**High-Order Quadratures for the Solution of
Scattering Problems in Two Dimensions**

Ran Duan and Vladimir Rokhlin
Technical Report YALEU/DCS/TR-1401
April 22, 2008

We construct an iterative algorithm for the solution of forward scattering problems in two dimensions. The scheme is based on the combination of high-order quadrature formulae, fast application of integral operators in Lippmann-Schwinger equations, and the stabilized biconjugate gradient method (BI-CGSTAB). While the FFT-based fast application of integral operators and the BI-CGSTAB for the solution of linear systems are fairly standard, a large part of this paper is devoted to constructing a class of high-order quadrature formulae applicable to a wide range of singular functions in two and three dimensions; these are used to obtain rapidly convergent discretizations of Lippmann-Schwinger equations. The performance of the algorithm is illustrated with several numerical examples.

**High-Order Quadratures for the Solution of
Scattering Problems in Two Dimensions**

Ran Duan and Vladimir Rokhlin
Technical Report YALEU/DCS/TR-1401
April 22, 2008

1   Introduction

Forward scattering has been an active field of research in science, mathematics, and engineering over the past several decades (see e.g. [3], [4]). The most straightforward method for the solution of a forward scattering problem is to discretize the underlying PDEs directly, replace the derivatives with finite differences, and solve numerically the resulting system of linear algebraic equations. However, discretization of differential equations leads to matrices with high condition numbers, with the attendant loss of accuracy, deterioration in the performance of iterative methods, etc. Another approach is to convert the underlying PDEs into integral equations of the second kind (normally referred to as the Lippmann-Schwinger equation), discretize the latter via appropriate quadrature formulae, and deal numerically with the resulting linear systems. This paper constructs a class of high-order quadrature formulae applicable to the Lippmann-Schwinger equation in two and three dimensions.

1.1   Statement of the Problem

The forward scattering problem is the problem of determining the scattered field given the parameters of the scattering structure and the incident field. In this section, we formulate the two-dimensional forward scattering problem for the Helmholtz equation, and derive the corresponding Lippmann-Schwinger equation.

The forward scattering problem we investigate arises from the time domain wave equation

$$\frac{\partial^2}{\partial^2 t}\psi(x,t) = c^2(x) \cdot \nabla^2 \psi(x,t), \tag{1}$$

where $\psi(x,t)$ is the value of the scalar field at a point x at time t, and $c(x)$ is the local speed of wave propagation at a point x. In order to solve (1), we assume that

$$\psi(x,t) = \psi_k(x)\, e^{i\,k\,c_0\,t}, \tag{2}$$

where k is a complex number with non-negative imaginary part, and c_0 is the speed of wave propagation outside of the scattering structure. Substituting (2) into (1), we obtain

$$(\nabla^2 + k^2)\,\psi_k(x) = k^2\, V(x)\,\psi_k(x), \tag{3}$$

where

$$V(x) = 1 - \left(\frac{c_0}{c(x)}\right)^2. \tag{4}$$

Equation (3) is the well-known Helmholtz equation, and the operator $(\nabla^2 + k^2)$ is known as the Helmholtz operator. For any point x outside the scattering object, $c(x) = c_0$; therefore, $V(x) = 0$ outside the scattering object. We represent the field $\psi_k(x)$ at a point x as a sum of two parts: the incident field $\psi_k^{in}(x)$ and the scattered field $\psi_k^{scat}(x)$, i.e.,

$$\psi_k(x) = \psi_k^{in}(x) + \psi_k^{scat}(x). \tag{5}$$

The incident field satisfies the homogenous Helmholtz equation

$$(\nabla^2 + k^2)\psi_k^{in}(x) = 0, \tag{6}$$

3

in some open region in $\mathbb{R}^2$ containing the scatterer; the scattered field satisfies the Sommerfeld radiation condition

$$\lim_{|x|\to\infty} \sqrt{|x|}\left(\frac{\partial \psi_k^{scat}(x)}{\partial |x|} - i\,k\,\psi_k^{scat}(x)\right) = 0. \tag{7}$$

Combining equations (3), (5), and (6), we obtain the equation for the scattered field

$$(\nabla^2 + k^2)\,\psi_k^{scat}(x) - k^2\,V(x)\,\psi_k^{scat}(x) = k^2\,V(x)\,\psi_k^{in}(x). \tag{8}$$

In this paper, we view the equation (8) with ψ_k^{scat} satisfying the Sommerfeld condition (7) as the principal formulation of the forward scattering problem. A standard approach to the numerical solution of (8) is to convert (8) into the well-known Lippmann-Schwinger equation, which is an integral equation of the second kind, as follows (see, for example, [5]).

Convolving (8) with a Green's function for the equation

$$(\nabla^2 + k^2)\,G_k(x, y) = \delta(x - y), \tag{9}$$

we obtain

$$\psi_k^{scat}(x) - k^2 \int_D G_k(x, y)\,V(y)\,\psi_k^{scat}(y)\,dy = k^2 \int_D G_k(x, y)\,V(y)\,\psi_k^{in}(y)\,dy, \tag{10}$$

which is an integral equation of the second kind; in (10) above, D denotes the region in space where the scatterer is located. As is well-known, in two dimensions, the Green's function $G_k(x, y)$ satisfying the condition (7) is

$$G_k(x, y) = -\frac{i}{4} H_0^{(1)}(k\|x - y\|), \tag{11}$$

where $H_0^{(1)}(k\|x - y\|)$ is the Hankel function of the first kind of order zero. We will define the operator $L : L^2(D) \to L^2(D)$ by the formula

$$L(\psi)(x) = \int_D G_k(x, y)\,V(y)\,\psi(y)\,dy, \tag{12}$$

and observe that a large part of this paper is devoted to the construction of accurate discretizations of L.

1.2 Overview

A number of algorithms exist for the modeling of acoustic scattering; since we are interested in frequency domain results, we have concentrated on frequency domain (as opposed to time-domain) models. The usual approach to such problems is to convert the scattering problem into the Lippmann-Schwinger equation, and solve the latter iteratively (integral equations of the second kind being much more amenable to iterative techniques than the straightforward discretizations of underlying partial differential equations (PDEs)). In addition, the use of the Lippmann-Schwinger equation obviates the need to impose the radiation (Sommerfeld) condition at the boundary of the grid, since the "background" Green's function (11) imposes the Sommerfeld condition automatically.

Historically, there have been two problems associated with the numerical use of integral equations in scattering calculations. First, the kernels of Lippmann-Schwinger equations are dense, except when the background is extremely attenuating; since iterative techniques require application of the matrix of the discretized integral operator to a sequence of recursively generated vectors, the cost of the procedure is prohibitive, except for extremely small-scale problems. This difficulty was overcome almost 40 years ago via the observation that the free-space Green's function for the Helmholtz equation is translation invariant; appropriately chosen discretizations of Lippmann-Schwinger equations result in Toeplitz matrices, and the latter can be rapidly applied to arbitrary vectors via the FFT (Fast Fourier Transform), resulting in algorithms with CPU time requirements proportional to $N \cdot \log(N)$, with N the number of nodes in the discretization of the problem. Various forms of this approach have been widely used in electrical engineering and other fields, under the name "k-space" methods; some of the existing codes are quite fast, even for discretizations involving hundreds of millions of nodes. However, the resulting solvers for the underlying PDEs are usually not very accurate, due to the problem discussed in the following paragraph.

The second difficulty associated with numerical use of Lippmann-Schwinger equations is due to the singular character of the Green's function for the Helmholtz equation; in two dimensions, the principal term of the singularity is of the form $\log(r)$, and in three dimensions, it is of the form $1/r$. As a result, kernels of Lippmann-Schwinger equations are singular; the singularities are located on the diagonal, and in two dimensions are of the form

$$K(x,y) = \log(|x-y|) + P(x,y) \cdot \log(|x-y|) + Q(x,y), \qquad (13)$$

with P, Q two smooth functions, and $P(x,x) = 0$ for all $x \in R^2$; the corresponding form in three dimensions is

$$K(x,y) = \frac{1}{|x-y|} + P(x,y) \cdot \frac{1}{|x-y|} + Q(x,y). \qquad (14)$$

It is important to observe that in most cases, we do not have access to each of the functions P, Q separately, but can only evaluate the whole kernel K given a pair of points (x,y). In other words, standard integration techniques (such as product integration, etc.) can not be used efficiently. The standard procedure in the literature (referred to as the "singularity extraction") is to subtract the principal singularity and treat it analytically, and apply the trapezoidal quadrature rule to the remaining function. Since the latter is not smooth (having infinite derivatives at $x = y$), the procedure converges slowly, normally behaving like a second order scheme.

We introduce a class of quadrature formulae for functions of the form (13) in two dimensions and (14) in three dimensions. The approach is somewhat related to the Ewald summation [6], and leads to quadratures that can be viewed as a version of the corrected trapezoidal rule; it is easily combined with the FFT to obtain fast algorithms. While in principle corrections of arbitrarily high order could be constructed, in practice both the complexity of derivation and the number of corrections grow rapidly with the order. We have designed corrections of orders 4, 6, 8, and 10; they require 1, 5, 13, and 25 corrected nodes respectively.

The paper is organized as follows. In Section 2, we summarize several well-known mathematical facts to be used in the paper. In Section 3, we introduce analytical tools to be used

in the construction of the algorithm. Section 4 describes the algorithm in detail, and contains a complexity analysis. In Section 5, several numerical examples are used to illustrate the performance of the algorithm. Finally, Section 6 contains generalizations and conclusions.

2   Analytical Preliminaries

In this section, we summarize several well-known mathematical facts to be used in the sections below. All of these are either well known or easily derived from well-known results.

2.1   Notation

For an integer $N \geq 1$, the two-dimensional discrete Fourier transform $\mathcal{F}^N$ is a mapping converting a two-dimensional complex sequence $a = \{a_{j_1 j_2}\}$, $j_1, j_2 = -N, ..., N$, into another two-dimensional complex sequence $A = \{A_{k_1 k_2}\}$, $k_1, k_2 = -N, ..., N$, defined by the formula

$$A_{k_1 k_2} = \sum_{j_1=-N}^{N} \sum_{j_2=-N}^{N} a_{j_1 j_2} \, e^{-\frac{2\pi i}{(2N+1)} k_1 j_1} \, e^{-\frac{2\pi i}{(2N+1)} k_2 j_2}. \tag{15}$$

It is easily verified that the inverse $(\mathcal{F}^N)^{-1}$ of the mapping $\mathcal{F}^N$ is given by the formula

$$(\mathcal{F}^N)^{-1}(A)_{j_1 j_2} = a_{j_1 j_2} = \frac{1}{(2N+1)^2} \sum_{k_1=-N}^{N} \sum_{k_2=-N}^{N} A_{k_1 k_2} \, e^{\frac{2\pi i}{(2N+1)} k_1 j_1} \, e^{\frac{2\pi i}{(2N+1)} k_2 j_2}, \tag{16}$$

with $j_1 = -N, ..., N$, $j_2 = -N, ..., N$.

For a Helmholtz equation

$$\nabla^2 \phi + k^2 \phi = 0 \tag{17}$$

in two dimensions, the potential ϕ at a point x produced by a unit point source at x_0 is given by the formula

$$\phi(x) = -\frac{i}{4} H_0(k \| x - x_0 \|), \tag{18}$$

where k is a complex number such that $\text{Im}(k) \geq 0$, and H_0 is the Hankel function of the first kind of order zero. The well-known Sommerfeld formula states that

$$H_0(kr) = \frac{1}{\pi} \cdot \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot e^{i\sqrt{k^2 - \lambda^2} x} \cdot e^{i\lambda y} \, d\lambda \tag{19}$$

for any $k \in \mathbb{C}^+$, $r, x, y \geq 0$, and $r = \sqrt{x^2 + y^2}$ (see, for example, [9]).

Finally, we will need the identity

$$\sum_{j=0}^{n} f_j g_j = f_n \sum_{k=0}^{n} g_k - \sum_{j=0}^{n-1} (f_{j+1} - f_j) \cdot \left(\sum_{k=0}^{j} g_k \right), \tag{20}$$

valid for two arbitrary finite sequences $\{f_j\}$, $j = 0, 1, 2, \ldots, n,$, $\{g_j\}$, $j = 0, 1, 2, \ldots, n,$. By analogy with integration by parts, (20) is normally referred to as summation by parts; it is easily verified by a substitution.

2.2 High-Order Corrected Trapezoidal Quadrature Rules for Singular Functions in One Dimension

For a function $f : [a, b] \rightarrow R^1$ and integer $n \geq 2$, the n-point trapezoidal rule T_n is defined by the formula

$$T_n(f) = h\left(\sum_{i=0}^{n-1} f(a + ih) - \left(\frac{f(a) + f(b)}{2} \right) \right), \tag{21}$$

where

$$h = \frac{b - a}{n - 1}, \tag{22}$$

and is widely used as an approximation to the integral $\int_a^b f(x)\,dx$. It is second order convergent, as long as the second derivative of f is continuous on $[a, b]$. In other words, if $f \in C^2[a, b]$, then

$$\int_a^b f(x)\,dx = T_n(f) + O(h^2). \tag{23}$$

For any function $f \in C^{2m+2}[a, b]$ with integer $m \geq 1$, the well-known Euler-Maclaurin formula (see, for example, [1]) states that there exists a real number ξ with $a < \xi < b$, such that

$$\int_a^b f(x)\,dx = T_n(f) + \sum_{l=1}^{m} \frac{h^{2l} B_{2l}}{(2l)!}(f^{(2l-1)}(b) - f^{(2l-1)}(a)) - \frac{h^{2m+2} B_{2m+2}}{(2m+2)!} f^{(2m+2)}(\xi), \tag{24}$$

where $B_k, k = 0, 1, 2, \ldots$ denote the Bernoulli numbers (see [1]). It is easily seen from (24) that for any function $f \in C^m[a - mh, b + mh]$ with integer $m \geq 3$, it is possible to construct quadratures of the form

$$T_{\beta^m}^n(f) = T_n(f) + h \sum_{k=-\frac{m-1}{2}}^{\frac{m-1}{2}} (f(b + kh) - f(a + kh))\beta_k^m, \tag{25}$$

where β_k^m are coefficients such that

$$\int_a^b f(x)\,dx = T_{\beta^m}^n(f) + O(h^{m+1}), \tag{26}$$

with h defined by (22). The quadrature $T_{\beta^m}^n$ is referred to as the $(m + 1)^{th}$-order endpoint-corrected trapezoidal rule; for any given k and m, where $m \geq 3$, and is odd, the coefficient β_k^m can be obtained via a direct calculation (see [7]).

