FAST MULTIPOLE ACCELERATION OF PERIODIC GREEN’S
FUNCTION USING SPHERICAL HARMONICS AND EWALD
SUMMATION

BY

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THESIS

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ABSTRACT

In this thesis, we present a fast multipole algorithm (FMA) for solving a periodic scattering problem using method of moments (MOM). The difference between the standard integral equations (EFIE and MFIE) and the ones used for periodic geometry is the use of periodic Green’s function (PGF) over free-space Green’s function (FGF). When expressed as a spatial sum, PGF converges slowly making this representation unsuitable for numerical implementation. An alternative representation known as Ewald summation can be used to evaluate PGF with exponential convergence and high accuracy. Despite the use of Ewald summation to evaluate PGF quickly, the MOM solution for a periodic scattering problem is still too slow. The matrix fill time for a scatterer with only a few thousand unknowns requires several hours to complete. The same geometry treated as a single scatterer (as opposed to a unit cell in a periodic array) requires only seconds to compute. This means that even problems with a small number of unknowns can benefit from a fast method. The PGF can be factorized using usual methods of factorization. The convergence problems of PGF do not simply vanish in this factorization—instead they manifest in the form of a lattice constant. These constants are commonly found in low energy electron diffraction (LEED). The lattice constants can also be evaluated using Ewald summation and has been well documented by researchers. In this thesis, we present a fast algorithm for scattering by a 2-D lattice in 3-D. Using the factorization of PGF, we develop a multi-level periodic fast multipole algorithm (MLP-FMA) which performs on par with existing ML-FMA algorithms. The MLP-FMA is applied to some example geometry and compared to periodic MOM computed using Ewald summation.
To my parents, for their love and support.
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<tr>
<td>ACA</td>
<td>Adaptive Cross Approximation</td>
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<tr>
<td>CEM</td>
<td>Computational Electromagnetics</td>
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<td>DGF</td>
<td>Dyadic Green’s Function</td>
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<td>EFIE</td>
<td>Electric Field Integral Equation</td>
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<td>Finite-Difference Time Domain</td>
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<td>MFIE</td>
<td>Magnetic Field Integral Equation</td>
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<td>MOM</td>
<td>Method of Moments</td>
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<td>ML-FMA</td>
<td>Multilevel Fast Multipole Algorithm</td>
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<td>MLP-FMA</td>
<td>Multilevel Periodic Fast Multipole Algorithm</td>
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<tr>
<td>NTNN</td>
<td>Non-Touching Near-Neighbors</td>
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<tr>
<td>PBC</td>
<td>Periodic Boundary Condition</td>
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<tr>
<td>PEC</td>
<td>Perfect Electric Conductor</td>
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Periodic structures have many useful applications in engineering, such as frequency selective surfaces, reflectors, photonic crystals, metamaterials, and resonators. The design of such structures is aided by various EM solvers such as finite difference time-domain method (FDTD), finite element method (FEM), and method of moments (MOM). While periodic structures are theoretically infinite; in reality, only finite periodic structures can be fabricated. Fortunately, one only needs a finite number of periods to achieve near-periodic behavior. This gives us two paths for simulation of periodic structures: (1) assume the structure is finite and model a sufficient number of periods to exhibit the behaviors of an infinitely periodic structure, and (2) assume the structure is truly periodic.

The first assumption requires that an EM solver models several unit cells of the periodic structure, which increases the number of unknowns by a multiple of the number of periods. The second assumption isolates the number of unknowns to a single unit cell and instead requires the use of periodic boundary conditions. The first approach, while memory intensive, is ultimately closer to reality due to the finite structure being modeled. However, it is difficult to know apriori the number of unit cells that need to be modeled. The second approach is less memory intensive, but does not permit the exploration of fringe effects in regions where the periodicity conditions are non-ideal.

MOM can be used to solve the scattering by a periodic structure more accurately and efficiently than FDTD or FEM. The types of periodic structure we want to solve are crystalline structures which can be defined by a Bravais lattice. More specifically, we want to solve for the scattering in 3-D space by a 2-D periodic lattice. This situation can be modeled using the electric field integral equation (EFIE) coupled with periodic Green’s function (PGF). Like FGF, PGF represents the field due to a point charge in a periodic medium.
The representation for this field is not unique. Mathematically, there exists a litany of representations, all of which exhibit different convergence behavior when evaluated numerically. Some representations do not converge at all under certain conditions, such as when the observation point lies on the lattice plane. Therefore, a viable numerical implementation should utilize the representation of PGF which converges fast in all situations.

