpha)}| |g_k^\alpha| \rho^{-2k} + \sum_{k=m+1}^N |d_{N,k}^{(\alpha)}| |g_k^\alpha| \rho^{-2k} + \sum_{k=N+1}^{\infty} |g_k^\alpha| \rho^{-2k} \\ &\leq |d_{N,m}^{(\alpha)}| \sum_{k=1}^m |g_k^\alpha| \rho^{-2k} + \sum_{k=m+1}^{N-1} \rho^{-2k} + |d_{N,N}^{(\alpha)} g_N^\alpha| \rho^{-2N} + \sum_{k=N+1}^{\infty} \rho^{-2k} \\ &\leq |d_{N,m}^{(\alpha)}| \left| (1 - \rho^{-2})^{-\alpha-1/2} - 1 \right| + \frac{\rho^{-2m}}{\rho^2 - 1} + \rho^{-2N}, \end{aligned}$$

where in the last step, we used the following facts:

$$\sum_{k=1}^m |g_k^\alpha| \rho^{-2k} \leq \text{sign}(\alpha + 1/2) \sum_{k=1}^{\infty} g_k^\alpha \rho^{-2k} = \text{sign}(\alpha + 1/2) \left((1 - \rho^{-2})^{-\alpha-1/2} - 1 \right),$$

for $\rho > 1$ (note that $\text{sign}(\alpha + 1/2)$ is the sign of $\alpha + 1/2$), and $|d_{N,N}^{(\alpha)} g_N^\alpha| = |g_N^\alpha - 1| < 2$, thanks to (4.43). $\square$

The estimate in Lemma 4.4 is quite tight and is valid even for small N . By choosing a suitable m to balance the two error terms in the upper bound, we are able to derive the anticipated estimate.

Theorem 4.4. *For any $z \in \mathcal{E}_\rho$ with $|w| = \rho > 1$, and any $\alpha > -1$ and $\alpha \neq -1/2$, there exists $0 < \varepsilon \leq 1/2$ such that*

$$\left| F_\alpha(w) - \frac{P_N^{(\alpha, \alpha)}(z)}{A_N^\alpha g_N^\alpha w^N} \right| \leq A(\rho, \alpha) N^{\varepsilon-1} + O(N^{-1}), \quad (4.51)$$

where

$$A(\rho, \alpha) = |\alpha - 1/2| \left| (1 - \rho^{-2})^{-\alpha-1/2} - 1 \right|. \quad (4.52)$$

Proof. We first estimate $|d_{N,m}^{(\alpha)}|$ in Lemma 4.4, when $N - m$ is large. Using (4.36) and (2.21)-(2.22) that

$$\begin{aligned} \frac{g_{N-m}^\alpha}{g_N^\alpha} &= \frac{\Gamma(N - m + \alpha + 1/2)}{\Gamma(N - m + 1)} \frac{\Gamma(N + 1)}{\Gamma(N + \alpha + 1/2)} \\ &\leq \left(1 - \frac{m}{N} \right)^{\alpha-1/2} \exp \left(\Upsilon_{N-m}^{\alpha+1/2, 1} + \Upsilon_N^{1, \alpha+1/2} \right); \\ \frac{g_{N-m}^\alpha}{g_N^\alpha} &\geq \left(1 - \frac{m}{N} \right)^{\alpha-1/2} \exp \left(-\Upsilon_{N-m}^{1, \alpha+1/2} - \Upsilon_N^{\alpha+1/2, 1} \right); \\ \implies \frac{g_{N-m}^\alpha}{g_N^\alpha} &= \left\{ 1 + \frac{(1/2 - \alpha)m}{N} + O\left(\frac{m^2}{N^2}\right) \right\} \left\{ 1 + O\left(\frac{1}{N - m}\right) \right\}. \end{aligned}$$

Hereafter, taking $m = [N^\varepsilon]$ with $0 < \varepsilon \leq 1/2$ yields

$$\begin{aligned} \frac{g_{N-m}^\alpha}{g_N^\alpha} &= 1 + (1/2 - \alpha)N^{\varepsilon-1} + O\left(\frac{1}{N - N^\varepsilon}\right) \\ \implies d_{N,m}^{(\alpha)} &= 1 - \frac{g_{N-m}^\alpha}{g_N^\alpha} = (\alpha - 1/2)N^{\varepsilon-1} + O(N^{-1}). \end{aligned} \quad (4.53)$$

One verifies readily that for $\alpha > 1/2$ and any $0 < \varepsilon \leq 1/2$,

$$\frac{m^{[\alpha+1/2]}}{\rho^{2m}} \leq \frac{1}{N} \iff \frac{\ln N}{N^\varepsilon} \leq \frac{2 \ln \rho}{1 + \varepsilon[\alpha + 1/2]}, \quad (4.54)$$

which, together with (4.48) and (4.53), implies (4.51) with $\alpha > 1/2$.

If $-1 < \alpha < 1/2$ and $\alpha \neq -1/2$, it follows from (4.54) that $\rho^{-2m} \leq N^{-1}$ for any $0 < \varepsilon \leq 1/2$. This validates the desired estimate. $\square$

A direct consequence of Theorem 4.4 is that

$$\lim_{N \rightarrow \infty} \frac{P_N^{(\alpha, \alpha)}(z)}{A_N^\alpha g_N^\alpha w^N} = \lim_{N \rightarrow \infty} \sum_{k=0}^N \frac{g_{N-k}^\alpha}{g_N^\alpha} g_k^\alpha w^{-2k} = (1 - w^{-2})^{-\alpha-1/2}, \quad (4.55)$$

for all $z \in \mathcal{E}_\rho$ with $|w| = \rho > 1$, and any $\alpha > -1$ and $\alpha \neq -1/2$.

With the tight estimate in Theorem 4.4, now we can obtain the lower bound of $|P_N^{(\alpha, \alpha)}(z)|$ with $z \in \mathcal{E}_\rho$.

Theorem 4.5. *Let $N \gg 1$, then we have*

$$\min_{z \in \mathcal{E}_\rho} |P_N^{(\alpha, \alpha)}(z)| \geq \frac{c_N D(\rho, \alpha)}{\Gamma(\alpha + 1)} \frac{|\Gamma(2\alpha + 1)|}{|\Gamma(\alpha + 1/2)|} \frac{\rho^N}{N^{1/2}}, \quad (4.56)$$

where $c_N \cong 1$ is a constant, and

$$D(\rho, \alpha) = \begin{cases} (1 + \rho^{-2})^{-\alpha-1/2}, & \alpha > -1/2, \\ (1 - \rho^{-2})^{-\alpha-1/2}, & \alpha < -1/2. \end{cases} \quad (4.57)$$

Proof. Recall that for any two complex numbers z_1 and z_2 , we have $||z_1| - |z_2|| \leq |z_1 - z_2|$. It follows from (4.51) that

$$\left| |1 - w^{-2}|^{-\alpha-1/2} - \frac{|P_N^{(\alpha, \alpha)}(z)|}{|A_N^\alpha| |g_N^\alpha| \rho^N} \right| \leq A(\rho, \alpha) N^{\varepsilon-1} + O(N^{-1}),$$

which implies

$$\begin{aligned} \left|1 - w^{-2}\right|^{-\alpha-1/2} - A(\rho, \alpha)N^{\varepsilon-1} - O(N^{-1}) &\leq \frac{|P_N^{(\alpha, \alpha)}(z)|}{|A_N^\alpha||g_N^\alpha|\rho^N} \\ &\leq \left|1 - w^{-2}\right|^{-\alpha-1/2} + A(\rho, \alpha)N^{\varepsilon-1} + O(N^{-1}). \end{aligned} \quad (4.58)$$

By (4.36) and (2.21)-(2.22), we have

$$\begin{aligned} |g_N^\alpha| &= \frac{\Gamma(N + \alpha + 1/2)}{|\Gamma(\alpha + 1/2)|\Gamma(N + 1)} \geq \frac{N^{\alpha-1/2}}{|\Gamma(\alpha + 1/2)|} \exp(-\Upsilon_N^{1, \alpha+1/2}), \\ |A_N^\alpha| &= \frac{|\Gamma(2\alpha + 1)|\Gamma(N + \alpha + 1)}{\Gamma(\alpha + 1)\Gamma(N + 2\alpha + 1)} \geq \frac{|\Gamma(2\alpha + 1)|}{\Gamma(\alpha + 1)} \exp(-\Upsilon_N^{2\alpha+1, \alpha+1}) N^{-\alpha}, \end{aligned} \quad (4.59)$$

and notice that

$$1 - \rho^{-2} \leq |1 - w^{-2}| \leq 1 + \rho^{-2}, \quad (4.60)$$

consequently, a combination of (4.58)-(4.60) leads to the estimate (4.56). $\square$

As the end of this subsection, we provide some numerical results to illustrate the tightness of the upper bound in (4.51). Denote by

$$E_N(\rho; \alpha) := \frac{1}{A(\rho, \alpha)} \max_{z \in \mathcal{E}_\rho} \left| (1 - w^{-2})^{-\alpha-1/2} - \frac{P_N^{(\alpha, \alpha)}(z)}{A_N^\alpha g_N^\alpha w^N} \right|. \quad (4.61)$$

To approximate the maximum value, we sample a set of points dense on the ellipse $\mathcal{E}_\rho$ based on the Joukowski transformation $z = \frac{1}{2}(w + w^{-1})$ of the Fourier points on the circle $w = \rho e^{i\theta}$. We plot in Figure 4.1 in (Matlab) log-log scale of $E_N(\rho; \alpha)$, N^{-1} and $N^{\varepsilon-1}$ (with $\varepsilon = 0.1$) for several sets of parameters α and ρ , and for large N . According to Theorem 4.4, E_N should be bounded by $N^{\varepsilon-1}$ from above, and it is anticipated to be bounded below by N^{-1} , if the estimate is tight. Indeed, we observe from Figure 4.1 such a behavior when N is large.

4.3.2 Main results

Now, we are ready to estimate the spectral interpolation and differentiation of analytic functions at Gegenbauer-Gauss-type points.

We start with the estimate of spectral interpolation at Gegenbauer-Gauss points, i.e., zeros of the Gegenbauer polynomial $P_{N+1}^{(\alpha, \alpha)}(x)$.

Figure 4.1: E_N against $N^{\varepsilon-1}$ (with $\varepsilon = 0.1$) and N^{-1} for large N .

Theorem 4.6. For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, let $(I_N u)(x)$ be the interpolant of $u(x)$ at the Gegenbauer-Gauss points $\{x_j\}_{j=0}^N$. Then

(i) for the interpolation error, we have

$$\max_{|x| \leq 1} |(u - I_N u)(x)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{2\pi d_\rho D(\rho, \alpha)} \frac{1}{\rho^{N+1}} \times \begin{cases} 2^{1/2-\alpha}, & \alpha < -1/2, \\ \frac{\Gamma(\alpha+1)}{\Gamma(2\alpha+1)} N^{\alpha+1/2}, & \alpha > -1/2; \end{cases} \quad (4.62)$$

(ii) for the first derivative, we have

$$\max_{0 \leq j \leq N} |(u - I_N u)'(x_j)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{\pi d_\rho D(\rho, \alpha)} \frac{\Gamma(\alpha+3/2)}{\Gamma(2\alpha+3)} \frac{N^{\alpha+5/2}}{\rho^{N+1}}, \quad (4.63)$$

and at the corresponding superconvergence points $\{y_j\}_{j=1}^N$, we have

$$\begin{aligned} \max_{1 \leq j \leq N} |(u - I_N u)'(y_j)| &\leq \frac{c_N M L(\mathcal{E}_\rho)}{2\pi d_\rho^2 D(\rho, \alpha)} \frac{1}{\rho^{N+1}} \\ &\times \begin{cases} 2^{1/2-\alpha}, & \alpha < -1/2, \\ \frac{\Gamma(\alpha+1)}{\Gamma(2\alpha+1)} N^{\alpha+1/2}, & \alpha > -1/2; \end{cases} \end{aligned} \quad (4.64)$$

(iii) for the second derivative, we have

$$\max_{0 \leq j \leq N} |(u - I_N u)''(x_j)| \leq \frac{2c_N M L(\mathcal{E}_\rho)}{\pi d_\rho D(\rho, \alpha)} \frac{\Gamma(\alpha+5/2)}{\Gamma(2\alpha+5)} \frac{N^{\alpha+9/2}}{\rho^{N+1}}, \quad (4.65)$$

and at the corresponding superconvergence points $\{z_j\}_{j=1}^{N-1}$, we have

$$\max_{1 \leq j \leq N-1} |(u - I_N u)''(z_j)| \leq \frac{2c_N M L(\mathcal{E}_\rho)}{\pi d_\rho^2 D(\rho, \alpha)} \frac{\Gamma(\alpha+3/2)}{\Gamma(2\alpha+3)} \frac{N^{\alpha+5/2}}{\rho^{N+1}}. \quad (4.66)$$

Here, $D(\rho, \alpha)$ is defined in (4.57), $M = \max_{z \in \mathcal{E}_\rho} |u(z)|$, the constants $L(\mathcal{E}_\rho)$ and d_ρ are defined in (2.5) and (2.6), respectively, and $c_N \cong 1$ is a generic positive constant.

Proof. For $\alpha > 1/2$, we derive from (4.14) that

$$M_Q = \max_{|x| \leq 1} |P_{N+1}^{(\alpha, \alpha)}(x)| = \frac{\Gamma(N+\alpha+2)}{\Gamma(N+2)\Gamma(\alpha+1)} \leq \frac{\exp(\Upsilon_N^{\alpha+2,2})}{\Gamma(\alpha+1)} N^\alpha, \quad (4.67)$$

For $\alpha < -1/2$, by [108, Theorem 7.33.1, Eq. (7.33.2) and Eq. (7.33.3)], we have

$$\max_{|x| \leq 1} |P_{N+1}^{(\alpha, \alpha)}(x)| \leq \frac{|A_{N+1}^\alpha|}{|\Gamma(\alpha+1/2)|} \begin{cases} \frac{\Gamma(N/2+\alpha+1)}{\Gamma(N/2+3/2)}, & N \text{ odd}; \\ \frac{2\Gamma(N/2+\alpha+3/2)}{\Gamma(N/2+1)\sqrt{(N+1)(N+2\alpha+2)}}, & N \text{ even}. \end{cases} \quad (4.68)$$

Using (2.21)-(2.22) and (4.59) leads to

$$\max_{|x| \leq 1} |P_{N+1}^{(\alpha, \alpha)}(x)| \leq \frac{c_N |\Gamma(2\alpha+1)| N^{-1/2}}{|\Gamma(\alpha+1/2)| \Gamma(\alpha+1) 2^{\alpha-1/2}}, \quad c_N \cong 1, \quad \alpha < -1/2. \quad (4.69)$$

Replacing q by α in the estimates (4.15) of $M_{Q'}$ and $M_{Q''}$, leads to

$$\begin{aligned} M_{Q'} &\leq \frac{1}{2}(N + 2\alpha + 2) \frac{\exp(\Upsilon_N^{\alpha+2,1})}{\Gamma(\alpha + 2)} N^{\alpha+1}; \\ M_{Q''} &\leq \frac{1}{4}(N + 2\alpha + 2)(N + 2\alpha + 3) \frac{\exp(\Upsilon_N^{\alpha+2,0})}{\Gamma(\alpha + 3)} N^{\alpha+2}. \end{aligned} \quad (4.70)$$

A combination of (4.56), (4.67), (4.69), (4.70) and Theorem 4.1 yields the desired estimates. $\square$

Next, we estimate the Gegenbauer-Gauss-Lobatto spectral interpolation. In this case, we have $Q_{N+1}(x) = (1 - x^2)P_{N-1}^{(\alpha+1, \alpha+1)}(x)$.

The main result is stated as follows.

Theorem 4.7. *For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, let $(I_N u)(x)$ be the interpolant of $u(x)$ at the Gegenbauer-Gauss-Lobatto points $\{x_j\}_{j=0}^N$.*

(a) *For the interpolation error, we have*

$$\max_{|x| \leq 1} |(u - I_N u)(x)| \leq c_N \frac{2ML(\mathcal{E}_\rho)(1 + \rho^{-2})^{\alpha+3/2}}{\pi d_\rho(1 - \rho^{-2})^2} \frac{\Gamma(\alpha + 3/2)}{\Gamma(2\alpha + 3)} \frac{N^{\alpha+3/2}}{\rho^{N+1}}. \quad (4.71)$$

(b) *For the first derivative, we have*

$$\max_{0 \leq j \leq N} |(u - I_N u)'(x_j)| \leq c_N \frac{4ML(\mathcal{E}_\rho)(1 + \rho^{-2})^{\alpha+3/2}}{\pi d_\rho(1 - \rho^{-2})^2} \frac{\Gamma(\alpha + 5/2)}{\Gamma(2\alpha + 5)} \frac{N^{\alpha+7/2}}{\rho^{N+1}}, \quad (4.72)$$

and at the corresponding superconvergence points $\{y_j\}_{j=1}^N$,

$$\max_{1 \leq j \leq N} |(u - I_N u)'(y_j)| \leq c_N \frac{2ML(\mathcal{E}_\rho)(1 + \rho^{-2})^{\alpha+3/2}}{\pi d_\rho^2(1 - \rho^{-2})^2} \frac{\Gamma(\alpha + 3/2)}{\Gamma(2\alpha + 3)} \frac{N^{\alpha+3/2}}{\rho^{N+1}}. \quad (4.73)$$

(c) *For the second derivative, we have*

$$\max_{0 \leq j \leq N} |(u - I_N u)''(x_j)| \leq c_N \frac{8ML(\mathcal{E}_\rho)(1 + \rho^{-2})^{\alpha+3/2}}{\pi d_\rho(1 - \rho^{-2})^2} \frac{\Gamma(\alpha + 7/2)}{\Gamma(2\alpha + 7)} \frac{N^{\alpha+11/2}}{\rho^{N+1}}, \quad (4.74)$$

and at the corresponding superconvergence points $\{z_j\}_{j=1}^{N-1}$,

$$\max_{1 \leq j \leq N-1} |(u - I_N u)''(z_j)| \leq c_N \frac{8ML(\mathcal{E}_\rho)(1 + \rho^{-2})^{\alpha+3/2}}{\pi d_\rho^2(1 - \rho^{-2})^2} \frac{\Gamma(\alpha + 5/2)}{\Gamma(2\alpha + 5)} \frac{N^{\alpha+7/2}}{\rho^{N+1}}. \quad (4.75)$$

Proof. For any $z \in \mathcal{E}_\rho$, one verifies that

$$\frac{1}{4}(\rho - \rho^{-1})^2 \leq |z^2 - 1| \leq \frac{1}{4}(\rho + \rho^{-1})^2,$$

which, together with (4.56), leads to

$$m_Q = \min_{z \in \mathcal{E}_\rho} \left| (1 - z^2) P_{N-1}^{(\alpha+1, \alpha+1)}(x) \right| \geq \frac{c_N}{4} (1 - \rho^{-2})^2 \frac{\Gamma(2\alpha + 3)(1 + \rho^{-2})^{-\alpha-3/2} \rho^{N+1}}{\Gamma(\alpha + 2)\Gamma(\alpha + 3/2)} \frac{1}{\sqrt{N}}.$$

The estimates in (4.23)-(4.25) with $q = \alpha, \beta = \alpha$, imply that

$$\begin{aligned} M_Q &\leq \frac{\exp(\Upsilon_N^{\alpha+1,0})}{\Gamma(\alpha + 2)} N^{\alpha+1}, \\ M_{Q'} &\leq \frac{2 \exp(\Upsilon_N^{\alpha+1,0})}{\Gamma(\alpha + 2)} N^{\alpha+1} + \frac{\exp(\Upsilon_N^{\alpha+1,-1})}{2\Gamma(\alpha + 3)} (N + 2\alpha + 2) N^{\alpha+2}, \\ M_{Q''} &\leq \frac{2 \exp(\Upsilon_N^{\alpha+1,0})}{\Gamma(\alpha + 2)} N^{\alpha+1} + 2(N + 2\alpha + 2) \frac{\exp(\Upsilon_N^{\alpha+1,-1})}{\Gamma(\alpha + 3)} N^{\alpha+2} \\ &\quad + \frac{\exp(\Upsilon_N^{\alpha+1,-2})}{4\Gamma(\alpha + 4)} (N + 2\alpha + 2)(N + 2\alpha + 3) N^{\alpha+3}. \end{aligned}$$

Inserting the above estimates into Theorem 4.1 leads to the desired results. $\square$

Remark 4.4. For the Gegenbauer-Gauss-Radau interpolation, by (2.15), we have

$$Q_{N+1}(x) = P_N^{(\alpha, \alpha)}(x) + \frac{N + 1}{N + 2\alpha + 1} P_{N+1}^{(\alpha, \alpha)}(x). \quad (4.76)$$

By (4.14), (4.68) and (2.21)-(2.22), we can easily obtain the estimates of $M_Q, M_{Q'}$ and $M_{Q''}$. For the estimate of m_Q , we cannot follow the proof of Theorem 4.4 directly. In fact, in this case, we need to analyze the upper bound of the remainder:

$$\left| F_\alpha(w) - \frac{Q_{N+1}(z)}{A_{N+1}^\alpha g_{N+1}^\alpha w^{N+1}} \right|, \quad \text{with } F_\alpha(w) = (1 - w^{-2})^{-\alpha-1/2} (1 + w^{-1}),$$

and the argument is similar to that in Subsection 4.3.1. For clarity of presentation, we just state the result (for the first derivative): For any $u \in \mathcal{A}_\rho$ with $\rho > 1$, let $(I_N u)(x)$ be the interpolant of $u(x)$ at the Gegenbauer-Gauss-Radau points $\{x_j\}_{j=0}^N$. Then we have

$$\max_{0 \leq j \leq N} \left| (u - I_N u)'(x_j) \right| \leq \frac{2c_N M L(\mathcal{E}_\rho)}{\pi d_\rho (\rho - 1) D(\rho, \alpha)} \frac{\Gamma(\alpha + 3/2)}{\Gamma(2\alpha + 3)} \frac{N^{\alpha+5/2}}{\rho^N}, \quad (4.77)$$

and at the corresponding superconvergence points $\{y_j\}_{j=1}^N$, we have

$$\max_{1 \leq j \leq N} |(u - I_N u)'(y_j)| \leq \frac{c_N M L(\mathcal{E}_\rho)}{\pi d_\rho^2 (\rho - 1) D(\rho, \alpha)} \frac{1}{\rho^N} \begin{cases} 2^{1/2-\alpha}, & \alpha < -1/2, \\ \frac{\Gamma(\alpha + 1)}{\Gamma(2\alpha + 1)} N^{\alpha+1/2}, & \alpha > -1/2, \end{cases}$$

where $D(\rho, \alpha)$ is given in (4.57), $d_\rho, M, L(\mathcal{E}_\rho)$ and c_N are the same as before. We provide the detailed proof in our paper [116] for the Legendre-Gauss-Radau case. The Gegenbauer-Gauss-Radau case can be proved in a similar fashion, but the analysis is much more involved. $\square$

4.4 Numerical results

In this section, we provide two numerical examples to demonstrate the sharpness of the estimates established in Theorems 4.6 and 4.7.

Example 1: We take

$$u(x) = \frac{1}{x^2 + 1}, \quad (4.78)$$

which has two simple poles at $\pm i$. We are free to choose $\mathcal{E}_\rho$ with ρ in the range

$$b = \frac{1}{2}(\rho - \rho^{-1}) \implies 1 < \rho < 1 + \sqrt{2} \approx 2.414, \quad (4.79)$$

such that u is analytic on and within $\mathcal{E}_\rho$. To compare the (discrete) maximum error of spectral differentiation with the upper bound, we sample about 2000 values of ρ equally from $(1, 1 + \sqrt{2})$, and find a tighter upper bound (which is usually attained when ρ is close to $1 + \sqrt{2}$). In Figure 4.2 (a)-(b), we plot the (discrete) maximum errors of spectral differentiation against the upper bounds. We visualize the exponential decay of the errors, and the upper bounds and the errors decay at almost the same rate. Moreover, it seems that the bounds are slightly sharper in the Gegenbauer-Gauss case.

Example 2: The estimates indicates that the errors essentially depend on the location of singularity (although it affects the constant M) rather than the

(a) Upper bound vs Max.-error (Example 1) (b) Upper bound vs Max.-error (Example 1)

(c) Upper bound vs Max.-error (Example 2) (d) Upper bound vs Max.-error (Example 2)

Figure 4.2: The (discrete) maximum errors of GG and GGL spectral differentiation against the upper bounds in Theorems 4.6 and 4.7 with $\alpha = 1, 2$. Example 1 (a)-(b), and Example 2 (c)-(d). In the legend, GG SP err (resp. GGL SP err) represents the Gegenbauer-Gauss (resp. Gegenbauer-Gauss-Lobatto) spectral differentiation error.

behavior of the singularity. To show this, we test the function with poles at $\pm i$ of order 2 :

$$u(x) = \frac{1}{(x^2 + 1)^2}. \quad (4.80)$$

We plot in Figure 4.2 (c)-(d) the errors and upper bounds as in (a)-(b). Indeed, a similar convergence behavior is observed. Indeed, Boyd [17] pointed out that the type of singularity might change the rate of convergence by a power of N , but not an exponential function of N .

Part II

Time-Domain Computation of
Scattering Problems

Acoustic Scattering Problems[†]

Wave propagation and scattering problems in unbounded media arise from diverse application areas such as acoustics, aerodynamics, electromagnetics, antenna design, oceanography and among others (see, e.g., [47, 103, 31]). Various approaches have been proposed for their numerical simulation as addressed in Section 1.2. An important method is to truncate an unbounded domain to a bounded domain by imposing an exact or approximate nonreflecting (absorbing or transparent) boundary condition at the outer artificial boundary, where the NRBC is designed to prevent spurious wave reflection from the artificial boundary (cf. the review papers [47, 48] and the references therein). The frequency-domain approaches using such boundary conditions for e.g., the time-harmonic Helmholtz problems have been intensively investigated, while the time-domain simulations, which are capable of capturing wide-band signals and modeling more general material inhomogeneities and nonlinearities (cf. [4, 30]), have been relatively less studied.

In this chapter, we restrict our attention to the exact time-domain circular/spherical NRBC. As described in Section 1.2, one major difficulty lies in that such an NRBC is *global* in space and time in nature, as it involves the

[†]The main part of this chapter is based on the paper [115]: “L.L. Wang, B. Wang and X.D. Zhao. Fast and accurate computation of time-domain acoustic scattering problems with exact nonreflecting boundary conditions. *SIAM J. Appl. Math.*, 72(6):1869–1898, 2012.”

Fourier/spherical harmonic expressions in space, and history dependence in time induced by a convolution. The convolution kernel NRBK is the inverse Laplace transform of an expression that includes the logarithmic derivative of a modified Bessel function. We derive an analytic formula for the NRBK based on a direct inversion of the Laplace transform (see Theorem 5.1 below). We show that with these formulas, we can evaluate the temporal convolution recursively and rapidly with $O(N_t)$ operations and almost without extra memory for the history dependence as in [3]. The analytic expression provides a useful apparatus for the stability and convergence analysis. We also propose an efficient spectral-Galerkin method with Newmark scheme for the truncated problem in an annulus or a spherical shell. We provide a practical approach to significantly reduce the computational cost for computing the NRBC via the analytic formulas.