While (21) and (25) are widely used for the numerical integration of smooth functions, their use for singular integrands tends to encounter difficulties (see, for example, [11]). In [7], a class of quadrature formulae is constructed for approximating integrals of singular functions of the form

$$f(x) = \phi(x)\,s(x), \tag{27}$$

7

where $\phi \in C^m[-b-mh, b+mh]$ with $m \geq 3$, and s is an integrable function on $[-b, b]$ with a singularity at zero. For integers $n \geq 1$, $p \geq 1$, and odd $m \geq 3$, the quadrature $U_{\tau^h \beta m}$ for the functions with separable singularities (i.e., functions defined by (27)) is given by the formula

$$U_{\tau^h \beta m}(f) = T''^{n}_{\beta m}(f) + \sum_{j=-p}^{p} \tau_j^h \, \phi(jh). \tag{28}$$

In (28),

$$T''^{n}_{\beta m}(f) = h \left(\sum_{\substack{j=-n \\ j \neq 0}}^{n} f(jh) - \left(\frac{f(-b) + f(b)}{2} \right) \right) + h \sum_{k=-\frac{m-1}{2}}^{\frac{m-1}{2}} (f(b+kh) - f(-b+kh))\beta_k^m, \tag{29}$$

where the coefficients β_k^m can be obtained via direct calculation (see [7]), $h = \frac{b}{n}$, and the coefficients τ_j^h can be obtained by solving the system of linear equations

$$\sum_{j=-p}^{p} x_j^{i-1} \tau_j^h = \int_{-b}^{b} (x^{i-1} s(x)) \, dx - T''^{n}_{\beta m}(x^{i-1} s), \tag{30}$$

with $x_j = jh$, and $i = 1, 2, \ldots, 2p + 1$. The quadrature formula (28) is of order $2p + 2$.

Remark 2.1 While (21) is the standard trapezoidal rule, and (25) is the trapezoidal rule with endpoints corrections, (28) is the trapezoidal rule with corrections at both endpoints and a singular point inside the interval. Here, the singular point is the center point, so the scheme is sometimes called a "center-corrected trapezoidal rule." The coefficients τ_j^h are called correction coefficients.

Remark 2.2 The only difference between $T''^{n}_{\beta m}(f)$ and $T^n_{\beta m}(f)$ is that $T''^{n}_{\beta m}(f)$ does not contain the term $h \cdot f(0)$, which may become infinite for f of the form (27).

2.3 Toeplitz Convolution

This section introduces two-dimensional Toeplitz convolutions and a procedure for the calculation of two-dimensional Toeplitz convolutions via the two-dimensional discrete Fourier transform. The Toeplitz convolution $a * b$ of finite two-dimensional complex sequences $a = \{a_{j_1 j_2}\}$, $j_1, j_2 = -N, ..., N$, and $b = \{b_{j_1 j_2}\}$, $j_1, j_2 = -2N, ..., 2N$, is defined by the formula

$$(a * b)_{k_1 k_2} = \sum_{j_1=-N}^{N} \sum_{j_2=-N}^{N} a_{j_1 j_2} b_{k_1 - j_1, \, k_2 - j_2}, \tag{31}$$

where $k_1, k_2 = -N, ..., N$. The well-known convolution theorem states that the Toeplitz convolution $a * b$ is equal to the inverse Fourier transform of the product of the Fourier transform of a' and b, where a' is a two-dimensional sequence obtained by padding the two-dimensional sequence a with zeros. In other words,

$$(a * b)_{k_1 k_2} = (\mathcal{F}^{2N})^{-1} \big(\mathcal{F}^{2N}(a') \cdot \mathcal{F}^{2N}(b) \big)_{k_1 k_2}, \tag{32}$$

where $k_1, k_2 = -N, ..., N$, and the coefficients of the two-dimensional complex sequence $a' = \{a'_{i_1 i_2}\}, i_1, i_2 = -2N, ..., 2N$ are defined by the formulae

$$a'_{i_1 i_2} = a_{i_1 i_2}, \tag{33}$$

when $-N \leq i_1, i_2 \leq N$, otherwise

$$a'_{i_1 i_2} = 0. \tag{34}$$

Remark 2.3 While direct calculation of Toeplitz convolution (31) leads to time cost of order $O(N^4)$, which is prohibitive for large scale problems, application of FFT to the formula (32) reduces the time cost to $O(N^2 \cdot \log N)$ (see, for example, [2]). In this paper, FFT is used for the fast calculation of Toeplitz convolution.

3 Mathematical Apparatus

In this section, we introduce analytical tools to be used in the construction of the algorithms.

3.1 Endpoint Corrected Trapezoidal Quadrature Rules in Two Dimensions

This section can be viewed as the extension of results of Section 2.2 to two dimensions.

For a function $f : [a, b] \times [a, b] \to R^1$ and integer $n \geq 2$, the two-dimensional trapezoidal rule T_n^{2D} is defined by the formula

$$T_n^{2D}(f) = \sum_{i=0}^{n-1} \sum_{j=0}^{n-1} f(a + ih, a + jh) \cdot h^2 \cdot \beta_{ij}, \tag{35}$$

where

$$h = \frac{b - a}{n - 1}, \tag{36}$$

and β_{ij} equals 1 in the interior of the square $[a, b] \times [a, b]$, equals $\frac{1}{2}$ in the interior of the edge, and equals $\frac{1}{4}$ on the corners of the square.

Further, if $f \in C^2[a, b] \times [a, b]$, then

$$\int_a^b \int_a^b f(x, y) \, dx \, dy = T_n^{2D}(f) + O(h^2). \tag{37}$$

The proof consists of a straightforward application of one-dimensional trapezoidal rule (21) to both directions in two dimensions, and thus omitted.

The following Lemma provides the two-dimensional version of the Euler-Maclaurin formula.

Lemma 3.1 *Suppose that a function $f \in C^{2m+2}[a,b] \times [a,b]$, integers $m \geq 1$, $n \geq 2$. Then,*

$$\int_a^b \int_a^b f(x,y)\,dx\,dy = T_n^{2D}(f) + \sum_{i=0}^{i=n-1} \sum_{l=1}^m \frac{h^{2l+1} \cdot B_{2l} \cdot \beta_i}{(2l)!} \cdot$$

$$\left(\frac{\partial^{2l-1}}{\partial x^{2l-1}} f(b, a+ih) - \frac{\partial^{2l-1}}{\partial x^{2l-1}} f(a, a+ih) - \frac{\partial^{2l-1}}{\partial y^{2l-1}} f(a+ih, b) - \frac{\partial^{2l-1}}{\partial y^{2l-1}} f(a+ih, a) \right)$$

$$+ \sum_{l=1}^m \sum_{l'=1}^m \frac{h^{2l+2l'} \cdot B_{2l} \cdot B_{2l'}}{(2l!)(2l'!)} \cdot \left(\frac{\partial^{2l+2l'-2}}{\partial x^{2l-1} \partial y^{2l'-1}} \Big(f(b,b) + f(a,a) - f(a,b) - f(b,a) \Big) \right) + O(h^{2m+2}),$$
(38)

where $T_n^{2D}(f)$ is defined in (35), h is defined in (36),

$$\beta_i = \begin{cases} 1 & 0 < i < n-1 \\ 1/2 & i = 0 \ or \ i = n-1 \end{cases},$$
(39)

and $B_k, k = 0, 1, 2, \ldots$ denote the Bernoulli numbers.

Proof. The Euler-Maclaurin formula (24) can be rewritten as

$$\int_a^b f(x)\,dx = T_n(f) + \sum_{l=1}^m \frac{h^{2l} B_{2l}}{(2l)!} (f^{(2l-1)}(b) - f^{(2l-1)}(a)) + O(h^{2m+2}).$$
(40)

Hence,

$$\int_a^b \int_a^b f(x,y)\,dx\,dy =$$

$$\int_a^b \left(\sum_{i=0}^{n-1} f(a+ih, y) \cdot \beta_i + \sum_{l=1}^m \frac{h^{2l} B_{2l}}{(2l)!} (f^{(2l-1)}(b) - f^{(2l-1)}(a)) + O(h^{2m+2}) \right) dy. \quad (41)$$

The conclusion of the Lemma follows immediately from applying the formula (40) to the integrals in (41). $\qquad \square$

The following Lemma provides a $(2m+2)^{th}$-order endpoint-corrected trapezoidal rule in two dimensions.

Lemma 3.2 *Suppose that a function $f \in C^{2m+2}[a,b] \times [a,b]$ with integers $m \geq 1$, $n \geq 2$, $h = \frac{b-a}{n-1}$. Then,*

$$\int_a^b \int_a^b f(x,y)\,dx\,dy = T_{\beta^{2m+1}}^{2D,n}(f) + O(h^{2m+2}),$$
(42)

In (42),

$$T_{\beta^{2m+1}}^{2D,n}(f) = T_n^{2D}(f) + h^2 \sum_{i=0}^{n-1} \sum_{k=-m}^m \left(\beta_k^{2m+1} \beta_i \cdot \right.$$

$$\Big(f(b+kh, ih) + f(ih, b+kh) - f(a+kh, ih) - f(ih, a+kh) \Big) \Big) + h^2 \sum_{k=-m}^m \sum_{k'=-m}^m \Big(\beta_k^{2m+1} \beta_{k'}^{2m+1} \cdot$$

$$\Big(f(a+kh, a+k'h) + f(b+kh, b+k'h) - f(a+kh, b+k'h) - f(b+kh, a+k'h) \Big) \Big), \quad (43)$$

T_n^{2D}, β_k^{2m+1}, and β_i are defined by (35), (25) and (39).

Proof. It is easily observed from the formulae (24), (25) that

$$\sum_{l=1}^{m} \frac{h^{2l+1} B_{2l}}{(2l!)} f^{(2l-1)}(a) = \sum_{k=-m}^{m} f(a+kh) \cdot \beta_k^{2m+1} \cdot h^2. \tag{44}$$

Therefore,

$$\sum_{k=-m}^{m} h^2 \cdot f(a+kh, a+ih) \cdot \beta_k^{2m+1} = \sum_{l=1}^{m} \frac{h^{2l+1} B_{2l}}{(2l!)} \frac{\partial^{2l+1}}{\partial x^{2l+1}} f(a, a+ih), \tag{45}$$

and

$$\sum_{l=1}^{m} \sum_{l'=1}^{m} \frac{h^{2l+2l'} \cdot B_{2l} \cdot B_{2l'}}{(2l!)(2l'!)} \left(\frac{\partial^{2l+2l'-2}}{\partial x^{2l-1} \partial y^{2l'-1}} f(a, a) \right)$$
$$= \sum_{l'=1}^{m} \frac{h^{2l'} B_{2l'}}{(2l'!)} \cdot \left(\sum_{k=-m}^{m} h \cdot \beta_k^{2m+1} \frac{\partial^{2l'-1}}{\partial y^{2l'-1}} f(a+kh, a) \right)$$
$$= \sum_{k=-m}^{m} h^2 \beta_k^{2m+1} \cdot \left(\sum_{l'=1}^{m} \frac{h^{2l'-1} B_{2l'}}{(2l'!)} \cdot \frac{\partial^{2l'-1}}{\partial y^{2l'-1}} f(a+kh, a) \right)$$
$$= \sum_{k=-m}^{m} \sum_{k'=-m}^{m} h^2 \cdot \beta_k^{2m+1} \beta_{k'}^{2m+1} f(a+kh, a+k'h). \tag{46}$$

Now, (43) follows immediately from the combination of (45), (46). $\qquad\square$

3.2   High-Order Center Corrected Trapezoidal Quadrature Rules for the Singular Functions in Two Dimensions

The following Lemma provides an estimate of the difference between the integral and the end-point corrected trapezoidal quadrature for functions of the form $x^{2p+2} \cdot \log(x^2 + y^2)$.

Lemma 3.3 *Suppose that n is a positive integer, a, h are two positive real numbers such that $h = a/n$, and integers m, p are such that $m \geq p+1 \geq 1$. Then,*

$$\int_{-a}^{a} \int_{-a}^{a} (x^{2p+2} \cdot \log(x^2 + y^2)) \, dx \, dy = T_{\beta^{2m+1}}^{2D,n}(x^{2p+2} \cdot \log(x^2 + y^2)) + O(h^{2p+4}), \tag{47}$$

with $T_{\beta^{2m+1}}^{2D,n}$ defined by (43).

