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High-order quadratures for the solution of scattering problems in two dimensions

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ABSTRACT

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 bi-conjugate 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.

1. Introduction

Forward scattering has been a remarkably active subject of research for the past several decades (see e.g. [2,3]). 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 (such as the Lippmann–Schwinger equation), discretize the latter via appropriate quadrature formulae, and deal numerically with the resulting linear systems. This paper focuses on the problem of discretization; we construct a class of high-order quadrature formulae applicable to the Lippmann–Schwinger equation in two dimensions. Our techniques generalize straightforwardly to three dimensions.

1.1. Statement of the problem

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

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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 start with the ansatz

$$\psi(x,t) = \psi_k(x)e^{ikc_0t}, \tag{2}$$

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

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

where

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

Eq. (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 homogeneous Helmholtz equation

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

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

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

where $i = \sqrt{-1}$ is the imaginary unit. Combining Eqs. (3), (5), and (6), we obtain the equation for the scattered field

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

In this paper, we view Eq. (8) with ψ_k^{scat} satisfying the Sommerfeld condition (7) as the principal formulation of the forward scattering problem. The following standard approach to the numerical solution of (8) converts (8) into the well-known Lippmann–Schwinger equation, which is an integral equation of the second kind (see, for example, [4]):

Convolving (8) with a Green's function G_k satisfying

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

where δ is the Dirac delta function, 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

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

where $H_0(k\|x-y\|)$ is the Hankel function of the first kind of order zero, and $\|x-y\|$ is the Euclidean norm of $x-y$. A large part of this paper is devoted to the construction of accurate discretizations of the operator $L : L^2(D) \to L^2(D)$ defined by the formula

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

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 a Lippmann–Schwinger equation, and solve the latter iteratively (integral equations of the second kind are much more amenable to iterative techniques than the straightforward discretizations of the 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 applications of the matrices 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 fast Fourier transform (FFT), resulting in algorithms with CPU time requirements proportional to $N\log(N)$, with N being 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 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 $1/r$, where r is the distance to the origin. 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

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

with $P,\ Q$ being two smooth functions, such that $P(x,x) = 0$ for all $x \in \mathbb{R}^2$; the corresponding form in three dimensions is

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

Importantly, we usually 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). Therefore, standard integration techniques (such as product integration, etc.) can not be used efficiently. The standard procedure in the literature (referred to as "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 when $x = y$), 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; similar techniques would yield quadrature formulae for functions of the form (14) in three dimensions. Our approach is related to Ewald summation [5], and leads to quadratures that can be viewed as a version of the corrected trapezoidal rule; the approach is easily combined with the FFT to obtain fast algorithms. Our quadratures can be viewed as a special case of those constructed in [11], and are extensions of those in [6]. While in principle corrections of arbitrarily high-order could be constructed, in practice both the complexity of the construction and the number of corrections grow rapidly with the order. We have designed corrections of orders approximately 4, 6, 8, and 10; they require 1, 5, 13, and 25 corrected nodes, respectively. (We say "approximately" since we prove that the quadrature errors are $O((\log(1/h))^2h^4)$, $O((\log(1/h))^2h^6)$, $O((\log(1/h))^2h^8)$, and $O((\log(1/h))^2h^{10})$ as the discretization step length h approaches zero.)

This 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

We denote the upper half of the complex plane (not including the real line) by $\mathbb{C}^+$, that is,

$$\mathbb{C}^+ = \{z \in \mathbb{C} : \mathrm{Im}\, z > 0\}. \tag{15}$$

For any non-negative integer k and subset D of the two-dimensional plane $\mathbb{R}^2$, we write $\phi \in C^k(D)$ to mean that ϕ is a function on D having continuous derivatives of all orders $\leqslant k$ at every point in the interior of D. (The order of a two-dimensional derivative is the sum of the orders of the constituent partial derivatives.)

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

$$A_{k_1k_2} = \sum_{j_1=-N}^{N}\sum_{j_2=-N}^{N} a_{j_1j_2} e^{-\frac{2\pi i}{(2N+1)}k_1j_1} e^{-\frac{2\pi i}{(2N+1)}k_2j_2}. \tag{16}$$

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

$$(\mathscr{F}^N)^{-1}(A)_{j_1j_2} = a_{j_1j_2} = \frac{1}{(2N+1)^2}\sum_{k_1=-N}^{N}\sum_{k_2=-N}^{N} A_{k_1k_2} e^{\frac{2\pi i}{(2N+1)}k_1j_1} e^{\frac{2\pi i}{(2N+1)}k_2j_2}, \tag{17}$$

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

For the Helmholtz equation

$$\nabla^2\phi + k^2\phi = 0 \tag{18}$$

in two dimensions, where k is a complex number such that $\mathrm{Im}(k) \geqslant 0$, the potential ϕ at a point x produced by a unit point source at x_0 is given by the formula

$$\phi(x) = -\frac{i}{4}H_0(k\|x - x_0\|), \tag{19}$$

where H_0 is the Hankel function of the first kind of order zero, and $\|x - x_0\|$ is the Euclidean norm of $x - x_0$. The well-known Sommerfeld formula states that

$$H_0(kr) = \frac{1}{\pi}\cdot\int_{-\infty}^{\infty}\frac{1}{\sqrt{k^2-\lambda^2}}\cdot e^{i\sqrt{k^2-\lambda^2}x}\cdot e^{i\lambda y}d\lambda \tag{20}$$

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

Finally, we will need the elementary identity

$$\sum_{j=0}^{n} f_j g_j = f_n\sum_{k=0}^{n} g_k - \sum_{j=0}^{n-1}(f_{j+1} - f_j)\cdot\left(\sum_{k=0}^{j} g_k\right), \tag{21}$$

valid for two arbitrary finite sequences $\{f_j\},\ j = 0,1,2,\dots,n$, $\{g_j\},\ j = 0,1,2,\dots,n$. By analogy with integration by parts, (21) is normally called summation by parts.

2.2. 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 $a = \{a_{j_1j_2}\},\ j_1, j_2 = -N, \dots, N$, and $b = \{b_{j_1j_2}\},\ j_1, j_2 = -2N, \dots, 2N$, is defined by the formula

$$(a * b)_{k_1k_2} = \sum_{j_1=-N}^{N}\sum_{j_2=-N}^{N} a_{j_1j_2} b_{k_1-j_1,k_2-j_2}, \tag{22}$$

where $k_1, k_2 = -N, \dots, N$. 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 transforms of a' and b, where a' is the two-dimensional sequence obtained by padding the two-dimensional sequence a with zeros. In other words,

$$(a * b)_{k_1k_2} = (\mathscr{F}^{2N})^{-1}(\mathscr{F}^{2N}(a')\cdot\mathscr{F}^{2N}(b))_{k_1k_2}, \tag{23}$$

where $k_1, k_2 = -N, \dots, N$, and the coefficients of the two-dimensional complex sequence $a' = \{a'_{i_1i_2}\},\ i_1, i_2 = -2N, \dots, 2N$ are defined by the formulae

$$a'_{i_1i_2} = a_{i_1i_2} \tag{24}$$

when $-N \leqslant i_1, i_2 \leqslant N$, and

$$a'_{i_1i_2} = 0 \tag{25}$$

otherwise.

Remark 2.1. While direct calculation of the Toeplitz convolution (22) leads to a cost of order $O(N^4)$ floating-point operations, which is prohibitive for large-scale problems, application of the FFT to the formula (23) reduces the cost to $O(N^2\cdot\log N)$ (see, for example, [1]). In this paper, the FFT is used for the fast calculation of Toeplitz convolutions.

2.3. Classical quadratures

This section summarizes basic facts about multidimensional quadratures.

Suppose that q is a non-negative integer, a and h are positive real numbers, and $f : [-a,a] \times [-a,a] \to \mathbb{R}$. We define the boundary-corrected trapezoidal quadrature $T^h_{a,q}(f)$ by the formula

$$T^h_{a,q}(f) = \sum_{(i,j)\in M} f(ih,jh)\cdot h^2 + C^h_{a,q}(f), \tag{26}$$

where

$$M = \{i,j \in \mathbb{Z} : (i,j) \neq (0,0), -a \leqslant ih \leqslant a, \text{ and } -a \leqslant jh \leqslant a\} \tag{27}$$

and $C^h_{a,q}(f)$ is the linear combination of values of f and its derivatives of orders $\leqslant q$ on the perimeter of the square $[-a,a]\times[-a,a]$ that appears in the two-dimensional Euler–Maclaurin formula (see, for example, Theorem 2.6 of [7]). (The order of a derivative of a two-dimensional function is the sum of the orders of its constituent partial derivatives.) We will not need to know the particular values of the coefficients in the linear combination $C^h_{a,q}(f)$, but only that they involve only positive powers of h, do not depend on f, and are symmetric about the origin (that is, they do not change when reflected through the origin).

The following lemma is a reformulation of Theorem 2.6 of [7]. The lemma provides a bound on the accuracy of a two-dimensional Euler–Maclaurin quadrature.

Lemma 2.1. *Suppose that q and r are positive integers, a is a positive real number, and $f \in C^r([-a,a]\times[-a,a])$.*

Then, the quadrature $T^h_{a,q}$ defined in (26) satisfies

$$\left|\int_{-a}^{a}\int_{-a}^{a} f(x,y)dxdy - T^h_{a,q}(f) - h^2 f(0,0)\right| = O(\max\{h^r, h^{q+3}\}) \tag{28}$$

for all positive real numbers $h < a$.

The following lemma is a reformulation of Theorem 6.14 of [7].

Lemma 2.2. *Suppose that l and q are positive integers, a is a positive real number, and $\varphi : \mathbb{R}^2 \to \mathbb{R}$ is real-analytic and depends only on the angular variable in polar coordinates, that is, $\varphi(cx,cy) = \varphi(x,y)$ for any real numbers c, x, and y such that $c > 0$.*

Then, the quadrature $T^h_{a,q}$ defined in (26) satisfies

$$\begin{aligned}&\left|\int_{-a}^{a}\int_{-a}^{a}(x^2+y^2)^{l/2}\varphi(x,y)\log(x^2+y^2)dxdy - T^h_{a,q}((x^2+y^2)^{l/2}\varphi(x,y)\log(x^2+y^2))\right|\\ &\quad = O(\max\{(\log(1/h))^2 h^{l+2}, h^{q+3}\})\end{aligned} \tag{29}$$

for all positive real numbers $h < a$.

3. Mathematical apparatus

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

3.1. High-order center-corrected trapezoidal quadrature rules for singular functions in two dimensions

For any non-negative integer p and positive real number a, Theorem 3.2 below supplies an approximately $(2p+4)$th-order center-corrected quadrature formula on $[-a,a]\times[-a,a]$ for the functions of the form

$$f(x,y) = \phi(x,y)\cdot s(x,y), \tag{30}$$

where $\phi : [-a,a]\times[-a,a] \to \mathbb{R}$, and

$$s(x,y) = \gamma(x,y)\cdot\log(x^2+y^2) + \delta(x,y) \tag{31}$$

with γ, δ being smooth real-valued functions. To prove Theorem 3.2, we will need the following lemma. This lemma bounds the accuracy of the quadrature defined in (26) when applied to functions of the form $x^k y^{l-k} s(x,y)$, where k and l are integers with $k \leqslant l$ and $l > 0$.

Lemma 3.1. *Suppose that k, l, and p are non-negative integers with $k \leqslant l$ and $l > 0$. Suppose further that $a > 0$ is a real number, and s is a function on $[-a,a]\times[-a,a]$ with a possible logarithmic singularity at $(0,0)$, i.e., of the form (31), with γ and δ in (31) being $l+4$ times continuously differentiable.*

Then,

$$\left|\int_{-a}^{a}\int_{-a}^{a} x^k y^{l-k} s(x,y)dxdy - T^h_{a,2p+1}(x^k y^{l-k} s)\right| = O(\max\{(\log(1/h))^2 h^{l+2}, h^{2p+4}\}) \tag{32}$$

for all positive real numbers $h < a$, where $T^h_{a,2p+1}$ is defined in (26).

