The diagonal forms are constructed for the translation operators for the Helmholtz equation in three dimensions. While the operators themselves have a fairly complicated structure (described somewhat incompletely by the classical addition theorems for the Bessel functions), their diagonal forms turn out to be quite simple. These diagonal forms are realized as generalized integrals, possess straightforward physical interpretations, and admit stable numerical implementation. This paper uses the obtained analytical apparatus to construct an algorithm for the rapid application to arbitrary vectors of matrices resulting from the discretization of integral equations of the potential theory for the Helmholtz equation in three dimensions. It is an extension to the three-dimensional case of the results of [13], where a similar apparatus is developed in the two-dimensional case.

Diagonal Forms of Translation Operators for the Helmholtz Equation in Three Dimensions

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1. Introduction

One of standard approaches to numerical treatment of boundary value problems for elliptic partial differential equations (PDEs) calls for converting them into second kind integral equations (SKIEs) with subsequent discretization of the latter via appropriate quadrature formulae. Discretization of the resulting SKIEs usually leads to dense large-scale systems of linear algebraic equations, which are in turn solved by means of some iterative technique, such as Generalized Conjugate Residual algorithm. Most iterative schemes for the solution of linear systems of this type require application of the matrix of the system to a sequence of recursively generated vectors. Applying a dense matrix to a vector is an order n^2 procedure, where n is the dimension of the matrix, which in this case is equal to the number of nodes in the discretization of the domain of the integral equation. As a result, the whole process is at least of the order n^2, and for many large scale problems, this estimate is prohibitively large.

During the last several years, a group of algorithms has been introduced for the rapid application to arbitrary vectors of matrices resulting from the discretization of integral equations from several areas of applied mathematics. The schemes include the Fast Multipole Method for the Laplace equation in two and three dimensions (see, for example, [7]), the fast Gauss transform (see [9]), the Fast Laplace Transform (see [13, 16]), and several other schemes. In all cases, the resulting algorithms have asymptotic CPU time estimates of either $O(n)$ or $O(n \cdot log(n))$, and are a dramatic improvement over the classical ones for large-scale problems.

All such schemes are based on one of two approaches.

1. The first approach utilizes the fact that the kernel of the integral operator to be applied is smooth (away from the diagonal or some other small part of the matrix), and decomposes it into some appropriately chosen set of functions (Chebychev polynomials in [13] and [2], wavelets in [4], wavelet-like objects in [3], etc.). This approach is extremely general and easy to use, since a single scheme is applicable to a wide class of operators.

2. The second approach is restricted to the cases when the integral operator has some special analytical structure, and uses the corresponding special functions (multipole expansions for the Laplace equation in [7], [8], Hermite polynomials in [9], Laguerre polynomials in [16], etc.

In this approach, a special-purpose algorithm has to be constructed for each narrow class of kernels, and in each case the appropriate special functions and translation operators for them (historically known as Addition Theorems) have to be available. However, once constructed, such algorithms tend to be extremely efficient. In addition, there are several important situations where the first approach fails, but the second can be used (a typical example is the n-body graviational problem with a highly non-uniform distribution of particles, as in [5]).

Both of the above approaches fail when the kernel is highly oscillatory, and simple counter-examples show that it is impossible to construct a scheme that would work in the general oscillatory case (the Nyquist theorem being the basic obstacle). However, several oscillatory problems are of sufficient importance that it is worth-while to construct special purpose methods for them. A typical example are kernels satisfying the Helmholtz equation in two and three dimensions, since this is the equation controlling the propagation of acoustic and electromagnetic waves, and many quantum-mechanical phenomena. Unlike the non-oscillatory case, the oscillatory one requires a fairly subtle mathematical apparatus, and for the Helmholtz equation in two dimensions, such an apparatus is constructed in [14].

The present paper presents an extension of the results of [14] to the three-dimensional case, and a description of an algorithm for the rapid application to arbitrary vectors of matrices resulting from the discretization of integral equations of the potential theory for the Helmholtz equation in three dimensions. The principal purpose of this paper are Theorems 3.1 - 3.3, describing the diagonal forms of the well-known translation operators for the Helmholtz equation in three dimensions.

2. Analytical and Numerical Preliminaries

2.1. Notation. We will be denoting by (ρ, θ, ϕ) the spherical coordinates in R^3, with the Euclidean coordinates denoted by (x, y, z). Given a point s on the two-dimensional sphere S^2, we will denote its spherical coordinates by $(\theta(s), \phi(s))$, and note that the north pole s_N has the coordinates $(\pi, *)$, while the coordinates of the south pole s_S are $(0, *)$.

We will denote by E the natural embedding $S^2 \rightarrow R^3$, defined by the formula

$$E(s) = (cos(\theta(s)) \cdot cos(\phi(s)), cos(\theta(s)) \cdot sin(\phi(s)), sin(\theta(s))). \tag{1}$$

For a non-zero vector $u \in R^3$, we will denote by $P(u)$ the point on S^2 defined by the formula

$$P(u) = E^{-1}(\frac{u}{||u||}). \tag{2}$$

Sometimes, we will use a more invariant notation, saying that the pair $(r \in R^1, s \in S^2)$ is the spherical coordinates of the point $u \in R^3$, with r, s defined by the formulae

$$r = ||u|| \tag{3}$$

$$s = P(u). \tag{4}$$

For a pair of points $s_0, s \in S^2$, we will denote by $A_{s_0}(s)$ the angle between the vectors $E(s_0)$, $E(s)$.

Finally, for any $s_0, s \in S^2$, we will denote by $c(s_0, s)$ the cosine of the angle between the vectors $E(s_0)$, $E(s)$, so that

$$c(s_0, s) = (E(s_0), E(s)) = cos(A_{s_0}(s)). \tag{5}$$

2.2. Charges and dipoles. For a Helmholtz equation

$$\nabla^2 f + k^2 f = 0 \tag{6}$$

we will define the potential $f^k_{x_0} : R^3 \setminus \{x_o\} \rightarrow C^1$ of a unit charge located at the point $x_0 \in R^3$ by the formula

$$f^k_{x_0}(x) = h_0(k||x - x_0||), \tag{7}$$

where h_0 denotes the spherical Hankel function of order zero (see (16) below). For any $h \in R^3$ such that $||h|| = 1$, we will define the potential $f^k_{x_0,h}$ of a unity dipole located at x_0 and oriented in the direction h by the formula

$$f^k_{x_0,h}(x) = -h_1(k||x - x_0||) \cdot \frac{k(x - x_0, h)}{||x - x_0||}. \tag{8}$$

As is well known, both potentials $f^k_{x_0}$, $f^k_{x_0,h}$ (as well as most other physically meaningful potentials for the equation (6)), satisfy the radiation condition at ∞, i.e., for any $x \in R^3$, there exists $c \in C^1$ such that when $t \to \infty$,

$$\psi(t \cdot x) = c \cdot \frac{e^{ikt \cdot |x|}}{t} + O(\frac{1}{t^2}). \tag{9}$$

The following theorem is well-known, and is a direct consequence of the Gauss theorem.

Theorem 2.1

Suppose that $\tilde{D} \subset D$ are two balls in R^3, and that D is bounded by a sphere S. Suppose further that $f : R^3 \setminus \tilde{D} \to C$ is a radiation field satisfying the equation (6)) in $R^3 \setminus \tilde{D}$ and the radiation condition (9)) at ∞. Then there exist two analytical functions $\sigma, \eta : S \to C$, such that for all $x \in R^3 \setminus D$,

$$f(x) = \int_S \sigma(s) \cdot f^k_s(x) ds, \tag{10}$$

and

$$f(x) = \int_S \eta(s) \cdot f^k_{s,N(s)}(x) ds, \tag{11}$$

where $N(s)$ denotes the exterior normal to S at the point s.

