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Solution of Helmholtz Equation in the Exterior Domain by Elementary Boundary Integral Methods

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In this paper *elementary boundary integral equations* for the Helmholtz equation in the exterior domain, based on Green's formula or through representation of the solution by layer potentials, are considered. Even when the partial differential equation has a unique solution, for any given closed boundary Γ, these elementary boundary integral equations can be shown to be singular at a countable set of characteristic wavenumbers. Spectral properties and conditioning of the boundary integral operators and their discrete boundary element counterparts are studied near characteristic wavenumbers, with a view to assessing the suitability of these formulations for the solution of the exterior Helmholtz equation. Collocation methods are used for the discretisation of the boundary integral equations which are either of the Fredholm first kind, second kind, or hyper-singular type. The effect of quadrature errors on the accuracy of the *discrete collocation methods* is systematically investigated. © 1995 Academic Press, Inc.

1. INTRODUCTION

The underlying problem that is considered in this paper is the solution of the Helmholtz equation,

$$\nabla^2\varphi(\mathbf{p}) + k^2\varphi(\mathbf{p}) = 0, \quad \mathbf{p} \in D_+, \tag{1}$$

in two space dimensions, where D_+ is the infinite region exterior to a closed boundary Γ, with k being the complex wavenumber and $\mathrm{Im}(k) \geq 0$. The majority of the results in this paper extend in a simple manner to the three-dimensional case. However, the numerical analysis of boundary integral equations in three dimensions is not as yet complete. For simplicity the boundary Γ will be assumed to be in C^∞.

In this paper we will be mainly concerned with the Dirichelt or Neumann boundary conditions

$$\varphi(\mathbf{p}) = f(\mathbf{p}) \quad \text{or} \quad \frac{\partial\varphi}{\partial\mathbf{n}}(\mathbf{p}) = f(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{2}$$

For (1)–(2) to possess a unique solution, φ needs to satisfy a suitable decaying condition at infinity such as the Sommerfeld radiation condition,

$$\frac{\partial\varphi(\mathbf{p})}{\partial r} - ik\varphi(\mathbf{p}) = o(r^{-1/2}), \quad \text{as } r \to \infty, \tag{3}$$

where $r = |\mathbf{p} - \mathbf{p}_0|$ and $\mathbf{p}_0$ is a fixed origin inside Γ.

The numerical solution of the exterior Helmholtz equation through first reformulating it as a *boundary integral equation* (BIE) has been of interest to researchers for several decades. The approach has the beneficial effects of reducing the dimension of the problem by one and transforming it from an infinite domain problem into a finite domain problem [26, 16]. In Section 2 *direct* and *indirect* boundary integral equations of the elementary type, derived using Green's second theorem or by layer potential representation, will be discussed. Even though the Helmholtz problem in the exterior domain has a unique solution, these elementary formulations are known to be singular for a countable set of real, positive values of the wavenumber. These are precisely the values for which $-k^2$ are the eigenvalues of the Laplacian operator in the interior region, D_-, with homogeneous Dirichlet or homogeneous Neumann boundary conditions, respectively. These values of k give the frequencies for the standing wave solutions of the Helmholtz equation in the region D_- [46]. Various more complex boundary integral formulations of this exterior problem have been proposed since 1965 in order to eliminate the difficulties with the elementary formulations. These reformulations are reviewed in Burton [14] and Kleinmann and Roach [29] and Amini *et al.* [5]. It is our purpose here to analyse the elementary formulations, in particular their conditioning close to characteristic wavenumbers, and assess their usefulness as a basis for numerical computation.

The application of finite element type discretisation schemes to the boundary integral equation gives rise to methods termed *boundary element methods* (BEM). In Section 3 the collocation method based on piecewise polynomial approximation of the boundary functions will be considered. The practical case where the integrations are carried out numerically, the so-called *discrete collocation* methods will also be discussed in that section. In Section 4, by studying the spectral properties of the Helmholtz integral operators over a unit circle, we are able to analyse the conditioning of the elementary boundary integral equations

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near their singularities. The behaviour of the *boundary element equations* (BEE), the discrete counterparts of the BIE, will also be investigated. In Section 5 extensive numerical experiments are reported for the case where the boundary Γ is a unit circle. The behaviour of the eigenvalues of the discrete operators and their conditioning near and away from characteristic wavenumbers are also discussed. Numerical results are presented for the solution of several Dirichlet and Neumann problems using different boundary integral equations with the collocation method with exact and approximate BEE. Finally the results of the paper are summarised, together with a discussion on the practical applications of these elementary boundary integral equations for the solution of the exterior Helmholtz equation.

2. ELEMENTARY INTEGRAL EQUATION FORMULATIONS

To define the various boundary integral formulations we require the Helmholtz integral operators which are here denoted by L_k, M_k, M_k^t, and N_k and defined as

$$(L_k\mu)(\mathbf{p}) \equiv \int_\Gamma G_k(\mathbf{p}, \mathbf{q})\mu(\mathbf{q})\, d\Gamma_q \quad (\mathbf{p} \in D_- \cup \Gamma \cup D_+),$$

$$(M_k\mu)(\mathbf{p}) \equiv \int_\Gamma \frac{\partial G_k}{\partial \mathbf{n}_q}(\mathbf{p}, \mathbf{q})\mu(\mathbf{q})\, d\Gamma_q \quad (\mathbf{p} \in D_- \cup \Gamma \cup D_+),$$

$$(M_k^t\mu)(\mathbf{p}) \equiv \frac{\partial}{\partial \mathbf{n}_p}\int_\Gamma G_k(\mathbf{p}, \mathbf{q})\mu(\mathbf{q})\, d\Gamma_q \quad (\mathbf{p} \in \Gamma),$$

$$(N_k\mu)(\mathbf{p}) \equiv \frac{\partial}{\partial \mathbf{n}_q}\int_\Gamma \frac{\partial G_k}{\partial \mathbf{n}_q}(\mathbf{p}, \mathbf{q})\mu(\mathbf{q})\, d\Gamma_q \quad (\mathbf{p} \in \Gamma),$$

where the element of integration is at $\mathbf{q}$ and $\mathbf{n}_q$ is the unit outward normal to the boundary at $\mathbf{q}$. The density function $\mu(\mathbf{q})$ is defined for $\mathbf{q} \in \Gamma$, and its smoothness requirements will be discussed shortly. $G_k(\mathbf{p}, \mathbf{q})$ is the free-space Green's function or *fundamental solution* for the Helmholtz equation and is given by

$$G_k(\mathbf{p}, \mathbf{q}) = \frac{i}{4} H_0^{(1)}(kr), \tag{4}$$

where $\mathbf{r} = \mathbf{p} - \mathbf{q}$, $r = |\mathbf{r}|$, and $H_0^{(1)}$ is the Hankel function of the first kind of order zero.

We shall now discuss the continuity properties of the Helmholtz potential operators. We note that M_k^t and N_k are the normal derivatives of the single and double layer potentials, respectively. The Green's function, the kernel of L_k, satisfies

$$H_0^{(1)}(x) = \frac{2i}{\pi}\ln(x) + \mathcal{O}(1), \quad \text{as } x \to 0, \tag{5}$$

and therefore as $\mathbf{p} \in D_+ \to \mathbf{q} \in \Gamma$ along $\mathbf{n}_q$ has a logarithmic singularity, whilst the kernel of M_k has the stronger *Cauchy* singularity. In the derivation of boundary integral equations the following jump conditions, as $\mathbf{p}$ crosses the boundary Γ, are useful.

THEOREM 1. *Let $\mathbf{p}_+$, $\mathbf{p}_-$, and $\mathbf{p}$ denote general points in D_+, D_-, and Γ, respectively. Then if $\sigma(\mathbf{p})$ is a bounded density function,*

$$\lim_{\mathbf{p}_+\to\mathbf{p}} (L_k\sigma)(\mathbf{p}_+) = (L_k\sigma)(\mathbf{p}) = \lim_{\mathbf{p}_-\to\mathbf{p}} (L_k\sigma)(\mathbf{p}_-).$$

If $\sigma(\mathbf{p})$ is Hölder-continuous on Γ (i.e., $\sigma \in \mathscr{C}^{0,\alpha}(\Gamma)$, $0 < \alpha < 1$) then

$$\lim_{\mathbf{p}_+\to\mathbf{p}} (M_k\sigma)(\mathbf{p}_+) = (M_k\sigma)(\mathbf{p}) + \tfrac{1}{2}\sigma(\mathbf{p})$$

and

$$\lim_{\mathbf{p}_-\to\mathbf{p}} (M_k\sigma)(\mathbf{p}_-) = (M_k\sigma)(\mathbf{p}) - \tfrac{1}{2}\sigma(\mathbf{p}).$$

If we assume that $\mathbf{n}_p$ is defined not only on Γ but also in a neighbourhood of Γ as a smooth extension of $\mathbf{n}_p$, for $\mathbf{p} \in \Gamma$, we can define the derivative operators M_k^t and N_k also in a neighbourhood of Γ. It can be proved [20, 19] that

THEOREM 2. *If $\sigma \in \mathscr{C}^{0,\alpha}(\Gamma)$ then*

$$\lim_{\mathbf{p}_+\to\mathbf{p}} (M_k^t\sigma)(\mathbf{p}_+) = (M_k^t\sigma)(\mathbf{p}) - \tfrac{1}{2}\sigma(\mathbf{p})$$

and

$$\lim_{\mathbf{p}_-\to\mathbf{p}} (M_k^t\sigma)(\mathbf{p}_-) = (M_k^t\sigma)(\mathbf{p}) + \tfrac{1}{2}\sigma(\mathbf{p}).$$