This chapter is organized as follows. In Section 5.1, we present the formulation of NRBCs, and derive analytic formulas for NRBKs. In Section 5.2, we present some properties of the NRBKs and analyze the well-posedness of the truncated wave equation. In Section 5.3, we outline the notion of the transformed field expansion (TFE) method and propose an efficient spectral-Galerkin and Newmark scheme for the truncated problem in regular domains. In Section 5.4, we provide ample numerical results to show the accuracy and efficiency of the proposed approach.

5.1 Evaluation of NRBKs

We consider the time-domain acoustic scattering problem with sound-soft boundary conditions on the bounded obstacle:

$$\partial_t^2 U = c^2 \Delta U + F, \quad \text{in } \Omega_\infty := \mathbb{R}^d \setminus \bar{D}, \quad t > 0, \quad d = 2, 3; \quad (5.1)$$

$$U = U_0, \quad \partial_t U = U_1, \quad \text{in } \Omega_\infty, \quad t = 0; \quad (5.2)$$

$$U = G, \quad \text{on } \Gamma_D, \quad t > 0; \quad \partial_t U + c \partial_{\mathbf{n}} U = o(|\mathbf{x}|^{(1-d)/2}), \quad |\mathbf{x}| \rightarrow \infty, \quad t > 0, \quad (5.3)$$

where D is a bounded obstacle (scatterer) with Lipschitz boundary Γ_D , $c > 0$ is the wave speed, and $\mathbf{n} = \mathbf{x}/|\mathbf{x}|$. Assume that the data F, U_0 and U_1 are compactly supported in a 2-D disk or a 3-D ball B of radius b , which contains the obstacle D .

A common way is to reduce this exterior problem to the problem in a bounded domain by imposing an exact or approximate NRBC at the artificial boundary $\Gamma_b := \partial B$. In what follows, we are concerned with the wave equation truncated by the exact circular/spherical NRBC:

$$\partial_t^2 U = c^2 \Delta U + F, \quad \text{in } \Omega := B \setminus \bar{D}, \quad t > 0, \quad d = 2, 3; \quad (5.4)$$

$$U = U_0, \quad \partial_t U = U_1, \quad \text{in } \Omega, \quad t = 0; \quad U = G, \quad \text{on } \Gamma_D, \quad t > 0; \quad (5.5)$$

$$\partial_r U = T_d(U), \quad \text{at } r = b, \quad t > 0, \quad (5.6)$$

where $T_d(U)$ is the so-called time-domain DtN map, to be specified below.

5.1.1 Formulation of the DtN map

We briefly review the derivation and formulation of the NRBC (5.6) (see, e.g., [61, 4]). Consider the “auxiliary” exterior problem:

$$\begin{aligned} \partial_t^2 U^e &= c^2 \Delta U^e, \quad \text{in } \Omega_{\text{ext}} := \mathbb{R}^d \setminus \bar{B}, \quad t > 0, \quad d = 2, 3; \\ U^e|_{r=b} &= U|_{r=b}, \quad t > 0; \quad U^e|_{t=0} = \partial_t U^e|_{t=0} = 0, \quad \text{in } \Omega_{\text{ext}}, \end{aligned} \quad (5.7)$$

together with the radiation condition (5.3) at infinity, where the Dirichlet data $U|_{r=b}$ is taken from the interior problem (5.4)-(5.6). The problem (5.7) can be solved analytically by using Laplace transform in time and separation of variables in space.

Let $u = \mathcal{L}[U^e]$ be the Laplace transform of U^e , defined by

$$u(\mathbf{x}, s) = \mathcal{L}[U^e](\mathbf{x}, s) = \int_0^\infty e^{-st} U^e(\mathbf{x}, t) dt, \quad s \in \mathbb{C}, \quad \text{Re}(s) > 0, \quad \mathbf{x} \in \Omega_{\text{ext}}, \quad (5.8)$$

and likewise for $\psi = \mathcal{L}[U|_{r=b}]$. Applying Laplace transform to (5.7) leads to

$$\begin{aligned} -c^2 \Delta u + s^2 u &= 0, \quad \text{in } \Omega_{\text{ext}}, \quad s \in \mathbb{C}, \quad \text{Re}(s) > 0; \\ u|_{r=b} &= \psi; \quad c \partial_r u + s u = o(r^{(1-d)/2}), \quad d = 2, 3, \end{aligned} \quad (5.9)$$

which can be solved by separation of variables.

In the 3-D case, the equation (5.9) admits the series solution:

$$u(r, \theta, \phi, s) = \sum_{n=0}^{\infty} \frac{k_n(sr/c)}{k_n(sb/c)} \sum_{|m|=0}^n \hat{\psi}_{nm}(s) Y_n^m(\theta, \phi), \quad (5.10)$$

where $(r, \theta, \phi) \in [b, \infty) \times [0, \pi] \times [0, 2\pi)$ is the spherical coordinates, and $\{Y_n^m\}$ are the spherical harmonics, which are orthonormal as defined in the book [87]. In (5.10), k_n is the modified spherical Bessel function of the second kind, defined by

$$k_n(z) = \sqrt{\frac{2}{\pi z}} K_{n+1/2}(z), \quad n \geq 0, \quad (5.11)$$

where $K_{n+1/2}$ is the modified Bessel function of the second kind (see, e.g., [1, 118]), and $\{\hat{\psi}_{nm}\}$ are the spherical harmonic expansion coefficients of the Laplace transformed Dirichlet data in (5.9):

$$\mathcal{L}[U|_{r=b}] = \psi(\theta, \phi, s) = \sum_{n=0}^{\infty} \sum_{|m|=0}^n \hat{\psi}_{nm}(s) Y_n^m(\theta, \phi). \quad (5.12)$$

Therefore, the Neumann data at Γ_b (in the Laplace transformed domain) can be obtained by

$$\left. \frac{\partial u}{\partial r} \right|_{r=b} = \sum_{n=0}^{\infty} \frac{s k'_n(sb/c)}{c k_n(sb/c)} \sum_{|m|=0}^n \hat{\psi}_{nm}(s) Y_n^m(\theta, \phi). \quad (5.13)$$

Applying the inverse Laplace transform on both sides of (5.13) leads to the time-domain DtN map:

$$\left. \frac{\partial U^e}{\partial r} \right|_{r=b} = T_d(U) := -\frac{1}{c} \left. \frac{\partial U}{\partial t} \right|_{r=b} + \frac{1}{c} \sum_{n=0}^{\infty} \sum_{|m|=0}^n \omega_{n+1/2}(t) * \partial_t \widehat{U}_{nm}(b, t) Y_n^m(\theta, \phi), \quad (5.14)$$

where $\{\widehat{U}_{nm}\}$ are the spherical harmonic expansion coefficients of $U|_{r=b}$, “ $*$ ” is the convolution operation defined as usual: $(f * g)(t) = \int_0^t f(t - \tau)g(\tau)d\tau$, and

$$\omega_{n+1/2}(t) := \mathcal{L}^{-1} \left[1 + \frac{k'_n(sb/c)}{k_n(sb/c)} \right] (t) = \mathcal{L}^{-1} \left[1 - \frac{c}{2bs} + \frac{K'_{n+1/2}(sb/c)}{K_{n+1/2}(sb/c)} \right] (t), \quad (5.15)$$

for $n \geq 0$.

By requiring $\partial_r U = \partial_r U^e$ at $r = b$, we derive the NRBC with $d = 3$ in (5.6).

Remark 5.1. To derive (5.14) from (5.13), we used the property $\mathcal{L}^{-1}[s\hat{\psi}_{nm}] = \partial_t \widehat{U}_{nm}(b, t)$, and added 1 to the ratio k'_n/k_n in $\omega_{n+1/2}(t)$ for the purpose of removing its singular part. Indeed, recall the asymptotic formula for fixed $\nu \geq 0$ and large $|z|$ (see [1, Formula 9.7.2]):

$$K_\nu(z) \sim \sqrt{\frac{\pi}{2z}} e^{-z} \left\{ 1 + \frac{4\nu^2 - 1}{8z} + O(z^{-2}) \right\}, \quad (5.16)$$

for $|\arg z| < 3\pi/2$, and the recurrence relation:

$$zK'_\nu(z) = \nu K_\nu(z) - zK_{\nu+1}(z). \quad (5.17)$$

One verifies that

$$\frac{K'_\nu(z)}{K_\nu(z)} \sim -1 - \frac{1}{2z} + O(z^{-2}), \quad (5.18)$$

and

$$\frac{k'_n(z)}{k_n(z)} = -\frac{1}{2z} + \frac{K'_{n+1/2}(z)}{K_{n+1/2}(z)} \sim -1 - \frac{1}{z} + O(z^{-2}). \quad (5.19)$$

Therefore, $1 + k'_n/k_n$ tends to zero as $|z| \rightarrow \infty$. $\square$

Similarly, in the 2-D case, applying the method of separation of variables to solve (5.9) leads to the series solution outside B :

$$u(r, \phi, s) = \sum_{|n|=0}^{\infty} \frac{K_n(sr/c)}{K_n(sb/c)} \hat{\psi}_n(s) e^{in\phi}, \quad (5.20)$$

where $(r, \phi) \in [b, \infty) \times [0, 2\pi)$ is the polar coordinate, K_n is the modified Bessel function of the second kind of order n (cf. [1]), and $\{\hat{\psi}_n\}$ are the Fourier expansion coefficients of ψ in (5.9). Thus, we can obtain the DtN map for $d = 2$:

$$T_d(U) = -\frac{1}{c} \frac{\partial U}{\partial t} \Big|_{r=b} + \frac{1}{c} \sum_{|n|=0}^{\infty} \omega_n(t) * \partial_t \widehat{U}_n(b, t) e^{in\phi}, \quad (5.21)$$

where

$$\omega_n(t) := \mathcal{L}^{-1} \left[1 + \frac{K'_n(sb/c)}{K_n(sb/c)} \right] (t). \quad (5.22)$$

Hence, a combination of (5.14), (5.15) and (5.21)-(5.22) yields that

$$T_d(U) = -\frac{1}{c} \frac{\partial U}{\partial t} \Big|_{r=b} + \frac{1}{c} \begin{cases} \sum_{|n|=0}^{\infty} \omega_n(t) * \partial_t \widehat{U}_n(b, t) e^{in\phi}, & d = 2, \\ \sum_{n=0}^{\infty} \sum_{|m|=0}^n \omega_{n+1/2}(t) * \partial_t \widehat{U}_{nm}(b, t) Y_n^m(\theta, \phi), & d = 3, \end{cases} \quad (5.23)$$

where for $d = 2, 3$,

$$\omega_\nu(t) = \mathcal{L}^{-1} \left[1 - \frac{(d-2)c}{2bs} + \frac{K'_\nu(sb/c)}{K_\nu(sb/c)} \right] (t), \quad \nu = n, n + 1/2. \quad (5.24)$$

It is seen that the time-domain DtN maps (5.23) involve the convolution of the temporal derivative of the Dirichlet data, and accordingly, the NRBC (5.6) corresponds to the DtN boundary condition of the Helmholtz equation in the frequency domain (see, e.g., [32, 87]). Alternatively, we can reformulate (5.23) as the convolution involving only the Dirichlet data on Γ_b as in [61, 4]:

$$T_d(U) = \begin{cases} \left(-\frac{1}{c} \frac{\partial U}{\partial t} - \frac{U}{2r} \right) \Big|_{r=b} + \sum_{|n|=0}^{\infty} \sigma_n(t) * \widehat{U}_n(b, t) e^{in\phi}, & d = 2, \\ \left(-\frac{1}{c} \frac{\partial U}{\partial t} - \frac{U}{r} \right) \Big|_{r=b} + \sum_{n=0}^{\infty} \sum_{|m|=0}^n \sigma_{n+1/2}(t) * \widehat{U}_{nm}(b, t) Y_n^m(\theta, \phi), & d = 3, \end{cases} \quad (5.25)$$

where

$$\sigma_\nu(t) := \mathcal{L}^{-1} \left[\frac{s}{c} + \frac{1}{2b} + \frac{s}{c} \frac{K'_\nu(sb/c)}{K_\nu(sb/c)} \right], \quad \nu = n, n + 1/2. \quad (5.26)$$

Once again, in view of (5.18) and (5.19), we removed the singular part by subtracting the first two terms of the ratio $sK'_\nu/(cK_\nu)$.

In fact, these two nonreflecting boundary kernels have the following relation.

Lemma 5.1. *We have*

$$\omega_\nu(t) = \begin{cases} -\frac{c}{2b} + c \int_0^t \sigma_\nu(\tau) d\tau, & \text{for } d = 2, \\ -\frac{c}{b} + c \int_0^t \sigma_\nu(\tau) d\tau, & \text{for } d = 3. \end{cases} \quad (5.27)$$

Proof. We first consider the kernels for $d = 2$. It follows from (5.22), (5.26) and the properties of Laplace transform that

$$\begin{aligned}\omega_n(t) &= \mathcal{L}^{-1} \left[\left(\frac{s}{c} + \frac{1}{2b} + \frac{s K'_n(sb/c)}{c K_n(sb/c)} \right) \frac{c}{s} - \frac{c}{2bs} \right] = \sigma_n(t) * \mathcal{L}^{-1} \left[\frac{c}{s} \right] - \frac{c}{2b} \mathcal{L}^{-1} \left[\frac{1}{s} \right] \\ &= \sigma_n(t) * c - \frac{c}{2b} = c \int_0^t \sigma_n(\tau) d\tau - \frac{c}{2b}.\end{aligned}$$

Similarly, we can derive (5.27) for $d = 3$. $\square$

Remark 5.2. *We find that the use of the NRBC involving ω_ν is more convenient, if one reformulates (5.4) into a first-order (with respect to the time variable) system (cf. [25]), and it is also more suitable for analysis, while the latter involving σ_ν is more appropriate for computation.* $\square$

Hereafter, we term σ_ν and ω_ν as the nonreflecting boundary kernels (NRBKs). Since $K_{-n}(z) = K_n(z)$ (see [1, Formula 9.6.6]), it suffices to consider ω_n and σ_n with $n \geq 0$, for $d = 2$.

We see that NRBCs are global in both time and space. To solve the truncated problem (5.4)-(5.6) efficiently, we need to (i) invert the Laplace transform to compute NRBKs; (ii) deal with temporal convolutions efficiently; and (iii) handle the nonlocality of the NRBC in space effectively. The rest of this chapter will address these issues.

5.1.2 Analytic formulas of NRBKs

Our starting point is to invert the Laplace transform via evaluating the Bromwich contour integral:

$$\begin{aligned}\sigma_\nu(t) &= \frac{1}{2\pi i} \int_{\gamma-\infty i}^{\gamma+\infty i} \left(\frac{s}{c} + \frac{1}{2b} + \frac{s K'_\nu(sb/c)}{c K_\nu(sb/c)} \right) e^{ts} ds \\ &= \frac{c}{2b^2 \pi i} \int_{\gamma-\infty i}^{\gamma+\infty i} F_\nu(z) e^{czt/b} dz,\end{aligned}\tag{5.28}$$

for $\nu = n, n + 1/2$ with $n \geq 0$, where

$$F_\nu(z) = z + \frac{1}{2} + z \frac{K'_\nu(z)}{K_\nu(z)},\tag{5.29}$$

and γ is the Laplace convergence abscissa, which is a generic constant greater than the real part of any singularity of $F_\nu(z)$.

In order to use the residue theorem to evaluate (5.28), it is essential to understand the behavior of the poles of $F_\nu(z)$, i.e., the zeros of $K_\nu(z)$.

Lemma 5.2. *Let $\nu \geq 0$ be a real number.*

- (i) *If z is a zero of $K_\nu(z)$, then its complex conjugate $\bar{z}$ is also a zero. Moreover, all complex conjugate pairs of zeros lie in the second and third quadrants with $\operatorname{Re}(z) < 0$.*
- (ii) *The total number of zeros of $K_\nu(z)$ is the even integer nearest to $\nu - 1/2$, if $\nu - 1/2$ is not an integer, or exactly $\nu - 1/2$, if $\nu - 1/2$ is an integer.*
- (iii) *All zeros of $K_n(z)$ and $K_{n+1/2}(z)$ are simple, and lie approximately along the left half of the boundary of an eye-shaped domain around $z = 0$ (see Figure 5.1).*

Proof. The properties (i) and (ii) can be found from [118, Page 511]. We now consider the property (iii). As a consequence of (i), it suffices to consider the zeros of $K_\nu(z)$ in the third quadrant and on the negative real axis (i.e., with $-\pi \leq \arg z < -\pi/2$) of the complex plane. According to [1, Formula 9.6.4], we have the following relation between $K_\nu(z)$ and the Hankel function of the first kind:

$$K_\nu(z) = \frac{\pi i}{2} e^{\frac{1}{2}\nu\pi i} H_\nu^{(1)}(iz), \quad -\pi < \arg z \leq \frac{\pi}{2}, \quad (5.30)$$

which implies that all zeros of $K_\nu(z)$ in the third quadrant (i.e., with $-\pi < \arg z < -\pi/2$) are obtained by rotating all zeros of $H_\nu^{(1)}(z)$ in the fourth quadrant (i.e., with $-\pi/2 < \arg z < 0$) by an angle $-\pi/2$. Recall that the zeros of $H_\nu^1(z)$ in the fourth quadrant lie approximately along the boundary of an eye-shaped domain around $z = 0$ (see [1, Figure 9.6 and Page 441]), whose boundary curve intersects the real axis at $z = n$ and the imaginary axis at $z = -ina$, where $a = \sqrt{t_0^2 - 1} \approx 0.66274$ and $t_0 \approx 1.19968$ is the positive root of $\coth t = t$. $\square$

Figure 5.1: Distributions of $\{z_j^\nu\}_{j=1}^{M_\nu}$ of K_n (left) and $K_{n+1/2}$ (right) for various n .

For clarity, let M_ν be the total number of zeros of $K_\nu(z)$ with $\nu = n, n + 1/2$, that is,

$$M_\nu = \begin{cases} \text{the largest even integer nearest to } n - 1/2, & \text{for } K_n(z), \\ n, & \text{for } K_{n+1/2}(z). \end{cases} \quad (5.31)$$

We plot in Figure 5.1 some samples of zeros of $K_n(z)$ and $K_{n+1/2}(z)$ for various n , and visualize that for a given n , the zeros sit on the left half boundary of an eye-shaped domain that intersects the imaginary axis approximately at $\pm ni$, and the negative real axis at $-na$ with $a \approx 0.66274$ (see the dashed coordinate grids) as predicted by Lemma 5.2 (iii).

With the above understanding of the poles of the integrand $F_\nu(z)$ in (5.29), we now present the exact formula for the NRBKs $\sigma_\nu(t)$ with $\nu = n, n + 1/2$.

Theorem 5.1. *Let $\nu = n, n + 1/2$ with $n \geq 0$, and let $\{z_j^\nu\}_{j=1}^{M_\nu}$ be the zeros of $K_\nu(z)$. Then*

- for $d = 2$,

$$\sigma_n(t) = \frac{c}{b^2} \left\{ \sum_{j=1}^{M_n} z_j^n e^{ctz_j^n/b} + (-1)^n \int_0^\infty \frac{e^{-ctr/b}}{K_n^2(r) + \pi^2 I_n^2(r)} dr \right\}, \quad (5.32)$$

- for $d = 3$,

$$\sigma_\nu(t) = \frac{c}{b^2} \sum_{j=1}^{M_\nu} z_j^\nu e^{ctz_j^\nu/b}, \quad \nu = n + 1/2, \quad (5.33)$$

where $I_n(z)$ is the modified Bessel function of the first kind (cf. [1]).

Proof. We first consider $d = 2$. Note that $F_n(z)$ is a multi-valued function with branch points at $z = 0$ and infinity. The contour L for (5.28) is depicted in Figure 5.2 (left) with the branch-cut along the negative real axis.

Figure 5.2: Contour L for the inverse Laplace transform. Left: $d = 2$. Right: $d = 3$.

We know from Lemma 5.2 that $F_n(z)$ has a finite number of simple poles in the second and third quadrants. Therefore, for any $n \geq 0$, it follows from the residue theorem that

$$\begin{aligned} \lim_{\substack{R \rightarrow +\infty \\ r \rightarrow 0^+}} \oint_L F_n(z) e^{czt/b} dz &= 2\pi i \sum_{j=1}^{M_n} \text{Res} [F_n(z) e^{czt/b}, z_j^n] \\ &= 2\pi i \sum_{j=1}^{M_n} \lim_{z \rightarrow z_j^n} \left\{ (z - z_j^n) e^{czt/b} \left[z + \frac{1}{2} + z \frac{K'_n(z)}{K_n(z)} \right] \right\} = 2\pi i \sum_{j=1}^{M_n} e^{ctz_j^n/b} z_j^n. \end{aligned} \quad (5.34)$$

Thus, by (5.28) and (5.34),

$$\begin{aligned} \frac{2b^2\pi i}{c} \sigma_n(t) &= 2\pi i \sum_{j=1}^{M_n} e^{ctz_j^n/b} z_j^n - \lim_{\substack{R \rightarrow +\infty \\ r \rightarrow 0^+}} \left[\int_{\widehat{BC}} F_n(z) e^{czt/b} dz \right. \\ &\quad + \int_{\widehat{CD}} F_n(z) e^{czt/b} dz + \int_{\widehat{DEF}} F_n(z) e^{czt/b} dz \\ &\quad \left. + \int_{\widehat{FG}} F_n(z) e^{czt/b} dz + \int_{\widehat{GA}} F_n(z) e^{czt/b} dz \right]. \end{aligned} \quad (5.35)$$

In view of (5.18), we find from the Jordan's lemma (cf. [35, 29]) and a direct calculation that

$$\lim_{\substack{R \rightarrow +\infty \\ r \rightarrow 0^+}} \left[\int_{\widehat{BC}} F_n(z) e^{czt/b} dz + \int_{\widehat{DEF}} F_n(z) e^{czt/b} dz + \int_{\widehat{GA}} F_n(z) e^{czt/b} dz \right] = 0, \quad (5.36)$$

since each contour integral tends to zero. Thus, we only need to evaluate the integrals along the line segments $\overline{CD}$ and $\overline{FG}$. We have

$$\begin{aligned} & \lim_{\substack{R \rightarrow +\infty \\ r \rightarrow 0^+}} \left[\int_{\overline{CD}} F_n(z) e^{czt/b} dz + \int_{\overline{FG}} F_n(z) e^{czt/b} dz \right] \\ &= \int_0^\infty r e^{-ctr/b} \left[\frac{K'_n(re^{-i\pi})}{K_n(re^{-i\pi})} - \frac{K'_n(re^{i\pi})}{K_n(re^{i\pi})} \right] dr. \end{aligned}$$

By [1, Formula 9.6.31],

$$K_n(re^{\pi i}) = e^{-n\pi i} K_n(r) - \pi i I_n(r), \quad K_n(re^{-\pi i}) = e^{n\pi i} K_n(r) + \pi i I_n(r),$$

which, together with (5.17), implies

$$\begin{aligned} & \frac{K'_n(re^{i\pi})}{K_n(re^{i\pi})} - \frac{K'_n(re^{-i\pi})}{K_n(re^{-i\pi})} = \frac{K_{n+1}(re^{-i\pi})}{K_n(re^{-i\pi})} - \frac{K_{n+1}(re^{i\pi})}{K_n(re^{i\pi})} \\ &= \frac{e^{(n+1)\pi i} K_{n+1}(r) + \pi i I_{n+1}(r)}{e^{n\pi i} K_n(r) + \pi i I_n(r)} - \frac{e^{-(n+1)\pi i} K_{n+1}(r) - \pi i I_{n+1}(r)}{e^{-n\pi i} K_n(r) - \pi i I_n(r)} \\ &= \frac{(-1)^n 2\pi i [K_{n+1}(r) I_n(r) + K_n(r) I_{n+1}(r)]}{K_n^2(r) + \pi^2 I_n^2(r)} = \frac{(-1)^n 2\pi i}{r [K_n^2(r) + \pi^2 I_n^2(r)]}, \end{aligned} \quad (5.37)$$

where we used the Wronskian identity (see [1, Formula 9.6.15]):

$$I_n(z) K_{n+1}(z) + I_{n+1}(z) K_n(z) = z^{-1}. \quad (5.38)$$

A combination of (5.34)-(5.37) leads to

$$\sigma_n(t) = \frac{c}{b^2} \left\{ \sum_{j=1}^{M_n} z_j^n e^{ctz_j^n/b} + \int_0^\infty \frac{(-1)^n e^{-ctr/b}}{K_n^2(r) + \pi^2 I_n^2(r)} dr \right\}, \quad (5.39)$$

which is the expression (5.32).

Now, we turn to the three dimensional case. It is important to notice that the kernel function $F_{n+1/2}(z)$ is not a multi-valued complex function, as opposed

to the two dimensional case. Indeed, although $K_{n+1/2}(z)$ is multi-valued, in view of the formula (see [118, Page 80]):

$$K_{n+1/2}(z) = \sqrt{\frac{\pi}{2z}} \sum_{k=0}^n \frac{(n+k)!e^{-z}}{k!(n-k)!(2z)^k}, \quad \forall n \geq 0, \quad (5.40)$$

the fact $1/\sqrt{z}$ can be eliminated from the ratio $K'_{n+1/2}/K_{n+1/2}$. Thanks to this property, we use the contour in Figure 5.2 (right), by the residue theorem and Jordan's lemma, we have

$$\begin{aligned} \lim_{R \rightarrow +\infty} \oint_L F_{n+1/2}(z) e^{czt/b} dz &= \int_{\gamma-\infty i}^{\gamma+\infty i} F_{n+1/2}(z) e^{czt/b} dz \\ &= 2\pi i \sum_{j=1}^{M_\nu} \text{Res} [F_{n+1/2}(z) e^{czt/b}, z_j^\nu] = 2\pi i \sum_{j=1}^{M_\nu} e^{ctz_j^\nu/b} z_j^\nu, \end{aligned} \quad (5.41)$$

for $\nu = n + 1/2$. This leads to the formula (5.33). $\square$

We remark that Sofronov [105] derived formulas of similar type by working on much more complicated expressions in terms of Tricomi's confluent hypergeometric functions. However, the formulas in the above theorem are more compact and informative.