Using MOM to discretize EFIE (augmented with PGF) results in an $N^2$ dense matrix where $N$ is the number of unknowns. This matrix equation can be solved using direct matrix solvers such as LU factorization or iterative methods such as BiCGSTAB, GMRES, or TFQMR. The MOM matrix can be viewed as a discretization of Green’s function, which generally leads to a diagonally dominant, well-conditioned matrix. For this type of matrix, the solution can be obtained much faster using iterative methods than direct methods. The drawback of MOM discretization is that even moderately large problems require a significant amount of memory. To alleviate this problem, multilevel fast multipole algorithm (ML-FMA) can be used to reduce the storage and matrix-vector product cost to $O(N)$ and $O(N \log N)$, respectively [1], [2]. Fast methods for solving scattering by periodic structures were presented as early as 1987 by Greengard and Rohklin [3], who investigated scattering by groups of particles governed by Laplace’s equation using the fast multipole method (FMM). Recent work on ML-FMA for periodic structures has been conducted by two separate groups. Nishimura and Otani have gone with a traditional spherical multipole-based method [4] while Shanker uses accelerated Cartesian expansion (ACE) which uses Cartesian multipoles to factorize the field [5], [6]. A common obstacle encountered by both approaches is the evaluation of a term called the lattice constant.

The lattice constant can be written as an infinite sum over the entire lattice. This sum does not converge numerically and requires special treatment in order to evaluate it [7]. Nishimura and Otani use Fourier analysis to evaluate the lattice constant while Shanker uses a technique called Ewald summation [8]. The method used by Nishimura and Otani divides the lattice sum into six different sums and evaluates them using techniques which can be found in [9]. Contrastingly, Ewald summation is exponentially convergent and only divides the lattice sum into two sums, requiring less work to implement. Other methods such as Linton summation can be used to evaluate the lattice constant even faster than Ewald summation [10]. The use of Schlömilch series...
and presence of artificial singularities in Linton summation make it more difficult to implement compared to Ewald.

In addition to determining a suitable method for evaluating lattice constants, one must also decide how to implement the oct-tree and interactions between near lattice cells and far lattice cells. In total, there are three main design choices we consider in our implementation of periodic ML-FMA: (1) the type of expansion used for factorization, (2) the acceleration method for evaluation of lattice constants, and (3) treatment of near and far lattice cells. The basis we chose to factorize PGF is spherical harmonics, owing to its longstanding use in computational electromagnetics (CEM) and modern MOM-based EM solvers. The method we use for acceleration of lattice constants is Ewald summation due to its ease of implementation and minimal use of special functions. The equations we derive for evaluating the lattice constants differ from ones presented in [7], [13], [14], [15]. Specifically, no complex incomplete gamma functions are used in our derivation. The incomplete gamma function has been replaced by erfc(z), the complex complementary error function. From our experience, it is easier to obtain a software library that provides the complex complementary error function than the complex incomplete gamma function. In our implementation, we use the Faddeeva C++ library developed at MIT [16].

In this thesis, we first cover the PGF in its spatial and spectral representations. Next, we present the Ewald summation for PGF and apply it to EFIE and MFIE. The use of PGF in EFIE and MFIE will be referred to as the MOM representation of PGF. We then explain how PGF is factorized and introduce the lattice constant. It will be shown how evaluation of lattice constants can also be accelerated using Ewald summation. After presenting the factorized form of PGF with Ewald summation, the major components of our periodic ML-FMA implementation will be explained, followed by a comparison with the MOM representation of PGF (which can be considered the exact solution). Finally, we explain the merits of our method over previous methods and conclude with suggestions for future work.
CHAPTER 2
PERIODIC GREEN’S FUNCTION