Furthermore, if $\sigma \in \mathscr{C}^{1,\alpha}$ then

$$\lim_{\mathbf{p}_+\to\mathbf{p}} (N_k\sigma)(\mathbf{p}_+) = (N_k\sigma)(\mathbf{p}) = \lim_{\mathbf{p}_-\to\mathbf{p}} (N_k\sigma)(\mathbf{p}_-).$$

In Theorems 1 and 2, the values of the operators $(L_k\sigma)(\mathbf{p})$, $(M_k\sigma)(\mathbf{p})$, $(M_k^t\sigma)(\mathbf{p})$, and $(N_k\sigma)(\mathbf{p})$ are the so-called direct values of the integrals, obtained by putting $\mathbf{p} \in \Gamma$ in the definitions of the operators and evaluating them as improper integrals. For the direct values, the single layer operator has a logarithmic type singularity whilst the kernel of the double layer potential and its transpose are continuous. On the other hand, the operator N_k, the normal derivative of the double layer potential, is an integro-differential operator. It can be shown that

$$\frac{\partial^2 G_k}{\partial \mathbf{n}_p \partial \mathbf{n}_q}(\mathbf{p}, \mathbf{q}) = \mathcal{O}(|\mathbf{p} - \mathbf{q}|^{-2})$$

and, therefore, in the definition of N_k, if the derivative outside the integral sign is taken inside, the integrand is *hyper-singular* and the integral does not exist as an improper integral even in the sense of Cauchy and needs to be interpreted in the sense of Hadamard finite-part [23, 34, 33, 39, 12].

Clearly the operator N_k, unlike the other three, is not a smoothing one. It can be shown that (see, for example, [36])

$$(N_k\sigma)(\mathbf{p}) = -\frac{\partial}{\partial t_p} \oint_\Gamma \sigma(\mathbf{q}) \frac{\partial}{\partial t_q} G_k(\mathbf{p}, \mathbf{q})\, d\Gamma_q + k^2 \int_\Gamma \mathbf{n}_p \cdot \mathbf{n}_q \sigma(q) G_k(\mathbf{p}, \mathbf{q})\, d\Gamma_q, \tag{6}$$

where $\partial/\partial t_p$ and $\partial/\partial t_q$ represent the tangential derivatives at $\mathbf{p}$ and $\mathbf{q}$, respectively. The kernel of the first integral operator in (6), $(\partial/\partial t_q)G_k(\mathbf{p}, \mathbf{q})$, is of Cauchy singular type and therefore the N_k operator is essentially a first-order differentiation operator or a classical pseudo-differential operator of order $+1$. The concept of *pseudo-differential* operators was introduced in order to allow the study of differential and integral operators within the same algebras of operators [45, 41]. As we shall see shortly a unified treatment of all boundary integral equations arising here is possible within this framework.

An interesting result [40] often used in the regularisation of the hyper-singular operator is

$$(L_k N_k)\sigma(\mathbf{p}) = (-\tfrac{1}{4}I + M_k^2)\sigma(\mathbf{p}), \quad \mathbf{p} \in \Gamma, \tag{7}$$

which shows that the operator $-4N_k$ is the inverse of L_k to within a compact operator. As the eigenvalues of the compact operator M_k accumulate at zero, we refer to $-4N_k$ as the asymptotic spectral inverse of L_k. It is therefore possible to deduce much about the spectral properties of L_k or N_k from the knowledge of the other.

In the case where $k = 0$, the Helmholtz equation reduces to Laplace's equation with a *fundamental solution* $G(\mathbf{p}, \mathbf{q}) = -(1/2\pi)\ln(|\mathbf{p} - \mathbf{q}|)$. In this case the properties of the single and double layer potential operators and their respective normal derivatives are well established. Due to the smoothness of the function $G_k - G$, by writing $G_k = G + (G_k - G)$, it is easily shown that the essential properties of the Helmholtz operators are the same as those for the Laplacian operator [43]. These properties can be stated in terms of the classical Hölder spaces $\mathscr{C}^{r,\alpha}$ or, since we are interested in the variational solution of the problem, more naturally these may be stated in Sobolev spaces $H^r(\Gamma)$. In Section 3 we shall define these Sobolev spaces more fully. The following theorem states the essential properties of the four operators that we need in our analysis here [43, 48].

THEOREM 3. *If* $\Gamma \in \mathscr{C}^\infty$ *then the pseudo-differential operators* L_k, M_k, $M_k^t : H^r(\Gamma) \to H^{r+1}(\Gamma)$ *and* $N_k : H^{r+1}(\Gamma) \to H^r(\Gamma)$ *are continuous bijective mappings.*

2.1. The Interior Problem

At this stage it is advantageous to consider boundary integral formulations of the Helmholtz equation in the interior domain, as these are closely related to those for the exterior domain. Application of Green's second theorem using the $\mathscr{C}^2$ functions φ and $G_k(\mathbf{p}, \cdot)$ over D_- yields the solution to the Helmholtz equation in the interior domain in the form

$$\varphi(\mathbf{p}) = -(M_k\varphi)(\mathbf{p}) + \left(L_k \frac{\partial\varphi}{\partial n}\right)(\mathbf{p}), \quad \mathbf{p} \in D_-, \tag{8}$$

which is referred to as the *Helmholtz integral representation*. In (8), we require the pair of Cauchy data $\varphi(\mathbf{p})$ and $(\partial\varphi/\partial n)(\mathbf{p})$ for $\mathbf{p} \in \Gamma$. The boundary condition (2) provides φ or $\partial\varphi/\partial n$ or in the case of spring-like scatterers a relationship between the two. We need another relationship between the two parts of the Cauchy data to solve for them simultaneously with (2). In boundary integral equations this second relationship is obtained by taking the limit in Eq. (8) as $\mathbf{p} \in D_- \to \Gamma$. Using the jump properties of the single and double layer operators (Theorem 1) we obtain

$$\varphi(\mathbf{p}) = -(M_k\varphi)(\mathbf{p}) + \tfrac{1}{2}\varphi(\mathbf{p}) + \left(L_k \frac{\partial\varphi}{\partial n}\right)(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{9}$$

We may write the above equation in the form

$$(\tfrac{1}{2}I + M_k)\varphi(\mathbf{p}) = \left(L_k \frac{\partial\varphi}{\partial n}\right)(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{10}$$

Equation (9) or (10) is known as the *surface Helmholtz equation* for the interior problem. This is the boundary integral equation which should be solved, together with the boundary condition (2), to yield the Cauchy data required in (8). On differentiating (8) along $\mathbf{n}_p$, the outward normal at $\mathbf{p}$ and using the jump conditions in Theorem 2 we obtain another relationship between the Cauchy data, referred to as the *differentiated surface Helmholtz equation*, in the form

$$(N_k\varphi)(\mathbf{p}) = (-\tfrac{1}{2}I + M_k^t)\frac{\partial\varphi}{\partial n}(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{11}$$

It is well known that for any given closed boundary Γ, the interior Helmholtz equation fails to have a unique solution at a countable set of wavenumbers. To be precise we have the following.

THEOREM 4. *The interior Helmholtz (eigenvalue) problem*

$$\nabla^2\varphi(\mathbf{p}) + k^2\varphi(\mathbf{p}) = 0, \quad \mathbf{p} \in D_-,$$

with the homogeneous Dirichlet boundary condition ($\varphi(\mathbf{p}) \equiv 0$, $\mathbf{p} \in \Gamma$) *has non-trivial solutions, provided* $k \in I_{D,\Gamma}$, *where* $I_{D,\Gamma}$ *is a countable set of positive real values. Similarly, the interior Helmholtz equation with a homogeneous Neumann* *boundary condition has non-trivial solutions if* $k \in I_{N,\Gamma}$, *where* $I_{N,\Gamma}$ *is a countable set of real positive values.*

The values of k in these two sets can easily be seen from (10) and (11) to be related to the singularities of certain BIE as follows.

THEOREM 5. $I_{D,\Gamma}$ *is precisely the set of values of k for which the operators* L_k *and* $-\frac{1}{2}I + M_k^t$ *are singular. Also* $k \in I_{N,\Gamma}$ iff *the operators* $\frac{1}{2}I + M_k$ *and* N_k *are singular.*

2.2. The Exterior Problem

We are now able to discuss the boundary integral equations for the Helmholtz equation in the exterior domain. Similar to the interior problem, a careful application of the Green's second theorem, this time over the unbounded domain D_+ yields the solution to the exterior problem in the form of the *Helmholtz integral representation formula*,

$$\varphi(\mathbf{p}) = (M_k\varphi)(\mathbf{p}) - \left(L_k \frac{\partial\varphi}{\partial n}\right)(\mathbf{p}), \quad \mathbf{p} \in D_+. \tag{12}$$

To obtain a relationship between $\varphi(\mathbf{p})$ and $(\partial\varphi/\partial n)(\mathbf{p})$ for $\mathbf{p} \in \Gamma$, we take the limit as $\mathbf{p} \in D_+ \to \Gamma$. Using the jump properties in Theorem 1, this yields

$$(-\tfrac{1}{2}I + M_k)\varphi(\mathbf{p}) = \left(L_k \frac{\partial\varphi}{\partial n}\right)(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{13}$$

Similar to the derivation of (11) we obtain from (12)

$$(N_k\varphi)(\mathbf{p}) = (\tfrac{1}{2}I + M_k^t)\frac{\partial\varphi}{\partial n}(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{14}$$

The above two boundary integral equations (13) and (14), are referred to as the *direct elementary formulations* for the exterior problem. We can now prove the following nonuniqueness results about these elementary formulations.