Remark 5.3. Based on a delicate study of the logarithmic derivative of the Hankel function $H_\nu^{(1)}(z)$, Alpert et al. [3] (see [3, Theorem 4.1 and Lemma 4.2]) obtained the following formula:

$$\begin{aligned} z \frac{H_\nu^{(1)'}(z)}{H_\nu^{(1)}(z)} &= iz - \frac{1}{2} + \sum_{j=1}^{N_\nu} \frac{h_{\nu,j}}{z - h_{\nu,j}} \\ &\quad - \frac{1}{\pi i} \int_0^\infty \frac{\pi \cos(\nu\pi)}{\cos^2(\nu\pi) K_\nu^2(r) + (\pi I_\nu(r) + \sin(\nu\pi) K_\nu(r))^2} \frac{1}{ir + z} dr, \end{aligned} \quad (5.42)$$

for any $\nu \neq n + 1/2$, where $h_{\nu,1}, h_{\nu,2}, \dots, h_{\nu,N_\nu}$ are the zeros of $H_\nu^{(1)}(z)$, which number N_ν . $\square$

Interestingly, (5.32) can be derived from (5.42), which is justified as follows.

Justification: Thanks to (5.30), we have

$$z \frac{H_\nu^{(1)'}(z)}{H_\nu^{(1)}(z)} = -iz \frac{K'_\nu(-iz)}{K_\nu(-iz)}.$$

Thus, by (5.42) with $\nu = n$ and $-iz = bs/c$, we find

$$\frac{s}{c} + \frac{1}{2b} + \frac{s K'_n(bs/c)}{c K_n(bs/c)} = -\frac{ic}{b^2} \sum_{j=1}^{N_n} \frac{h_{n,j}}{s + \frac{ich_{n,j}}{b}} + \frac{c}{b^2} \int_0^\infty \frac{(-1)^n}{K_n^2(r) + \pi^2 I_n^2(r)} \frac{1}{\frac{cr}{b} + s} dr.$$

Applying the inverse Laplace transform to both sides of the above identity leads to

$$\begin{aligned} \mathcal{L}^{-1} \left[\frac{s}{c} + \frac{1}{2b} + \frac{s K'_n(bs/c)}{c K_n(bs/c)} \right] &= \frac{c}{b^2} \sum_{j=1}^{N_n} (-ih_{n,j}) e^{-ict h_{n,j}/b} \\ &\quad + \frac{c}{b^2} \int_0^\infty \frac{(-1)^n e^{-crt/b}}{K_n^2(r) + \pi^2 I_n^2(r)} dr, \end{aligned}$$

which turns out to be (5.39), since $-ih_{n,j}$ are zeros of $K_n(z)$ and $N_n = M_n$. $\square$

Thanks to Lemma 5.1, we obtain from Theorem 5.1 the following exact expressions of the NRBK $\omega_\nu(t)$ in (5.24).

Remark 5.4. Thanks to (5.27), we obtain from Theorem 5.1 the expression of $\omega_\nu(t)$:

- for $d = 2$,

$$\omega_n(t) = -\frac{c}{2b} + \frac{c}{b} \left\{ \sum_{j=1}^{M_n} (e^{ctz_j^n/b} - 1) + (-1)^n \int_0^\infty \frac{1 - e^{-ctr/b}}{r \{K_n^2(r) + \pi^2 I_n^2(r)\}} dr \right\}, \quad (5.43)$$

- for $d = 3$,

$$\omega_\nu(t) = -\frac{c}{b} + \frac{c}{b} \sum_{j=1}^{M_\nu} (e^{ctz_j^\nu/b} - 1), \quad \nu = n + 1/2. \quad \square \quad (5.44)$$

5.1.3 Computation of the improper integral in (5.32)

The computation of the two-dimensional NRBK requires to evaluate the improper integral involving the kernel function:

$$W_n(r) := \frac{1}{K_n^2(r) + \pi^2 I_n^2(r)} := \frac{1}{G_n(r)}, \quad n \geq 0, \quad r > 0, \quad (5.45)$$

whose important properties are characterized below.

Lemma 5.3. For any $n \geq 0$ and any real $r > 0$, we have

- (i) $G_n(r)$ is a convex function on the positive real axis, and $W_n(r)$ attains its maximum at a unique point.
- (ii) For large n , we have the uniform asymptotic estimate:

$$W_n(n\kappa) \sim \frac{n\sqrt{1+\kappa^2}}{\pi} \operatorname{sech}(2n\Theta) := \widetilde{W}_n(n\kappa), \quad \kappa > 0, \quad (5.46)$$

where

$$\Theta = \Theta(\kappa) := \sqrt{1+\kappa^2} + \ln \frac{\kappa}{1+\sqrt{1+\kappa^2}}. \quad (5.47)$$

Approximately, the maximum value of $W_n(r)$ is attained at $r = na$ with $a \approx 0.66274$ being the root of Θ , and the maximum value is approximately $n\sqrt{1+a^2}/\pi \approx 0.38187n$.

Proof. (i). We find from [1, Page 374] that for a given n , $K_n(r), I_n(r) > 0$, and $K_n(r)$ (resp. $I_n(r)$) is monotonically descending (resp. ascending) with respect to r . From the series representation (see [1, Formula 9.6.10]):

$$I_n(r) = \frac{r^n}{2^n} \sum_{k=0}^{\infty} \frac{r^{2k}}{2^{2k} k! (n+k)!}, \quad n \geq 0,$$

we conclude that $I_n''(r) > 0$.

Moreover, since $K_n(r)$ satisfies (see [1, Formula 9.6.1])

$$r^2 K_n''(r) + r K_n'(r) - (r^2 + n^2) K_n(r) = 0,$$

we have $K_n''(r) > 0$. Therefore, a direct calculation shows that $G_n''(r) > 0$, so $G_n(r)$ is convex.

One verifies that $G_n(0+) = G_n(+\infty) = +\infty$ for all n , which follows from

$$K_\nu(r) \sim \sqrt{\frac{\pi}{2r}} e^{-r} \left\{ 1 + \frac{4\nu^2 - 1}{8r} + O(r^{-2}) \right\},$$

(cf. (5.16)), and the asymptotic properties (see [1] again):

$$K_\nu(r) \sim \begin{cases} -\ln r, & \text{if } \nu = 0, \\ \frac{\Gamma(\nu)}{2} \left(\frac{r}{2}\right)^{-\nu}, & \text{if } \nu > 0, \end{cases} \quad I_\nu(r) \sim \frac{1}{\Gamma(\nu+1)} \left(\frac{r}{2}\right)^\nu, \quad \nu \geq 0, \quad (5.48)$$

for $0 < r \ll 1$, and

$$I_\nu(r) \sim \sqrt{\frac{1}{2\pi r}} e^r, \quad r \gg 1, \quad \nu \geq 0. \quad (5.49)$$

Since $G_n(r)$ is convex, $G_n(r)$ attains its minimum at a unique point r_0 . Thanks to $G'_n(r) = -W'_n(r)/W_n^2(r)$, $W_n(r)$ has a unique maximum at the same point r_0 .

(ii). Recall that for large n (see [1, Formulas (9.7.7)-(9.7.11)]):

$$\begin{aligned} K_n(n\kappa) &\sim \sqrt{\frac{\pi}{2n}} \frac{e^{-n\Theta}}{(1+\kappa^2)^{1/4}}, & I_n(n\kappa) &\sim \frac{1}{\sqrt{2\pi n}} \frac{e^{n\Theta}}{(1+\kappa^2)^{1/4}}, \\ K'_n(n\kappa) &\sim -\sqrt{\frac{\pi}{2n}} \frac{(1+\kappa^2)^{1/4}}{\kappa} e^{-n\Theta}, & I'_n(n\kappa) &\sim \frac{1}{\sqrt{2\pi n}} \frac{(1+\kappa^2)^{1/4}}{\kappa} e^{n\Theta}, \end{aligned} \quad (5.50)$$

which, together with (5.45), leads to the asymptotic estimate (5.46). Thus, the maximum value of $W_n(r)$ is approximately attained at the unique root of $\Theta(\kappa)$, which turns out to be $a \approx 0.66274$ as in Figure 5.1, and the maximum value is about $n\sqrt{1+a^2}/\pi \approx 0.38187n$. $\square$

Figure 5.3: Left: graph of $\Theta(\kappa)$, $\kappa \in (0, 8]$ defined in (5.47). Right: W_n against the asymptotic estimate $\widetilde{W}_n$ (“•”) for $n = 5, 15, 30, 45$.

We depict in Figure 5.3 (left) the graph of $\Theta(\kappa)$, and highlight the zero point $(a, 0)$. Observe that $\Theta(\kappa)$ grows like κ , when $\kappa > a$. We plot in Figure 5.3 (right) several sample graphs of W_n (solid lines) and the asymptotic estimate $\widetilde{W}_n$ (“•”), and particularly mark the asymptotic point $(na, n\sqrt{1+a^2}/\pi)$ of the maximum of

$W_n(r)$ obtained in Lemma 5.3 (ii). Observe that even for small n , the asymptotic estimate provides a very accurate approximation of W_n .

As $W_n(r)$ behaves like a spike, we can truncate the improper integral in (5.32) and approximate it very accurately. For $n \geq n_0$ (e.g., $n_0 = 8$ in our computation), we truncate $(0, \infty)$ to a narrow interval $[L_1, L_2] := [(a - \delta_1)n, (a + \delta_2)n]$ around the maximum point $r = na$, where δ_1 and δ_2 are chosen such that for a preassigned tolerance $\varepsilon > 0$, $\delta_1 = \sup_{\delta} \widetilde{W}_n((a - \delta)n) < \varepsilon$, and $\delta_2 = \inf_{\delta} \widetilde{W}_n((a + \delta)n) < \varepsilon$. For small $n < n_0$, we simply take $L_1 = 0$ and choose $L_2 = \inf_r W_n(r) < \varepsilon$. We tabulate in Table 5.1 the truncated interval with $\varepsilon = 10^{-13}$ for various n , and see that the length of the interval of interest is around 18. For the readers' reference, we provide in Table 5.2 some samples of $\sigma_n(t)$ with $b = c = 1$.

Table 5.1: Truncation of the improper integral.

n	L_1	L_2	$L_2 - L_1$	n	L_1	L_2	$L_2 - L_1$	n	L_1	L_2	$L_2 - L_1$
0	0	16.1	16.1	8	0.81	18.0	17.2	30	12.2	30.5	18.3
2	0	16.3	16.3	10	1.49	18.9	17.4	40	18.4	36.9	18.5
4	0	16.7	16.7	15	3.71	21.4	17.7	50	24.8	43.5	18.7
6	0	17.2	17.2	20	6.35	24.3	18.0	60	31.2	50.2	19.0

Table 5.2: Some samples of $\sigma_n(t)$.

n	$\sigma_n(0)$	$\sigma_n(1)$	$\sigma_n(2)$	$\sigma_n(3)$
0	1.250000000000e-1	5.684288622608e-2	3.351856052343e-2	2.266050114914e-2
5	-1.237500000000e+1	2.202467951276e-1	-4.319989183539e-2	5.379927213148e-3
10	-4.987500000000e+1	-7.484612960447e-1	7.405362971595e-3	1.794812888151e-3
30	-4.498750000000e+2	-4.436774439706e-1	2.776460499307e-3	2.472420517813e-5
80	-3.199875000000e+3	-9.903043482030e-2	-1.941146013844e-4	-2.697087894087e-7
120	-7.199875000000e+3	-7.499180003657e-2	4.237771379095e-5	-8.100282555699e-9

5.1.4 Rapid evaluation of the temporal convolution

The presence of the time variable t in the exponentials in (5.32) and (5.33) allows us to eliminate the burden of history dependence of temporal convolution as in [4]. More precisely, given a function $g(t)$, we define

$$f(t; r) := e^{-ctr/b} * g(t) = \int_0^t e^{-c(t-\tau)r/b} g(\tau) d\tau.$$

One verifies readily that

$$f(t + \Delta t; r) = e^{-c\Delta tr/b} f(t; r) + \int_t^{t+\Delta t} e^{-c(t+\Delta t-\tau)r/b} g(\tau) d\tau, \quad (5.51)$$

so $f(t; r)$ can march in t with step size Δt recursively. This enables us to compute the time convolution rapidly. For example, in the 2-D case,

$$\begin{aligned} [\sigma_n * g](t) &= \int_0^t \sigma_n(t - \tau) g(\tau) d\tau = \frac{c}{b^2} \sum_{j=1}^{M_n} z_j^n \int_0^t e^{c(t-\tau)z_j^n/b} g(\tau) d\tau \\ &\quad + \frac{(-1)^n c}{b^2} \int_0^\infty \frac{1}{K_n^2(r) + \pi^2 I_n^2(r)} \left[\int_0^t e^{-c(t-\tau)r/b} g(\tau) d\tau \right] dr \\ &= \frac{c}{b^2} \sum_{j=1}^{M_n} z_j^n f(t; -z_j^n) + \frac{(-1)^n c}{b^2} \int_0^\infty f(t; r) W_n(r) dr. \end{aligned} \quad (5.52)$$

Thanks to (5.51), $[\sigma_n * g](t + \Delta t)$ can be computed recursively from the previous step and the history dependence is then narrowed down to $[t, t + \Delta t]$. We also refer to Subsections 5.3.4-5.3.5 for more detailed discussions.

5.2 A priori estimates

In this section, we analyze the well-posedness of the truncated problem (5.4)-(5.6), and provide *a priori* estimates for its solution.

We first recall the Plancherel or Parseval results for the Laplace transform.

Lemma 5.4. *Let $s = s_1 + is_2$ with $s_1, s_2 \in \mathbb{R}$. If f, g are Laplace transformable, then*

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathcal{L}[f](s) \mathcal{L}[\bar{g}](s) ds_2 = \int_0^\infty e^{-2s_1 t} f(t) \bar{g}(t) dt, \quad \forall s_1 > \gamma, \quad (5.53)$$

where γ is the abscissa of convergence for both f and g , and $\bar{g}$ is the complex conjugate of g .

Proof. This identity can be proved by following the same lines as for (2.46) in [29] (or [35]). $\square$

By (5.11), we know that

$$\frac{k'_n(z)}{k_n(z)} = -\frac{1}{2z} + \frac{K'_{n+1/2}(z)}{K_{n+1/2}(z)}. \quad (5.54)$$

The following properties are also indispensable for the analysis.

Lemma 5.5. *Let $s = s_1 + is_2$ with $s_1, s_2 \in \mathbb{R}$. Then for any $s_1 > 0$,*

$$\begin{aligned} \text{(i)} \quad & \operatorname{Re}\left(s \frac{Z'_n(sb/c)}{Z_n(sb/c)}\right) \leq 0, \quad \operatorname{Re}\left(\frac{Z'_n(sb/c)}{Z_n(sb/c)}\right) \leq 0; \\ \text{(ii)} \quad & \operatorname{Im}\left(s \frac{Z'_n(sb/c)}{Z_n(sb/c)}\right) \leq 0, \quad \forall s_2 \geq 0, \end{aligned} \quad (5.55)$$

where $Z_n(z) = K_n(z)$ or $k_n(z)$.

Proof. The results with $Z_n = K_n$ were proved in Chen [25]. We next prove (5.55) with $Z_n = k_n$ by using a similar argument. Multiplying the first equation of (5.9) by $\bar{u}$ and integrating over $\Omega_{b,\rho} := B_\rho \setminus \bar{B}$, where B_ρ is a ball of radius $\rho > b$, the imaginary part of the resulting equation reads

$$2s_1s_2 \int_{\Omega_{b,\rho}} |u|^2 d\mathbf{x} - c^2 \operatorname{Im} \int_{\partial\Omega_{b,\rho}} \frac{\partial u}{\partial \mathbf{n}} \bar{u} d\gamma = 0, \quad (5.56)$$

where $\mathbf{n}$ is the unit outer normal of $\partial\Omega_{b,\rho}$.

Since $s_1 > 0$, multiplying (5.56) by s_2 yields

$$s_2 \operatorname{Im} \int_{\{r=b\}} \frac{\partial u}{\partial r} \bar{u} d\gamma \leq s_2 \operatorname{Im} \int_{\{r=\rho\}} \frac{\partial u}{\partial r} \bar{u} d\gamma. \quad (5.57)$$

It is clear that $u = k_n(sr/c)/k_n(sb/c) \hat{\psi}_{nm}(s) Y_n^m(\theta, \phi)$ (where $\hat{\psi}_{nm}$ is the same as in (5.10)) is a solution of (5.9), so using the orthogonality of $\{Y_n^m\}$, and the fact $\bar{k}_n/|k_n|^2 = 1/k_n$, we obtain from (5.57) that

$$\frac{b}{c} \operatorname{Im}\left(s_2 s \frac{k'_n(sb/c)}{k_n(sb/c)}\right) |\hat{\psi}_{nm}|^2 \leq \frac{\rho}{c} \operatorname{Im}\left(s_2 s \frac{k'_n(s\rho/c)}{k_n(sb/c)}\right) |\hat{\psi}_{nm}|^2. \quad (5.58)$$

We find from (5.11) and (5.16) that $k'_n(s\rho/c)$ decays exponentially if $s_1 > 0$, so the right hand side of (5.57) tends to zero as $\rho \rightarrow +\infty$. Thus, letting $\rho \rightarrow +\infty$ in (5.58) leads to

$$\operatorname{Im}\left(s_2 s \frac{k'_n(sb/c)}{k_n(sb/c)}\right) \leq 0. \quad (5.59)$$

If $s_2 \geq 0$, then we obtain (ii) in (5.55). Next, we prove the first inequality of (5.55). Recall the formula (see [25, Lemma 2.3]):

$$|K_{n+1/2}(sr)|^2 = \frac{1}{2} \int_0^{+\infty} e^{-\frac{|s|^2 r^2}{2r} - \frac{s^2 + \bar{s}^2}{2|s^2|}} K_{n+1/2}(\tau) \frac{d\tau}{\tau}, \quad s_1 > 0,$$

which implies that $|K_{n+1/2}(sr)|^2$ is monotonically descending with respect to r . The property $\frac{d}{dr}|K_{n+1/2}(sr)|^2 \leq 0$, together with (5.54), implies $\operatorname{Re}\left(s \frac{k'_n(sb/c)}{k_n(sb/c)}\right) \leq 0$. Denoting $s \frac{k'_n(sb/c)}{k_n(sb/c)} = \gamma_1 + i\gamma_2$ with $\gamma_1, \gamma_2 \in \mathbb{R}$, we know from (5.59) that $\gamma_1 \leq 0$ and $s_2\gamma_2 \leq 0$. Therefore,

$$\operatorname{Re}\left(\frac{k'_n(sb/c)}{k_n(sb/c)}\right) = \operatorname{Re}\left(\frac{\gamma_1 + i\gamma_2}{s}\right) = \frac{1}{|s|^2}(s_1\gamma_1 + s_2\gamma_2) \leq 0.$$

This ends the proof. $\square$

With the above preparations, we can derive the following important property.

Theorem 5.2. *For any $v \in L^2(0, T)$, we have*

$$\operatorname{Re} \int_0^T [\omega_\nu * v](t) \bar{v}(t) dt \leq \int_0^T |v(t)|^2 dt, \quad \forall T > 0, \quad (5.60)$$

for $\nu = n, n + 1/2$, where ω_ν is the NRBK given by (5.24).

Proof. Let $\tilde{v} = v \mathbf{1}_{[0, T]}$, where $\mathbf{1}_{[0, T]}$ is the characteristic function of $[0, T]$. Then we obtain from Lemma 5.4 that for $d = 3$,

$$\begin{aligned} \int_0^T e^{-2s_1 t} [\omega_{n+1/2} * v](t) \bar{v}(t) dt &= \int_0^\infty e^{-2s_1 t} [\omega_{n+1/2} * \tilde{v}](t) \bar{\tilde{v}}(t) dt \\ &= \frac{1}{2\pi} \int_{-\infty}^\infty \left[\frac{k'_n(sb/c)}{k_n(sb/c)} + 1 \right] |\mathcal{L}[\tilde{v}](s)|^2 ds_2 \\ &= \frac{1}{2\pi} \int_{-\infty}^\infty \frac{k'_n(sb/c)}{k_n(sb/c)} |\mathcal{L}[\tilde{v}](s)|^2 ds_2 + \frac{1}{2\pi} \int_{-\infty}^\infty |\mathcal{L}[\tilde{v}](s)|^2 ds_2. \end{aligned}$$

It is clear that by Lemma 5.4 with $f = g = \tilde{v}$,

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} |\mathcal{L}[\tilde{v}](s)|^2 ds_2 = \int_0^{+\infty} e^{-2s_1 t} |\tilde{v}(t)|^2 dt = \int_0^T e^{-2s_1 t} |v(t)|^2 dt.$$

On the other hand, we have

$$\begin{aligned} \frac{1}{2\pi} \operatorname{Re} \int_{-\infty}^{\infty} \frac{k'_n(sb/c)}{k_n(sb/c)} |\mathcal{L}[\tilde{v}](s)|^2 ds_2 &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \operatorname{Re} \left(\frac{k'_n(sb/c)}{k_n(sb/c)} \right) |\mathcal{L}[\tilde{v}](s)|^2 ds_2 \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \operatorname{Re} \left(\frac{k'_n(sb/c)}{k_n(sb/c)} \right) \left| \mathcal{L} \left[\int_0^t \tilde{v}(\tau) d\tau \right] (s) \right|^2 |s|^2 ds_2. \end{aligned} \quad (5.61)$$

Thus, we conclude from Lemma 5.5 and the above identities that for $s_1 > 0$,

$$\operatorname{Re} \int_0^T e^{-2s_1 t} [\omega_{n+1/2} * v](t) \bar{v}(t) dt \leq \int_0^T e^{-2s_1 t} |v(t)|^2 dt. \quad (5.62)$$

Notice that the asymptotic formulas in (5.48) are also valid for complex r (see [1, Formula 9.6.9]), which, together with Lemma 5.2, implies that $k'_n(sb/c)/k_n(sb/c)$ is analytic for all $\operatorname{Re}(s) \geq 0$ but $|s| \neq 0$, and $\lim_{s_1 \rightarrow 0^+} |s|^2 k'_n(sb/c)/k_n(sb/c)$ exists for all s_2 . Hence, the integral in (5.61) is finite. By letting $s_1 \rightarrow 0^+$ in (5.62) leads to the desired result for $d = 3$.

The result (5.60) with $d = 2$ can be proved in a similar fashion. $\square$

Corollary 5.1. *Suppose that $v' \in L^2(0, T)$ with $v(0) = 0$. Then we have*

$$\operatorname{Re} \int_0^T [\sigma_\nu * v](t) \bar{v}'(t) dt \leq \frac{1}{c} \int_0^T |v'(t)|^2 dt + \frac{d-1}{4b} |v(T)|^2, \quad \forall T > 0, \quad (5.63)$$

for $\nu = n, n + 1/2$, where $\sigma_\nu(t)$ is the NRBK defined in (5.26).

Proof. By (5.27), we have $\omega'_\nu(t) = c\sigma_\nu(t)$, $\omega_\nu(0) = -\frac{(d-1)c}{2b}$. Thus, we obtain from integration by parts and the fact $v(0) = 0$ that

$$[\omega_\nu * v'](t) = -\frac{(d-1)c}{2b} v(t) + c[\sigma_\nu * v](t).$$

By Theorem 5.2 with v' in place of v ,

$$\begin{aligned} \operatorname{Re} \int_0^T [\omega_\nu * v'](t) \bar{v}'(t) dt &= -\frac{(d-1)c}{2b} \operatorname{Re} \int_0^T v(t) \bar{v}'(t) dt + c \operatorname{Re} \int_0^T [\sigma_\nu * v](t) \bar{v}'(t) dt \\ &= -\frac{(d-1)c}{4b} |v(T)|^2 + c \operatorname{Re} \int_0^T [\sigma_\nu * v](t) \bar{v}'(t) dt \leq \int_0^T |v'(t)|^2 dt. \end{aligned}$$

This gives (5.63). $\square$

Now, we are ready to analyze the stability of the solution of the truncated problem (5.4)-(5.6). To this end, we assume that the scatterer D is a simply connected domain with Lipschitz boundary Γ_D , and the Dirichlet data $G = 0$ on Γ_D . More precisely, the problem of interest is

$$\partial_t^2 U = c^2 \Delta U + F, \quad \text{in } \Omega := B \setminus \bar{D}, \quad t > 0, \quad d = 2, 3; \quad (5.64)$$

$$U = U_0, \quad \partial_t U = U_1, \quad \text{in } \Omega, \quad t = 0; \quad U = 0, \quad \text{on } \Gamma_D, \quad t > 0; \quad (5.65)$$

$$\partial_r U - T_d(U) = H, \quad \text{at } r = b, \quad t > 0, \quad (5.66)$$

where the given data H may result from lifting of nonhomogeneous Dirichlet data or the boundary perturbation to be described in Subsection 5.3.1. Denote $X := \{U \in H^1(\Omega) : U|_{\Gamma_D} = 0\}$, and let $(\cdot, \cdot)_{L^2(\Omega)}$ and $\|\cdot\|_{L^2(\Omega)}$ be the inner product and norm of $L^2(\Omega)$, respectively, and likewise, we define $\langle \cdot, \cdot \rangle_{L^2(\Gamma_b)}$ and $\|\cdot\|_{L^2(\Gamma_b)}$, where $\Gamma_b = \{r = b\}$ and b is the radius of the artificial boundary.