2.1 Spatial and Spectral Lattice Domains

A periodic structure can be described using a Bravais lattice, which is a discrete set of points defined by spatial lattice vector $\mathbf{R}_n \in \Lambda$ (see Figure 2.1). If we let $d_\Lambda$ be the dimension of periodicity, then a general expression for $\Lambda$ is

$$\Lambda \equiv \left\{ n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + \cdots + n_{d_\Lambda} \mathbf{a}_{d_\Lambda} : n_i \in \mathbb{Z} \text{ for } i = 1, \ldots, d_\Lambda \right\}, \quad (2.1)$$

where $\mathbf{R}_n$ is written as a superposition of primitive vectors $\mathbf{a}_i$. A lattice cell (or unit cell) represents an elementary volume in the lattice which can be replicated to form the rest of the lattice. We shall denote functions of $\mathbf{R}_n$ as being in the spatial lattice domain and the representation of PGF associated with a sum over just $\mathbf{R}_n$ as the spatial representation of PGF. One may also
derive a spectral representation of PGF using the reciprocal lattice domain.

A reciprocal lattice can be derived from the primitive vectors of the spatial lattice. The points in the reciprocal lattice are defined by a reciprocal lattice vector $\mathbf{K}_l \in \Lambda^*$ where

$$\Lambda^* \equiv \{ l_1 \mathbf{b}_1 + l_2 \mathbf{b}_2 + \cdots + l_{d_\Lambda} \mathbf{b}_{d_\Lambda} : l_i \in \mathbb{Z} \text{ for } i = 1, \ldots, d_\Lambda \}. \quad (2.2)$$

In this thesis, we focus specifically on the case $d_\Lambda = 2$. The ensuing mathematics assumes that the lattice lies in the $x - y$ plane. For this case, the primitive vectors in the reciprocal lattice domain are

$$\mathbf{b}_1 = \frac{2\pi}{A} \mathbf{a}_2 \times \mathbf{\hat{z}}, \quad (2.3)$$

$$\mathbf{b}_2 = \frac{2\pi}{A} \mathbf{\hat{z}} \times \mathbf{a}_1, \quad (2.4)$$

$$A = |\mathbf{a}_1 \times \mathbf{a}_2|, \quad (2.5)$$

where $A$ is the area of a unit cell. The primitive vectors $\mathbf{a}_i$ and $\mathbf{b}_i$ satisfy the orthogonality condition $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}$. This orthogonality leads to the definition of a generalized Fourier series. It is often useful to expand fields using the generalized Fourier series for non-orthonormal basis and we will use it to derive a spectral representation of PGF which converges much faster than the spatial representation of PGF.

2.2 Spatial Representation

PGF can be derived from EFIE for a periodic structure. An important assumption which leads to this derivation is that the incident field is a plane wave with wavevector $\mathbf{k}$. This implies that PGF is also a function of $\mathbf{k}$. The EFIE for a plane wave excitation is

$$\mathbf{E}_0 e^{i\mathbf{k} \cdot \mathbf{r}} = -i\omega \mu \int_S \mathbf{G}_0(k, \mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_s(\mathbf{r}') \, d\mathbf{r}' + \nabla \times \int_S \mathbf{G}_0(k, \mathbf{r}, \mathbf{r}') \cdot \mathbf{M}_s(\mathbf{r}') \, d\mathbf{r}', \quad (2.6)$$
where $\mathbf{G}_0(k, r, r')$ is the dyadic Green’s function (DGF) defined as

$$
\mathbf{G}_0(k, r, r') = \left(\mathbf{I} + \nabla^2 \frac{k^2}{k^2}\right) g_0(k, r, r'),
$$

(2.7)

and $g_0(k, r, r')$ is the FGF. Let us introduce a coordinate shift by the lattice vector $\mathbf{R}_n$ of both the observation point and source such that $r \rightarrow r + \mathbf{R}_n$, $r' \rightarrow r' + \mathbf{R}_n$. Doing so gives us

$$
E_0 e^{i k \cdot (r + \mathbf{R}_n)} = -i \omega \mu \int_S \mathbf{G}_0(k, r + \mathbf{R}_n, r' + \mathbf{R}_n) \cdot \mathbf{J}_s(r' + \mathbf{R}_n) \, dr' 
+ \nabla \times \int_S \mathbf{G}_0(k, r + \mathbf{R}_n, r' + \mathbf{R}_n) \cdot \mathbf{M}_s(r' + \mathbf{R}_n) \, dr'.
$$