THEOREM 6. • *If* $k \in I_{D,\Gamma}$ *then the boundary integral equation* (13) *fails to yield a unique relationship between* φ *and* $\partial\varphi/\partial n$.

• *If* $k \in I_{N,\Gamma}$ *then* (14) *fails to provide a unique relationship between* φ *and* $\partial\varphi/\partial n$.

Proof. The results follow from Theorem 5. We need only to remember that the eigenvalues of transposed operators such as M_k and M_k^t are the same.

Similar boundary integral equations referred to as *indirect boundary integral equations* are obtained if we assume a representation for the solution to the problem (1)–(3) in terms of single or double layer potentials. As a way of an example we may write the solution to (1)–(3), in the case of a Neumann boundary condition, in the form

$$\varphi(\mathbf{p}) = (L_k\sigma)(\mathbf{p}), \quad \mathbf{p} \in D_+, \tag{15}$$

where $\sigma(\mathbf{p})$ for $\mathbf{p} \in \Gamma$ is an as yet unknown density function belonging to the Hölder space $\mathscr{C}^{0,\alpha}_{(\Gamma)}$. Clearly for any σ, the function $L_k\sigma$ is a *radiating wave function*, i.e., a solution of (1) and (3). To ensure that this solution also satisfies a Neumann boundary condition such as $(\partial\varphi/\partial n)(\mathbf{p}) = f(\mathbf{p})$, we differentiate (15) along $\mathbf{n}_p$ in the neighbourhood of Γ and take the limit as $\mathbf{p} \to \Gamma$ and use the jump conditions in Theorem 2, to obtain

$$(-\tfrac{1}{2}I + M_k^t)\sigma(\mathbf{p}) = f(\mathbf{p}), \quad \mathbf{p} \in \Gamma. \tag{16}$$

Once σ is found from (16), we use it in (15) to obtain φ in D_+. The indirect boundary integral equation (16) should be compared with its direct counterpart (13). The indirect counterpart of (14) can be found if in (15) we represent φ, instead of a single layer with unknown density as a double layer with unknown density. In this paper we concentrate mainly on the direct formulations but similar results can be deduced trivially for the indirect ones.

Many alternative boundary integral equations have been suggested in order to avoid the problems with the direct and indirect elementary formulations at characteristic wavenumbers, notably [44, 11, 35, 40, 15, 27, 47]. An example of these modified formulations is the direct boundary integral equation due to Burton and Miller [15],

$$\begin{aligned}\{(-\tfrac{1}{2}I + M_k) + i\eta N_k\}\varphi(\mathbf{p}) \\ = \{L_k + i\eta(\tfrac{1}{2}I + M_k^t)\}\left(\frac{\partial\varphi}{\partial n}\right)(\mathbf{p}), \quad \mathbf{p} \in \Gamma,\end{aligned} \tag{17}$$

which is obtained by coupling (13) and (14). Equation (17) has a unique solution, provided the real coupling parameter η is non-zero for real values of k. For reviews of these methods the reader is referred to [14, 29, 5].

The elementary methods have the advantages of being easier to implement and are computationally less expensive than the alternative methods. Reports on results of implementations of the elementary methods first appeared in the 1960s: Banaugh and Goldsmith [10], Chen and Schweikert [17], Chertock [18], and Brundrit [13]. All but the last of these references seem to have been unaware of the potential difficulties with these methods at $k \in I_{D,\Gamma} \cup I_{N,\Gamma}$. The computational performance of elementary methods is compared with various alternative methods in Schenck [44], Meyer *et al.* [37], and Sayhi *et al.* [42], for example. Because of the perceived computational difficulties at or near these characteristic wavenumbers, research has generally moved away from the elementary methods to the alternative methods, although fairly recent articles (e.g., Hall and Robertson [24]) still advocate the use of elementary methods.

The purpose of this paper is to present a formal analysis and appraisal of the elementary methods. Much of our results can also be used for the investigation of the uniquely solvable nonelementary formulations such as Burton and Miller [15] or Brakhage and Werner [11], or [35, 40, 27, 47].

3. ANALYSIS OF COLLOCATION METHODS

Collocation methods are perhaps the most popular discretisation techniques for the solution of boundary integral equations. We are interested in the solution of the elementary boundary integral equations (13) and (14). As an equation for φ, (13) is a second kind Fredholm type, whilst (14) is a *hyper-singular* or integro-differential type. On the other hand, as an equation for $\partial\varphi/\partial n$, (13) is a first kind Fredholm type, whilst (14) is a second kind Fredholm type. In the classical analysis of numerical methods for integral equations in the continuous or square integrable spaces, it is the *compactness* of the integral operator which is often exploited. The analysis of projection methods for smooth boundary integral equations of the second kind follows from [8]. In the case of the first kind equations the reader is referred to [22] and references therein. The numerical analysis of the hyper-singular integral equation (14) has received very little attention in the classical subspaces of continuous functions.

In appropriate Sobolev space setting, the numerical analysis of the above equations can be carried out in a unified manner [6, 7, 43], as all the operators involved can be shown to be examples of *strongly elliptic* pseudo-differential operators. *Strong ellipticity* is essentially equivalent to the positivity of the principal symbol of the operator (see [48] and references therein) and from which the Gärding inequality follows, a result which is essential in establishing the stability of projection type solutions.

Let us consider

$$\mathscr{A}\phi = \mathscr{F}, \tag{18}$$

where $\mathscr{A}: H^r(\Gamma) \rightarrow H^{r-2\beta}(\Gamma)$ is a strongly elliptic operator of order 2β. It follows from Theorem 3, that for the first kind equation with L_k as the operator we have $\beta = -\frac{1}{2}$, for the second kind equations $\beta = 0$ and for the hyper-singular equation $\beta = +\frac{1}{2}$.

If we assume a global 2π periodic mapping from Γ to $[0, 2\pi]$, the Sobolev space of $H^r(\Gamma)$ is equivalent to the space of 2π periodic distributions, $H^r[0, 2\pi]$, which can be elegantly defined in terms of Fourier coefficients as follows [31]:

Let $\phi \in \mathscr{L}^2[0, 2\pi]$ be a 2π periodic function with the Fourier expansion

$$\phi(t) = \frac{1}{\sqrt{2\pi}} \sum_{m=-\infty}^{\infty} \hat{\phi}_m e^{imt},$$

where

$$\hat{\phi}_m = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \phi(t) e^{-imt}\, dt$$

are the Fourier coefficients. For any $r \in (0, \infty)$ the Sobolev space $H^r[0, 2\pi]$ is the subspace of the 2π periodic distributions in $\mathscr{L}^2[0, 2\pi]$ such that

$$\|\phi\|_{H^r}^2 = \sum_{m=-\infty}^{\infty} (1 + m^2)^r |\hat{\phi}_m|^2 < \infty. \tag{19}$$

Here we will state a generic result on the convergence of the collocation methods, the proof of which is given in [7]. Other generalisation of this result is possible for a wider class of approximation spaces.

Following [7], to define our collocation solution for the boundary integral equations, we denote by $\mathscr{S}_h^d$ the space of periodic smoothest splines of degree d, that is, piecewise polynomials of degree d which are subsets of $\mathscr{C}^{d-1}$ space. For the moment we assume that the meshes are uniform, with $\mathscr{S}_h^d$ having dimension $n = 2\pi/h$. The collocation approximation to (18) may be written as an interpolatory projection in the form

$$\mathscr{P}_h \mathscr{A} \phi_h = \mathscr{P}_h \mathscr{F}, \tag{20}$$

where

$$\phi_h(\mathbf{p}) = \sum_{i=1}^{n} a_i \psi_i(\mathbf{p}) \tag{21}$$

with $\mathscr{S}_h^d = \text{span}\{\psi_1, \psi_2, ..., \psi_n\}$. Equivalently we may write (20) as

$$(\mathscr{A}\phi_h)(p_i) = \mathscr{F}(p_i), \quad i = 1, 2, ..., n, \tag{22}$$

where for odd values of d we choose the collocation points as $p_i = (i - 1)h$ and for even values of d we choose $p_i = (i - \frac{1}{2})h$ with $h = 2\pi/n$.

THEOREM 7. *Let d be either a positive odd integer exceeding 2β or a nonnegative even integer exceeding $2\beta - \frac{1}{2}$. Then there exist $h_0 > 0$ such that for $0 < h \leq h_0$ and any continuous function $\mathscr{F}$ the collocation equations* (22) *are uniquely solvable for ϕ_h and if $s, t \in \mathbb{R}$ satisfy*

$$2\beta \leq s \leq t \leq d + 1, \quad s < d + \tfrac{1}{2}, \quad 2\beta + \tfrac{1}{2} < t,$$

and the solution ϕ of (18) is in H^t, then there holds the optimal error estimate

$$\|\phi - \phi_h\|_{H^s} \leq Ch^{t-s} \|\phi\|_{H^t}. \tag{23}$$

For practical problems the integrals over each element, the components of the boundary element equations, $(\mathscr{A}\psi_j)(p_i)$ need to be evaluated numerically. In this case in place of ϕ_h we obtain the discrete collocation solution $\hat{\phi}_h$, where

$$\hat{\phi}_h(\mathbf{p}) = \sum_{i=1}^{n} \hat{a}_i \psi_i(\mathbf{p}). \tag{24}$$

If we denote the $n \times n$ collocation matrix by $\mathscr{A}_n$ and the discrete collocation matrix, i.e., including quadrature errors, by $\hat{\mathscr{A}}_n$, the boundary element equations and the discrete boundary element equations are

$$\mathscr{A}_n \mathbf{a}_n = \mathscr{F}_n \quad \text{and} \quad \hat{\mathscr{A}}_n \hat{\mathbf{a}}_n = \mathscr{F}\Im m \mathscr{F}_n. \tag{25}$$