Proof. Here, we prove the case of $p = 0$ as an illustration; the proof for $p > 0$ is quite similar. For simplicity, we will be denoting $x^2 \cdot \log(x^2 + y^2)$ by $g(x, y)$. Then,

$$\frac{\partial g(x, y)}{\partial y} = \frac{2x^2 y}{x^2 + y^2}, \tag{48}$$

11

$$\frac{\partial^3 g(x,y)}{\partial y^3} = \frac{16x^2 y^3}{(x^2+y^2)^3} - \frac{12x^2 y}{(x^2+y^2)^2}, \tag{49}$$

and

$$\frac{\partial^6 g(x,y)}{\partial y^6} = -\frac{7680x^2 y^6}{(x^2+y^2)^6} + \frac{11520x^2 y^4}{(x^2+y^2)^5} - \frac{4320x^2 y^2}{(x^2+y^2)^4} + \frac{240x^2}{(x^2+y^2)^3}. \tag{50}$$

Replacing the derivatives in (24) with the appropriate finite differences, we rewrite (24) in the form

$$\int_a^b g(x)\, dx = T_n(g) + \frac{1}{12}h \cdot (-g(b+h) + g(a+h) + g(b-h) - g(a-h)) +$$
$$C_1 \cdot h^4 \cdot (g^{(3)}(b) - g^{(3)}(a)) - C_2 \cdot h^6 \cdot g^{(6)}(\xi)$$
$$= T_{\beta^3}^n(g) + C_1 \cdot h^4 \cdot (g^{(3)}(b) - g^{(3)}(a)) + C_2 \cdot h^6 \cdot g^{(6)}(\xi), \quad (51)$$

where C_1 and C_2 are two constants independent of g, and $\xi \in [a,b]$. Therefore, for any fixed x and $g(x,y) = x^2 \cdot \log(x^2 + y^2)$, the error $\epsilon(x)$ of the end-point corrected trapezoidal quadrature in the y direction is

$$\epsilon(x) = \int_{-a}^a g(x,y)\, dy - T_{\beta^3}^n(g) = C_1 \cdot h^4 \left(\frac{16x^2 a^3}{(x^2+a^2)^3} - \frac{12x^2 a}{(x^2+a^2)^2} \right) + C_2 \cdot h^6 \cdot g^{(6)}(x,\xi). \tag{52}$$

Summing up all the errors along the x axis, we obtain

$$\epsilon = \int_{-a}^a \int_{-a}^a (x^2 \cdot \log(x^2 + y^2))\, dx dy - T_{\beta^3}^{2D,n}(x^2 \cdot \log(x^2 + y^2)) \sim 2 \cdot \sum_{i=1}^n h \cdot \epsilon(ih)$$

$$\leq h \cdot \sum_{i=1}^n \left(C_1 \cdot h^4 \left(\frac{16(ih)^2 a^3}{((ih)^2 + a^2)^3} - \frac{12(ih)^2 a}{((ih)^2 + a^2)^2} \right) \right) + h \cdot \sum_{i=1}^n C_2 \cdot h^6 \cdot |g^{(6)}(\xi)|_{max}$$

$$\leq C_1 h^4 \int_0^a \left(\frac{16x^2 a^3}{(x^2+a^2)^3} - \frac{12x^2 a}{(x^2+a^2)^2} \right) dx + C_2 \cdot h^7 \sum_{i=1}^n \frac{240}{(ih)^4}$$

$$\sim C_1 \cdot (3 - \pi) \cdot h^4 + C_2 \cdot h^6 \cdot \log(h) \sim O(h^4). \tag{53}$$

$\square$

Theorem 3.4 below is an extension of the formula (28) to two dimensions. For an integer $p \geq 0$, it supplies a $(2p+4)^{th}$-order center-corrected quadrature formula on $\mathbb{R}^2$ for the functions of the form

$$f(x,y) = \phi(x,y) \cdot s(x,y), \tag{54}$$

where $\phi : R^2 \to R$, and

$$s(x,y) = \log(x^2 + y^2) + P(x,y) \cdot \log(x^2 + y^2) + Q(x,y), \tag{55}$$

with P, Q two smooth functions, and $P(0,0) = 0$. Suppose that n, m are positive integers, and a, h are two positive real numbers such that $h = a/n$. We define $T'^{2D,n}_{\beta^{2m+1}}(f)$ by the

12

formula

$$T'^{2D,n}_{\beta^{2m+1}}(f) = \sum_{(i,j)\in M} f(ih,jh) \cdot h^2 \cdot \beta_{ij} + h^2 \sum_{i=-n}^{n} \sum_{k=-m}^{m} \Big(\beta_k^{2m+1}\beta_i \cdot$$

$$(f(a+kh,ih) + f(ih,a+kh) - f(-a+kh,ih) - f(ih,-a+kh)) \Big) + h^2 \sum_{k=-m}^{m} \sum_{k'=-m}^{m} \Big(\beta_k^{2m+1}\beta_{k'}^{2m+1} \cdot$$

$$(f(-a+kh,-a+k'h) + f(a+kh,a+k'h) - f(-a+kh,a+k'h) - f(a+kh,-a+k'h)) \Big),$$
(56)

where

$$M = \{i,j \in \mathbb{Z} : |i| \leq n, |j| \leq n, (i,j) \neq (0,0)\}, \tag{57}$$

$$\beta_i = \begin{cases} 1 & |i| < n \\ 1/2 & |i| = n \end{cases} ; \tag{58}$$

in (56), coefficients β_{ij} equal 1 in the interior of the square $[-a,a] \times [-a,a]$, equal $\frac{1}{2}$ in the interior of the edge, and equal $\frac{1}{4}$ on the corners of the square, and β_k^{2m+1} are defined in (25).

Theorem 3.4 *Suppose that $\phi \in C^{2p+2}(\mathbb{R}^2)$ with $p \geq 0$, integer $m \geq p+1$, and s is a singular function on R^2 with a logarithmic singularity at $(0,0)$, i.e., of the form (55). Suppose further that*

$$U^{2D}_{\tau^h\beta^{2m+1}}(\phi \cdot s) = T'^{2D,n}_{\beta^{2m+1}}(\phi \cdot s) + \sum_{(i,j)\in W} \tau_{ij}^h \phi(ih,jh), \tag{59}$$

where $T'^{2D,n}_{\beta^{2m+1}}(\phi \cdot s)$ is defined by the formula (56),

$$W = \{i,j \in \mathbb{Z} : |i+j| \leq p \text{ and } |i-j| \leq p\}, \tag{60}$$

and the coefficients τ_{ij}^h in (59) satisfy the system of linear equations

$$\sum_{(i,j)\in W} x_i^{i'-1} y_j^{j'-1} \tau_{ij}^h = \int_{-a}^{a}\int_{-a}^{a} (x^{i'-1}y^{j'-1}s(x,y))\, dx\, dy - T'^{2D,n}_{\beta^{2m+1}}(x^{i'-1}y^{j'-1}s), \tag{61}$$

with $x_i = ih$, $y_j = jh$, and $(i',j') \in H$, where $H = \{i',j', \in Z : i' \geq 1, j' \geq 1, i'+j' \leq 2p+2\}$. Then,

$$\int_{-a}^{a}\int_{-a}^{a} (\phi(x,y) \cdot s(x,y))\, dx\, dy = U^{2D}_{\tau^h\beta^{2m+1}}(\phi \cdot s) + O(h^{2p+4}). \tag{62}$$

Proof. Applying the Taylor expansion to the function $\phi(x,y)$ at the point $(0,0)$ we have

$$\phi(x,y) = P(x,y) + R(x,y), \tag{63}$$

where

$$P(x,y) = \sum_{j=0}^{2p+1} \sum_{i=0}^{j} \frac{1}{j!}\binom{j}{i} x^i y^{j-i} \frac{\partial^j}{\partial x^i \partial y^{j-i}}\phi(x,y)|_{x=0,\,y=0}, \tag{64}$$

13

and

$$R(x, y) = \frac{1}{(2p + 2)!} \sum_{i=0}^{2p+2} \binom{2p + 2}{i} x^i y^{2p+2-i} \frac{\partial^{2p+2}}{\partial x^i \partial y^{2p+2-i}} \phi(x, y)|_{x=\xi_1, y=\xi_2}, \tag{65}$$

where $\xi_1, \xi_2 \in [-a, a] \times [-a, a]$. Thus,

$$|\int_{-a}^{a} \int_{-a}^{a} (\phi(x, y) \cdot s(x, y)) \, dx \, dy - U^{2D}_{\tau^h \beta^{2m+1}}(\phi \cdot s)|$$
$$\leq |\int_{-a}^{a} \int_{-a}^{a} (P(x, y) \cdot s(x, y)) \, dx \, dy - U^{2D}_{\tau^h \beta^{2m+1}}(P \cdot s)| +$$
$$|\int_{-a}^{a} \int_{-a}^{a} (R(x, y) \cdot s(x, y)) \, dx \, dy - U^{2D}_{\tau^h \beta^{2m+1}}(R \cdot s)|. \tag{66}$$

Now, we make the following three observations. Due to (61),

$$\int_{-a}^{a} \int_{-a}^{a} (P(x, y) \cdot s(x, y)) \, dx \, dy - U^{2D}_{\tau^h \beta^{2m+1}}(P \cdot s) = 0, \tag{67}$$

and due to (59),

$$|\int_{-a}^{a} \int_{-a}^{a} (R(x, y) \cdot s(x, y)) \, dx \, dy - U^{2D}_{\tau^h \beta^{2m+1}}(R \cdot s)|$$
$$\leq |\int_{-a}^{a} \int_{-a}^{a} (R(x, y) \cdot s(x, y)) \, dx \, dy - T'^{2D,n}_{\beta^{2m+1}}(R \cdot s)| + |\sum_{(i,j) \in W} \tau^h_{ij} R(ih, jh)|. \tag{68}$$

Due to formulae (47) and (61), it is obvious that

$$|\int_{-a}^{a} \int_{-a}^{a} (R(x, y) \cdot s(x, y)) \, dx \, dy - T'^{2D,n}_{\beta^{2m+1}}(R \cdot s)| \sim O(h^{2p+4}),$$
$$\tag{69}$$

and the coefficients τ^h_{ij} are of the order h^2, hence,

$$|\sum_{(i,j) \in W} \tau^h_{ij} R(ih, jh)| \sim O(h^{2p+4}). \tag{70}$$

Finally, the conclusion of the Lemma follows from the combination of (66) – (70). $\qquad \square$

3.3 High-Order Center Corrected Trapezoidal Quadrature Rules for the Green's Function for the Helmholtz equation

In this section, we prove Theorem 3.10, which is the principal analytical tool of this paper. Theorem 3.10 describes the 10th-order center-corrected trapezoidal quadrature formulae for the Hankel function. It can be viewed as a special case of Theorem 3.4 with $p = 3$, and the singular function s the Hankel function H_0.

In the remainder of this paper, we will be using the following notation. For any $k \in C^+$ and $h > 0$, we will define the complex numbers D_0, D_1, D_2, D_3, D_4, D_5, via the formulae

$$D_0 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2, \tag{71}$$

$$D_1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)x^2\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^2 \cdot h^2, \tag{72}$$

$$D_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)x^4\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^4 \cdot h^2, \tag{73}$$

$$D_3 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)x^2 y^2\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^2 (qh)^2 \cdot h^2, \tag{74}$$

$$D_4 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)x^6\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^6 \cdot h^2, \tag{75}$$

$$D_5 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)x^4 y^2\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^4 (qh)^2 \cdot h^2. \tag{76}$$

The following Lemma is a simple consequence of the Sommerfeld formula (19).

Lemma 3.5 *For any $k \in \mathbb{C}^+$, r, x, $y \geq 0$, and $r = \sqrt{x^2 + y^2}$,*

$$H_0(kr) = \frac{1}{\pi} \cdot \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot x} \cdot e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot y}\, d\lambda, \tag{77}$$

where $r^2 = x^2 + y^2$, $x, y \geq 0$.

The following two technical lemmas follow immediately from the Sommerfeld formula (19).

Lemma 3.6 *For any $k \in \mathbb{C}^+$, and $a \geq 0$,*

$$\int_{-a}^{a} \int_{-a}^{a} H_0(kr)\, dx\, dy = \frac{4}{\pi} \cdot \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot$$
$$\frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a} - 1}{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda)} \cdot \frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a} - 1}{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda)}\, d\lambda, \tag{78}$$

with $r = \sqrt{x^2 + y^2}$.

Proof. Substituting (77) into the left side of (78), and changing the order of integration, we obtain

$$\int_{-a}^{a} \int_{-a}^{a} H_0(kr)\, dx\, dy = 4 \int_{0}^{a} \int_{0}^{a} H_0(kr)\, dx\, dy$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \int_{0}^{a} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot x}\, dx \cdot \int_{0}^{a} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot y}\, dy$$

$$= \frac{4}{\pi} \cdot \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot \frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a} - 1}{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda)} \cdot \frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a} - 1}{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda)}\, d\lambda. \tag{79}$$

$$\square$$

Lemma 3.7 *For any $k \in \mathbb{C}^+$, integer $n \geq 1$, and $a > 0$,*

$$\sum_{p=-n}^{n} \sum_{q=-n}^{n} H_0(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2 \cdot \beta_{pq} \tag{80}$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot h^2 \cdot \left(\frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a} - 1}{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot h} - 1} - \frac{1}{2} + \frac{1}{2} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a} \right)$$

$$\cdot \left(\frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a} - 1}{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot h} - 1} - \frac{1}{2} + \frac{1}{2} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a} \right) d\lambda, \tag{81}$$

with

$$h = a/n, \tag{82}$$

and β_{pq} equals 1 in the interior of the $(2n+1) \times (2n+1)$ square, equals $\frac{1}{2}$ in the interior of the edge, and equals $\frac{1}{4}$ on the corners of the square.

Proof. The trapezoidal sum (84) over the domain $[-a, a] \times [-a, a]$ is equal to four times the trapezoidal sum over the domain $[0, a] \times [0, a]$. In other words,

$$\sum_{p=-n}^{n} \sum_{q=-n}^{n} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2 \cdot \beta_{pq}$$

$$= 4 \cdot \sum_{p=0}^{n} \sum_{q=0}^{n} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2 \cdot \beta'_{pq}, \tag{83}$$

where β'_{pq} equals 1 in the interior of the $(n+1) \times (n+1)$ square, equals $\frac{1}{2}$ in the interior of the edge, and equals $\frac{1}{4}$ on the corners of the square. Substituting (77) into (83), and exchanging the order of integration and summation, we obtain

$$\sum_{p=-n}^{n} \sum_{q=-n}^{n} H_0(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2 \cdot \beta_{pq} \tag{84}$$

$$\frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot h^2 \cdot \left(\sum_{p=0}^{n} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot p \cdot h} - \frac{1 + e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a}}{2} \right)$$

$$\cdot \left(\sum_{q=0}^{n} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot q \cdot h} - \frac{1 + e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a}}{2} \right) \tag{85}$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot h^2 \cdot \left(\frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a} - 1}{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot h} - 1} - \frac{1}{2} + \frac{1}{2} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} - \lambda) \cdot a} \right)$$

$$\cdot \left(\frac{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a} - 1}{e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot h} - 1} - \frac{1}{2} + \frac{1}{2} e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} + \lambda) \cdot a} \right) d\lambda. \tag{86}$$

$$\square$$

.