(2.9)

By reciprocity of Green’s function [17], $\mathbf{G}_0(k, r + \mathbf{R}_n, r' + \mathbf{R}_n) = \mathbf{G}_0(k, r, r')$, which leads to

$$
E_0 e^{i k \cdot (r + \mathbf{R}_n)} = -i \omega \mu \int_S \mathbf{G}_0(k, r, r') \cdot \mathbf{J}_s(r' + \mathbf{R}_n) \, dr' 
+ \nabla \times \int_S \mathbf{G}_0(k, r, r') \cdot \mathbf{M}_s(r' + \mathbf{R}_n) \, dr'.
$$

(2.10)

The lattice phase from the incident plane wave can be moved to the other side of the equation, resulting in

$$
E_0 e^{i k \cdot r} = -i \omega \mu \int_S \mathbf{G}_0(k, r, r') \cdot \mathbf{J}_s(r' + \mathbf{R}_n) e^{-i \mathbf{k} \cdot \mathbf{R}_n} \, dr' 
+ \nabla \times \int_S \mathbf{G}_0(k, r, r') \cdot \mathbf{M}_s(r' + \mathbf{R}_n) e^{-i \mathbf{k} \cdot \mathbf{R}_n} \, dr'.
$$

(2.11)

Comparing (2.6) and (2.11), Bloch conditions for the surface current can be deduced.

$$
\mathbf{J}_s(r' + \mathbf{R}_n) = e^{i \mathbf{k} \cdot \mathbf{R}_n} \mathbf{J}_s(r')
$$

(2.12)

$$
\mathbf{M}_s(r' + \mathbf{R}_n) = e^{i \mathbf{k} \cdot \mathbf{R}_n} \mathbf{M}_s(r')
$$

(2.13)

The currents in one unit cell can be derived from the currents in another cell through (2.12) and (2.13). Additionally, since the surface $S$ refers to all cells in $\Lambda$, we can isolate the integration over $S$ to just the surface in one unit cell,
The lattice cell that contains \( S_0 \) will be referred to as the reference cell. Performing a sum over \( \mathbf{R}_n \),

\[
\mathbf{E}_0 e^{i\mathbf{k} \cdot \mathbf{r}} = -i \omega \mu \int_{S_0} \mathbf{J}_s(\mathbf{r}') \cdot \sum_{\mathbf{R}_n \in \Lambda} \overline{\mathbf{G}}_0(k, \mathbf{r}, \mathbf{r}' + \mathbf{R}_n) e^{i\mathbf{k} \cdot \mathbf{R}_n} d\mathbf{r}'
\]

\[
+ \nabla \times \int_{S_0} \mathbf{M}_s(\mathbf{r}') \cdot \sum_{\mathbf{R}_n \in \Lambda} \overline{\mathbf{G}}_0(k, \mathbf{r}, \mathbf{r}' + \mathbf{R}_n) e^{i\mathbf{k} \cdot \mathbf{R}_n} d\mathbf{r}'.
\]

(2.14)

The result is dyadic PGF (DPGF) expressed in terms of PGF

\[
\overline{\mathbf{G}}_\Lambda(k, \mathbf{k}, \mathbf{R}) = \left( \mathbf{I} + \frac{\nabla \nabla}{k^2} \right) g_\Lambda(k, \mathbf{k}, \mathbf{R}),
\]

(2.15)

\[
g_\Lambda(k, \mathbf{k}, \mathbf{R}) = \sum_{\mathbf{R}_n \in \Lambda} \frac{e^{i|\mathbf{R} - \mathbf{R}_n|}}{4\pi|\mathbf{R} - \mathbf{R}_n|} e^{i\mathbf{k} \cdot \mathbf{R}_n},
\]

(2.16)

where \( \mathbf{R} = \mathbf{r} - \mathbf{r}' \).