Theorem 5.3. *Let $U \in X$ be the solution of (5.64)-(5.66). If $U_0 \in H^1(\Omega)$, $U_1 \in L^2(\Omega)$, $H \in L^\infty(0, T; L^2(\Gamma_b))$, $\partial_t H \in L^1(0, T; L^2(\Gamma_b))$, and $F \in L^1(0, T; L^2(\Omega))$ for any $T > 0$, then we have $\nabla U \in L^\infty(0, T; (H^1(\Omega))^d)$, $\partial_t U \in L^\infty(0, T; L^2(\Omega))$, and there holds*

$$\begin{aligned} \|\partial_t U\|_{L^\infty(0, T; L^2(\Omega))} + c \|\nabla U\|_{L^\infty(0, T; L^2(\Omega))} &\leq C(\|U_1\|_{L^2(\Omega)} + c \|\nabla U_0\|_{L^2(\Omega)} \\ &\quad + \|H\|_{L^\infty(0, T; L^2(\Gamma_b))} + \|\partial_t H\|_{L^1(0, T; L^2(\Gamma_b))} + \|F\|_{L^1(0, T; L^2(\Omega))}), \end{aligned} \quad (5.67)$$

where C is a positive constant independent of any functions and c . Moreover, if $F \equiv 0$ and $H \equiv 0$, we have the conservation of the energy: $E'(t) = 0$ for all $t \geq 0$, where

$$E(t) = \int_{\Omega} (|\partial_t U|^2 + c^2 |\nabla U|^2) d\mathbf{x} - 2c^2 \operatorname{Re} \int_0^t \int_{\Gamma_b} T_d(U) \partial_\tau \bar{U} d\gamma d\tau. \quad (5.68)$$

Proof. Multiplying (5.64) by $2\partial_t \bar{U}$, integrating over Ω , and taking the real part of the resulted equation, we derive from the Green's formula that for any $t > 0$,

$$\begin{aligned} \frac{d}{dt} \left(\|\partial_t U\|_{L^2(\Omega)}^2 + c^2 \|\nabla U\|_{L^2(\Omega)}^2 \right) - 2c^2 \operatorname{Re} \int_{\Gamma_b} T_d(U) \partial_t \bar{U} d\gamma \\ = 2\operatorname{Re}(F, \partial_t U)_{L^2(\Omega)} + 2c^2 \operatorname{Re}\langle H, \partial_t U \rangle_{\Gamma_b}. \end{aligned} \quad (5.69)$$

Integrating the above equation over $(0, t)$, we find that for any $t > 0$,

$$\begin{aligned}
& \|\partial_t U\|_{L^2(\Omega)}^2 + c^2 \|\nabla U\|_{L^2(\Omega)}^2 - 2c^2 \operatorname{Re} \int_0^t \int_{\Gamma_b} T_d(U) \partial_\tau \bar{U} d\gamma d\tau \\
&= 2 \operatorname{Re} \int_0^t (F, \partial_\tau U)_{L^2(\Omega)} d\tau + 2c^2 \operatorname{Re} \int_0^t \langle H, \partial_\tau U \rangle_{\Gamma_b} d\tau + \|U_1\|_{L^2(\Omega)}^2 + c^2 \|\nabla U_0\|_{L^2(\Omega)}^2 \\
&\leq 2 \|\partial_t U\|_{L^\infty(0,T;L^2(\Omega))} \|F\|_{L^1(0,T;L^2(\Omega))} \\
&\quad + 2c^2 \operatorname{Re} \int_0^t \langle H, \partial_\tau U \rangle_{\Gamma_b} d\tau + \|U_1\|_{L^2(\Omega)}^2 + c^2 \|\nabla U_0\|_{L^2(\Omega)}^2.
\end{aligned}$$

Using integration by parts leads to

$$\begin{aligned}
\operatorname{Re} \int_0^t \langle H, \partial_\tau U \rangle_{\Gamma_b} d\tau &= \operatorname{Re} \langle H, U \rangle_{\Gamma_b} - \operatorname{Re} \langle H, U \rangle_{\Gamma_b} \Big|_{t=0} - \operatorname{Re} \int_0^t \langle \partial_\tau H, U \rangle_{\Gamma_b} d\tau \\
&\leq 2 \|H\|_{L^\infty(0,T;L^2(\Gamma_b))} \|U\|_{L^\infty(0,T;L^2(\Gamma_b))} \\
&\quad + \|\partial_t H\|_{L^1(0,T;L^2(\Gamma_b))} \|U\|_{L^\infty(0,T;L^2(\Gamma_b))} \\
&\leq C (\|H\|_{L^\infty(0,T;L^2(\Gamma_b))} + \|\partial_t H\|_{L^1(0,T;L^2(\Gamma_b))}) \|\nabla U\|_{L^\infty(0,T;L^2(\Omega))},
\end{aligned} \tag{5.70}$$

where we used the following estimate derived from the trace inequality (see, e.g., [19, Eq. (1.6.2)]) and the Poincaré inequality (see, e.g., [27, Theorem 1.2.1]):

$$\|U\|_{L^\infty(0,T;L^2(\Gamma_b))} \leq C \|U\|_{L^\infty(0,T;L^2(\Omega))}^{1/2} \|U\|_{L^\infty(0,T;H^1(\Omega))}^{1/2} \leq C \|\nabla U\|_{L^\infty(0,T;L^2(\Omega))}.$$

We next show that for any $t > 0$,

$$\operatorname{Re} \int_0^t \int_{\Gamma_b} T_d(U) \partial_\tau \bar{U} d\gamma d\tau \leq 0. \tag{5.71}$$

For $d = 3$, it follows from (5.23), Theorem 5.2 and the orthogonality of $\{Y_n^m\}$ that

$$\begin{aligned}
\operatorname{Re} \int_0^t \int_{\Gamma_b} T_d(U) \partial_\tau \bar{U} d\gamma d\tau &= -\frac{1}{c} \int_0^t \|\partial_\tau U\|_{L^2(\Gamma_b)}^2 d\tau \\
&\quad + \frac{1}{c} \sum_{n=0}^{\infty} \sum_{|m|=0}^n \operatorname{Re} \int_0^t [\omega_{n+1/2} * \partial_\tau \widehat{U}_{nm}(b, \tau)] \partial_\tau \overline{\widehat{U}_{nm}}(b, \tau) d\tau \\
&\leq -\frac{1}{c} \int_0^t \|\partial_\tau U\|_{L^2(\Gamma_b)}^2 d\tau + \frac{1}{c} \sum_{n=0}^{\infty} \sum_{|m|=0}^n \int_0^t |\partial_\tau \widehat{U}_{nm}(b, \tau)|^2 d\tau = 0.
\end{aligned}$$

This verifies (5.71) with $d = 3$. Similarly, one can justify (5.71) with $d = 2$.

Consequently, the estimate (5.67) follows from (5.69)-(5.70) and the Cauchy-Schwarz inequality.

Letting $F \equiv 0$ and $H \equiv 0$ in (5.69) leads to the conservation of energy. $\square$

Remark 5.5. *Note that (i) if $T_d(U)$ is given by (5.25), we can use Corollary 5.1 to verify (5.71); (ii) a similar estimate for $d = 2$ was derived by [25] with a slightly different argument; and (iii) it is seen from (5.67) that the validation of this estimate requires $\partial_t H \in L^1(0, T; L^2(\Gamma_b))$, which appears restrictive. This is largely due to the lack of the uniform Kreiss-Lopatinski conditions (cf. [100]) for the truncated wave equation (also refer to the Appendix of [3]). $\square$*

5.3 Spectral-Galerkin approximation and Newmark scheme

This section is devoted to numerical approximation of the truncated problem (5.4)-(5.6) with a focus on the treatment for the global NRBC imposed at the circular/spherical boundary $r = b$. Given the series representation of the NRBC in (5.25), it is known that if the scatterer D is a disk/ball (i.e., the computational domain Ω is an annulus or a spherical shell), the NRBC in space becomes local in the space of Fourier/spherical harmonic coefficients. The use of polar/spherical coordinates allows to reduce the truncated problem to a sequence of decoupled one-dimensional problems (see (5.74) below), which therefore leads to fast spatial Fourier/spherical harmonic-Legendre spectral solvers. It is driven by this that efficient spectral-Galerkin methods integrated with a boundary perturbation technique have been successfully applied to simulate of the time-harmonic acoustic scattering waves by an irregular bounded obstacle with moderate to large wave numbers (see, e.g., [90, 40]). The boundary perturbation method (termed as “method of variation of boundary” sometimes) had its root in the monumental work of Rayleigh [95] and Rice [97] with a flurry of subsequent improvements and enhancements (by, e.g., Bruno, Reitich and/or Nicholls (cf. [20, 89] and a series of papers by these groups)). Within its domain of applicability, this method is fast and accurate, and in particular, an enhanced version, called “transformed field expansion (TFE) method”, is proved to be robust for large and/or rough

boundary perturbations. The key to success lies in the convergence property: “the scattered field depends analytically on the domain perturbations under reasonable assumptions on the geometry of the scatterer surface and regularity of boundary data” (see [91] for a rigorous analysis). While the major requisite pieces are in order for frequency-domain computation, the process of assembling them to design high-order time-domain methods is far from trivial. Here, we intend to construct one of the major building blocks, that is, the efficient space-time solver for (5.4)-(5.6) in an annulus or a spherical shell, but leave the combination with the TFE method to a future work as the implementation is rather involved.

5.3.1 Notion of transformed field expansion

We outline this technique for (5.4)-(5.6) with $d = 2$ and

$$\Gamma_D = \{r = b_0 + \eta(\phi) : 0 \leq \phi < 2\pi\}, \quad b > b_0 + \max_{\phi \in [0, 2\pi]} |\eta(\phi)|,$$

where $r(\phi) = b_0 + \eta(\phi)$ is the parametric form of the boundary of the scatterer D . As before, the outer artificial disk $\{r = b\}$ contains the scatterer D , and supports of the source term and initial data. Based on the general setup for the TFE method in [91], we assume η is smooth (in certain Sobolev space with regularity index $\geq 3/2$ in [91, Theorem 5.5]), and assume that the domain Ω is “close” to a regular simple domain Ω_0 .

- As the name suggests, we first make a change of variables

$$r' = \frac{(b - b_0)r - b\eta(\phi)}{(b - b_0) - \eta(\phi)}, \quad \phi' = \phi,$$

which maps Ω to the annulus $\Omega_0 = \{(r', \phi') : b_0 < r' < b, 0 \leq \phi' < 2\pi\}$. To simplify the notation, we still use U, F, r, ϕ etc. to denote the transformed functions or variables. Then the problem (5.4)-(5.6) becomes

$$\partial_t^2 U = c^2 \Delta U + F + J(\eta, U), \quad \text{in } \Omega_0, \quad t > 0;$$

$$U = U_0, \quad \partial_t U = U_1, \quad \text{in } \Omega_0, \quad t = 0;$$

$$U|_{r=b_0} = G, \quad t > 0; \quad (\partial_r U - T_d(U))|_{r=b} = L(\eta, U)|_{r=b}, \quad t > 0,$$

where $J(\eta, U)$ and $L(\eta, U)$ contain differential operators with nonconstant coefficients.

- Considering the smooth boundary deformation $\eta = \varepsilon\zeta$, the scattering field, U , has the strongly convergent expansion:

$$U(r, \phi, t; \varepsilon) = \sum_{l=0}^{\infty} U_l(r, \phi, t) \varepsilon^l, \quad t > 0, \quad (5.72)$$

which depends analytically on ε . Formally, by expanding the data in similar series, we obtain the sequence of equations after collecting the terms of ε^l (similar to the derivations in [90]):

$$\begin{aligned} \partial_t^2 U_l &= c^2 \Delta U_l + F_l + \tilde{J}(\eta, U_{l-4}, \dots, U_{l-1}), \quad \text{in } \Omega_0, \quad t > 0; \\ U_l &= U_{0,l}, \quad \partial_t U_l = U_{1,l}, \quad \text{in } \Omega_0, \quad t = 0; \\ U_l|_{r=b_0} &= G_l, \quad t > 0; \quad (\partial_r U_l - T_d(U_l))|_{r=b} = \tilde{L}(\eta, U_{l-1})|_{r=b}, \quad t > 0. \end{aligned}$$

- Solve the above equation for $l = 0, 1, \dots$, and sum up the series by using a Padé approximation.

We remark that the parameter ε , which measures the size of perturbation, is not necessary to be small [89], and numerical evidences in [90] show that the method in frequency-domain produces satisfactory results for very rough scatterer of Lipschitz C^0 (star-like) shape. We also point out that in this context, we have extra time derivatives in the functionals $\tilde{J}$ and $\tilde{L}$. Under this notion, the whole algorithm boils down to solving a sequence of prototype equations, so it becomes crucial to develop a fast, stable solver for the problem (5.73) below.

5.3.2 Prototype equation and dimension reduction

Consider

$$\begin{aligned} \partial_t^2 U &= c^2 \Delta U + F, \quad \text{in } \Omega_0 = \{\mathbf{x} \in \mathbb{R}^d : b_0 < |\mathbf{x}| < b\}, \quad t > 0; \\ U &= U_0, \quad \partial_t U = U_1, \quad \text{in } \Omega_0, \quad t = 0; \\ U|_{r=b_0} &= 0, \quad (\partial_r U - T_d(U))|_{r=b} = H, \quad t > 0, \end{aligned} \quad (5.73)$$

where $T_d(U)$ is the DtN map as before. By expanding the solution and given data in Fourier series/spherical harmonic series, the problem (5.73), after a polar (in 2-D) and spherical (in 3-D) transform, reduces to a sequence of one-dimensional problems (for brevity, we use u to denote the Fourier/spherical harmonic expansion coefficients of U , and likewise, we use u_0, u_1, h and f to denote the expansion coefficients of U_0, U_1, H and F , respectively):

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{c^2}{r^{d-1}} \frac{\partial}{\partial r} \left(r^{d-1} \frac{\partial u}{\partial r} \right) + c^2 \beta_n \frac{u}{r^2} &= f, \quad b_0 < r < b, \quad t > 0; \\ u|_{t=0} &= u_0, \quad \frac{\partial u}{\partial t} \Big|_{t=0} = u_1, \quad b_0 < r < b; \quad u|_{r=b_0} = 0, \quad t > 0; \\ \left(\frac{1}{c} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial r} + \frac{d-1}{2r} u \right) \Big|_{r=b} &= \int_0^t \sigma_\nu(t-\tau) u(b, \tau) d\tau + h, \quad t > 0, \end{aligned} \quad (5.74)$$

where $\beta_n = n^2, n(n+1)$ and $\nu = n, n+1/2$ for $d = 2, 3$, respectively. Since σ_ν is real, the real and imaginary parts of u and the given data can be decoupled. In what follows, we assume they are real.

5.3.3 Spectral-Galerkin approximation in space

We apply the Legendre spectral-Galerkin method to approximate (5.74) in space. For convenience of implementation, we transform the interval (b_0, b) to the reference interval $I = (-1, 1)$ by $r = \frac{b-b_0}{2}x + \frac{b+b_0}{2}$ with $x \in I$, and denote the transformed functions by $v(x, t) = u(r, t)$, $g(x, t) = f(r, t)$ and $v_i(x) = u_i(r)$ with $i = 0, 1$, respectively. Then (5.74) can be reformulated as

$$\begin{aligned} \frac{\partial^2 v}{\partial t^2} - \frac{\tilde{c}^2}{(x+c_0)^{d-1}} \frac{\partial}{\partial x} \left((x+c_0)^{d-1} \frac{\partial v}{\partial x} \right) + \tilde{c}^2 \beta_n \frac{v}{(x+c_0)^2} &= g, \quad x \in I, \quad t > 0; \\ v(x, 0) &= v_0(x), \quad \frac{\partial v}{\partial t}(x, 0) = v_1(x), \quad x \in I; \quad v(-1, t) = 0, \quad t > 0; \\ \left(\frac{1}{c} \frac{\partial v}{\partial t} + \frac{2}{b-b_0} \frac{\partial v}{\partial x} + \frac{d-1}{2b} v \right) (1, t) &= \int_0^t \sigma_\nu(t-\tau) v(1, \tau) d\tau + h(t), \quad t > 0, \end{aligned} \quad (5.75)$$

where the constants $\tilde{c} = \frac{2c}{b-b_0}$ and $c_0 = \frac{b+b_0}{b-b_0}$.

Let $V_N := \{\psi \in \mathbb{P}_N : \psi(-1) = 0\}$, where $\mathbb{P}_N$ is the set of all algebraic polynomials of degree at most N . The semi-discretization Legendre spectral-Galerkin

approximation of (5.75) is to find $v_N(x, t) \in V_N$ for all $t > 0$ such that for all $w \in V_N$,

$$\begin{aligned}
& (\ddot{v}_N, w)_\varpi + \tilde{c}(1 + c_0)^{d-1} \dot{v}_N(1, t)w(1) + \tilde{c}^2(\partial_x v_N, \partial_x w)_\varpi \\
& + \tilde{c}^2 \beta_n (v_N(x + c_0)^{-2}, w)_\varpi \\
& + \frac{2c^2}{b - b_0} (1 + c_0)^{d-1} \left(\frac{d-1}{2b} v_N(1, t) - \sigma_\nu(t) * v_N(1, t) \right) w(1) \quad (5.76) \\
& = (I_N g, w)_\varpi + \frac{2c^2}{b - b_0} (1 + c_0)^{d-1} h(t)w(1), \quad t > 0, \\
& v_N(x, 0) = v_{0,N}(x), \quad \dot{v}_N(x, 0) = v_{1,N}(x), \quad x \in I,
\end{aligned}$$

where $(\cdot, \cdot)_\varpi$ is the (weighted) inner product of $L^2_\varpi(I)$ with the weight function $\varpi = (x + c_0)^{d-1}$, $\ddot{v}$ denotes $\partial_t^2 v$ or $\frac{d^2 v}{dt^2}$ as usual, I_N is the interpolation operator on $(N + 1)$ Legendre-Gauss-Lobatto points, and $v_{0,N}, v_{1,N} \in \mathbb{P}_N$ are suitable approximations of the initial values.

Like Theorem 5.3, we have the following *a priori* estimates.

Theorem 5.4. *Let v_N be the solution of (5.76). If $h \in L^\infty(0, T)$, $\partial_t h \in L^1(0, T)$ and $g(\cdot, t) \in C(I)$. Then for all $T > 0$,*

$$\begin{aligned}
& \|\partial_t v_N\|_{L^\infty(0,T;L^2_\varpi(I))}^2 + \tilde{c}^2 (\|\partial_x v_N\|_{L^\infty(0,T;L^2_\varpi(I))}^2 + \beta_n \|v_N/(x + c_0)\|_{L^\infty(0,T;L^2_\varpi(I))}^2) \\
& \leq C (\|v_{1,N}\|_{L^2_\varpi(I)}^2 + \tilde{c}^2 (\|\partial_x v_{0,N}\|_{L^2_\varpi(I)}^2 + \beta_n \|v_{0,N}/(x + c_0)\|_{L^2_\varpi(I)}^2) \quad (5.77) \\
& + \|h\|_{L^\infty(0,T)}^2 + \|\partial_t h\|_{L^1(0,T)}^2 + \|I_N g\|_{L^1(0,T;L^2_\varpi(I))}^2),
\end{aligned}$$

where C is a positive constant independent of N .

Proof. Taking $w = \partial_t v_N$ in (5.76), and integrating the resulted equation with respect to t , we use Corollary 5.1 and the argument similar to that for Theorem 5.3 to derive the estimate. $\square$

Remark 5.6. *Equipped with Theorem 5.4, we can analyze the convergence of the semi-discretized scheme (5.76) as on [102, Page 341].* $\square$

We next examine the linear system of (5.76). As shown in [101, 102], it is advantageous to construct basis functions satisfying the underlying homogeneous

Dirichlet boundary conditions. Let $P_l(x)$ be the Legendre polynomial of degree l (see, e.g., [108]), and define

$$\begin{aligned}\phi_k(x) &= P_k(x) + P_{k+1}(x), \\ \Rightarrow \phi_k(-1) &= 0 \text{ and } V_N = \text{span}\{\phi_k : 0 \leq k \leq N-1\}.\end{aligned}\tag{5.78}$$

Note that $\phi_k(1) = 2$. Setting

$$\begin{aligned}v_N(x, t) &= \sum_{j=0}^{N-1} \hat{v}_j(t) \phi_j(x), \quad \mathbf{v} = (\hat{v}_0, \hat{v}_1, \dots, \hat{v}_{N-1})^t, \quad m_{ij} = (\phi_j, \phi_i)_\varpi, \\ \tilde{m}_{ij} &= (\phi_j(x + c_0)^{-2}, \phi_i)_\varpi, \quad s_{ij} = (\phi'_j, \phi'_i)_\varpi, \quad \mathbf{1} = (1, 1, \dots, 1)^t, \\ \tilde{h}_i &= (I_N g, \phi_i)_\varpi + \frac{c\alpha}{2} h, \quad \mathbf{h} = (\tilde{h}_0, \tilde{h}_1, \dots, \tilde{h}_{N-1})^t,\end{aligned}$$

we obtain the system:

$$M\ddot{\mathbf{v}} + \alpha E\dot{\mathbf{v}} + \tilde{c}^2(S + \beta_n \widetilde{M})\mathbf{v} + \mu E\mathbf{v} - c\alpha \left(\sigma_\nu * \sum_{j=0}^{N-1} \hat{v}_j \right) \mathbf{1} = \mathbf{h},\tag{5.79}$$

with $\mathbf{v}(0) = \mathbf{v}_0$ and $\dot{\mathbf{v}}(0) = \mathbf{v}_1$, where $M = (m_{ij})$, $S = (s_{ij})$, $\widetilde{M} = (\tilde{m}_{ij})$ and $E = \mathbf{1}\mathbf{1}^t$ is an $N \times N$ matrix of all ones. In (5.79), $\mathbf{v}_0$ and $\mathbf{v}_1$ are column- N vectors of the expansion coefficients of $v_{0,N}$ and $v_{1,N}$ in terms of $\{\phi_k\}$, and the constants $\alpha = 8c(1 + c_0)^{d-1}/(b - b_0)$ and $\mu = 4c^2(d - 1)(1 + c_0)^{d-1}/(b(b - b_0))$.

5.3.4 Newmark scheme

To discretize the second-order ordinary differential system (5.79), we resort to the implicit second-order Newmark scheme, which has wide applications in the field of structural mechanics (see [88, 119]). To this end, let Δt be the time-stepping size, and let $\{\mathbf{v}^m, \dot{\mathbf{v}}^m, \ddot{\mathbf{v}}^m\}$ be the approximation of $\{\mathbf{v}, \dot{\mathbf{v}}, \ddot{\mathbf{v}}\}$ at $t = t_m = m\Delta t$, and $\mathbf{h}^m = \mathbf{h}(t_m)$.

We first take care of the convolution term $[\sigma_\nu * \sum_{j=0}^{N-1} \hat{v}_j](t_{m+1})$ in (5.79):

$$\begin{aligned}
& \left[\sigma_\nu * \sum_{j=0}^{N-1} \hat{v}_j \right](t_{m+1}) \\
&= \sum_{j=0}^{N-1} \int_{t_m}^{t_{m+1}} \sigma_\nu(t_{m+1} - \tau) \hat{v}_j(\tau) d\tau + \sum_{j=0}^{N-1} \int_0^{t_m} \sigma_\nu(t_{m+1} - \tau) \hat{v}_j(\tau) d\tau \\
&\approx \frac{\Delta t}{2} \left(\sigma_\nu(0) \sum_{j=0}^{N-1} \hat{v}_j^{m+1} + \sigma_\nu(\Delta t) \sum_{j=0}^{N-1} \hat{v}_j^m \right) + \int_0^{t_m} \sigma_\nu(t_{m+1} - \tau) \left(\sum_{j=0}^{N-1} \hat{v}_j \right)(\tau) d\tau \\
&\approx \frac{\Delta t}{2} \sigma_\nu(0) E \mathbf{v}^{m+1} + \mathbf{g}^m,
\end{aligned} \tag{5.80}$$

where we used the Trapezoidal rule to approximate the integral over (t_m, t_{m+1}) , and denoted by $\mathbf{g}^m$ the approximation of the remaining terms. Note that $\mathbf{g}^m$ depends on the history $\mathbf{v}^l (0 \leq l \leq m)$, but fortunately, it can be evaluated recursively and rapidly as described in Subection 5.1.4. Moreover, only $\sum_{j=0}^{N-1} \hat{v}_j^m$ needs to be stored as an input for computing $\mathbf{v}^{m+1}$. As a result, the burden of the history dependence can be eliminated.

Denoting

$$A = M, \quad B = \alpha E, \quad C = \tilde{c}^2 (S + \beta_n \widetilde{M}) + \left(\mu - c\alpha \frac{\Delta t}{2} \sigma_\nu(0) \right) E, \tag{5.81}$$

and $\mathbf{f}^{m+1} = \mathbf{h}^{m+1} + c\alpha \mathbf{g}^m$, we carry out the full scheme for (5.75) as follows.

(i) Set $\mathbf{v}^0 = \mathbf{v}_0$ and $\dot{\mathbf{v}}^0 = \mathbf{v}_1$, and compute $\ddot{\mathbf{v}}^0$ from the system (5.79) by

$$\ddot{\mathbf{v}}^0 = M^{-1} \{ \mathbf{h}^0 - \alpha E \dot{\mathbf{v}}^0 - \tilde{c}^2 (S + \beta_n \widetilde{M}) \mathbf{v}^0 - \mu E \mathbf{v}^0 \}, \tag{5.82}$$

where the convolution term vanishes at $t = 0$.

(ii) For $m \geq 0$, compute $\mathbf{v}^{m+1}$ from

$$\begin{aligned}
(A + \vartheta \Delta t B + \theta \Delta t^2 C) \ddot{\mathbf{v}}^{m+1} &= \mathbf{f}^{m+1} - B(\dot{\mathbf{v}}^m + (1 - \vartheta) \Delta t \ddot{\mathbf{v}}^m) \\
&\quad - C \left(\mathbf{v}^m + \Delta t \dot{\mathbf{v}}^m + \frac{1 - 2\theta}{2} \Delta t^2 \ddot{\mathbf{v}}^m \right),
\end{aligned} \tag{5.83}$$

and update $\mathbf{v}^{m+1}$ and $\dot{\mathbf{v}}^{m+1}$ by

$$\mathbf{v}^{m+1} = \mathbf{v}^m + \Delta t \dot{\mathbf{v}}^m + \frac{1 - 2\theta}{2} \Delta t^2 \ddot{\mathbf{v}}^m + \theta \Delta t^2 \ddot{\mathbf{v}}^{m+1}, \tag{5.84}$$

$$\dot{\mathbf{v}}^{m+1} = \dot{\mathbf{v}}^m + (1 - \vartheta) \Delta t \ddot{\mathbf{v}}^m + \vartheta \Delta t \ddot{\mathbf{v}}^{m+1}, \tag{5.85}$$

respectively. It is known that in general, the Newmark scheme is of second-order and unconditionally stable, if the parameters satisfy $\vartheta \geq \frac{1}{2}$ and $\theta \geq \frac{1}{4}(\frac{1}{2} + \vartheta)^2$ (see, e.g., [119]).

5.3.5 Computational complexity

Let N_r and N_ϕ be the cutoff numbers in the radial and angular directions, respectively, and N_t be the consecutive time steps. We approximate the solution of (5.73) by

$$\begin{aligned} U_{\mathbf{N}}(r, \phi, t_m) &= \sum_{|n|=0}^{N_\phi} u_{N_r, n}(r, t_m) e^{in\phi} \quad \text{or} \quad U_{\mathbf{N}}(r, \theta, \phi, t_m) \\ &= \sum_{n=0}^{N_\phi} \sum_{|l|=0}^n u_{N_r, nl}(r, t_m) Y_n^l(\theta, \phi), \end{aligned} \quad (5.86)$$

where $\mathbf{N} = (N_r, N_\phi)$, and $\{u_{N_r, n}, u_{N_r, nl}\}$ are computed from the proposed Legendre spectral-Galerkin and Newmark scheme.

Some remarks on the complexity of the algorithm for (5.73) are in order.

(i) Discrete Fourier and spherical harmonic transforms are needed to assemble the solutions (in (5.86)) and transform the given data in (5.73) to the frequency space. It is known that Fourier transform can be carried out by fast Fourier transform (FFT) with $O(N_\phi \log N_\phi)$ operations. The software, SpherePack [107], can be used to perform the discrete spherical harmonic transform, though it is not optimal in computational complexity. However, substantial progress with $O(N_\phi^2 \log N_\phi)$ operations (cf. [106, 99]), has been made by using ideas stemming from the fast multipole method.

(ii) The coefficients $\{u_{N_r, n}, u_{N_r, nl}\}$ are computed from (5.83), so the major computational cost at each time step lies in inverting the coefficient matrix and evaluating the vectors in the right-hand side of (5.83).