Using the triangular inequality, for the actual error, we have

$$\|\phi - \hat{\phi}_h\|_{H^s} \le \|\phi - \phi_h\|_{H^s} + \|\phi_h - \hat{\phi}_h\|_{H^s}. \tag{26}$$

The first part of the error-bound in (26), the *discretisation error*, is governed by (23). We refer to the second part as the *quadrature induced error*, although the error could arise from methods other than quadrature [28]. Briefly, we have

$$\begin{aligned} \|\phi_h - \hat{\phi}_h\|_{H^s} &= \left\| \sum_{i=1}^{n} (a_i - \hat{a}_i)\psi_i \right\|_{H^s} \\ &\le Ch^{-s} \left\| \sum_{i=1}^{n} (a_i - \hat{a}_i)\psi_i \right\|_{H^0} \qquad (27) \\ &\le Ch^{-s} \|a_n - \hat{a}_n\|_2 \sum_{i=1}^{n} \|\psi_i\|_{H^0} \le Ch^{-s-1/2} \|a_n - \hat{a}_n\|_2. \end{aligned}$$

The first inequality above follows from the *inverse property* [43] satisfied by our regular spline space which essentially allows us to bound, for functions in $\mathscr{S}_h^d$ "stronger norms" with "weaker norms." We have also used the fact that for spline basis functions $\sum \|\psi_i\|_{H^0} = \mathbb{O}(h^{-1/2})$. In practice it is difficult to measure the quadrature error accurately, as often some elements of the discrete collocation matrix are computed more accurately than others. However, we may assume that the maximum relative error in the quadrature approximation of any of the elements is $\mathbb{O}(h^l)$. From (25) we have [9, 21]

$$\frac{\|\hat{\mathbf{a}}_n - \mathbf{a}_n\|}{\|\mathbf{a}_n\|} \le \frac{\text{cond}(\mathscr{A}_n)}{1 - \gamma} \left\{ \frac{\|\mathscr{A}_n - \hat{\mathscr{A}}_n\|}{\|\mathscr{A}_n\|} + \frac{\|\mathscr{F}_n - \hat{\mathscr{F}}_n\|}{\|\mathscr{F}_n\|} \right\},$$

where $\gamma = \|\mathscr{A}_n - \hat{\mathscr{A}}_n\| \, \|\mathscr{A}_n^{-1}\| < 1$. We may deduce that

$$\|\mathbf{a}_n - \hat{\mathbf{a}}_n\| \le C \, \text{cond}(\mathscr{A}_n) h^l.$$

It can be shown [48, 6, 7, 43] that $\text{cond}(\mathscr{A}_n) = \mathbb{O}(h^{-2|\beta|})$ which, together with (27), leads to a bound for the quadrature induced error of the form

$$\|\phi_h - \hat{\phi}_h\|_{H^s} = \mathbb{O}(h^{l-s-1/2-2|\beta|}). \tag{28}$$

Therefore, provided the quadrature errors are sufficiently small, that is, l is sufficiently large, the error in the discrete collocation method is dominated by the collocation discretisation error (23) and it should remain $\mathbb{O}(h^{t-s})$. In our boundary integral equations the value of $2|\beta|$ is either 0 or 1 and, therefore, the condition number of the collocation matrix is only either $\mathbb{O}(1)$ or $\mathbb{O}(n)$.

4. SPECTRAL PROPERTIES OF THE HELMHOLTZ OPERATORS

In this section the properties of the Helmholtz integral operators will be studied. In particular we are seeking to obtain results on the conditioning of the operators in (13) and (14) as $k \to k^* \in I_{D,\Gamma} \cup I_{N,\Gamma}$. In order to carry out analytically such investigation we restrict ourselves to the case where Γ is a unit circle. In this case we can find the eigensystems of these operators exactly and use asymptotic expansions to estimate the condition number of the operators in appropriate Sobolev space setting. We are also able to investigate the conditioning of the resulting collocation matrices, the discrete counterpart of these operators.

If $\mathscr{A} : H^r \to H^{r-2\beta}$ then

$$\text{cond}(\mathscr{A}) = \|\mathscr{A}\|_{H^r \to H^{r-2\beta}} \|\mathscr{A}^{-1}\|_{H^{r-2\beta} \to H^r},$$

where

$$\|\mathscr{A}\|_{H^r \to H^{r-2\beta}} = \sup_m \frac{\|\mathscr{A}\Psi_m\|_{H^{r-2\beta}}}{\|\Psi_m\|_{H^r}},$$

provided $\{\Psi_m\}$ forms a complete set in H^r.

For the case of the periodic Sobolev spaces $H^r[0, 2\pi]$, the functions $\{\Psi_m = e^{im\theta}; m = 0, \pm 1, \pm 2, \ldots\}$ form a complete set, [31]. It follows from (19) that

$$\|\Psi_m\|_{H^r}^2 = (1 + m^2)^r.$$

We shall shortly show that in the case where Γ is a circle, the functions $\Psi_m = e^{im\theta}$ are the eigenfunctions of all four operators L_k, $M_k = M_k^t$ and N_k. In this case, with $\mathscr{A}$ representing any of these operators with $\mathscr{A}\Psi_m = \lambda_m \Psi_m$, it follows that

$$\begin{aligned} \|\mathscr{A}\|_{H^r \to H^{r-2\beta}} &= \sup_m \frac{|\lambda_m| \, \|\Psi_m\|_{H^{r-2\beta}}}{\|\Psi_m\|_{H^r}} \\ &= \sup_m \frac{|\lambda_m|}{(1 + m^2)^\beta} = \sup_m \mu_m = \mu_{\text{sup}}. \end{aligned} \tag{29}$$

Similarly we can find that

$$\|\mathscr{A}^{-1}\|_{H^{r-2\beta} \to H^r} = \sup_m \frac{1}{\mu_m} = \frac{1}{\inf_m \mu_m} = \frac{1}{\mu_{\text{inf}}},$$

from which it follows that

$$\text{cond}(\mathcal{A}) = \frac{\mu_{\text{sup}}}{\mu_{\text{inf}}}. \tag{30}$$

Let us now state a result giving the eigensystem of the Helmholtz operators, the proof of which may be found in [30]; see also [32, 2] for a similar result in three dimensions with Γ a unit sphere.

THEOREM 8. *For* $m = 0, 1, 2, \ldots,$

$$L_k e^{\pm im\theta} = \left\{\frac{i\pi}{2} J_m(k)H_m(k)\right\} e^{\pm im\theta} = \lambda_{L_{k,m}} e^{\pm im\theta}$$

$$M_k e^{\pm im\theta} = \left\{-\frac{1}{2} + \frac{i\pi}{2} kJ'_m(k)H_m(k)\right\} e^{\pm im\theta}$$

$$= \left\{\frac{1}{2} + \frac{i\pi}{2} kJ_m(k)H'_m(k)\right\} e^{\pm im\theta} = \lambda_{M_{k,m}} e^{\pm im\theta}$$

$$M_k^t e^{\pm im\theta} = M_k e^{\pm im\theta} = \lambda_{M_{k,m}} e^{\pm im\theta} = \lambda_{M_{k,m}^t} e^{\pm im\theta}$$

$$N_k e^{\pm im\theta} = \left\{\frac{i\pi}{2} k^2 J'_m(k)H'_m(k)\right\} e^{\pm im\theta} = \lambda_{N_{k,m}} e^{\pm im\theta},$$

where J_m *denotes the Bessel function of order m and* H_m *denotes the Hankel function of the first kind of order m. Note that in the above a prime (′) denotes the derivative with respect to k.*

The following results now follows from Theorems 5 and 8.

THEOREM 9. *If* Γ *is a unit circle then*

$$I_{\text{D},\Gamma} = \{k_{mj} | J_m(k_{mj}) = 0, m = 0, 1, 2, \ldots \textit{ and } k = 1, 2, \ldots\}$$

and

$$I_{\text{N},\Gamma} = \{k'_{mj} | J'_m(k'_{mj}) = 0, m = 0, 1, 2, \ldots \textit{ and } k = 1, 2, \ldots\}$$

The zeros of the integer order Bessel functions and their derivatives are listed in [1]. These form the values of the wave-number k at which the elementary boundary integral equations for the Helmholtz equation in the exterior domain such as (13) and (14) become singular when Γ is a unit circle. The number of elements in the sets $I_{\text{D},\Gamma}$ or $I_{\text{N},\Gamma}$ less than a given value of k grows rapidly as k increases [14]. For large real values of k, Eqs. (13) and (14) are in general ill-conditioned. We wish to investigate the precise conditioning of these boundary integral equations and their discrete counterparts, near and also away from these singularities.