The PGF in its spatial representation is described by (2.16). This representation is considered to be the most intuitive description of PGF. EFIE and MFIE for periodic geometry can be found in a straightforward manner by replacing FGF with the PGF defined in (2.16) in addition to the requirement that the incident field be a plane wave. Equation (2.16) is known to converge slowly due to the decay rate of \(|\mathbf{R} - \mathbf{R}_n|^{-1}\). For efficient numerical evaluation, it becomes necessary to find fast ways to evaluate this summation.

### 2.3 Spectral Representation

The PGF has a spectral representation which converges much faster in many situations than its spatial representation. The spectral representation uses Poisson summation, which is derived from Fourier theory [18]. Poisson summation formula depends on the dimension of the Fourier transform. For our case, the appropriate form of Poisson summation formula is

\[
\sum_{\mathbf{R}_n \in \Lambda} e^{i\mathbf{k}_s \cdot \mathbf{R}_n} f(\mathbf{R}_s - \mathbf{R}_n) = \frac{1}{(2\pi)^2} \sum_{\mathbf{k}_l \in \Lambda^*} F(\mathbf{k}_s + \mathbf{K}_l) e^{i(\mathbf{k}_s + \mathbf{K}_l) \cdot \mathbf{R}_s},
\]

(2.17)
where \( \mathbf{k}_s = \hat{x}_k \mathbf{k}_x + \hat{y}_k \mathbf{k}_y, \mathbf{R}_s = \hat{x}_R \mathbf{R}_s + \hat{y}_R \mathbf{R}_s\), and \( F(\mathbf{k}_s) \) is the Fourier transform of \( f(\mathbf{R}_s) \). Using the Weyl identity, FGF can be expressed as

\[
\frac{e^{i k R}}{4 \pi R} = \frac{i}{8 \pi^2} \int \int_{-\infty}^{\infty} \frac{e^{i k_s \mathbf{R}_s + i k_z |z - z'|}}{k_z} \, dk_s,
\]

(2.18)

where \( R = |\mathbf{R}_s + \hat{z} z| \) and

\[
k_z = \begin{cases} \sqrt{k^2 - (\mathbf{k}_s + \mathbf{K}_l) \cdot (\mathbf{k}_s + \mathbf{K}_l)}, & |\mathbf{k}_s + \mathbf{K}_l| < k \\ i \sqrt{(\mathbf{k}_s + \mathbf{K}_l) \cdot (\mathbf{k}_s + \mathbf{K}_l) - k^2}, & |\mathbf{k}_s + \mathbf{K}_l| > k. \end{cases}
\]

(2.19)

Inserting (2.18) into (2.16) gives us

\[
g_\Lambda(k, \mathbf{k}, \mathbf{R}) = \frac{i}{8 \pi^2} \sum_{\mathbf{R}_n \in \Lambda} e^{i k \cdot \mathbf{R}_n} \int \int_{-\infty}^{\infty} \frac{e^{i k_s \cdot (\mathbf{R}_s - \mathbf{R}_n) + i k_z |z - z'|}}{k_z} \, dk_s,
\]

(2.20)

which has the same form as the LHS of (2.17). Comparing (2.20) to (2.17), \( f(\mathbf{R}_s) \) is identified to be

\[
f(\mathbf{R}_s) = \frac{1}{4 \pi^2} \int \int_{-\infty}^{\infty} i e^{i k_s \cdot \mathbf{R}_s + i k_z |z - z'|} \, 2k_z \, dk_s.
\]

(2.21)

Equation (2.21) is the inverse Fourier transform of a Gaussian. Therefore, by inspection, \( F(\mathbf{k}_s) \) must be

\[
F(\mathbf{k}_s) = \frac{i e^{i k_z |z - z'|}}{2 k_z}.
\]

(2.22)

Since we know \( F(\mathbf{k}_s) \), we can write PGF as a sum over \( \mathbf{K}_l \) using Poisson summation formula. Thus,

\[
g_\Lambda(k, \mathbf{k}, \mathbf{R}) = \frac{i}{8 \pi^2} \sum_{\mathbf{K}_l \in \Lambda^*} \frac{e^{i k_z |z - z'|}}{k_z} e^{i (\mathbf{k}_s + \mathbf{K}_l) \cdot \mathbf{R}_s}.
\]

(2.23)