Proof. The two-dimensional Euler–Maclaurin formula (28) allows us to assume without loss of generality that $\gamma(0,0)\neq 0$ and

$$s(x,y) = \gamma(x,y)\cdot \log(x^2+y^2) \tag{33}$$

in place of (31).

Using the Taylor expansion of γ at the point $(0,0)$, we obtain

$$\gamma(x,y) = P(x,y) + R(x,y), \tag{34}$$

where

$$P(x,y) = \sum_{j=0}^{l+3}\sum_{i=0}^{j}\frac{1}{j!}\binom{j}{i}x^i y^{j-i}\frac{\partial^j}{\partial x^i \partial y^{j-i}}\gamma(0,0), \tag{35}$$

$$R(x,y) = \frac{1}{(l+4)!}\sum_{i=0}^{l+4}\binom{l+4}{i}x^i y^{l+4-i}\frac{\partial^{l+4}}{\partial x^i \partial y^{l+4-i}}\gamma(\xi_1(x,y),\xi_2(x,y)) \tag{36}$$

with $(\xi_1(x,y),\xi_2(x,y)) \in [-a,a]\times[-a,a]$, and

$$\frac{\partial^{i+j}}{\partial x^i \partial y^j}R(0,0) = 0 \tag{37}$$

for all non-negative integers i and j such that $i+j \leqslant l+3$.

To simplify notation, we define $\lambda : \mathbb{R}^2 \to \mathbb{R}$ via the formula

$$\lambda(x,y) = \log(x^2+y^2). \tag{38}$$

It follows from (34) that

$$\left|\int_{-a}^{a}\int_{-a}^{a}(x^k y^{l-k}\gamma(x,y)\lambda(x,y))dxdy - T^h_{a,2p+1}(x^k y^{l-k}\gamma\lambda)\right| \leqslant \left|\int_{-a}^{a}\int_{-a}^{a}(x^k y^{l-k}P(x,y)\lambda(x,y))dxdy - T^h_{a,2p+1}(x^k y^{l-k}P\lambda)\right| + \left|\int_{-a}^{a}\int_{-a}^{a}(x^k y^{l-k}R(x,y)\lambda(x,y))dxdy - T^h_{a,2p+1}(x^k y^{l-k}R\lambda)\right|. \tag{39}$$

Combining (37) and the fact that $R \in C^{l+3}([-a,a]\times[-a,a])$ yields that $R\cdot\lambda \in C^{l+2}([-a,a]\times[-a,a])$. Combining the two-dimensional Euler–Maclaurin formula (28) and the fact that $x^k y^{l-k}R\cdot\lambda \in C^{l+2}([-a,a]\times[-a,a])$ yields

$$\left|\int_{-a}^{a}\int_{-a}^{a}(x^k y^{l-k}R(x,y)\cdot\lambda(x,y))dxdy - T^h_{a,2p+1}(x^k y^{l-k}R\cdot\lambda)\right| = O(\max\{h^{l+2},h^{2p+4}\}). \tag{40}$$

Formula (40) provides a bound on the second term in the right-hand side of (39).

To bound the first term in the right-hand side of (39), we use polar coordinates (r,θ), observing that

$$x^k y^{l-k} x^i y^{j-i} = r^{j+l}\cos^{i+k}(\theta)\sin^{j+l-i-k}(\theta) = r^{j+l}\varphi(\theta), \tag{41}$$

where $\varphi(\theta) = \cos^{i+k}(\theta)\sin^{j+l-i-k}(\theta)$. Combining (29) and (41) yields

$$\left|\int_{-a}^{a}\int_{-a}^{a}(x^k y^{l-k}x^i y^{j-i}\lambda(x,y))dxdy - T^h_{a,2p+1}(x^k y^{l-k}x^i y^{j-i}\lambda)\right| = O(\max\{(\log(1/h))^2 h^{j+l+2},h^{2p+4}\}). \tag{42}$$

Combining (33)–(42) yields (32). □

Theorem 3.2. *Suppose that p is a non-negative integer, a is a positive real number, $\phi : [-a,a]\times[-a,a] \to \mathbb{R}$ with $\phi \in C^{2p+6}([-a,a]\times[-a,a])$, and s is a function on $[-a,a]\times[-a,a]$ with a possible logarithmic singularity at $(0,0)$, i.e., of the form (31), with γ and δ in (31) being $2p+9$ times continuously differentiable. Suppose in addition that $s(x,y) = s(y,x)$ and $s(-x,-y) = s(x,y)$ for any x and y from $[-a,a]$, and*

$$U^h_{a,p,s}(\phi\cdot s) = T^h_{a,2p+1}(\phi\cdot s) + \sum_{(i,j)\in W}\tau^h_{ij}\phi(ih,jh) \tag{43}$$

for any positive real number $h < a/p$, where $T^h_{a,2p+1}(\phi\cdot s)$ is defined in (26),

$$W = \{i,j \in \mathbb{Z} : |i+j| \leqslant p \text{ and } |i-j| \leqslant p\}, \tag{44}$$

and the coefficients τ^h_{ij} in (43) satisfy the system of linear equations

$$\sum_{(i,j)\in W} x_i^{i'-1}y_j^{j'-1}\tau^h_{ij} = \int_{-a}^{a}\int_{-a}^{a}(x^{i'-1}y^{j'-1}\cdot s(x,y))dxdy - T^h_{a,2p+1}(x^{i'-1}y^{j'-1}\cdot s) \tag{45}$$

with $x_i = ih$, $y_j = jh$, and $(i',j') \in H$, where $H = \{i',j', \in \mathbb{Z} : i' \geqslant 1, j' \geqslant 1, i'+j' \leqslant 2p+2\}$, and $\tau^h_{ij} = \tau^h_{ji}$ and $\tau^h_{-i,-j} = \tau^h_{i,j}$ for all $(i,j) \in W$.

Then,

$$\left|\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot s(x,y)dxdy - U^h_{a,p,s}(\phi\cdot s)\right| = O((\log(1/h))^2h^{2p+4}) \quad (46)$$

for all positive real numbers $h < a/p$.

Proof. Using the Taylor expansion of ϕ at the point $(0,0)$, we obtain

$$\phi(x,y) = P(x,y) + Q(x,y) + R(x,y), \quad (47)$$

where

$$P(x,y) = \sum_{j=0}^{2p+1}\sum_{i=0}^{j}\frac{1}{j!}\binom{j}{i}x^iy^{j-i}\frac{\partial^j}{\partial x^i\partial y^{j-i}}\phi(0,0), \quad (48)$$

$$Q(x,y) = \sum_{j=2p+2}^{2p+5}\sum_{i=0}^{j}\frac{1}{j!}\binom{j}{i}x^iy^{j-i}\frac{\partial^j}{\partial x^i\partial y^{j-i}}\phi(0,0), \quad (49)$$

$$R(x,y) = \frac{1}{(2p+6)!}\sum_{i=0}^{2p+6}\binom{2p+6}{i}x^iy^{2p+6-i}\frac{\partial^{2p+6}}{\partial x^i\partial y^{2p+6-i}}\phi(\xi_1(x,y),\xi_2(x,y)), \quad (50)$$

with $(\xi_1(x,y),\xi_2(x,y))\in\mathbb{R}^2$, and

$$\frac{\partial^{i+j}}{\partial x^i\partial y^j}R(0,0) = 0 \quad (51)$$

for all non-negative integers i and j such that $i+j\leqslant 2p+5$.

It follows from (47) that

$$\begin{aligned}\left|\int_{-a}^{a}\int_{-a}^{a}(\phi(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(\phi\cdot s)\right| \leqslant &\left|\int_{-a}^{a}\int_{-a}^{a}(P(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(P\cdot s)\right| \\ &+\left|\int_{-a}^{a}\int_{-a}^{a}(Q(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(Q\cdot s)\right| \\ &+\left|\int_{-a}^{a}\int_{-a}^{a}(R(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(R\cdot s)\right|. \end{aligned} \quad (52)$$

First, we derive a bound on the first term in the right-hand side of (52). It follows from the supposition that $s(-x,-y) = s(x,y)$ for any x and y from $[-a,a]$ that $x^iy^{2p+1-i}s(x,y)$ changes sign when reflected through the origin for $i = 1,2,\ldots,2p+1$, while (by assumption) $\tau^h_{-i,-j} = \tau^h_{i,j}$ for all $(i,j)\in W$. Therefore,

$$\int_{-a}^{a}\int_{-a}^{a}(x^iy^{2p+1-i}\cdot s(x,y))dxdy = 0 = U^h_{a,p,s}(x^iy^{2p+1-i}\cdot s) \quad (53)$$

for $i = 1,2,\ldots,2p+1$. Combining (48), (45), and (53) yields

$$\int_{-a}^{a}\int_{-a}^{a}(P(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(P\cdot s) = 0. \quad (54)$$

Next, we derive bounds on the second and third terms in the right-hand side of (52). It follows from (43) that

$$\left|\int_{-a}^{a}\int_{-a}^{a}(Q(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(Q\cdot s)\right| \leqslant \left|\int_{-a}^{a}\int_{-a}^{a}(Q(x,y)\cdot s(x,y))dxdy - T^h_{a,2p+1}(Q\cdot s)\right| + \left|\sum_{(i,j)\in W}\tau^h_{ij}Q(ih,jh)\right| \quad (55)$$

and

$$\left|\int_{-a}^{a}\int_{-a}^{a}(R(x,y)\cdot s(x,y))dxdy - U^h_{a,p,s}(R\cdot s)\right| \leqslant \left|\int_{-a}^{a}\int_{-a}^{a}(R(x,y)\cdot s(x,y))dxdy - T^h_{a,2p+1}(R\cdot s)\right| + \left|\sum_{(i,j)\in W}\tau^h_{ij}R(ih,jh)\right|. \quad (56)$$

It follows from (32) that

$$\left|\int_{-a}^{a}\int_{-a}^{a}(x^iy^{j-i}\cdot s(x,y))dxdy - T^h_{a,2p+1}(x^iy^{j-i}\cdot s)\right| = O(\max\{(\log(1/h)^2)h^{j+2}, h^{2p+4}\}), \quad (57)$$

whence

$$\left|\int_{-a}^{a}\int_{-a}^{a}(x^iy^{j-i}\cdot s(x,y))dxdy - T^h_{a,2p+1}(x^iy^{j-i}\cdot s)\right| = O((\log(1/h))^2h^{2p+4}) \quad (58)$$

for any integer $j \geqslant 2p+2$ such that $j \leqslant 2p+5$, with $i = 0, 1, \ldots, j$. Combining (49) and (58) yields

$$\left| \int_{-a}^{a} \int_{-a}^{a} (Q(x,y) \cdot s(x,y)) dxdy - T^h_{a,2p+1}(Q \cdot s) \right| = O((\log(1/h))^2 h^{2p+4}). \tag{59}$$

Due to formulae (32) and (45), the coefficients τ^h_{ij} are no greater than a constant times $(\log(1/h))^2 h^2$; combining this fact with (49) yields

$$\left| \sum_{(i,j)\in W} \tau^h_{ij} Q(ih, jh) \right| = O((\log(1/h))^2 h^{2p+4}). \tag{60}$$

Combining (51) and the fact that $R \in C^{2p+5}([-a,a] \times [-a,a])$ yields that $R \cdot s \in C^{2p+4}([-a,a] \times [-a,a])$. Combining the two-dimensional Euler–Maclaurin formula (28) and the fact that $R \cdot s \in C^{2p+4}([-a,a] \times [-a,a])$ yields

$$\left| \int_{-a}^{a} \int_{-a}^{a} (R(x,y) \cdot s(x,y)) dxdy - T^h_{a,2p+1}(R \cdot s) \right| = O(h^{2p+4}). \tag{61}$$

As mentioned above, the coefficients τ^h_{ij} are no greater than a constant times $(\log(1/h))^2 h^2$ (due to formulae (32) and (45)); combining this fact with (50) yields

$$\left| \sum_{(i,j)\in W} \tau^h_{ij} R(ih, jh) \right| = O((\log(1/h))^2 h^{2p+8}). \tag{62}$$

Finally, combining (52)–(62) yields (46). □

Remark 3.1. The suppositions of the theorem that $s(x,y) = s(y,x)$ for any x and y from $[-a,a]$, and that $\tau^h_{ij} = \tau^h_{ji}$ for any $(i,j) \in W$, ensure that the number of independent constraints is at most the number of independent variables in the system of linear Eq. (45), guaranteeing that the system has a solution.

