# A New Spectral Boundary Integral Collocation Method for Three-Dimensional Potential Problems

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**Abstract**

In this work we propose and analyse a new global collocation method for classical second-kind boundary integral equations of potential theory on smooth simple closed surfaces $\Gamma \subset \mathbb{R}^3$. Under the assumption that $\Gamma$ is diffeomorphic to the unit sphere $\partial B$, the original equation is transferred to an equivalent one on $\partial B$ which is solved using collocation onto a non-standard set of basis functions. The collocation points are situated on lines of constant latitude and longitude. The interpolation operator used in the collocation method is equivalent to a certain discrete orthogonal (pseudospectral) projection and this equivalence allows us to establish the fundamental properties of the interpolation process and subsequently to prove that our collocation method is stable and super-algebraically convergent. In addition we describe a fast method for computing the weakly singular collocation integrals and present some numerical experiments illustrating the use of the method. These show that at least for model problems the method attains an exponential rate of convergence and exhibits a good accuracy for very small numbers of degrees of freedom.

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# 1 Introduction

In this work we present a new spectrally convergent collocation method for second-kind boundary integral equations of potential theory. Our method is the result of a search for a three-dimensional analogue of well-known discrete global Galerkin or "pseudospectral" schemes for integral equations on planar contours (see, e.g., [15], [19], [4] or [14]). In these two-dimensional methods the contour is parametrized by a periodic univariate function and the basis functions used to approximate the solution are constructed from trigonometric polynomials with respect to this parameter. With an appropriate choice of quadrature rule the discrete orthogonal projection is then also an interpolation operator, the discrete Galerkin method is equivalent to a collocation scheme and hence is relatively cheap to implement. Stability and spectral orders of convergence are then proved using reasonably standard arguments.

It is interesting to consider the extension of such ideas to three dimensions. In that case a spectral method may be quite attractive since it has the potential to achieve an acceptable accuracy with a significantly smaller linear algebra overhead than that required by conventional (piecewise) methods. In line with spectral methods in general, we consider here only problems with smooth solutions and hence (in common with the two-dimensional case) we assume that our boundary integral equation is posed on a smooth surface.

Although most boundaries of interest in structural or mechanical engineering are not smooth, there are many applications of smooth boundaries in other branches of science — such as biology and medicine, where problems with corners and edges are rare.

We make the further assumption that our boundary is diffeomorphic to the unit sphere, which means that the sphere may be used as a parametrization of the boundary. Although this does restrict the range of problems which can be treated, it is in some sense a natural generalisation of the fact that in two dimensions all simple closed contours may be parametrized by the unit circle. Moreover there exists quite a lot of interest already in the literature on problems of this form.

Applications of boundary value problems on spherical or nearly spherical geometries are found for example in global weather prediction and in geodesy see, e.g. [21], [11]. Numerical analyses of various methods for such problems and further applications can be found in [2], [1], [5], [7, §3.6], [8], [9], [12], [16], [23], [24], [25] and the associated references. For a recent review of spectral methods in general see [10].

For boundary integral equations of the type considered in this paper, *nondiscrete* (and therefore not fully practical) Galerkin methods using spherical harmonic basis functions are the only global approximation schemes whose convergence has been proved ([2], [1], [16]).

Two questions then naturally arise:

(a) whether these (or related) Galerkin methods still converge when quadrature rules are used to compute the Galerkin integrals, and

(b) whether any such discrete Galerkin method is equivalent to a collocation scheme.

A discrete method using spherical harmonics and closely related to those used for *implementation* (but not covered by the proofs) in [2], [3], [1] and [16] is analysed completely in [12] for boundaries which are exactly spherical.

However the convergence proof used there fails when the boundary is merely diffeomorphic to the sphere. This is essentially because the corresponding discrete Galerkin projection has a bound which grows so fast that the usual stability proof fails. Thus the answer to (a) is still unknown in this case. With regard to (b), it is known from [22] that the answer is "no" when the underlying basis functions are spherical harmonics.

The very interesting unpublished Ph.D. thesis of Wienert [25] (see also [7]) suggested some fully discrete variants of Galerkin's method with both spherical harmonics and other basis sets and proved some new approximation theory (yielding exponential convergence rates) for the discrete integral operators. However Wienert did not give a convergence analysis for the corresponding approximate integral equations and thus does not provide an answer to (a). Nevertheless one of his methods suggests the use of a discrete orthogonal projection, with basis functions chosen as Fourier modes on $\mathbb{R}^2$ (mapped to the unit sphere with polar coordinates). This happens also to be an interpolatory projection and hence satisfies (b).

Our method takes Wienert's idea as starting point. We construct a basis set by choosing a distinguished set of Fourier modes on the plane and mapping them to the unit sphere, again with spherical polar coordinates. However unlike Wienert, we only choose those Fourier modes which map to continuous functions on the sphere and which have a certain reflectional symmetry. (Similar ideas are in [21].) Our choice ensures that the spherical polar coordinate transformation forms a bijection between our basis set and the distinguished set of Fourier modes and that the usual discrete orthogonal projection onto these Fourier modes corresponds to a discrete orthogonal projection on the sphere. Both are interpolatory and have norm growing with $O(\log^2(N))$, when the number of degrees of freedom is $O(N^2)$. This growth is slow enough to allow stability of the corresponding discrete Galerkin method to be proved. So the answer to both (a) and (b) is "yes" for this new method. These results and the implementation of the method are the principal aim of this paper.

The layout of the paper is as follows. In Section 2 we describe our basis set on the sphere and prove the required properties of the corresponding discrete orthogonal projection. The space spanned by our basis functions has dimension $2N(N-1)+2$. It contains, as a proper subset, spherical polynomials (which are smooth on the sphere) as well as extra functions which are continuous on the sphere but lack smoothness at the poles. Once Section 2 is done the convergence of the collocation method is obtained very easily in Section 3. The method is proved to be super-algebraically convergent. It should be possible also to show exponential convergence in an appropriate analytic setting (similar to that in [25]), but we do not attempt that here.

Computation of the collocation integrals is considered in Section 4. Here were are again influenced by [25]. If the basis functions were smooth on the sphere there is a very nice way of evaluating the required weakly singular integrals using a rotational change of variables and then polar coordinates, which eliminates the weak singularity in the integrand (see also [7, §3.6]). In Section 4 we consider this transformation applied to our collocation integrals and we show that it yields integrands on polar coordinate space $(\theta, \phi) \in [0, \pi] \times [0, 2\pi]$ with a mild singularity in the second derivative at certain points.

Fortunately this singularity seems not to affect the empirical convergence of standard quadrature rules for the collocation integrals. These perform as if the kernel were smooth, as is seen in Section 5 where we use the tensor product Gauss-Legendre rule for the integrals (after having transformed the singularities to the edges of the domain of integration) and observe exponential convergence. This would be difficult to prove because of the mild singularity in the integrands. We also observe exponential convergence of the solutions to the integral equation and to the corresponding solution to the underlying harmonic boundary value problem, provided the number of quadrature points increases appropriately with the number of degrees of freedom. For regular problems the method is extremely accurate: relative errors of about $10^{-3}$ are obtained by inverting linear systems of dimension about 40. Because of the relatively small linear algebra requirements of this method we are able to code it using MATLAB ([18]). On modern machines this has been found to yield accurate solutions of potential problems quickly enough to be usable as an interactive tool.

We finish this section by describing in more detail the problem to be solved. Let $\Omega \subset \mathbb{R}^3$ be a bounded domain with simple smooth closed boundary $\Gamma$. For any $\boldsymbol{\eta} \in \Gamma$ let $\mathbf{N}(\boldsymbol{\eta})$ denote the outward unit normal to $\Gamma$ and let $d\Sigma(\boldsymbol{\eta})$ denote surface measure on $\Gamma$. Let $|\cdot|$ denote the Euclidean norm on $\mathbb{R}^3$. We are primarily concerned in this paper with fast (spectrally accurate) solutions of the boundary integral equation

$$u(\boldsymbol{\xi}) - \int_\Gamma \frac{1}{2\pi} \frac{(\boldsymbol{\xi}-\boldsymbol{\eta})^T \mathbf{N}(\boldsymbol{\eta})}{|\boldsymbol{\xi}-\boldsymbol{\eta}|^3} u(\boldsymbol{\eta}) d\Sigma(\boldsymbol{\eta}) = f(\boldsymbol{\xi}) \ , \quad \boldsymbol{\xi} \in \Gamma. \tag{1.1}$$

This is the classical second kind equation which arises when the indirect boundary integral method with a double layer potential *ansatz* is used to solve the Dirichlet problem for Laplace's equation on $\Omega$. The method of this paper can also be used to solve the Neumann problem on $\Omega$ or the corresponding (exterior) problems on $\Omega' = \mathbb{R}^3 \backslash \bar{\Omega}$.

Our method for solving (1.1) is based upon expanding the solution $u$ in terms of a certain set of global basis functions, with the coefficients in the expansion determined by collocation. We make the following assumptions which are fundamental to the construction of this collocation method.

(A.1) There exists a smooth map $\boldsymbol{q} : D \subset \mathbb{R}^3 \to \mathbb{R}^3$ (where $D$ is a domain containing the unit sphere $\partial B = \{\boldsymbol{x} \in \mathbb{R}^3 : |\boldsymbol{x}| = 1\}$) with $\boldsymbol{q} \in (\mathcal{C}^\infty(D))^3$.

(A.2) $\boldsymbol{q} : \partial B \to \Gamma$ is bijective and its Jacobian $d\boldsymbol{q}$ is assumed to satisfy

$$\det d\boldsymbol{q}(\boldsymbol{x}) \neq 0, \quad \boldsymbol{x} \in \partial B \ .$$

Since $\partial B \subset D$ is compact it follows from (A.1) that:

$$\text{All derivatives of } \boldsymbol{q} \text{ are bounded on } \partial B \ . \tag{1.2}$$

With the change of variable $\boldsymbol{\eta} = \boldsymbol{q}(\boldsymbol{y})$, $\boldsymbol{y} \in \partial B$ the directed measures on $\Gamma$ and $\partial B$ are related by *Nanson's formula* ([20, p.88]):

$$\mathbf{N}(\boldsymbol{\eta}) d\Sigma(\boldsymbol{\eta}) = \mathrm{Adj}(d\boldsymbol{q}(\boldsymbol{y}))^T \boldsymbol{n}(\boldsymbol{y}) \ d\sigma(\boldsymbol{y}), \tag{1.3}$$

where $d\sigma(\boldsymbol{y})$ denotes surface measure on $\partial B$ at $\boldsymbol{y} \in \partial B$, $\boldsymbol{n}(\boldsymbol{y}) = \boldsymbol{y}$ is the unit normal to $\partial B$ at $\boldsymbol{y}$ and $\mathrm{Adj}(M)$ denotes the adjugate of the $3 \times 3$ matrix $M$ (i.e. the transposed matrix of its cofactors).

Now, with the substitution $\boldsymbol{\xi} = \boldsymbol{q}(\boldsymbol{x})$, $\boldsymbol{\eta} = \boldsymbol{q}(\boldsymbol{y})$, and using (1.3), we can transplant (1.1) onto $\partial B$ to obtain

$$(u \circ \boldsymbol{q})(\boldsymbol{x}) - \int_{\partial B} k(\boldsymbol{x}, \boldsymbol{y})(u \circ \boldsymbol{q})(\boldsymbol{y}) d\sigma(\boldsymbol{y}) = (f \circ \boldsymbol{q})(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial B \tag{1.4}$$

where

$$k(\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{2\pi} \frac{(\boldsymbol{q}(\boldsymbol{x}) - \boldsymbol{q}(\boldsymbol{y}))^T \mathrm{Adj}(d\boldsymbol{q}(\boldsymbol{y}))^T \boldsymbol{n}(\boldsymbol{y})}{|\boldsymbol{q}(\boldsymbol{x}) - \boldsymbol{q}(\boldsymbol{y})|^3}. \tag{1.5}$$

We will be concerned with the solution of (1.4), which is equivalent to (1.1). Thus we rewrite $u \circ \boldsymbol{q}$ as $u$ and $f \circ \boldsymbol{q}$ as $f$ and we abbreviate (1.4) as

$$(I - K)u = f \ , \tag{1.6}$$

where $K$ is the integral operator on $\partial B$ induced by the kernel $k$. It is well known that (1.6) has a unique solution $u$ which is smooth when $f$ is smooth.

# 2 Discrete Fourier series and interpolation on the unit sphere

## 2.1 Functions on the unit sphere

Let $\mathcal{C}^r(\partial B), r \geq 0$, denote the usual space of $r$-times continuously differentiable functions on the unit sphere $\partial B$ with norm $\|.\|_{\infty,r,\partial B}$. Let $\mathcal{D} = [0, 2\pi] \times [0, 2\pi]$ and let $\mathcal{C}^r(\mathcal{D}), r \geq 0$ denote the space of $r$-times continuously differentiable functions on $\mathbb{R}^2$ which are $2\pi$-periodic in each argument with norm $\|.\|_{\infty,r,\mathcal{D}}$. In addition, for $r \in \mathbb{N} \cup \{0\}$ and $\alpha \in [0, 1]$ we let $\mathcal{C}^{r,\alpha}(\partial B)$ denote the functions in $\mathcal{C}^r(\partial B)$ whose $r$th partial derivatives (defined with respect to a suitable chart) satisfy a Hölder condition of order $\alpha$. ($\mathcal{C}^{r,0}(\partial B) \equiv \mathcal{C}^r(\partial B)$.) Also, let $\mathcal{C}^{r,\alpha}(\mathcal{D})$ denote the analogous space on the Euclidean domain $\mathcal{D}$. Let $\|.\|_{\infty,r,\alpha,\partial B}$ and $\|.\|_{\infty,r,\alpha,\mathcal{D}}$ denote the corresponding norms. When $r = 0$ we drop the index $r$ in the above notations.