4.1. Behaviour of High Order Eigenvalues

Let us now consider the asymptotic behaviour of the eigenvalues of the operators on either side of Eqs. (13) and (14). We use the asymptotic expansions given in Section 9.3.1 of [1]

$$J_m(k) \sim \frac{1}{\sqrt{2\pi m}}\left(\frac{ek}{2m}\right)^m, \tag{31}$$

$$Y_m(k) \sim -\sqrt{\frac{2}{\pi m}}\left(\frac{ek}{2m}\right)^{-m}, \tag{32}$$

where $Y_m(k)$ is a Bessel function of the second kind. Since $H_m(k) = J_m(k) + iY_m(k)$ it follows that

$$H_m(k) \sim -i\sqrt{\frac{2}{\pi m}}\left(\frac{ek}{2m}\right)^{-m}. \tag{33}$$

Differentiating (31) and (33) with respect to k gives

$$J'_m(k) \sim \frac{1}{\sqrt{2\pi m}}\, m\frac{e}{2m}\left(\frac{ek}{2m}\right)^{m-1} \sim \frac{m}{k} J_m(k), \tag{34}$$

$$H'_m(k) \sim -i\sqrt{\frac{2}{\pi m}}(-m)\frac{e}{2m}\left(\frac{ek}{2m}\right)^{-m-1} \sim -\frac{m}{k} H_m(k). \tag{35}$$

Let us denote by $\lambda_m(\mathcal{A})$, the eigenvalues of the operator $\mathcal{A}$. Using the above asymptotic expansions in Theorem 8, we can show that in the limit as $m \to \infty$,

$$\lambda_m(L_k) \approx \frac{1}{2m}, \tag{36}$$

$$\lambda_m\left(M_k - \frac{1}{2}I\right) = \lambda_m\left(M_k^t - \frac{1}{2}I\right) \approx -\frac{1}{2}, \tag{37}$$

$$\lambda_m\left(M_k + \frac{1}{2}I\right) = \lambda_m\left(M_k^t + \frac{1}{2}I\right) \approx +\frac{1}{2}, \tag{38}$$

$$\lambda_m(N_k) \approx -\frac{m}{2}. \tag{39}$$

We refer the interested reader to [3] for a more detailed asymptotic expansion of the eigenvalues of the operators obtained by using a series representation of J_m and Y_m. Note from (39) and (36) that for large m, $\lambda_m(L_k N_k) \approx -\frac{1}{4}$ as predicted by (7).

4.2. Eigenvalues near Characteristic Wavenumbers

Let k be sufficiently close to k_{lj}, the j-th zero of the l-th order Bessel function, J_l, for some $l \in \{0, 1, 2, \ldots\}$ and some $j \in \{1, 2, \ldots\}$. Then, from Theorem 8, $\lambda_l(L_k) = (i\pi/2)J_l(k)H_l(k)$ is the smallest eigenvalue of L_k. Similarly $\lambda_l(M_k - \frac{1}{2}I) = (i\pi/2)kJ_l(k)H'_l(k)$ is the smallest eigenvalue of $M_k - \frac{1}{2}I$. A Taylor series expansion about k_{lj} shows that they have the asymptotic form

$$\lambda_l(L_k) = i\frac{\pi}{2}H_l(k_{lj})J_l'(k_{lj})(k - k_{lj}) + \mathbb{O}((k - k_{lj})^2), \tag{40}$$

$$\lambda_l\left(M_k - \frac{1}{2}I\right) = i\frac{\pi}{2}k_{lj}H_l'(k_{lj})J_l'(k_{lj})(k - k_{lj}) + \mathbb{O}((k - k_{lj})^2). \tag{41}$$

Similarly, when k is sufficiently close to k_{lj}', the jth zero of J_l' then $\lambda_l(M_k + \frac{1}{2}I)$ is the smallest eigenvalue of $M_k + \frac{1}{2}I$ and $\lambda_l(N_k)$ is the smallest eigenvalue of N_k and they have the asymptotic form

$$\lambda_l\left(M_k + \frac{1}{2}I\right) = i\frac{\pi}{2}k_{lj}'H_l(k_{lj}')J_l''(k_{lj}')(k - k_{lj}') + \mathbb{O}((k - k_{lj}')^2), \tag{42}$$

$$\lambda_l(N_k) = i\frac{\pi}{2}k_{lj}'^2H_l'(k_{lj}')J_l''(k_{lj})(k - k_{lj}') + \mathbb{O}((k - k_{lj}')^2). \tag{43}$$

In all cases, therefore, the absolute value of the smallest eigenvalue behaves as $\mathbb{O}(d^{-1})$, where d is the distance of k from the appropriate singular sets $I_{\mathrm{D},\Gamma}$ or $I_{\mathrm{N},\Gamma}$.

4.3. Conditioning of the Operators

We are now in a position to look at the condition numbers of Eqs. (13) and (14). It follows from (29) that

$$\mu_m(L_k) = |\lambda_m(L_k)|\sqrt{m^2 + 1}, \tag{44}$$

$$\mu_m(M_k - \tfrac{1}{2}I) = \mu_m(M_k' - \tfrac{1}{2}I) = |\lambda_m(M_k - \tfrac{1}{2}I)| \tag{45}$$

$$\mu_m(M_k + \tfrac{1}{2}I) = \mu_m(M_k' + \tfrac{1}{2}I) = |\lambda_m(M_k - \tfrac{1}{2}I)| \tag{46}$$

$$\mu_m(N_k) = \frac{|\lambda_m(N_k)|}{\sqrt{m^2 + 1}}. \tag{47}$$

Substituting the results of (36)–(39) into the expressions above gives the following results as $m \to \infty$:

$$\mu_m(L_k) \approx \tfrac{1}{2}, \tag{48}$$

$$\mu_m(M_k - \tfrac{1}{2}I) = \mu_m(M_k' - \tfrac{1}{2}I) \approx \tfrac{1}{2}, \tag{49}$$

$$\mu_m(M_k + \tfrac{1}{2}I) = \mu_m(M_k' + \tfrac{1}{2}I) \approx \tfrac{1}{2}, \tag{50}$$

$$\mu_m(N_k) \approx \tfrac{1}{2}. \tag{51}$$

Therefore, the condition numbers of our operators are likely to be dominated, not by the high order eigenvalues as $m \to \infty$, but by their proximity to their respective characteristic wavenumbers. For Eq. (13), near to a characteristic wavenumber k_{lj}, it follows from (40), (41), (44), and (45) that

$$\mu_{\inf}(L_k) = \mu_l(L_k) = \frac{\pi}{2}\sqrt{l^2 + 1}\,|H_l(k_{lj})J_l'(k_{lj})|\,|k - k_{lj}| + |\mathbb{O}((k - k_{lj})^2)|, \tag{52}$$

$$\mu_{\inf}\left(M_k - \frac{1}{2}I\right) = \mu_l\left(M_k - \frac{1}{2}I\right) = \frac{\pi}{2}k_{lj}|H_l'(k_{lj})J_l'(k_{lj})|\,|k - k_{lj}| + |\mathbb{O}((k - k_{lj})^2)|. \tag{53}$$

Similarly, near the characteristic wavenumbers k_{lj}', it follows from (42), (43), (46), and (47) that

$$\mu_{\inf}\left(M_k + \frac{1}{2}I\right) = \mu_l\left(M_k + \frac{1}{2}I\right) = \frac{\pi}{2}k_{lj}'|H_l(k_{lj}')J_l''(k_{lj}')|\,|k - k_{lj}'| + |\mathbb{O}((k - k_{lj})^2)|, \tag{54}$$

$$\mu_{\inf}(N_k) = \mu_l(N_k) = \frac{\pi}{2}k_{lj}'^2\frac{|H_l'(k_{lj}')J_l''(k_{lj})|\,|k - k_{lj}'|}{\sqrt{l^2 + 1}} + |\mathbb{O}((k - k_{lj})^2)|. \tag{55}$$

Hence, near to the characteristic wavenumbers k_{lj}, the condition of the operators may be written in the form

$$\mathrm{cond}(L_k) \approx \frac{\mu_{\sup}(L_k)}{(\pi/2)\sqrt{l^2 + 1}\,|H_l(k_{lj})J_l'(k_{lj})|}\frac{1}{|k - k_{lj}|}, \tag{56}$$

$$\mathrm{cond}\left(M_k - \frac{1}{2}I\right) = \mathrm{cond}\left(M_k' - \frac{1}{2}I\right) \approx \frac{\mu_{\sup}(M_k - (1/2)I)}{(\pi/2)k_{lj}|H_l'(k_{lj})J_l'(k_{lj})|}\frac{1}{|k - k_{lj}|}, \tag{57}$$

and near to the characteristic wavenumbers k_{lj}', we have

$$\mathrm{cond}\left(M_k + \frac{1}{2}I\right) = \mathrm{cond}\left(M_k' + \frac{1}{2}I\right) \approx \frac{\mu_{\sup}(M_k + (1/2)I)}{(\pi/2)k_{lj}'|H_l(k_{lj}')J_l''(k_{lj}')|}\frac{1}{|k - k_{lj}'|}, \tag{58}$$

$$\mathrm{cond}(N_k) \approx \frac{\mu_{\sup}(N_k)\sqrt{l^2 + 1}}{(\pi/2)k_{lj}'^2|H_l'(k_{lj}')J_l''(k_{lj})|}\frac{1}{|k - k_{lj}'|}. \tag{59}$$

It can be seen that the condition number of all the operators involved behave as $\mathcal{O}(d^{-1})$, where d is the distance of k from the operators' singular set $I_{D,\Gamma}$ or $I_{N,\Gamma}$. We shall observe these numerically in Section 5.

4.4 Properties of the Boundary Element Matrices

In order to study the conditioning of the boundary element equations which are the discrete counterparts of the boundary integral operators, let us assume that we have a uniform discretisation of the boundary functions with N degrees of freedom. Let us assume that the resulting matrix representation of the operator approximates the n most fundamental eigenvalues of the continuous operators. Note that for a given N, the value of n will be different for the different matrices.

As a measure of the conditioning of the boundary element equations we use the ratio of the largest to smallest, in absolute value, of the eigenvalues of $\mathcal{A}_n$. That is,

$$\text{cond}_*(\mathcal{A}_n) = \frac{\lambda_{\max}(\mathcal{A}_n)}{\lambda_{\min}(\mathcal{A}_n)}. \tag{60}$$

This would be the 2-norm condition number of the matrix, if $\mathcal{A}_n$ was a *normal* matrix. However, for our collocation matrices the above will in general only be a good indication of the conditioning of the boundary element equations [9].