Equation (2.23) is referred to as the spectral representation of PGF. One can observe that when \( K_{\perp,l} = 0, g_\Lambda(k, \mathbf{k}, \mathbf{R}) \) becomes infinite. This is not a byproduct of the spectral representation, but an actual physical phenomenon known as Wood’s anomaly [19]. When computing values for PGF, one must be judicious in avoiding Wood’s anomaly. For the case where \( K_{\perp,l} \) is imaginary, (2.23) becomes an exponentially decaying function of \( \mathbf{K}_l \), leading to fast
convergence. A large $K_l$ results in a faster onset of this exponentially decaying behavior. Since $K_l \sim \frac{1}{R_n}$, (2.23) decays faster for small spatial lattices. When $|z - z'| = 0$, the PGF decays with respect to $K_{\perp l}$, which is comparable to the spatial PGF representation. This deficiency makes the spectral representation unfeasible. Ewald summation can be used as a remedy.

2.4 Ewald Representation

An exponentially convergent representation of PGF was derived by Ewald in 1916 [20]. Ewald summation leverages both spatial and spectral domains to achieve fast convergence. We shall refer to the corresponding PGF representation as the Ewald representation of PGF. To derive this representation, we need to use a complex integral representation of FGF,

$$g_0(k, R) = \frac{1}{2\pi\sqrt{\pi}} \int_0^\infty e^{-R^2\xi^2 + \frac{k^2}{4\xi^2}} d\xi,$$

(2.24)

which can be found in [18].

Using the expression in (2.24), PGF can be written as

$$g_\Lambda(k, k, R) = \frac{1}{2\pi\sqrt{\pi}} \sum_{R_n \in \Lambda} e^{ikR_n} \int_0^\infty e^{-|R - R_n|^2\xi^2 + \frac{k^2}{4\xi^2}} d\xi.$$  

(2.25)

We mentioned earlier that Ewald summation leverages both spatial and spectral domains. This is done by dividing the integral into two parts using the Ewald splitting parameter $\eta$. The PGF can be re-written as

$$g_\Lambda(k, k, R) = \frac{1}{2\pi\sqrt{\pi}} \sum_{R_n \in \Lambda} e^{ikR_n} \int_0^\eta e^{-|R - R_n|^2\xi^2 + \frac{k^2}{4\xi^2}} d\xi$$ 

$$+ \frac{1}{2\pi\sqrt{\pi}} \sum_{R_n \in \Lambda} e^{ikR_n} \int_\eta^\infty e^{-|R - R_n|^2\xi^2 + \frac{k^2}{4\xi^2}} d\xi.$$  

(2.26)

Denoting the first and second sum in (2.26) as $g_K(k, k, R)$ and $g_R(k, k, R)$, respectively, $g_K(k, k, R)$ can be evaluated in the reciprocal lattice domain using Poisson summation. To apply Poisson summation, the order of inte-
gration and summation are exchanged so that

\[ g_K(k, k, R) = \frac{1}{2\pi \sqrt{\pi}} \int_0^\eta \frac{k^2}{4\xi^2} e^{i k R_n} e^{-|R - R_n|^2 \xi^2} d\xi. \]  

(2.27)

Assuming that \( R_n \) lies in the \( x-y \) plane, we can separate the Gaussian term in (2.27) in the following manner:

\[ e^{-|R - R_n|^2 \xi^2} = e^{-|R_x - R_n|\xi^2} e^{-|z - z'|^2 \xi^2}. \]  

(2.28)

This lets us write (2.27) as

\[ g_\Lambda(k, k, R) = \frac{1}{2\pi \sqrt{\pi}} \int_0^\eta \frac{k^2}{4\xi^2} |z - z'|^2 \xi^2 \sum_{R_n \in \Lambda} e^{i k R_n} e^{-|R_x - R_n|^2 \xi^2} d\xi. \]  

(2.29)

Using (2.17), let \( f(R_s - R_n) = e^{-|R_s - R_n|^2 \xi^2} \) such that

\[ F(k_s) = \pi e^{-\frac{k_s^2}{4\xi^2}} \xi^{-2}. \]  

(2.30)