The standard mapping from $\mathbb{R}^2$ to $\partial B$ is the *spherical polar coordinate transformation*

$$\boldsymbol{p}(\theta, \phi) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T, \quad (\theta, \phi) \in \mathbb{R}^2.$$

This is invertible when considered as a map from $(0, \pi) \times [0, 2\pi)$ onto the *punctured sphere* $\partial B \backslash \{\boldsymbol{n}, \boldsymbol{s}\}$, where

$$\begin{aligned} \boldsymbol{n} = &\quad (0, 0, 1)^T &= \boldsymbol{p}(0, \phi), \\ \boldsymbol{s} = &\quad (0, 0, -1)^T &= \boldsymbol{p}(\pi, \phi) \end{aligned} \tag{2.1}$$

(for any $\phi \in \mathbb{R}$) are the north and south poles, respectively. On $\partial B \backslash \{\boldsymbol{n}, \boldsymbol{s}\}$, $\boldsymbol{p}$ has a continuous inverse given by $\boldsymbol{p}^{-1}(\boldsymbol{x}) = (\theta, \phi)$, where $(\theta, \phi) \in (0, \pi) \times [0, 2\pi)$ is the solution of the equations

$$\cos\theta = x_3, \quad \cos\phi = \frac{x_1}{\sqrt{1 - x_3^2}}, \quad \sin\phi = \frac{x_2}{\sqrt{1 - x_3^2}}. \tag{2.2}$$

The function $\boldsymbol{p}$ is smooth and $2\pi$-periodic in $(\theta, \phi)$ and any $v \in \mathcal{C}(\partial B)$ thus induces a function $\mathcal{J}v \in \mathcal{C}(\mathcal{D})$ given by

$$(\mathcal{J}v)(\theta, \phi) = v(\boldsymbol{p}(\theta, \phi)). \tag{2.3}$$

Analogously, for all $r \in \mathbb{N} \cup \{0\}$ and $\alpha \in (0, 1]$, $\mathcal{J} : \mathcal{C}^r(\partial B) \to \mathcal{C}^r(\mathcal{D})$, $\mathcal{J} : \mathcal{C}^{r,\alpha}(\partial B) \to \mathcal{C}^{r,\alpha}(\mathcal{D})$ and

$$\|\mathcal{J}v\|_{\infty,r,\mathcal{D}} \leq \|v\|_{\infty,r,\partial B} \quad , \quad \|\mathcal{J}v\|_{\infty,r,\alpha,\mathcal{D}} \leq \|v\|_{\infty,r,\alpha,\partial B} \ . \tag{2.4}$$

It is clear that $\mathcal{J}$ is an isometry from $\mathcal{C}(\partial B)$ into $\mathcal{C}(\mathcal{D})$, i.e.

$$\|\mathcal{J}v\|_{\infty,\mathcal{D}} = \|v\|_{\infty,\partial B}, \quad v \in \mathcal{C}(\partial B).$$

Since $\boldsymbol{p}$ has *reflectional symmetry*:

$$\boldsymbol{p}(-\theta, \phi + \pi) = \boldsymbol{p}(\theta, \phi), \quad (\theta, \phi) \in \mathbb{R}^2 \tag{2.5}$$

and is independent of $\phi \in \mathbb{R}$ at $\theta = 0$ or $\theta = \pi$ (see (2.1)), it is natural to introduce the proper subspaces of $\mathcal{C}(\mathcal{D})$:

$$\begin{aligned} \mathcal{R}(\mathcal{D}) &= \{w \in \mathcal{C}(\mathcal{D}) : w(-\theta, \phi + \pi) = w(\theta, \phi), \ (\theta, \phi) \in \mathbb{R}^2\}, \\ \mathcal{S}(\mathcal{D}) &= \{w \in \mathcal{R}(\mathcal{D}) : w(0, \phi), \ w(\pi, \phi) \text{ are independent of } \phi \in \mathbb{R}\}. \end{aligned}$$

Then it is easy to show that $\mathcal{J} : \mathcal{C}(\partial B) \to \mathcal{S}(\mathcal{D})$ is an isometric isomorphism with inverse given by $\mathcal{J}^{-1}w = v$, where

$$v(\boldsymbol{x}) = \begin{cases} w(0, \phi), & \boldsymbol{x} = \boldsymbol{n} \\ (w \circ \boldsymbol{p}^{-1})(\boldsymbol{x}), & \boldsymbol{x} \in \partial B \backslash \{\boldsymbol{n}, \boldsymbol{s}\} \\ w(\pi, \phi), & \boldsymbol{x} = \boldsymbol{s}. \end{cases} \tag{2.6}$$

We shall use (2.6) to define our approximation procedure in $\mathcal{C}(\partial B)$. We do this by first recalling the discrete Fourier projection on $\mathcal{C}(\mathcal{D})$. Provided this is carefully defined it turns out also to be a projection operator in $\mathcal{S}(\mathcal{D})$. Using the isometry (2.6) this gives us an analogue of discrete Fourier approximation in $\mathcal{C}(\partial B)$. The details are explored in the following subsections.

## 2.2 Discrete Fourier series in $\mathcal{C}(\mathcal{D})$

The *Fourier modes*

$$e_n^m(\theta, \phi) = \frac{1}{2\pi} \exp(in\theta) \exp(im\phi), \ (\theta, \phi) \in \mathbb{R}^2, \ n, m \in \mathbb{Z} \tag{2.7}$$

are orthonormal with respect to the usual inner product

$$(w_1, w_2) = \int_0^{2\pi} \int_0^{2\pi} w_1(\theta, \phi) \overline{w_2(\theta, \phi)} d\theta d\phi. \tag{2.8}$$

We shall use a corresponding discrete inner product defined using the quadrature points

$$\theta_j = j\frac{\pi}{N} = \phi_j, \quad j, k = 0, \cdots, 2N. \tag{2.9}$$

Throughout the paper we assume that $N$ is odd, so that $\pi/2$ is never a quadrature point. The commonly used discrete analogue of (2.8) is then obtained by applying the tensor product trapezoidal rule based at the nodes (2.9) to obtain

$$\langle w_1, w_2 \rangle_N = \frac{\pi^2}{N^2} \sum_{j=0}^{2N}{}' \sum_{k=0}^{2N}{}' w_1(\theta_j, \phi_k) \overline{w_2(\theta_j, \phi_k)} \tag{2.10}$$

for $w_1, w_2 \in \mathcal{C}(\mathcal{D})$. Throughout the paper $\sum'$ means the usual summation with only half the first and last terms included and $C$ denotes a generic constant which is independent of $N$.

The truncated discrete Fourier series of a function $w \in \mathcal{C}(\mathcal{D})$ is then defined by

$$\mathcal{E}_N w = \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' \langle w, e_n^m \rangle_N \; e_n^m \ , \tag{2.11}$$

The following lemma discusses various properties of $\mathcal{E}_N$. Before we prove it we recall the following useful formula

$$\frac{1}{2N} \sum_{n=-N}^{N}{}' \exp(ik\theta_n) = \begin{cases} 1, & k = 0 \pmod{2N} \\ 0, & k \neq 0 \pmod{2N} \ . \end{cases} \tag{2.12}$$

**Lemma 2.1**

(i) $\mathcal{E}_N(\mathcal{C}(\mathcal{D}))$

$$= \left\{ \sum_{|n|,|m|=0}^{N} \alpha_n^m e_n^m \ : \ \alpha_N^m = \alpha_{-N}^m, \ \alpha_n^N = \alpha_n^{-N}, \ 0 \leq |m|, |n| \leq N \right\}. \tag{2.13}$$

(ii) $\mathcal{E}_N^2 = \mathcal{E}_N$ *and* $\mathcal{E}_N w_N = w_N$ *for all* $w_N \in \mathcal{E}_N(\mathcal{C}(\mathcal{D}))$.

(iii) $(\mathcal{E}_N w)(\theta_p, \phi_q) = w(\theta_p, \phi_q), \quad p, q = 0, \ldots, 2N-1, \ w \in \mathcal{C}(\mathcal{D})$.

(iv) $\|\mathcal{E}_N w\|_{\infty,\mathcal{D}} \leq C \log^2 N \|w\|_{\infty,\mathcal{D}}, \quad w \in \mathcal{C}(\mathcal{D})$.

(v) $\|w - \mathcal{E}_N w\|_{\infty,\mathcal{D}} \leq C \dfrac{\log^2 N}{N^{r+\alpha}} \|w\|_{\infty,r,\alpha,\mathcal{D}}, \quad w \in \mathcal{C}^{r,\alpha}(\mathcal{D}), \ r \geq 0, \ \alpha \in [0,1]$

**Proof** Let $\mathfrak{E}_N$ denote the set defined on the right hand side of (2.12) and let $w \in \mathcal{C}(\mathcal{D})$. Note first that

$$\exp(iN\phi_j) = \exp(iN\theta_j) = \exp(-iN\theta_j) = \exp(-iN\phi_j), \quad j \in \mathbb{Z}. \tag{2.14}$$

Hence, for $m, j, k \in \mathbb{Z}$ we have $e_N^m(\theta_j, \phi_k) = e_{-N}^m(\theta_j, \phi_k)$ and thus it follows that $\langle w, e_N^m \rangle_N = \langle w, e_{-N}^m \rangle_N, \ 0 \leq |m| \leq N$. Similarly $\langle w, e_n^N \rangle_N = \langle w, e_n^{-N} \rangle_N, \ 0 \leq |n| \leq N$. Hence from the definition of $\mathcal{E}_N$, we get

$$\mathcal{E}_N(\mathcal{C}(\mathcal{D})) \subseteq \mathfrak{E}_N. \tag{2.15}$$

Moreover, using the identity

$$\langle e_n^m, e_p^q \rangle_N = \begin{cases} 1, & n \equiv p \pmod{2N} \text{ and } m \equiv q \pmod{2N} \\ 0, & \text{otherwise} \end{cases}$$

we obtain, for $0 \le |m|, |n| \le N-1$,

$$\mathcal{E}_N e_n^m = e_n^m,$$
$$\mathcal{E}_N(e_N^m + e_{-N}^m) = e_N^m + e_{-N}^m, \qquad \mathcal{E}_N(e_n^N + e_n^{-N}) = e_n^N + e_n^{-N},$$

together with

$$\mathcal{E}_N(e_N^N + e_{-N}^N + e_N^{-N} + e_{-N}^{-N}) = e_N^N + e_{-N}^N + e_N^{-N} + e_{-N}^{-N}.$$

Hence a short calculation shows that

$$\mathcal{E}_N w_N = w_N, \quad w_N \in \mathfrak{E}_N. \tag{2.16}$$

Thus (i) and (ii) follow from (2.15) and (2.16). Also observe that for $p, q = 0, \cdots, 2N-1$,

$$\begin{aligned}&(\mathcal{E}_N w)(\theta_p, \phi_q)\\ &= \frac{1}{4N^2} \sum_{j,k=0}^{2N-1} w(\theta_j, \phi_k) \left[ \sum_{n=-N}^{N}{}' \exp\left(i(p-j)\theta_n\right) \right] \left[ \sum_{m=-N}^{N}{}' \exp\left(i(q-k)\phi_m\right) \right]. \end{aligned}\tag{2.17}$$

Then (iii) follows on using (2.12). For (iv), let $w \in \mathcal{C}(\mathcal{D})$ and $(\theta, \phi) \in \mathcal{D}$. Then

$$\begin{aligned}&(\mathcal{E}_N w)(\theta, \phi)\\ &\quad = \frac{1}{N^2} \sum_{j=0}^{2N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \left[ \sum_{n=0}^{N}{}' \cos n(\theta - \theta_j) \right] \left[ \sum_{m=0}^{N}{}' \cos m(\phi - \phi_k) \right]\\ &\quad = \frac{1}{N^2} \sum_{j=0}^{2N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) D_N^*(\theta - \theta_j) D_N^*(\phi - \phi_k),\end{aligned}$$

where $D_N^*$ is the modified Dirichlet kernel [26, Vol I, p.50] given by

$$D_N^*(t) = \sum_{l=0}^{N}{}' \cos lt, \quad t \in \mathbb{R}. \tag{2.18}$$

Hence

$$\|\mathcal{E}_N w\|_{\infty,\mathcal{D}} \le \left( \frac{1}{N} \sup_{0 \le \theta \le 2\pi} \sum_{j=0}^{2N-1} |D_N^*(\theta - \theta_j)| \right)^2 \|w\|_{\infty,\mathcal{D}}. \tag{2.19}$$

We show in the Appendix that $\sup_{0 \le \theta \le 2\pi} \sum_{j=0}^{2N-1} |D_N^*(\theta - \theta_j)| = O(N \log N)$, as $N \to \infty$. (The proof is obtained by modifying the argument in [26, Vol.II, p.19]). Hence (iv) follows from (2.19).

Finally, to obtain (v), let $w \in \mathcal{C}^{r,\alpha}(\mathcal{D}), r \ge 0, \alpha \in (0,1]$. Then recall that for each $n \in \mathbb{N}$, there exists a trigonometric polynomial $T_n(\theta, \phi)$ of degree $n$ in each variable such that

$$\|w - T_n\|_{\infty,\mathcal{D}} \le C \frac{1}{n^{r+\alpha}} \|w\|_{\infty,r,\alpha,\mathcal{D}} \tag{2.20}$$

[17, p.89, Theorem 7]. Since $\mathcal{E}_N T_{N-1} = T_{N-1}$, it follows that

$$\|w - \mathcal{E}_N w\|_{\infty,\mathcal{D}} \le \|w - T_{N-1}\|_{\infty,\mathcal{D}} + \|\mathcal{E}_N(w - T_{N-1})\|_{\infty,\mathcal{D}}. \tag{2.21}$$

Using (iv) and (2.20) in (2.21), we get (v). □

## 2.3 Discrete Fourier series in $\mathcal{R}(\mathcal{D})$ and $\mathcal{C}(\mathcal{D})$

The next result shows that the discrete orthogonal projection $\mathcal{E}_N$ maps $\mathcal{R}(\mathcal{D})$ into itself with range a subspace of $\mathcal{E}_N(\mathcal{C}(\mathcal{D}))$. To show this, it is convenient to introduce functions

$$r_n^m = e_n^m + (-1)^m e_{-n}^m, \qquad n, m \in \mathbb{Z}. \tag{2.22}$$

Observe that $r_n^m \in \mathcal{R}(\mathcal{D})$ for all $n, m$.