Remark 3.1 As $a \to \infty$, the exponential terms $e^{(i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2 - \lambda^2} \pm \lambda) \cdot a)}$ in (78) and (81) tend to zero; this fact will be used in Lemma 3.8 below.

The following lemma provides an analytical form for the difference between the integral (78) and the trapezoidal sum (81). Its proof consists of combining Remark 3.1 with (78), (81).

Lemma 3.8 *For any $k \in \mathbb{C}^+$ and $h > 0$,*

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr) \, dx \, dy - \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \left(\frac{1}{(i\alpha_1)(i\alpha_2)} - \frac{h^2}{4} \frac{e^{i\alpha_1 h} + 1}{e^{i\alpha_1 h} - 1} \frac{e^{i\alpha_2 h} + 1}{e^{i\alpha_2 h} - 1} \right), \quad (87)$$

where

$$r = \sqrt{x^2 + y^2}, \quad (88)$$

$$\alpha_1 = \frac{\sqrt{2}}{2}(\sqrt{k^2 - \lambda^2} - \lambda), \alpha_2 = \frac{\sqrt{2}}{2}(\sqrt{k^2 - \lambda^2} + \lambda). \quad (89)$$

The following Lemma follows immediately from Lemma 3.8. It supplies an analytical form for the difference

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \left(x^{i-1} y^{j-1} H_0(k\sqrt{x^2 + y^2}) \right) dx \, dy - \sum_{(p,q) \neq (0,0)} \left((ph)^{i-1} (qh)^{j-1} H_0(k\sqrt{(ph)^2 + (qh)^2}) \right) \cdot h^2,$$

$$(90)$$

with $i = 1$, $j = 1$.

Remark 3.2 (90) is the right hand side of the equation (61), and thus is directly used in the calculation of coefficients τ_{ij}^h. Direct numerical subtraction of the integral and the sum in (90) leads to loss of accuracy because of cancellation errors, especially when i, j are relatively large. Lemma 3.9 below and Lemmas 6.1 – 6.5 in Appendix A, provide analytical formulae for (90) with $(i, j) = \{(1, 1), (3, 1), (5, 1), (3, 3), (7, 1), (5, 3)\}$, i.e., $D_0 - D_5$ defined by (71) – (76), so that cancellation errors are reduced.

Lemma 3.9 *For any $k \in \mathbb{C}^+$ and $h > 0$,*

$$D_0 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr) \, dx \, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \left(\frac{1}{(i\alpha_1)(i\alpha_2)} - \frac{h^2}{2} \cdot \frac{e^{i\alpha_1 h} + e^{i\alpha_2 h}}{(e^{i\alpha_1 h} - 1)(e^{i\alpha_2 h} - 1)} \right) \quad (91)$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \frac{(\frac{\lambda^2}{4} - \frac{k^2}{24})h^2 + z_1 + z_2 + i\sqrt{\frac{1}{2}}\lambda h(y_1 - y_2) + y_1 y_2}{(i\alpha_1)(i\alpha_2)(1 + x_1)(1 + x_2)}, \quad (92)$$

where the complex numbers x_1, x_2, y_1, y_2, z_1, z_2 are defined by the formulae

$$x_1 = \frac{e^{i\alpha_1 h} - 1}{i\alpha_1 h} - 1 = \sum_{n=1}^{\infty} \frac{(i\alpha_1 h)^n}{(n+1)!}, \qquad x_2 = \frac{e^{i\alpha_2 h} - 1}{i\alpha_2 h} - 1 = \sum_{n=1}^{\infty} \frac{(i\alpha_2 h)^n}{(n+1)!}, \quad (93)$$

17

$$y_1 = x_1 - \frac{i\alpha_1 h}{2} = \sum_{n=2}^{\infty} \frac{(i\alpha_1 h)^n}{(n+1)!}, \qquad y_2 = x_2 - \frac{i\alpha_2 h}{2} = \sum_{n=2}^{\infty} \frac{(i\alpha_2 h)^n}{(n+1)!}, \qquad (94)$$

$$z_1 = y_1 - \frac{(i\alpha_1 h)^2}{6} = \sum_{n=3}^{\infty} \frac{(i\alpha_1 h)^n}{(n+1)!}, \qquad z_2 = y_2 - \frac{(i\alpha_2 h)^2}{6} = \sum_{n=3}^{\infty} \frac{(i\alpha_2 h)^n}{(n+1)!}, \qquad (95)$$

and r, α_1, and α_2 are defined by (88), (89).

Proof. Substituting (77) into

$$\sum_{(p,q)\neq(0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2, \qquad (96)$$

and exchanging the order of integration and summation, we obtain

$$\sum_{(p,q)\neq(0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \left(\frac{h^2}{4} \frac{e^{i\alpha_1 h} + 1}{e^{i\alpha_1 h} - 1} \frac{e^{i\alpha_2 h} + 1}{e^{i\alpha_2 h} - 1} - \frac{h^2}{4} \right)$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \frac{h^2}{2} \cdot \frac{e^{i\alpha_1 h} + e^{i\alpha_2 h}}{(e^{i\alpha_1 h} - 1)(e^{i\alpha_2 h} - 1)}. \qquad (97)$$

Now, (91) follows immediately from the combination of (97), (78), and Remark 3.1. Substituting (93) into (91), we obtain

$$\frac{1}{(i\alpha_1)(i\alpha_2)} - \frac{h^2}{2} \cdot \frac{e^{i\alpha_1 h} + e^{i\alpha_2 h}}{(e^{i\alpha_1 h} - 1)(e^{i\alpha_2 h} - 1)}$$

$$= \frac{1}{(i\alpha_1)(i\alpha_2)} - \frac{1}{2} \cdot \frac{2 + i\alpha_1 h(1 + x_1) + i\alpha_2 h(1 + x_2)}{(i\alpha_1)(i\alpha_2)(1 + x_1)(1 + x_2)}$$

$$= \frac{x_1 + x_2 + x_1 x_2 - \frac{1}{2}i\alpha_1 h(1 + x_1) - \frac{1}{2}i\alpha_1 h(1 + x_1)}{(i\alpha_1)(i\alpha_2)(1 + x_1)(1 + x_2)}. \qquad (98)$$

Finally, (92) follows from the combination of (93), (94), (95) and (98). $\qquad \square$

Remark 3.3 Introducing the notation $z = \frac{\lambda}{k}$, we rewrite D_0 in the form

$$D_0 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr) \, dx \, dy - \sum_{(p,q)\neq(0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot h^2$$

$$= \frac{4h^2}{\pi} \int_{-\infty}^{\infty} \frac{d z}{\sqrt{1 - z^2}} \cdot \left(\frac{1}{(z^2 - 0.5) \cdot (kh)^2} - \frac{1}{2} \cdot \frac{e^{i\frac{\sqrt{2}}{2}(\sqrt{1-z^2}-z)kh} + e^{i\frac{\sqrt{2}}{2}(\sqrt{1-z^2}+z)kh}}{(e^{i\frac{\sqrt{2}}{2}(\sqrt{1-z^2}-z)kh} - 1)(e^{i\frac{\sqrt{2}}{2}(\sqrt{1-z^2}+z)kh} - 1)} \right). \qquad (99)$$

Thus, D_0 is entirely determined by k and h, and is of the form $h^2 \cdot f(k \cdot h)$. Similarly, D_1 is of the form $h^4 \cdot f(k \cdot h)$; D_2 and D_3 are of the form $h^6 \cdot f(k \cdot h)$; D_4 and D_5 are of the form $h^8 \cdot f(k \cdot h)$. In other words, except for the multiplicative factors (h^2, h^4, h^6, or h^8), $D_0 - D_5$ only depend on the product $k \cdot h$.

18

Remark 3.4 Even when Lemmas 6.1 – 6.5 are used, a certain loss of accuracy in the calculation of $D_1 - D_5$ is encountered (see Remark 3.2 above). Thus, evaluating D_0 in double precision, one obtains roughly 13 digits; for D_1 one gets 9 digits, and D_2 D_3 D_4 D_5 yield even fewer digits.

To avoid this difficulty, we utilized extended (real *32) precision to precompute the coefficients $D_0 - D_5$ for values of kh at appropriately chosen nodes on the boundary of the square $\Omega = [0, 1] \times [0, 1]$ in the complex plane, and used Lagrange interpolation to evaluate D_0 – D_5 for arbitrary points in Ω to 13 digits (see [8] for a detailed description of the technique). Thus, in all of our numerical experiments reported in Section 5 below, the coefficients $D_0 -$ D_5 were obtained by interpolation, rather than computed "from scratch".

Now, we are ready to formulate Theorem 3.10, which is the principal analytical tool of this paper (together with Lemmas 6.6, 6.7, 6.8). Theorem 3.10 describes the 10th-order center-corrected quadrature formula for the Green's function for the Helmholtz equation in two dimensions; this theorem is a special case of the high-order center-corrected trapezoidal rule for singular functions in two dimensions (see Theorem 3.4) with $p = 3$, and $s(x, y) = H_0^{(1)}(k\sqrt{x^2 + y^2})$. The 4th-order, 6th-order, and 8th-order center-corrected quadratures are similar and listed in Appendix B (see Lemma 6.6, 6.7 and 6.8). All the proofs are quite similar to that of Theorem 3.4, and are omitted.

Theorem 3.10 *Suppose that $n \geq 1$ is an integer, and a, h are two positive real numbers such that $h = a/n$. Suppose further that $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in c^8(R \times R)$, and that ϕ is zero outside the square $[-a, a] \times [-a, a]$. Then, for any $k \in \mathbb{C}^+$,*

$$\int_{-a}^{a} \int_{-a}^{a} \phi(x, y) \cdot H_0(k\sqrt{x^2 + y^2}) \, dx \, dy = U_{\tau^h}(\phi \cdot H_0) + O(h^{10}). \tag{100}$$

In (100),

$$U_{\tau^h}(\phi \cdot H_0) = T'^{2D}(\phi \cdot H_0) + \sum_{p,q \in S} \tau_{pq}^h \phi(ph, qh), \tag{101}$$

where

$$S = \{p, q \in Z : |p + q| \leq 3 \text{ and } |p - q| \leq 3\}, \tag{102}$$

$$T'^{2D}(\phi \cdot H_0) = \sum_{(p,q) \neq (0,0)} \left(\phi(ph, qh) \cdot H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \right) \cdot h^2, \tag{103}$$

and

$$\tau_{00}^h = D_0 - \frac{49}{18} \frac{D_1}{h^2} + \frac{7}{9} \frac{D_2}{h^4} + \frac{3}{2} \frac{D_3}{h^4} - \frac{1}{18} \frac{D_4}{h^6} - \frac{1}{2} \frac{D_5}{h^6}, \tag{104}$$

$$\tau_{\pm 10}^h = \tau_{0 \pm 1}^h = \frac{3}{4} \frac{D_1}{h^2} - \frac{13}{48} \frac{D_2}{h^4} - \frac{19}{24} \frac{D_3}{h^4} + \frac{1}{48} \frac{D_4}{h^6} + \frac{7}{24} \frac{D_5}{h^6}, \tag{105}$$

$$\tau_{\pm 20}^h = \tau_{0 \pm 2}^h = -\frac{3}{40} \frac{D_1}{h^2} + \frac{1}{12} \frac{D_2}{h^4} + \frac{1}{24} \frac{D_3}{h^4} - \frac{1}{120} \frac{D_4}{h^6} - \frac{1}{24} \frac{D_5}{h^6}, \tag{106}$$

$$\tau_{\pm 30}^h = \tau_{0 \pm 3}^h = \frac{1}{180} \frac{D_1}{h^2} - \frac{1}{144} \frac{D_2}{h^4} + \frac{1}{720} \frac{D_4}{h^6}, \tag{107}$$

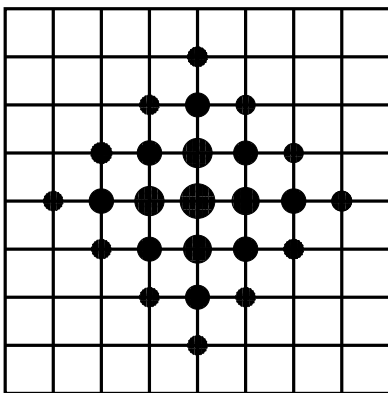$$\tau_{\pm 1 \pm 1}^h = \frac{5}{12} \frac{D_3}{h^4} - \frac{1}{6} \frac{D_5}{h^6}, \tag{108}$$

Figure 1: The 25 correction nodes

$$\tau^h_{\pm 1 \pm 2} = \tau^h_{\pm 2 \pm 1} = -\frac{1}{48}\frac{D_3}{h^4} + \frac{1}{48}\frac{D_5}{h^6}. \tag{109}$$

Remark 3.5 For simplicity, we assume here the function ϕ to be zero outside the square $[-a, a] \times [-a, a]$. Thus, the endpoint corrected trapezoidal rule $T'^{2D,n}_{\beta^{2m+1}}(\phi \cdot H_0)$ in Theorem 3.4 reduces to the standard trapezoidal rule $T'^{2D}(\phi \cdot H_0)$, and the integral and the sum on the square $[-a, a] \times [-a, a]$ are identical to those in R^2. This simplification allows the direct use of the analytical formulae for $D_0 - D_5$ (see Lemma 3.9 above and Lemmas 6.1 – 6.5 in Appendix A).

Remark 3.6 Combining Remark 3.3 with the definitions (104)–(109), we observe that each of the coefficients τ^h_{pq} in (104)–(109) has the form $h^2 \cdot f(k \cdot h)$; we will refer to the coefficients τ^h_{pq} as correction coefficients.

Remark 3.7 The set S defined in (102) contains 25 pairs of integers (p, q); in other words, corrections at 25 points around the singularity are required to construct a 10th-order quadrature formula (see Figure 1). In general, for any integer $p \geq 0$, $2p^2 + 2p + 1$ correction nodes are needed to obtain a quadrature of order $2p + 4$.

3.4 Fast Numerical Application of Discretized Lippmann-Schwinger Operators

In this section, we combine the 10th-order quadrature formula for the integral (100) with the FFT to obtain a fast procedure for the application of discretizations of the operator (12). We will denote by D the square $[-a, a] \times [-a, a]$ in R^2.