Applying the Poisson summation formula,

\[ g_K(k, k, R) = \frac{1}{2\pi \sqrt{\pi}} \int_0^\eta \frac{k^2}{4\xi^2} \sum_{K_l \in \Lambda^*} e^{-|k_s - K_l|^2 \xi^2} \frac{\pi}{A} \sum_{K_l \in \Lambda^*} e^{-\frac{(k_s + K_l)\cdot R_s}{4\xi^2}} e^{i(k_s + K_l)\cdot R_s} \xi^{-2} d\xi, \]  

(2.31)

\[ = \frac{A^{-1}}{2\sqrt{\pi}} \sum_{K_l \in \Lambda^*} e^{i(k_s + K_l)\cdot R_s} \]  

\[ \times \int_0^\eta \frac{k^2}{4\xi^2} |z - z'|^2 \xi^2 \frac{e^{-\frac{(k_s + K_l)\cdot (k_s + K_l)}{4\xi^2}}}{4\xi^2} \xi^{-2} d\xi. \]  

(2.32)

Additionally, let \( s = \frac{1}{\xi} \) such that

\[ g_K(k, k, R) = \frac{A^{-1}}{2\sqrt{\pi}} \sum_{K_l \in \Lambda^*} e^{i(k_s + K_l)\cdot R_s} \]  

\[ \times \int_1^\infty e^{-\frac{|z - z'|^2}{s^2}} e^{s^2 \frac{k^2 - (k_s + K_l)\cdot (k_s + K_l)}{2}} ds. \]  

(2.33)
Equation (2.33) is the desired form of the $g_K(k, k, R)$. In summary,

$$g_\Lambda(k, k, R) = g_K(k, k, R) + g_R(k, k, R), \quad (2.34)$$

where

$$g_K(k, k, R) = \frac{A^{-1}}{2\sqrt{\pi}} \sum_{\mathbf{K}_l \in \Lambda^*} e^{i(k_z + K_l) \cdot \mathbf{R}_s} \times \int_{1/\eta}^\infty e^{-\frac{|z - z'|^2}{s^2}} e^{\frac{k^2}{4}(k_z + K_l)^2} ds, \quad (2.35)$$

$$g_R(k, k, R) = \frac{1}{2\pi \sqrt{\pi}} \sum_{\mathbf{R}_n \in \Lambda} e^{i\mathbf{k} \cdot \mathbf{R}_n} \int_{\eta}^\infty e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi. \quad (2.36)$$

The integrals in $g_K(k, k, R)$ and $g_R(k, k, R)$ can be evaluated using Gaussian quadrature as is. They can also be converted into complementary error functions. The integral term in $g_K(k, k, R)$ can be manipulated as follows:

$$\int_{1/\eta}^\infty e^{s \cdot \frac{k^2}{4}(k_z + K_l)^2} ds$$

$$= \frac{i}{K_{\perp, l}} \left[ \int_{1/\eta}^\infty \left( -\frac{iK_{\perp, l}}{2} - \frac{|z - z'|}{s^2} \right) e^{s \cdot \frac{k^2}{4} + \frac{|z - z'|^2}{s^2}} ds \right.$$  

$$+ \int_{1/\eta}^\infty \left( -\frac{iK_{\perp, l}}{2} + \frac{|z - z'|}{s^2} \right) e^{s \cdot \frac{k^2}{4} - \frac{|z - z'|^2}{s^2}} ds \left. \right], \quad (2.38)$$

$$= \frac{i}{K_{\perp, l}} \left[ e^{iK_{\perp, l} |z - z'|} \int_{1/\eta}^\infty \left( -\frac{iK_{\perp, l}}{2} - \frac{|z - z'|}{s^2} \right) e^{-\left( -\frac{is K_{\perp, l}}{2} + \frac{|z - z'|}{s} \right)^2} ds \right.$$  

$$+ e^{-iK_{\perp, l} |z - z'|} \int_{1/\eta}^\infty \left( -\frac{iK_{\perp, l}}{2} + \frac{|z - z'|}{s^2} \right) e^{-\left( -\frac{is K_{\perp, l}}{2} - \frac{|z - z'|}{s} \right)^2} ds \right], \quad (2.39)$$

$$= \frac{i}{K_{\perp, l}} \sum_{\pm} e^{\pm iK_{\perp, l} |z - z'|} \int_{\eta |z - z'|}^\infty e^{-w^2} dw. \quad (2.40)$$