2.3. Spherical Bessel and Hankel functions. In agreement with standard practice, we will denote by j_m the spherical Bessel function of the first kind of order m, and by h_m, the spherical Hankel function of order m. As is well known (see, for example [18]), j_m are analytic on the whole complex plane for all values of m, while h_m have a branch cut along the negative real axis, and become infinite at the origin. The asymptotic behaviour of the functions j_m, h_m for large m is given by the formulae

$$\lim_{m \to \infty} j_m(z) \cdot \frac{2 \cdot (2n+1)^{n+1}}{z^n \cdot e^{n+\frac{1}{2}}} = 1, \tag{12}$$

and

$$\lim_{m \to \infty} h_m(z) \cdot \frac{e^{n+\frac{1}{2}} \cdot z^{n+1}}{\sqrt{2} \cdot (2n+1)^n} = 1 \tag{13}$$

(see [1], 9.3.1, 9.3.2, 9.1.3). For large z and fixed m, the asymptotic behavior of $j_m(z)$, $h_m(z)$ is given by the formulae

$$z \cdot j_m(z) - \cos(z - \frac{m\pi}{2} - \frac{\pi}{2}) = O(\frac{e^{|Im(z)|}}{|z|^2}), \tag{14}$$

$$z \cdot h_m(z) - e^{i\cdot(z - \frac{m\pi}{2} - \frac{\pi}{2})} = O(\frac{e^{-Im(z)}}{|z|^2}) \tag{15}$$

when $z \to \infty$, as long as $Im(z) \geq 0$ (see [1], 9.2.5, 9.2.7).

All spherical Bessel functions are 'elementary functions'. In particular,

$$\begin{aligned} j_0(z) &= \frac{sin(z)}{z}, \\ h_0(z) &= -\frac{i \cdot e^{i\cdot z}}{z}, \\ j_1(z) &= \frac{sin(z)}{z^2} - \frac{cos(z)}{z}, \\ h_1(z) &= -(\frac{1}{z} + \frac{i}{z^2}) \cdot e^{i\cdot z}, \\ \frac{d}{dz} j_0(z) &= -j_1(z), \\ \frac{d}{dz} h_0(z) &= -h_1(z). \end{aligned} \tag{16}$$

The following theorem is known as the Addition Theorem for spherical Bessel functions, and is one of principal analytical tools of this paper. It can be found, for example, in [1].

Theorem 2.2

Suppose that r, ρ, θ, λ are arbitrary complex numbers, $\eta = \pi - \theta$, and that $R \in C$ is defined by the formula

$$R = (r^2 + \rho^2 - 2 \cdot r \cdot \rho \cdot cos(\theta))^{\frac{1}{2}} = (r^2 + \rho^2 + 2 \cdot r \cdot \rho \cdot cos(\eta))^{\frac{1}{2}} \tag{17}$$

(see Figure 1). Then

$$\begin{aligned} &\sum_{n=0}^{\infty} (2n+1) \cdot j_n(\lambda \cdot r) \cdot j_n(\lambda \cdot \rho) \cdot P_n(cos(\theta)) = \\ &\sum_{n=0}^{\infty} (-1)^n \cdot (2n+1) \cdot j_n(\lambda \cdot r) \cdot j_n(\lambda \cdot \rho) \cdot P_n(cos(\eta)) = \\ &j_0(\lambda \cdot R) = \frac{sin(\lambda \cdot R)}{\lambda \cdot R}. \end{aligned} \tag{18}$$

and

$$\sum_{n=0}^{\infty}(2n+1)\cdot e^{\frac{1}{2}\cdot n\pi\cdot i}\cdot j_n(\rho)\cdot P_n(cos(\theta)) =$$
$$\sum_{n=0}^{\infty}(2n+1)\cdot i^n\cdot j_n(\rho)\cdot P_n(cos(\theta)) = e^{i\cdot\rho\cdot cos(\theta)}. \tag{19}$$

If, in addition, $| r\cdot e^{\pm i\cdot\theta} |<| \rho |$, then

$$\sum_{n=0}^{\infty}(2n+1)\cdot j_n(\lambda\cdot r)\cdot h_n(\lambda\cdot\rho)\cdot P_n(cos(\theta)) =$$
$$\sum_{n=0}^{\infty}(-1)^n\cdot(2n+1)\cdot j_n(\lambda\cdot r)\cdot h_n(\lambda\cdot\rho)\cdot P_n(cos(\eta)) = \tag{20}$$
$$h_0(\lambda\cdot R) = \frac{-i\cdot e^{i\cdot\lambda\cdot R}}{\lambda\cdot R}.$$

2.4. Integrals of spherical harmonics.

A function $\omega : S^2 \to C$ is referred to as a spherical harmonic of degree n if the function $f : R^3 \to C$ defined by the formula

$$f(x,y,z) = \omega(\theta,\phi)\cdot\rho^m \tag{21}$$

satisfies the Laplace equation in R^3 (see, for example, [10]).

Remark 2.1

As is well-known (see, for example, [11]), for any integer $n \geq 0$, there exist exactly $2n+1$ linearly independent spherical harmonics of order n, and a standard representation of a spherical harmonic of order n is by an expression

$$\omega(\theta,\phi) = \sum_{m=-n}^{n}\gamma_i\cdot P_n^m(cos(\theta))\cdot e^{i\cdot m\cdot\phi}, \tag{22}$$

with P_n^m the associated Legendre function of degree n and order m (see, for example, [1]), and $\gamma_i, i = 0, \pm1, \pm2, \cdots, \pm n$ a finite sequence of complex numbers. However, in this paper we will not be using the representation (22), remembering only that the spherical harmonics of order n constitute a complex linear space of dimension $2n+1$.

We will need the following three well-known lemmas involving the integration of spherical harmonics over the surface of the sphere. Lemmas 2.1, 2.2 below can be found, for example, in [10]), [1], respectively. Lemma 2.3 is a simple consequence of Lemma 2.2, and can be found in [1].

Lemma 2.1.

For any spherical harmonic Y of degree $n \geq 0$,

$$\int_{S^2} Y(s) \cdot P_n(cos(\theta(s)))ds = \frac{4 \cdot \pi}{2n+1} \cdot Y(s_N) \tag{23}$$

Lemma 2.2.

For any $n \geq 0$ and $z \in C$,

$$j_n(z) = \frac{(-i)^n}{2} \cdot \int_{S^2} e^{i \cdot z \cdot cos(\theta(s))} \cdot P_n(cos(\theta(s)))ds. \tag{24}$$

The following theorem is a simple consequence of the preceeding two lemmas, Theorem 2.2, and the formulae (12), (13).

Theorem 2.3.

Suppose that $\rho \in R$, n is a natural number, and $k \in C$ is such that $Im(k) \geq 0$. Suppose further that $u \in R^3$ is such that $\|u\| < \rho$, and that the functions $T_n : S^2 \rightarrow C$, $F_n : R^3 \rightarrow C$ are defined by the formulae

$$T_n(s) = T_n(\theta, \phi) = \sum_{m=0}^{n} i^m \cdot (2m+1) \cdot h_m(k \cdot \rho) \cdot P_m(cos(\theta)), \tag{25}$$

$$F_n(u) = \frac{1}{4 \cdot \pi} \cdot \int_{S^2} T_n(s) \cdot e^{i \cdot k \cdot (E(s), u)} ds. \tag{26}$$

Then

$$\lim_{n \rightarrow \infty} F_n(u) = h_0(k \cdot (\rho^2 + \|u\|^2 + 2 \cdot \rho \cdot \|u\| \cdot cos(\eta))^{\frac{1}{2}}), \tag{27}$$

with η the angle between the vector u and the z axis. Furthermore, for large n,

$$| F_n(u) - h_0(k \cdot (\rho^2 + \|u\|^2 + 2 \cdot \rho \cdot \|u\| \cdot cos(\eta))^{\frac{1}{2}}) = O((\frac{\|u\|}{\rho})^n). \tag{28}$$

Proof.