(a) Notice that under the basis $\{\phi_k\}$ (cf. (5.78)), the matrices M and $\widetilde{M}$ (for $d = 3$ or $d = 2$ and $b_0 = 0$) are sparse with small bandwidth and their entries

can be evaluated exactly by using the properties of Legendre polynomials (cf. [102, Ch. 4]). For $d = 2$ and $b_0 > 0$, one may take $\varpi = (x+c_0)^2$ in (5.76) (note: the “weight function” is bounded below away from 0), so that $\widetilde{M}$ will be tridiagonal. Although the matrices E and S in (5.81) are full, they can be converted to sparse matrices coincidentally by a simultaneous elimination. Let Q be an $N_r \times N_r$ fundamental matrix for elementary row operations, whose entries on the main diagonal (resp. lower off-diagonal) are all 1 (resp. -1), and the other entries are 0. One finds $QEQ^t = \text{diag}(1, 0, \dots, 0)$, and

$$(QS)_{ij} = s_{ij} - s_{i-1,j}, \quad (QSQ^t)_{ij} = s_{ij} - s_{i,j-1} + s_{i-1,j-1} - s_{i-1,j},$$

where $(\cdot)_{ij}$ denotes the entry of the involved matrix, and we set $s_{ij} = 0$ if i or j is negative. By the definition of s_{ij} , we obtain from (5.78) that

$$\begin{aligned} (QSQ^t)_{ij} &= \int_{-1}^1 (\phi_i - \phi_{i-1})'(\phi_j - \phi_{j-1})'(x+c_0)^{d-1} dx \\ &= (2i+1)(2j+1) \int_{-1}^1 P_i(x)P_j(x)(x+c_0)^{d-1} dx, \end{aligned} \quad (5.87)$$

where we used the property: $(2k+1)P_k(x) = P'_{k+1}(x) - P'_{k-1}(x)$ (cf. [102, Eq. (3.176a)]). Then one verifies readily from the three-term recurrence relation and orthogonality of Legendre polynomials that QSQ^t is tridiagonal for $d = 2$ and is pentadiagonal for $d = 3$. It is clear that the operations acting on the matrices M and $\widetilde{M}$, i.e., QMQ^t and $Q\widetilde{M}Q^t$ only increases two more non-zero off-diagonals. In summary, with this simple preprocessing, the coefficient matrix of (5.83) becomes sparse with small bandwidth, which can be inverted efficiently with nearly $O(N_r)$ operations (cf. [102, Ch. 4]).

- (b) As a typical spectral approximation using a modal basis, discrete Legendre transforms between the physical and frequency spaces are necessary for computing, e.g., $\mathbf{f}^{m+1}$, which can be done by matrix-vector multiplication in $O(N_r^2)$ operations (cf. [102]). Alpert and Rokhlin [5] developed an $O(N_r \log N_r)$ algorithm by evaluating Legendre coefficients and physical values on Chebyshev nodes, and Iserles [70] proposed a fast and simple algorithm with similar complexity for functions analytic in a sizable ellipse.

(c) We reiterate the overheads for evaluating the temporal convolution in (5.80).

Firstly, the zeros $\{z_j^\nu\}_{j=1}^{M_\nu}$ of $K_\nu(z)$ ($\nu = n, n + 1/2$) must be pre-computed to evaluate $\sigma_\nu(0)$ and $\sigma_\nu(\Delta t)$ in (5.80) and the temporal convolution. Note that the symmetry of the zeros (cf. Lemma 5.2) enables to halve the computational cost, if we use the Newton's method with initial guess in [34]. Another practical algorithm (cf. [77]) could be used to find the zeros of $K_{n+1/2}(z)$ for any $n \leq 1000$ accurately in negligible time, which can be extended to compute zeros of $K_n(z)$ easily. Secondly, armed with the zeros, the vector $\mathbf{g}^m$, computed by recurrence marching as in (5.51)-(5.52), requires $O(m)$ operators for the factor f in the sum and integral, so the cost for the convolution at $t = t_m$ in (5.52) is $O(mN_\phi)$ (note: $M_\nu \sim N_\phi$). Moreover, it's seen from (5.80) that we only need to store the sum of Legendre coefficients at previous steps.

(iii) In a nutshell, the computational cost of the solver consists of the overheads for the Legendre spectral-Galerkin-Newmark scheme for each mode $\{u_{N_r,n}, u_{N_r,nl}\}$ and Fourier/spherical harmonic transforms:

$$\{[O(N_r^2) + O(N_\phi)] \times (2N_\phi + 1)\} \times N_t + O(N_\phi \log N_\phi), \quad \text{for } d = 2, \quad (5.88)$$

$$\{[O(N_r^2) + O(N_\phi)] \times (N_\phi + 1)^2\} \times N_t + O(N_\phi^2 \log N_\phi), \quad \text{for } d = 3, \quad (5.89)$$

where $O(N_t N_\phi)$ counts the contribution of computing the temporal convolution of each mode. As mentioned before, $O(N_r^2)$ for the Legendre transforms can be reduced to $O(N_r \log N_r)$ (cf. [5]), and with the matrix operations shown in (ii)(a), the system (5.83) can be solved in nearly $O(N_r)$ operations. It is important to point out that the modes $\{u_{N_r,n}, u_{N_r,nl}\}$ can be computed parallelly, as they are decoupled.

Remark 5.7. *As outlined in Subsection 5.3.1, the coupling with the TFE method for general scatterers requires a truncation of (5.72), e.g., for $d = 2$: the numerical solution: $U_{\text{sol}} = \sum_{l=0}^{N_\varepsilon} U_{l,\mathbf{N}} \varepsilon^l$, for a given cut-off N_ε , where $\{U_{l,\mathbf{N}}\}$ are obtained*

from (5.86) by the solver. Hence, an N_ε multiple of the cost in (5.88)-(5.89) is expected. $\square$

The spectral solver should be of optimal complexity (cf. [102, Ch. 8]). However, in this context, extra price is paid for the temporal convolution, where the number of zeros (poles) grows linearly with N_ϕ . One idea to reduce the cost is to use the compressed rational approximation proposed in [3] to approximate σ_ν , which may result in a reduction to $O(N_t \log^2 N_\phi + N_t \log N_\phi \log \frac{1}{\varepsilon})$ for a prescribed accuracy threshold ε in the sense as in [3].

Here, we describe a simple approach based on the observation that for slightly large t , the contribution of the zeros z_j^n far away from the imaginary axis to the value of σ_n is exponentially small, as $\min_j \{\operatorname{Re}(z_j^n)\} \sim -na$ (where $a \approx 0.66274$) for large order n . Moreover, the zeros are much denser near the left-side of the eye-shaped curve (see Figure 5.1). Hence, we propose to modify the two-dimensional convolution kernel as $\tilde{\sigma}_n(t) = \sigma_n(t)$ for $0 \leq t < t_0$ and

$$\tilde{\sigma}_n(t) = \frac{c}{b^2} \left\{ \sum_{j \in \Upsilon_n^\delta} z_j^n e^{ctz_j^n/b} + (-1)^n \int_0^\infty \frac{e^{-ctr/b}}{K_n^2(r) + \pi^2 I_n^2(r)} dr \right\}, \quad (5.90)$$

$\forall t \geq t_0, n \gg 1$, where $\Upsilon_n^\delta = \{j : \operatorname{Re}(z_j^n) \geq -\delta(na)\}$ for some $\delta \in (0, 1)$ (note: δ tunes the number of zeros used for the summation). Notice that the integral term can be computed via (5.46) in negligible time. Accordingly, we denote the modified DtN operator (cf. (5.25)) by $\tilde{T}_d(U)$. We now examine the error induced by this approximation. If the solution $U \in H_p^s(0, 2\pi)$ (in ϕ direction and p means the periodicity), it is known that the Fourier coefficients $\widehat{U}_n \sim n^{-s}$ for all t . Then we have

$$\begin{aligned} T_d(\widehat{U}_n) - \tilde{T}_d(\widehat{U}_n) &= (\sigma_n - \tilde{\sigma}_n) * \widehat{U}_n = \frac{c}{b^2} \sum_{j \notin \Upsilon_n^\delta} z_j^n \int_{t_0}^t e^{c\tau z_j^n/b} \widehat{U}_n(b, t - \tau) d\tau \\ &\sim \frac{1}{bn^s} \sum_{j \notin \Upsilon_n^\delta} (e^{ctz_j^n/b} - e^{ct_0 z_j^n/b}) \sim \left(\sum_{j \notin \Upsilon_n^\delta} e^{ct_0 z_j^n/b} \right) n^{-s}. \end{aligned} \quad (5.91)$$

Roughly, the factor in the parentheses is dominated by $e^{-c\delta na t_0/b}$. In practice we can choose $t_0 \sim (c\delta na/b)^{-\mu}$ for some $0 < \mu < 1$ so that the factor will

be uniformly bounded. The 3D NRBK can be treated in a similar fashion. This allows to significantly reduce the cost for computing temporal convolution without lose of accuracy. This will be further confirmed by the numerical results in the forthcoming section.

5.4 Numerical results

In this section, we present various numerical results to show the accuracy and convergence of the proposed algorithm, and to demonstrate the efficiency of the reduction by (5.90).

Typically, we test the algorithm on computing the waves scattered by a disk of radius $r = b_0$ and by the impedance data $G(\phi, t)$, $\phi \in [0, 2\pi)$ and $t \geq 0$. It is known that this problem admits a series solution, which can be used as a reference solution to examine various aspects of the algorithm.

Proposition 5.1. *The exterior problem (5.1)-(5.3) with $d = 2$, $D = \{\mathbf{x} \in \mathbb{R}^2 : |\mathbf{x}| < b_0\}$, $F = U_0 = U_1 \equiv 0$, and $U|_{r=b_0} = G$, admits the solution: $U(r, \phi, t) = \sum_{|n|=0}^{\infty} \widehat{U}_n(r, t) e^{in\phi}$, for $r > b_0$, $\phi \in [0, 2\pi)$, $t > 0$, where*

$$\widehat{U}_n(r, t) = \begin{cases} 0, & t < \beta_0, \\ H_n(r, t) * \widehat{G}_n(t - \beta_0) + \sqrt{b_0/r} \widehat{G}_n(t - \beta_0), & t \geq \beta_0, \end{cases} \quad (5.92)$$

with $\beta_0 = (r - b_0)/c$, $\widehat{G}_n(t)$ being the Fourier expansion coefficient of $G(\phi, t)$, and

$$\begin{aligned} H_n = & \frac{c}{b_0} \sum_{j=1}^{M_n} \frac{K_n(r z_j^n / b_0)}{K'_n(z_j^n)} e^{tc z_j^n / b_0} \\ & + (-1)^n \frac{c}{b_0} \int_0^\infty \frac{I_n(r\rho/b_0) K_n(\rho) - K_n(r\rho/b_0) I_n(\rho)}{K_n^2(\rho) + \pi^2 I_n^2(\rho)} e^{-c\rho/b_0} d\rho, \end{aligned} \quad (5.93)$$

where $\{z_j^n\}$ are zeros of $K_n(z)$.

Proof. This problem can be solved by Laplace transform and separation of variables. Indeed, the Fourier coefficients $\{\widehat{U}_n\}$ in (5.92) can be expressed as

$$\widehat{U}_n(r, t) = \mathcal{L}^{-1} \left(\frac{K_n(sr/c)}{K_n(sb_0/c)} \right) (t) * \widehat{G}_n(t), \quad r > b_0. \quad (5.94)$$

We next sketch the evaluation of the inverse Laplace transform by using the residue theorem as in Theorem 5.1 for $\sigma_n(t)$. Using (5.16), we find $\frac{K_n(sr/c)}{K_n(sb_0/c)} \sim \sqrt{\frac{b_0}{r}} e^{-s\beta_0}$, where $\beta_0 = (r - b_0)/c$. In order to use the Jordan's lemma (cf. [35, 29]), we write

$$\begin{aligned} \mathcal{L}^{-1}\left(\frac{K_n(sr/c)}{K_n(sb_0/c)}\right)(t) &= \mathcal{L}^{-1}\left(e^{-\beta_0 s} \left\{ e^{\beta_0 s} \frac{K_n(sr/c)}{K_n(sb_0/c)} - \sqrt{\frac{b_0}{r}} \right\}\right) \\ &\quad + \mathcal{L}^{-1}\left(e^{-\beta_0 s} \sqrt{\frac{b_0}{r}}\right)(t) \\ &= \widetilde{H}_n(r, t - \beta_0) U_{\beta_0}(t) + \sqrt{\frac{b_0}{r}} \delta(t - \beta_0), \end{aligned} \quad (5.95)$$

where $\widetilde{H}_n(r, t) = \mathcal{L}^{-1}\left(e^{\beta_0 s} \frac{K_n(sr/c)}{K_n(sb_0/c)} - \sqrt{b_0/r}\right)(t)$, $U_{\beta_0}(t)$ is the unit step function (which takes 1 for $t \geq \beta_0$, and 0 for $t < \beta_0$), and $\delta(t)$ is the Dirac delta function. By applying the residue theorem and Jordan's lemma to the Bromwich's contour integral:

$$\widetilde{H}_n(r, t) = \frac{1}{2\pi i} \int_{\gamma - \infty i}^{\gamma + \infty i} \left(e^{\beta_0 s} \frac{K_n(sr/c)}{K_n(sb_0/c)} - \sqrt{\frac{b_0}{r}} \right) e^{ts} ds, \quad (5.96)$$

we obtain (5.93) by using the contour in Figure 5.2 (left) and the same argument as Theorem 5.1. Denoting $H_n(r, t) := \widetilde{H}_n(r, t - \beta_0)$, the desired expression follows from (5.95). $\square$

Remark 5.8. *Similarly, the exact solution of the 3D exterior problem can be obtained by using the same approach as in Proposition 5.1 but with the right contour in Figure 5.2.* $\square$

We take the Dirichlet data:

$$G(\phi, t) = A_1 e^{-\iota((b_0 \cos \phi - x_s)^2 + (b_0 \sin \phi - y_s)^2)} \sin^p(\omega t), \quad (5.97)$$

where $A_1 = 10$, $\iota = 0.1$, $x_s = y_s = 2.1$, $b_0 = 2$, and ω, p are to be specified later. We compute the Fourier coefficient

$$\widehat{G}_n(t) = \frac{A_1}{2\pi} \sin^p(\omega t) \int_0^{2\pi} e^{-\iota((b_0 \cos \phi - x_s)^2 + (b_0 \sin \phi - y_s)^2)} e^{-in\phi} d\phi,$$

via the fast Fourier transform with sufficient Fourier points so that the error of numerical integration can be neglected.

The first important issue is to compute the exact solution and σ_n very accurately. We point out that the convolution in (5.93) can be computed exactly, and the improper integral in (5.93) can be treated by a similar manner as the improper integral of $\sigma_n(t)$ in Subsection 5.1.3. We adopt a Newton's iteration method to compute the zeros of $K_n(z)$ accurately for moderate large n , and use a (composite) Legendre-Gauss quadrature to evaluate the integral with high precision.

We plot in Figure 5.4 the exact solution with $p = 2, b_0 = 2, b = 4$ and two different ω at various t . We see that the Dirichlet data $G(\phi, t)$ acts as a dynamical wave-maker.

Figure 5.4: Time evolution of exact solution for $\omega = 10\pi$ and $\omega = 20\pi$.

5.4.1 Accuracy of the NRBC

Now, we examine accuracy of the NRBC by computing the error of the NRBC for the problem in Proposition 5.1:

$$E_{N_\phi}(t) = \max_{|n| \leq N_\phi} \left| \left(\frac{1}{c} \frac{\partial \widehat{U}_n}{\partial t} + \frac{\partial \widehat{U}_n}{\partial r} + \frac{\widehat{U}_n}{2r} \right) \Big|_{r=b} - \sigma_n(t) * \widehat{U}_n(b, t) \right|, \quad t > 0, \quad (5.98)$$

where $\{\widehat{U}_n(b, t)\}$ are computed from (5.92), and we take $N_\phi = 32$ so that $\{|\widehat{U}_n(b, t)|\}$ are sufficiently small for all modes $|n| > N_\phi$ and all t of interest.

We tabulate in Table 5.3 the errors with various parameters and time t , where we choose the radius b so that the reference solution: $U_{N_\phi}(b, \phi, t) = \sum_{|n|=0}^{N_\phi} \widehat{U}_n(b, t) e^{in\phi}$ has a bigger magnitude. We see that in all cases, the errors are almost machine zero. This validates the formula for σ_n in Theorem 5.1 and shows the super-high accuracy of its numerical treatment.

Table 5.3: The errors $E_{N_\phi}(t)$.

t	$\omega = 10\pi$		$\omega = 20\pi$	
	$b = 2.22$	$b = 2.75$	$b = 2.38$	$b = 2.87$
0.5	2.637e-16	7.026e-17	6.245e-17	8.327e-17
1	4.684e-16	2.099e-16	9.021e-17	2.272e-16
5	2.567e-16	1.131e-15	7.251e-16	1.318e-15
10	7.772e-16	2.207e-15	1.457e-15	2.387e-15

As a comparison study, we demonstrate the accuracy of three different approaches for computing the NRBC σ_ν , i.e., the accurate formula in (5.33), the modified formula in (5.90), and the compressed rational approximation in [3]. Here, we extract the available data (for spherical kernel with 10^{-6} accuracy in [3]) from Hagstrom's website: "<http://faculty.smu.edu/thagstrom/sph6.txt>". The intention is to compare their performance for large mode n . Hence, we choose the spherical harmonic expansion coefficient of the data at the scatterer's surface, which generates the 3D exact solution (cf. Proposition 5.1 and Remark 5.8), to

be $\sin^6(\pi t)$. In Table 5.4, we listed the accuracy measured as in (5.98), but for $d = 3$ and each fixed mode. We see that the use of a comparable number of zeros (compressed poles in [3]) leads to a very similar accuracy. We reiterate that the simple modified approach in (5.90) requires to use all zeros for $0 \leq t < t_0$.

Table 5.4: Comparison of three approaches ($t = 3.5, t_0 = 0.2, b = 2.1, c = 5$).

n (total zeroes)	Approach by (5.33)		Approach by (5.90)		Approach in [3]	
	accuracy	used zeros	accuracy	used zeros	accuracy	used poles
60	1.3223e-12	60	1.6646e-07	10	1.6763e-07	11
70	1.7082e-12	70	4.2907e-08	12	2.6160e-07	11
90	2.6909e-12	90	1.1889e-09	12	6.8482e-08	12
100	7.5346e-12	100	2.6676e-09	12	6.9170e-08	12

5.4.2 Convergence of the algorithm for smooth solutions

The second task is to demonstrate the accuracy and convergence of the spectral-Galerkin-Newmark scheme described in Section 5.3. Let $\{u_{N_r,n}(r, t_m)\}$ be the numerical solutions (as defined in (5.86)) computed by the scheme, which approximate the corresponding reference solutions $\{\widehat{U}_n(r, t_m)\}$ in Proposition 5.1. Here, we take N_ϕ so that the magnitudes of the truncated modes $\{|\widehat{U}_n|\}_{|n| > N_\phi}$ are sufficiently small, and the parameters are taken as before. The numerical errors are measured by

$$\begin{aligned}\widehat{E}_{\mathbf{N}}(t) &= \max_{|n| \leq N_\phi} \|u_{N_r,n}(\cdot, t) - \widehat{U}_n(\cdot, t)\|_{L^2, N_r}, \\ \widetilde{E}_{\mathbf{N}}(t) &= \max_{|n| \leq N_\phi} \|u_{N_r,n}(\cdot, t) - \widehat{U}_n(\cdot, t)\|_{L^\infty, N_r},\end{aligned}$$

where $\mathbf{N} = (N_r, N_\phi)$, $\|\cdot\|_{L^2, N_r}$ is the discrete L^2 -norm associated with the Legendre-Gauss-Lobatto points, and $\|\cdot\|_{L^\infty, N_r}$ is the corresponding discrete maximum norm.

We list in Table 5.5 the errors and convergence order in time discretization, where we choose $N_r = 50, N_\phi = 15$ so that the error of spatial discretization is

Table 5.5: The errors $\widehat{E}_N(t)$ and $\widetilde{E}_N(t)$, and order of convergence in time.

t	Δt	$\widehat{E}_N(t)$	order	$\widetilde{E}_N(t)$	order	t	Δt	$\widehat{E}_N(t)$	order	$\widetilde{E}_N(t)$	order
1	1e-3	1.21e-5		1.93e-5		3	1e-3	1.23e-5		2.01e-5	
	5e-4	3.02e-6	2.0001	4.83e-6	1.9999		5e-4	3.07e-6	2.0001	5.02e-6	2.0000
	1e-4	1.21e-7	1.9999	1.93e-7	1.9999		1e-4	1.23e-7	2.0000	2.01e-7	2.0000
	5e-5	3.02e-8	2.0001	4.83e-8	1.9991		5e-5	3.07e-8	2.0001	5.02e-8	2.0000
2	1e-3	1.23e-5		2.01e-5		4	1e-3	1.23e-5		2.01e-5	
	5e-4	3.07e-6	2.0000	5.02e-6	2.0000		5e-4	3.07e-6	2.0001	5.02e-6	2.0000
	1e-4	1.23e-7	2.0000	2.01e-7	2.0000		1e-4	1.23e-7	2.0000	2.01e-7	2.0000
	5e-5	3.07e-8	2.0000	5.02e-8	1.9999		5e-5	3.07e-8	2.0001	5.02e-8	2.0000

negligible, and the other parameters are $b = 5$, $\omega = \pi$, and $p = 6$. As expected, we observe a second-order convergence of the Newmark scheme.

To see the spectral accuracy of the Legendre-Galerkin approximation, we take $\Delta t = 10^{-5}$, and fix other parameters, but vary N_r . Observe from Table 5.6 a fast decay of the errors as a typical spectral approximation, which also shows the scheme is quite stable.

Table 5.6: The errors $\widehat{E}_N(t)$ and $\widetilde{E}_N(t)$.

t	$N_r = 8$		$N_r = 10$		$N_r = 16$		$N_r = 32$	
	$\widehat{E}_N(t)$	$\widetilde{E}_N(t)$	$\widehat{E}_N(t)$	$\widetilde{E}_N(t)$	$\widehat{E}_N(t)$	$\widetilde{E}_N(t)$	$\widehat{E}_N(t)$	$\widetilde{E}_N(t)$
0.5	2.349e-4	2.687e-4	2.253e-5	2.846e-5	8.224e-7	1.207e-6	9.229e-9	1.639e-8
1.0	3.877e-4	4.179e-4	1.708e-5	2.042e-5	1.833e-7	2.777e-7	1.959e-9	2.673e-9
1.5	3.276e-4	3.596e-4	5.965e-6	7.146e-6	3.072e-8	5.238e-8	1.508e-9	1.762e-9
2.0	4.105e-4	4.368e-4	1.092e-5	1.188e-5	7.353e-9	1.238e-8	1.237e-9	2.119e-9
2.5	3.239e-4	3.607e-4	5.724e-6	6.997e-6	2.381e-9	3.182e-9	1.488e-9	1.734e-9
3.0	4.113e-4	4.380e-4	1.095e-5	1.189e-5	1.404e-9	2.893e-9	1.227e-9	2.009e-9
3.5	3.238e-4	3.608e-4	5.747e-6	7.036e-6	1.554e-9	2.063e-9	1.488e-9	1.732e-9
4.0	4.113e-4	4.380e-4	1.095e-5	1.189e-5	1.269e-9	2.061e-9	1.227e-9	2.007e-9

Finally, we plot in Figure 5.5 the numerical solution (red nets) against the

Figure 5.5: Propagation of exact and numerical solutions.

exact solution (blue smooth surface), where the exact solution in (a) and (b) is in the annulus: $2 \leq r \leq 10$, while the numerical solution within $2 \leq r \leq 5$. Figure 5.5 (c) shows the wave propagation through the artificial boundary at $b = 5, 0 \leq \phi \leq 2\pi$ for $0 \leq t \leq 4$ (numerical solution) against $0 \leq t \leq 4.5$ (exact solution). We see that the red nets and blue surfaces agree well in these plots. Moreover, we observe the waves pass the boundary transparently. This shows that the proposed scheme is very stable and accurate.

5.4.3 Test for the modification of NRBCs

To illustrate the effectiveness of the modification in (5.90)-(5.91), we take the Dirichlet data G to be less regular in ϕ -direction:

$$G = y^\lambda e^{xy/2} \sin^6(\pi t) = e^{b_0^2 \cos \phi \sin \phi/2} (b_0 \sin \phi)^\lambda \sin^6(\pi t), \quad (5.99)$$

where $\lambda > 0$ is a non-integer constant. One verifies that $G \in H_p^{\lambda+1/2-\varepsilon}(0, 2\pi)$ (for small $\varepsilon > 0$) and its Fourier coefficients decay like $O(N_\phi^{\varepsilon-(\lambda+1/2)})$. The Fourier coefficients of the exact solution in Proposition 5.1 are expected to decay in a similar fashion.

Hereafter, we take $\lambda = 2.5, b_0 = 2, b = c = 3$, and use the modified NBRK $\tilde{\sigma}_n$ in (5.90) for $n \geq 20$, and $t \geq t_0 = (c\delta na/b)^{-\mu}$ (cf. (5.91), note: $a = 0.66274$) with $\mu = 0.9$. Recall that the poles $\{z_j^n\}$ are dropped, if $\text{Re}(z_j^n) < -\delta na$. As $\{z_j^n\}$

are very dense on the left portion of the eye-shaped curve (cf. Figure 5.1), many poles can be dropped (about 90% as shown in Table 5.7) for large n and all $t \geq t_0$. Moreover, equipped with the guideline in (5.90)-(5.91), such a modification does not deteriorate the accuracy and stability of the algorithm as shown in Figure 5.6.

Table 5.7: The number of used poles and the starting time of modification.

n	$\delta = 0.4$			$\delta = 0.5$		
	used	total	t_0	used	total	t_0
55	6	54	0.090	10	54	0.073
65	8	64	0.077	10	64	0.063
75	8	74	0.068	12	74	0.055
90	10	90	0.058	16	90	0.047
100	12	100	0.052	18	100	0.043
110	12	110	0.048	18	110	0.039

Figure 5.6: Left: $\log_{10}(L^2\text{-error})$ against $\log_{10}(N_\phi)$ with $N_r = 30$ and $\Delta t = 5e - 5$ at $t = 2.5$. Right: stability of “without modification” (marked by “ $\diamond$ ”) and “with modification” (marked by “ $\circ$ ”), where $N_\phi = 100$, $N_r = 30$, and $\delta = 0.4$.

5.4.4 Test for three-dimensional case

Now, we examine the performance of the proposed algorithm for 3D case. In the following test, we take

$$G(\theta, \phi, t) = 50[1 - \tanh(2 \cos \phi \sin(5\theta))] \sin^6(\pi t), \quad (5.100)$$

and choose $b_0 = 2, b = c = 3$. The reference exact solution (cf. Remark 5.8) is evaluated by a very fine mesh and the numerical solution is computed by the spherical harmonic expansion (5.86), where the coefficients are computed by the one-dimensional solver (5.76). We tabulate in Table 5.8 the (discrete) L^2 -errors with $N_r = 30, N_\phi = 100$, and various time step sizes Δt at different time t , which indicates a convergence behavior similar to the two-dimensional case (cf. Table 5.5).