Suppose that $N \geq 1$ is an integer, h is a positive real number, and S is a set defined in (102). Suppose further that the coefficients $\tau^h_{i_1 i_2}$ are defined in (104)–(109). Then, we define a two-dimensional complex sequence $H = \{H_{i_1 i_2}\}$, $i_1, i_2 = -2N, ..., 2N$, as follows:

$$H_{i_1 i_2} = H_0(k\sqrt{(i_1 h)^2 + (i_2 h)^2}) + \tau^h_{i_1 i_2}/h^2, \tag{110}$$

when $(i_1, i_2) \in S$ and $(i_1, i_2) \neq (0, 0)$;

$$H_{00} = \tau_{00}^h / h^2, \tag{111}$$

and

$$H_{i_1 i_2} = H_0(k\sqrt{(i_1 h)^2 + (i_2 h)^2}), \tag{112}$$

otherwise. We define a complex sequence $\Phi = \{\Phi_{i_1 i_2}\}$, $i_1, i_2 = -N, ..., N$, to be the two-dimensional sequence defined by the formula

$$\Phi_{i_1 i_2} = \phi(i_1 h, i_2 h), \tag{113}$$

where $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a two-dimensional c^8-function which is zero outside D.

Lemma 3.11 *Suppose that the integers n, l_1, l_2 are such that $n \geq 1$, $-n \leq l_1 \leq n$, $-n \leq l_2 \leq n$, and that the real numbers a, x, y are such that $a > 0$, $-a \leq x \leq a$, $-a \leq y \leq a$. Suppose further that $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a c^8-function which is zero outside the square $[-a, a] \times [-a, a]$. Then for any $k \in \mathbb{C}^+$,*

$$\int_{-a}^{a} \int_{-a}^{a} \phi(x', y') \cdot H_0^{(1)}(k\sqrt{(x - x')^2 + (y - y')^2})\, dx'\, dy'$$

$$= \sum_{-n \leq i_1 \leq n} \sum_{-n \leq i_2 \leq n} \Phi_{i_1 i_2} \cdot H_{(l_1 - i_1)(l_2 - i_2)} + O(h^{10}), \tag{114}$$

where $h = a/n$, $x = l_1 h$, $y = l_2 h$, the two-dimensional sequence $\Phi = \{\Phi_{i_1 i_2}\}$, $i_1, i_2 = -n, ..., n$ is defined in (113), and the two-dimensional sequence $H = \{H_{j_1 j_2}\}$, $j_1, j_2 = -2n, ..., 2n$ is defined in (110) – (112).

Proof. Due to (100), (101),

$$\int_{-a}^{a} \phi(x', y') \cdot H_0^{(1)}(k\sqrt{(x - x')^2 + (y - y')^2})\, dx'\, dy'$$

$$= \sum_{(i_1, i_2) \in I'} \phi(i_1 h, i_2 h) \cdot H_0^{(1)}(k\sqrt{(l_1 h - i_1 h)^2 + (l_2 h - i_2 h)^2}) \cdot h^2$$

$$+ \sum_{(p,q) \in S} \tau_{pq}^h \, \phi(l_1 h + ph, l_2 h + qh) + O(h^{10}), \tag{115}$$

where

$$I' = \{i_1, i_2 \in \mathbb{Z} : |i_1| \leq n,\ |i_2| \leq n,\ (i_1, i_2) \neq (l_1, l_2)\}, \tag{116}$$

and S is defined in (102). Now, (114) follows immediately from the combination of (115) and the definitions in (110) – (113). $\qquad\square$

Remark 3.8 Obviously, (114) is the Toeplitz convolution of the two-dimensional sequences Φ, H, and as such, it can be rapidly calculated via the FFT (see Section 2.3 above). Thus,

$$\sum_{-n \leq i_1 \leq n} \sum_{-n \leq i_2 \leq n} \Phi_{i_1 i_2} \cdot H_{(l_1 - i_1)(l_2 - i_2)} = (\mathcal{F}^{2n})^{-1} (\mathcal{F}^{2n}(\Phi') \cdot \mathcal{F}^{2n}(H))_{l_1 l_2}, \tag{117}$$

where $-n \le l_1 \le n$, $-n \le l_2 \le n$, and the two-dimensional sequence $\Phi' = \{\Phi'_{ij}\}$, $i, j = -2n, ..., 2n$, is defined by

$$\Phi'_{ij} = \begin{cases} \Phi_{ij} & \text{if } |i| \le n \text{ and } |j| \le n \\ 0 & \text{if } |i| > n \text{ or } |j| > n \end{cases}. \tag{118}$$

Remark 3.9 For any point x outside the square $[-a, a] \times [-a, a]$, integral (12) is approximated via the standard trapezoidal rule. This approximation is 10th-order convergent, as long as $\phi \in c^{10}(R^2)$.

4 Description of the Procedure

This section describes the algorithm of the present paper in some detail. We start with an informal description, follow with a more detailed one, and finish with a complexity analysis.

4.1 Informal Description of the Algorithm

Below, we describe an FFT-based 10th-order iterative algorithm for the solution of the Lippmann-Schwinger equation

$$\psi(x) - k^2 \int_D G_k(x, y) V(y) \psi(y) \, dy = k^2 \int_D G_k(x, y) V(y) \phi(y) \, dy \tag{119}$$

in two dimensions, where $D = [-a, a] \times [-a, a]$, G_k is the Green's function for the Helmholtz equation in two dimension, i.e., $G_k(x, y) = -\frac{i}{4} \cdot H_0^{(1)}(k\|x - y\|)$, and $V(x)$ denotes the potential at a point x. Here, $\psi(x)$ and $\phi(x)$ are the scattered and the incident fields at a point x, respectively.

As discussed in Remark 3.9, once the scattered field ψ in the domain D is known, the scattered field ψ outside D can be calculated via the standard trapezoidal rule applied to (119). Therefore, we focus on obtaining the solution of (119) for $x \in D$. Obviously, (119) can be written as the linear system

$$(\mathbb{1} - A)\psi = A\phi, \tag{120}$$

where ψ is the unknown scattered field in D, ϕ is the given incident field in D, $\mathbb{1}$ is the identity operator, and A is the integral operator in (119). As discussed in Section 3, we use (114) to approximate the integral operator A on the functions ψ, ϕ. With the help of FFT (see Remark 3.8), we apply the discretized version of A rapidly to arbitrary vectors, and solve the linear system (120) iteratively. We use one of the most popular iterative solvers, BI-CGSTAB (the stabilized bi-conjugate gradient method) (see [10], [12]).

4.2 Detailed Description of the Algorithm

Comment [Choose principal parameters.]

22

Set the size of the scattering structure to $[-a, a] \times [-a, a]$.

Set the initial position of a point source to (x_0, y_0) to generate the incident field.

Choose precision ϵ to be achieved for the iterative solver.

Choose an integer n; set $h = \frac{a}{n}$; set the number of nodes discretizing a side of the square to $2n + 1$, so that the total number of nodes in the discretization is $N = (2n + 1)^2$.

Choose the wave number k for the incident and the scattered fields.

Construct a two-dimensional sequence $\{V_{ij}\}$, $i, j = -n, ..., n$ via the formula $V_{ij} = V(ih, jh)$.

Stage 1

Comment [Construct the values of the the Green's function.]

For the user-specified h and k, calculate the correction coefficients $D_0, D_1, D_2, D_3, D_4, D_5$ in (71)–(76) via interpolation (see Remark 3.4).

Construct the two-dimensional sequence H via the formulae (110) – (112) on the square $[-2a, 2a] \times [-2a, 2a]$, and calculate its Fourier transform using the two-dimensional FFT.

Stage 2

Comment [Construct the right hand side of the linear system (120).]

For a point source (x_0, y_0), construct a two-dimensional sequence $\Phi = \{\Phi_{ij}\}$, $i, j = -n, ..., n$ for the discretized incident field on the domain $[-a, a] \times [-a, a]$ via the formula (113). Construct the two-dimensional sequence $f = \{\Phi_{ij} \cdot V_{ij}\}$, $i, j = -n, ..., n$.

As in Remark 3.8, use the two-dimensional FFT to calculate the Toeplitz convolution of the sequences H and f.

Stage 3

Comment [Solve the linear system using iterative solvers.]

Use the iterative solver BI-CGSTAB to solve the linear system $(\mathbb{1} - A)\,\psi = A\,\phi$ to the predetermined precision ϵ. The multiplication $A\psi$ is done via the combination of FFT and the Toeplitz convolution of the two-dimensional sequences H and g, where $g = \{\Psi_{ij} \cdot V_{ij}\}$, $i, j = -n, \cdots, n$ with $\Psi_{ij} = \psi(ih, jh)$ (see Remark 3.8).

The solution is the scattered field at the N discretization points in the square $[-a, a] \times [-a, a]$.

Stage 4

Comment [Calculate the scattered field at any point in the two-dimensional plane.]

Use interpolation to obtain the scattered field at any arbitrary point in the square $[-a, a] \times [-a, a]$, based on the scattered field at the N discretization points. As in Remark 3.9, apply the trapezoidal rule to (119) to obtain the scattered field at any arbitrary point outside the square $[-a, a] \times [-a, a]$.

4.3 Complexity Analysis

A brief analysis of the complexity of the algorithm is given below.

In stage 1, the construction of the two-dimensional sequence H costs $O(N)$, where N is the total number of the discretization points on the square $[-a, a] \times [-a, a]$, i.e., $N = (2n+1)^2$. The two-dimensional FFT costs $O(N \log(N))$. Thus, the CPU time cost of the stage 1 is of the order $O(N \log(N))$.

In stage 2, the construction of the two dimensional sequences Φ, f costs $O(N)$, and the two-dimensional FFT costs $O(N \log(N))$. Thus, the CPU time cost of the stage 2 is of order $O(N \log(N))$.

The CPU time cost of the stage 3 is of order $O(N_{iter} \cdot N \log(N))$, where N_{iter} is the number of iterations required by the iterative solver to get the pre-determined precision ϵ.

In stage 4, the CPU time cost of interpolating the field at any point in $[-a, a] \times [-a, a]$ $O(N)$.

Summing up the CPU times above, we obtain the time estimate for the algorithm

$$T = \alpha(N_{iter} \cdot N \log(N)) + \beta \cdot N + \gamma, \tag{121}$$

where N is the total number of discretization points, N_{iter} is the number of iterations required by the iterative solvers to reach the precision ϵ, and the coefficients α, β, γ are determined by the computer system, implementation, etc.

The storage requirements of the algorithm are determined by the total number of discretization points N and the number of iterations K performed before restarting the iterative solvers, and are of the form

$$S = O(K \cdot N). \tag{122}$$

5   Numerical Examples

The algorithm of Section 4 has been implemented in FORTRAN 77 in double precision. In this section, we illustrate the performance of the scheme as applied to two scattering objects: a Gaussian and a crude model of the human skull. The experiments were carried out on a 2.8 GHz Pentium D desktop with 2 Gb of RAM and an L2 cache of 1 Mb. The calculations reported in Tables 1 and 3 were carried out with a requested accuracy of 10^{-13}; the calculations reported in Tables 2 and 4 were carried out with a requested accuracy of 10^{-9}. We restarted the BI-CGSTAB every 5 steps.

Tables 1 - 4 illustrate the numerical behavior of the scattered field at arbitrary far-field points, generated by the potential V defined in (3); the incident field is produced by a single point source. In Tables 1 and 2, we set the potential $V(x, y) = e^{-40(x^2+y^2)}$. Tables 3 and 4 illustrate the numerical behavior of the scattered field, generated by a model of the human skull, as shown in Figures 2 and 3. The headings of the Tables are as follows:

k is the wave number defined in (2);

the computational grid is $N \times N$ for a total of N^2 discretization points;

the computational grid is $size_{obj}$ wavelengths $\times$ $size_{obj}$ wavelengths;

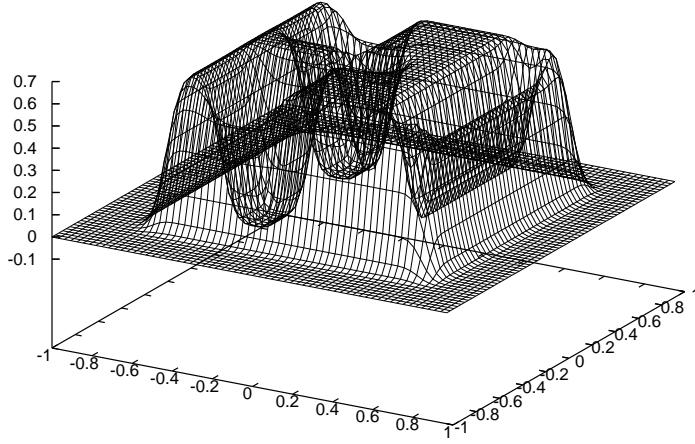N_λ is the number of discretization points per wavelength;
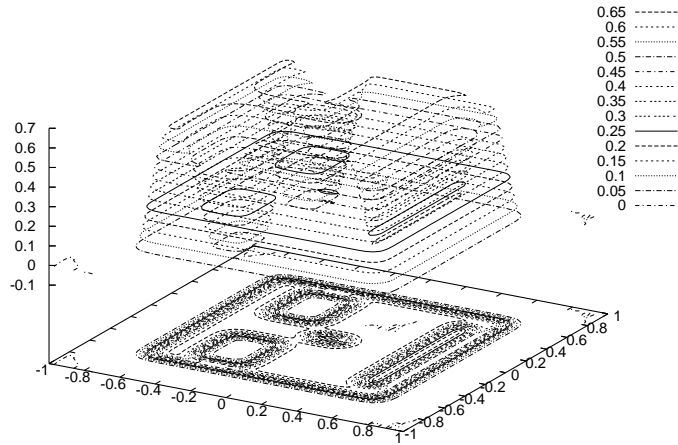
Figure 2: The human skull model