**Lemma 2.2**

$$\begin{aligned}&\mathcal{E}_N(\mathcal{R}(\mathcal{D}))\\ &= \left\{ \sum_{n=0}^{N} \sum_{m=-N}^{N} \alpha_n^m r_n^m : \ \alpha_n^{-N} = \alpha_n^N, \ 0 \le n \le N, \quad \alpha_N^m = 0, \ 0 \le |m| \le N, \ \ |m| \text{ odd} \right\}\end{aligned} \tag{2.23}$$

*and hence* $\mathcal{E}_N : \mathcal{R}(\mathcal{D}) \to \mathcal{R}(\mathcal{D})$.

**Proof** Let $\mathfrak{R}_N$ denote the set defined by the right hand side of (2.23). We prove first that $\mathcal{E}_N(\mathcal{R}(\mathcal{D})) \subseteq \mathfrak{R}_N$, using essentially the method of [25, p.26] but in a slightly different setting.

Let $w \in \mathcal{R}(\mathcal{D})$. We write

$$\mathcal{E}_N w = \frac{\pi}{2N^2} \left( w_N^{(1)} + w_N^{(2)} \right) \tag{2.24}$$

where

$$w_N^{(1)}(\theta, \phi) = \sum_{j=0}^{N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' e_n^m(\theta - \theta_j, \phi - \phi_k), \tag{2.25}$$

and

$$\begin{aligned} w_N^{(2)}(\theta, \phi) &= \sum_{j=N}^{2N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' e_n^m(\theta - \theta_j, \phi - \phi_k) \\ &= \sum_{j=0}^{N}{}' \sum_{k=0}^{2N}{}' w(\theta_{N+j}, \phi_k) \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' e_n^m(\theta - \theta_{N+j}, \phi - \phi_k). \end{aligned}$$

Using the fact that $w \in \mathcal{R}(\mathcal{D})$, and the $2\pi$ periodicity of $w$ and $e_n^m$ we have

$$\begin{aligned} w_N^{(2)}(\theta, \phi) &= \sum_{j=0}^{N}{}' \sum_{k=0}^{2N}{}' w(\theta_{N-j}, \phi_{N+k}) \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' e_n^m(\theta + \theta_{N-j}, \phi - \phi_k) \\ &= \sum_{j=0}^{N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' e_n^m(\theta + \theta_j, \phi - \phi_{k-N}) \, . \end{aligned}$$

Using this together with (2.24) and (2.25), we have

$$(\mathcal{E}_N w)(\theta, \phi) = \frac{\pi^2}{N^2} \sum_{j=0}^{N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \sum_{n=-N}^{N}{}' \sum_{m=-N}^{N}{}' e_n^m(\theta, \phi) \overline{r_n^m(\theta_j, \phi_k)}$$

Since $r_{-n}^m = (-1)^m r_n^m$, this yields

$$(\mathcal{E}_N w)(\theta, \phi) = \sum_{m=-N}^{N}{}' \sum_{n=0}^{N}{}' \alpha_n^m r_n^m(\theta, \phi), \tag{2.26}$$

where

$$\alpha_n^m = \frac{\pi^2}{N^2} \sum_{j=0}^{N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \overline{r_n^m(\theta_j, \phi_k)}. \tag{2.27}$$

By (2.13) it follows easily that $r_n^N(\theta_j, \phi_k) = r_n^{-N}(\theta_j, \phi_k)$, for $n, k, j \in \mathbb{Z}$. Hence we have $\alpha_n^N = \alpha_n^{-N}$ for $0 \le n \le N$. Also for $0 \le |m| \le N$ with $m$ odd we have

$$r_N^m(\theta_j, \phi_k) = \frac{i}{\pi} \sin(N\theta_j) \exp(im\phi_k) = 0,$$

which implies $\alpha_N^m = 0$. Thus we have shown

$$\mathcal{E}_N(\mathcal{R}(\mathcal{D})) \subseteq \mathfrak{R}_N. \tag{2.28}$$

The fact that $\mathfrak{R}_N \subseteq \mathcal{E}_N(\mathcal{R}(\mathcal{D}))$ follows from the following four identities, which can be proved using standard arguments.

$$\mathcal{E}_N r_p^q = r_p^q, \quad 0 \le |q| \le N-1, \quad 0 \le p \le N-1,$$
$$\mathcal{E}_N(r_p^{-N} + r_p^N) = r_p^{-N} + r_p^N, \quad 0 \le p \le N-1,$$
$$\mathcal{E}_N r_N^q = \begin{cases} r_N^q\ , & |q| \le N-1,\ |q| \text{ even}, \\ 0\ , & |q| \le N-1,\ |q| \text{ odd}, \end{cases} .$$
$$\mathcal{E}_N(r_N^{-N} + r_N^N) = \begin{cases} r_N^{-N} + r_N^N & , \quad N \text{ even}, \\ 0 & , \quad N \text{ odd}. \end{cases}$$

□

The next result shows that in fact $\mathcal{E}_N$ leaves $\mathcal{S}(\mathcal{D})$ invariant.

**Lemma 2.3** *For all $w \in \mathcal{S}(\mathcal{D})$, and all $\phi \in \mathbb{R}$, we have $(\mathcal{E}_N w)(0, \phi) = w(0, \phi)$ and $(\mathcal{E}_n w)(\pi, \phi) = w(\pi, \phi)$. Hence $\mathcal{E}_N : \mathcal{S}(\mathcal{D}) \to \mathcal{S}(\mathcal{D})$.*

**Proof** Let $w \in \mathcal{S}(\mathcal{D})$ and set $w(0, \phi) = C_1$ for all $\phi \in \mathbb{R}$. Then by (2.10), (2.11) and (2.12) we have, for all $\phi \in \mathbb{R}$,

$$\begin{aligned} (\mathcal{E}_N w)(0, \phi) &= \frac{1}{4N^2} \sum_{j=0}^{2N}{}' \sum_{k=0}^{2N}{}' w(\theta_j, \phi_k) \sum_{n=-N}^{N}{}' \exp(-ij\theta_n) \sum_{m=-N}^{N}{}' \exp(im(\phi - \phi_k)) \\ &= \frac{1}{2N} \sum_{k=0}^{2N}{}' w(0, \phi_k) \sum_{m=-N}^{N}{}' \exp(im(\phi - \phi_k)) \\ &= \frac{C_1}{2N} \sum_{m=-N}^{N}{}' \exp(im\phi) \sum_{k=0}^{2N}{}' \exp(-im\phi_k) = C_1 = w(0, \phi). \end{aligned}$$

Similarly $(\mathcal{E}_N w)(\pi,\phi) = w(\pi,\phi)$, $\phi \in \mathbb{R}$. Since $\mathcal{E}_N w \in \mathcal{R}(\mathcal{D})$ by Lemma 2.2, we have $\mathcal{E}_N w \in \mathcal{S}(\mathcal{D})$ also. $\square$

The previous lemmas show that $\mathcal{E}_N$ is an interpolatory projection operator on $\mathcal{S}(\mathcal{D})$. Its image $\mathcal{E}_N(\mathcal{S}(\mathcal{D}))$ constitutes a distinguished subspace of the space spanned by the Fourier modes. It is from this subspace that a basis of interpolating trigonometric polynomials in $\mathcal{S}(\mathcal{D})$ can be constructed. Using $\mathcal{J}^{-1}$ given by (2.6) this leads directly to an interpolatory basis in $\mathcal{C}(\partial B)$.

To define the basis in $\mathcal{S}(\mathcal{D})$, define a function $j : \mathbb{N}\cup 0 \to \{0,\pm 1\}$ by

$$j(m) = \begin{cases} 1 & m \text{ even} \quad , \quad m \geq 2 \\ 0 & m \text{ odd} \\ -1 & m = 0\ . \end{cases}$$

Then, for $n,m \in \mathbb{N}\cup\{0\}$, define $s_n^m,\ c_n^m : \mathbb{R}\times\mathbb{R} \to \mathbb{R}$ by

$$\left.\begin{array}{rcl} s_n^m(\theta,\phi) & = & \sin n\theta(\sin\theta)^{j(m)}\sin m\phi \\ c_n^m(\theta,\phi) & = & \sin n\theta(\sin\theta)^{j(m)}\cos m\phi \end{array}\right\} \tag{2.29}$$

Clearly $s_n^m, c_n^m \in \mathcal{S}(\mathcal{D})$ for all $n,m \in \mathbb{N}\cup\{0\}$. Moreover the sets $\{s_n^m\ : n,m = 1,2,\ldots\}$ and $\{c_n^m\ : n = 1,2,\ldots; m = 0,1,\ldots\}$ are orthogonal with respect to the inner product (2.8). The spaces

$$\begin{array}{rcl} \Sigma_N & = & \mathrm{span}\{s_n^m : n,m = 1,\ldots N-1\} \\ \Xi_N & = & \mathrm{span}\{c_n^m : n = 1,\ldots N-1\ ,\ m = 1,\ldots N\} \oplus \mathrm{span}\{c_n^0 : n = 1,\ldots,N+1\} \end{array}$$

are mutually orthogonal and have dimension $(N-1)^2$ and $N(N-1)+(N+1)$ respectively. Hence the space

$$\Lambda_N := \Sigma_M \oplus \Xi_N \tag{2.30}$$

is a subspace of $\mathcal{S}(\mathcal{D})$ with dimension $2N^2-2N+2$. We shall show in Theorem 2.6 below that for each $w \in \mathcal{S}(\mathcal{D})$, $\mathcal{E}_N w$ is the unique element of $\Lambda_N$ which interpolates $w$ at a certain set of $2N^2-2N+2$ points. Thus $\mathcal{E}_N$ is an interpolation operator. The proof is obtained with the help of the following two lemmas.

**Lemma 2.4**

$$\mathcal{E}_N(\mathcal{R}(\mathcal{D})) = \Lambda_N \oplus \Delta_N \tag{2.31}$$

*where*

$$\begin{array}{rl} \Delta_N = & \mathrm{span}\{\cos m\phi, \cos\theta\cos m\phi,\quad m = 1,\ldots,N,\ m \text{ even}\} \\ \oplus & \mathrm{span}\{\sin m\phi, \cos\theta\sin m\phi,\quad m = 1,\ldots,N,\ m \text{ even}\} \end{array} \tag{2.32}$$

**Proof** Observe first that, since the basis functions for $\Lambda_N$ are independent of those for $\Delta_N$ we have $\Lambda_N \cap \Delta_N = \{0\}$. Now, by examining each of the basis functions for $\Lambda_N \oplus \Delta_N$ in turn and using the characterisation (2.13) and the definition of $\mathcal{R}(\mathcal{D})$ we can show that

$$\Lambda_N \oplus \Delta_N \subseteq \mathcal{E}_N(\mathcal{C}(\mathcal{D})) \cap \mathcal{R}(\mathcal{D}). \tag{2.33}$$

Hence if $w_N \in \Lambda_N \oplus \Delta_N$ then by Lemma 2.1 (ii), $w_N = \mathcal{E}_N w_N \in \mathcal{E}_N(\mathcal{R}(\mathcal{D}))$. So

$$\Lambda_N \oplus \Delta_N \subseteq \mathcal{E}_N(\mathcal{R}(\mathcal{D})). \tag{2.34}$$

Conversely, suppose $w_N \in \mathcal{E}_N(\mathcal{R}(\mathcal{D}))$. Then from Lemma 2.2 there exist constants $\alpha_n^m$ with $\alpha_n^{-N} = \alpha_n^N$ and $\alpha_N^m = 0$ when $|m|$ is odd such that

$$w_N = \sum_{n=0}^{N} \sum_{m=-N}^{N} \alpha_n^m r_n^m.$$

Thus, recalling (2.22),

$$\begin{aligned} w_N(\theta,\phi) &= \frac{1}{\pi}\sum_{n=0}^{N} \sum_{\substack{m=-N \\ m \text{ even}}}^{N} \alpha_n^m \cos n\theta \exp im\phi + \frac{1}{\pi}\sum_{n=0}^{N} \sum_{\substack{m=-N \\ m \text{ odd}}}^{N} \alpha_n^m \sin n\theta \exp im\phi. \\ &:= w_N^{(1)} + w_N^{(2)}, \end{aligned}$$

where

$$\begin{aligned} w_N^{(1)} \in \quad & \operatorname{span}\{\sin n\theta \sin m\phi : \quad n,m = 1,...,N-1, \;\; m \text{ odd}\} \\ \oplus \quad & \operatorname{span}\{\sin n\theta \cos m\phi : \quad n = 1,...,N-1, \;\; m = 1,...,N \;\; m \text{ odd}\} \end{aligned}$$

and

$$\begin{aligned} w_N^{(2)} \in \quad & \operatorname{span}\{\cos n\theta \cos m\phi : \quad n,m = 0,...,N, \;\; m \text{ even}\} \\ \oplus \quad & \operatorname{span}\{\cos n\theta \sin m\phi : \quad n = 0,...,N, \;\; m = 2,...,N-1, \;\; m \text{ even}\}. \end{aligned}$$