Table 5.8: Second-order convergence in time.

t	Δt	error	order	t	Δt	error	order
1	1e-3	3.61e-5		2	1e-3	3.53e-5	
	5e-4	9.04e-6	2.00		5e-4	8.81e-6	2.00
	1e-4	3.61e-7	2.00		1e-4	3.53e-7	2.00
	5e-5	9.04e-8	1.99		5e-5	8.81e-8	1.99
3	1e-3	3.52e-5		4	1e-3	3.52e-5	
	5e-4	8.81e-6	2.00		5e-4	8.81e-6	2.00
	1e-4	3.52e-7	2.00		1e-4	3.52e-7	2.00
	5e-5	8.81e-8	2.00		5e-5	8.81e-8	2.00

We depict in Figure 5.7 (a)-(d) spherical plots of the waves on the artificial spherical boundary $r = b$, across which the outgoing waves propagate seamlessly. Finally, we compare the convergence and accuracy of the algorithm using exact NRBCs and the low-order boundary conditions in [11] at $r = b$:

Figure 5.7: Numerical solution at different time t at $r = b$: (a)-(c): function plot on the outer spherical surface; (d): surf-plot on spherical coordinates. Contour of numerical solution at $t = 2$ sliced by $\theta = 15\pi/199$: (e)-(g): BT1, BT2, NRBC. (h): L^2 -errors obtained by three boundary conditions and the full algorithm with $\Delta t = 10^{-4}$, $N_r = 30$ and $N_\phi = 100$.

$$\begin{aligned}
 \text{BT1 : } & \left(\frac{\partial}{\partial r} + \frac{\partial}{\partial t} \right) [ru] = 0; \\
 \text{BT2 : } & \left(\frac{\partial}{\partial r} + \frac{\partial}{\partial t} \right) \left(\frac{\partial}{\partial r} + \frac{\partial}{\partial t} + \frac{2}{r} \right) [ru] = 0.
 \end{aligned} \tag{5.101}$$

We plot in Figure 5.7 (e)-(g) the contour of the numerical solution sliced in θ , and in Figure 5.7 (h) the convergence of the boundary conditions. We see that the NRBC produces very accurate numerical solution, while BT1 and BT2 give very poor results.

Time-Dependent Maxwell's Equations[†]

For the three-dimensional Maxwell's equations, the existing formulations for the NRBC (see, e.g., [61, 26]) present a great challenge for evaluation. Therefore, in this chapter, we reformulate the NRBC for Maxwell's equations, and use the techniques in Chapter 5 to compute the temporal convolutions in a fast and accurate manner. We also use the algorithm proposed in Chapter 5, i.e., spectral-Galerkin in space and Newmark scheme in time, to solve the interior truncated problem with a spherical scatterer. However, the extension appears much more involved due to the involvement of vector spherical harmonics.

This chapter is organized as follows. In Section 6.1, we reformulate the NRBC and provide the analytic formulas for NRBKs, which allow us to use the fast temporal techniques in Chapter 5 to compute the involved convolutions. We present the variational formulation of the interior problem and prove its well-posedness in Section 6.2. In Section 6.3, we use the Newmark-spectral-Galerkin solver with updated Richardson extrapolation (fourth order in time) for the interior problem with a spherical scatterer. We provide some numerical results in the last section

[†]The main part of this chapter is based on the conference paper: “X.D. Zhao and L.L. Wang. Fast and accurate computation of exact nonreflecting boundary condition for Maxwell's equations. Accepted by the Conference: The 29th International Review of Progress in Applied and Computational Electromagnetics, 2013.”

to show the exactness of our NRBC, and the convergence orders of the algorithm.

6.1 New formulation of NRBC

We consider the electromagnetic scattering problem with the perfect conducting boundary condition on a bounded obstacle:

$$\left\{ \begin{array}{l} \varepsilon \frac{\partial \mathbf{E}}{\partial t} - \nabla \times \mathbf{H} = \mathbf{J}, \quad \text{in } \mathbb{R}^3 \setminus \bar{D}, \quad t > 0, \end{array} \right. \quad (6.1a)$$

$$\left\{ \begin{array}{l} \mu \frac{\partial \mathbf{H}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0}, \quad \text{in } \mathbb{R}^3 \setminus \bar{D}, \quad t > 0, \end{array} \right. \quad (6.1b)$$

$$\left\{ \begin{array}{l} \mathbf{E} \times \hat{\mathbf{x}} = \mathbf{g}, \quad \text{at } \Gamma_D, \quad t > 0, \end{array} \right. \quad (6.1c)$$

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{E}_T}{\partial t} + \sqrt{\frac{\mu}{\varepsilon}} \hat{\mathbf{x}} \times \frac{\partial \mathbf{H}}{\partial t} = o(|\mathbf{x}|^{-1}), \quad t > 0, \end{array} \right. \quad (6.1d)$$

$$\left\{ \begin{array}{l} \mathbf{E}|_{t=0} = \mathbf{E}_0, \quad \mathbf{H}|_{t=0} = \mathbf{H}_0, \quad \text{in } \mathbb{R}^3 \setminus \bar{D}. \end{array} \right. \quad (6.1e)$$

Here, D is a bounded domain with Lipschitz boundary Γ_D , the vector functions $\mathbf{E}, \mathbf{H}$ are respectively the electric and magnetic fields, $\hat{\mathbf{x}} = \mathbf{x}/|\mathbf{x}|$, and $\mathbf{E}_T = \hat{\mathbf{x}} \times (\mathbf{E} \times \hat{\mathbf{x}})$ is the tangential component of $\mathbf{E}$. The source current $\mathbf{J}$ and the initial data $\mathbf{E}_0, \mathbf{H}_0$ are assumed to be supported in a ball $B := \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| < b\}$. The electric permittivity ε and magnetic permeability μ are assumed to be positive constants, and throughout this chapter, we define $c = 1/\sqrt{\varepsilon\mu}, \eta = \sqrt{\mu/\varepsilon}$.

To solve this exterior problem, it is critical to truncate the unbounded domain into a bounded one, and accordingly, an appropriate boundary condition should be imposed at the outer boundary to prevent the reflection of waves. Here, we are mostly interested in the imposition of exact nonreflecting boundary conditions (or transparent boundary conditions). Moreover, to reduce the number of unknowns, we eliminate $\mathbf{H}$ from the system and focus on the truncated problem:

$$\left\{ \begin{array}{l} \frac{\partial^2 \mathbf{E}}{\partial t^2} + c^2 \nabla \times \nabla \times \mathbf{E} = \mathbf{F}, \quad \text{in } \Omega, \quad t > 0, \end{array} \right. \quad (6.2a)$$

$$\left\{ \begin{array}{l} \mathbf{E} \times \hat{\mathbf{x}} = \mathbf{g}, \quad \text{at } \Gamma_D, \quad t > 0, \end{array} \right. \quad (6.2b)$$

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{E}_T}{\partial t} - c \hat{\mathbf{x}} \times (\nabla \times \mathbf{E}) = \mathcal{T}_b[\mathbf{E}], \quad \text{at } r = b, \quad t > 0, \end{array} \right. \quad (6.2c)$$

$$\left\{ \begin{array}{l} \mathbf{E}|_{t=0} = \mathbf{E}_0, \quad \frac{\partial \mathbf{E}}{\partial t} \Big|_{t=0} = \mathbf{E}_1, \quad \text{in } \Omega, \end{array} \right. \quad (6.2d)$$

where $\Omega = B \setminus \bar{D}$, $\mathbf{F} = c\eta \partial_t \mathbf{J}$ and the boundary condition (6.2c) is referred to exact NRBC, which involves the electric-to-magnetic (EtM) operator $\mathcal{T}_b$ to be specified later.

6.1.1 Vector spherical harmonics

The expression of the EtM operator requires the use of vector spherical harmonics (VSH), and we collect some relevant properties to be used later.

The spherical coordinates (r, θ, φ) are related to the Cartesian coordinates $\mathbf{x} = (x_1, x_2, x_3)$ via

$$x_1 = r \sin \theta \cos \varphi, \quad x_2 = r \sin \theta \sin \varphi, \quad x_3 = r \cos \theta, \quad (6.3)$$

with the moving (right-handed) orthonormal coordinate basis $\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{e}_\varphi\}$:

$$\begin{aligned} \mathbf{e}_r &= \frac{\mathbf{x}}{r}, \quad \mathbf{e}_\theta = (\cos \theta \cos \varphi, \cos \theta \sin \varphi, -\sin \theta), \\ \mathbf{e}_\varphi &= (-\sin \varphi, \cos \varphi, 0). \end{aligned} \quad (6.4)$$

Let S be the unit spherical surface. Recall that the Laplace-Beltrami operator Δ_S and tangent gradient operator ∇_S on S are defined as

$$\Delta_S u = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 u}{\partial \varphi^2}, \quad \nabla_S u = \frac{\partial u}{\partial \theta} \mathbf{e}_\theta + \frac{1}{\sin \theta} \frac{\partial u}{\partial \varphi} \mathbf{e}_\varphi. \quad (6.5)$$

The operator Δ_S is self-adjoint, positive compact in $L^2(S)$, the (complex) Hilbert space of square-integrable functions on S , equipped with the inner product

$$(u, v)_{0,S} := \int_S u \bar{v} d\sigma = \int_0^{2\pi} \int_0^\pi u \bar{v} \sin \theta d\theta d\varphi. \quad (6.6)$$

The spherical harmonics $\{Y_l^m\}$ (as normalized in [87]) are eigenfunctions of Δ_S :

$$\Delta_S Y_l^m = -l(l+1)Y_l^m, \quad l \geq 0, \quad 0 \leq |m| \leq l; \quad \int_S Y_l^m \overline{Y_{l'}^{m'}} dS = \delta_{ll'} \delta_{mm'}. \quad (6.7)$$

The VSH are built upon the spherical harmonics $\{Y_l^m\}$. We remark that several versions of VSH have been used in the literature (see, e.g., [66, 87, 86, 33, 85]).

In this context, we adopt two families of equivalent VSH bases. The first family, up to a constant multiple, is from Hill [66, 87]:

$$\left\{ \begin{array}{l} \mathbf{T}_l^m = \nabla_S Y_l^m \times \mathbf{e}_r = \frac{1}{\sin \theta} \frac{\partial Y_l^m}{\partial \varphi} \mathbf{e}_\theta - \frac{\partial Y_l^m}{\partial \theta} \mathbf{e}_\varphi, \quad l \geq 1, \quad 0 \leq |m| \leq l, \end{array} \right. \quad (6.8a)$$

$$\left\{ \begin{array}{l} \mathbf{V}_l^m = (l+1)Y_l^m \mathbf{e}_r - \nabla_S Y_l^m, \quad l \geq 0, \quad 0 \leq |m| \leq l, \end{array} \right. \quad (6.8b)$$

$$\left\{ \begin{array}{l} \mathbf{W}_l^m = lY_l^m \mathbf{e}_r + \nabla_S Y_l^m, \quad l \geq 1, \quad 0 \leq |m| \leq l. \end{array} \right. \quad (6.8c)$$

Notice that $\mathbf{V}_0^0 = \mathbf{e}_r / \sqrt{4\pi}$. With the understanding of $\mathbf{T}_0^0 = \mathbf{W}_0^0 = \mathbf{0}$, the indexes $\{l, m\}$ run over $\{(l, m) : l \geq 0, 0 \leq |m| \leq l\}$.

We will also utilize the VSH $\{Y_l^m \mathbf{e}_r, \nabla_S Y_l^m, \nabla_S Y_l^m \times \mathbf{e}_r\}$, which can be found in Morse and Feshbach [86], and has been used in the Spherepack [107]. One easily finds the correspondence:

$$Y_l^m \mathbf{e}_r = \frac{\mathbf{W}_l^m + \mathbf{V}_l^m}{2l+1}, \quad \nabla_S Y_l^m = \frac{(l+1)\mathbf{W}_l^m - l\mathbf{V}_l^m}{2l+1}, \quad \nabla_S Y_l^m \times \mathbf{e}_r = \mathbf{T}_l^m. \quad (6.9)$$

By (6.7), (6.8) and (6.9), we have

$$\begin{aligned} \int_S \mathbf{T}_l^m \cdot \overline{\mathbf{V}_{l'}^{m'}} dS &= \int_S \mathbf{T}_l^m \cdot \overline{\mathbf{W}_{l'}^{m'}} dS = \int_S \mathbf{V}_l^m \cdot \overline{\mathbf{W}_{l'}^{m'}} dS = 0, \\ \int_S \mathbf{V}_l^m \cdot \overline{\mathbf{V}_{l'}^{m'}} dS &= (l+1)(2l+1)\delta_{ll'}\delta_{mm'}, \\ \int_S \mathbf{T}_l^m \cdot \overline{\mathbf{T}_{l'}^{m'}} dS &= l(l+1)\delta_{ll'}\delta_{mm'}, \quad \int_S \mathbf{W}_l^m \cdot \overline{\mathbf{W}_{l'}^{m'}} dS = l(2l+1)\delta_{ll'}\delta_{mm'}, \end{aligned} \quad (6.10)$$

and

$$\begin{aligned} \int_S Y_l^m \mathbf{e}_r \cdot \overline{\mathbf{T}_{l'}^{m'}} dS &= \int_S Y_l^m \mathbf{e}_r \cdot \overline{\nabla_S Y_{l'}^{m'}} dS = \int_S \mathbf{T}_l^m \cdot \overline{\nabla_S Y_{l'}^{m'}} dS = 0, \\ \int_S \nabla_S Y_l^m \cdot \overline{\nabla_S Y_{l'}^{m'}} dS &= l(l+1)\delta_{ll'}\delta_{mm'}, \\ \int_S Y_l^m \mathbf{e}_r \cdot \overline{Y_{l'}^{m'} \mathbf{e}_r} dS &= \delta_{ll'}\delta_{mm'}. \end{aligned} \quad (6.11)$$

Therefore, either $\{\mathbf{T}_l^m, \mathbf{V}_l^m, \mathbf{W}_l^m\}$ or $\{Y_l^m \mathbf{e}_r, \nabla_S Y_l^m, \nabla_S Y_l^m \times \mathbf{e}_r\}$ forms a complete orthogonal basis of $(L^2(S))^3$.

Remark 6.1. *It is worthwhile to point out the correspondence between (6.8a)-(6.8c) and the notation and definition in [66, 87, 86, 33, 85].*

- Hill [66] used the notation $\{\mathbf{V}_{lm}, \mathbf{X}_{lm}, \mathbf{W}_{lm}\}$, and there holds

$$\mathbf{V}_{lm} = \frac{-\mathbf{V}_l^m}{\sqrt{(l+1)(2l+1)}}, \quad \mathbf{X}_{lm} = \frac{i\mathbf{T}_l^m}{\sqrt{l(l+1)}}, \quad \mathbf{W}_{lm} = \frac{\mathbf{W}_l^m}{\sqrt{l(2l+1)}}. \quad (6.12)$$

- Nédélec [87] used the notation $\{I_l^m, T_l^m, N_l^m\}$, and we have the relationship

$$N_{l+1}^m = \mathbf{V}_l^m, \quad T_l^m = \mathbf{T}_l^m, \quad I_{l-1}^m = \mathbf{W}_l^m. \quad (6.13)$$

- Colton and Kress [33, Eq. (6.530)] and Monk [85, Eq. (9.56)] adopted

$$U_l^m = \frac{1}{\sqrt{l(l+1)}} \nabla_S Y_l^m, \quad V_l^m = \hat{\mathbf{x}} \times U_l^m, \quad (6.14)$$

to expand the tangential fields on S .

For any vector field $\mathbf{v} = (v_1, v_2, v_3)$, denote by v_r, v_θ and v_φ the projections of $\mathbf{v}$ onto $\mathbf{e}_r, \mathbf{e}_\theta$ and $\mathbf{e}_\varphi$, respectively, that is,

$$v_r = \mathbf{v} \cdot \mathbf{e}_r, \quad v_\theta = \mathbf{v} \cdot \mathbf{e}_\theta, \quad v_\varphi = \mathbf{v} \cdot \mathbf{e}_\varphi \quad \Rightarrow \quad \mathbf{v} = v_r \mathbf{e}_r + v_\theta \mathbf{e}_\theta + v_\varphi \mathbf{e}_\varphi. \quad (6.15)$$

Let $\mathbf{v}$ be differentiable vector function. Recall that in spherical coordinates (6.4) (cf. [1]):

$$\begin{aligned} \mathbf{curl} \mathbf{v} = \nabla \times \mathbf{v} &= \frac{1}{r \sin \theta} \left(\frac{\partial(\sin \theta v_\varphi)}{\partial \theta} - \frac{\partial v_\theta}{\partial \varphi} \right) \mathbf{e}_r \\ &+ \frac{1}{r} \left(\frac{1}{\sin \theta} \frac{\partial v_r}{\partial \varphi} - \frac{\partial(r v_\varphi)}{\partial r} \right) \mathbf{e}_\theta + \frac{1}{r} \left(\frac{\partial(r v_\theta)}{\partial r} - \frac{\partial v_r}{\partial \theta} \right) \mathbf{e}_\varphi. \end{aligned} \quad (6.16)$$

For ease of notation, we define

$$d_l^+ = \frac{d}{dr} + \frac{l}{r}, \quad d_l^- = \frac{d}{dr} - \frac{l}{r}.$$

The following properties stem from Hill [66]:

$$\begin{aligned} \mathbf{curl}(f \mathbf{V}_l^m) &= (d_{l+2}^+ f) \mathbf{T}_l^m, \quad \mathbf{curl}(f \mathbf{W}_l^m) = -(d_{l-1}^- f) \mathbf{T}_l^m, \\ (2l+1) \mathbf{curl}(f \mathbf{T}_l^m) &= (l+1)(d_{l+1}^+ f) \mathbf{W}_l^m - l(d_l^- f) \mathbf{V}_l^m. \end{aligned} \quad (6.17)$$

6.1.2 Formulation of the EtM operator

Let $\{E_{lm}^r, E_{lm}^{(1)}, E_{lm}^{(2)}\}$ be the VSH expansion coefficients of the electric field $\mathbf{E}$ in terms of VSH $\{Y_l^m \mathbf{e}_r, \nabla_S Y_l^m, \mathbf{T}_l^m\}$ at the artificial spherical surface $r = b$, i.e.,

$$\mathbf{E} = \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(E_{lm}^r Y_l^m \mathbf{e}_r + E_{lm}^{(1)} \nabla_S Y_l^m + E_{lm}^{(2)} \mathbf{T}_l^m \right). \quad (6.18)$$

Note that in [61], the exact NRBC is expressed as a system of $\mathbf{E}$ and $\mathbf{H}$, which is actually equivalent to the formulation (cf. [26]) by using the VSH $\{Y_l^m \mathbf{e}_r, \nabla_S Y_l^m, \mathbf{T}_l^m\}$, and the electric-to-magnetic (EtM) operator is given by

$$\mathcal{T}_b[\mathbf{E}] = \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l \left((\rho_l * E_{lm}^{(1)}) \nabla_S Y_l^m + (\sigma_l * E_{lm}^{(2)}) \mathbf{T}_l^m \right). \quad (6.19)$$

Here, ρ_l and σ_l , termed as the nonreflecting boundary kernels (NRBKs), are defined by

$$\rho_l(t) = \mathcal{L}^{-1} \left[z \left(\frac{z k_l(z)}{k_l(z) + z k_l'(z)} + 1 \right) \right](t), \quad z = \frac{sb}{c}, \quad (6.20)$$

$$\sigma_l(t) = \mathcal{L}^{-1} \left[1 + z + z \frac{k_l'(z)}{k_l(z)} \right](t), \quad z = \frac{sb}{c}, \quad (6.21)$$

where $\mathcal{L}^{-1}$ is the inverse Laplace transform, and $k_l(z)$ is the modified spherical Bessel function defined by $k_l(z) = \sqrt{2/(\pi z)} K_{l+1/2}(z)$, with $K_{l+1/2}$ being the modified Bessel function of the second kind of order $l + 1/2$ (cf. [118]). The involved convolution is defined as usual: $(f * g)(t) = \int_0^t f(\tau)g(t - \tau)d\tau$.

The NRBK σ_l appears in the NRBC for the transient wave equation, which has an explicit formula (see (5.33) in Chapter 5) derived from the Residue theory (see e.g., [61, 115]). However, this analytic tool for inverse Laplace transform can not be applied to compute ρ_l , since we lack information on the zeros of $k_l(z) + z k_l'(z)$ (i.e., the poles of the integrand in the inverse Laplace transform), while that of $k_l(z)$ is available.

Observe from (6.19) that the EtM operator only involves the VSH expansion coefficients $\{E_{lm}^{(1)}, E_{lm}^{(2)}\}$ in (6.18). In fact, there holds the following relation

between E_{lm}^r and $E_{lm}^{(1)}$:

$$\widehat{E}_{lm}^r(s) = l(l+1) \frac{k_l(z)}{k_l(z) + z k_l'(z)} \widehat{E}_{lm}^{(1)}(s), \quad z = \frac{sb}{c}, \quad \text{at } r = b, \quad (6.22)$$

where $\{\widehat{E}_{lm}^r(s), \widehat{E}_{lm}^{(1)}(s)\}$ are Laplace transforms of $\{E_{lm}^r, E_{lm}^{(1)}\}$, respectively. Using the relation in (6.22) leads to the following alternative formulation, and we provide the derivation of (6.19) and (6.23) at the end of this section.

Theorem 6.1. *The EtM operator $\mathcal{T}_b[\mathbf{E}]$ in (6.19) can be reformulated as:*

$$\mathcal{T}_b[\mathbf{E}] = \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\frac{\omega_l * E_{lm}^r}{l(l+1)} \nabla_s Y_l^m + (\sigma_l * E_{lm}^{(2)}) \mathbf{T}_l^m \right), \quad (6.23)$$

where σ_l is defined in (6.21), and ω_l is given by

$$\omega_l(t) = \mathcal{L}^{-1} \left[z \left(1 + z + z \frac{k_l'(z)}{k_l(z)} \right) \right] (t) = \frac{b}{c} (\sigma_l'(t) + \sigma_l(0) \delta(t)), \quad z = \frac{sb}{c}, \quad (6.24)$$

with δ being the Dirac delta function.

It is seen from (6.19) and (6.23) that the exact NRBC (6.2c) is global in both time and space, due to the involvement of the VSH expansion coefficients and temporal convolutions. Moreover, it requires to compute the inverse Laplace transform of the ratio of modified Bessel functions. Hence, some care needs to be taken to deal with the non-localness of NRBCs.

As already mentioned, the NRBC σ_l appears in the exact NRBC for the wave equation, and the explicit formula derived from the Residue theory (see (5.33)) is of the form:

$$\sigma_l(t) = \frac{c}{b} \sum_{j=1}^l z_j^l e^{\frac{c}{b} z_j^l t}, \quad l \geq 1, \quad t \geq 0, \quad (6.25)$$

where $\{z_j^l\}_{j=1}^l$ are the zeros of $K_{l+1/2}(z)$. Hence, it follows from (6.24) that

$$\omega_l(t) = \frac{c}{b} \sum_{j=1}^l (z_j^l)^2 e^{\frac{c}{b} z_j^l t} + \delta(t) \sum_{j=1}^l z_j^l, \quad l \geq 1, \quad t \geq 0. \quad (6.26)$$

Observe from (6.25)-(6.26) that the time variable t merely appears in the exponentials. This allows for a fast recursive temporal convolution as shown in

(5.51) in Chapter 5, therefore, we can eliminate the nonlocality of NRBC in time. Thanks to this notion, we deduce from (6.25)-(6.26) that

$$\begin{aligned} [\sigma_l * g](t) &= \int_0^t \sigma_l(t - \tau) g(\tau) d\tau \\ &= \frac{c}{b} \sum_{j=1}^l z_j^l \int_0^t e^{c(t-\tau)z_j^l/b} g(\tau) d\tau = \frac{c}{b} \sum_{j=1}^l z_j^l f(t; z_j^l), \end{aligned} \quad (6.27)$$

and

$$\begin{aligned} [\omega_l * g](t) &= \frac{c}{b} \sum_{j=1}^l (z_j^l)^2 \int_0^t e^{c(t-\tau)z_j^l/b} g(\tau) d\tau + g(t) \sum_{j=1}^l z_j^l \\ &= \frac{c}{b} \sum_{j=1}^l (z_j^l)^2 f(t; z_j^l) + g(t) \sum_{j=1}^l z_j^l. \end{aligned} \quad (6.28)$$

For clarity, we summarize the whole algorithm for the computation of $\mathcal{T}_b[\mathbf{E}]$ in (6.23). The algorithm is intended to compute $\mathcal{T}_b[\mathbf{E}](t)$ in (6.23) at $t = t_n = n\Delta t, n \geq 0$, and on the colatitude-longitude grids adopted by the Spherepack [2] from $\mathbf{E}$ on the same grids.

Algorithm for computing $\mathcal{T}_b[\mathbf{E}]$ in (6.23)

Step 1. Use the Spherepack to compute $\{E_{lm}^r, E_{lm}^{(2)}\}$ from $\mathbf{E}$ in (6.18).

Step 2. Compute the zeros $\{z_j^l\}$ for $l \geq 1$.

Step 3. Compute $\sigma_l * E_{lm}^{(2)}$ and $\omega_l * E_{lm}^r$ via (6.27)-(6.28).

Step 4. Use the Spherepack to compute $\mathcal{T}_b[\mathbf{E}]$ via (6.23).

It is clear that the number of zeros to be used is determined by the truncation of the expansion (6.18). If l is large, we can adopt the strategies: (i) dropping insignificant zeros (see Subsection 5.3.5 in Chapter 5) and (ii) compression algorithm (cf. [3]) to reduce the complexity in Step 3.