3.2. High-order center-corrected trapezoidal quadratures for the green's function of the helmholtz equation

The main point of this section is Theorem 3.7, which is the principal analytical tool of this paper. Theorem 3.7 describes an approximately 10th-order center-corrected trapezoidal quadrature formula for the Hankel function. It can be viewed as a special case of Theorem 3.2 with $p = 3$ and $s(x,y) = H_0(k\sqrt{x^2+y^2})$, where H_0 is the Hankel function of the first kind of order 0, and $k \in \mathbb{C}^+$.

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

$$D_0 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0(kr) dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2 + (qh)^2}\right) \cdot h^2, \tag{63}$$

$$D_1 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0(kr) x^2 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2 + (qh)^2}\right) \cdot (ph)^2 \cdot h^2, \tag{64}$$

$$D_2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0(kr) x^4 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2 + (qh)^2}\right) \cdot (ph)^4 \cdot h^2, \tag{65}$$

$$D_3 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0(kr) x^2 y^2 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2 + (qh)^2}\right) \cdot (ph)^2 (qh)^2 \cdot h^2, \tag{66}$$

$$D_4 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0(kr) x^6 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2 + (qh)^2}\right) \cdot (ph)^6 \cdot h^2, \tag{67}$$

$$D_5 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} H_0(kr) x^4 y^2 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2 + (qh)^2}\right) \cdot (ph)^4 (qh)^2 \cdot h^2. \tag{68}$$

The following lemma is a simple consequence of the Sommerfeld formula (20).

Lemma 3.3. *For any $k \in \mathbb{C}^+$, $r, x, y \geqslant 0$, and $r = \sqrt{x^2+y^2}$,*

$$H_0(kr) = \frac{1}{\pi} \cdot \int_{-\infty}^{\infty} \frac{1}{\sqrt{k^2 - \lambda^2}} \cdot e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2-\lambda^2} - \lambda) \cdot x} \cdot e^{i \cdot \frac{\sqrt{2}}{2} \cdot (\sqrt{k^2-\lambda^2} + \lambda) \cdot y} d\lambda, \tag{69}$$

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

The following two technical lemmas follow immediately from (69).

Lemma 3.4. *For any $k \in \mathbb{C}^+$, and $a \geqslant 0$,*

$$\int_{-a}^{a}\int_{-a}^{a} H_0(kr)dxdy = \frac{4}{\pi}\cdot\int_{-\infty}^{\infty}\frac{1}{\sqrt{k^2-\lambda^2}}\cdot\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}-1}{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)}\cdot\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}-1}{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)}d\lambda \tag{70}$$

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

Proof. Substituting (69) into the left-hand side of (70), and changing the order of integration, we obtain

$$\begin{aligned}\int_{-a}^{a}\int_{-a}^{a} H_0(kr)dxdy &= 4\int_0^a\int_0^a H_0(kr)dxdy = \frac{4}{\pi}\cdot\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\int_0^a e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot x}dx\cdot\int_0^a e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot y}dy\\ &= \frac{4}{\pi}\cdot\int_{-\infty}^{\infty}\frac{1}{\sqrt{k^2-\lambda^2}}\cdot\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}-1}{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)}\cdot\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}-1}{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)}d\lambda. \qquad \square\end{aligned} \tag{71}$$

Lemma 3.5. *For any $k \in \mathbb{C}^+$, integer $n \geqslant 1$, and $a > 0$,*

$$\sum_{p=-n}^{n}\sum_{q=-n}^{n} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2\cdot\beta_{pq} \tag{72}$$

$$\begin{aligned}&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{h^2}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}-1}{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot h}-1}-\frac{1}{2}-\frac{1}{2}e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}\right)\\ &\quad\cdot\left(\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}-1}{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot h}-1}-\frac{1}{2}-\frac{1}{2}e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}\right)d\lambda\end{aligned} \tag{73}$$

with

$$h = a/n, \tag{74}$$

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

Proof. The trapezoidal sum (72) 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,

$$\sum_{p=-n}^{n}\sum_{q=-n}^{n} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2\cdot\beta_{pq} = 4\cdot\sum_{p=0}^{n}\sum_{q=0}^{n} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2\cdot\beta'_{pq}, \tag{75}$$

where β'_{pq} equals 1 in the interior of the $(n+1)\times(n+1)$ square, equals $\frac{1}{2}$ in the interior of an edge, and equals $\frac{1}{4}$ on the corners of the square. Substituting (69) into (75), and exchanging the order of integration and summation, we obtain

$$\sum_{p=-n}^{n}\sum_{q=-n}^{n} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2\cdot\beta_{pq} \tag{76}$$

$$\begin{aligned}&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{h^2}{\sqrt{k^2-\lambda^2}}\cdot\left(\sum_{p=0}^{n} e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot p\cdot h}-\frac{1+e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}}{2}\right)\\ &\quad\cdot\left(\sum_{q=0}^{n} e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot q\cdot h}-\frac{1+e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}}{2}\right)d\lambda\end{aligned} \tag{77}$$

$$\begin{aligned}&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{h^2}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}-1}{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot h}-1}-\frac{1}{2}-\frac{1}{2}e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}-\lambda\right)\cdot a}\right)\\ &\quad\cdot\left(\frac{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}-1}{e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot h}-1}-\frac{1}{2}-\frac{1}{2}e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}+\lambda\right)\cdot a}\right)d\lambda. \qquad \square\end{aligned} \tag{78}$$

Remark 3.2. As $a\to\infty$, the exponential terms $e^{i\cdot\frac{\sqrt{2}}{2}\cdot\left(\sqrt{k^2-\lambda^2}\pm\lambda\right)\cdot a}$ in (70) and (73) tend to zero; this fact will be used in Lemma 3.6 below.

The following lemma supplies an analytical form for the difference

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(x^{i-1}y^{j-1}H_0\left(k\sqrt{x^2+y^2}\right)\right)dxdy-\sum_{(p,q)\neq(0,0)}\left((ph)^{i-1}(qh)^{j-1}H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\right)\cdot h^2 \tag{79}$$

with $i=1, j=1, k\in\mathbb{C}^+$.

Remark 3.3. (79) is the right-hand side of (45) in the limit as $a\to\infty$ (after all, the integrand in (79) decays exponentially at infinity with $k\in\mathbb{C}^+$), and thus is directly used in the calculation of coefficients τ_{ij}^h. Direct numerical subtraction of the integral and the sum in (79) loses accuracy because of cancellation errors, especially when i, j are relatively large. Lemma 3.6 below and Lemmas 6.1–6.5 in Appendix A provide analytical formulae for (79) with $(i,j)=\{(1,1),(3,1),(5,1),(3,3),(7,1),(5,3)\}$, i.e., for D_0–D_5 defined by (63)–(68), so that cancellation errors are reduced.

Lemma 3.6. *For any $k\in\mathbb{C}^+$ and $h>0$,*

$$\begin{aligned}D_0&=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}H_0(kr)dxdy-\sum_{(p,q)\neq(0,0)}H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2\\&=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{1}{(i\alpha_1)(i\alpha_2)}-\frac{h^2}{2}\cdot\frac{e^{i\alpha_1h}+e^{i\alpha_2h}}{(e^{i\alpha_1h}-1)(e^{i\alpha_2h}-1)}\right) &(80)\\&=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{\left(\frac{\lambda^2}{4}-\frac{k^2}{24}\right)h^2+z_1+z_2+i\sqrt{\frac{1}{2}}\lambda h(y_1-y_2)+y_1y_2}{(i\alpha_1)(i\alpha_2)(1+x_1)(1+x_2)}, &(81)\end{aligned}$$

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

$$x_1=\frac{e^{i\alpha_1h}-1}{i\alpha_1h}-1=\sum_{n=1}^{\infty}\frac{(i\alpha_1h)^n}{(n+1)!},\quad x_2=\frac{e^{i\alpha_2h}-1}{i\alpha_2h}-1=\sum_{n=1}^{\infty}\frac{(i\alpha_2h)^n}{(n+1)!}, \tag{82}$$

$$y_1=x_1-\frac{i\alpha_1h}{2}=\sum_{n=2}^{\infty}\frac{(i\alpha_1h)^n}{(n+1)!},\quad y_2=x_2-\frac{i\alpha_2h}{2}=\sum_{n=2}^{\infty}\frac{(i\alpha_2h)^n}{(n+1)!}, \tag{83}$$

$$z_1=y_1-\frac{(i\alpha_1h)^2}{6}=\sum_{n=3}^{\infty}\frac{(i\alpha_1h)^n}{(n+1)!},\quad z_2=y_2-\frac{(i\alpha_2h)^2}{6}=\sum_{n=3}^{\infty}\frac{(i\alpha_2h)^n}{(n+1)!}, \tag{84}$$

and

$$r=\sqrt{x^2+y^2}, \tag{85}$$

$$\alpha_1=\frac{\sqrt{2}}{2}\left(\sqrt{k^2-\lambda^2}-\lambda\right),\quad \alpha_2=\frac{\sqrt{2}}{2}\left(\sqrt{k^2-\lambda^2}+\lambda\right). \tag{86}$$

Proof. Substituting (69) into

$$\sum_{(p,q)\neq(0,0)}H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2, \tag{87}$$

and exchanging the order of integration and summation, we obtain

$$\begin{aligned}\sum_{(p,q)\neq(0,0)}H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2&=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{h^2}{4}\frac{e^{i\alpha_1h}+1}{e^{i\alpha_1h}-1}\frac{e^{i\alpha_2h}+1}{e^{i\alpha_2h}-1}-\frac{h^2}{4}\right)\\&=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{h^2}{2}\cdot\frac{e^{i\alpha_1h}+e^{i\alpha_2h}}{(e^{i\alpha_1h}-1)(e^{i\alpha_2h}-1)}. &(88)\end{aligned}$$

Now, (80) follows immediately from the combination of (88), (70), and Remark 3.2. Substituting (82) into the expression in parentheses in (80), we obtain

$$\begin{aligned}\frac{1}{(i\alpha_1)(i\alpha_2)}-\frac{h^2}{2}\cdot\frac{e^{i\alpha_1h}+e^{i\alpha_2h}}{(e^{i\alpha_1h}-1)(e^{i\alpha_2h}-1)}&=\frac{1}{(i\alpha_1)(i\alpha_2)}-\frac{1}{2}\cdot\frac{2+i\alpha_1h(1+x_1)+i\alpha_2h(1+x_2)}{(i\alpha_1)(i\alpha_2)(1+x_1)(1+x_2)}\\&=\frac{x_1+x_2+x_1x_2-\frac{1}{2}i\alpha_1h(1+x_1)-\frac{1}{2}i\alpha_1h(1+x_1)}{(i\alpha_1)(i\alpha_2)(1+x_1)(1+x_2)}. &(89)\end{aligned}$$

Finally, (81) follows from the combination of (82), (83), (84) and (89). □

Remark 3.4. Introducing the notation $z = \frac{\lambda}{k}$ in (80), we rewrite D_0 in the form

$$\begin{aligned} D_0 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_0(kr)dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot h^2 \\ &= \frac{4h^2}{\pi}\cdot\int_{-\infty}^{\infty}\frac{dz}{\sqrt{1-z^2}}\left(\frac{1}{(z^2-\frac{1}{2})(kh)^2} - \frac{e^{i\frac{\sqrt{2}}{2}\left(\sqrt{1-z^2}-z\right)kh}+e^{i\frac{\sqrt{2}}{2}\left(\sqrt{1-z^2}+z\right)kh}}{2\left(e^{i\frac{\sqrt{2}}{2}\left(\sqrt{1-z^2}-z\right)kh}-1\right)\left(e^{i\frac{\sqrt{2}}{2}\left(\sqrt{1-z^2}+z\right)kh}-1\right)}\right). \end{aligned} \tag{90}$$

Thus, D_0 is entirely determined by k and h, and is of the form h^2 times a function of $k\cdot h$. Similarly, D_1 is of the form h^4 times a function of $k\cdot h$; D_2 and D_3 are of the form h^6 times functions of $k\cdot h$; D_4 and D_5 are of the form h^8 times functions of $k\cdot h$. In other words, except for the multiplicative factors (h^2, h^4, h^6, or h^8), D_0–D_5 depend only on the product $k\cdot h$. Fig. 4 and Tables 5, 6 in Appendix B provide plots and several representative numerical values of the functions $\frac{D_0}{h^2}, \frac{D_1}{h^4}, \frac{D_2}{h^6}, \frac{D_3}{h^6}, \frac{D_4}{h^8}, \frac{D_5}{h^8}$ for $k\cdot h\in[0,1]$.