Since $w_N^{(1)} \in \Lambda_N$ it remains to show

$$w_N^{(2)} \in \Lambda_N \oplus \Delta_N. \tag{2.35}$$

To obtain (2.35) let $m \in \{0,...,N\}$ be even. Then observe that for $n \in \{1,...,N\}$ with $n$ odd,

$$\begin{aligned} \cos n\theta \cos m\phi &= (\cos n\theta - \cos\theta)\cos m\phi + \cos\theta \cos m\phi \\ &= \sum_{j=1}^{n-1} \sin j\theta \sin\theta \cos m\phi + \cos\theta\cos m\phi \\ &\in \Lambda_N \oplus \Delta_N. \end{aligned} \tag{2.36}$$

In addition if $n \in \{0,...,N\}$ with $n$ even then

$$\begin{aligned} \cos n\theta \cos m\phi &= (\cos n\theta - 1)\cos m\phi + \cos m\phi \\ &= \sum_{j=1}^{n-1} \sin j\theta \sin\theta \cos m\phi + \cos m\phi \\ &\in \Lambda_N \oplus \Delta_N. \end{aligned} \tag{2.37}$$

Similarly when $m \in \{2, ..., N-1\}$ is even and $n \in \{0, ..., N\}$

$$\cos n\theta \sin m\phi \in \Lambda_N \oplus \Delta_N. \tag{2.38}$$

Now (2.36)–(2.38) imply (2.35) and $w_N \in \Lambda_N \oplus \Delta_N$. Hence

$$\mathcal{E}_N(\mathcal{R}(\mathcal{D})) \subseteq \Lambda_N \oplus \Delta_N$$

and, together with (2.34) this proves the result. □

**Lemma 2.5** $\mathcal{E}_N(\mathcal{S}(\mathcal{D})) = \Lambda_N$.

**Proof** Let $w_N \in \Lambda_N$. It is easily checked that $w_N \in \mathcal{S}(\mathcal{D})$. Since by (2.33), $w_N \in \mathcal{E}_N(\mathcal{C}(\mathcal{D}))$, Lemma 2.1 (ii) yields $w_N \in \mathcal{E}_N(\mathcal{S}(\mathcal{D}))$ and so

$$\Lambda_N \subseteq \mathcal{E}_N(\mathcal{S}(\mathcal{D})). \tag{2.39}$$

On the other hand suppose $w_N \in \mathcal{E}_N(\mathcal{S}(\mathcal{D}))$. Then also $w_N \in \mathcal{E}_N(\mathcal{R}(\mathcal{D}))$ and by Lemma 2.4 there exist unique $w_N^{(1)} \in \Lambda_N$ and $w_N^{(2)} \in \Delta_N$ such that $w_N = w_N^{(1)} + w_N^{(2)}$. Also, by Lemma 2.3, $w_N \in \mathcal{S}(\mathcal{D})$ and, since $\Lambda_N \subseteq \mathcal{S}(\mathcal{D})$, we have $w_N^{(2)} = w_N - w_N^{(1)} \in \mathcal{S}(\mathcal{D})$. Hence there exist $C_2, C_2$ such that

$$w_N^{(2)}(0, \phi) = C_1, \quad w_N^{(2)}(\pi, \phi) = C_2$$

for all $\phi \in \mathbb{R}$. From the definition of $\Delta_N$ it follows easily that $w_N^{(2)} \equiv 0$ and so $w_N \in \Lambda_N$. Hence $\mathcal{E}_N(\mathcal{S}(\mathcal{D})) \subseteq \Lambda_N$ and the result follows from this and (2.39). □

These lemmas then lead to the following theorem describing the interpolatory properties of $\mathcal{E}_N$.

**Theorem 2.6** *For all $w \in \mathcal{S}(\mathcal{D})$, $\mathcal{E}_N w$ is the unique element of $\Lambda_N$ which satisfies*

$$\begin{aligned} (\mathcal{E}_N w)(0, \phi) &= w(0, \phi), \ \ \phi \in \mathbb{R}, & (2.40)\\ (\mathcal{E}_N w)(\pi, \phi) &= w(\pi, \phi), \ \ \phi \in \mathbb{R}, & (2.41)\\ (\mathcal{E}_N w)(\theta_j, \phi_k) &= w(\theta_j, \phi_k), \ \ j = 1, \ldots, N-1, \ \ k = 0, \ldots 2N-1. & (2.42) \end{aligned}$$

**Proof** Let $w \in \mathcal{S}(\mathcal{D})$. From Lemmas 2.1 and 2.5, $\mathcal{E}_N w \in \Lambda_N$ has the interpolation property (2.40) -(2.42). To establish uniqueness, suppose $w_N \in \Lambda_N$ satisfies $w_N(0, \phi) = 0 = w_N(\pi, \phi)$, $\phi \in \mathbb{R}$ and $w_N(\theta_j, \phi_k) = 0$, for $j = 1, \ldots, N-1$ and $k = 0, \ldots, 2N-1$. Then since $\Lambda_N \subset \mathcal{S}(\mathcal{D})$ we have in fact $w_N(\theta_j, \phi_k) = 0$ for all $j, k = 1, \ldots, 2N$ and thus $\mathcal{E}_N w_N = 0$. Since $w_N = \mathcal{E}_N w$ for some $w \in \mathcal{S}(\mathcal{D}))$ we have (using Lemma 2.1 (ii)),

$$w_N = \mathcal{E}_N w = \mathcal{E}_N^2 w = \mathcal{E}_N w_N = 0,$$

as required. □

### 2.4 A discrete orthogonal projection on $\mathcal{C}(\partial B)$

Finally in this section we study the interpolatory operator on $\mathcal{C}(\partial B)$ induced by the operator $\mathcal{E}_N$ on $\mathcal{S}(\mathcal{D})$. That is we set

$$E_N = \mathcal{J}^{-1}\mathcal{E}_N\mathcal{J}$$

where $\mathcal{J} : \mathcal{C}(\partial B) \to \mathcal{S}(\mathcal{D})$ is the isometric isomorphism introduced in (2.3). We introduce the interpolation points on the sphere

$$\boldsymbol{x}_{jk} = p(\theta_j, \phi_k), \quad j = 1, ..., N-1, \quad k = 0, ..., 2N-1.$$

Together with the north pole $\boldsymbol{n}$ and the south pole $\boldsymbol{s}$ these form a set of $2N^2 - 2N + 2$ points on $\partial B$. Similarly we introduce the interpolation space

$$S_N = \mathcal{J}^{-1}\Lambda_N. \tag{2.43}$$

**Theorem 2.7**

*(i)* $E_N^2 = E_N$ *and* $E_N v_N = v_N$ *for all* $v_N \in S_N$.

*(ii) For* $v \in \mathcal{C}(\partial B)$, $E_N v$ *is the unique element of* $S_N$ *with the property*

$$\begin{aligned} E_N v(\boldsymbol{x}_{jk}) &= v(\boldsymbol{x}_{jk}), \quad j = 1, ..., N-1, \quad k = 0, ..., 2N-1, \\ E_N v(\boldsymbol{n}) &= v(\boldsymbol{n}), \\ E_N v(\boldsymbol{s}) &= v(\boldsymbol{s}). \end{aligned}$$

*(iii)* $\|E_N v\|_{\infty,\partial B} \le C \log^2 N \|v\|_{\infty,\partial B}, \quad v \in \mathcal{C}(\partial B).$

*(iv) For* $v \in \mathcal{C}^{r,\alpha}(\partial B), \quad r \ge 0, \quad \alpha \in [0,1]$,

$$\|v - E_N v\|_{\infty,\partial B} \le C \frac{\log^2 N}{N^{r+\alpha}} \|v\|_{\infty,r,\alpha,\partial B}.$$

**Proof** This is immediate from Lemma 2.1, Theorem 2.6 and the properties of $\mathcal{J}$. $\square$

# 3 The Collocation (Pseudospectral) Method

In this section we introduce our pseudospectral method for (1.6) and prove its convergence. First we give an algorithmic description of the method. Let $d = 2N^2 - 2N + 2$ denote the dimension of the space $S_N = \mathcal{J}^{-1}\Lambda_N$ introduced in (2.30) and (2.43). A basis for this space is

$$\bigcup_{n=1}^{N-1} \Big\{ \{\mathcal{J}^{-1} s_n^m : m = 1, ..., N-1\} \cup \{\mathcal{J}^{-1} c_n^m : m = 0, ..., N\} \Big\} \cup \{\mathcal{J}^{-1} c_N^0, \mathcal{J}^{-1} c_{N+1}^0\}. \tag{3.1}$$

For convenience we denote this basis $\{\psi_p : p \equiv 1, ..., d\}$. It is natural to choose the ordering implicit in (3.1), i.e. to choose the first $2N$ basis functions $\psi_1, ..., \psi_{2N}$ to be

$$\mathcal{J}^{-1} s_1^m, \quad m = 1, ..., N-1, \quad \mathcal{J}^{-1} c_1^m, \; m = 0, ..., N\ .$$

Then $\psi_{2N+1}, ..., \psi_{4N}$ are

$$\mathcal{J}^{-1}s_2^m, \ m = 1, ...N-1, \ \ \mathcal{J}^{-1}c_2^m, \ m = 0, ..., N,$$

and so on with $\psi_{d-1}, \ \psi_d$ being the last two basis functions $\mathcal{J}^{-1}c_N^0, \ \mathcal{J}^{-1}c_{N+1}^0$.

The collocation points are the set

$$C_N = \bigcup_{j=1}^{N-1} \{\boldsymbol{x}_{jk} : k = 0, ..., 2N-1\} \cup \{\boldsymbol{n}, \boldsymbol{s}\}. \tag{3.2}$$

These have a corresponding natural ordering $\boldsymbol{x}_{1k}, \ k = 0, ..., 2N-1$; $\boldsymbol{x}_{2k}, \ k = 0, ..., 2N-1$, and so on, with $\boldsymbol{n}$ and $\boldsymbol{s}$ being the last two collocation points.

Our method for (1.6) then consists of seeking a numerical solution

$$u_N = \sum_{p=1}^{d} a_p \psi_p$$

where the $\{a_p\}$ are scalars chosen so that

$$(I-K)u_N(\boldsymbol{x}) = f(\boldsymbol{x}), \quad \boldsymbol{x} \in C_N, \tag{3.3}$$

or equivalently

$$\sum_{p=1}^{d} a_p\{\psi_p(\boldsymbol{x}) - K\psi_p(\boldsymbol{x})\} = f(\boldsymbol{x}), \quad \boldsymbol{x} \in C_N. \tag{3.4}$$

We discuss the calculation of the matrix entries

$$K\psi_p(\boldsymbol{x}), \quad p = 1, ..., d, \quad \boldsymbol{x} \in C_N$$

in the next section.

The proof of convergence of (3.3) is straightforward from the results of §2.

**Theorem 3.1** *Let $f \in \mathcal{C}(\partial B)$. For $N$ sufficiently large (3.3) has a unique solution $u_N \in S_N$. If, in addition, $f \in \mathcal{C}^r(\partial B)$ with $r \geq 1$ then, for $N$ sufficiently large,*

$$\|u - u_N\|_{\infty,\partial B} \leq C\frac{\log^2 N}{N^r}\|u\|_{\infty,r,\partial B}.$$

**Proof** Observe that by Theorem 2.7, $u_N$ satisfies (3.3) if and only if

$$(I - E_N K)u_N = E_N f.$$

It is well known e.g. [13, §6.4] that $(I-K)^{-1}$ exists and is bounded on $\mathcal{C}(\partial B)$. Moreover [6, §2.4], $K : \mathcal{C}(\partial B) \to \mathcal{C}^{0,\alpha}(\partial B)$ is bounded for $\alpha \in (0,1)$. Hence, for all $u \in \mathcal{C}(\partial B)$, Theorem 2.7 (iv) yields

$$\begin{aligned} \|(K - E_N K)u\|_\infty &\leq C\frac{\log^2 N}{N^\alpha}\|Ku\|_{\infty,\alpha,\partial B} \\ &\leq C\frac{\log^2 N}{N^\alpha}\|u\|_{\infty,\partial B} \end{aligned}$$

for any $\alpha \in (0,1)$. Hence $\|K - E_N K\|_\infty \to 0$ and standard perturbation theory shows that $(I - E_N K)^{-1}$ exists for $N$ sufficiently large and is uniformly bounded. Then, since $u - u_N = (I - E_N K)^{-1}(I - E_N)u$, we have

$$\|u - u_N\|_\infty \leq C\|(I - E_N)u\|_\infty. \tag{3.5}$$

If $f \in \mathcal{C}^r(\partial B)$ then since $I - K$ is also invertible on $\mathcal{C}^r(\partial B)$, $u \in \mathcal{C}^r(\partial B)$ and the result follows from Theorem 2.7 (iv). $\Box$

# 4 Collocation Integrals

To implement the collocation method we must calculate integrals of the form

$$(Kv)(\boldsymbol{x}) = \int_{\partial B} k(\boldsymbol{x}, \boldsymbol{y}) v(\boldsymbol{y}) d\sigma(\boldsymbol{y}) \ , \tag{4.1}$$

where $v$ is one of the basis functions for $S_N$ introduced in Section 2 and $k$ is given by (1.5).