6.1.3 Derivation of the EtM operators in (6.19) and (6.23)

Consider the Maxwell's equations exterior to the artificial ball B :

$$\left\{ \begin{array}{l} \varepsilon \frac{\partial \mathbf{E}^e}{\partial t} - \nabla \times \mathbf{H}^e = \mathbf{0}, \quad \text{in } \Omega^e := \mathbb{R}^3 \setminus \bar{B}, \quad t > 0, \end{array} \right. \quad (6.29a)$$

$$\left\{ \begin{array}{l} \mu \frac{\partial \mathbf{H}^e}{\partial t} + \nabla \times \mathbf{E}^e = \mathbf{0}, \quad \text{in } \Omega^e, \quad t > 0, \end{array} \right. \quad (6.29b)$$

$$\left\{ \begin{array}{l} \hat{\mathbf{x}} \times \mathbf{E}^e|_{r=b} = \mathbf{\Psi}, \quad t > 0, \end{array} \right. \quad (6.29c)$$

with the initial data $\mathbf{E}^e|_{t=0} = \mathbf{H}^e|_{t=0} = \mathbf{0}$, and the far-field radiational condition (cf. (6.1d)). This problem can be solved by Laplace transform in time and separation of variables in space. Hereafter, we denote by a wide-hat the Laplace transform of the underlying functions, e.g., $\widehat{\mathbf{E}}^e = \mathcal{L}[\mathbf{E}^e]$ and $\widehat{\mathbf{H}}^e = \mathcal{L}[\mathbf{H}^e]$. Applying the Laplace transform to the above exterior problem yields

$$\left\{ \begin{array}{l} s\varepsilon \widehat{\mathbf{E}}^e - \nabla \times \widehat{\mathbf{H}}^e = \mathbf{0}, \quad \text{in } \Omega^e, \quad \text{Re}(s) > 0, \end{array} \right. \quad (6.30a)$$

$$\left\{ \begin{array}{l} s\mu \widehat{\mathbf{H}}^e + \nabla \times \widehat{\mathbf{E}}^e = \mathbf{0}, \quad \text{in } \Omega^e, \quad \text{Re}(s) > 0, \end{array} \right. \quad (6.30b)$$

$$\left\{ \begin{array}{l} \hat{\mathbf{x}} \times \widehat{\mathbf{E}}^e|_{r=b} = \widehat{\mathbf{\Psi}}, \end{array} \right. \quad (6.30c)$$

$$\left\{ \begin{array}{l} s\widehat{\mathbf{E}}_T^e + s\eta \hat{\mathbf{x}} \times \widehat{\mathbf{H}}^e = o(r^{-1}). \end{array} \right. \quad (6.30d)$$

Now, we use the method of separation of variables in spherical coordinates to solve (6.30). For this purpose, we expand the vector fields in terms of VSH in (6.9) as

$$\begin{aligned} \{\widehat{\mathbf{E}}^e, \widehat{\mathbf{H}}^e\} &= \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\{\widehat{E}_{lm}^r, \widehat{H}_{lm}^r\} Y_l^m \mathbf{e}_r + \{\widehat{E}_{lm}^{(1)}, \widehat{H}_{lm}^{(1)}\} \nabla_S Y_l^m + \{\widehat{E}_{lm}^{(2)}, \widehat{H}_{lm}^{(2)}\} \mathbf{T}_l^m \right), \\ \widehat{\mathbf{\Psi}} &= \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\widehat{\Psi}_{lm}^{(1)} \nabla_S Y_l^m + \widehat{\Psi}_{lm}^{(2)} \mathbf{T}_l^m \right), \end{aligned} \quad (6.31)$$

where with a little abuse of notation, we still used $\{E_{lm}^r, E_{lm}^{(1)}, E_{lm}^{(2)}\}$ to denote the expansion coefficients of $\mathbf{E}$ exterior to B . Inserting the first expansion into (6.30a)-(6.30b), we obtain from (6.9) and (6.17) the algebraic equations:

$$s\varepsilon \widehat{E}_{lm}^r = \frac{l(l+1)}{r} \widehat{H}_{lm}^{(2)}, \quad s\mu \widehat{H}_{lm}^r = -\frac{l(l+1)}{r} \widehat{E}_{lm}^{(2)}, \quad (6.32)$$

and the system of differential equations:

$$\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\widehat{E}_{lm}^{(1)} = s\mu\widehat{H}_{lm}^{(2)} + \frac{1}{r}\widehat{E}_{lm}^r, \quad \left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\widehat{E}_{lm}^{(2)} = -s\mu\widehat{H}_{lm}^{(1)}, \quad (6.33)$$

$$\left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\widehat{H}_{lm}^{(1)} = -s\varepsilon\widehat{E}_{lm}^{(2)} + \frac{1}{r}\widehat{H}_{lm}^r, \quad \left(\frac{\partial}{\partial r} + \frac{1}{r}\right)\widehat{H}_{lm}^{(2)} = s\varepsilon\widehat{E}_{lm}^{(1)}. \quad (6.34)$$

Eliminating $\widehat{E}_{lm}^r$ and $\widehat{H}_{lm}^r$ in (6.33)-(6.34) by using (6.32), we obtain the matrix form

$$\left(\frac{\partial}{\partial r} + \frac{1}{r}\right) \begin{pmatrix} \widehat{E}_{lm}^{(1)} \\ \widehat{E}_{lm}^{(2)} \\ \widehat{H}_{lm}^{(1)} \\ \widehat{H}_{lm}^{(2)} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & s\mu + \frac{l(l+1)}{s\varepsilon r^2} \\ 0 & 0 & -s\mu & 0 \\ 0 & -s\varepsilon - \frac{l(l+1)}{s\mu r^2} & 0 & 0 \\ s\varepsilon & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \widehat{E}_{lm}^{(1)} \\ \widehat{E}_{lm}^{(2)} \\ \widehat{H}_{lm}^{(1)} \\ \widehat{H}_{lm}^{(2)} \end{pmatrix}. \quad (6.35)$$

Notice that (6.35) reduces to [61, Eq. (2.25)], if $\varepsilon = \mu = c^{-1}$. As in [61], the general solution that meets the far-field radiation condition (6.30d) is

$$\begin{pmatrix} \widehat{E}_{lm}^{(1)} \\ \widehat{E}_{lm}^{(2)} \\ \widehat{H}_{lm}^{(1)} \\ \widehat{H}_{lm}^{(2)} \end{pmatrix} = A_{lm}(s) \begin{pmatrix} k'_l(sr/c) + \frac{k_l(sr/c)}{sr/c} \\ 0 \\ 0 \\ k_l(sr/c)/\eta \end{pmatrix} + B_{lm}(s) \begin{pmatrix} 0 \\ -\eta k_l(sr/c) \\ k'_l(sr/c) + \frac{k_l(sr/c)}{sr/c} \\ 0 \end{pmatrix}, \quad (6.36)$$

where $\{A_{lm}, B_{lm}\}$ are arbitrary functions. Using the properties: $\hat{\mathbf{x}} \times \mathbf{T}_l^m = \nabla_s Y_l^m$ and $\hat{\mathbf{x}} \times \nabla_s Y_l^m = -\mathbf{T}_l^m$, and imposing the boundary condition (6.30c), we find

$$A_{lm}(s) = -\frac{sb/c}{Z_l(sb/c)}\widehat{\Psi}_{lm}^{(2)}(s), \quad B_{lm}(s) = -\frac{1}{\eta k_l(sb/c)}\widehat{\Psi}_{lm}^{(1)}(s), \quad (6.37)$$

where $Z_l(z) = k_l(z) + zk'_l(z)$. Consequently, we derive the solution of (6.35):

$$\widehat{E}_{lm}^{(1)}(r, s) = -\frac{b}{r} \frac{Z_l(sr/c)}{Z_l(sb/c)}\widehat{\Psi}_{lm}^{(2)}(s), \quad \widehat{E}_{lm}^{(2)}(r, s) = \frac{k_l(sr/c)}{k_l(sb/c)}\widehat{\Psi}_{lm}^{(1)}(s), \quad (6.38)$$

$$\widehat{H}_{lm}^{(1)}(r, s) = -\frac{1}{\eta sr/c} \frac{Z_l(sr/c)}{k_l(sb/c)}\widehat{\Psi}_{lm}^{(1)}(s), \quad (6.39)$$

$$\widehat{H}_{lm}^{(2)}(r, s) = -\frac{sb/c}{\eta} \frac{k_l(sr/c)}{Z_l(sb/c)}\widehat{\Psi}_{lm}^{(2)}(s), \quad (6.40)$$

and the other two components can be obtained from the above and (6.32). Substituting them into (6.31) leads to the solution of (6.30). In particular, we have

$$\begin{aligned} \widehat{\mathbf{H}}^e = & - \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\left[l(l+1) \frac{k_l(sr/c)}{k_l(sb/c)} Y_l^m \mathbf{e}_r + \frac{Z_l(sr/c)}{k_l(sb/c)} \nabla_s Y_l^m \right] \frac{\widehat{\Psi}_{lm}^{(1)}}{\eta sr/c} \right. \\ & \left. + \frac{sb/c}{\eta} \frac{k_l(sr/c)}{Z_l(sb/c)} \widehat{\Psi}_{lm}^{(2)} \mathbf{T}_l^m \right). \end{aligned} \quad (6.41)$$

We remark that with a change of VSH to (6.13), the special case of the solution ($b = 1$ and pure imaginary s) coincides with [87, Eqs. (5.3.28)-(5.3.29)]. Then by (6.30b) with $r = b$, we have the electric-to-magnetic Calderon relation:

$$\begin{aligned} -c \hat{\mathbf{x}} \times (\nabla \times \widehat{\mathbf{E}}^e) \Big|_{r=b} &= s\eta \hat{\mathbf{x}} \times \widehat{\mathbf{H}}^e \Big|_{r=b} \\ &= \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\frac{1}{sb/c} \frac{Z_l(sb/c)}{k_l(sb/c)} (s\widehat{\Psi}_{lm}^{(1)}) \mathbf{T}_l^m - sb/c \frac{k_l(sb/c)}{Z_l(sb/c)} (s\widehat{\Psi}_{lm}^{(2)}) \nabla_s Y_l^m \right). \end{aligned} \quad (6.42)$$

By requiring the interior fields $\{\mathbf{E}, \mathbf{H}\}$ to be identical to the exterior fields $\{\mathbf{E}^e, \mathbf{H}^e\}$ across the artificial boundary $r = b$, and setting $\hat{\mathbf{x}} \times \mathbf{E}|_{r=b} = \Psi$, we obtain

$$\begin{aligned} -c \hat{\mathbf{x}} \times (\nabla \times \widehat{\mathbf{E}}) \Big|_{r=b} &= \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(sb/c \frac{k_l(sb/c)}{Z_l(sb/c)} s\widehat{E}_{lm}^{(1)} \nabla_s Y_l^m + \frac{1}{sb/c} \frac{Z_l(sb/c)}{k_l(sb/c)} s\widehat{E}_{lm}^{(2)} \mathbf{T}_l^m \right) \\ &= \sum_{l=1}^{\infty} \sum_{m=-l}^l \left\{ \left(\frac{c}{b} \mathcal{L}[\rho_l] - s \right) \widehat{E}_{lm}^{(1)} \nabla_s Y_l^m + \left(\frac{c}{b} \mathcal{L}[\sigma_l] - s \right) \widehat{E}_{lm}^{(2)} \mathbf{T}_l^m \right\} \\ &= \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l \left\{ \mathcal{L}[\rho_l] \widehat{E}_{lm}^{(1)} \nabla_s Y_l^m + \mathcal{L}[\sigma_l] \widehat{E}_{lm}^{(2)} \mathbf{T}_l^m \right\} - s\widehat{\mathbf{E}}_T, \end{aligned} \quad (6.43)$$

where ρ_l and σ_l are given in (6.20)-(6.21). Transforming back to t -domain leads to the NRBC (6.2c) with $\mathcal{T}_b[\mathbf{E}]$ given by (6.19).

We now turn to the derivation of (6.23). Our standing point is to obtain from (6.38)-(6.40) that

$$s \left(\frac{1}{c\eta} \widehat{E}_{lm}^{(1)} + \frac{1}{c} \widehat{H}_{lm}^{(2)} \right) = \frac{1}{r} Q_l(sr/c) \widehat{H}_{lm}^{(2)}, \quad (6.44)$$

$$s \left(\frac{1}{c\eta} \widehat{E}_{lm}^{(2)} - \frac{1}{c} \widehat{H}_{lm}^{(1)} \right) = \frac{1}{r\eta} Q_l(sr/c) \widehat{E}_{lm}^{(2)}, \quad (6.45)$$

where $\eta = \sqrt{\mu/\varepsilon}$ as before, and

$$Q_l(z) = 1 + z + z \frac{k'_l(z)}{k_l(z)} = z + \frac{Z_l(z)}{k_l(z)}. \quad (6.46)$$

Multiplying (6.44) (resp. (6.45)) by $\nabla_S Y_l^m$ (resp. $\mathbf{T}_l^m$), and summing the resulted equations, together with (6.32), leads to

$$\begin{aligned} \frac{s}{c\eta} \widehat{\mathbf{E}}_T^e + \frac{s}{c} \hat{\mathbf{x}} \times \widehat{\mathbf{H}}^e &= \frac{1}{r} \sum_{l=1}^{\infty} \sum_{m=-l}^l Q_l(sr/c) \left(\widehat{H}_{lm}^{(2)} \nabla_S Y_l^m + \frac{1}{\eta} \widehat{E}_{lm}^{(2)} \mathbf{T}_l^m \right) \\ &= \frac{1}{\eta r} \sum_{l=1}^{\infty} \sum_{m=-l}^l Q_l(sr/c) \left(\frac{sr/c}{l(l+1)} \widehat{E}_{lm}^r \nabla_S Y_l^m + \widehat{E}_{lm}^{(2)} \mathbf{T}_l^m \right). \end{aligned} \quad (6.47)$$

Letting $r = b$, we find from the first identity of (6.42) and $\widehat{\mathbf{E}}_T^e|_{r=b} = \widehat{\mathbf{E}}_T|_{r=b}$ that

$$\begin{aligned} \left[s \widehat{\mathbf{E}}_T - c \hat{\mathbf{x}} \times (\nabla \times \widehat{\mathbf{E}}) \right] \Big|_{r=b} \\ = \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l Q_l(sb/c) \left(\frac{sb/c}{l(l+1)} \widehat{E}_{lm}^r \nabla_S Y_l^m + \widehat{E}_{lm}^{(2)} \mathbf{T}_l^m \right). \end{aligned} \quad (6.48)$$

Performing inverse Laplace transform on (6.48) leads to the alternative formulation of NRBC with the EtM given in (6.23):

$$\begin{aligned} \left[\frac{\partial \mathbf{E}_T}{\partial t} - c \hat{\mathbf{x}} \times (\nabla \times \mathbf{E}) \right] \Big|_{r=b} \\ = \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\frac{\omega_l * E_{lm}^r}{l(l+1)} \nabla_S Y_l^m + (\sigma_l * E_{lm}^{(2)}) \mathbf{T}_l^m \right), \end{aligned} \quad (6.49)$$

where σ_l is given by (6.21).

Comparing the first identity in (6.43) with (6.48), we obtain the relation (6.22).

6.2 Variational formulation and well-posedness

To this end, we show the well-posedness of the truncated problem (6.2). Without loss of generality, we assume $\mathbf{g} = \mathbf{0}$ since the nonhomogeneous boundary condition at Γ_D can be simply converted to a homogeneous one by subtracting a suitable

function from the solution, and this yields an additional term $\mathbf{G}$ in the NRBC. To be precise, the problem of interest takes the following form

$$\left\{ \begin{array}{l} \frac{\partial^2 \mathbf{E}}{\partial t^2} + c^2 \nabla \times \nabla \times \mathbf{E} = \mathbf{F}, \quad \text{in } \Omega, \quad t > 0, \end{array} \right. \quad (6.50a)$$

$$\left\{ \begin{array}{l} \mathbf{E} \times \hat{\mathbf{x}} = \mathbf{0}, \quad \text{at } \Gamma_D, \quad t > 0, \end{array} \right. \quad (6.50b)$$

$$\left\{ \begin{array}{l} \frac{\partial \mathbf{E}_T}{\partial t} - c \hat{\mathbf{x}} \times (\nabla \times \mathbf{E}) = \mathcal{T}_b[\mathbf{E}] + \mathbf{G}, \quad \text{at } r = b, \quad t > 0, \end{array} \right. \quad (6.50c)$$

$$\left\{ \begin{array}{l} \mathbf{E}|_{t=0} = \mathbf{E}_0, \quad \frac{\partial \mathbf{E}}{\partial t} \Big|_{t=0} = \mathbf{E}_1, \quad \text{in } \Omega, \end{array} \right. \quad (6.50d)$$

Define $H(\mathbf{curl}; \Omega) := \{\mathbf{v} \in (L^2(\Omega))^3 : \nabla \times \mathbf{v} \in (L^2(\Omega))^3\}$, and the space of surface tangential vector fields in $L^2(\partial B)$:

$$\mathbf{TL}^2(\partial B) = \{\mathbf{u} \in (L^2(\partial B))^3 : \mathbf{u} \cdot \hat{\mathbf{x}} = 0 \text{ a.e. on } \partial B\}. \quad (6.51)$$

Let $\mathbf{X} := \{\mathbf{v} \in L^2(0, T; H(\mathbf{curl}; \Omega)) \cap H^1(0, T; (L^2(\Omega))^3) : \mathbf{v} \times \hat{\mathbf{x}}|_{\Gamma_D} = \mathbf{0}\}$, and $(\cdot, \cdot)$ and $\|\cdot\|$ be the complex inner product and norm of $(L^2(\Omega))^3$, respectively. Likewise, we define $\langle \cdot, \cdot \rangle_{r=b}$ with b being the radius of the artificial boundary. By [85, Theorem 3.31], we know that for any $\mathbf{v} \in H(\mathbf{curl}; \Omega)$ and $\phi \in H(\mathbf{curl}; \Omega)$,

$$(\nabla \times \mathbf{v}, \phi) - (\mathbf{v}, \nabla \times \phi) = \langle \boldsymbol{\nu} \times \mathbf{v}, (\boldsymbol{\nu} \times \phi) \times \boldsymbol{\nu} \rangle_{\partial \Omega}, \quad (6.52)$$

where $\boldsymbol{\nu}$ is the unit normal outward to Ω .

Take $\mathbf{v} = \nabla \times \mathbf{E}$, and $\phi \in \mathbf{X}$ in (6.52). By (6.50b) and (6.50c), we have

$$\begin{aligned} & (\nabla \times \nabla \times \mathbf{E}, \phi) - (\nabla \times \mathbf{E}, \nabla \times \phi) \\ &= \langle \hat{\mathbf{x}} \times (\nabla \times \mathbf{E}), (\hat{\mathbf{x}} \times \phi) \times \hat{\mathbf{x}} \rangle_{r=b} - \langle \hat{\mathbf{x}} \times (\nabla \times \mathbf{E}), (\hat{\mathbf{x}} \times \phi) \times \hat{\mathbf{x}} \rangle_{\Gamma_D} \\ &= \frac{1}{c} \left\langle \frac{\partial \mathbf{E}_T}{\partial t} - \mathcal{T}_b[\mathbf{E}], \phi_T \right\rangle_{r=b} - \frac{1}{c} \langle \mathbf{G}, \phi_T \rangle_{r=b}, \end{aligned}$$

where ϕ_T is the tangential component of ϕ .

We define a bilinear form on $\mathbf{X} \times \mathbf{X}$:

$$\begin{aligned} \mathcal{B}(\mathbf{E}, \mathbf{V}) &= \left(\frac{\partial^2 \mathbf{E}}{\partial t^2}, \mathbf{V} \right) + c^2 (\nabla \times \mathbf{E}, \nabla \times \mathbf{V}) \\ &\quad + c \left\langle \frac{\partial \mathbf{E}_T}{\partial t} - \mathcal{T}_b[\mathbf{E}], \mathbf{V}_T \right\rangle_{r=b}. \end{aligned} \quad (6.53)$$

The variational formulation of (6.50) is as follows: Given $\mathbf{F} \in L^\infty(0, T; (L^2(\Omega))^3)$ and $\mathbf{G} \in H^1(0, T; \mathbf{TL}^2(\partial B))$, find $\mathbf{E} \in \mathbf{X}$, such that

$$\mathcal{B}(\mathbf{E}, \mathbf{V}) = c \langle \mathbf{G}, \mathbf{V}_T \rangle_{r=b} + (\mathbf{F}, \mathbf{V}), \quad \forall \mathbf{V} \in \mathbf{X}. \quad (6.54)$$

The existence and uniqueness of the solution for (6.50) follow from the energy conservation, which is stated in the following theorem.

Theorem 6.2. *Assume that $\mathbf{F} = \mathbf{G} = \mathbf{0}$ in (6.50), $\mathbf{E}_0 \in H(\mathbf{curl}; \Omega)$ and $\mathbf{E}_1 \in (L^2(\Omega))^3$. Then we have the energy conservation: $\mathbb{E}(t) = \mathbb{E}_0$ for all $t \geq 0$, where*

$$\begin{aligned} \mathbb{E}(t) = & \int_{\Omega} (|\partial_t \mathbf{E}|^2 + c^2 |\nabla \times \mathbf{E}|^2) d\mathbf{x} \\ & + 2c \operatorname{Re} \int_0^t \int_{\{r=b\}} (\partial_\tau \mathbf{E}_T - \mathcal{T}_b[\mathbf{E}]) \cdot \partial_\tau \overline{\mathbf{E}}_T dS d\tau, \end{aligned} \quad (6.55)$$

and

$$\mathbb{E}_0 = \int_{\Omega} (|\mathbf{E}_1|^2 + c^2 |\nabla \times \mathbf{E}_0|^2) d\mathbf{x}. \quad (6.56)$$

Hence, the truncated problem has a unique solution such that $\mathbf{E} \in L^\infty(0, T; H(\mathbf{curl}; \Omega))$ and $\partial_t \mathbf{E} \in L^\infty(0, T; (L^2(\Omega))^3)$ for all $T > 0$.

Proof. Let $\mathbf{V} = 2\partial_t \mathbf{E}$ in (6.53), and take the real part of the resulted equation, we arrive at

$$\frac{d}{dt} \int_{\Omega} (|\partial_t \mathbf{E}|^2 + c^2 |\nabla \times \mathbf{E}|^2) d\mathbf{x} + 2c \operatorname{Re} \int_{\{r=b\}} (\partial_\tau \mathbf{E}_T - \mathcal{T}_b[\mathbf{E}]) \cdot \partial_\tau \overline{\mathbf{E}}_T dS = 0.$$

Integrating the above equation over $(0, t)$ leads to $\mathbb{E}(t) = \mathbb{E}_0$ for all $t \geq 0$, where $\mathbb{E}(t)$ and $\mathbb{E}_0$ are defined in (6.55) and (6.56), respectively. $\square$

Remark 6.2. *One may further show the stability of the truncated problem (6.50) with $\mathbf{F} \neq \mathbf{0}$ and $\mathbf{G} \neq \mathbf{0}$. The argument is similar to Theorem 5.3 in Chapter 5. In the following, we provide some analysis tools for readers' reference.* $\square$

The main tools for the proof of stability include (i) the Plancherel or Parseval identity for the Laplace transform (see Lemma 5.4), (ii) some properties of the ratio of modified Bessel functions (see [26]), and (iii) the energy method.

The following properties, which can be derived from [26, Lemma 2.5], are indispensable for the analysis.

Lemma 6.1. *Let $s = s_1 + is_2$ with $s_1, s_2 \in \mathbb{R}$ and $s_1 > 0$. Then we have*

$$\operatorname{Re}\left(\frac{Z_l(z)}{zk_l(z)}\right) < 0, \quad \operatorname{Re}\left(\frac{zk_l(z)}{Z_l(z)}\right) < 0, \quad (6.57)$$

where $Z_l(z) = zk'_l(z) + k_l(z)$ with $z = sb/c$.

Proof. From the proof of Lemma 2.5 in [26], for $k = is/c$ with $\operatorname{Im}(k) > 0$, we have that

$$\operatorname{Re}\left(\frac{z_l^{(1)}(kb)}{ikbh_l^{(1)}(kb)}\right) > 0, \quad \operatorname{Re}\left(\frac{ikbh_l^{(1)}(kb)}{z_l^{(1)}(kb)}\right) > 0, \quad (6.58)$$

where $z_l^{(1)}(z) = z(h_l^{(1)}(z))' + h_l^{(1)}(z)$ with $h_l^{(1)}(z)$ is the spherical Hankel function of the first kind of order l .

By the relation $k_l(z) = -i^l h_l^{(1)}(iz)$ (cf. [92, Eq. (10.47.13)]), we have

$$Z_l(sb/c) = sb/ck'_l(sb/c) + k_l(sb/c) = -i^l(kbh_l^{(1)'}(kb) + h_l^{(1)}(kb)) = -i^l z_l^{(1)}(kb).$$

This implies

$$\begin{aligned} \frac{Z_l(z)}{zk_l(z)} &= \frac{Z_l(sb/c)}{sb/ck_l(sb/c)} = -\frac{z_l^{(1)}(kb)}{ikbh_l^{(1)}(kb)}, \\ \frac{zk_l(z)}{Z_l(z)} &= \frac{sb/ck_l(sb/c)}{Z_l(sb/c)} = -\frac{ikbh_l^{(1)}(kb)}{z_l^{(1)}(kb)}, \end{aligned}$$

which, together with $\operatorname{Im}(k) = s_1/c$ and (6.58), lead to the desired results. $\square$

With the aid of the above lemma and Lemma 5.4, we can obtain the following important results.

Lemma 6.2. *Let ρ_l and σ_l be the NRBKs defined in (6.20) and (6.21), respectively. Then for any $v, w \in H^1(0, T)$ with $v(0) = w(0) = 0$, and all $T > 0, l \geq 1$, we have*

$$\operatorname{Re} \int_0^T [\sigma_l * v](t) \bar{v}'(t) dt \leq \frac{b}{c} \int_0^T |v'(t)|^2 dt, \quad (6.59)$$

$$\operatorname{Re} \int_0^T [\rho_l * w](t) \bar{w}'(t) dt \leq \frac{b}{c} \int_0^T |w'(t)|^2 dt. \quad (6.60)$$

Proof. We can follow the same lines as the proof of Lemma 5.2 by using the properties in Lemma 6.1. $\square$

An important consequence of Lemma 6.2 is the following property of the EtM operator, which is essential for the analysis.

Lemma 6.3. *For any $t > 0$, if $\partial_\tau \mathbf{E} \in L^2(0, t; \mathbf{TL}^2(\partial B))$, then we have*

$$\operatorname{Re} \int_0^t \int_{\{r=b\}} \mathcal{T}_b[\mathbf{E}] \cdot \partial_\tau \overline{\mathbf{E}}_T dS d\tau \leq \int_0^t \int_{\{r=b\}} |\partial_\tau \mathbf{E}_T|^2 dS d\tau. \quad (6.61)$$

Proof. This inequality follows from (6.19), the orthogonality of $\{\nabla_S Y_l^m, \mathbf{T}_l^m\}$ (cf. (6.10)-(6.11)) and Lemma 6.2, since

$$\begin{aligned} \operatorname{Re} \int_0^t \int_{\{r=b\}} \mathcal{T}_b[\mathbf{E}] \cdot \partial_\tau \overline{\mathbf{E}}_T dS d\tau &= \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l l(l+1) \left(\operatorname{Re} \int_0^t (\rho_l * E_{lm}^{(1)})(\tau) \partial_\tau \overline{E_{lm}^{(1)}} d\tau \right) \\ &\quad + \frac{c}{b} \sum_{l=1}^{\infty} \sum_{m=-l}^l l(l+1) \left(\operatorname{Re} \int_0^t (\sigma_l * E_{lm}^{(2)})(\tau) \partial_\tau \overline{E_{lm}^{(2)}} d\tau \right) \\ &\leq \sum_{l=1}^{\infty} \sum_{m=-l}^l l(l+1) \int_0^t \left(|\partial_\tau E_{lm}^{(1)}|^2 + |\partial_\tau E_{lm}^{(2)}|^2 \right) d\tau \\ &= \int_0^t \int_{\{r=b\}} |\partial_\tau \mathbf{E}_T|^2 dS d\tau. \end{aligned}$$

This ends the proof. $\square$

It is clear that by Lemma 6.3, the term involving the outer artificial spherical surface $\{r = b\}$ in $\mathbb{E}(t)$ is non-negative. Then we can follow the argument in Theorem 5.3 to prove the stability of (6.50) with $\mathbf{F} \neq \mathbf{0}, \mathbf{G} \neq \mathbf{0}$.