Remark 3.5. 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 3.3 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. In our computations, we utilized extended (complex *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 3.7, which is the principal analytical tool of this paper (together with Lemmas 6.6–6.8). Theorem 3.7 describes an approximately 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 3.2) with $p=3$, and $s(x,y)=H_0\left(k\sqrt{x^2+y^2}\right)$. Approximately fourth-order, sixth-order, and eighth-order center-corrected quadratures are similar and are listed in Appendix C (see Lemmas 6.6–6.8). All the proofs are quite similar to that of Theorem 3.2, and are omitted.

Theorem 3.7. *Suppose that a is a positive real number, and* $\phi:\mathbb{R}^2\to\mathbb{C}$ *is a function such that* $\phi\in C^{12}(\mathbb{R}\times\mathbb{R})$ *and* ϕ *is zero outside the square* $[-a,a]\times[-a,a]$.

Then, for any $k\in\mathbb{C}^+$,

$$\left|\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)dxdy - U_{a,s}^h(\phi\cdot H_0)\right| = O((\log(1/h))^2h^{10}) \tag{91}$$

for all positive real numbers $h<a/p$.

In (91),

$$U_{a,s}^h(\phi\cdot H_0) = T_a^h(\phi\cdot H_0) + \sum_{p,q\in S}\tau_{pq}^h\phi(ph,qh), \tag{92}$$

where

$$S=\{p,q\in\mathbb{Z}: |p+q|\leqslant 3 \text{and} |p-q|\leqslant 3\}, \tag{93}$$

$$T_a^h(\phi\cdot H_0) = \sum_{(p,q)\neq(0,0)}\left(\phi(ph,qh)\cdot H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\right)\cdot h^2, \tag{94}$$

and

$$\tau_{0,0}^h = D_0 - \frac{49}{18}\frac{D_1}{h^2} + \frac{7}{9}\frac{D_2}{h^4} + \frac{3}{2}\frac{D_3}{h^4} - \frac{1}{18}\frac{D_4}{h^6} - \frac{1}{2}\frac{D_5}{h^6}, \tag{95}$$

$$\tau_{\pm1,0}^h = \tau_{0,\pm1}^h = \frac{3}{4}\frac{D_1}{h^2} - \frac{13}{48}\frac{D_2}{h^4} - \frac{19}{24}\frac{D_3}{h^4} + \frac{1}{48}\frac{D_4}{h^6} + \frac{7}{24}\frac{D_5}{h^6}, \tag{96}$$

$$\tau_{\pm2,0}^h = \tau_{0,\pm2}^h = -\frac{3}{40}\frac{D_1}{h^2} + \frac{1}{12}\frac{D_2}{h^4} + \frac{1}{24}\frac{D_3}{h^4} - \frac{1}{120}\frac{D_4}{h^6} - \frac{1}{24}\frac{D_5}{h^6}, \tag{97}$$

$$\tau_{\pm3,0}^h = \tau_{0,\pm3}^h = \frac{1}{180}\frac{D_1}{h^2} - \frac{1}{144}\frac{D_2}{h^4} + \frac{1}{720}\frac{D_4}{h^6}, \tag{98}$$

$$\tau_{\pm1,\pm1}^h = \frac{5}{12}\frac{D_3}{h^4} - \frac{1}{6}\frac{D_5}{h^6}, \tag{99}$$

$$\tau^h_{\pm1,\pm2} = \tau^h_{\pm2,\pm1} = -\frac{1}{48}\frac{D_3}{h^4} + \frac{1}{48}\frac{D_5}{h^6}, \tag{100}$$

where D_0–D_5 are defined in formulae (63)–(68).

Remark 3.6. For simplicity, we assume here that the function ϕ is zero outside the square $[-a,a]\times[-a,a]$. Thus, the integral and the sum on the square $[-a,a]\times[-a,a]$ are identical to those in $\mathbb{R}^2$. This simplification allows the direct use of the analytical formulae for D_0–D_5 (see Lemma 3.6 above and Lemmas 6.1–6.5 in Appendix A).

Remark 3.7. Theorem 3.7 is valid in the limit when k is real-valued, too, as seen in the numerical examples of Section 5.

Remark 3.8. Combining Remark 3.4 with the definitions (95)–(100), we observe that each of the coefficients τ^h_{pq} in (95)–(100) has the form h^2 times a function of $k\cdot h$; we will refer to the coefficients τ^h_{pq} as correction coefficients.

Remark 3.9. The set S defined in (93) contains 25 pairs of integers (p,q); in other words, corrections at 25 points around the singularity are required to construct a nearly 10th-order quadrature formula (see Fig. 1). In general, for any integer $p\geqslant 0$, $2p^2+2p+1$ correction nodes are needed to obtain a quadrature of order approximately $2p+4$.

3.3. Fast numerical application of discretized Lippmann–Schwinger operators

In this section, we combine the approximately 10th-order quadrature formula (91) 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 $\mathbb{R}^2$, where a is a positive real number.

Suppose that N is a positive integer, $h=a/N$, and S is the set defined in (93). Suppose further that the coefficients $\tau^h_{i_1i_2}$ are defined in (95)–(100). Then, we define a two-dimensional complex sequence $H=\{H_{i_1i_2}\},\ i_1,i_2=-2N,\dots,2N$, as follows:

$$H_{i_1i_2} = H_0\left(k\sqrt{(i_1h)^2+(i_2h)^2}\right) + \tau^h_{i_1i_2}/h^2, \tag{101}$$

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

$$H_{00} = \tau^h_{00}/h^2, \tag{102}$$

and

$$H_{i_1i_2} = H_0\left(k\sqrt{(i_1h)^2+(i_2h)^2}\right) \tag{103}$$

otherwise. We define $\Phi=\{\Phi_{i_1i_2}\}$, $i_1,i_2=-N,\dots,N$, to be the complex sequence given by the formula

$$\Phi_{i_1i_2} = \phi(i_1h, i_2h), \tag{104}$$

where $\phi:\mathbb{R}^2\to\mathbb{C}$ is a function such that $\phi\in C^{12}(\mathbb{R}^2)$ and ϕ is zero outside D.

Lemma 3.8. *Suppose that $N,\ l_1,\ l_2$ are integers such that $N\geqslant 1$, $-N\leqslant l_1\leqslant N$, $-N\leqslant l_2\leqslant N$, and that a,x,y are real numbers such that $a>0$, $-a\leqslant x\leqslant a$, $-a\leqslant y\leqslant a$. Suppose further that $\phi:\mathbb{R}^2\to\mathbb{C}$ is a function such that $\phi\in C^{12}(\mathbb{R}^2)$ and ϕ is zero outside the square $[-a,a]\times[-a,a]$. Then, for any $k\in\mathbb{C}^+$,*

$$\left|\int_{-a}^{a}\int_{-a}^{a}\phi(x',y')\cdot H_0\left(k\sqrt{(x-x')^2+(y-y')^2}\right)dx'dy' - \sum_{-N\leqslant i_1\leqslant N}\ \sum_{-N\leqslant i_2\leqslant N}\Phi_{i_1i_2}\cdot H_{(l_1-i_1),(l_2-i_2)}\right| = O((\log(1/h))^2h^{10}), \tag{105}$$

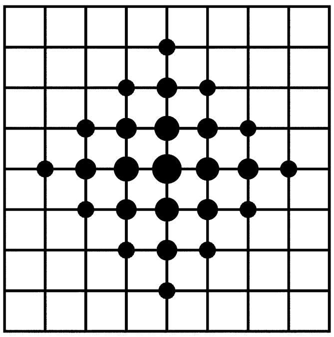

Fig. 1. The 25 correction nodes.

where $h = a/N$, $x = l_1 h$, $y = l_2 h$, the two-dimensional sequence $\Phi = \{\Phi_{i_1 i_2}\}$, $i_1, i_2 = -N, \ldots, N$ is defined in (104), and the two-dimensional sequence $H = \{H_{j_1 j_2}\}$, $j_1, j_2 = -2N, \ldots, 2N$ is defined in (101)–(103).

Proof. Due to (91) and (92),

$$\left| \int_{-a}^{a} \int_{-a}^{a} \phi(x', y') \cdot H_0\left(k\sqrt{(x-x')^2 + (y-y')^2}\right) dx'dy' - \sum_{(i_1,i_2)\in I'} \phi(i_1 h, i_2 h) \cdot H_0\left(k\sqrt{(l_1 h - i_1 h)^2 + (l_2 h - i_2 h)^2}\right) \cdot h^2 \right.$$
$$\left. - \sum_{(p,q)\in S} \tau_{pq}^h \phi(l_1 h + ph, l_2 h + qh) \right| = O((\log(1/h))^2 h^{10}), \tag{106}$$

where

$$I' = \{i_1, i_2 \in \mathbb{Z} : |i_1| \leqslant N, |i_2| \leqslant N, (i_1, i_2) \neq (l_1, l_2)\}, \tag{107}$$

and S is defined in (93). Now, (105) follows immediately from the combination of (106) and the definitions in (101)–(104). □

Remark 3.10. Obviously, the sum in the left-hand side of (105) is the Toeplitz convolution of the two-dimensional sequences Φ, H, and as such, it can be rapidly calculated via the FFT (see Section 2.2 above). Thus,

$$\sum_{-N\leqslant i_1\leqslant N} \sum_{-N\leqslant i_2\leqslant N} \Phi_{i_1 i_2} \cdot H_{(l_1-i_1),(l_2-i_2)} = (\mathscr{F}^{2N})^{-1} (\mathscr{F}^{2N}(\Phi') \cdot \mathscr{F}^{2N}(H))_{l_1 l_2}, \tag{108}$$

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

$$\Phi'_{ij} = \begin{cases} \Phi_{ij}, & \text{if } |i| \leqslant N \text{ and } |j| \leqslant N, \\ 0, & \text{if } |i| > N \text{ or } |j| > N. \end{cases} \tag{109}$$

Remark 3.11. 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 $\psi \in C^{10}(\mathbb{R}^2)$.

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 approximately 10th-order iterative algorithm for the solution of the Lippmann–Schwinger equation

$$\psi(x) - k^2 \int_D G_k(x,y)V(y)\psi(y)dy = k^2 \int_D G_k(x,y)V(y)\phi(y)dy \tag{110}$$

in two dimensions, where $D = [-a,a] \times [-a,a]$, G_k is the Green's function for the Helmholtz equation in two dimensions, i.e., $G_k(x,y) = -\frac{i}{4} \cdot H_0(k\|x-y\|)$, 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 3.11, 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 (110). Therefore, we focus on obtaining the solution of (110) for $x \in D$. Obviously, (110) can be written as the linear system

$$(I - A)\psi = A\phi, \tag{111}$$

where ψ is the unknown scattered field in D, ϕ is the given incident field in D, I is the identity operator, and A is the integral operator in (110). As discussed in Section 3, we use (105) to approximate the integral operator A acting on the functions ψ, ϕ. With the help of the FFT (see Remark 3.10), we apply the discretized version of A rapidly to arbitrary vectors, and solve the linear system (111) 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.]
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.