To compute the weakly singular integrals (4.1) we follow the approach of Wienert ([25]) and introduce the *Householder matrix* defined for $\boldsymbol{x} \in \partial B$ by

$$H(\boldsymbol{x}) = (I - 2\boldsymbol{u}(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x})^T), \tag{4.2}$$

where

$$\boldsymbol{u}(\boldsymbol{x}) = \frac{(\boldsymbol{x} - (0,0,\tau(\boldsymbol{x}))^T)}{|\boldsymbol{x} - (0,0,\tau(\boldsymbol{x})^T)|} \tag{4.3}$$

and

$$\tau(\boldsymbol{x}) = \begin{cases} 1, & x_3 \leq 0 \\ -1, & x_3 > 0 \end{cases}$$

Since $|\boldsymbol{u}(\boldsymbol{x})| = 1$ we have

$$H(\boldsymbol{x}) = H(\boldsymbol{x})^{-1} = H(\boldsymbol{x})^T, \quad \boldsymbol{x} \in \partial B, \tag{4.4}$$

and

$$H(\boldsymbol{x})\boldsymbol{x} = (0,0,\tau(\boldsymbol{x}))^T, \qquad H(\boldsymbol{x})(0,0,\tau(\boldsymbol{x}))^T = \boldsymbol{x} \ . \tag{4.5}$$

Moreover, since $H(\boldsymbol{x})$ has eigenvalues $-1$ and $1$ in directions $\boldsymbol{u}(\boldsymbol{x})$ and $\{\boldsymbol{u}(\boldsymbol{x})\}^\perp$, it follows that

$$\det(H(\boldsymbol{x})) = -1. \tag{4.6}$$

Thus $H(\boldsymbol{x}) : \partial B \to \partial B$ and, geometrically, multiplication by $H(\boldsymbol{x})$ represents reflection in the plane perpendicular to the line joining $\boldsymbol{x}$ to $(0,0,\tau(\boldsymbol{x}))^T$, passing through the mid-point of that line. Since surface measure on $\partial B$ is unaffected by an orthogonal change of variable, we may rewrite (4.1) as

$$Kv(\boldsymbol{x}) = \int_{\partial B} k(\boldsymbol{x}, H(\boldsymbol{x})\boldsymbol{y}) v(H(\boldsymbol{x})\boldsymbol{y}) d\sigma(\boldsymbol{y}) \ . \tag{4.7}$$

By virtue of (4.5) the integrand in (4.7) now has a singularity at $\boldsymbol{y} = (0, 0, \tau(\boldsymbol{x}))^T$. We handle this by taking polar coordinates $\boldsymbol{y} = \boldsymbol{p}(\theta, \phi)^T$ to obtain

$$(Kv)(\boldsymbol{x}) = \int_0^{\pi} \int_0^{2\pi} \kappa(\boldsymbol{x}, \theta, \phi) v(H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi)) d\phi d\theta \tag{4.8}$$

with

$$\kappa(\boldsymbol{x}, \theta, \phi) = \sin\theta \; k(\boldsymbol{x}, H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi)).$$

We shall approximate the integrals (4.8) by quadrature. As we shall see in Lemmas 4.1–4.3 below, $\kappa(\boldsymbol{x}, \theta, \phi)$ is smooth on $(\theta, \phi) \in \mathcal{D}$ with all its derivatives uniformly bounded in $\boldsymbol{x} \in \partial B$. This is obtained using the arguments of Wienert [25] (see also [7]) but in the context of $\mathcal{C}^\infty$ rather than analytic function spaces.

We shall also examine below the behaviour of $v(H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi))$. As a function of $(\theta, \phi) \in \mathcal{D}$ this may have a very mild singularity when $\boldsymbol{p}(\theta, \phi) = \boldsymbol{x}$. We characterise this behaviour in results from Lemma 4.4 below onwards. Together these results show that the integrand in (4.8) is smooth except for a mild singularity at a single point. We devise a suitable method for approximating these integrals in the context of a model example in Section 5.

When examining the properties of $\kappa$ it is useful to define the function

$$\mathbf{Q}(\boldsymbol{x}, \theta, \phi) = \boldsymbol{q} \circ H(\boldsymbol{x}) \circ \boldsymbol{p}(\theta, \phi) = \boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi)). \tag{4.9}$$

We can then write

$$\kappa(\boldsymbol{x}, \theta, \phi) = \kappa_1(\boldsymbol{x}, \theta, \phi)\kappa_2(\boldsymbol{x}, \theta, \phi), \tag{4.10}$$

with (for $x_3 \leq 0$)

$$\kappa_1(\boldsymbol{x}, \theta, \phi) = \frac{1}{2\pi} \frac{\sin\theta}{|\mathbf{Q}(\boldsymbol{x}, 0, \phi) - \mathbf{Q}(\boldsymbol{x}, \theta, \phi)|}, \tag{4.11}$$

and

$$\kappa_2(\boldsymbol{x}, \theta, \phi) = \frac{(\mathbf{Q}(\boldsymbol{x}, 0, \phi) - \mathbf{Q}(\boldsymbol{x}, \theta, \phi))^T}{|\mathbf{Q}(\boldsymbol{x}, 0, \phi) - \mathbf{Q}(\boldsymbol{x}, \theta, \phi)|^2} \left\{ \mathrm{Adj}(d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi)))^T H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi) \right\}. \tag{4.12}$$

(If $x_3 > 0$ then we replace 0 by $\pi$ in (4.11) and (4.12).)

Before we analyse $\kappa_1$ and $\kappa_2$ we point out a useful simpler expression for the last factor on the right-hand side of (4.12) This is obtained by recalling the formula (valid for any $n \times n$ matrix $A$ and any two vectors $\mathbf{v}$, $\boldsymbol{w} \in \mathbb{R}^n$):

$$\mathrm{Adj(A)}^T \, \mathbf{v} \wedge \boldsymbol{w} = A\mathbf{v} \wedge A\boldsymbol{w} \, . \tag{4.13}$$

Then (as is easily verified),

$$\boldsymbol{p}(\theta, \phi) = \frac{1}{\sin\theta} \left\{ \frac{\partial \boldsymbol{p}}{\partial \theta} \wedge \frac{\partial \boldsymbol{p}}{\partial \theta} \right\} \tag{4.14}$$

and using (4.4), (4.6) we have

$$\mathrm{Adj}(H(\boldsymbol{x})) = \det(H(\boldsymbol{x}))H(\boldsymbol{x})^{-1} = -H(\boldsymbol{x}). \tag{4.15}$$

Hence (4.4) and (4.13)–(4.15) yield

$$H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi) = -\frac{1}{\sin\theta}\left\{H(\boldsymbol{x})\frac{\partial \boldsymbol{p}}{\partial\theta} \wedge H(\boldsymbol{x})\frac{\partial \boldsymbol{p}}{\partial\phi}(\theta,\phi)\right\}.$$

Using (4.13) again together with the chain rule, we have

$$\begin{aligned}
&\mathrm{Adj}(d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi))^T H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi) \\
&\quad = -\frac{1}{\sin\theta}\left\{d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi))H(\boldsymbol{x})\frac{\partial \boldsymbol{p}}{\partial\theta}(\theta,\phi) \wedge d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi))H(\boldsymbol{x})\frac{\partial \boldsymbol{p}}{\partial\phi}(\theta,\phi)\right\} \\
&\quad = -\frac{1}{\sin\theta}\left\{\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},\theta,\phi) \wedge \frac{\partial \mathbf{Q}}{\partial\phi}(\boldsymbol{x},\theta,\phi)\right\}. \qquad (4.16)
\end{aligned}$$

To examine the smoothness of the first factor in the integrand of (4.8) it is convenient to make the following definition.

**Definition** Given $v : \partial B \times \mathcal{D} \to \mathbb{R}$, we say $v(\boldsymbol{x},\theta,\phi)$ is $\mathcal{C}^\infty(\mathcal{D})$ *uniformly on* $\partial B$ if the function $(\theta,\phi) \mapsto v(\boldsymbol{x},\theta,\phi)$ is in $\mathcal{C}^\infty(\mathcal{D})$ and all its derivatives are uniformly bounded in $\boldsymbol{x} \in \partial B$.

Our first lemma is the following.

**Lemma 4.1** $\mathbf{Q}(\boldsymbol{x},\theta,\phi)$ *is* $\mathcal{C}^\infty(\mathcal{D})$ *uniformly on* $\partial B$.

**Proof** From (1.2) it is clear that the function $(\theta,\phi) \mapsto \mathbf{Q}(\boldsymbol{x},\theta,\phi)$ is in $\mathcal{C}^\infty(\mathcal{D})$. By the chain rule, its $(\theta,\phi)$ derivatives are products of the Euclidean derivatives of $\boldsymbol{q}$ evaluated at $H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi) \in \partial B$ and $(\theta,\phi)$ derivatives of $H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)$. The former are bounded independently of $\boldsymbol{x}$ (by (1.2)). For the latter, observe that for all $\boldsymbol{x} \in \partial B$, we have, using (4.4),

$$\left|\frac{d^{k+l}}{d\theta^k d\phi^l}(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi))\right| = \left|H(\boldsymbol{x})\frac{d^{k+l}\boldsymbol{p}}{d\theta^k d\phi^l}(\theta,\phi)\right| = \left|\frac{d^{k+l}\boldsymbol{p}}{d\theta^k d\phi^l}(\theta,\phi)\right| \le 1, \qquad \boldsymbol{x} \in \partial B \qquad (4.17)$$

and the results follow. □

The next two lemmas treat the two factors on the right-hand side of (4.10).

**Lemma 4.2** $\kappa_1(\boldsymbol{x},\theta,\phi)$ *is* $\mathcal{C}^\infty(\mathcal{D})$ *uniformly on* $\partial B$.

**Proof** Let $\boldsymbol{x} \in \partial B$ and without loss of generality assume $x_3 \le 0$. Then using (4.11), we have

$$\kappa_1(\boldsymbol{x},\theta,\phi)^2 = \frac{1}{4\pi^2}\frac{(\sin\theta/\theta)^2}{|\mathbf{Q}(\boldsymbol{x},0,\phi) - \mathbf{Q}(\boldsymbol{x},\theta,\phi)|^2/\theta^2} =: \frac{1}{4\pi^2}\frac{(\sin\theta/\theta)^2}{\hat{Q}(\boldsymbol{x},\theta,\phi)^2}$$

The result then follows from the following properties of $\hat{Q}$ which we shall establish below

$$\hat{Q}(\boldsymbol{x},\theta,\phi) \text{ is } \mathcal{C}^\infty(\mathcal{D}) \text{ uniformly in } \boldsymbol{x}\ , \qquad (4.18)$$

$$\hat{Q}(\boldsymbol{x},\theta,\phi) \ge \underline{\hat{Q}} > 0, \quad \boldsymbol{x} \in \partial B, \quad (\theta,\phi) \in \mathcal{D}, \ \underline{\hat{Q}} \text{ constant} \ . \qquad (4.19)$$

(If $x_3 > 0$ we write

$$\kappa_1(\boldsymbol{x},\theta,\phi)^2 = \frac{1}{4\pi^2}\frac{(\sin\theta/(\pi-\theta))^2}{|\mathbf{Q}(\boldsymbol{x},\pi,\phi)-\mathbf{Q}(\boldsymbol{x},\theta,\phi)|^2/(\pi-\theta)^2}$$

and proceed analogously.)

To obtain (4.18), observe that

$$\begin{aligned}\mathbf{Q}(\boldsymbol{x},0,\phi)-\mathbf{Q}(\boldsymbol{x},\theta,\phi) &= \int_0^1 \frac{d}{dt}\{(\mathbf{Q}(\boldsymbol{x},(1-t)\theta,\phi)\}\;dt \\ &= (-\theta)\int_0^1 \frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},(1-t)\theta,\phi)\,dt\ . \end{aligned} \tag{4.20}$$

Hence

$$\hat{Q}(\boldsymbol{x},\theta,\phi) = \int_0^1 \frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},(1-t)\theta,\phi)^T\,dt \int_0^1 \frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},(1-t)\theta,\phi)\,dt\ , \tag{4.21}$$

and (4.18) follows from Lemma 4.1.

To obtain (4.19) observe that $\hat{Q}(\boldsymbol{x},\theta,\phi) > 0$ for $\boldsymbol{x}\in\partial B$ and $(\theta,\phi)\in\mathcal{D}$ with $\theta\neq 0$. Since $\mathcal{D}$ is compact we simply have to show that

$$\lim_{\theta\to 0}\hat{Q}(\boldsymbol{x},\theta,\phi) > 0\ ,\quad \boldsymbol{x}\in\partial B,\quad \phi\in[0,2\pi]\ . \tag{4.22}$$

However by (4.21), $\hat{Q}(\boldsymbol{x},0,\phi)$ is well-defined and non-negative. Thus, if (4.22) is not true, then (4.21) implies

$$\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},0,\phi) = \mathbf{0}\ ,$$

for some $\phi\in[0,2\pi]$. By (4.9) and (4.5) this implies

$$d\boldsymbol{q}(\boldsymbol{x})H(\boldsymbol{x})\begin{bmatrix}\cos\phi\\ \sin\phi\\ 0\end{bmatrix} = d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(0,\phi))H(\boldsymbol{x})\begin{bmatrix}\cos\phi\\ \sin\phi\\ 0\end{bmatrix} = \mathbf{0}\ .$$

Hence $d\boldsymbol{q}(\boldsymbol{x})$ has a zero eigenvalue. However this is ruled out by assumption (A.2) of the Introduction and so (4.19) (and hence the result) follows. □

**Lemma 4.3** *$\kappa_2(\boldsymbol{x},\theta,\phi)$ is $\mathcal{C}^\infty(\mathcal{D})$ uniformly on $\partial B$.*

**Proof** As in Lemma 4.2, without loss of generality, let $\boldsymbol{x}\in\partial B$ with $x_3\le 0$. By (4.20), we have

$$\begin{aligned}&\mathbf{Q}(\boldsymbol{x},0,\phi)-\mathbf{Q}(\boldsymbol{x},\theta,\phi)\\ &\quad = \theta\int_0^1\left\{\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},0,\phi)-\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},(1-t)\theta,\phi)\right\}\,dt - \theta\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},0,\phi)\\ &\quad = \theta\int_0^1\int_0^1\frac{d}{ds}\left\{\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},(1-t)(1-s)\theta,\phi)\right\}\,ds\,dt - \theta\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},\theta,\phi)\\ &\quad = \theta^2\int_0^1\int_0^1\frac{\partial^2 \mathbf{Q}}{\partial\theta^2}(\boldsymbol{x},(1-t)(1-s)\theta,\phi)\,ds\,(t-1)\,dt - \theta\frac{\partial \mathbf{Q}}{\partial\theta}(\boldsymbol{x},\theta,\phi)\,.\end{aligned}$$