For our example of a circle, each eigenvalue λ_m of the continuous integral operator has two linearly independent eigenfunctions $e^{\pm im\theta}$, except for $m = 0$, where it has one. For N sufficiently large, we would expect their discrete counterparts to provide approximations to $\lambda_0, \lambda_1, \ldots, \lambda_{[N/2]}$, in which case $n = [N/2] + 1$.

In what follows we assume that our discretisation is sufficiently accurate (i.e., N/k is sufficiently large) so that the boundary element matrices can be expected to mimic appropriate spectral properties of the continuous operators. We denote the matrix approximation to a given operator with N degrees of freedom with a superscript $[N]$.

Recall that, $\lambda_m(L_k)$, the eigenvalues of L_k go to zero as $1/2m$ and therefore provided k is not very close to an element of $I_{D,\Gamma}$, we would expect

$$\lambda_{\min}(L_k^{[N]}) \approx \lambda_n(L_k). \tag{61}$$

On the other hand, if k is close to k_{lj} then L_k and hence $L_k^{[N]}$ will have a nearly zero eigenvalue of order $\mathcal{O}(|k - k_{lj}|^{-1})$. In general, therefore,

$$\lambda_{\min}(L_k^{[N]}) \approx \min\{\lambda_l(L_k), \lambda_n(L_k)\}. \tag{62}$$

As far as the minimum eigenvalues of the other boundary element matrices are concerned they can only be small if the value of k is close to a corresponding element of $I_{D,\Gamma}$ or $I_{N,\Gamma}$. Therefore if k is close to k_{lj} then

$$\lambda_{\min}(M_k^{[N]} - \tfrac{1}{2}I^{[N]}) \approx \lambda_l(M_k - \tfrac{1}{2}I) = \mathcal{O}(|k - k_{lj}|^{-1}). \tag{63}$$

Similarly, if k is close to k'_{lj}

$$\lambda_{\min}(M_k^{[N]} + \tfrac{1}{2}I^{[N]}) \approx \lambda_l(M_k + \tfrac{1}{2}I) = \mathcal{O}(|k - k'_{lj}|^{-1}) \tag{64}$$

and

$$\lambda_{\min}(N_k^{[N]}) \approx \lambda_l(N_k)\} = \mathcal{O}(|k - k'_{lj}|^{-1}). \tag{65}$$

The maximum eigenvalues of the matrices $L_k^{[N]}, M_k^{[N]} - \frac{1}{2}I$ and $M_k^{[N]} + \frac{1}{2}I$ are $\mathcal{O}(1)$ and rapidly convergent as $N \to \infty$. However, the maximum eigenvalue of the hyper-singular operator N_k is not bounded. We have

$$\lambda_{\max}(N_k^{[N]}) \approx \lambda_n(N_k) = \mathcal{O}(N). \tag{66}$$

It now follows from (60)–(66) that the condition numbers of $M_k^{[N]} - \frac{1}{2}I^{[N]}$ and $M_k^{[N]} + \frac{1}{2}I^{[N]}$ behave as $\mathcal{O}(d^{-1})$, where d is the distance of k from the set $I_{D,\Gamma}$ or the set $I_{N,\Gamma}$, respectively. For the matrix $L_k^{[N]}$, because of (62), its condition number behaves as $\mathcal{O}(d^{-1})$, for a fixed N as $d \to 0$, whilst for k fixed it behaves as $\mathcal{O}(N)$ as $N \to \infty$ (see Table II in Section 5). For the hyper-singular operator, it can be seen from (65) and (66) that the condition number of the matrix $N_k^{[N]}$ behaves as $\mathcal{O}(Nd^{-1})$, where d is the distance of k from $I_{N,\Gamma}$.

5. NUMERICAL EXPERIMENTS

In this section the results of the analysis in the previous sections are illustrated through applying the boundary element method to radiation and scattering problems from a unit circle. The boundary element method is derived through dividing the boundary into N uniform elements and approximating the boundary functions by a constant on each element.

5.1. Conditioning of the Boundary Element Equations

Properties of the boundary element matrices are considered at three nearby wavenumbers, $k = 6.00000$, $k = 6.38016 \in I_{D,\Gamma}$, $k = 6.70613 \in I_{N,\Gamma}$ (to six significant figures). In all cases, the eigenvalues are computed using routine F02AKF from the NAG library [38].

Let the approximations based on the formulation (13) be identified by SHE, the surface Helmholtz equation, and those based on the differentiated surface Helmholtz equation (14) be identified by DSHE. Therefore we identify by SHE-Dirichlet, the solution of the Dirchlet problem, using the formulation (13), yielding a first kind boundary integral equation for $\partial\varphi/\partial n$ and so on.

5.1.1. *Eigenvalues at a Non-characteristic Wavenumber*

For ease of notation, from now on, we shall drop the superscript $[N]$ when referring to the $N \times N$ matrix approximation

TABLE I

Properties of Matrices, $k = 6.0$

Matrix	N	$\lvert\lambda_{max}\rvert$	$\lvert\lambda_{min}\rvert$	Condition number
L_k	64	0.23220	0.01858	12.49862
	128	0.23389	0.00915	25.54818
	156	0.23432	0.00456	51.37426
	512	0.23443	0.00228	102.88801
$M_k - \frac{1}{2}I$	64	0.97517	0.33166	2.94026
or	128	0.97770	0.33227	2.94251
$M_k^t - \frac{1}{2}I$	256	0.97833	0.33242	2.94306
	512	0.97849	0.33246	2.94320
$M_k + \frac{1}{2}I$	64	0.98219	0.21746	4.51669
or	128	0.98358	0.21725	4.52735
$M_k^t + \frac{1}{2}I$	256	0.98392	0.21721	4.52986
	512	0.98401	0.21720	4.53047
N_k	64	9.85444	0.83729	11.76938
	128	20.20744	0.84629	23.87757
	256	40.66163	0.84820	47.93867
	512	81.44633	0.84863	95.97376

of an operator. In Table I the modulus of the largest and the smallest eigenvalues of the matrices L_k, $M_k - \frac{1}{2}I\ (=M_k^t - \frac{1}{2}I)$, $M_k + \frac{1}{2}I\ (=M_k^t + \frac{1}{2}I)$, and N_k are given for $k = 6.00000$ and with 64, 128, 256, and 512 elements. The matrix condition number, as defined by (60), which is simply the modulus of the maximum divided by the minimum eigenvalue, is also listed.

The results confirm the analysis of Section 4. The minimum and maximum eigenvalues and hence the condition number of the matrices $M_k - \frac{1}{2}I$ and $M_k^t - \frac{1}{2}I$ converge to a finite value as $N \to \infty$. For the matrix L_k, however, the maximum eigenvalue converges but the minimum eigenvalue behaves as $\mathcal{O}(1/N)$ as $N \to \infty$. For the matrix N_k, the minimum eigenvalue converges as $N \to \infty$ but the maximum eigenvalue behaves as $\mathcal{O}(N)$. The condition numbers of the matrices $M_k - \frac{1}{2}I$ and $M_k + \frac{1}{2}I$ mimic those of their respective boundary operators but the condition number of the matrices L_k and N_k are $\mathcal{O}(N)$.

TABLE II

Condition Numbers of L_k, $k \approx k^* = 6.38016$

$N\downarrow/k\to$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	2.31(1)	9.44(1)	4.10(2)	3.60(3)	3.34(2)	8.98(1)	2.29(1)
128	2.49(1)	9.27(1)	3.74(2)	3.03(4)	3.66(2)	9.23(1)	2.45(1)
256	5.01(1)	9.26(1)	3.71(2)	3.38(5)	3.70(2)	9.26(1)	4.92(1)
512	1.00(2)	9.98(1)	3.70(2)	1.29(6)	3.71(2)	9.93(1)	9.86(1)
$N\downarrow/k\to$	$k^*-\frac{i}{16}$	$k^*-\frac{i}{64}$	$k^*-\frac{i}{256}$	k^*	$k^*+\frac{i}{256}$	$k^*+\frac{i}{64}$	$k^*+\frac{i}{16}$
64	2.27(1)	9.17(1)	3.66(2)	3.60(3)	3.67(2)	9.24(1)	2.33(1)
128	2.58(1)	9.22(1)	3.70(2)	3.03(4)	3.70(2)	9.28(1)	2.37(1)
256	5.19(1)	9.23(1)	3.70(2)	3.38(5)	3.71(2)	9.29(1)	4.77(1)
512	1.00(2)	9.98(1)	3.70(2)	1.29(6)	3.71(2)	9.85(1)	9.56(1)

TABLE III

Condition Numbers of $M_k - \frac{1}{2}I$ or $M_k^t - \frac{1}{2}I$, $k \approx k^* = 6.38016$