Table 1
Tenth-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 discretization 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
Tenth-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 discretization 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

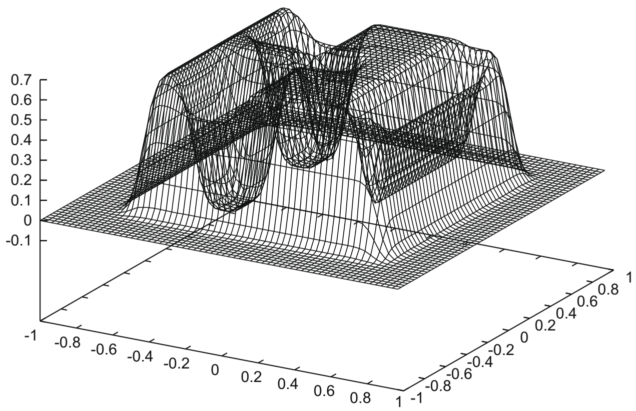

Fig. 2. The human skull model.

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 $N_2 = (2N+1)^2$.

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

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

Stage 1. *Comment* [Construct the values of 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 (63)–(68) via interpolation (see Remark 3.5).

Construct the two-dimensional sequence H via the formulae (101)–(103) 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 (111).]

For a point source (x_0, y_0), construct a two-dimensional sequence $\Phi = \{\Phi_{ij}\}$, $i,j = -N,\ldots,N$ for the discretized incident field on the domain $[-a,a] \times [-a,a]$ via the formula (104). Construct the two-dimensional sequence $f = \{\Phi_{ij} \cdot V_{ij}\}$, $i,j = -N,\ldots,N$. (We require $V \in C^{12}(\mathbb{R}^2)$ and that V vanishes outside $[-a,a] \times [-a,a]$, so that $V \cdot \phi \in C^{12}(\mathbb{R}^2)$ and $V \cdot \phi$ vanishes outside $[-a,a] \times [-a,a]$.)

As in Remark 3.10, 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 $(I - A)\psi = A\phi$ to the pre-determined precision ϵ. A is applied to vectors via the FFT, as in Remark 3.10.

The solution produced by BI-CGSTAB is the scattered field ψ at the N_2 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_2 discretization points. As in Remark 3.11, apply the trapezoidal rule to (110) 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 $O(N_2)$, where N_2 is the total number of discretization points on the square $[-a,a] \times [-a,a]$, i.e., $N_2 = (2N+1)^2$. The two-dimensional FFT costs $O(N_2 \log(N_2))$. Thus, the CPU time cost of Stage 1 is of the order $O(N_2 \log(N_2))$.

In Stage 2, the construction of the two-dimensional sequences Φ, f costs $O(N_2)$, and the two-dimensional FFT costs $O(N_2 \log(N_2))$. Thus, the CPU time cost of the Stage 2 is of order $O(N_2 \log(N_2))$.

The CPU time cost of Stage 3 is of order $O(N_{iter} \cdot N_2 \log(N_2))$, where N_{iter} is the number of iterations required by the iterative solver to produce the pre-determined precision ϵ.

In Stage 4, the CPU time cost of interpolating the field at any point in $\mathbb{R}^2$ is $O(N_2)$.

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

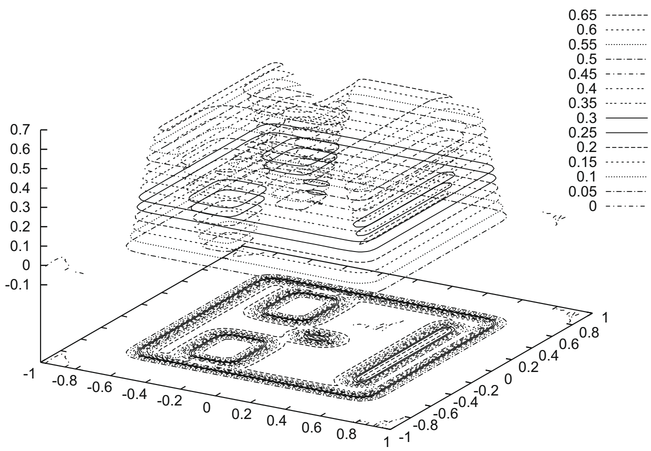

Fig. 3. The human skull model viewed from the top.

$$T = \alpha(N_{iter} \cdot N_2 \log(N_2)) + \beta \cdot N_2 + \gamma, \tag{112}$$

where N_2 is the total number of discretization points, N_{iter} is the number of iterations required by the iterative solver to reach the precision ϵ, and the coefficients $\alpha,\ \beta,\ \gamma$ are determined by the computer system, implementation, etc.

The storage (memory) requirements of the algorithm are determined by the total number of discretization points N_2 and the number of iterations N_{its} performed before restarting the iterative solver, and are of the form

$$S = O(N_{its} \cdot N_2). \tag{113}$$

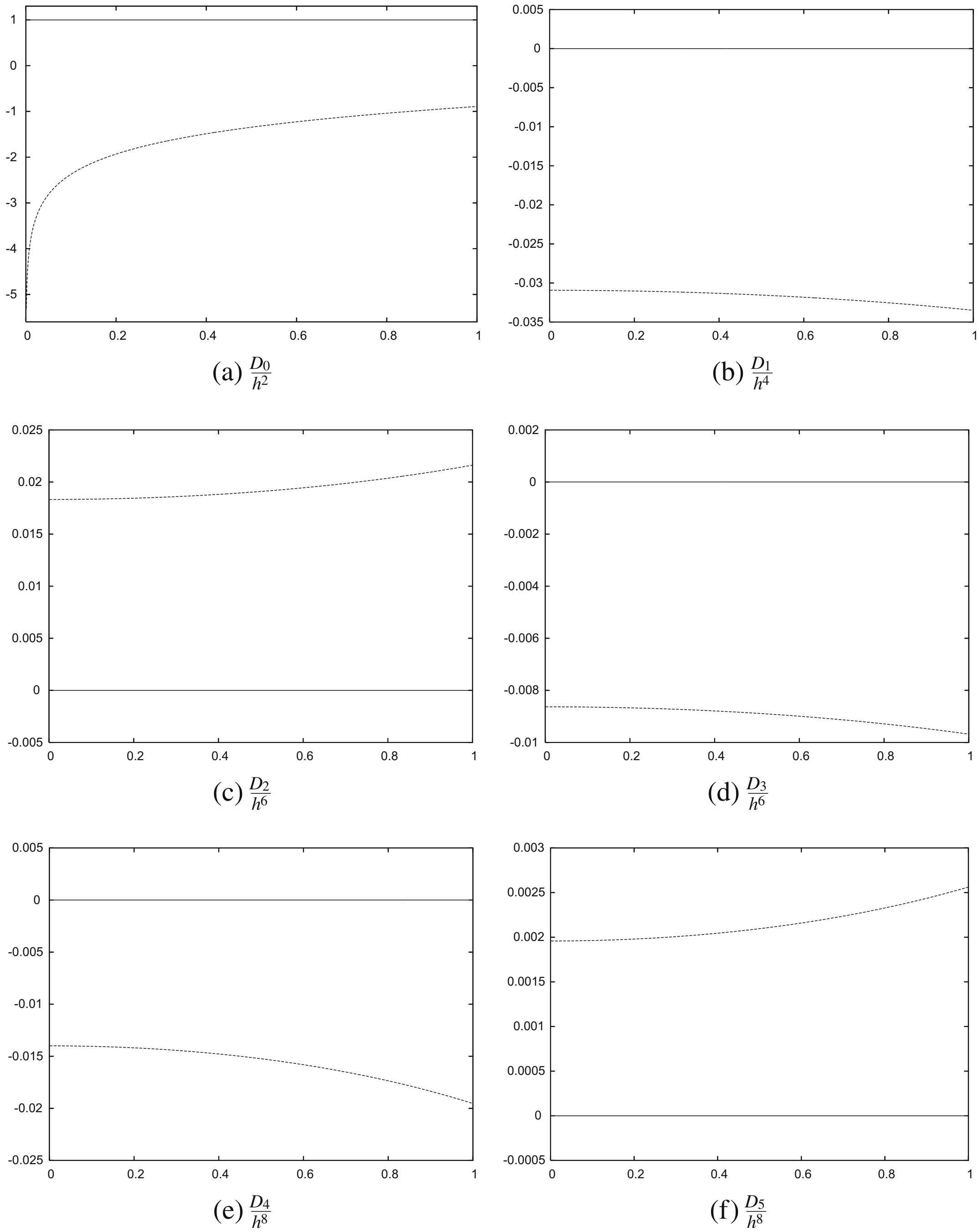

Fig. 4. The real and imaginary parts of $\frac{D_0}{h^2}, \frac{D_1}{h^4}, \frac{D_2}{h^6}, \frac{D_3}{h^6}, \frac{D_4}{h^8}, \frac{D_5}{h^8}$. The horizontal axis is $k \cdot h$. The solid lines are the real parts; the dotted lines are the imaginary parts. (a) $\frac{D_0}{h^2}$ (b) $\frac{D_1}{h^4}$ (c) $\frac{D_2}{h^6}$ (d) $\frac{D_3}{h^6}$ (e) $\frac{D_4}{h^8}$ (f) $\frac{D_5}{h^8}$.

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} for the BI-CGSTAB iterations; the calculations reported in Tables 2 and 4 were carried out with a requested accuracy of 10^{-9}. We restarted the BI-CGSTAB iterations every 5 steps.

Tables 1–4 illustrate the numerical behavior at arbitrary far-field points of the scattered field generated by the potential V from (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. The skull model is shown in Figs. 2 and 3. The headings of the tables are as follows:

k is the wave number from (2);
N — the computational grid is $N \times N$, for a total of N^2 discretization points;
$size_{obj}$ — the computational grid is ($size_{obj}$ wavelengths) $\times$ ($size_{obj}$ wavelengths);
N_λ is the number of discretization points per wavelength;
E_{rel} is the average of the relative errors of the solution for the scattered field at twenty randomly chosen far-field points (the errors are estimated as the relative differences between the computed solution and the solution computed using four times as many discretization points in the domain $[-1,1] \times [-1,1]$ containing the scatterer);
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 more detailed numerical tests performed by the authors:

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

Table 5
$\frac{D_0}{h^2}, \frac{D_1}{h^4}, \frac{D_2}{h^6}$ for several real values of $k \cdot h$.

$k \cdot h$	$\frac{D_0}{h^2}$	$\frac{D_1}{h^4}$	$\frac{D_2}{h^6}$
1	1.00E+00 − $i \cdot$ 8.92E–01	4.16E–17 − $i \cdot$ 3.35E–02	−2.60E–17 + $i \cdot$ 2.16E–02
$\frac{1}{2}$	1.00E+00 − $i \cdot$ 1.35E+00	1.12E–16 − $i \cdot$ 3.15E–02	−7.11E–17 + $i \cdot$ 1.91E–02
$\frac{1}{4}$	1.00E+00 − $i \cdot$ 1.79E+00	5.20E–17 − $i \cdot$ 3.11E–02	−2.95E–17 + $i \cdot$ 1.85E–02
$\frac{1}{8}$	1.00E+00 − $i \cdot$ 2.23E+00	2.60E–17 − $i \cdot$ 3.10E–02	−1.56E–17 + $i \cdot$ 1.84E–02
$\frac{1}{16}$	1.00E+00 − $i \cdot$ 2.67E+00	9.32E–17 − $i \cdot$ 3.09E–02	−6.95E–17 + $i \cdot$ 1.83E–02
$\frac{1}{32}$	1.00E+00 − $i \cdot$ 3.11E+00	4.23E–17 − $i \cdot$ 3.09E–02	−2.65E–17 + $i \cdot$ 1.83E–02

Table 6
$\frac{D_3}{h^6}, \frac{D_4}{h^8}, \frac{D_5}{h^8}$ for several real values of $k \cdot h$.