Combining (25) with (26), we have

$$F_n(u) = \frac{1}{4 \cdot \pi} \cdot \sum_{m=0}^{n} i^m \cdot (2m+1) \cdot h_m(k \cdot \rho) \cdot \int_{S^2} T_n(s) \cdot P_m(cos(\theta)) \cdot e^{i \cdot k \cdot (E(s),u)} ds, \quad (29)$$

and, substituting (19) into (29), obtain

$$\begin{aligned} F_n(u) &= \frac{1}{4 \cdot \pi} \cdot \sum_{m=0}^{n} i^m \cdot (2m+1) \cdot h_m(k \cdot \rho) \cdot \qquad (30) \\ \int_{S^2} P_m(cos(\theta(s))) &\cdot \sum_{l=0}^{\infty} (2l+1) \cdot e^{\frac{l \cdot \pi \cdot i}{2}} \cdot j_l(k \cdot \|u\|) \cdot P_l(c(P(u), s)) ds \end{aligned}$$

For any $m \neq l$,

$$\int_{S^2} P_m(cos(\theta(s))) \cdot P_l(c(P(u), s)) ds = 0, \quad (31)$$

since in this case $P_m(cos(\theta(s)))$, $P_l(c(P(u), s))$ are two spherical harmonics of different degrees, and, therefore, orthogonal on S^2. Combining (30) with (31), we have

$$\begin{aligned} F_n(u) &= \frac{1}{4 \cdot \pi} \cdot \sum_{m=0}^{n} (2m+1)^2 \cdot h_m(k \cdot \rho) \cdot j_m(k \cdot \|u\|) \qquad (32) \\ &\cdot \int_{S^2} P_m(cos(\theta(s))) \cdot P_m(c(P(u), s)) ds. \end{aligned}$$

Due to Lemma 2.1,

$$\int_{S^2} P_m(cos(\theta(s))) \cdot P_m(c(P(u), s)) ds = \frac{4 \cdot \pi}{(2m+1)} \cdot P_m(cos(\theta(P(u))), \quad (33)$$

and (32) assumes the form

$$F_n(u) = \sum_{m=0}^{n} (2m+1) \cdot h_m(k \cdot \rho) \cdot j_m(k \cdot \|u\|) \cdot P_m(cos(\theta(P(u))). \quad (34)$$

Now (27) follows from the combination of (34) and Theorem 2.2, and (28) follows from the combination of (27) with (12), (13).

2.5. Partial wave expansions of radiation fields. Suppose that the function $\phi : R^3 \to C^1$ satisfies the Helmholtz equation (6) outside an open ball D of radius R with the center at the point $x_0 \in R^3$, and also satisfies the radiation condition (9) at ∞. Then there exists a unique sequence of spherical harmonics $\alpha = \{\alpha_m\}$, $m = 0, 1, 2, \cdots$, such that for any $x \in R^3 \setminus \bar{D}$,

$$\phi(x) = \sum_{m=0}^{\infty} \alpha_m(s) \cdot h_m(k\rho), \tag{35}$$

with (ρ, s) the spherical coordinates of the vector $x - x_0$, and for each $m \in [0, \infty)$, α_m a spherical harmonic of degree m.

If a function ψ satisfies the equation (6) inside D, then there exists a unique sequence of spherical harmonics $\beta = \{\beta_m\}, m = 0, 1, 2, \cdots$, such that for each m, β_m is a harmonic of degree m, and for any $x \in D$,

$$\psi(x) = \sum_{m=0}^{\infty} \beta_m(s) \cdot j_m(k\rho). \tag{36}$$

A derivation of the formulae (35), (36) can be found, for example, in [11], and we will refer to functions satisfying the Helmholtz equation as radiation fields, to expansions of forms (35), (36) as h-expansions and j-expansions respectively, and to the point x_0 as the center of the expansions (35) (36).

The following lemma is a direct consequence of the formulae (12), (13). It establishes the convergence rates of the expansions (35), (36).

Lemma 2.4

If $D_1 \subset D$ is a ball of radius $R_1 < R$ with the center at x_0 then there exists $c > 0$ such that for any $x \in D_1$ and $N > |k| \cdot R_1$,

$$|\phi(x) - \sum_{m=0}^{N} \alpha_m(\theta, \phi) j_m(k\rho)| < (\frac{R_1}{R})^N. \tag{37}$$

If $D_2 \supset D$ is a ball of radius $R_2 > R$ with the center at x_0 then there exists $c > 0$ such that for any $x \in R^2 \setminus \bar{D}_2$ and $N > |k| \cdot R$,

$$|\psi(x) - \sum_{m=0}^{N} \beta_m(\theta, \phi) h_m(k\rho)| < c(\frac{R}{R_2})^N. \tag{38}$$

Remark 2.2

In numerical calculations, expansions (35), (36) are truncated after a finite number of terms, and the resulting expressions are viewed as approximations to the fields ϕ, ψ. If we want to approximate ϕ by an expansion of the form (37) with an accuracy ϵ then according to the above lemma, we have to choose

$$N \geq \max(|k| \cdot R_1, \frac{-\ln(\epsilon) + \ln(c)}{\ln(R) - \ln(R_1)}). \tag{39}$$

Since logarithm is a very slowly growing function, for medium and large scale problems,

$$\max(R_1 \cdot |k|, \frac{-\ln(\epsilon) + \ln(c)}{\ln(R) - \ln(R_1)}) \sim R_1 \cdot |k|, \tag{40}$$

i.e. the number of terms in the approximation is almost independent of ϵ, and must be roughly equal to $|k|\ R_1$. A similar calculation shows that for medium to large scale problems, the expansion (36) can be truncated after approximately $N \geq |k|R$ terms.

2.6. Numerical integration on S^2.

In this subsection we formulate two lemmas describing the optimum quadrature formulas for two situations: smooth functions on a circle, and smooth functions on an interval. Then, we use these lemmas to construct a high-order quadrature formula on S^2 (Theorem 2.4 below). Both Lemmas 2.5, 2.6 are well-known, and can be found, for example, in [15].

Lemma 2.5

For any integer m, n such that $n \geq 2|m|$, the n-point trapezoidal quadrature rule on the interval $[0, 2\pi]$ integrates the function e^{imx} exactly.

Lemma 2.6

For any natural n, there exist a unique pair of finite sequences $\{\chi_i^n\}$, $\{w_i^n\}, i = 1, 2, \cdots, n$, such that for any integer $k \in [1, 2n-1]$,

$$\sum_{i=1}^{n} w_i^n \cdot (\chi_i^n)^k = \int_{-1}^{1} t^k dt. \tag{41}$$

Furthermore, $\chi_i^n \in [-1, 1]$ and $w_i^n \in [0, 1]$ for all $i = 1, 2, \cdots n$.

The points χ_i^n and the coefficients w_i^n are known as the nodes and coefficients of the n-point Gaussian quadrature rule, which is the unique n-point quadrature rule that integrates exactly all polynomials of order up to $2n-1$.

For a natural n, we will define a finite sequence $\phi_1, \phi_2, \cdots, \phi_n$ by the formula

$$\phi_j = \frac{2 \cdot \pi}{n} \cdot (j-1), \tag{42}$$

and the finite sequence $\theta_1, \theta_2, \cdots, \theta_n$ by the formula

$$\theta_j = arccos(w_j^n). \tag{43}$$

Now, we define a discretization of $D^n \subset S^2$ as a collection of n^2 points $s_{j,k}^n$ defined by the formula

$$s_{j,k}^n = (\theta_j, \phi_k), \tag{44}$$

and given a function $f : S^2 \to C$, will be approximately representing it by a table of n^2 values

$$f_{j,k}^n = f(\theta_j, \phi_k). \tag{45}$$

Our choice of this discretization scheme is motivated by the following theorem, which is an immediate consequence of Lemmas 2.5, 2.6.

Theorem 2.4.

Suppose that the function $f : S^2 \to C$ is a spherical harmonic of degree n. Then

$$\int_{S^2} f(s)ds = \sum_{j,k=1}^{n} w_{j,k}^n \cdot f_{j,k}^n, \tag{46}$$

with the coefficients $w_{j,k}$ defined by the formula

$$w_{j,k}^n = \frac{2 \cdot \pi}{n} \cdot w_j^n. \tag{47}$$

Furthermore, the condition (46) defines the nodes $s_{j,k}^n$ and the weights $w_{j,k}^n$ uniquely, except for obvious transpositions and rotations.