Figure 3: The human skull model viewed from the top

Table 1: 10th order convergence of the algorithm for Gaussian objects

k	N	$size_{obj}$	N_λ	E_{rel}	N_{iter}	t_{CPU}
25	50	8λ	6.28	6.33E-06	16	1.2E-01
25	100	8λ	12.6	6.63E-09	16	5.9E-01
25	200	8λ	25.1	6.04E-12	16	2.6E+00
25	400	8λ	50.2	7.25E-13	16	1.1E+01
25	800	8λ	100	6.32E-13	16	5.5E+01
25	1600	8λ	201	-	16	2.4E+02

Table 2: Gaussian objects with a fixed number of points per wavelength

k	N	$size_{obj}$	N_λ	E_{rel}	N_{iter}	t_{CPU}
25	50	8λ	6.28	6.33E-06	14	1.1E-01
50	100	16λ	6.28	3.80E-06	20	7.2E-01
100	200	32λ	6.28	4.44E-06	33	5.2E+00
200	400	64λ	6.28	8.26E-06	61	4.4E+01
400	800	128λ	6.28	1.60E-05	171	6.2E+02
800	1600	255λ	6.28	-	891	1.4E+04

Table 3: 10th order convergence of the algorithm for the simulated human skull

k	N	$size_{obj}$	N_λ	E_{rel}	N_{iter}	t_{CPU}
25	50	8λ	6.28	1.18E-04	134	1.1E+00
25	100	8λ	12.6	1.91E-07	133	4.7E+00
25	200	8λ	25.1	2.05E-10	134	2.1E+01
25	400	8λ	50.2	4.56E-12	135	9.7E+01
25	800	8λ	100	7.55E-12	132	4.7E+02
25	1600	8λ	201	-	132	2.0E+03

Table 4: The simulated human skull with a fixed number of points per wavelength

k	N	$size_{obj}$	N_λ	E_{rel}	N_{iter}	t_{CPU}
25	50	8λ	6.28	1.17E-04	97	7.6E-01
50	100	16λ	6.28	1.55E-05	165	5.8E+00
100	200	32λ	6.28	1.03E-05	328	5.2E+01
200	400	64λ	6.28	1.69E-05	756	5.5E+02
400	800	128λ	6.28	2.21E-05	3286	1.2E+04
800	1600	255λ	6.28	-	13568	2.1E+05

E_{rel} is the average of the relative errors of the solution for the scattered field at twenty chosen far-field points;

N_{iter} is the number of iterations used by the BI-CGSTAB;

t_{CPU} is the CPU time required in seconds.

The following observations can be made from the tables above, and from the more detailed numerical tests performed by the authors.

1. For smooth scattering objects, the numerical algorithm of Section 4 displays 10th-order convergence; the CPU time required to obtain requested precision is proportional to $N_{iter} \cdot N^2 \log N$, where N^2 is the total number of discretization points, N_{iter} is determined by the requested precision, the number of iterations before restarting the iterative solver, the size and the structure of the scattering objects.

2. For sufficiently smooth scatterers, the relative precision of the solution is determined by the number of discretization points per wavelength. For example, to obtain 5-digit precision, we need roughly 6.5 points per wavelength. Thus, with our constraint of 2 GB RAM, five digits can be obtained for scattering objects as large as 300 wavelengths $\times$ 300 wavelengths.

3. The number of iterations increases dramatically as the size of the scattering object increases, as shown in Tables 2, 4.

6 Conclusions

In this paper, we construct an iterative algorithm for the solution of two-dimensional forward scattering problems. The scheme is based on the combination of high-order quadrature formulae, rapid numerical application of the integral operator in the Lippmann-Schwinger equation, and the stabilized bi-conjugate gradient method (BI-CGSTAB). As illustrated via several numerical examples, the scheme is $(2p+4)^{th}$ $(p = 0, 1, 2, 3, ...)$ order convergent; the computational complexity of the algorithm is $O(N_{iter} \cdot N^2 \log N)$, where N_{iter} is the number of iterations used by the iterative solver, and N^2 is the total number of discretization points.

The approach we use for the design of high order center-corrected quadrature formulae introduced in this paper is not limited to functions of the form (13) in two dimensions; it is also applicable to functions of the form (14) in three dimensions, as well as many similar situations. Furthermore, the method does not require access to each of the functions P, Q separately in (13) and (14); it only requires the evaluation of the whole kernel K given a pair of points (x, y). Quadrature formulae of order higher than 10 can also be constructed, though the derivations become more tedious. Finally, the scheme is easily extended to rectangular regions of the form $[-a, a] \times [-b, b]$, even though this paper only discusses on the square region $[-a, a] \times [-a, a]$.

Appendix A

Lemmas 6.1 – 6.5 below provide analytical formulae for

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(x^{i-1}y^{j-1}\,H_0(k\sqrt{x^2+y^2})\right)dx\,dy - \sum_{(p,q)\neq(0,0)}\left((ph)^{i-1}(qh)^{j-1}\,H_0(k\sqrt{(ph)^2+(qh)^2})\right)\cdot h^2,$$

(123)

with $(i,j)=\{(3,1),(5,1),(3,3),(7,1),(5,3)\}$. The proofs are straightforward and tedious, and use the help of Mathematica.

Lemma 6.1 *For any $k\in\mathbb{C}^+$ and $h>0$,*

$$D_1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_0^{(1)}(kr)x^2\,dx\,dy - \sum_{(p,q)\neq(0,0)} H_0^{(1)}(k\sqrt{(ph)^2+(qh)^2})\cdot(ph)^2\cdot h^2$$

$$= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{2}{(i\alpha_1)^3(i\alpha_2)}-\frac{h^4}{2}\cdot\frac{e^{i\alpha_1 h}(e^{i\alpha_1 h}+1)(e^{i\alpha_2 h}+1)}{(e^{i\alpha_1 h}-1)^3(e^{i\alpha_2 h}-1)}\right) \tag{124}$$

$$= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{2}{\alpha_1^3\alpha_2(1+x_1)^3(1+x_2)}$$

$$\cdot\left(\frac{(\alpha_2 h)^2}{12}+3z_1+z_2+3y_1^2+\frac{3}{2}y_1(i\alpha_1 h)+3y_1y_2+\frac{3}{2}y_1(i\alpha_2 h)+\frac{3}{2}y_2(i\alpha_1 h)\right.$$

$$+x_1^3+3x_1^2x_2+x_1^3x_2-\frac{1}{2}i\alpha_2 hy_2+\frac{1}{2}\alpha_1^2h^2(x_1^2+2x_1)$$

$$\left.+\frac{3}{4}\alpha_1\alpha_2 h^2(x_1x_2+x_1+x_2)+\frac{1}{4}i\alpha_1^2\alpha_2 h^3(1+x_1)^2(1+x_2)\right), \tag{125}$$

where $r,\alpha_1,\alpha_2,x_1,x_2,y_1,y_2,z_1,z_2$ are defined by (88), (89), and (93)–(95).

Lemma 6.2 *For any $k \in \mathbb{C}^+$ and $h > 0$,*

$$D_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)\, x^4\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^4 \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}}$$

$$\cdot \left(\frac{24}{(i\alpha_1)^5(i\alpha_2)} - \frac{h^6}{2} \cdot \frac{e^{i\alpha_1 h} + 11e^{2i\alpha_1 h} + 11e^{3i\alpha_1 h} + e^{4i\alpha_1 h}}{(e^{i\alpha_1 h} - 1)^5} \cdot \frac{e^{i\alpha_2 h} + 1}{e^{i\alpha_2 h} - 1} \right)$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \frac{1}{\alpha_1^5 \alpha_2 (1 + x_1)^5 (1 + x_2)}$$

$$\cdot \Bigg(2(i\alpha_2 h)^2 + (i\alpha_2 h)^3 + 5(i\alpha_1 h)(i\alpha_2 h)^2 + \frac{3}{10}(i\alpha_2 h)^4 + \frac{20}{3}(i\alpha_1 h)^2(i\alpha_2 h)^2$$

$$+ \frac{5}{2}(i\alpha_1 h)(i\alpha_2 h)^3 + \frac{1}{2}(i\alpha_1 h)^4(i\alpha_2 h) + 4x_1(i\alpha_1 h)^4 + \frac{45}{2}x_1(i\alpha_1 h)^3(i\alpha_2 h)$$

$$+ 2x_1(i\alpha_1 h)^4(i\alpha_2 h) + 45x_1^2(i\alpha_1 h)^3 + 25x_1^2(i\alpha_1 h)^2(i\alpha_2 h) + 6x_1^2(i\alpha_1 h)^4$$

$$+ \frac{45}{2}x_1^2(i\alpha_1 h)^3(i\alpha_2 h) + 3x_1^2(i\alpha_1 h)^4(i\alpha_2 h) + 15x_1^3(i\alpha_1 h)^3 + 4x_1^3(i\alpha_1 h)^4$$

$$+ \frac{15}{2}x_1^3(i\alpha_1 h)^3(i\alpha_2 h) + 2x_1^3(i\alpha_1 h)^4(i\alpha_2 h) + x_1^4(i\alpha_1 h)^4 + \frac{1}{2}x_1^4(i\alpha_1 h)^4(i\alpha_2 h)$$

$$+ \frac{15}{2}x_2(i\alpha_1 h)^3(i\alpha_2 h) + \frac{1}{2}x_2(i\alpha_1 h)^4(i\alpha_2 h) + 50x_1 x_2(i\alpha_1 h)^2(i\alpha_2 h)$$

$$+ \frac{45}{2}x_1 x_2(i\alpha_1 h)^3(i\alpha_2 h) + 2x_1 x_2(i\alpha_1 h)^4(i\alpha_2 h) + 25x_1^2 x_2(i\alpha_1 h)^2(i\alpha_2 h)$$

$$+ \frac{45}{2}x_1^2 x_2(i\alpha_1 h)^3(i\alpha_2 h) + 3x_1^2 x_2(i\alpha_1 h)^4(i\alpha_2 h) + \frac{15}{2}x_1^3 x_2(i\alpha_1 h)^3(i\alpha_2 h)$$

$$+ 2x_1^3 x_2(i\alpha_1 h)^4(i\alpha_2 h) + \frac{1}{2}x_1^4 x_2(i\alpha_1 h)^4(i\alpha_2 h) + 12w_2(i\alpha_2 h) + 30z_2(i\alpha_1 h)(i\alpha_2 h)$$

$$+ 40y_2(i\alpha_1 h)^2(i\alpha_2 h) + 15y_1(i\alpha_1 h)(i\alpha_2 h)^2 + 30y_1 y_2(i\alpha_1 h)(i\alpha_2 h) - 120u_1 - 24u_2$$

$$- 180w_1(i\alpha_1 h) - 60w_2(i\alpha_1 h) - 60w_1(i\alpha_2 h) - 160z_1(i\alpha_1 h)^2 - 90z_1(i\alpha_1 h)(i\alpha_2 h)$$

$$- 80z_2(i\alpha_1 h)^2 + 35y_1(i\alpha_1 h)^3 - 40y_1(i\alpha_1 h)^2(i\alpha_2 h) - 130y_1^2(i\alpha_1 h)^2$$

$$- 180y_1^2(i\alpha_1 h)(i\alpha_2 h) - 240y_1^3(i\alpha_1 h) - 120y_1^3(i\alpha_2 h) - 120y_1^4 - 30y_2(i\alpha_1 h)^3$$

$$- 180y_1 y_2(i\alpha_1 h)^2 - 360y_1^2 y_2(i\alpha_1 h) - 240y_1^3 y_2 - 20z_1(i\alpha_2 h)^2 - 240z_1^2 - 120z_1 z_2$$

$$- 360y_1^2(i\alpha_1 h) - 240y_1^3 - 120y_1^2(i\alpha_2 h) - 240y_1 y_2(i\alpha_1 h) - 240y_1^2 y_2$$

$$- 24x_1^5 - 120x_1^4 x_2 - 24x_1^5 x_2 \Bigg), \tag{126}$$

where

$$w_1 = z_1 - \frac{(i\alpha_1 h)^3}{24} = \sum_{n=4}^{\infty} \frac{(i\alpha_1 h)^n}{(n+1)!}, \ w_2 = z_2 - \frac{(i\alpha_2 h)^3}{24} = \sum_{n=4}^{\infty} \frac{(i\alpha_2 h)^n}{(n+1)!}, \tag{127}$$

$$u_1 = w_1 - \frac{(i\alpha_1 h)^4}{120} = \sum_{n=5}^{\infty} \frac{(i\alpha_1 h)^n}{(n+1)!}, \ u_2 = w_2 - \frac{(i\alpha_2 h)^4}{120} = \sum_{n=5}^{\infty} \frac{(i\alpha_2 h)^n}{(n+1)!}, \tag{128}$$

and $r, \alpha_1, \alpha_2, x_1, x_2, y_1, y_2, z_1, z_2$ are defined by (88), (89) and (93)–(95).