$k \cdot h$	$\frac{D_3}{h^6}$	$\frac{D_4}{h^8}$	$\frac{D_5}{h^8}$
1	−1.47E–17 − $i \cdot$ 9.68E–03	2.95E–17 − $i \cdot$ 1.95E–02	−3.25E–18 + $i \cdot$ 2.56E–03
$\frac{1}{2}$	3.30E–17 − $i \cdot$ 8.88E–03	5.55E–17 − $i \cdot$ 1.52E–02	−7.91E–18 + $i \cdot$ 2.10E–03
$\frac{1}{4}$	1.82E–17 − $i \cdot$ 8.69E–03	1.56E–17 − $i \cdot$ 1.43E–02	−3.25E–18 + $i \cdot$ 1.99E–03
$\frac{1}{8}$	9.11E–18 − $i \cdot$ 8.65E–03	1.30E–17 − $i \cdot$ 1.41E–02	−2.17E–18 + $i \cdot$ 1.97E–03
$\frac{1}{16}$	2.81E–17 − $i \cdot$ 8.64E–03	3.62E–17 − $i \cdot$ 1.40E–02	−4.04E–18 + $i \cdot$ 1.96E–03
$\frac{1}{32}$	1.74E–17 − $i \cdot$ 8.63E–03	1.81E–17 − $i \cdot$ 1.40E–02	−2.58E–18 + $i \cdot$ 1.96E–03

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 proven above and illustrated via several numerical examples, the scheme is nearly $(2p+4)$th $(p = 0, 1, 2, 3, \ldots)$ 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, for example. Furthermore, the method does not require access to each of the functions P, Q 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 discusses only the square region $[-a, a] \times [-a, a]$.

Acknowledgments

The authors would like to thank Mark Tygert and the referees for helpful suggestions.

Appendix A. Lemmas 6.1–6.5 below provide analytical formulae for

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\left(x^{i-1}y^{j-1}H_0\left(k\sqrt{x^2+y^2}\right)\right)dxdy - \sum_{(p,q)\neq(0,0)}\left((ph)^{i-1}(qh)^{j-1}H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\right)\cdot h^2, \tag{114}$$

with $(i,j) = \{(3,1),(5,1),(3,3),(7,1),(5,3)\}$. The proofs are straightforward, but tedious; we used the software package Mathematica for help.

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

$$\begin{aligned}
D_1 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_0(kr)x^2 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot(ph)^2\cdot h^2 \\
&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{2}{(i\alpha_1)^3(i\alpha_2)} - \frac{h^4}{2}\cdot\frac{e^{i\alpha_1 h}(e^{i\alpha_1 h}+1)(e^{i\alpha_2 h}+1)}{(e^{i\alpha_1 h}-1)^3(e^{i\alpha_2 h}-1)}\right) \\
&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{2}{\alpha_1^3\alpha_2(1+x_1)^3(1+x_2)}\cdot\left(\frac{(\alpha_2 h)^2}{12} + 3z_1 + z_2 + 3y_1^2 + \frac{3}{2}y_1(i\alpha_1 h)\right. \\
&\quad + 3y_1y_2 + \frac{3}{2}y_1(i\alpha_2 h) + \frac{3}{2}y_2(i\alpha_1 h) + x_1^3 + 3x_1^2x_2 + x_1^3x_2 - \frac{1}{2}i\alpha_2 h y_2 + \frac{1}{2}\alpha_1^2h^2(x_1^2+2x_1) \\
&\quad \left.+ \frac{3}{4}\alpha_1\alpha_2h^2(x_1x_2+x_1+x_2) + \frac{1}{4}i\alpha_1^2\alpha_2h^3(1+x_1)^2(1+x_2)\right),
\end{aligned} \tag{115}$$

where r, α_1, α_2, x_1, x_2, y_1, y_2, z_1, z_2 are defined by (85), (86), and (82), (83), (84).

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

$$\begin{aligned}
D_2 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_0(kr)x^4 dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot(ph)^4\cdot h^2 \\
&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{24}{(i\alpha_1)^5(i\alpha_2)} - \frac{h^6}{2}\cdot\frac{e^{i\alpha_1 h}+11e^{2i\alpha_1 h}+11e^{3i\alpha_1 h}+e^{4i\alpha_1 h}}{(e^{i\alpha_1 h}-1)^5}\cdot\frac{e^{i\alpha_2 h}+1}{e^{i\alpha_2 h}-1}\right) \\
&= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{1}{\alpha_1^5\alpha_2(1+x_1)^5(1+x_2)}\cdot\left(2(i\alpha_2 h)^2 + (i\alpha_2 h)^3 + 5(i\alpha_1 h)(i\alpha_2 h)^2\right. \\
&\quad + \frac{3}{10}(i\alpha_2 h)^4 + \frac{20}{3}(i\alpha_1 h)^2(i\alpha_2 h)^2 + \frac{5}{2}(i\alpha_1 h)(i\alpha_2 h)^3 + \frac{1}{2}(i\alpha_1 h)^4(i\alpha_2 h) + 4x_1(i\alpha_1 h)^4 \\
&\quad + \frac{45}{2}x_1(i\alpha_1 h)^3(i\alpha_2 h) + 2x_1(i\alpha_1 h)^4(i\alpha_2 h) + 45x_1^2(i\alpha_1 h)^3 + 25x_1^2(i\alpha_1 h)^2(i\alpha_2 h) \\
&\quad + 6x_1^2(i\alpha_1 h)^4 + \frac{45}{2}x_1^2(i\alpha_1 h)^3(i\alpha_2 h) + 3x_1^2(i\alpha_1 h)^4(i\alpha_2 h) + 15x_1^3(i\alpha_1 h)^3 + 4x_1^3(i\alpha_1 h)^4 \\
&\quad + \frac{15}{2}x_1^3(i\alpha_1 h)^3(i\alpha_2 h) + 2x_1^3(i\alpha_1 h)^4(i\alpha_2 h) + x_1^4(i\alpha_1 h)^4 + \frac{1}{2}x_1^4(i\alpha_1 h)^4(i\alpha_2 h)
\end{aligned}$$

$$+\frac{15}{2}x_2(i\alpha_1h)^3(i\alpha_2h)+\frac{1}{2}x_2(i\alpha_1h)^4(i\alpha_2h)+50x_1x_2(i\alpha_1h)^2(i\alpha_2h)$$
$$+\frac{45}{2}x_1x_2(i\alpha_1h)^3(i\alpha_2h)+2x_1x_2(i\alpha_1h)^4(i\alpha_2h)+25x_1^2x_2(i\alpha_1h)^2(i\alpha_2h)$$
$$+\frac{45}{2}x_1^2x_2(i\alpha_1h)^3(i\alpha_2h)+3x_1^2x_2(i\alpha_1h)^4(i\alpha_2h)+\frac{15}{2}x_1^3x_2(i\alpha_1h)^3(i\alpha_2h)$$
$$+2x_1^3x_2(i\alpha_1h)^4(i\alpha_2h)+\frac{1}{2}x_1^4x_2(i\alpha_1h)^4(i\alpha_2h)+12w_2(i\alpha_2h)+30z_2(i\alpha_1h)(i\alpha_2h)$$
$$+40y_2(i\alpha_1h)^2(i\alpha_2h)+15y_1(i\alpha_1h)(i\alpha_2h)^2+30y_1y_2(i\alpha_1h)(i\alpha_2h)-120u_1-24u_2$$
$$-180w_1(i\alpha_1h)-60w_2(i\alpha_1h)-60w_1(i\alpha_2h)-160z_1(i\alpha_1h)^2-90z_1(i\alpha_1h)(i\alpha_2h)$$
$$-80z_2(i\alpha_1h)^2+35y_1(i\alpha_1h)^3-40y_1(i\alpha_1h)^2(i\alpha_2h)-130y_1^2(i\alpha_1h)^2$$
$$-180y_1^2(i\alpha_1h)(i\alpha_2h)-240y_1^3(i\alpha_1h)-120y_1^3(i\alpha_2h)-120y_1^4-30y_2(i\alpha_1h)^3$$
$$-180y_1y_2(i\alpha_1h)^2-360y_1^2y_2(i\alpha_1h)-240y_1^3y_2-20z_1(i\alpha_2h)^2-240z_1^2-120z_1z_2$$
$$-360y_1^2(i\alpha_1h)-240y_1^3-120y_1^2(i\alpha_2h)-240y_1y_2(i\alpha_1h)-240y_1^2y_2-24x_1^5-120x_1^4x_2-24x_1^5x_2\Big), \tag{116}$$

where

$$w_1=z_1-\frac{(i\alpha_1h)^3}{24}=\sum_{n=4}^{\infty}\frac{(i\alpha_1h)^n}{(n+1)!},\quad w_2=z_2-\frac{(i\alpha_2h)^3}{24}=\sum_{n=4}^{\infty}\frac{(i\alpha_2h)^n}{(n+1)!}, \tag{117}$$

$$u_1=w_1-\frac{(i\alpha_1h)^4}{120}=\sum_{n=5}^{\infty}\frac{(i\alpha_1h)^n}{(n+1)!},\quad u_2=w_2-\frac{(i\alpha_2h)^4}{120}=\sum_{n=5}^{\infty}\frac{(i\alpha_2h)^n}{(n+1)!}, \tag{118}$$

and $r,\alpha_1,\alpha_2,x_1,x_2,y_1,y_2,z_1,z_2$ *are defined by (85), (86) and (82), (83), (84).*

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

$$D_3=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}H_0(kr)x^2y^2dxdy-\sum_{(p,q)\neq(0,0)}H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot(ph)^2(qh)^2\cdot h^2$$
$$=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\left(\frac{4}{(i\alpha_1)^3(i\alpha_2)^3}-h^6\cdot\frac{e^{i\alpha_1h}(e^{i\alpha_1h}+1)}{(e^{i\alpha_1h}-1)^3}\cdot\frac{e^{i\alpha_1h}(e^{i\alpha_1h}+1)}{(e^{i\alpha_1h}-1)^3}\right)$$
$$=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{-4}{\alpha_1^3\alpha_2^3(1+x_1)^3(1+x_2)^3}\cdot\Big(\frac{1}{240}(i\alpha_1h)^4+\frac{1}{240}(i\alpha_2h)^4$$
$$+\frac{3}{4}z_1(i\alpha_1h)^2+\frac{3}{4}z_2(i\alpha_2h)^2+\frac{9}{2}(i\alpha_1h)(i\alpha_2h)(z_1+z_2)$$
$$+\frac{15}{4}z_1(i\alpha_2h)^2+\frac{15}{4}z_2(i\alpha_1h)^2-\frac{3}{2}y_1(i\alpha_1h)^2(i\alpha_2h)-\frac{3}{2}y_2(i\alpha_1h)(i\alpha_2h)^2$$
$$+3u_1+3u_2+\frac{9}{2}w_2(i\alpha_1h)+\frac{9}{2}w_1(i\alpha_2h)+\frac{3}{2}w_1(i\alpha_1h)+\frac{3}{2}w_2(i\alpha_2h)$$
$$-\frac{9}{4}(i\alpha_1h)(i\alpha_2h)(z_1+z_2)+3z_1^2+3z_2^2+9z_1z_2-\frac{1}{2}y_1(i\alpha_1h)^3-\frac{1}{2}y_2(i\alpha_2h)^3$$
$$-\frac{1}{2}y_1^2(i\alpha_1h)^2-\frac{1}{2}y_2^2(i\alpha_2h)^2+\frac{9}{4}(i\alpha_1h)(i\alpha_2h)(3y_1y_2+\frac{1}{6}y_1(i\alpha_2h)+\frac{1}{6}y_2(i\alpha_1h))$$
$$+\frac{9}{8}y_1(i\alpha_1h)^2(i\alpha_2h)+\frac{3}{8}y_1(i\alpha_2h)^3+\frac{9}{4}y_1^2(i\alpha_1h)(i\alpha_2h)+\frac{9}{4}y_1^2(i\alpha_2h)^2+\frac{3}{2}y_1^3(i\alpha_2h)$$
$$+\frac{3}{8}y_2(i\alpha_1h)^3+\frac{9}{8}y_2(i\alpha_1h)(i\alpha_2h)^2+\frac{9}{4}y_1y_2(i\alpha_1h)^2+\frac{9}{4}y_1y_2(i\alpha_2h)^2$$
$$+\frac{9}{2}y_1^2y_2(i\alpha_1h)+9y_1^2y_2(i\alpha_2h)+3y_1^3y_2+\frac{9}{4}y_2^2(i\alpha_1h)^2+\frac{9}{4}y_2^2(i\alpha_1h)(i\alpha_2h)$$
$$+9y_1y_2^2(i\alpha_1h)+\frac{9}{2}y_1y_2^2(i\alpha_2h)+9y_1^2y_2^2+\frac{3}{2}y_2^3(i\alpha_1h)+3y_1y_2^3$$