3. Translation Operators For h and j Expansions.

3.1. Sequences of spherical harmonics and functions on S^2. We will denote by Y the set of all sequences $\alpha = \{\alpha_m\}, \quad m = 0, 1, 2, \cdots$, such that for each m, α_m is a spherical harmonic of degree m. We will define a norm on Y via the formula

$$\|\alpha\| = \sqrt{(\sum_{m=0}^{\infty} \|\alpha_m\|^2)}, \tag{48}$$

denote by X the subspace of Y consisting of such sequences α that $\|\alpha\| < \infty$, and observe that the norm (48) converts X into a Hilbert space. For a real number $r > 0$, we will denote by X_r the subspace of X consisting of all sequences $\alpha = \{\alpha_m\}, m = 0, 1, 2, \cdots$, such that

$$\|\alpha_m\| \cdot (\frac{2m}{er})^m \cdot \sqrt{m} < c \tag{49}$$

for all $m \geq r$. We will denote by Y_r the subspace of Y consisting of all complex sequences $\beta = \{\beta_m\}, m = 0, 1, 2, \cdots$, such that for some $c > 0$,

$$\|\beta_m\| \cdot (\frac{er}{2m})^m \cdot \sqrt{m} < c \tag{50}$$

for all $m \geq r$. It is easy to see that $X_r \subset Y_r$, and that the condition (49) is a very restrictive one, since in order to satisfy it, the elements of the sequence $\{\alpha_m\}$ must decay roughly as $(r/2)^m/m!$, while the condition (49) is a very mild one - it prohibits the elements of $\{\beta_m\}$ from growing faster than approximately $(2/r)^m \cdot m!$. By applying formulae (9.3.1), (9.3.2) from [1], it is easy to show that in (35) (36), $\alpha \in Y_{|k|R}$ and $\beta \in Y_{|k|\ R}$. Conversely, for any sequence $\alpha \in Y_{|k|\ R}$, the expansion (35) converges inside D, and for any $\beta \in Y_{|k|\ R}$, the expansion (36), converges outside D. For a natural n, we will denote by T_n a linear mapping $Y_r \to Y_r$ converting a sequence $\alpha = \{\alpha_m\}, m = 0, 1, 2, \cdots$ into a sequence $\tilde{\alpha} = \{\tilde{\alpha}_m\}, m = 0, 1, 2, \cdots$, defined by the formulae

$$\begin{aligned} \tilde{\alpha}_m &= \alpha_m \ \ for \ \ |m| \leq n \\ \tilde{\alpha}_m &= 0 \ \ for \ \ |m| \geq n + 1. \end{aligned} \tag{51}$$

Clearly, $T_n(Y_r) \subset X_r$, and for obvious reasons, we will refer to T_n as truncation.

We will define the mapping $F : X \to L^2(S^2)$ by the formula

$$F(\alpha)(s) = \sum_{m=0}^{\infty} \alpha_m(s) \cdot e^{-i \cdot \frac{(m+1) \cdot \pi)}{2}}, \tag{52}$$

with $\alpha = \{\alpha_0, \alpha_1, \cdots\} \in X$, and the mapping $F_- : X \to L^2(S^2)$ by the formula

$$F_-(\alpha)(s) = \sum_{m=0}^{\infty} \alpha_m(s) \cdot e^{i \cdot \frac{(m+1)\cdot\pi)}{2}}. \tag{53}$$

It is easy to see that the mappings F, F_- are unitary in the norm on X defined by (48), since the expansion into spherical harmonics is a unitary transformation, and any two spherical harmonics of different degrees are orthogonal to each other (see, for example, [10])).

The following obvious lemma can be found, for example, in [6]. It connects the speed of convergence of an expansion of the form (52) with the analyticity of its sum.

Lemma 3.1

Suppose that $\alpha \in X_r$ with some (arbitrarily large) r. Then $F(\alpha) : S^2 \to C$ is an analytic function on S^2.

While the definitions (52), (53) might seem arbitrary, they are motivated by the following two lemmas, which are a direct consequence of the formulae (14), (15).

Lemma 3.2

If $\phi : R^3 \setminus \bar{D} \to C^1$ is defined by (35), then

$$\lim_{t\to\infty} \phi(x_0 + t \cdot E(s)) \cdot t \cdot e^{-i \cdot k \cdot t} = F(\alpha)(s). \tag{54}$$

Lemma 3.3

Suppose that $\psi : D \to C^1$ is defined by (36), and that, in addition, $\beta \in X_a$ for some (arbitrarily large) a. Then

$$\lim_{t\to\infty} t \cdot (\psi(x_0 + t \cdot E(s)) - (F(\beta)(s) \cdot e^{i \cdot k \cdot t}) + F_-(\beta)(s) \cdot e^{-i \cdot k \cdot t}). \tag{55}$$

Remark 3.1

The above two lemmas can be viewed as describing the far-field behavior of the potentials ϕ, ψ in terms of the mappings $F(\alpha), F(\beta) : S^2 \to C$, and we will refer to $F(\alpha), F(\beta)$ as far-field representations of ϕ, ψ, respectively. Alternatively, we will be calling $F(\alpha), F(\beta)$ far-field forms of expansions (35), (36).

For a point $s_0 \in S^2$, a natural n, and a complex z, we will define the function $\lambda_{s_0}^{z,n} : S^2 \rightarrow C^1$ by the formula

$$\lambda_{s_0}^{z,n}(s) = \sum_{m=0}^{n} i^m \cdot (2m+1) \cdot P_m(c(s_0, s) \cdot j_m(z). \tag{56}$$

It immediately follows from (19) that

$$\sum_{m=0}^{\infty} i^m \cdot (2m+1) \cdot P_j(c(s_0, s)) \cdot j_m(z) = e^{i \cdot z \cdot c(s_0, s)}, \tag{57}$$

and for $n = \infty$, (56) assumes the form

$$\lambda_{s_0}^{z,\infty}(s) = e^{i \cdot z \cdot c(s_0, s)}. \tag{58}$$

For a point $s_0 \in S^2$, a natural n, and a complex z, we will define the function $\mu_{s_0}^{z,n} : S^2 \rightarrow C^1$ by the formula

$$\mu_{s_0}^{z,n}(s) = \sum_{m=0}^{n} i^m \cdot (2m+1) \cdot P_m(c(s_0, s)) \cdot h_m(z), \tag{59}$$

and observe that no analogue of the formula (58) is possible in this case (at least in the proper sense), since the series

$$\sum_{m=0}^{\infty} i^m \cdot (2m+1) \cdot P_j(c(s_0, s)) \cdot h_m(z) \tag{60}$$

does not converge.

Finally, we will define mappings $\Lambda_{s_0}^{z,n}, M_{s_0}^{z,n} : L^2(S^2) \rightarrow L^2(S^2)$ via the formulae

$$\Lambda_{s_0}^{z,n}(f)(s) = \lambda_{s_0}^{z,n}(s) \cdot f(s), \tag{61}$$

$$M_{s_0}^{z,n}(f)(s) = \mu_{s_0}^{z,n}(s) \cdot f(s) \tag{62}$$

respectively, with $f \in L^2(S^2)$.

3.3. Definition of translation operators. For the remainder of this section, D_1, D_2, D_3 will denote three balls in R^3 such that $D_2 \subset D_1$ and $D_1 \cap D_3 = \emptyset$ (see Figure 2). The centers and radii of these disks will be denoted by c_1, c_2, c_3 and R_1, R_2, R_3 respectively. We will denote the spherical coordinates of the vector $c_2 - c_1$ by (ρ_{12}, s_{12}), the spherical coordinates of the vector $c_1 - c_2$ by (ρ_{21}, s_{21}), the spherical coordinates of the vector $c_3 - c_1$ by (ρ_{13}, s_{13}), and the spherical coordinates of the vector $c_1 - c_3$ by (ρ_{31}, s_{31}). For a point $x \in R^3$, we will denote by (ρ_1, s_1), (ρ_2, s_2), (ρ_3, s_3) its spherical coordinates with respect to the centers c_1, c_2, c_3 respectively.