6.3 A Newmark-spectral-Galerkin solver for spherical scatterer

In this section, we describe a mixed VSH-Legendre spectral-Galerkin approximation in space and Newmark discretization with Richardson extrapolation in time for the truncated Maxwell's equations (6.50) with a spherical scatterer

$D = \{\mathbf{x} \in \mathbb{R}^3 : r = |\mathbf{x}| < a\}$. While it appears of limited interest to consider a special regular scatterer, we feel it worthy of care for twofold reasons:

- (i) It's an ideal situation to test the proposed algorithm for treating exact NRBC. As we will see, the nonlocality of NRBC in space can be completely eliminated, if one approximates the problem in the frequency space (of VSH expansion coefficients).
- (ii) Such a solver plays an utmost important role in solving the scattering problem with an irregular bounded scatterer. The methodology is similar to Subsection 5.3.1 in Chapter 5, but the implementation is much more involved and complicated.

6.3.1 Dimension reduction

Previously, we used the VSH in (6.9) to represent the EtM operator and reformulate the NRBC, but computationally, we find it more conveniently to express $\mathbf{E}$ in terms of $\{\mathbf{V}_l^m, \mathbf{W}_l^m, \mathbf{T}_l^m\}$ defined in (6.8). Let

$$\{\mathbf{E}, \mathbf{F}\} = \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\{v_l^m, f_{l,0}^m\} \mathbf{V}_l^m + \{w_l^m, f_{l,1}^m\} \mathbf{W}_l^m + \{u_l^m, f_{l,2}^m\} \mathbf{T}_l^m \right),$$

and

$$\mathbf{H} = \sum_{l=1}^{\infty} \sum_{m=-l}^l \left(\hat{h}_l^m \nabla_S Y_l^m + \tilde{h}_l^m \mathbf{T}_l^m \right).$$

From (6.9), we find that

$$E_{lm}^r = (l+1)v_l^m + lw_l^m, \quad E_{lm}^{(1)} = -v_l^m + w_l^m, \quad E_{lm}^{(2)} = u_l^m. \quad (6.62)$$

Next, we take special test function $\mathbf{V} \in \mathbf{X}$ in the variational formulation (6.54) to get rid of the nonlocality in space. For each fixed l and $0 \leq |m| \leq l$,

- (i) we take $\mathbf{V} = \phi_{l,0}^m \mathbf{V}_l^m + \phi_{l,1}^m \mathbf{W}_l^m$ with $(\phi_{l,0}^m - \phi_{l,1}^m)(a) = 0$ in (6.54), and for convenience of notations, we use $v, w, \phi_0, \phi_1, f_0, f_1, \hat{h}$ to denote $v_l^m, w_l^m, \phi_{l,0}^m,$

$\phi_{l,1}^m, f_{l,0}^m, f_{l,1}^m, \hat{h}_l^m$, respectively. By the curl formulas in (6.17), the orthogonality of $\{\mathbf{V}_l^m, \mathbf{W}_l^m, \mathbf{T}_l^m\}$ (cf. (6.10)) and the expression of EtM operation in (6.23), we arrive at

$$\begin{aligned}
& (l+1) \left(\frac{\partial^2 v}{\partial t^2}, \phi_0 \right)_{\varpi} + l \left(\frac{\partial^2 w}{\partial t^2}, \phi_1 \right)_{\varpi} \\
& + b^2 c \frac{l(l+1)}{2l+1} \frac{\partial}{\partial t} (v-w)(b, t) (\overline{\phi_0 - \phi_1})(b) \\
& + c^2 \frac{l(l+1)}{2l+1} (d_{l+2}^+ v - d_{l-1}^- w, d_{l+2}^+ \phi_0 - d_{l-1}^- \phi_1)_{\varpi} \\
& = -bc^2 \frac{l(l+1)}{2l+1} \left(\frac{1}{l} \omega_l * v(b, t) + \frac{1}{l+1} \omega_l * w(b, t) \right) (\overline{\phi_0 - \phi_1})(b) \\
& - b^2 c \frac{l(l+1)}{2l+1} \hat{h}(\overline{\phi_0 - \phi_1})(b) + (l+1)(f_0, \phi_0)_{\varpi} + l(f_1, \phi_1)_{\varpi},
\end{aligned} \tag{6.63}$$

where $d_l^{\pm} = \frac{d}{dr} \pm \frac{l}{r}$;

(ii) we take $\mathbf{V} = \phi_{l,2}^m \mathbf{T}_l^m$ with $\phi_{l,2}^m(a) = 0$ in (6.54), and use $u, \phi_2, \tilde{h}, f_2$ to denote $u_l^m, \phi_{l,2}^m, \tilde{h}_l^m, f_{l,2}^m$, respectively. By the curl formulas in (6.17), the orthogonality of $\mathbf{T}_l^m$ and the expression of EtM operation in (6.23), we have

$$\begin{aligned}
& \left(\frac{\partial^2 u}{\partial t^2}, \phi_2 \right)_{\varpi} + c^2 (\partial_r u, \partial_r \phi_2)_{\varpi} + c^2 l(l+1)(u, \phi_2) \\
& + b^2 c \frac{\partial}{\partial t} u(b, t) \overline{\phi_2}(b) + bc^2 u(b, t) \overline{\phi_2}(b) \\
& = bc^2 (\sigma_l * u(b, t)) \overline{\phi_2}(b) + b^2 c \tilde{h} \overline{\phi_2}(b) + (f_2, \phi_2)_{\varpi}.
\end{aligned} \tag{6.64}$$

Here, $(u, v)_{\varpi} = \int_a^b u(r) \bar{v}(r) \varpi dr$ with $\varpi = r^2$.

Notice that the weak formulation (6.64) is the same as that for the wave equation (cf. (5.76) in Chapter 5), therefore, we mainly present the numerical approximation for (6.63) with each fixed l and m . Since ω_l is real, in the following, we assume v and w are real.

6.3.2 Spectral-Galerkin approximation in space

We apply the Legendre spectral-Galerkin method to approximate (6.63) in space.

Denote $V_N = \{(\phi, \psi)^t \in (\mathbb{P}_N)^2 : (\phi - \psi)(a) = 0\}$, where $\mathbb{P}_N$ is the set of all algebraic polynomials of degree at most N . The semi-discretization Legendre spectral-Galerkin approximation for (6.63) is to find $(v_N(\cdot, t), w_N(\cdot, t))^t \in V_N$, such that for any $(\xi_0, \xi_1)^t \in V_N$,

$$\begin{aligned}
 & (l+1) \left(\frac{\partial^2 v_N}{\partial t^2}, \xi_0 \right)_\varpi + l \left(\frac{\partial^2 w_N}{\partial t^2}, \xi_1 \right)_\varpi + b^2 c \frac{l(l+1)}{2l+1} \frac{\partial}{\partial t} (v_N - w_N)(b, t) (\xi_0 - \xi_1)(b) \\
 & + c^2 \frac{l(l+1)}{2l+1} (d_{l+2}^+ v_N - d_{l-1}^- w_N, d_{l+2}^+ \xi_0 - d_{l-1}^- \xi_1)_\varpi \\
 & = -bc^2 \frac{l(l+1)}{2l+1} \left(\frac{1}{l} \omega_l * v_N(b, t) + \frac{1}{l+1} \omega_l * w_N(b, t) \right) (\xi_0 - \xi_1)(b) \\
 & - b^2 c \frac{l(l+1)}{2l+1} \hat{h}(\xi_0 - \xi_1)(b) + (l+1) (I_N f_0, \xi_0)_\varpi + l (I_N f_1, \xi_1)_\varpi, \\
 & v_N(x, 0) = v_{0,N}(x), \quad \dot{v}_N(x, 0) = v_{1,N}(x), \\
 & w_N(x, 0) = w_{0,N}(x), \quad \dot{w}_N(x, 0) = w_{1,N}(x),
 \end{aligned} \tag{6.65}$$

where I_N is the interpolation operator on $N+1$ Legendre-Gauss-Lobatto points, and $v_{0,N}, v_{1,N}, w_{0,N}, w_{1,N}$ are suitable approximations of the initial values.

Theorem 6.3. *Let $(v_N(\cdot, t), w_N(\cdot, t))^t$ be the solution of (6.65). If $\hat{h} \in L^\infty(0, T)$, $\partial_t \hat{h} \in L^1(0, T)$ and $f_0(\cdot, t), f_1(\cdot, t) \in C(a, b)$. Then for all $T > 0$,*

$$\begin{aligned}
 & (l+1) \|\partial_t v_N\|_{L^\infty(0, T; L^2_\varpi(a, b))}^2 + l \|\partial_t w_N\|_{L^\infty(0, T; L^2_\varpi(a, b))}^2 \\
 & + c^2 \frac{l(l+1)}{2l+1} \|d_{l+2}^+ v_N - d_{l-1}^- w_N\|_{L^\infty(0, T; L^2_\varpi(a, b))}^2 \\
 & \leq C \left((l+1) \|v_{1,N}\|_{L^2_\varpi(a, b)}^2 + l \|w_{1,N}\|_{L^2_\varpi(a, b)}^2 \right. \\
 & + c^2 \frac{l(l+1)}{2l+1} \|d_{l+2}^+ v_{0,N} - d_{l-1}^- w_{0,N}\|_{L^2_\varpi(a, b)}^2 + \|\hat{h}\|_{L^\infty(0, T)}^2 \\
 & \left. + \|\partial_t \hat{h}\|_{L^1(0, T)}^2 + \|I_N f_0\|_{L^1(0, T; L^2_\varpi(a, b))}^2 + \|I_N f_1\|_{L^1(0, T; L^2_\varpi(a, b))}^2 \right),
 \end{aligned} \tag{6.66}$$

where C is a positive constant independent of N .

Proof. Take $\xi_0 = \partial_t v_N, \xi_1 = \partial_t w_N$ in (6.65), and integrate the resulted equation with respect to t . By using the relation (6.22), (6.60) and (6.62), we could easily get the following estimate:

$$\operatorname{Re} \int_0^t \omega_l * \left(\frac{v_N}{l} + \frac{w_N}{l+1} \right) (b, \tau) \partial_\tau (v_N - w_N)(b, \tau) d\tau \leq \frac{b}{c} \int_0^t |\partial_t (v_N - w_N)(b, \tau)|^2 d\tau.$$

Then we use the argument similar to [26] to derive the estimate. $\square$

Let P_l be the Legendre polynomial of degree l (see, e.g., [108]), and define $\tilde{P}_l(r) = P_l(\frac{2}{b-a}r - \frac{b+a}{b-a})$, $a < r < b$. Let $\phi_j(r) = \tilde{P}_j(r) + \tilde{P}_{j+1}(r)$, and this implies $\phi_j(a) = 0$. Choose the basis functions of V_N to be

$$\boldsymbol{\psi}_j(r) = \begin{pmatrix} \phi_j \\ 0 \end{pmatrix}, \quad \boldsymbol{\psi}_{j+N}(r) = \begin{pmatrix} 0 \\ \phi_j \end{pmatrix}, \quad 0 \leq j \leq N-1, \quad \boldsymbol{\psi}_{2N}(r) = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad (6.67)$$

and write

$$\begin{pmatrix} v_N(r, t) \\ w_N(r, t) \end{pmatrix} = \sum_{j=0}^{2N} \hat{u}_j(t) \boldsymbol{\psi}_j(r) = \sum_{j=0}^{2N} \hat{u}_j(t) \begin{pmatrix} \psi_j^0(r) \\ \psi_j^1(r) \end{pmatrix}. \quad (6.68)$$

By taking $(\xi_0, \xi_1)^t = \boldsymbol{\psi}_k = (\psi_k^0, \psi_k^1)^t$ in (6.65), and setting

$$\begin{aligned} \mathbf{u}(t) &= (\hat{u}_0, \hat{u}_1, \dots, \hat{u}_{2N})^t, \quad m_{kj} = (l+1)(\psi_j^0, \psi_k^0)_{r^2} + l(\psi_j^1, \psi_k^1)_{r^2}; \\ c_{kj} &= cb^2 \frac{l(l+1)}{2l+1} (\psi_j^0 - \psi_j^1)(b) (\psi_k^0 - \psi_k^1)(b); \\ s_{kj} &= c^2 \frac{l(l+1)}{2l+1} (d_{l+2}^+ \psi_j^0 - d_{l-1}^- \psi_j^1, d_{l+2}^+ \psi_k^0 - d_{l-1}^- \psi_k^1)_{r^2}; \\ \tilde{s}_{kj} &= -\frac{bc^2}{2l+1} ((l+1)\psi_j^0(b) + l\psi_j^1(b)) (\psi_k^0 - \psi_k^1)(b); \\ \tilde{f}_k &= (l+1)(I_N f_0, \psi_k^0)_{r^2} + l(I_N f_1, \psi_k^1)_{r^2} - cb^2 \frac{l(l+1)}{2l+1} \hat{h}(\psi_k^0 - \psi_k^1)(b); \\ \mathbf{f}(t) &= (\tilde{f}_0, \tilde{f}_1, \dots, \tilde{f}_{2N})^t, \quad M = (m_{kj}), \quad C = (c_{kj}), \quad K = (s_{kj}), \quad \tilde{K} = (\tilde{s}_{kj}), \end{aligned}$$

we obtain the system

$$M\ddot{\mathbf{u}} + C\dot{\mathbf{u}} + K\mathbf{u} = \omega_l * (\tilde{K}\mathbf{u}) + \mathbf{f}, \quad (6.69)$$

with $\mathbf{u}(0) = \mathbf{u}_0$ and $\dot{\mathbf{u}}(0) = \mathbf{u}_1$. Here, $\mathbf{u}_0, \mathbf{u}_1$ are expansion coefficients of $(v_{0,N}, w_{0,N})^t, (v_{1,N}, w_{1,N})^t$ in terms of the basis $\{\boldsymbol{\psi}_j\}_{j=0}^{2N}$, respectively.

6.3.3 Newmark scheme and Richardson extrapolation

To discretize the second-order ordinary differential system (6.69), we resort to the implicit second-order Newmark scheme, which has wide applications in the field

of structural mechanics (see [88, 119]). To this end, let Δt be the time-stepping size, and let $\{\mathbf{u}^m, \dot{\mathbf{u}}^m, \ddot{\mathbf{u}}^m\}$ be the approximation of $\{\mathbf{u}, \dot{\mathbf{u}}, \ddot{\mathbf{u}}\}$ at $t = t_m = m\Delta t$, and $\mathbf{f}^m = \mathbf{f}(t_m)$, and then at $t = t_m$, (6.69) becomes

$$M\ddot{\mathbf{u}}^m + C\dot{\mathbf{u}}^m + K\mathbf{u}^m = \omega_l * (\widetilde{K}\mathbf{u}^m) + \mathbf{f}^m. \quad (6.70)$$

The implementation of Newmark scheme for (6.70) is very similar to the wave equation, we refer to Subsection 5.3.4 in Chapter 5 for the details.

In order to upgrade the second order to higher order, we implement the Richardson extrapolation technique. Let $\mathbf{u}_N(\cdot, t)$ (resp. $\mathbf{u}_N^R(\cdot, t)$) be the numerical solution computed by the Newmark scheme with time step Δt (resp. $\Delta t/2$, refined in time). Then the Richardson extrapolation improves the accuracy by

$$\mathbf{v}_N(\cdot, t) = \frac{4}{3}\mathbf{u}_N^R(\cdot, t) - \frac{1}{3}\mathbf{u}_N(\cdot, t). \quad (6.71)$$

As to be shown (see Table 6.2), this leads to a fourth-order scheme in time.

6.4 Numerical results

In this section, we will show the exactness of our nonreflecting boundary condition, and the convergence order of the algorithm proposed in Section 6.3.

In the following tests, we generate the exact solution through the field: $(\mathbf{E} \times \hat{\mathbf{x}})|_{r=a} = \mathbf{g}$, and with homogeneous initial data and source term. More precisely, we take

$$\begin{aligned} \mathbf{g}(\theta, \phi, t) = \sum_{l=1}^{\infty} \sum_{m=-l}^l \left[\sin^6(6t) g_{l,1}^m \nabla_S Y_l^m \right. \\ \left. + \left(\mathcal{L}^{-1} \left[\frac{c}{sa} + \frac{k_l'(sa/c)}{k_l(sa/c)} \right] (t) * \sin^8(4t) \right) g_{l,2}^m \mathbf{T}_l^m \right], \end{aligned}$$

where $\{g_{l,1}^m, g_{l,2}^m\}$ are the expansion coefficients in terms of $\{\nabla_S Y_l^m, \mathbf{T}_l^m\}$, of the function

$$\tilde{\mathbf{g}}(\theta, \phi) = b \left(\left(\cos(x_1^2 x_2 x_3) + 2 \right)^{\frac{5}{2}}, x_3^2 \left(\sin(x_1 x_2) + 1 \right)^{\frac{3}{2}}, x_1 \left(0.5 \cos(x_2 x_3) + 1 \right)^{\frac{7}{2}} \right).$$

Table 6.1: The error $e(b, t)$ and the magnitude $\|\mathbf{E}\|$.

b	t	$\ \mathbf{E}\ $	$e(b, t)$	b	t	$\ \mathbf{E}\ $	$e(b, t)$
3	1.0	20.3730526964564	7.732E-14	5	1.0	9.00913663235211	1.646E-14
	2.0	20.7676168833996	7.019E-14		2.0	2.13838020370519	4.309E-14
	4.0	10.7362772069814	1.306E-13		4.0	18.7689414530879	8.158E-14
	10.0	29.5839763557074	3.353E-13		10.0	8.35297606167613	2.324E-13
4	1.0	3.67103876161396	2.677E-14	6	1.0	14.5066847348693	1.015E-14
	2.0	4.73647016565852	4.431E-14		2.0	4.79485815318372	9.582E-14
	4.0	9.30939040495999	7.076E-14		4.0	4.07128321534483	9.563E-14
	10.0	14.0411399157792	1.871E-13		10.0	11.5015473517173	2.747E-13

Table 6.2: Convergence of the Newmark scheme and Richardson extrapolation.

t	Δt	Err	order	Err ^R	order
0.5	5.00e-3	2.3090E-2		2.0719E-5	
	2.50e-3	5.7684E-3	2.001	1.2870E-6	4.009
	1.25e-3	1.4419E-3	2.000	8.0317E-8	4.002
	1.00e-3	9.2276E-4	2.000	3.2912E-8	3.998
1.0	5.00e-3	2.1041E-2		2.6540E-5	
	2.50e-3	5.2591E-3	2.000	1.6500E-6	4.008
	1.25e-3	1.3147E-3	2.000	1.0299E-7	4.001
	1.00e-3	8.4140E-4	2.000	4.2178E-8	4.009
1.5	5.00e-3	1.6912E-2		2.8491E-5	
	2.50e-3	4.2193E-3	2.003	1.7754E-6	4.004
	1.25e-3	1.0543E-3	2.000	1.1088E-7	4.001
	1.00e-3	6.7470E-4	2.001	4.5411E-8	4.009
2.0	5.00e-3	2.2117E-2		2.3189E-5	
	2.50e-3	5.5142E-3	2.004	1.4467E-6	4.003
	1.25e-3	1.3776E-3	2.001	9.0376E-8	4.001
	1.00e-3	8.8159E-4	2.000	3.7016E-8	4.000

Note that $\mathbf{x} = (x_1, x_2, x_3)$ (with $|\mathbf{x}| = 1$) is the corresponding Cartesian coordinates. Here, we compute $\{g_{l,1}^m, g_{l,2}^m\}$ accurately by using the Spherpak [2].

We first test the accuracy of the algorithm for the NRBC (6.49). Let $\mathbf{E}^N$ be the truncated exact solution $\mathbf{E}$ (the included modes are $1 \leq l \leq N_\theta; |m| \leq l$). Define the error:

$$e(b, t) = \left\| \left(\partial_t \mathbf{E}_T^N - c \hat{\mathbf{x}} \times (\nabla \times \mathbf{E}^N) \right) - \mathcal{T}_b[\mathbf{E}^N] \right\|_{N_\theta, N_\phi}, \quad (6.72)$$

where $\|\cdot\|_{N_\theta, N_\phi}$ denotes the discrete L^2 -norm associated with $N_\theta \times N_\phi$ colatitude and longitude grids. Here, we take $a = 2, c = 5, N_\theta = 40$ and $N_\phi = 2N_\theta$. We aim to test the accuracy for computing $\mathcal{T}_b[\mathbf{E}^N]$, so the differentiations in t and curl are calculated analytically. In Table 6.1, we tabulate $e(b, t)$ and the magnitude of $\mathbf{E}$ for different t and b (note that the magnitude of $\mathbf{E}$ is actually between 1 and 20, so the waves cross the artificial boundary). We see that in all cases, the computation of the NRBC is very accurate.

Next, we test the convergence order of the system with homogeneous initial conditions and free source in a spherical shell, which is solved by the spectral-Galerkin and Newmark scheme algorithm. Under the same setting of the reference solution and other data, we provide in Table 6.2, the discrete L^2 -norm errors (in space with sufficient resolution): $\text{Err}(t)$ (Newmark scheme), $\text{Err}^R(t)$ (Richardson extrapolation), and the convergence order in time at different time t . As expected, we observe the second-order convergence for the Newmark scheme and the fourth-order convergence for the extrapolation.

Conclusion and Future Works

In this chapter, we give a summary of the works done in this thesis and explore some relevant topics for further investigation.

7.1 Conclusion

The thesis was focused on two parts: (i) exponential convergence of spectral approximations of analytic functions; (ii) time-domain computation of scattering problems.

In the first part, we derived sharp error bounds of Jacobi expansion coefficients, and estimated the exponential convergence of spectral interpolation and differentiation, provided that the underlying function is analytic on and within the Bernstein ellipse. Following the principle in [125], we identified the superconvergence points for the first and second derivatives of Jacobi-Gauss-type interpolation, and obtained the superconvergence estimates directly from the spectral interpolation.

- (i) In Chapter 2, we derived various new and sharp error bounds for Jacobi polynomial expansions and Gegenbauer-Gauss quadrature of analytic functions with analyticity characterized by the Bernstein ellipse. We adopted an argument that could recover the best known bounds, and attempted to

make the dependence of the estimates on the parameters explicitly. Both analytic estimates and numerical comparisons with available ones demonstrated the sharpness of the error bounds.

- (ii) In Chapter 3, we studied the superconvergence of Jacobi-Gauss-type spectral interpolation. Following [125], we identified superconvergence points from the interpolation error remainder represented by Hermite's contour integral under analytic assumption, and for the first time, we had useful insights into the superconvergence of functions with limited regularity.
- (iii) In Chapter 4, the general framework of error estimates for spectral interpolation was provided, which straightforwardly lead to the superconvergence estimates. The exponential convergence of Gegenbauer spectral interpolation and differentiation of functions analytic on and within the Bernstein ellipse was analyzed. Sharp estimates in the maximum norm with explicit dependence on the important parameters were obtained. Illustrative numerical results were provided to support the analysis.

In the second part of this thesis, we tackled the longstanding issue with exact circular/spherical NRBC for wave equations and time-dependent Maxwell's equations. We provided efficient techniques to overcome the nonlocality of the exact NRBCs in both space and time. In particular, we derived new computable formulation of NRBC for Maxwell's equations.

- (i) In Chapter 5, we proposed analytic and accurate numerical means for the time-domain wave propagation with exact and global nonreflecting boundary conditions. We derived the analytic expressions of the convolution kernels and presented highly accurate methods for their evaluations. We analyzed the stability of the truncated problem and provided efficient numerical schemes, and gave ample numerical results to demonstrate the features of the method.

- (ii) In Chapter 6, we derived an alternative formula of the NRBC for the three dimensional time-dependent Maxwell's equations, and used the techniques and algorithms proposed in Chapter 5 to compute the temporal convolutions and the interior systems with a spherical scatterer. Moreover, we used the updated Richardson extrapolation to improve the temporal accuracy to fourth order. The numerical results showed the exactness of our NRBC, and the convergence orders of the proposed algorithm.

7.2 Future works

We explore some relevant topics for further investigation in this section.

- (i) In Chapter 5, we used the second order Newmark scheme in time to discretize the time direction, and used Richardson extrapolation to upgrade the accuracy in Chapter 6 for the Maxwell's equations. One of the future works is to develop some fast and high-order schemes in time to solve the interior truncated problems with regular scatterers. Moreover, in Subsection 5.3.1, we introduced the notion of the transformed field expansion (TFE) method, which, together with the fast high-order scheme in time, will be another research topic in the future. The same process also applies to time-dependent Maxwell's equations.
- (ii) In Chapter 6, we reformulated the NRBC for the three dimensional time-dependent Maxwell's equations. It is quite generic to integrate the NRBC with any solver for the interior truncated problem (for example, the finite element/spectral element methods, and the boundary perturbation technique [91]), with the aid of the Spherepack [2] or certain hybrid mesh interpolation [78]. These could be explored as well in the future.

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List of Publications

Papers published in referred Journals

- (i) L.L. Wang, B. Wang, and X.D. Zhao. Fast and accurate computation of time-domain acoustic scattering problems with exact nonreflecting boundary conditions. *SIAM J. Appl. Math.*, 72(6):1869–1898, 2012.
- (ii) Z.Q. Xie, L.L. Wang, and X.D. Zhao. On exponential convergence of Gegenbauer interpolation and spectral differentiation. *Math. Comp.*, 82(282):1017–1036, 2013.
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- (iv) X.D. Zhao and L.L. Wang. An efficient spectral-Galerkin method for a waveguide problem in an infinite domain. *Communication on Applied Mathematics and Computation*, 27(1):87–100, 2013. Dedicated to Professor Ben-yu Guo on the occasion of his 70th Birthday.
- (v) L.L. Wang, X.D. Zhao, and Z. Zhang. Superconvergence of Jacobi-Gauss-type spectral interpolation. *J. Sci. Comput.*, DOI: 10.1007/s10915-013-9777-x, 2013.

Conference paper

- (i) X.D. Zhao and L.L. Wang. Fast and accurate computation of exact nonreflecting boundary condition for Maxwell’s equations. Accepted by the Conference: The 29th International Review of Progress in Applied and Computational Electromagnetics, 2013.

Paper in Revision

L.L. Wang, M. Samson, and X.D. Zhao. A well-conditioned collocation method using pseudospectral integration matrix. Submitted to *SIAM J. Sci. Comput.*, 2013.