Thus, in view of (4.16),

$$\begin{aligned}(\mathbf{Q}(\boldsymbol{x},0,\phi)-\mathbf{Q}(\boldsymbol{x},\theta,\phi))^T&\left\{\mathrm{Adj}(d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)))^T H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)\right\}\\ &=\left\{\theta^2\int_0^1\int_0^1\frac{\partial^2\mathbf{Q}}{\partial\theta^2}(\boldsymbol{x},(1-t)(1-s)\theta,\phi)^T\,ds\,(t-1)\,dt\right\}\\ &\qquad\times\left\{\mathrm{Adj}(d\boldsymbol{q}(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)))^T H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)\right\}.\end{aligned}$$

Hence dividing (4.12) top and bottom by $\theta^2$ we have a numerator which is $\mathcal{C}^\infty(\mathcal{D})$ uniformly on $\partial B$ and a denominator which is precisely $\hat{Q}(\boldsymbol{x},\theta,\phi)$. Then (4.18) and (4.19) complete the proof. $\square$

Our next set of results concerns the second factor in the integrand of (4.8), namely the function

$$v(\boldsymbol{x},\theta,\phi):=v(H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)), \tag{4.23}$$

where $v$ is one of the basis functions for the space $S_N$ defined in (2.43), i.e.

$$v=\mathcal{J}^{-1}w, \tag{4.24}$$

where $w$ is one of the basis functions for $\Lambda_N$ listed in (2.29). It turns out to be convenient to study the function $v(\boldsymbol{x},\theta,\phi)$ as $(\theta,\phi)$ ranges over all of $\mathbb{R}^2$. Then, recalling (2.6) motivates us to introduce the set $\mathcal{P}(\boldsymbol{x})=\{(\theta,\phi)\in\mathbb{R}^2 : H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)\in\{\boldsymbol{n},\boldsymbol{s}\}\}$. Then $(\theta,\phi)\in\mathcal{P}(\boldsymbol{x})$ if and only if $\boldsymbol{p}(\theta,\phi)\in\{-\boldsymbol{x},\boldsymbol{x}\}$. If, in particular,

$$\boldsymbol{x}=\boldsymbol{p}(\tilde{\theta},\tilde{\phi}) \tag{4.25}$$

then it is easy to see that

$$\mathcal{P}(\boldsymbol{x})=\{(\tilde{\theta}+k\pi,\tilde{\phi}+2l\pi):k,l\in\mathbb{Z}\}\ \cup\{(-\tilde{\theta}+k\pi,\tilde{\phi}+(2\ell+1)\pi):k,\ell\in\mathbb{Z}\}. \tag{4.26}$$

Then by (2.43) and (2.6), we have, for $(\theta,\phi)\in\mathbb{R}^2\backslash\mathcal{P}(\boldsymbol{x})$,

$$v(\boldsymbol{x},\theta,\phi)=w((\boldsymbol{p}^{-1}\circ H(\boldsymbol{x})\circ\boldsymbol{p})(\theta,\phi)). \tag{4.27}$$

Moreover if $(\theta,\phi)\in\mathcal{P}(\boldsymbol{x})$, then either $H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi)=\boldsymbol{n}$ or $\boldsymbol{s}$ in which case

$$v(\boldsymbol{x},\theta,\phi)=w(0,\phi)\quad\text{or}\quad v(\boldsymbol{x},\theta,\phi)=w(\pi,\phi)\quad\text{respectively.} \tag{4.28}$$

It follows easily that $(\theta,\phi)\mapsto v(\boldsymbol{x},\theta,\phi)$ defines a function in $\mathcal{S}(\mathcal{D})$ for each fixed $\boldsymbol{x}\in\partial B$. It is convenient to write (4.27) as

$$v(\boldsymbol{x},\theta,\phi)=w\circ\boldsymbol{G}(\boldsymbol{x},\theta,\phi):=w(g_1(\boldsymbol{x},\theta,\phi),g_2(\boldsymbol{x},\theta,\phi)),\quad(\theta,\phi)\in\mathbb{R}^2\backslash\mathcal{P}(\boldsymbol{x}), \tag{4.29}$$

where

$$\boldsymbol{G}(\boldsymbol{x},\theta,\phi)=(g_1(\boldsymbol{x},\theta,\phi),g_2(\boldsymbol{x},\theta,\phi))=(\boldsymbol{p}^{-1}\circ H(\boldsymbol{x})\circ\boldsymbol{p})(\theta,\phi). \tag{4.30}$$

The first step in characterising the smoothness of $v$ is to examine the properties of $\boldsymbol{G}$. Here some care must be taken, since (as well as being undefined at $\boldsymbol{n}$ and $\boldsymbol{s}$), the second component of $\boldsymbol{p}^{-1}$ suffers a jump discontinuity of amplitude $2\pi$ along the line $\ell = \{\boldsymbol{p}(\theta, 0) : \ \theta \in (0, \pi)\}$ on $\partial B$, This motivates the introduction of the set

$$\mathcal{L}(\boldsymbol{x}) = \left\{(\theta, \phi) \in \mathbb{R}^2 : H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi) \in \ell\right\}.$$

Then $\boldsymbol{G}(\boldsymbol{x}, \theta, \phi)$ is well-defined for $(\theta, \phi) \in \mathbb{R}^2 \backslash \mathcal{Z}(\boldsymbol{x})$, where

$$\mathcal{Z}(\boldsymbol{x}) = \mathcal{P}(\boldsymbol{x}) \cup \mathcal{L}(\boldsymbol{x}).$$

and in fact is smooth there, as is shown in the following lemma.

**Lemma 4.4** *Let $\boldsymbol{x} \in \partial B$. Then the function $(\theta, \phi) \mapsto \boldsymbol{G}(\boldsymbol{x}, \theta, \phi)$ is in $(\mathcal{C}^\infty(\mathbb{R}^2 \backslash \mathcal{Z}(\boldsymbol{x})))^2$.*

**Proof** If $(\theta, \phi) \in \mathbb{R}^2 \backslash \mathcal{Z}(\boldsymbol{x})$ then $\boldsymbol{y} = \boldsymbol{G}(\boldsymbol{x}, \theta, \phi) \in \mathbb{R}^2$ is a solution of the parameter-dependent problem:

$$\boldsymbol{F}(\boldsymbol{y}, \theta, \phi) := \boldsymbol{p}(\boldsymbol{y}) - H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi) = \boldsymbol{0}.$$

$\boldsymbol{F}$ is infinitely continuously differentiable in $\boldsymbol{y}$ and $(\theta, \phi)$. The Jacobian of $\boldsymbol{F}$ with respect to $\boldsymbol{y} \in \mathbb{R}^2$ is the $3 \times 2$ matrix $\left(\dfrac{\partial p_i}{\partial y_j}\right)$ which may easily be shown to have rank 2 when evaluated at $\boldsymbol{G}(\boldsymbol{x}, \theta, \phi)$ for all $(\theta, \phi) \in \mathbb{R}^2 \backslash \mathcal{Z}(\boldsymbol{x})$. Hence the result follows from the implicit function theorem. $\square$

Our next result obtains formulae for the first partial derivatives of $\boldsymbol{G}$.

**Notation** If $\boldsymbol{a}, \boldsymbol{b}$ are vectors in $\mathbb{R}^n$ then $[\boldsymbol{a}, \boldsymbol{b}]$ denotes the $n \times 2$ matrix which has $\boldsymbol{a}$ as its first column and $\boldsymbol{b}$ as its second column.

**Lemma 4.5** *Let $\boldsymbol{x} \in \partial B$. Then, for $(\theta, \phi) \in \mathbb{R}^2 \backslash \mathcal{Z}(\boldsymbol{x})$, we have*

$$\begin{pmatrix} \frac{\partial g_1}{\partial \theta} & \frac{\partial g_1}{\partial \phi} \\ \sin g_1 \frac{\partial g_2}{\partial \theta} & \sin g_1 \frac{\partial g_2}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \cos g_1 \cos g_2 & \cos g_1 \sin g_2 & -\sin g_1 \\ -\sin g_2 & \cos g_2 & 0 \end{pmatrix} H(\boldsymbol{x}) \left[\frac{\partial \boldsymbol{p}}{\partial \theta}(\theta, \phi), \frac{\partial \boldsymbol{p}}{\partial \phi}(\theta, \phi)\right], \quad (4.31)$$

*where the components of $\boldsymbol{G}$ and their derivatives are evaluated at $(\boldsymbol{x}, \theta, \phi)$. Moreover $\dfrac{\partial \boldsymbol{G}}{\partial \theta}(\boldsymbol{x}, \theta, \phi)$, $\dfrac{\partial \boldsymbol{G}}{\partial \phi}(\boldsymbol{x}, \theta, \phi)$ extend as continuous functions to $(\theta, \phi) \in \mathbb{R}^2 \backslash \mathcal{P}(\boldsymbol{x})$.*

**Proof** Since $\boldsymbol{p}(\boldsymbol{G}(\boldsymbol{x}, \theta, \phi)) = H(\boldsymbol{x})\boldsymbol{p}(\theta, \phi)$, we can differentiate this with respect to $\theta$ first and then $\phi$ to obtain

$$\begin{pmatrix} \cos g_1 \cos g_2 & -\sin g_1 \sin g_2 \\ \cos g_1 \sin g_2 & \sin g_1 \cos g_2 \\ -\sin g_1 & 0 \end{pmatrix} \left[\frac{\partial \boldsymbol{G}}{\partial \theta}, \ \frac{\partial \boldsymbol{G}}{\partial \phi}\right] = H(\boldsymbol{x}) \left[\frac{\partial \boldsymbol{p}}{\partial \theta}(\theta, \phi), \ \frac{\partial \boldsymbol{p}}{\partial \phi}(\theta, \phi)\right]. \quad (4.32)$$

Then, multiplying both sides of (4.32) by the matrix

$$\begin{pmatrix} \cos g_1 \cos g_2 & \cos g_1 \sin g_2 & -\sin g_1 \\ -\sin g_2 & \cos g_2 & 0 \end{pmatrix}$$

yields (4.31). Since the right-hand side of (4.31) is continuous across $\mathcal{L}(\boldsymbol{x})$ the result follows. $\square$

Our next result concerns the smoothness of the function $v(\boldsymbol{x},\theta,\phi)$ given by (4.29). We use the following standard multi-index notation : Given $\alpha = (\alpha_1,\alpha_2)$ with $\alpha_1,\alpha_2 \in \mathbb{N}\cup\{0\}$, $D^\alpha\psi$ denotes the partial derivative $\partial^{|\alpha|}\psi/\partial\theta^{\alpha_1}\partial\phi^{\alpha_2}$ where $|\alpha| = \alpha_1+\alpha_2$.

**Theorem 4.6** *(i) For fixed $\boldsymbol{x}\in\partial B$ the function $(\theta,\phi)\mapsto v(\boldsymbol{x},\theta,\phi)$ is infinitely continuously differentiable on $\mathbb{R}^2\backslash\mathcal{Z}(\boldsymbol{x})$.*

*(ii) If $\boldsymbol{x}\in\{\boldsymbol{n},\boldsymbol{s}\}$ all the partial derivatives of $v(\boldsymbol{x},\cdot)$ on $\mathbb{R}^2\backslash\mathcal{Z}(\boldsymbol{x})$ have a continuous extension to $\mathbb{R}^2\backslash\mathcal{P}(\boldsymbol{x})$ and are bounded on $\mathbb{R}^2\backslash\mathcal{P}(\boldsymbol{x})$.*

*(iii) If $\boldsymbol{x}\in\partial B\backslash\{\boldsymbol{n},\boldsymbol{s}\}$ then for each $\alpha$ with $|\alpha|\geq 1$, $D^\alpha v(\boldsymbol{x},\cdot)$ has a continuous extension to $\mathbb{R}^2\backslash\mathcal{P}(\boldsymbol{x})$ and there exists a function $R_{\boldsymbol{x},\alpha}\in\mathcal{C}^\infty(\mathbb{R}^4)$ which is $2\pi$-periodic in each argument such that*

$$D^\alpha v = (\sin g_1)^{1-|\alpha|}R_{\boldsymbol{x},\alpha}(g_1,g_2,\theta,\phi),\quad (\theta,\phi)\in\mathbb{R}^2\backslash\mathcal{Z}(\boldsymbol{x}), \tag{4.33}$$

*where $v, g_1$ and $g_2$ are evaluated at $(\boldsymbol{x},\theta,\phi)$.*

**Proof** By (4.29), Lemma 4.4 and the fact that $w\in\mathcal{C}^\infty(\mathcal{D})$, part (i) follows directly. To obtain (ii), observe that if $\boldsymbol{x}\in\{\boldsymbol{n},\boldsymbol{s}\}$ then, for $(\theta,\phi)\in(0,\pi)\times[0,2\pi)$, $H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi) = \boldsymbol{p}(\pi-\theta,\phi)$ and $\boldsymbol{G}(\boldsymbol{x},\theta,\phi) = (\pi-\theta,\phi)$. Hence, we have $v(\boldsymbol{x},\theta,\phi) = w(\pi-\theta,\phi)$, which is smooth and $2\pi$-periodic on $(0,\pi)\times\mathbb{R}$. Also, since $v(\boldsymbol{x},\cdot)\in\mathcal{S}(\mathcal{D})$, if $(\theta,\phi)\in(-\pi,0)\times\mathbb{R}$, then

$$v(\boldsymbol{x},\theta,\phi) = v(\boldsymbol{x},-\theta,\phi+\pi) = w(\pi+\theta,\phi+\pi).$$

Then $v(\boldsymbol{x},\theta,\phi)$ is defined by extending these formulae $2\pi$-periodically and part (ii) follows.