Suppose now that $\psi : R^3 \to C^1$ is a radiation field analytical in $R^3 \setminus \bar{D}_2$ and satisfying the radiation condition (9) at ∞. Suppose further that ψ is represented by an expansion

$$\psi(x) = \sum_{m=0}^{\infty} \beta_m(s_2) \cdot h_m(k\rho_2) \tag{63}$$

valid in $R^3 \setminus \bar{D}_2$, and by an expansion

$$\psi(x) = \sum_{m=0}^{\infty} \tilde{\beta}_m(s_1) \cdot h_m(k\rho_1) \tag{64}$$

valid in $R^3 \setminus \bar{D}_1$. It is easy to see that $\tilde{\beta} \in X_{|k| \cdot R_1}$ depends linearly on $\beta \in X_{|k| \cdot R_2}$, and we will denote by $U_{c2,c1}$ the operator $X_{|k| \cdot R_2} \to X_{|k| \cdot R_1}$ such that

$$\tilde{\beta} = U_{c2,c1}(\beta). \tag{65}$$

Suppose that $\phi : R^3 \to C^1$ is a radiation field analytical in D_1 and represented by an expansion

$$\phi(x) = \sum_{m=0}^{\infty} \alpha_m(s_1) \cdot j_m(k\rho_1) \tag{66}$$

valid in D_1, and by an expansion

$$\phi(x) = \sum_{m=0}^{\infty} \tilde{\alpha}_m(s_2) \cdot j_m(k\rho_2), \tag{67}$$

valid in D_2. Again, it is easy to see that $\tilde{\alpha} \in Y_{|k| \cdot R_2}$ depends linearly on $\alpha \in Y_{|k| \cdot R_1}$, and we will denote by $V_{c1,c2}$ the operator $Y_{|k| \cdot R_1} \to Y_{|k| \cdot R_2}$ such that

$$\tilde{\alpha} = V_{c1,c2}(\alpha). \tag{68}$$

For any $r > 0$, we will denote by $V^r_{c1,c2}$ the restriction of $V_{c1,c2}$ on the subspace X_r of $Y_{|k| \cdot R_1}$, so that

$$V^r_{c1,c2} = (V_{c1,c2})_{|X_r}. \tag{69}$$

Finally, suppose that $\psi : R^3 \setminus \bar{D}_1 \to C^1$ is a radiation field analytical outside the ball D_1 and satisfying the radiation condition (9) and that it is represented in $R^3 \setminus \bar{D}_1$ by the expansion (63). Then inside the ball D_3, the function ψ can be represented in the form

$$\psi(x) = \sum_{m=0}^{\infty} \gamma_m(s_3) \cdot j_m(k\rho_3) \tag{70}$$

with $\gamma \in Y_{|k|\cdot R_3}$ a linear function of $\alpha \in X_{|k|\cdot R_2}$, and we define the operator $W_{c1,c2} : X_{|k|\cdot R_1} \to Y_{|k|\cdot R_3}$ via the formula

$$\gamma = W_{c1,c3}(\alpha). \tag{71}$$

3.4. Diagonal Forms of Translation Operators. This subsection describes the diagonal forms of the translation operators U, V, W for the Helmholtz equation. These diagonal forms are provided by the Theorems 3.1 - 3.3 below, and are the principal purpose of this paper.

Theorem 3.1.

If the operator $U_{c2,c1} : X_{|k|\cdot R_2} \to X_{|k|\cdot R_1}$ is defined by the formula (65), then

$$U_{c2,c1} = F^{-1} \circ \Lambda_{s_{12}}^{k\cdot\rho_{12},\infty} \circ F. \tag{72}$$

Proof.

We will prove (72) by showing that

$$F \circ U_{c2,c1} = \Lambda_{s_{12}}^{k\cdot\rho_{12},\infty} \circ F. \tag{73}$$

Suppose that $s \in S^2$, and $\beta \in X_{kR_2}$. Combining (61) with (58), we have

$$\Lambda_{s_{12}}^{k\cdot\rho_{12},\infty}(s) = F(\beta(s) \cdot e^{i\cdot k\cdot R_{21}\cdot c(P(c_1-c_2),s)}. \tag{74}$$

On the other hand, due to Lemma 3.1,

$$\begin{aligned} F(\tilde{\beta})(s) &= \lim_{t\to\infty} \phi(c_1 + t\cdot E(s)) \cdot t \cdot e^{-i\cdot k\cdot t} \\ &= \lim_{t\to\infty} \phi(c_2 + (c_1 - c_2) + t\cdot E(s)) \cdot t \cdot e^{-i\cdot k\cdot t} \\ &= \lim_{t\to\infty} \phi(c_2 + \frac{u + t\cdot v}{\|u + t\cdot v\|} \cdot \|u + t\cdot v\|) \cdot t \cdot e^{-i\cdot k\cdot t}, \end{aligned} \tag{75}$$

with $u = c_1 - c_2$, and $v = E(s)$. Denoting $\|u + t \cdot v\|$ by τ, we obtain after simple analysis

$$t = \tau - (u, v) + O(\frac{1}{\tau}), \tag{76}$$

and (75) assumes the form

$$\begin{aligned} F(\tilde{\beta})(s) &= \lim_{\tau\to\infty} \phi(c_2 + \frac{u + (\tau - (u,v) + O(\frac{1}{\tau}))\cdot v}{\|u + (\tau - (u,v) + O(\frac{1}{\tau}))\cdot v\|}\cdot \tau) \\ &\cdot \quad (\tau - (u,v) + O(\frac{1}{\tau}))\cdot e^{-i\cdot k\cdot(\tau-(u,v)+O(\frac{1}{\tau}))}, \end{aligned} \tag{77}$$

which, due to the radiation condition (9) can be reduced to

$$\begin{aligned} F(\tilde{\beta})(s) &= \lim_{\tau\to\infty} \phi(c_2 + \frac{u + (\tau - (u,v))\cdot v}{\|u + (\tau - (u,v))\cdot v\|}\cdot \tau) \\ &\cdot \quad \tau \cdot e^{i\cdot k\cdot(u,v)} \cdot e^{-i\cdot k\cdot\tau}. \end{aligned} \tag{78}$$

Finally, combining Lemma 3.1 with (78) yelds

$$\begin{aligned} F(\tilde{\beta})(s) &= \lim_{\tau\to\infty} \phi(c_2 + \frac{v}{\|v\|}\cdot\tau)\cdot\tau\cdot e^{-i\cdot k\cdot\tau}\cdot e^{i\cdot k\cdot(u,v)} \\ &= \lim_{\tau\to\infty} \phi(c_2 + E(s)\cdot\tau)\cdot\tau\cdot e^{-i\cdot k\cdot\tau}\cdot e^{i\cdot k\cdot(c_1-c_2,E(s))} \\ &= F(\beta)(s)\cdot e^{i\cdot k\cdot(c_1-c_2,E(s))}. \end{aligned} \tag{79}$$

Now, the conclusion of the theorem follows from the combination of (79) with (74).

The above theorem provides the diagonal form of the operator U_{c_2,c_1} shifting the origin of an h - expansion. Theorem 3.2 below is the analogue of of Theorem 3.1 for the case of j-expansions. Since the proofs of the two theorems are virtually adentical, we omit the proof of the following theorem.

Theorem 3.2.

If the operator $V_{c1,c2} : Y_{|k|\cdot R_1} \to Y_{|k|\cdot R_2}$ is defined by the formula (68), then for any $r > 0$,

$$V_{c1,c2} = F^{-1} \circ \Lambda_{s_{12}}^{k\cdot\rho_{12},\infty} \circ F. \tag{80}$$

The following two lemmas are an immediate consequence of Theorems 3.1, 3.2. Lemma 3.4 provides the far-field representations of the potentials (7), (8) of charge and dipole. Given a far-field representation of a potential of the form (36), Lemma 3.5 provides an expression of its value (and the value of its gradient) at any point within the region of its validity.