Lemma 6.3 *For any $k \in \mathbb{C}^+$ and $h > 0$,*

$$D_3 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)\, x^2\, y^2\, dx\, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^2 (qh)^2 \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \left(\frac{4}{(i\alpha_1)^3 (i\alpha_2)^3} - h^6 \cdot \frac{e^{i\alpha_1 h}(e^{i\alpha_1 h} + 1)}{(e^{i\alpha_1 h} - 1)^3} \cdot \frac{e^{i\alpha_1 h}(e^{i\alpha_1 h} + 1)}{(e^{i\alpha_1 h} - 1)^3} \right) \qquad (129)$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \frac{-4}{\alpha_1^3 \alpha_2^3 (1 + x_1)^3 (1 + x_2)^3}$$

$$\cdot \Bigg(\frac{1}{240}(i\alpha_1 h)^4 + \frac{1}{240}(i\alpha_2 h)^4 + \frac{3}{4} z_1 (i\alpha_1 h)^2 + \frac{3}{4} z_2 (i\alpha_2 h)^2$$

$$+ \frac{9}{2}(i\alpha_1 h)(i\alpha_2 h)(z_1 + z_2) + \frac{15}{4} z_1 (i\alpha_2 h)^2 + \frac{15}{4} z_2 (i\alpha_1 h)^2 - \frac{3}{2} y_1 (i\alpha_1 h)^2 (i\alpha_2 h)$$

$$- \frac{3}{2} y_2 (i\alpha_1 h)(i\alpha_2 h)^2 + 3u_1 + 3u_2 + \frac{9}{2} w_2 (i\alpha_1 h) + \frac{9}{2} w_1 (i\alpha_2 h)$$

$$+ \frac{3}{2} w_1 (i\alpha_1 h) + \frac{3}{2} w_2 (i\alpha_2 h) - \frac{9}{4}(i\alpha_1 h)(i\alpha_2 h)(z_1 + z_2) + 3z_1^2 + 3z_2^2$$

$$+ 9z_1 z_2 - \frac{1}{2} y_1 (i\alpha_1 h)^3 - \frac{1}{2} y_2 (i\alpha_2 h)^3 - \frac{1}{2} y_1^2 (i\alpha_1 h)^2 - \frac{1}{2} y_2^2 (i\alpha_2 h)^2$$

$$+ \frac{9}{4}(i\alpha_1 h)(i\alpha_2 h)(3y_1 y_2 + \frac{1}{6} y_1 (i\alpha_2 h) + \frac{1}{6} y_2 (i\alpha_1 h)) + \frac{9}{8} y_1 (i\alpha_1 h)^2 (i\alpha_2 h)$$

$$+ \frac{3}{8} y_1 (i\alpha_2 h)^3 + \frac{9}{4} y_1^2 (i\alpha_1 h)(i\alpha_2 h) + \frac{9}{4} y_1^2 (i\alpha_2 h)^2 + \frac{3}{2} y_1^3 (i\alpha_2 h)$$

$$+ \frac{3}{8} y_2 (i\alpha_1 h)^3 + \frac{9}{8} y_2 (i\alpha_1 h)(i\alpha_2 h)^2 + \frac{9}{4} y_1 y_2 (i\alpha_1 h)^2 + \frac{9}{4} y_1 y_2 (i\alpha_2 h)^2$$

$$+ \frac{9}{2} y_1^2 y_2 (i\alpha_1 h) + 9 y_1^2 y_2 (i\alpha_2 h) + 3 y_1^3 y_2 + \frac{9}{4} y_2^2 (i\alpha_1 h)^2 + \frac{9}{4} y_2^2 (i\alpha_1 h)(i\alpha_2 h)$$

$$+ 9 y_1 y_2^2 (i\alpha_1 h) + \frac{9}{2} y_1 y_2^2 (i\alpha_2 h) + 9 y_1^2 y_2^2 + \frac{3}{2} y_2^3 (i\alpha_1 h) + 3 y_1 y_2^3$$

$$- \frac{1}{4}(i\alpha_1 h)^2 (i\alpha_2 h)^2 (2x_1 + x_1^2 + 2x_2 + 4x_1 x_2 + 2x_1^2 x_2 + x_2^2$$

$$+ 2x_1 x_2^2 + x_1^2 x_2^2) + \frac{3}{2} y_1^2 (i\alpha_1 h) + y_1^3 + \frac{3}{2} y_2^2 (i\alpha_2 h) + y_2^3 + \frac{9}{2} y_1^2 (i\alpha_2 h)$$

$$+ 9 y_1 y_2 (i\alpha_1 h + i\alpha_2 h) + 9 y_1^2 y_2 + \frac{9}{2} y_2^2 (i\alpha_1 h) + 9 y_1 y_2^2$$

$$- \frac{3}{4}(i\alpha_1 h)^2 (i\alpha_2 h)(x_1^2 + 2x_1 x_2 + x_1^2 x_2)$$

$$- \frac{3}{4}(i\alpha_1 h)(i\alpha_2 h)^2 (x_2^2 + 2x_1 x_2 + x_1 x_2^2) + 3 x_1^3 x_2^2 + 3 x_1^2 x_2^3 + x_1^3 x_2^3 \Bigg), \qquad (130)$$

where $r, \alpha_1, \alpha_2, x_1, x_2, y_1, y_2, z_1, z_2, w_1, w_2, u_1, u_2$ are defined by (88), (89), (93)–(95), (127) and (128).

Lemma 6.4 *For any $k \in \mathbb{C}^+$ and $h > 0$,*

$$D_4 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr) \, x^6 \, dx \, dy - \sum_{(p,q) \neq (0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^6 \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}}$$

$$\cdot \left(\frac{720}{\alpha_1^7 \alpha_2} - \frac{h^8}{2} \cdot \frac{e^{i\alpha_1 h} + 57 e^{2i\alpha_1 h} + 302 e^{3i\alpha_1 h} + 302 e^{4i\alpha_1 h} + 57 e^{5i\alpha_1 h} + e^{6i\alpha_1 h}}{(e^{i\alpha_1 h} - 1)^7} \cdot \frac{e^{i\alpha_2 h} + 1}{e^{i\alpha_2 h} - 1} \right)$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \frac{1}{\alpha_1^7 \alpha_2 (1 + x_1)^7 (1 + x_2)} \cdot (A + B), \tag{131}$$

where

$$\begin{aligned}
A =\ & 60(\alpha_2 h)^2 - 30(i\alpha_2 h)^3 - 210(i\alpha_1 h)(i\alpha_2 h)^2 - 9(\alpha_2 h)^4 - 105(\alpha_1 h)(\alpha_2 h)^3 \\
& -385(\alpha_1 h)^2(\alpha_2 h)^2 + 37800 y_1^2(i\alpha_1 h) + 25200 y_1^3 + 7560 y_1^2(i\alpha_2 h) \\
& +15120 y_1 y_2(i\alpha_1 h) + 15120 y_1^2 y_2 + 15120 x_1^5 + 5040 x_1^6 + 720 x_1^7 + 25200 x_1^4 x_2 \\
& +15120 x_1^5 x_2 + 5040 x_1^6 x_2 + 720 x_1^7 x_2 + 5040 u_1 + 720 u_2 + 12600 w_1(i\alpha_1 h) \\
& -360 w_2(i\alpha_2 h) + 2520 w_2(i\alpha_1 h) + 2520 w_1(i\alpha_2 h) - 17220(\alpha_1 h)^2 z_1 \\
& +6300 z_1(i\alpha_1 h)(i\alpha_2 h) + 1260 z_2(\alpha_1 h)(\alpha_2 h) - 4620(\alpha_1 h)^2 z_2 + 15120 z_1^2 \\
& +2940 y_1(i\alpha_1 h)^3 - 6090 y_1(\alpha_1 h)^2(i\alpha_2 h) - 34440 y_1^2(\alpha_1 h)^2 - 18900 y_1^2(\alpha_1 h)(\alpha_2 h) \\
& +50400 y_1^3(i\alpha_1 h) + 12600 y_1^3(i\alpha_2 h) + 25200 y_1^4 + 3150 y_2(i\alpha_1 h)^3 \\
& -18900 y_1 y_2(\alpha_1 h)^2 + 37800 y_1^2 y_2(i\alpha_1 h) + 25200 y_1^3 y_2 - 840 z_1(\alpha_2 h)^2 + 5040 z_1 z_2 \\
& +2310 y_2(\alpha_1 h)^2(i\alpha_2 h) + 630 y_1(i\alpha_1 h)(\alpha_2 h)^2 + 1260 y_1 y_2(\alpha_1 h)(\alpha_2 h) \\
& -63(i\alpha_1 h)^5 - 301(i\alpha_1 h)^4(i\alpha_2 h) + (\alpha_1 h)^6 + \frac{63}{2}(\alpha_1 h)^5(\alpha_2 h) + \frac{1}{2}(\alpha_1 h)^6(i\alpha_2 h) \\
& -2408 x_1(\alpha_1 h)^4 - 3150 x_1(\alpha_1 h)^3(\alpha_2 h) - 315 x_1(i\alpha_1 h)^5 - 1204 x_1(i\alpha_1 h)^4(i\alpha_2 h) \\
& +6 x_1(\alpha_1 h)^6 + \frac{315}{2} x_1(\alpha_1 h)^5(\alpha_2 h) + 3 x_1(\alpha_1 h)^6(i\alpha_2 h) - 6300 x_1^2(i\alpha_1 h)^3 \\
& +1680 x_1^2(\alpha_1 h)^2(i\alpha_2 h) - 3612 x_1^2(\alpha_1 h)^4 - 3150 x_1^2(\alpha_1 h)^3(\alpha_2 h) - 630 x_1^2(i\alpha_1 h)^5 \\
& -1806 x_1^2(i\alpha_1 h)^4(i\alpha_2 h) + 15 x_1^2(\alpha_1 h)^6 + 315 x_1^2(\alpha_1 h)^5(\alpha_2 h) + \frac{15}{2} x_1^2(\alpha_1 h)^6(i\alpha_2 h) \\
& -2100 x_1^3(i\alpha_1 h)^3 - 2408 x_1^3(\alpha_1 h)^4 - 1050 x_1^3(\alpha_1 h)^3(\alpha_2 h) - 630 x_1^3(i\alpha_1 h)^5 \\
& -1204 x_1^3(i\alpha_1 h)^4(i\alpha_2 h) + 20 x_1^3(\alpha_1 h)^6 + 315 x_1^3(\alpha_1 h)^5(\alpha_2 h) + 10 x_1^3(\alpha_1 h)^6(i\alpha_2 h) \\
& -602 x_1^4(\alpha_1 h)^4 - 315 x_1^4(i\alpha_1 h)^5 - 301 x_1^4(i\alpha_1 h)^4(i\alpha_2 h) + 15 x_1^4(\alpha_1 h)^6 \\
& +\frac{315}{2} x_1^4(\alpha_1 h)^5(\alpha_2 h) + \frac{15}{2} x_1^4(\alpha_1 h)^6(i\alpha_2 h) - 63 x_1^5(i\alpha_1 h)^5 + 6 x_1^5(\alpha_1 h)^6 \\
& +\frac{63}{2} x_1^5(\alpha_1 h)^5(\alpha_2 h) + 3 x_1^5(\alpha_1 h)^6(i\alpha_2 h) + x_1^6(\alpha_1 h)^6 + \frac{1}{2} x_1^6(\alpha_1 h)^6(i\alpha_2 h), \tag{132}
\end{aligned}$$

$$B = -1050x_2(\alpha_1 h)^3(\alpha_2 h) - 301x_2(\alpha_1 h)^4(i\alpha_2 h) + \frac{63}{2}x_2(\alpha_1 h)^5(\alpha_2 h)$$

$$+\frac{1}{2}x_2(\alpha_1 h)^6(i\alpha_2 h) + 3360x_1 x_2(\alpha_1 h)^2(i\alpha_2 h) - 3150x_1 x_2(\alpha_1 h)^3(\alpha_2 h)$$

$$-1204x_1 x_2(\alpha_1 h)^4(i\alpha_2 h) + \frac{315}{2}x_1 x_2(\alpha_1 h)^5(\alpha_2 h) + 3x_1 x_2(\alpha_1 h)^6(i\alpha_2 h)$$

$$+1680x_1^2 x_2(\alpha_1 h)^2(i\alpha_2 h) - 3150x_1^2 x_2(\alpha_1 h)^3(\alpha_2 h) - 1806x_1^2 x_2(\alpha_1 h)^4(i\alpha_2 h)$$

$$+315x_1^2 x_2(\alpha_1 h)^5(\alpha_2 h) + \frac{15}{2}x_1^2 x_2(\alpha_1 h)^6(i\alpha_2 h) - 1050x_1^3 x_2(\alpha_1 h)^3(\alpha_2 h)$$

$$-1204x_1^3 x_2(\alpha_1 h)^4(i\alpha_2 h) + 315x_1^3 x_2(\alpha_1 h)^5(\alpha_2 h) + 10x_1^3 x_2(\alpha_1 h)^6(i\alpha_2 h)$$

$$-301x_1^4 x_2(\alpha_1 h)^4(i\alpha_2 h) + \frac{315}{2}x_1^4 x_2(\alpha_1 h)^5(\alpha_2 h) + \frac{15}{2}x_1^4 x_2(\alpha_1 h)^6(i\alpha_2 h)$$

$$+\frac{63}{2}x_1^5 x_2(\alpha_1 h)^5(\alpha_2 h) + 3x_1^5 x_2(\alpha_1 h)^6(i\alpha_2 h) + \frac{1}{2}x_1^6 x_2(\alpha_1 h)^6(i\alpha_2 h), \tag{133}$$

and where $r, \alpha_1, \alpha_2, x_1, x_2, y_1, y_2, z_1, z_2, w_1, w_2, u_1, u_2$ are defined by (88), (89), (93)–(95), (127) and (128).