Part (iii) is proved by induction on $m = |\alpha|$. We first examine the case $m = 1$. A simple analysis of (2.29) shows that any basis function $w\in\Lambda_N$ satisfies either

$$w(\theta,\phi) = \sin\theta P(\theta,\phi),\quad (\theta,\phi)\in\mathbb{R}^2 \tag{4.34}$$

or

$$w(\theta,\phi) = Q(\theta),\quad (\theta,\phi)\in\mathbb{R}^2, \tag{4.35}$$

where $P,Q$ are $\mathcal{C}^\infty$ functions which are $2\pi$-periodic in each argument. We shall consider only the case (4.34). The case (4.35) is similar but slightly simpler. Substituting (4.34) into (4.29) and differentiating with respect to $\theta$ gives

$$\begin{aligned}\frac{\partial v}{\partial\theta} &= \frac{\partial}{\partial\theta}w\circ\boldsymbol{G}\\ &= \left(\cos g_1 P(g_1,g_2) + \sin g_1\frac{\partial P}{\partial\theta}(g_1,g_2)\right)\frac{\partial g_1}{\partial\theta} + \frac{\partial P}{\partial\phi}(g_1,g_2)\sin g_1\frac{\partial g_2}{\partial\theta}\ ,\end{aligned}$$

where $v, g_1$ and $g_2$ are evaluated at $(\boldsymbol{x},\theta,\phi)$. Now substituting the expressions for $\dfrac{\partial g_1}{\partial\theta}$ and $\sin g_1\dfrac{\partial g_2}{\partial\theta}$ found in (4.31) yields an expression of the form (4.33) in the case $|\alpha| = 1$. An identical argument can be used to obtain an analogous expression for $\dfrac{\partial v}{\partial \phi}$. This completes the proof of (4.33) when $m = 1$.

Now suppose (4.33) holds for all $|\alpha| = m \geq 1$, and suppose $\hat{\alpha} = (\hat{\alpha}_1, \hat{\alpha}_2)$ satisfies $|\hat{\alpha}| = m + 1$. If $\hat{\alpha}_1 \geq 1$ then set $\tilde{\alpha} = (\hat{\alpha}_1 - 1, \hat{\alpha}_2)$. By the inductive hypothesis we have

$$D^{\tilde{\alpha}} v = (\sin g_1)^{1-m} R_{\boldsymbol{x},\tilde{\alpha}}(g_1, g_2, \theta, \phi).$$

Differentiating with respect to $\theta$ yields

$$\begin{aligned} D^{\hat{\alpha}} v = (\sin g_1)^{1-(m+1)} \quad & \left[ (1-m) R_{\boldsymbol{x},\tilde{\alpha}} \cos g_1 \frac{\partial g_1}{\partial \theta} + \frac{\partial R_{\boldsymbol{x},\tilde{\alpha}}}{\partial g_1} \sin g_1 \frac{\partial g_1}{\partial \theta} \right. \\ & \left. + \frac{\partial R_{\boldsymbol{x},\tilde{\alpha}}}{\partial g_2} \sin g_1 \frac{\partial g_2}{\partial \theta} + \frac{\partial R_{\boldsymbol{x},\tilde{\alpha}}}{\partial \theta} \sin g_1 \right], \end{aligned}$$

with $R_{\boldsymbol{x},\tilde{\alpha}}$ evaluated at $(g_1, g_2, \theta, \phi)$. Again substituting the expressions for $\partial g_1/\partial\theta$ and $\sin g_1 \partial g_2/\partial\theta$ found in (4.31) yields an expression for $D^{\hat{\alpha}} v$ of the form (4.33).

If $\hat{\alpha}_1 = 0$ then we set $\tilde{\alpha} = (\hat{\alpha}_1, \hat{\alpha}_2 - 1)$ and proceed analogously with $\theta$ replaced by $\phi$. Hence (4.33) holds when $|\alpha| = m + 1$ and the assertion follows. $\square$

Theorem 4.6 (iii) allows the higher derivatives of $v(\boldsymbol{x}, \cdot)$ to blow up as $(\theta, \phi)$ approaches any point in $\mathcal{P}(\boldsymbol{x})$. In the following corollary we give more detail of the blow-up behaviour which may arise. Recall that $\mathcal{P}(\boldsymbol{x})$ is characterised by (4.26) when $\boldsymbol{x}$ satisfies (4.25).

**Corollary 4.7** *Let $\boldsymbol{x} \in \partial B \backslash \{\boldsymbol{n}, \boldsymbol{s}\}$. For any multi-index $\alpha$, $D^\alpha v(\boldsymbol{x}, \theta, \phi)$ has a continuous extension to $(\theta, \phi) \in \mathbb{R}^2 \backslash \mathcal{P}(\boldsymbol{x})$. Moreover there exists a constant $M_\alpha$ such that, if $(\hat{\theta}, \hat{\phi}) \in \mathcal{P}(\boldsymbol{x})$,*

$$|D^\alpha v(\boldsymbol{x}, \theta, \phi)| \leq M_\alpha \|(\theta, \phi) - (\hat{\theta}, \hat{\phi})\|^{1-|\alpha|}, \tag{4.36}$$

*for all $(\theta, \phi) \in \mathbb{R}^2$ sufficiently close (but not equal) to $(\hat{\theta}, \hat{\phi})$. (Here $\|\cdot\|$ denotes the Euclidean norm in $\mathbb{R}^2$.)*

**Proof** Since $R_{\boldsymbol{x},\alpha}$ defined in Theorem 4.6(iii) is $2\pi$ periodic in its second argument and $g_2$ has a jump discontinuity of amplitude $2\pi$ along the curves in $\mathcal{L}(\boldsymbol{x})$ the first assertion follows directly from (4.33). This yields the estimate

$$|D^\alpha v(\boldsymbol{x}, \theta, \phi)| \leq M_\alpha |\sin g_1|^{1-|\alpha|}, \tag{4.37}$$

for $(\theta, \phi)$ sufficiently close to $(\hat{\theta}, \hat{\phi})$, where

$$g_1 = g_1(\boldsymbol{x}, \theta, \phi) = ((\boldsymbol{p}^{-1} H(\boldsymbol{x}) \boldsymbol{p})(\theta, \phi))_1.$$

To obtain the second assertion from the bound (4.37), we observe that when $(\theta, \phi)$ is near to but not equal to $(\hat{\theta}, \hat{\phi})$ then $(\theta, \phi) \notin \mathcal{P}(\boldsymbol{x})$ and $g_1 \in (0, \pi)$ is uniquely defined by

$$\cos g_1 = (H(\boldsymbol{x}) \boldsymbol{p}(\theta, \phi))_3. \tag{4.38}$$

Suppose $\boldsymbol{x}$ is given by (4.25) and recall (4.26). It is then a simple calculation to show that

$$(H(\boldsymbol{x}) \boldsymbol{p}(\theta, \phi))_3 = \tau(\boldsymbol{x})(\cos\theta \cos\tilde{\theta} + \sin\theta \sin\tilde{\theta} \cos(\phi - \tilde{\phi})).$$

A Taylor expansion about $(\hat{\theta}, \hat{\phi}) \in \mathcal{P}(\boldsymbol{x})$ then yields

$$|(H(\boldsymbol{x})p(\theta,\phi))_3| \geq 1 - C\|(\theta,\phi) - (\hat{\theta},\hat{\phi})\|^2$$

for some constant $C$ and all $(\theta,\phi)$ sufficiently close to $(\hat{\theta},\hat{\phi})$. Hence from (4.38)

$$\sin g_1 = \sqrt{1-\cos^2 g_1} = O(\|(\theta,\phi) - (\hat{\theta},\hat{\phi})\|),$$

which, together with (4.37), yields (4.36). □

**Remark 4.8** It is not difficult to find an illustration of the sharpness of the estimates in Corollary 4.7. For example if $\boldsymbol{x} = (1,0,0)^T = \boldsymbol{p}(\tilde{\theta},\tilde{\phi})$ with $(\tilde{\theta},\tilde{\phi}) = (\pi/2, 0)$, then

$$H(\boldsymbol{x})\boldsymbol{p}(\theta,\phi) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \boldsymbol{p}(\theta,\phi) = \begin{bmatrix} \cos\theta \\ \sin\theta\sin\phi \\ \sin\theta\cos\phi \end{bmatrix}.$$

When examining the smoothness of $\boldsymbol{G}$ and $v$ we can consider the limit $(\theta,\phi) \to (\tilde{\theta},\tilde{\phi})$ along infinitely many paths. Two such paths are

$$\begin{aligned} &\text{Path 1}: \quad (\theta,\phi) = (\pi/2+\varepsilon, 0), \quad 0 \neq \varepsilon \to 0; \\ &\text{Path 2}: \quad (\theta,\phi) = (\pi/2, \delta), \quad 0 \neq \delta \to 0. \end{aligned}$$

Then a simple calculation shows that $\boldsymbol{G}(\boldsymbol{x},\theta,\phi) = (-\varepsilon, 0)$ on Path 1 whereas $\boldsymbol{G}(\boldsymbol{x},\theta,\phi) = (\delta, \pi/2)$ on Path 2. Making use of this and (4.31) shows that as $(\theta,\phi) \to (\tilde{\theta},\tilde{\phi})$ on Path 1,

$$g_1 \to 0, \quad g_2 \to 0, \quad \frac{\partial g_1}{\partial\theta} \to -1, \quad \sin g_1 \frac{\partial g_2}{\partial\theta} \to 0, \tag{4.39}$$

whereas if $(\theta,\phi) \to (\tilde{\theta},\tilde{\phi})$ on Path 2 then

$$g_1 \to 0, \quad g_2 \to \frac{\pi}{2}, \quad \frac{\partial g_1}{\partial\theta} \to 0, \quad \sin g_1 \frac{\partial g_2}{\partial\theta} \to 1. \tag{4.40}$$

Now let us consider, for example, the basis function

$$w(\theta,\phi) = \sin\theta\cos 3\phi \quad \in \Lambda_N.$$

Using (4.39), (4.40), it is then straightforward to check that $v(\boldsymbol{x},\theta,\phi) = w(g_1,g_2)$ (with $g_i = g_i(\boldsymbol{x},\theta,\phi)$) satisfies

$$\frac{\partial v}{\partial\theta} \to -1 \text{ as } (\theta,\phi) \to (\tilde{\theta},\tilde{\phi}) \text{ on Path 1}$$

whereas

$$\frac{\partial v}{\partial\theta} \to 3 \text{ as } (\theta,\phi) \to (\tilde{\theta},\tilde{\phi}) \text{ on Path 2.}$$

So $\partial v/\partial\theta$ is discontinuous at $(\theta,\phi) = (\tilde{\theta},\tilde{\phi})$. In this case the limiting values of $\partial^2 v/\partial\theta^2$ are actually equal along each of Paths 1 and 2. However if we consider instead $v(\boldsymbol{x},\theta,\phi) = w(g_1,g_2)$, where

$$w(\theta,\phi) = \sin\theta\sin 3\phi \quad \in \Lambda_N$$

then $\dfrac{\partial v}{\partial \theta}$ has the same limiting value along Paths 1 and 2 but an elementary calculation shows

$$(\sin g_1)\frac{\partial^2 v}{\partial \theta^2} \to 0 \text{ as } (\theta,\phi) \to (\tilde{\theta},\tilde{\phi}) \text{ along Path 1}$$

and

$$(\sin g_1)\frac{\partial^2 v}{\partial \theta^2} \to 8 \text{ as } (\theta,\phi) \to (\tilde{\theta},\tilde{\phi}) \text{ along Path 2.}$$

So the estimate $O((\sin g_1)^{1-|\alpha|})$ of Corollary 4.7 cannot, in general, be strengthened.

$\square$

# 5 Numerical Experiments

As a model case we solve (1.1) where $\Gamma$ is the ellipsoid

$$\frac{\xi_1^2}{A^2} + \frac{\xi_2^2}{B^2} + \xi_3^2 = 1$$

and $\Omega$ is the interior of $\Gamma$. This was converted to (1.6) using the mapping $\boldsymbol{q}(\boldsymbol{x}) = (Ax_1, Bx_2, x_3)^T, \boldsymbol{x} \in \partial B$. We used the method in §3 to solve (1.6) yielding the solution $u_N$ on $\partial B$ which is identified with a function on $\Gamma$ (also called $u_N$), defined using the inverse of $\boldsymbol{q}$. Having found this we can compute the potential in $\Omega$:

$$U_N(\boldsymbol{\xi}) = \int_{\partial B} \frac{1}{4\pi} \frac{(\boldsymbol{\xi} - \boldsymbol{q}(\boldsymbol{y}))^T \mathrm{Adj}(dq(\boldsymbol{y}))^T \boldsymbol{n}(\boldsymbol{y})}{|\boldsymbol{\xi} - \boldsymbol{q}(\boldsymbol{y})|^3} u_N(\boldsymbol{q}(\boldsymbol{y}))d\sigma(\boldsymbol{y}) \ , \quad \boldsymbol{\xi} \in \Omega \tag{5.1}$$

which approximates the solution $U$ of the boundary value problem $\triangle U = 0$ in $\Omega$, $U = \frac{1}{2}f$ on $\Gamma$. We consider two cases

- Case A : $f \equiv 2$.
- Case B : $f(\boldsymbol{\xi}) = \exp(\xi_1)\cos(\xi_3), \quad \boldsymbol{\xi} \in \Gamma$.

In Case A, (1.1) has the exact solution $u \equiv 1$ and the solution to the boundary value problem is $U \equiv 1$. Because of the quasioptimal estimate (3.5) and since the constant functions lie in the basis space for the collocation method we have $u_N \equiv 1$ for all $N$ provided the collocation integrals are computed exactly. Thus Case A can be used as a test of the accuracy of the quadrature method which we shall use for the collocation integrals.