Lemma 3.4

Suppose that in (35),

$$\phi = \phi^k_{x_1}, \tag{81}$$

with x_1 an arbitrary point in R^3. Then for any $s \in S^2$,

$$F(\alpha)(s) = \lambda^{k\cdot\|x_0-x_1\|,\infty}_{P(x_0-x_1)}(s) = e^{i\cdot k\cdot(x_0-x_1,E(s))}. \tag{82}$$

If $h \in R^3$ is such that $\|h\| = 1$, and

$$\phi = \phi^k_{x_1,h}, \tag{83}$$

then for any $s \in S^2$,

$$\begin{aligned} F(\alpha)(s) &= \lambda^{k\cdot\|x_0-x_1\|,\infty}_{P(x_0-x_1)}(s)\cdot i\cdot k\cdot\frac{(x_0-x_1,E(s))}{\|x_0-x_1\|} \\ &= e^{i\cdot k\cdot(x_0-x_1,E(s))}\cdot i\cdot k\cdot c(P(x_0-x_1),s). \end{aligned} \tag{84}$$

Lemma 3.5

Suppose that the potential ψ is defined by (36), and that $\beta \in X_r$, with some $0 < r < \infty$. Then for any $x \in D$ and $h \in R^3$ such that $\|h\| = 1$,

$$\psi(x) = \int_{S^2} F(\beta)(s)\cdot\lambda^{k\cdot\|x_0-x\|,\infty}_{P(x_0-x)}(s)ds = \int_{S^2} F(\beta)(s)\cdot e^{i\cdot k\cdot(x_0-x,E(s))}ds. \tag{85}$$

and

$$\begin{aligned} \frac{d}{dt}\psi(x+t\cdot h)|_{t=0} &= \int_{S^2} F(\beta)(s)\cdot\lambda^{k\cdot\|x_0-x\|,\infty}_{P(x_0-x)}(s)\cdot i\cdot k\cdot\frac{(x_0-x,E(s))}{\|x_0-x\|}ds \\ &= \int_{S^2} F(\beta)(s)\cdot e^{i\cdot k\cdot(x_0-x,E(s))}\cdot i\cdot k\cdot c(P(x_0-x),s)ds. \end{aligned} \tag{86}$$

While the preceeding two theorems are fairly obvious, and appear to be known (though in a somewhat different form) among certain groups of physicists, the following theorem is considerably more technical, and appears to be quite new.

Theorem 3.3.

Suppose that the operator $W_{c1,c3} : X_{|k|\cdot R_1} \to Y_{|k|\cdot R_3}$ is defined by the formula (71). Suppose further that $\psi : R^3 \setminus \bar{D}_1 \to C$ is a radiation field represented by the expansion (64) outside D_1, and by the expansion (70) inside D_3. For any $n \geq 1$, we will denote by ψ_n the radiation field $D_3 \to C$ defined by the formula

$$\psi_n(x) = \sum_{m=0}^{\infty} \gamma_m^n(s_3) \cdot j_m(k\rho_3), \tag{87}$$

with $\gamma^n = \{\gamma_1^n, \gamma_2^n, \gamma_3^n, \cdots\}$ defined by the formula

$$\gamma^n = F^{-1} \circ M_{s_{13}}^{k\cdot\rho_{13},n} \circ F(\alpha). \tag{88}$$

Then for any $x \in D_3$,

$$\lim_{n\to\infty} \psi_n(x) = \psi(x). \tag{89}$$

Furthermore,

$$\max_{D_3} |\ \psi_n(x) - \psi(x)\ | = O((\frac{R_1 + R_3}{R_{13}})^n \cdot \|\alpha\|). \tag{90}$$

Proof.

Due to Theorem 2.1, it is sufficient to prove (90) in the special case of

$$\psi = f_{x_0}^k, \tag{91}$$

with X_0 an arbitrary point in D_1. Combining (91) with (82), we have

$$F(\beta)(s) = e^{i\cdot k\cdot(x_0 - c_1, E(s))} \tag{92}$$

for all $s \in S^2$, and combining (92) with (62), (59), obtain

$$M_{s_{1,3}}^{k\cdot\rho_{13},n} \circ F(\beta)(x) = \tag{93}$$

$$e^{i\cdot k\cdot(x_0 - c_1, E(s))} \cdot \sum_{m=0}^{n} i^m \cdot (2m+1) \cdot P_m(c(s_{13}, s)) \cdot h_m(k \cdot \rho_{13}). \tag{94}$$

Now, combining (93) with (85), (87), we have

$$\psi_n(x) = \int_{S^2} e^{i\cdot k\cdot(x_0-c_1,E(s))} \cdot e^{i\cdot k\cdot(x-c_3,E(s))} \cdot \sum_{m=0}^{n} i^m \cdot (2m+1)\cdot P_m(c(s_{13},s))\cdot h_m(k\cdot\rho_{13}), \tag{95}$$

and (90) follows from the combination of (95) and Theorem 2.3.

3.5. Numerical evaluation of translation operators. For the rest of this paper, we will view the asymptotic representations $F(\alpha)$, $f(\beta)$ defined by (52) (as opposed to the expansions of the forms (35), (36)) as our principal tool for representing radiation fields. Lemma 3.4 permits one to calculate asymptotic representations of fields of distributions of charges and dipoles without evaluating the coefficients of their h-expansions, and Lemma 3.5 provides a tool for calculating the fields and derivatives of the fields with given asymptotic representations without having to evaluate the coefficients of j-expansions of these fields.

For a radiation field $\psi : R^3 \to C^1$ analytical outside D_1 given by the expansion (64), and an integer $n \geq 2$, we will denote by F^n_{ψ,c_1} the function $F(\tilde{\beta})$ tabulated at the n^2 nodes $s^n_{j,k}$ defined by the formulae (42) - (44), so that

$$F^n_{\psi,c_1}(j,k) = F(\tilde{\beta})(s^n_{j,k}). \tag{96}$$

Similarly, for a radiation field ϕ analytical inside D_1 defined by (66) and possessing an asymptotic representation $F(\alpha)$, we will denote by G^n_{ϕ,c_1} the table of n^2 complex numbers defined by the formula

$$G^n_{\phi,c_1}(j,k) = F(\alpha)(s^n_{j,k}). \tag{97}$$

and view F^n_{ψ,c_1}, G^n_{ϕ,c_1} as finite-dimensional projections of the asymptotic representations of the radiation fields ψ, ϕ.

Given a function $G : D^n \to C$ (see (44), we will consider a radiation field $\bar{G} : R^3 \to C^1$ defined by the formula

$$\bar{G}(x) = \sum_{j,k=1}^{n} w^n_{j,k} \cdot G^n_{\phi,c_1}(j,k)\cdot e^{i\cdot k\cdot(x_0-x,E(s^n_{j,k}))}. \tag{98}$$