$$
\begin{aligned}
&-\frac{1}{4}(i\alpha_1 h)^2(i\alpha_2 h)^2(2x_1+x_1^2+2x_2+4x_1x_2+2x_1^2x_2+x_2^2+2x_1x_2^2+x_1^2x_2^2)\\
&+\frac{3}{2}y_1^2(i\alpha_1 h)+y_1^3+\frac{3}{2}y_2^2(i\alpha_2 h)+y_2^3+\frac{9}{2}y_1^2(i\alpha_2 h)+9y_1y_2(i\alpha_1 h+i\alpha_2 h)\\
&+9y_1^2y_2+\frac{9}{2}y_2^2(i\alpha_1 h)+9y_1y_2^2-\frac{3}{4}(i\alpha_1 h)^2(i\alpha_2 h)(x_1^2+2x_1x_2+x_1^2x_2)\\
&-\frac{3}{4}(i\alpha_1 h)(i\alpha_2 h)^2(x_2^2+2x_1x_2+x_1x_2^2)+3x_1^3x_2^2+3x_1^2x_2^3+x_1^3x_2^3\Bigg),
\end{aligned}
\tag{119}
$$

where r, α_1, α_2, x_1, x_2, y_1, y_2, z_1, z_2, w_1, w_2, u_1, u_2 are defined by (85), (86), (82), (83), (84), (117) and (118).

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

$$
\begin{aligned}
D_4 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_0(kr)x^6\,dx\,dy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot(ph)^6\cdot h^2\\
&=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{720}{\alpha_1^7\alpha_2}-\frac{h^8}{2}\cdot\frac{e^{i\alpha_1 h}+57e^{2i\alpha_1 h}+302e^{3i\alpha_1 h}+302e^{4i\alpha_1 h}+57e^{5i\alpha_1 h}+e^{6i\alpha_1 h}}{(e^{i\alpha_1 h}-1)^7}\cdot\frac{e^{i\alpha_2 h}+1}{e^{i\alpha_2 h}-1}\right)\\
&=\frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{1}{\alpha_1^7\alpha_2(1+x_1)^7(1+x_2)}\cdot(A+B),
\end{aligned}
\tag{120}
$$

where

$$
\begin{aligned}
A &= 60(\alpha_2 h)^2-30(i\alpha_2 h)^3-210(i\alpha_1 h)(i\alpha_2 h)^2-9(\alpha_2 h)^4-105(\alpha_1 h)(\alpha_2 h)^3\\
&-385(\alpha_1 h)^2(\alpha_2 h)^2+37800y_1^2(i\alpha_1 h)+25200y_1^3+7560y_1^2(i\alpha_2 h)\\
&+15120y_1y_2(i\alpha_1 h)+15120y_1^2y_2+15120x_1^5+5040x_1^6+720x_1^7+25200x_1^4x_2\\
&+15120x_1^5x_2+5040x_1^6x_2+720x_1^7x_2+5040u_1+720u_2+12600w_1(i\alpha_1 h)\\
&-360w_2(i\alpha_2 h)+2520w_2(i\alpha_1 h)+2520w_1(i\alpha_2 h)-17220(\alpha_1 h)^2z_1\\
&+6300z_1(i\alpha_1 h)(i\alpha_2 h)+1260z_2(\alpha_1 h)(\alpha_2 h)-4620(\alpha_1 h)^2z_2+15120z_1^2\\
&+2940y_1(i\alpha_1 h)^3-6090y_1(\alpha_1 h)^2(i\alpha_2 h)-34440y_1^2(\alpha_1 h)^2-18900y_1^2(\alpha_1 h)(\alpha_2 h)\\
&+50400y_1^3(i\alpha_1 h)+12600y_1^3(i\alpha_2 h)+25200y_1^4+3150y_2(i\alpha_1 h)^3\\
&-18900y_1y_2(\alpha_1 h)^2+37800y_1^2y_2(i\alpha_1 h)+25200y_1^3y_2-840z_1(\alpha_2 h)^2+5040z_1z_2\\
&+2310y_2(\alpha_1 h)^2(i\alpha_2 h)+630y_1(i\alpha_1 h)(\alpha_2 h)^2+1260y_1y_2(\alpha_1 h)(\alpha_2 h)\\
&-63(i\alpha_1 h)^5-301(i\alpha_1 h)^4(i\alpha_2 h)+(\alpha_1 h)^6+\frac{63}{2}(\alpha_1 h)^5(\alpha_2 h)+\frac{1}{2}(\alpha_1 h)^6(i\alpha_2 h)\\
&-2408x_1(\alpha_1 h)^4-3150x_1(\alpha_1 h)^3(\alpha_2 h)-315x_1(i\alpha_1 h)^5-1204x_1(i\alpha_1 h)^4(i\alpha_2 h)\\
&+6x_1(\alpha_1 h)^6+\frac{315}{2}x_1(\alpha_1 h)^5(\alpha_2 h)+3x_1(\alpha_1 h)^6(i\alpha_2 h)-6300x_1^2(i\alpha_1 h)^3\\
&+1680x_1^2(\alpha_1 h)^2(i\alpha_2 h)-3612x_1^2(\alpha_1 h)^4-3150x_1^2(\alpha_1 h)^3(\alpha_2 h)-630x_1^2(i\alpha_1 h)^5\\
&-1806x_1^2(i\alpha_1 h)^4(i\alpha_2 h)+15x_1^2(\alpha_1 h)^6+315x_1^2(\alpha_1 h)^5(\alpha_2 h)+\frac{15}{2}x_1^2(\alpha_1 h)^6(i\alpha_2 h),
\end{aligned}
\tag{121}
$$

$$
\begin{aligned}
B &= -2100x_1^3(i\alpha_1 h)^3-2408x_1^3(\alpha_1 h)^4-1050x_1^3(\alpha_1 h)^3(\alpha_2 h)-630x_1^3(i\alpha_1 h)^5\\
&-1204x_1^3(i\alpha_1 h)^4(i\alpha_2 h)+20x_1^3(\alpha_1 h)^6+315x_1^3(\alpha_1 h)^5(\alpha_2 h)+10x_1^3(\alpha_1 h)^6(i\alpha_2 h)\\
&-602x_1^4(\alpha_1 h)^4-315x_1^4(i\alpha_1 h)^5-301x_1^4(i\alpha_1 h)^4(i\alpha_2 h)+15x_1^4(\alpha_1 h)^6\\
&+\frac{315}{2}x_1^4(\alpha_1 h)^5(\alpha_2 h)+\frac{15}{2}x_1^4(\alpha_1 h)^6(i\alpha_2 h)-63x_1^5(i\alpha_1 h)^5+6x_1^5(\alpha_1 h)^6\\
&+\frac{63}{2}x_1^5(\alpha_1 h)^5(\alpha_2 h)+3x_1^5(\alpha_1 h)^6(i\alpha_2 h)+x_1^6(\alpha_1 h)^6+\frac{1}{2}x_1^6(\alpha_1 h)^6(i\alpha_2 h)\\
&-1050x_2(\alpha_1 h)^3(\alpha_2 h)-301x_2(\alpha_1 h)^4(i\alpha_2 h)+\frac{63}{2}x_2(\alpha_1 h)^5(\alpha_2 h)\\
&+\frac{1}{2}x_2(\alpha_1 h)^6(i\alpha_2 h)+3360x_1x_2(\alpha_1 h)^2(i\alpha_2 h)-3150x_1x_2(\alpha_1 h)^3(\alpha_2 h)\\
&-1204x_1x_2(\alpha_1 h)^4(i\alpha_2 h)+\frac{315}{2}x_1x_2(\alpha_1 h)^5(\alpha_2 h)+3x_1x_2(\alpha_1 h)^6(i\alpha_2 h)
\end{aligned}
$$

$$+1680x_1^2x_2(\alpha_1h)^2(i\alpha_2h) - 3150x_1^2x_2(\alpha_1h)^3(\alpha_2h) - 1806x_1^2x_2(\alpha_1h)^4(i\alpha_2h)$$
$$+315x_1^2x_2(\alpha_1h)^5(\alpha_2h) + \frac{15}{2}x_1^2x_2(\alpha_1h)^6(i\alpha_2h) - 1050x_1^3x_2(\alpha_1h)^3(\alpha_2h)$$
$$-1204x_1^3x_2(\alpha_1h)^4(i\alpha_2h) + 315x_1^3x_2(\alpha_1h)^5(\alpha_2h) + 10x_1^3x_2(\alpha_1h)^6(i\alpha_2h)$$
$$-301x_1^4x_2(\alpha_1h)^4(i\alpha_2h) + \frac{315}{2}x_1^4x_2(\alpha_1h)^5(\alpha_2h) + \frac{15}{2}x_1^4x_2(\alpha_1h)^6(i\alpha_2h)$$
$$+\frac{63}{2}x_1^5x_2(\alpha_1h)^5(\alpha_2h) + 3x_1^5x_2(\alpha_1h)^6(i\alpha_2h) + \frac{1}{2}x_1^6x_2(\alpha_1h)^6(i\alpha_2h), \tag{122}$$

and where r, α_1, α_2, x_1, x_2, y_1, y_2, z_1, z_2, w_1, w_2, u_1, u_2 are defined by (85), (86), (82), (83), (84), (117) and (118).

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

$$\begin{aligned} D_5 &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} H_0(kr)x^4y^2dxdy - \sum_{(p,q)\neq(0,0)} H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\cdot(ph)^4(qh)^2\cdot h^2 \\ &= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\left(\frac{48}{\alpha_1^5\alpha_2^3} - h^8\cdot\frac{e^{i\alpha_1h}+11e^{2i\alpha_1h}+11e^{3i\alpha_1h}+e^{4i\alpha_1h}}{(e^{i\alpha_1h}-1)^5}\cdot\frac{e^{i\alpha_2h}\cdot(e^{i\alpha_2h}+1)}{(e^{i\alpha_2h}-1)^3}\right) \\ &= \frac{4}{\pi}\int_{-\infty}^{\infty}\frac{d\lambda}{\sqrt{k^2-\lambda^2}}\cdot\frac{1}{\alpha_1^5\alpha_2^3(1+x_1)^5(1+x_2)^3}\cdot(C+D), \end{aligned} \tag{123}$$