In Case B the solution of (1.1) is not known analytically but $U(\boldsymbol{\xi}) = \frac{1}{2}\exp(\xi_1)\cos(\xi_3)$, $\boldsymbol{\xi} \in \Omega$, which can be used for comparison with the computed value $U_N(\boldsymbol{\xi})$. In all the tables of results given below $\|u_N - 1\|_\infty$ is computed by finding the maximum of $u_N - 1$ at the collocation points on $\partial B$, and $\boldsymbol{\xi}^* = \boldsymbol{q}(\boldsymbol{x}^*)$ where $\boldsymbol{x}^*$ is the (randomly chosen) point $\boldsymbol{x}^* = (0.1589, 0.2542, 0.01058)^T$ on the unit sphere. For any table of results containing a sequence $(a_N)$ which tends to 0 as $N \to \infty$, *exponential convergence* is tested by conjecturing that

$$a_N = C\exp(-\alpha N)$$

and then computing $\alpha$ from results for two different values of $N$ by

$$\alpha = \left\{ \frac{1}{N_2 - N_1} \right\} \log(a_{N_1}/a_{N_2}).$$

It remains to explain how we use the information derived in §4 to devise an accurate method of computing the collocation integrals. Since the collocation method has a spectral convergence rate we do not want to use any quadrature rule which would destroy that fast rate and so this question is vitally important.

Recall that the collocation integrals are given by (4.8). The integrands have singularities (described by Corollary 4.7) if $\boldsymbol{x} \neq \boldsymbol{n}$ or $\boldsymbol{s}$. So suppose $\boldsymbol{x} = \boldsymbol{p}(\tilde{\theta}, \tilde{\phi})$ with $\tilde{\theta} \in (0, \pi)$ and $\tilde{\phi} \in (0, 2\pi]$. Then we are concerned with singularities in the integrand of (4.8) at any point in the region $[0, \pi] \times [0, 2\pi]$. By Corollary 4.7 these can only happen at points

$$(\tilde{\theta}, \tilde{\phi}), \quad (-\tilde{\theta} + \pi, \ \tilde{\phi} + \pi)$$

and at their translates through $2\pi$ in the $\phi$ direction.

Since the integrand in (4.8) is $2\pi$-periodic in $\phi$ we can write

$$(Kv)(\boldsymbol{x}) = \int_0^{\pi} \int_0^{2\pi} \kappa(\boldsymbol{x}, \theta, \phi + \tilde{\phi}) v(H(\boldsymbol{x}) \boldsymbol{p}(\theta, \phi + \tilde{\phi})) d\phi d\theta, \tag{5.2}$$

where the integrand now has singularities at three points in the domain of integration:

$$(\tilde{\theta}, 0), \qquad (-\tilde{\theta} + \pi, \pi), \qquad (\tilde{\theta}, 2\pi).$$

We split (5.2) into the sum of integrals over $[0, \pi] \times [0, \pi]$ and $[0, \pi] \times [\pi, 2\pi]$ and apply the tensor product Gauss-Legendre rule with $M$ points in each coordinate direction to each integral. Since the singularities lie on the boundaries of the integration domains we expect this to converge reasonably well.

We solved (1.1) with $A = 1, B = 2, N = 3$ for Case A above. The results are given in Table 1 and they indicate that in fact the quadrature rule yields solutions to the integral equation and approximate potentials which converge with order roughly $O(\exp(-1.2M))$. The convergence is less regular for the potential at the arbitrarily chosen point $\boldsymbol{\xi}^*$. These results are surprisingly good (we have no proof of the exponential convergence), and they indicate that we have no problems from the weak singularities in (4.8).

| $M$ | $\|u-1\|_\infty$ | $\alpha$ | $\|U(\mathbf{0})-1\|$ | $\alpha$ | $\|U(\boldsymbol{\xi}^*)-1\|$ | $\alpha$ |
|---|---|---|---|---|---|---|
| 5 | 9.826(-4) | | 3.081(-3) | | 7.236(-3) | |
| 10 | 8.606(-6) | 0.9 | 2.680(-6) | 1.4 | 2.396(-5) | 1.1 |
| 15 | 3.754(-8) | 1.1 | 6.787(-9) | 1.2 | 1.854(-6) | 0.5 |
| 20 | 9.122(-11) | 1.2 | 3.822(-11) | 1.0 | 3.049(-8) | 0.8 |
| 25 | 2.001(-13) | 1.2 | 1.101(-13) | 1.2 | 8.679(-11) | 1.2 |

**Table 1 :** $A = 1, B = 2, N = 3$, Case A.

Next, to check the performance of the collocation method in the absence of quadrature errors we solved (1.1) with $A = 1, B = 2$, and $M = 25$ for Case B above. From Table 1, we expect quadrature error to pollute at worst (about) the 11th decimal place of our solution. The results are in Table 2 and show a convergence rate for approximate potentials which is roughly of order $O(\exp(-2.5N))$.

| $N$ | $\|U_N(\mathbf{0}) - U(\mathbf{0})\|$ | $\alpha$ | $N$ | $\|U_N(\mathbf{0}) - U(\mathbf{0})\|$ | $\alpha$ |
|---|---|---|---|---|---|
| 3 | 1.563(-3) | | 2 | 1.853(-2) | |
| 5 | 2.466(-5) | 2.1 | 4 | 9.382(-5) | 2.6 |
| 7 | 1.681(-7) | 2.5 | 6 | 5.720(-7) | 2.5 |
| 9 | 8.051(-10) | 2.7 | 8 | 2.602(-9) | 2.7 |

**Table 2 :** $A = 1, B = 2, M = 25$, Case B

Table 2 shows that good solutions to the boundary value problem are obtained by solving a system of very small dimension (e.g. when $N = 7$ there are 86 degrees of freedom). A similar accuracy is reported in [2]. However since the method used there is a Galerkin method more quadrature is needed to assemble the stiffness matrix (for the same number of degrees of freedom). The program used to compute these solutions is very simple and compact, was written in MATLAB ([18]) and runs interactively on a Sun 4 workstation with many concurrent users and also on stand alone PC-486.

Finally it is interesting to try to reduce the overall cost of the method by balancing the quadrature error with the underlying error in the collocation method. To do this let $u_N^e$ denote the (theoretical) collocation solution (if the collocation integrals are done exactly) and let $u_N$ denote the corresponding solution in the presence of quadrature. Then

$$u - u_N = (u - u_N^e) + (u_N^e - u_N). \tag{5.3}$$

We know that the first term on the right-hand side of (5.3) converges exponentially. We want to ensure the second does also. Recall that from §3 $(I - E_N K)u_N^e = E_N f$ and suppose that $(I - K_{N,M})u_N = E_N f$ where $K_{N,M}$ denotes the quadrature approximation to $E_N K$ (using the $M$ point Gauss rule described above). Then a simple manipulation shows

$$(I - K_{N,M})(u_N^e - u_N) = (E_N K - K_{N,M})u_N^e.$$

Thus, assuming stability for $(I - K_{NM})$ and using the fact that $u_N^e \to u$, we expect that

$$\|u_N^e - u_N\|_\infty \le C\|(E_N K - K_{N,M})|_{S_N}\|_\infty \tag{5.4}$$

where $S_N$ is as in §3. The right-hand side of (5.4) is the uniform norm of a matrix with dimension $O(N^2)$, each entry of which is converging exponentially. Thus it is reasonable to conjecture

$$\|u_N^e - u_N\|_\infty \le CN^2 \exp(-\beta M). \tag{5.5}$$

for some $\beta$. We checked the sharpness of the $N$-dependence in this estimate by solving (1.1) with $A = 1, B = 2, M = 10$ in Case A. The results are in Table 3 and confirm the $N^2$ growth conjectured in (5.5). (Note $u_N^e = u$ in this example.)

| $N$ | $\|u - u_N\|_\infty$ |
|---|---|
| 3 | 8.606(-6) |
| 5 | 1.138(-4) |
| 7 | 5.316(-4) |
| 9 | 1.059(-3) |
| 11 | 1.602(-3) |

**Table 3 :** $A = 1, B = 2, M = 10$, Case A.

To ensure exponential convergence for $u_N^e - u_N$ (i.e. $\|u_N^e - u_N\|_\infty = O(\exp(-\alpha' N))$ for some $\alpha' > 0$) it is then clear from (5.5) that we must choose

$$M = \frac{1}{\beta}\{\alpha' N + 2\log N\}. \tag{5.6}$$

In principle we would choose $\alpha'$ equal to $\alpha$ where $\|u - u_N^e\|_\infty = O(\exp(-\alpha N))$ (see (5.3)), and then $M$ by (5.6), but in practice $\alpha$, and $\beta$ are unknown in general, and $\alpha'$, and $\beta$ in (5.6) would have to be chosen by experiment. Here we can verify this analysis since Table 1 shows $\beta \cong 1.2$ and Table 2 shows $\alpha \cong 2.5$. In (5.6) we put $\beta = 1, \alpha' = 2$. The results are in Table 4 and exhibit a very similar convergence and accuracy to Table 2, but much less quadrature is needed.

| $N$ | $M \cong 2(N + \log N)$ | $\|U_N(\mathbf{0}) - U(\mathbf{0})\|$ | $\alpha$ |
|---|---|---|---|
| 3 | 9 | 1.535(-3) | |
| 5 | 14 | 2.465(-5) | 2.1 |
| 7 | 18 | 1.678(-7) | 2.5 |
| 9 | 23 | 7.917(-10) | 2.7 |

**Table 4 :** $A = 1, B = 2$, Case B

Finally, we tried the method on the long slender ellipsoid $A = 2, B = 10$. The results are in Table 5 and exhibit similar convergence to Table 4 but with a somewhat larger asymptotic constant. The accuracy of $3 \times 10^{-6}$ with 86 degrees of freedom is still very good.

| $N$ | $M$ | $\|U_N(\mathbf{0}) - U(\mathbf{0})\|$ | $\alpha$ |
|---|---|---|---|
| 3 | 9 | 3.431(-2) | |
| 5 | 14 | 3.738(-4) | 2.3 |
| 7 | 18 | 3.459(-6) | 2.3 |
| 9 | 23 | 1.521(-7) | 1.6 |

**Table 5 :** $A = 2, B = 10$, Case B.

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# Appendix

In this section we prove the following lemma which is used in the proof of Lemma 2.1.
**Lemma A.1**

$$\frac{1}{N} \sup_{\theta \in [0,2\pi]} \sum_{j=0}^{2N-1} |D_N^*(\theta - \theta_j)| = O(\log N), \quad \text{as } N \to \infty,$$

*where $D_N^*$ is the modified Dirichlet kernel defined in (2.18).*

**Proof** It uses formulae and arguments from [26, Vol.I, p.50, 88, Vol.II, p.29]. Introduce the Dirichlet kernel

$$D_j(t) = \frac{1}{2} + \sum_{l=1}^{j} \cos lt = \frac{\sin(j+\frac{1}{2})\theta}{2\sin\theta/2}$$

and the Fejér kernel

$$K_n(t) = \frac{1}{n+1} \sum_{j=0}^{n} D_j(t).$$

Then

$$K_n(t) \geq 0, \quad n \geq 0 \tag{A.1}$$

and

$$\frac{1}{\pi} \int_{-\pi}^{\pi} K_n(t)dt = 1, \quad n \geq 1. \tag{A.2}$$

Moreover

$$2K_{2N-1}(t) - K_{N-1}(t) = \frac{1}{N} \sum_{j=N}^{2N-1} D_j(t). \tag{A.3}$$

If now $S_N$ is any trigonometric polynomial of degree $\leq N$ then it is easy to show that

$$S_N(\theta) = \frac{1}{\pi}\int_0^{2\pi} S_N(\phi)D_j(\theta-\phi)d\phi, \quad j \geq N. \tag{A.4}$$

Combining (A.3) and (A.4) we have

$$S_N(\theta) = \frac{1}{\pi}\int_0^{2\pi} S_N(\phi)\left\{2K_{2N-1}(\theta-\phi) - K_{N-1}(\theta-\phi)\right\}d\phi.$$

Thus

$$\begin{aligned}
\frac{1}{3N}\sum_{j=0}^{2N-1}|S_N(\theta_j)| &\leq \frac{2}{3\pi}\int_0^{2\pi}|S_N(\phi)|\frac{1}{N}\sum_{j=0}^{2N-1}|K_{2N-1}(\theta_j-\phi)|d\phi \\
&+ \frac{1}{3\pi}\int_0^{2\pi}|S_N(\phi)|\frac{1}{N}\sum_{j=0}^{2N-1}|K_{N-1}(\theta_j-\phi)|d\phi.
\end{aligned}$$

Then using (A.1), (A.2) and the precision properties of the trapezoidal rule,

$$\frac{1}{N}\sum_{j=0}^{2N-1}|K_m(\theta_j-\phi)| = \frac{1}{\pi}\int_{-\pi}^{\pi}K_m(\theta-\phi)d\phi = 1$$

for $m = N-1$ or $2N-1$. Hence

$$\frac{1}{N}\sum_{j=0}^{2N-1}|S_N(\theta_j)| \leq \frac{3}{\pi}\int_0^{2\pi}|S_N(\theta)|d\theta. \tag{A.5}$$

This is true for any trigonometric polynomial $S_N$ of degree $\leq N$. Hence for all $\theta \in [0, 2\pi]$,

$$\begin{aligned}
\frac{1}{N}\sum_{j=0}^{2N-1}|D_N^*(\theta-\theta_j)| &\leq \frac{3}{\pi}\int_0^{2\pi}|D_N^*(\theta-\phi)|d\phi \\
&= \frac{3}{\pi}\int_0^{2\pi}|D_N^*(\phi)|d\phi \\
&= O(\log N) \quad \text{as } N \to \infty,
\end{aligned}$$

where the final estimate is to be found in [26, Vol.I, p.67].