Clearly, (98) is a quadrature formula approximating the integral (85) and we will look upon (98) as an approximation to the field ϕ. Differentiating (98) with respect to x, we obtain the formula

$$\frac{d}{dt}\bar{G}(x+th)_{|t=h} =$$
$$i \cdot k \cdot \|h\| \cdot \sum_{j,k=1}^{n} w_{j,k}^n \cdot G_{\phi,c_1}^n(j,k) \cdot c(P(x_0-x),s) \cdot e^{i\cdot k\cdot(x_0-x,E(s_{j,k}^n))}, \tag{99}$$

with any $h \in R^3$. Finally, we will define mappings $P_{c_2c_1}^{mn}$, $Q_{c_1c_2}^{mn}$, $S_{c_1c_3}^{mn} : C^{n\times n} \to C^{n\times n}$ by the formulae

$$P_{c_2c_1}^{mn} = \Lambda_{c_2,c_1}^{k\cdot\rho_{12},m}{}_{|s_{j,k}^n}, \tag{100}$$

$$Q_{c_1c_2}^{mn} = \Lambda_{c_1,c_2}^{k\cdot\rho_{12},m}{}_{|s_{j,k}^n}, \tag{101}$$

$$S_{c_1c_3}^{mn} = M_{c_1,c_3}^{k\cdot\rho_{13},m}{}_{|s_{j,k}^n}. \tag{102}$$

Observing that $P_{c_2c_1}^{mn}$, $Q_{c_1c_2}^{mn}$, $S_{c_1c_3}^{mn}$ are restrictions to the nodes $s_{j,k}^n$ of the discretization (45) of the mappings $\Lambda_{c_2,c_1}^{k\cdot\rho_{12},m}$, $\Lambda_{c_1,c_2}^{k\cdot\rho_{12},m}$, $M_{c_1,c_3}^{k\cdot\rho_{13},m}$ respectively, we will look upon the operators $P_{c_2c_1}^{mn}$, $Q_{c_1c_2}^{mn}$, $S_{c_1c_3}^{mn}$ as approximate discretizations of diagonal forms of the operators $U_{c_2c_1}^{mn}$, $V_{c_1c_2}^{mn}$, $W_{c_1c_3}^{mn}$.

Remark 3.5

By combining the above lemma with Remark 2.2, it is easy see that the number n of nodes in the discretization G_{ϕ,c_1}^n of the function $G_{\phi,c_1} : S^2 \to C^1$ has to be approximately equal to $(2\cdot|k|\cdot R_1)^2$, and is almost independent of the accuracy ϵ with which the field ϕ is being calculated.

Theorems 3.1 - 3.3 provide a tool for shifting the origins of asymptotic expansions of radiation fields, and for converting asymptotic representations of the form (54) into asymptotic representations of the form (55) for a cost proportional to n, where n is the number of nodes in the discretization (45) of the interval S^2. In the following two sections, this apparatus is used to construct an algorithm for rapid evaluation of radiation fields of charge (and dipole) distributions.

4. Rapid Evaluation of Radiation Fields of Charge Distributions

In this section, we describe an algorithm for rapid evaluation of the field and the normal derivative of the field created on a surface $\Gamma \subset R^3$ by charge and dipole distributions on that same surface. For definitiveness, we will be discussing the evaluation of the field created by a charge distribution. The algorithms evaluating the normal derivative of the field created by a charge distribution, and the field and the normal derivative of the field created by a dipole distribution are quite similar.

4.1. Notation. We will consider the situation depicted in Figure 3. The surface $\Gamma \subset R^3$ is discretized into n nodes $x_1, x_2, \cdots, x_n$, and we will assume that these nodes are distributed on the surface in a roughly uniform manner. Suppose that for each $i = 1, 2, \cdots, n$, a charge a_i of strength σ_i is located at the point x_i. In this section, we describe an algorithm for rapid calculation of approximations $g_i = 1, 2, \cdots, n$ to the sums

$$G_\sigma(x_i) = \sum_{j=1,\ j\neq i}^{n} \sigma_j \phi^k_{x_j}(x_i) \tag{103}$$

for $i = 1, 2, \cdots, n$. Clearly, this is an order n^2 process (evaluating n fields at n points). However, if we are interested in evaluating (103) with a finite accuracy (which is always the case in practical calculations), Theorem 3.3 and Lemmas 3.4, 3.5 can be used to speed up the process.

For an integer $m \geq 4$, we will subdivide the surface Γ into m non-intersecting patches P_i, each patch roughly rectangular in shape, and containing approximately $\frac{N}{m}$ of the nodes x_i.

For each $i \in [1, m]$, we will denote by r_i the radius of the smallest circle containing P_i, and define $r \in R$ by the formula

$$r = \max_{i\in[1,m]} r_i. \tag{104}$$

Remark 4.1

Obviously, for sufficiently large m,

$$r \sim \frac{L}{\sqrt{m}}, \tag{105}$$

where L is the diameter of the surface Γ. This will be important in Subsection 4.3.

For each $i = 1, 2, \cdots, m$, we will denote by z_i the center of the $i-th$ patch, by A_i the set of all charges a_j such that $a_j \in A_i$, and by D_j the disk of radius r with the center at Z_j.

We will denote by W_j the union of all A_i such that $\|z_j - z_i\| > 3 \cdot r$, and by $\bar{W}_j$ the union of all A_i such that $\|z_j - z_i\| \leq 3 \cdot r$. Obviously, $A_j \subset D_j$ for any $j = 1, 2, \cdots, m$. Also, it follows from the triangle inequality that

$$\min_{x \in A_i,\ y \in A_j} \|x - y\| \geq r \tag{106}$$

for any i, j such that $A_i \subset W_j$. Finally, we will denote by ϕ_j the field of all charges a_i such that $x_i \subset A_j$ and observe that if $x_p \in A_j$ then

$$G_\sigma(x_p) = \sum_{A_i \subset W_j} \phi_i(x_p) + \sum_{x_i \in \bar{W}_j} \sigma_i \phi^k_{x_i}(x_p). \tag{107}$$

4.2. Detailed description of an order $N^{3/2}$ algorithm. In this subsection, M, N will denote "sufficiently large" integer numbers. The actual choice of the numbers M, N is discussed in the following subsection.

We will evaluate the fields (103) in five steps.

Step 1.

Using Lemma 3.4, obtain discretized asymptotic representations $F^N_{\phi_j, z_j}$ of the fields ϕ_j for all $j = 1, 2, \cdots, m$.

Step 2

For every pair of natural numbers $i, j \in [1, m]$ such that $A_i \subset W_j$, calculate the representation

$$G^N_{i,j} = S^{M,N}_{z_i, z_j}(F^N_{\phi_j, z_j}) \tag{108}$$

of the field $\psi_{ij} = \bar{G}^N_{i,j}$, and view it as a finite - dimensional approximation to the asymptotic representation of the field ϕ_i on D_j.

Step 3

For each natural $j \in [1, m]$, calculate the sum

$$G^N_{\psi_j, z_j} = \sum_{A_i \subset W_j} G^N_{\psi_{i,j}, z_j}, \tag{109}$$

and view the field $\psi_j = \sum_i \psi_{i,j}$ as an approximation to the field $\sum_{A_i \subset W_j} \phi_i$, and $G^N_{\psi_j, z_j}$ as a finite-dimensional approximation to the asymptotic representation of ψ_j on D_j.

Step 4

For each natural $j \in [1, m]$, evaluate

$$\tilde{\psi}_j(x_i) = \bar{G}_{\psi_j, z_j}(x_i)^N \tag{110}$$

for all i such that $x_i \in P_j$ and look upon (110) as an approximation to $\psi_j(x_i)$.

Step 5.

For each $j = 1, 2, \cdots, m$, evaluate the sum

$$\tilde{\psi}_j(x_i) + \sum_{x_p \in \bar{W}_j} \sigma_p \phi^k_{x_p}(x_i) \tag{111}$$

for all i such that $x_i \in P_j$, and view (111) as an approximation to $G_\sigma(x_i)$.

4.3. Choice of parameters and CPU time estimate. In the estimates below, a, b, c, d, e are coefficients determined by the computer system, language, particular implementation of the algorithm, etc.

Step 1

Obviously, this step will require order $n \cdot N^2$ operations (tabulating $F^N_{\phi_j, z_j}$ at N^2 nodes on D^n for each of the nodes $x_1, x_2, \cdots, x_n$). Combining Remarks 3.5, 4.1, we observe that $N \sim |k| \cdot L/\sqrt{m}$, and the CPU time estimate for this step becomes $a \cdot n \cdot (|k| \cdot L/m)^2 = a \cdot n \cdot (|k| \cdot L)^2/m$.

Step 2

For each of the pairs i, j such that $A_j \subset W_i$, evaluating (108) will require order N^2 operations (see (102)), and the total number of such pairs is less than m^2, which results in the CPU time estimate of $b \cdot m^2 \cdot n \sim b \cdot m^2 \cdot (|k| \cdot L/\sqrt{m})^2 = b \cdot m \cdot (|k| \cdot L)^2$ for this step.