$N\downarrow/k\to$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	1.76(1)	7.10(1)	2.63(2)	5.49(2)	2.41(2)	6.94(1)	1.77(1)
128	1.76(1)	7.10(1)	2.85(2)	2.20(3)	2.78(2)	7.08(1)	1.79(1)
256	1.76(1)	7.09(1)	2.85(2)	8.82(3)	2.83(2)	7.11(1)	1.79(1)
512	1.76(1)	7.09(1)	2.84(2)	3.54(4)	2.84(2)	7.11(1)	1.79(1)
$N\downarrow/k\to$	$k^*-\frac{i}{16}$	$k^*-\frac{i}{64}$	$k^*-\frac{i}{256}$	k^*	$k^*+\frac{i}{256}$	$k^*+\frac{i}{64}$	$k^*+\frac{i}{16}$
64	1.76(1)	7.10(1)	2.63(2)	5.49(2)	1.87(2)	6.31(1)	1.75(1)
128	1.76(1)	7.10(1)	2.85(2)	2.20(3)	2.51(2)	6.91(1)	1.80(1)
256	1.76(1)	7.09(1)	2.85(2)	8.82(3)	2.76(2)	7.08(1)	1.81(1)
512	1.76(1)	7.09(1)	2.84(2)	3.54(4)	2.84(2)	7.12(1)	1.81(1)

5.1.2. *Condition of Matrices near a Characteristic Wavenumber*

Tables II and III list the condition number of the matrices L_k and $M_k - \frac{1}{2}I\ (=M_k^t - \frac{1}{2}I)$ near a characteristic wavenumber of their respective continuous operators. Results are given for $k = 6.38016 \pm \delta$ and $k = 6.38016 \pm i\delta$ for $\delta = \frac{1}{16}, \frac{1}{64}, \frac{1}{256}$. The value $k^* = 6.38016$ is the first zero of $J_3(k)$, correct to six significant figures. Also, Tables IV and V list the condition number of the matrices $M_k + \frac{1}{2}I\ (=M_k^t + \frac{1}{2}I)$ and N_k near a characteristic wavenumber of their respective continuous operators. Results are given for $k = 6.70613 \pm \delta$ for $\delta = \frac{1}{16}, \frac{1}{64}, \frac{1}{256}$. The value $k^* = 6.70613$ is the second zero of $J_2'(k)$, correct to six significant figures. The results for $k = 6.70613 \pm i\delta$ are not given as these are almost identical to those for $k = 6.70613 \pm \delta$.

Several observations can be made from the tables. At the characteristic wavenumbers of the operators the condition number of their corresponding matrix approximations grows rapidly as $N \to \infty$.

For the L_k matrix in Table II, as discussed in Section 4.4, in

TABLE IV

Condition Numbers of $M_k + \frac{1}{2}I$ or $M_k^t + \frac{1}{2}I$, $k \approx k^* = 6.70613$

$N\downarrow/k\to$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	1.62(1)	6.54(1)	2.53(2)	1.21(3)	2.63(2)	6.65(1)	1.67(1)
128	1.63(1)	6.57(1)	2.62(2)	4.86(3)	2.65(2)	6.63(1)	1.67(1)
256	1.63(1)	6.57(1)	2.63(2)	1.93(4)	2.65(2)	6.63(1)	1.67(1)
512	1.63(1)	6.58(1)	2.63(2)	7.42(4)	2.65(2)	6.62(1)	1.67(1)

TABLE V

Condition Numbers of N_k, $k \approx k^* = 6.70613$

$N\downarrow/k\rightarrow$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	2.60(1)	1.03(2)	4.19(2)	1.97(4)	4.01(2)	1.02(2)	2.53(1)
128	5.34(1)	2.12(2)	8.46(2)	4.35(6)	8.45(2)	2.11(2)	5.23(2)
256	1.08(2)	4.27(2)	1.70(3)	1.11(6)	1.70(3)	4.25(2)	1.05(2)
512	2.16(2)	8.55(2)	3.41(3)	2.57(6)	3.41(3)	8.51(2)	2.11(2)

general the eigenvalues will tend towards zero as c/N. Near a characteristic wavenumber, the modulus of the smallest eigenvalue of the matrix L_k behaves as $\min\{c_1|k-k^*|, c_2/N\}$. Therefore the condition number L_k behaves as $\max\{d_1/|k-k^*|, d_2N\}$. Looking along the first column of Table II for the case $k = k^* - \frac{1}{16}$ we note that the doubling of the condition number occurs for $N > 128$, where it is dominated by d_2N with $d_2 \approx 0.2$. The first two numbers in that column and results in columns for $k = k^* - \frac{1}{64}$ and $k = k^* - \frac{1}{256}$ show that there the condition number is dominated by $d_1/|k-k^*|$ with the value of $d_1 \approx 1.5$.

For the matrices $M_k - \frac{1}{2}I$ and $M_k + \frac{1}{2}I$ in Tables III and IV, the smallest eigenvalues behave as $\mathcal{O}(|k-k^*|)$ and hence their condition numbers behave as $\mathcal{O}(1/|k-k^*|)$, remaining stable along each column but increasing as $k \rightarrow k^*$.

For the N_k matrix, its smallest eigenvalue behaves as $\mathcal{O}_1(|k-k^*|)$ and its largest eigenvalue as $\mathcal{O}_2(N)$ and therefore its condition number behaves as $\mathcal{O}(N/|k-k^*|)$. Moving down along each column in Table V we observe the doubling of the condition number and along each row the condition numbers increase by a factor of 4, in accordance with $1/|k-k^*|$.

These observations and results are valid for k varying along the real axis and into the complex plane.

5.2. Error in Solution

For the purpose of comparison with numerical solution, exact solutions can be generated for any boundary, for fields which are produced by point sources [25, 4]. Here we assume the boundary condition on the unit circle $x^2 + y^2 = 1$ produced by placing one point source at $\mathbf{p}_0 = (x_0, y_0) = (0, 0.5)$ with unit strength. The field generated by this point source is

$$\varphi(\mathbf{p}) = \frac{i}{4} H_0^{(1)}(k|\mathbf{p} - \mathbf{p}_0|), \quad \mathbf{p} \in \mathbb{R}^2. \tag{67}$$

The Dirichlet boundary condition generating the above field (67) for $\mathbf{p} \in D_+$ is obtained by choosing $\mathbf{p} \in \Gamma$ in (67). We obtain the Neumann boundary condition from (67) using $(\partial\varphi/\partial n)(\mathbf{p}) = \nabla\varphi \cdot \mathbf{n}_p$.

In this section we study the error in the numerical solution of Eqs. (13) and (14) for both the Dirichlet and the Neumann boundary conditions. In the tables we refer to these as SHE-Dirichlet, SHE-Neumann, DSHE-Dirichlet, and DSHE-Neumann. The measure of error that we use is the relative mean error (RME),

$$\text{RME}(\mathbf{f}) = \frac{\sum_{j=1}^{N} |f_i - \hat{f}_i|}{\sum_{j=1}^{N} |f_i|},$$

where $\hat{\mathbf{f}}$ is the numerical approximation to $\mathbf{f}$.

The numerical error is observed both for the *theoretical collocation method*, that is, when the collocation matrices are exactly (or very accurately) represented and also for the *discrete collocation method*, where the collocation matrices are obtained using quadrature rules.

TABLE VI

Log_2 RME in Solution

k	N	SHE-Dirichlet	DSHE-Dirichlet	SHE-Neumann	DSHE-Neumann
6.00000	64	−8.76	−8.98	−8.66	−8.65
	128	−10.77	−11.01	−10.66	−10.70
	256	−12.77	−13.02	−12.66	−12.72
	512	−14.77	−15.03	−14.66	−14.73
6.38016	64	1.13	−6.04	−1.14	−5.41
	128	2.18	−7.99	−1.15	−7.51
	256	3.66	−9.99	−1.14	−9.54
	512	3.59	−12.00	−1.14	−11.55
6.70613	64	−8.29	−0.67	−8.22	2.68
	128	−10.31	−0.69	−10.23	7.41
	256	−12.30	−0.70	−12.23	2.42
	512	−14.30	−0.76	−14.23	0.63

TABLE VII

Log_2 RME in SHE-Dirichlet, $k \approx k^* = 6.38016$

$N\downarrow / k\rightarrow$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	−6.17	−4.13	−2.01	1.13	−2.30	−4.20	−6.15
128	−8.19	−6.17	−4.16	2.18	−4.19	−6.17	−8.15
256	−10.19	−8.18	−6.17	3.66	−6.17	−8.16	−10.14
512	−12.19	−10.17	−8.17	3.59	−8.17	−10.16	−12.14

TABLE IX

Log_2 RME in DSHE-Dirichlet, $k \approx k^* = 6.70613$

$N\downarrow / k\rightarrow$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	−6.76	−4.87	−2.92	−0.67	−2.88	−4.87	−6.85
128	−8.78	−6.88	−4.89	−0.69	−4.88	−6.89	−8.87
256	−10.79	−8.88	−6.89	−0.70	−6.89	−8.90	−10.87
512	−12.78	−10.88	−8.89	−0.76	−8.89	−10.89	−12.87

5.2.1. *Results for Exact Matrices*

Table VI gives the RME for $N = 64, 128, 256$, and 512 for each of the surface Helmholtz equation, SHE-method (Eq. (13)) and the differentiated surface Helmholtz equation, DSHE-method (Eq. (14)) for the wavenumbers $k = 6.00000$, $k = 6.38016$, and $k = 6.70613$, with Dirichlet and Neumann boundary conditions.

The results in Table VI demonstrate the extremes in the results that arise from using the elementary methods. Away from their respective characteristic wavenumbers the methods converge at a rate proportional to $1/N^2$, demonstrating superconvergence of the collocation method at collocation points. However, at their respective characteristic wavenumbers no convergence is observed.

In Tables VII–X we explore the error in the methods close to the characteristic wavenumbers of the boundary integral equations. These results may be looked at in conjunction with Tables II–V for the condition number of the appropriate matrices.