where

$$\begin{aligned} C = &\frac{1}{5}(\alpha_2h)^4 + 240u_1 + 360w_1(i\alpha_1h) + 144u_2 + 360w_2(i\alpha_1h) + 360w_1(i\alpha_2h) \\ &+ 72w_2(i\alpha_2h) - 320z_1(\alpha_1h)^2 - 540z_1(\alpha_1h)(\alpha_2h) - 480z_2(\alpha_1h)^2 \\ &- 300z_1(\alpha_2h)^2 - 180z_2(\alpha_1h)(\alpha_2h) - 36z_2(\alpha_2h)^2 + 480z_1^2 + 720z_1z_2 + 144z_2^2 \\ &- 70y_1(i\alpha_1h)^3 - 240y_1(\alpha_1h)^2(i\alpha_2h) - 210y_1(i\alpha_1h)(\alpha_2h)^2 \\ &+ 30y_1(i\alpha_2h)^3 - 260y_1^2(\alpha_1h)^2 - 1080y_1^2(\alpha_1h)(\alpha_2h) - 360y_1^2(\alpha_2h)^2 \\ &+ 480y_1^3(i\alpha_1h) + 720y_1^3(i\alpha_2h) + 240y_1^4 + 180y_2(i\alpha_1h)^3 + 120y_2(i\alpha_1h)^2(i\alpha_2h) \\ &+ 30y_2(i\alpha_1h)(\alpha_2h)^2 - 1080y_1y_2(\alpha_1h)^2 - 1260y_1y_2(\alpha_1h)(\alpha_2h) \\ &- 180y_1y_2(\alpha_2h)^2 + 2160y_1^2y_2(i\alpha_1h) + 1440y_1^2y_2(i\alpha_2h) + 1440y_1^3y_2 - 360y_2^2(\alpha_1h)^2 \\ &- 180y_2^2(\alpha_1h)(\alpha_2h) + 1440y_1y_2^2(i\alpha_1h) + 360y_1y_2^2(i\alpha_2h) + 1440y_1^2y_2^2 + 120y_2^3(i\alpha_1h) \\ &+ 240y_1y_2^3 + 720y_1^2(i\alpha_1h) + 480y_1^3 + 720y_1^2(i\alpha_2h) + 1440y_1y_2(i\alpha_1h) + 1440y_1^2y_2 \\ &+ 720y_1y_2(i\alpha_2h) + 360y_2^2(i\alpha_1h) + 720y_1y_2^2 + 72y_2^2(i\alpha_2h) + 48y_2^3 + 48x_1^5 + 720x_1^4x_2 \\ &+ 144x_1^5x_2 + 1440x_1^3x_2^2 + 720x_1^4x_2^2 + 144x_1^5x_2^2 + 480x_1^2x_2^3 + 480x_1^3x_2^3 + 240x_1^4x_2^3 \\ &+ 48x_1^5x_2^3 - 24y_2(i\alpha_2h)^3 + 24y_2^2(\alpha_2h)^2 - 3(i\alpha_1h)^4(i\alpha_2h) - 15(i\alpha_1h)^3(i\alpha_2h)^2 \\ &+ (\alpha_1h)^4(\alpha_2h)^2 - 8x_1(\alpha_1h)^4 - 135x_1(\alpha_1h)^3(\alpha_2h) - 100x_1(\alpha_1h)^2(\alpha_2h)^2 \\ &- 12x_1(\alpha_1h)^4(i\alpha_2h) - 45x_1(i\alpha_1h)^3(i\alpha_2h)^2 + 4x_1(\alpha_1h)^4(\alpha_2h)^2 - 90x_1^2(i\alpha_1h)^3 \\ &- 150x_1^2(i\alpha_1h)^2(i\alpha_2h) - 12x_1^2(\alpha_1h)^4 - 135x_1^2(\alpha_1h)^3(\alpha_2h) - 50x_1^2(\alpha_1h)^2(\alpha_2h)^2 \\ &- 18x_1^2(\alpha_1h)^4(i\alpha_2h) - 45x_1^2(i\alpha_1h)^3(i\alpha_2h)^2 + 6x_1^2(\alpha_1h)^4(\alpha_2h)^2 - 30x_1^3(i\alpha_1h)^3 \\ &- 8x_1^3(\alpha_1h)^4 - 45x_1^3(\alpha_1h)^3(\alpha_2h) - 12x_1^3(\alpha_1h)^4(i\alpha_2h) - 15x_1^3(i\alpha_1h)^3(i\alpha_2h)^2 \\ &+ 4x_1^3(\alpha_1h)^4(\alpha_2h)^2 - 2x_1^4(\alpha_1h)^4 - 3x_1^4(\alpha_1h)^4(i\alpha_2h) + x_1^4(\alpha_1h)^4(\alpha_2h)^2 \\ &- 45x_2(\alpha_1h)^3(\alpha_2h) - 100x_2(\alpha_1h)^2(\alpha_2h)^2 - 3x_2(\alpha_1h)^4(i\alpha_2h) \\ &- 30x_2(i\alpha_1h)^3(i\alpha_2h)^2 + 2x_2(\alpha_1h)^4(\alpha_2h)^2 + 300x_1x_2(\alpha_1h)^2(i\alpha_2h) \\ &+ 120x_1x_2(i\alpha_1h)(\alpha_2h)^2 - 135x_1x_2(\alpha_1h)^3(\alpha_2h) - 200x_1x_2(\alpha_1h)^2(\alpha_2h)^2 \\ &- 12x_1x_2(\alpha_1h)^4(i\alpha_2h) - 90x_1x_2(i\alpha_1h)^3(i\alpha_2h)^2 + 8x_1x_2(\alpha_1h)^4(\alpha_2h)^2 \\ &+ 150x_1^2x_2(\alpha_1h)^2(i\alpha_2h) - 135x_1^2x_2(\alpha_1h)^3(\alpha_2h) - 100x_1^2x_2(\alpha_1h)^2(\alpha_2h)^2 \\ &- 18x_1^2x_2(\alpha_1h)^4(i\alpha_2h) - 90x_1^2x_2(i\alpha_1h)^3(i\alpha_2h)^2 + 12x_1^2x_2(\alpha_1h)^4(\alpha_2h)^2, \end{aligned} \tag{124}$$

$$\begin{aligned}D = {} & -45x_1^3x_2(\alpha_1 h)^3(\alpha_2 h) - 12x_1^3x_2(\alpha_1 h)^4(i\alpha_2 h) - 30x_1^3x_2(i\alpha_1 h)^3(i\alpha_2 h)^2 \\ & + 8x_1^3x_2(\alpha_1 h)^4(\alpha_2 h)^2 - 3x_1^4x_2(\alpha_1 h)^4(i\alpha_2 h) + 2x_1^4x_2(\alpha_1 h)^4(\alpha_2 h)^2 \\ & + 60x_2^2(i\alpha_1 h)(\alpha_2 h)^2 - 50x_2^2(\alpha_1 h)^2(\alpha_2 h)^2 - 15x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 \\ & + x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 + 60x_1x_2^2(i\alpha_1 h)(\alpha_2 h)^2 - 100x_1x_2^2(\alpha_1 h)^2(\alpha_2 h)^2 \\ & - 45x_1x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 4x_1x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 - 50x_1^2x_2^2(\alpha_1 h)^2(\alpha_2 h)^2 \\ & - 45x_1^2x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 + 6x_1^2x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 - 15x_1^3x_2^2(i\alpha_1 h)^3(i\alpha_2 h)^2 \\ & + 4x_1^3x_2^2(\alpha_1 h)^4(\alpha_2 h)^2 + x_1^4x_2^2(\alpha_1 h)^4(\alpha_2 h)^2,\end{aligned} \tag{125}$$

where r, α_1, α_2, x_1, x_2, y_1, y_2, z_1, z_2, w_1, w_2, u_1, u_2 are defined by (85), (86), (82), (83), (84), (117) and (118).

Appendix B. Fig. 4 provides plots of the functions $\frac{D_0}{h^2}, \frac{D_1}{h^4}, \frac{D_2}{h^6}, \frac{D_3}{h^6}, \frac{D_4}{h^8}, \frac{D_5}{h^8}$ for $k \cdot h \in [0,1]$. Tables 5 and 6 provide numerical values of $\frac{D_0}{h^2}, \frac{D_1}{h^4}, \frac{D_2}{h^6}, \frac{D_3}{h^6}, \frac{D_4}{h^8}, \frac{D_5}{h^8}$ for the values of $k \cdot h$ used in the numerical examples of Section 5. The values of $\frac{D_0}{h^2}, \frac{D_1}{h^4}, \frac{D_2}{h^6}, \frac{D_3}{h^6}, \frac{D_4}{h^8}, \frac{D_5}{h^8}$ were calculated via interpolation in double precision, as described in Remark 3.5.

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

$$\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)dxdy. \tag{126}$$

Lemma 6.6. (∼ 4th-order center-corrected quadrature formula) *Suppose that a is a positive real number, and $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in C^6(\mathbb{R}\times\mathbb{R})$ and ϕ is zero outside the square $[-a,a]\times[-a,a]$.*

Then, for any $k \in \mathbb{C}^+$,

$$\left|\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)dxdy - U_{a,s}^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right)\right| = O((\log(1/h))^2h^4) \tag{127}$$

for all positive real numbers $h < a/p$. In (127),

$$U_{a,s}^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) = T_a^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) + \sum_{p,q\in S}\tau_{pq}^h\phi(ph,qh), \tag{128}$$

where

$$S = \{p,q \in \mathbb{Z} : p = 0 \text{ and } q = 0\}, \tag{129}$$

$$T_a^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) = \sum_{(p,q)\neq(0,0)}\left(\phi(ph,qh)\cdot H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\right)\cdot h^2, \tag{130}$$

and

$$\tau_{00}^h = D_0. \tag{131}$$

Lemma 6.7. (∼ 6th-order center-corrected quadrature formula) *Suppose that a is a positive real number, and $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in C^8(\mathbb{R}\times\mathbb{R})$ and ϕ is zero outside the square $[-a,a]\times[-a,a]$.*

Then, for any $k \in \mathbb{C}^+$,

$$\left|\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)dxdy - U_{a,s}^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right)\right| = O((\log(1/h))^2h^6) \tag{132}$$

for all positive real numbers $h < a/p$. In (132),

$$U_{a,s}^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) = T_a^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) + \sum_{p,q\in S}\tau_{pq}^h\phi(ph,qh), \tag{133}$$

where

$$S = \{p,q \in \mathbb{Z} : |p+q| \leqslant 1 \text{ and } |p-q| \leqslant 1\}, \tag{134}$$

$$T_a^h\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) = \sum_{(p,q)\neq(0,0)}\left(\phi(ph,qh)\cdot H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\right)\cdot h^2, \tag{135}$$

and

$$\tau^h_{0,0} = D_0 - 2\frac{D_1}{h^2}, \tag{136}$$

$$\tau^h_{\pm1,0} = \tau^h_{0,\pm1} = \frac{1}{2}\frac{D_1}{h^2}. \tag{137}$$

Lemma 6.8. ($\sim$ 8th-order center-corrected quadrature formula) *Suppose that a is a positive real number, and $\phi : \mathbb{R}^2 \to \mathbb{C}$ is a function such that $\phi \in C^{10}(\mathbb{R}\times\mathbb{R})$ and ϕ is zero outside the square $[-a,a]\times[-a,a]$. Then, for any $k \in \mathbb{C}^+$,*

$$\left|\int_{-a}^{a}\int_{-a}^{a}\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)dxdy - U^h_{a,s}\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right)\right| = O((\log(1/h))^2h^8) \tag{138}$$

for all positive real numbers $h < a/p$. In (138),

$$U^h_{a,s}\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) = T^h_a\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) + \sum_{p,q\in S}\tau^h_{pq}\phi(ph,qh), \tag{139}$$

where

$$S = \{p,q \in \mathbb{Z} : |p+q| \leqslant 2 \text{and} |p-q| \leqslant 2\}, \tag{140}$$

$$T^h_a\left(\phi(x,y)\cdot H_0\left(k\sqrt{x^2+y^2}\right)\right) = \sum_{(p,q)\neq(0,0)}\left(\phi(ph,qh)\cdot H_0\left(k\sqrt{(ph)^2+(qh)^2}\right)\right)\cdot h^2, \tag{141}$$

and

$$\tau^h_{0,0} = D_0 - \frac{5}{2}\frac{D_1}{h^2} + \frac{1}{2}\frac{D_2}{h^4} + \frac{D_3}{h^4}, \tag{142}$$

$$\tau^h_{\pm1,0} = \tau^h_{0,\pm1} = \frac{2}{3}\frac{D_1}{h^2} - \frac{1}{6}\frac{D_2}{h^4} - \frac{1}{2}\frac{D_3}{h^4}, \tag{143}$$

$$\tau^h_{\pm2,0} = \tau^h_{0,\pm2} = -\frac{1}{24}\frac{D_1}{h^2} + \frac{1}{24}\frac{D_2}{h^4}, \tag{144}$$

$$\tau^h_{\pm1,\pm1} = \frac{1}{4}\frac{D_3}{h^4}. \tag{145}$$

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