Step 3

Obviously, evaluating the sums (109) for all $j = 1, 2, \cdots, m$ is an order $c \cdot m \cdot N^2 \sim c \cdot m \cdot (|k| \cdot L/\sqrt{m})^2 = c \cdot (|k| \cdot L)^2$ procedure.

Step 4

Evaluating (110) for each $i = 1, 2, \cdots, n$ is an order N^2 procedure, resulting in the total CPU time estimate for this step of $d \cdot n \cdot N^2 \sim d \cdot n \cdot (|k| \cdot L)^2/m$.

Step 5

Evaluating the sum (111) for each $i = 1, 2, \cdots, n$ is an order n/m procedure, with the resulting CPU time estimate of $e \cdot n^2/m$ for this step.

Summing up the time estimates for the steps 1-5, we obtain the following time estimate for the whole process:

$$T = \frac{A \cdot n \cdot (|k| \cdot L)^2}{m} + b \cdot m \cdot (|k| \cdot L)^2 + c \cdot (|k| \cdot L)^2 + \frac{e \cdot n^2}{m}, \tag{112}$$

with $A = a+d$, and we would like to choose m in such a manner that (112) would be minimized. Differentiating (112) with respect to m, and setting the resulting derivative to zero, we obtain

$$m_{\text{min}} = \sqrt{\frac{A \cdot n \cdot (|k| \cdot L)^2 + e \cdot n^2}{b \cdot (|k| \cdot L)^2}} \tag{113}$$

and the corresponding minimum of (112) is equal to

$$T_{\text{min}} = 2\sqrt{A \cdot n \cdot (|k| \cdot L)^2 + e \cdot n^2} \cdot \sqrt{b \cdot (|k| \cdot L)^2} + c \cdot (|k| \cdot L)^2. \tag{114}$$

If the calculations are performed with a fixed number of nodes per wavelength (which is often a reasonable assumption), n is proportional to $(|k|L)^2$, and (114) assumes the form

$$T_{\text{min}} \sim (|k| \cdot L)^3, \tag{115}$$

or

$$T_{\text{min}} \sim n^{\frac{3}{2}}, \tag{116}$$

which for large n is considerably smaller than n^2.

4.4. Further reduction of the CPU time estimate of the process. The approach of the above subsection can be used recursively by subdividing each of the sets A_i into subsets $\{B_{ij}\}, j = 1, 2, \cdots, \bar{m}$ with appropriately chosen $\bar{m}$ and representing the fields ϕ_i as sums $\phi_i = \sum_i \phi_{ij}$ where ϕ_{ij} is the field created by all charges a_p such that $a_p \in B_{ij}$. A calculation similar to the one in the preceeding section shows that such an algorithm will have an asymptotic CPU time estimate of $n^{4/3}$.

By continuing this process recursively until only a finite number of nodes is left on a surface patch on the finest lavel, one can obtain an order $n \log(n)$ algorithm for evaluating (103). However, our estimates indicate that for problems of practicable size ($n \leq 1000,000$), the improvement in actual computation times obtained by replacing an order $n^{4/3}$ algorithm with an order $n \log n$ algorithm would not be very significant.

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FIGURE 1

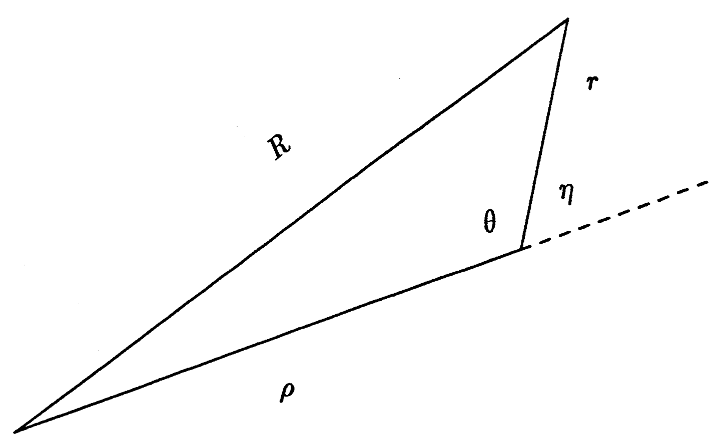


FIGURE 2

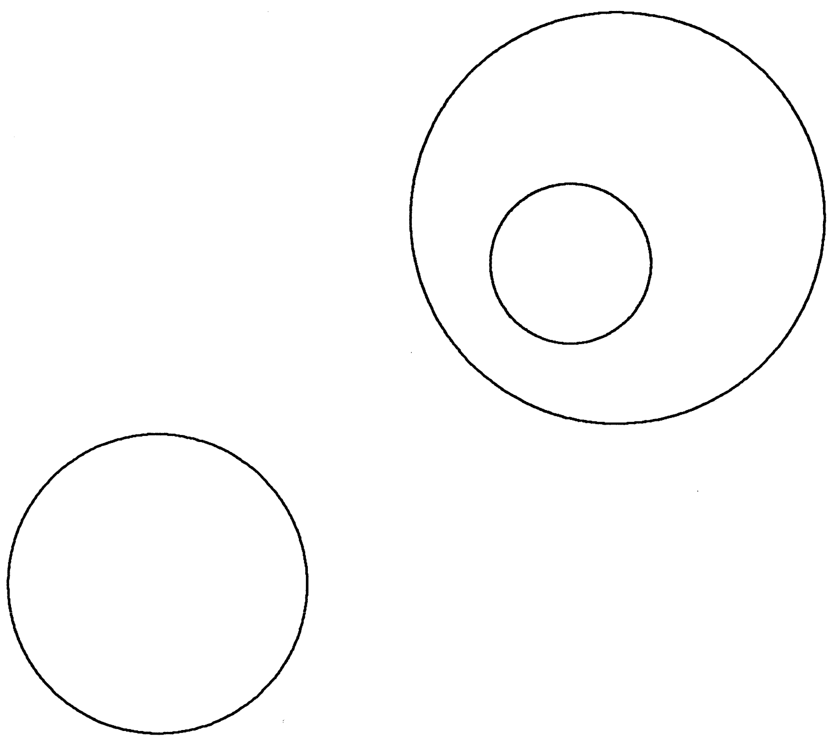
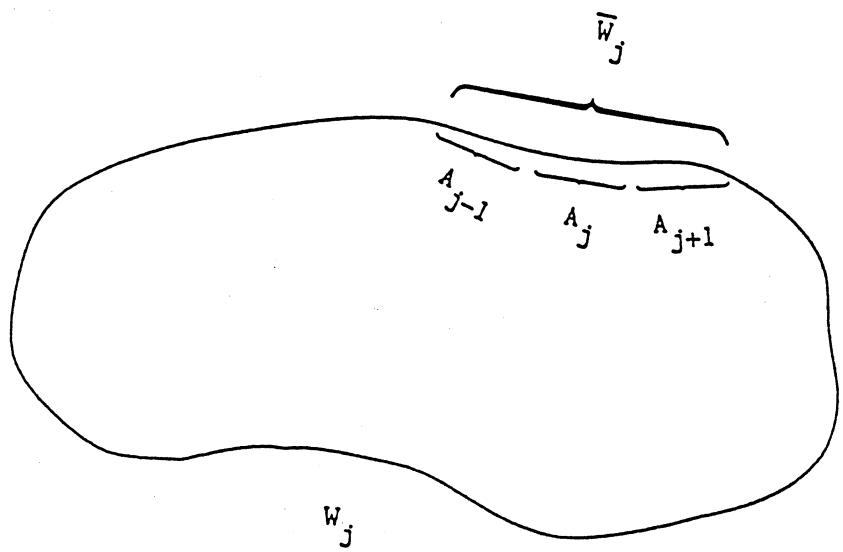


FIGURE 3



Definition of the Sets A_j, $\overline{W}_j$, W_j