Lemma 6.5 *For any* $k \in \mathbb{C}^+$ *and* $h > 0$,

$$D_5 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0^{(1)}(kr)\, x^4\, y^2\, dx\, dy - \sum_{(p,q)\neq(0,0)} H_0^{(1)}(k\sqrt{(ph)^2 + (qh)^2}) \cdot (ph)^4 (qh)^2 \cdot h^2$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \left(\frac{48}{\alpha_1^5 \alpha_2^3} - h^8 \cdot \frac{e^{i\alpha_1 h} + 11e^{2i\alpha_1 h} + 11e^{3i\alpha_1 h} + e^{4i\alpha_1 h}}{(e^{i\alpha_1 h} - 1)^5} \cdot \frac{e^{i\alpha_2 h} \cdot (e^{i\alpha_2 h} + 1)}{(e^{i\alpha_2 h} - 1)^3} \right)$$

$$= \frac{4}{\pi} \int_{-\infty}^{\infty} \frac{d\lambda}{\sqrt{k^2 - \lambda^2}} \cdot \frac{1}{\alpha_1^5 \alpha_2^3 (1 + x_1)^5 (1 + x_2)^3} \cdot (C + D) \tag{134}$$

where

$$C = \frac{1}{5}(\alpha_2 h)^4 + 240u_1 + 360w_1(i\alpha_1 h) + 144u_2 + 360w_2(i\alpha_1 h)$$

$$+360w_1(i\alpha_2 h) + 72w_2(i\alpha_2 h) - 320z_1(\alpha_1 h)^2 - 540z_1(\alpha_1 h)(\alpha_2 h)$$

$$-480z_2(\alpha_1 h)^2 - 300z_1(\alpha_2 h)^2 - 180z_2(\alpha_1 h)(\alpha_2 h) - 36z_2(\alpha_2 h)^2 + 480z_1^2$$

$$+720z_1 z_2 + 144z_2^2 - 70y_1(i\alpha_1 h)^3 - 240y_1(\alpha_1 h)^2(i\alpha_2 h) - 210y_1(i\alpha_1 h)(\alpha_2 h)^2$$

$$+30y_1(i\alpha_2 h)^3 - 260y_1^2(\alpha_1 h)^2 - 1080y_1^2(\alpha_1 h)(\alpha_2 h) - 360y_1^2(\alpha_2 h)^2$$

$$+480y_1^3(i\alpha_1 h) + 720y_1^3(i\alpha_2 h) + 240y_1^4 + 180y_2(i\alpha_1 h)^3 + 120y_2(i\alpha_1 h)^2(i\alpha_2 h)$$

$$+30y_2(i\alpha_1 h)(\alpha_2 h)^2 - 1080y_1 y_2(\alpha_1 h)^2 - 1260y_1 y_2(\alpha_1 h)(\alpha_2 h)$$

$$-180y_1 y_2(\alpha_2 h)^2 + 2160y_1^2 y_2(i\alpha_1 h) + 1440y_1^2 y_2(i\alpha_2 h) + 1440y_1^3 y_2 - 360y_2^2(\alpha_1 h)^2$$

$$-180y_2^2(\alpha_1 h)(\alpha_2 h) + 1440y_1 y_2^2(i\alpha_1 h) + 360y_1 y_2^2(i\alpha_2 h) + 1440y_1^2 y_2^2 + 120y_2^3(i\alpha_1 h)$$

$$+240y_1 y_2^3 + 720y_1^2(i\alpha_1 h) + 480y_1^3 + 720y_1^2(i\alpha_2 h) + 1440y_1 y_2(i\alpha_1 h)$$

$$+1440y_1^2 y_2 + 720y_1 y_2(i\alpha_2 h) + 360y_2^2(i\alpha_1 h) + 720y_1 y_2^2 + 72y_2^2(i\alpha_2 h) + 48y_2^3 + 48x_1^5$$

$$+720x_1^4 x_2 + 144x_1^5 x_2 + 1440x_1^3 x_2^2 + 720x_1^4 x_2^2 + 144x_1^5 x_2^2 + 480x_1^2 x_2^3 + 480x_1^3 x_2^3, \tag{135}$$

$$
\begin{aligned}
D ={}& 240x_1^4 x_2^3 + 48x_1^5 x_2^3 - 24y_2(i\alpha_2 h)^3 + 24y_2^2(\alpha_2 h)^2 - 3(i\alpha_1 h)^4(i\alpha_2 h) \\
& -15(i\alpha_1 h)^3(i\alpha_2 h)^2 + (\alpha_1 h)^4(\alpha_2 h)^2 - 8x_1(\alpha_1 h)^4 - 135x_1(\alpha_1 h)^3(\alpha_2 h) \\
& -100x_1(\alpha_1 h)^2(\alpha_2 h)^2 - 12x_1(\alpha_1 h)^4(i\alpha_2 h) - 45x_1(i\alpha_1 h)^3(i\alpha_2 h)^2 + 4x_1(\alpha_1 h)^4(\alpha_2 h)^2 \\
& -90x_1^2(i\alpha_1 h)^3 - 150x_1^2(i\alpha_1 h)^2(i\alpha_2 h) - 12x_1^2(\alpha_1 h)^4 - 135x_1^2(\alpha_1 h)^3(\alpha_2 h) \\
& -50x_1^2(\alpha_1 h)^2(\alpha_2 h)^2 - 18x_1^2(\alpha_1 h)^4(i\alpha_2 h) - 45x_1^2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 6x_1^2(\alpha_1 h)^4(\alpha_2 h)^2 \\
& -30x_1^3(i\alpha_1 h)^3 - 8x_1^3(\alpha_1 h)^4 - 45x_1^3(\alpha_1 h)^3(\alpha_2 h) - 12x_1^3(\alpha_1 h)^4(i\alpha_2 h) \\
& -15x_1^3(i\alpha_1 h)^3(i\alpha_2 h)^2 + 4x_1^3(\alpha_1 h)^4(\alpha_2 h)^2 - 2x_1^4(\alpha_1 h)^4 - 3x_1^4(\alpha_1 h)^4(i\alpha_2 h) \\
& +x_1^4(\alpha_1 h)^4(\alpha_2 h)^2 - 45x_2(\alpha_1 h)^3(\alpha_2 h) - 100x_2(\alpha_1 h)^2(\alpha_2 h)^2 - 3x_2(\alpha_1 h)^4(i\alpha_2 h) \\
& -30x_2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 2x_2(\alpha_1 h)^4(\alpha_2 h)^2 + 300x_1 x_2(\alpha_1 h)^2(i\alpha_2 h) \\
& +120x_1 x_2(i\alpha_1 h)(\alpha_2 h)^2 - 135x_1 x_2(\alpha_1 h)^3(\alpha_2 h) - 200x_1 x_2(\alpha_1 h)^2(\alpha_2 h)^2 \\
& -12x_1 x_2(\alpha_1 h)^4(i\alpha_2 h) - 90x_1 x_2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 8x_1 x_2(\alpha_1 h)^4(\alpha_2 h)^2 \\
& +150x_1^2 x_2(\alpha_1 h)^2(i\alpha_2 h) - 135x_1^2 x_2(\alpha_1 h)^3(\alpha_2 h) - 100x_1^2 x_2(\alpha_1 h)^2(\alpha_2 h)^2 \\
& -18x_1^2 x_2(\alpha_1 h)^4(i\alpha_2 h) - 90x_1^2 x_2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 12x_1^2 x_2(\alpha_1 h)^4(\alpha_2 h)^2 \\
& -45x_1^3 x_2(\alpha_1 h)^3(\alpha_2 h) - 12x_1^3 x_2(\alpha_1 h)^4(i\alpha_2 h) - 30x_1^3 x_2(i\alpha_1 h)^3(i\alpha_2 h)^2 \\
& +8x_1^3 x_2(\alpha_1 h)^4(\alpha_2 h)^2 - 3x_1^4 x_2(\alpha_1 h)^4(i\alpha_2 h) + 2x_1^4 x_2(\alpha_1 h)^4(\alpha_2 h)^2 \\
& +60x_2^2(i\alpha_1 h)(\alpha_2 h)^2 - 50x_2^2(\alpha_1 h)^2(\alpha_2 h)^2 - 15x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 + x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 \\
& +60x_1 x_2^2(i\alpha_1 h)(\alpha_2 h)^2 - 100x_1 x_2^2(\alpha_1 h)^2(\alpha_2 h)^2 - 45x_1 x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 \\
& +4x_1 x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 - 50x_1^2 x_2^2(\alpha_1 h)^2(\alpha_2 h)^2 - 45x_1^2 x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 \\
& +6x_1^2 x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 - 15x_1^3 x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 4x_1^3 x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 \\
& +x_1^4 x_2^2(\alpha_1 h)^4(\alpha_2 h)^2,
\end{aligned}
\tag{136}
$$

where $r, \alpha_1, \alpha_2, x_1, x_2, y_1, y_2, z_1, z_2, w_1, w_2, u_1, u_2$ are defined by (88), (89), (93)–(95), (127) and (128).

Appendix B

Here, we present the center-corrected quadrature formulae of orders 4, 6 and 8 for the integral

$$
\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0(k\sqrt{x^2+y^2})\,dx\,dy.
\tag{137}
$$

Lemma 6.6 (The 4th-Order Center-corrected Quadrature Formula). *Suppose that $n \geq 1$ is an integer, and a, h are two positive real numbers such that $h = a/n$. Suppose further that $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in c^2(R \times R)$, and that ϕ is zero outside the square $[-a, a] \times [-a, a]$. Then, for any $k \in \mathbb{C}^+$,*

$$
\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0(k\sqrt{x^2+y^2})\,dx\,dy = U_{\tau^h}\Big(\phi(x,y)\cdot H_0(k\sqrt{x^2+y^2})\Big) + O(h^4).
\tag{138}
$$

In (138),

$$
U_{\tau^h}\Big(\phi(x,y)\cdot H_0(k\sqrt{x^2+y^2})\Big) = T'^{h}\Big(\phi(x,y)\cdot H_0(k\sqrt{x^2+y^2})\Big) + \sum_{p,q\in S}\tau_{pq}^h\phi(ph,qh),
\tag{139}
$$

33

where

$$S = \{p, q \in Z : p = 0 \ and \ q = 0\}, \tag{140}$$

$$T'^h\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) = \sum_{(p,q)\neq(0,0)} \left(\phi(ph,qh) \cdot H_0(k\sqrt{(ph)^2+(qh)^2})\right) \cdot h^2, \tag{141}$$

and

$$\tau_{00}^h = D_0. \tag{142}$$

Lemma 6.7 (The 6th-Order Center-corrected Quadrature Formula). *Suppose that $n \geq 1$ is an integer, and a, h are two positive real numbers such that $h = a/n$. Suppose further that $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in c^4(R \times R)$, and that ϕ is zero outside the square $[-a, a] \times [-a, a]$. Then, for any $k \in \mathbb{C}^+$,*

$$\int_{-a}^{a}\int_{-a}^{a} \phi(x,y) \cdot H_0(k\sqrt{x^2+y^2}) \, dx \, dy = U_{\tau^h}\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) + O(h^6). \tag{143}$$

In (143),

$$U_{\tau^h}\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) = T'^h\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) + \sum_{p,q \in S} \tau_{pq}^h \phi(ph,qh), \tag{144}$$

where

$$S = \{p, q \in Z : |p+q| \leq 1 \ and \ |p-q| \leq 1\}, \tag{145}$$

$$T'^h\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) = \sum_{(p,q)\neq(0,0)} \left(\phi(ph,qh) \cdot H_0(k\sqrt{(ph)^2+(qh)^2})\right) \cdot h^2, \tag{146}$$

and

$$\tau_{00}^h = D_0 - 2\frac{D_1}{h^2}, \tag{147}$$

$$\tau_{\pm 10}^h = \tau_{0\pm 1}^h = \frac{1}{2}\frac{D_1}{h^2}. \tag{148}$$

Lemma 6.8 (The 8th-Order Center-corrected Quadrature Formula). *Suppose that $n \geq 1$ is an integer, and a, h are two positive real numbers such that $h = a/n$. Suppose further that $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in c^6(R \times R)$, and that ϕ is zero outside the square $[-a, a] \times [-a, a]$. Then, for any $k \in \mathbb{C}^+$,*

$$\int_{-a}^{a}\int_{-a}^{a} \phi(x,y) \cdot H_0(k\sqrt{x^2+y^2}) \, dx \, dy = U_{\tau^h}\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) + O(h^8). \tag{149}$$

In (149),

$$U_{\tau^h}\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) = T'^h\left(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\right) + \sum_{p,q \in S} \tau_{pq}^h \phi(ph,qh), \tag{150}$$

where

$$S = \{p, q \in Z : |p+q| \leq 2 \ and \ |p-q| \leq 2\}, \tag{151}$$

$$T'^h\Big(\phi(x,y) \cdot H_0(k\sqrt{x^2+y^2})\Big) = \sum_{(p,q)\neq(0,0)} \Big(\phi(ph,qh) \cdot H_0(k\sqrt{(ph)^2+(qh)^2})\Big) \cdot h^2, \quad (152)$$

and

$$\tau_{00}^h = D_0 - \frac{5}{2}\frac{D_1}{h^2} + \frac{1}{2}\frac{D_2}{h^4} + \frac{D_3}{h^4}, \tag{153}$$

$$\tau_{\pm10}^h = \tau_{0\pm1}^h = \frac{2}{3}\frac{D_1}{h^2} - \frac{1}{6}\frac{D_2}{h^4} - \frac{1}{2}\frac{D_3}{h^4}, \tag{154}$$

$$\tau_{\pm20}^h = \tau_{0\pm2}^h = -\frac{1}{24}\frac{D_1}{h^2} + \frac{1}{24}\frac{D_2}{h^4}, \tag{155}$$

$$\tau_{\pm1\pm1}^h = \frac{1}{4}\frac{D_3}{h^4}. \tag{156}$$

References

[1] M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions*, Applied Math. Series (National Bureau of Standards), Washington, DC, 1964.

[2] W. L. Briggs and V. E. Henson, *The DFT: An Owners' Manual for the Discrete Fourier Transform*, SIAM, Philadelphia, 1995.

[3] Y. Chen, A Fast Direct Algorithm for the Lippmann-Schwinger Integral Equation in Two Dimensions, Advances in Computational Mathematics. Vol. 16, pp. 175-190, 2002.

[4] D. L. Colton, R. Kress, *Integral equation methods in scattering theory*, Pure and Applied Mathematics, 1983.

[5] D. L. Colton, R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, Springer-Verlag, 1992.

[6] P. Ewald, *Die Berechnung Optischer und Eletrostatischer Gitterpotentiale*, Annals of Physics. Vol. 64, pp. 253-287, 1921.

[7] S. Kapur, V. Rokhlin, *High-Order Corrected Trapezoidal Quadrature Rule for Singular Functions*, Journal of Numerical Analysis, Vol. 34, No. 4, pp.1331-1356, 1997.

[8] J. Ma, *Interpolation on Arbitrary Regions in the Complex Plane*, Applied and Computational Harmonic Analysis, Vol. 4, Issue. 3, pp.264-292, 1997.

[9] P. M. Morse, H. Feshbach, *Methods of Theoretical Physics*, McGraw-Hill Book Company, USA, 1953.

[10] Y. Saad, *Iterative Methods for Sparse Linear Systems*, SIAM, USA, 2003.

[11] J. Stoer, R. Bulirsch, *Introduction to Numerical Analysis*, Springer-Verlag New York, Inc., USA, 1993.

[12] H. A. van der Vorst, *BI-CGSTAB: a Fast and Smoothly Converging Variant of BI-CG for the Solution of Nonsymmetric Linear Systems*, SIAM Journal on Scientific and Statistical Computing. Vol. 13, No. 2, pp.631-644, 1992.