The results in Tables VII–X show that for any given fixed number of elements the mean relative error is approximately proportional to $1/|k - k^*|$ for k varying along the real axis and into the complex plane, as in Tables II–V. This is due to the fact that the condition number of the relevant boundary integral operators behaves as $\mathcal{O}(1/|k - k^*|)$. Along each column we observe the $\mathcal{O}(N^{-2})$ convergence. The increase in the condition number of the matrices L_k and N_k as shown in Tables II and V, with increase in N, plays no role in the asymptotic behaviour of the collocation solution as one would expect from (22). In all cases, for a fixed value of k, the condition number of matrices for large N behaves as $\mathcal{O}(N^{2|\beta|})$, where 2β is the order of the underlying pseudo-differential operator. Recall that for L_k and N_k, the value of 2β equals -1 and $+1$, respectively, whilst for $\pm\frac{1}{2}I + M_k$ the value of 2β is zero. We shall see in the next section that the condition number of boundary element matrices play an important role in the case of the *discrete collocation methods*.

5.2.2. *Results for Approximate Matrices*

In order to study the effect of the quadrature error on the accuracy of the discrete collocation solution, a deliberate error is introduced into the elements of the boundary element matrices L_k, M_k, M_k^t, and N_k to give $\hat{L}_k$, $\hat{M}_k$, $\hat{M}_k^t$, and $\hat{N}_k$. The approximations are defined so that

$$[\hat{L}_k]_{ij} = \left(1 + \frac{(-1)^{i+j}}{256}\right)[L_k]_{ij}, \tag{68}$$

and similarly for the other matrices. The inclusion of an error of the form (68) simulates and structures the error that may be present in the computation of the matrices. In a discrete collocation method one would like to ensure that all the elements of the matrices have errors of similar size which are less than a prescribed value, $\varepsilon(N)$, say. Ideally $\varepsilon(N)$ should be chosen such that the *quadrature induced error* in the solution *is of the same size as the discretisation error,* $\delta(N)$.

Here by fixing $\varepsilon(N)$ at 2^{-8}, as N is increased we are able to study cases where the integration error is small, about the same and also large, compared to the discretisation error. The results are given in Tables XI–XIV. It is interesting and instructive to study these results alongside Tables II–V, on the condition number of the corresponding matrices and also alongside Tables

TABLE VIII

Log_2 RME in SHE-Neumann, $k \approx k^* = 6.38016$

$N\downarrow / k\rightarrow$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	−6.11	−4.09	−2.20	−1.14	−2.33	−4.12	−6.08
128	−8.12	−6.10	−4.10	−1.15	−4.13	−6.10	−8.08
256	−10.11	−8.10	−6.10	−1.14	−6.11	−8.10	−10.08
512	−12.11	−10.10	−8.10	−1.14	−8.10	−10.09	−12.08

TABLE X

Log_2 RME in DSHE-Neumann, $k \approx k^* = 6.70613$

$N\downarrow / k\rightarrow$	$k^*-\frac{1}{16}$	$k^*-\frac{1}{64}$	$k^*-\frac{1}{256}$	k^*	$k^*+\frac{1}{256}$	$k^*+\frac{1}{64}$	$k^*+\frac{1}{16}$
64	−6.74	−4.87	−2.87	2.68	−2.93	−4.92	−6.87
128	−8.76	−6.90	−4.92	7.41	−4.92	−6.93	−8.89
256	−10.77	−8.91	−6.93	2.42	−6.93	−8.93	−10.90
512	−12.77	−10.91	−8.92	0.63	−8.93	−10.93	−12.89

TABLE XI

Log$_2$ MRE in SHE-Dirichlet, $k \approx k^* = 6.38016$

$N \downarrow / k \rightarrow$	$k^* - \frac{1}{16}$	$k^* - \frac{1}{64}$	$k^* - \frac{1}{256}$	k^*	$k^* + \frac{1}{256}$	$k^* + \frac{1}{64}$	$k^* + \frac{1}{16}$
64	−5.54	−4.07	−2.01	1.13	−2.30	−4.12	−5.55
128	−4.78	−4.75	−3.94	2.18	−3.96	−4.75	−4.81
256	−3.79	−3.80	−3.79	3.66	−3.79	−3.80	−3.81
512	−2.79	−2.80	−2.80	3.59	−2.80	−2.81	−2.81

TABLE XIII

Log$_2$ MRE in DSHE-Dirichlet, $k \approx k^* = 6.70613$

$N \downarrow / k \rightarrow$	$k^* - \frac{1}{16}$	$k^* - \frac{1}{64}$	$k^* - \frac{1}{256}$	k^*	$k^* + \frac{1}{256}$	$k^* + \frac{1}{64}$	$k^* + \frac{1}{16}$
64	−6.04	−4.81	−2.96	−0.68	−2.91	−4.81	−6.08
128	−5.27	−5.25	−4.65	−0.58	−4.64	−5.27	−5.30
256	−4.28	−4.28	−4.08	1.78	−4.08	−4.29	−4.31
512	−3.29	−3.28	−3.07	5.95	−3.07	−3.29	−3.32

VII–X, for the respective collocation error for the case with negligible integration errors.

Because of the injected error of 2^{-8} in all the matrix elements, we cannot expect accuracies beyond this value and indeed this is observed in all tables.

For many of the results in the Tables XI–XIV, the observed error is much greater than the corresponding results in Tables VII–X. In these cases, it is clearly the error from the matrix approximation that is dominant. In general, provided the integration error is sufficiently small compared to the discretisation error, this has no adverse effect on the error in the *discrete collocation* approximation. This is because the condition numbers of the boundary element matrices are moderately small, either $\mathcal{O}(1)$, for $-\frac{1}{2}I + M_k$ and $\frac{1}{2}I + M_k^t$ or $\mathcal{O}(N)$, for L_k and N_k. However, if the numerical quadrature errors are of comparable size or larger than the discretisation error, doubling the number of collocation points may actually double the error in the discrete collocation approximation due to the $\mathcal{O}(N)$ condition number of the boundary element matrices (see Tables XI and XIII).

It follows from (23), (27), and (28) (with $s = 0$) that if the expected discretisation error is $\delta(N)$, to retain this level of accuracy in the discrete collocation solution we should aim for integration errors $\varepsilon(N)$ with $\varepsilon(N) \leq \delta(N).\ N^{-3/2}$. This follows from (28) with $2|\beta| = 1$. In our examples here $\delta(N) = CN^{-2}$; hence $\varepsilon(N) \leq CN^{-7/2}$ is recommended.

6. CONCLUSIONS

The results in Table VI show that the elementary methods simply do not work at characteristic wavenumbers. Tables VII–X show that near characteristic wavenumbers the error in the numerical approximation is inversely proportional to the distance of k from the characteristic sets. Even though the expected $\mathcal{O}(N^{-2})$ convergence is still observed near the characteristic wavenumbers, this nevertheless implies that in order to obtain the same level of accuracy when $|k - k^*| = \frac{1}{256}$ as when $|k - k^*| = \frac{1}{64}$ we need twice the number of elements. This deterioration of the accuracy with proximity to characteristic wavenumbers is undesirable, especially as one in general does not know *a priori* the characteristic sets $I_{D,\Gamma}$ and $I_{N,\Gamma}$.

The improved integral equations such as (17) can be well-conditioned for all values of k, provided an appropriate choice of an inherent coupling parameter is used; see [32, 30, 2]. Hence, at least when k is close to the characteristic values the improved integral equation formulations will provide more efficient methods than the elementary methods. Given that the characteristic wavenumbers become more and more clustered as real k increases, the improved methods such as (17) will be more efficient than the elementary methods for all real values of k sufficiently large. However, for complex values of k, sufficiently away from the real axis, the elementary equations are expected to be the most suitable for yielding efficient methods of solution.

Regarding the use of numerical quadrature, Tables XI–XIV show that, provided the integration error is sufficiently small compared to the discretisation error, this should not have a significant effect on the error in the *discrete collocation* approximation. However, if the quadrature errors are larger or of comparable size to the discretisation error, increasing the number of collocation points may actually increase the error in the discrete collocation approximation. This is because

TABLE XII

Log$_2$ MRE in SHE-Neumann, $k \approx k^* = 6.38016$

$N \downarrow / k \rightarrow$	$k^* - \frac{1}{16}$	$k^* - \frac{1}{64}$	$k^* - \frac{1}{256}$	k^*	$k^* + \frac{1}{256}$	$k^* + \frac{1}{64}$	$k^* + \frac{1}{16}$
64	−6.06	−4.10	−2.21	−1.14	−2.34	−4.13	−6.04
128	−7.59	−6.10	−4.14	−1.15	−4.18	−6.10	−7.57
256	−7.97	−7.66	−6.25	−1.15	−6.25	−7.65	−7.97
512	−8.00	−7.99	−7.89	−1.14	−7.89	−7.99	−8.00

TABLE XIV

Log$_2$ MRE in DSHE-Neumann, $k \approx k^* = 6.70613$

$N \downarrow / k \rightarrow$	$k^* - \frac{1}{16}$	$k^* - \frac{1}{64}$	$k^* - \frac{1}{256}$	k^*	$k^* + \frac{1}{256}$	$k^* + \frac{1}{64}$	$k^* + \frac{1}{16}$
64	−6.63	−4.86	−2.87	2.68	−2.93	−4.90	−6.73
128	−7.80	−6.76	−4.90	7.41	−4.91	−6.78	−7.78
256	−7.98	−7.83	−6.78	2.42	−6.78	−7.82	−7.97
512	−7.99	−7.98	−7.83	0.63	−7.83	−7.98	−7.99

in these cases the total error will be dominated by the *quadrature induced errors* which increase with N, due to $\mathcal{O}(N)$ behaviour of the condition number of certain boundary element matrices.

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