Defining the complementary error function as

$$\text{erfc}(z) = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-w^2} dw, \quad (2.41)$$

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the integral in (2.37) can be expressed compactly as

\[
\int_{1/\eta}^{\infty} e^{iK_{\perp,l}|z-z'|} \text{erfc} \left( -\frac{iK_{\perp,l}}{2\eta} \mp z-z'|\eta \right) \, ds
\]

Using the result from (2.42) in (2.35), \( g_K(k, k, R) \) can then be written as

\[
g_K(k, k, R) = \frac{i}{4A} \sum_{\mathbf{K}_l \in \Lambda^*} e^{i(k + \mathbf{K}_l) \cdot \mathbf{R}} \sum_{\pm} e^{\pm iK_{\perp,l}|z-z'|} \text{erfc} \left( -\frac{iK_{\perp,l}}{2\eta} \mp z-z'|\eta \right).
\]

(2.43)

The procedure for \( g_R(k, k, R) \) is similar. Let

\[
\int_{\eta}^{\infty} e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi
\]

\[
= \frac{1}{2|R-R_n|} \left[ \int_{\eta}^{\infty} \left( |\mathbf{R} - \mathbf{R}_n| - \frac{ik}{2\xi^2} \right) e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi + \int_{\eta}^{\infty} \left( |\mathbf{R} - \mathbf{R}_n| + \frac{ik}{2\xi^2} \right) e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi \right],
\]

(2.44)

\[
= \frac{1}{2|R-R_n|} \left[ e^{ik|\mathbf{R} - \mathbf{R}_n|} \int_{\eta}^{\infty} \left( |\mathbf{R} - \mathbf{R}_n| - \frac{ik}{2\xi^2} \right) e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi + e^{-ik|\mathbf{R} - \mathbf{R}_n|} \int_{\eta}^{\infty} \left( |\mathbf{R} - \mathbf{R}_n| + \frac{ik}{2\xi^2} \right) e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi \right],
\]

(2.45)

\[
= \frac{1}{2|R-R_n|} \left[ e^{ik|\mathbf{R} - \mathbf{R}_n|} \int_{|\mathbf{R} - \mathbf{R}_n| - \frac{i|\mathbf{R} - \mathbf{R}_n|}{2\eta}}^{\infty} e^{-w^2} dw + e^{-ik|\mathbf{R} - \mathbf{R}_n|} \int_{|\mathbf{R} - \mathbf{R}_n| - \frac{i|\mathbf{R} - \mathbf{R}_n|}{2\eta}}^{\infty} e^{-w^2} dw \right],
\]

(2.46)

\[
= \frac{\sqrt{\pi}}{4|R-R_n|} \sum_{\pm} e^{\pm ik|R-R_n|} \text{erfc} \left( |\mathbf{R} - \mathbf{R}_n| \eta \pm \frac{ik}{2\eta} \right).
\]

(2.47)

Using (2.47) in (2.36),

\[
g_R(k, k, R) = \frac{1}{8\pi} \sum_{\mathbf{R}_n \in \Lambda} e^{ik\mathbf{R}_n} \sum_{\pm} e^{\pm ik|R-R_n|} \text{erfc} \left( |\mathbf{R} - \mathbf{R}_n| \eta \pm \frac{ik}{2\eta} \right).
\]

(2.48)
2.5 Convergence

In this section, the convergence behavior of spatial, spectral, and Ewald representations of PGF are examined. The sums are evaluated in a spiral around the observation point which roughly adheres to the order of decreasing magnitude contribution by mirror sources (see Figure 2.2). The spatial PGF is expected to have the slowest convergence rate. The spectral PGF converges much faster than the spatial PGF when the observation point does not lie in the lattice plane. The Ewald PGF converges at the same rate as PGF as spectral PGF when the observation point is not on the lattice plane. The spectral PGF loses its exponential convergence when the observation point is on the lattice plane. The Ewald PGF has no trouble with this case.

Figure 2.2: The spiraling sum strategy used to evaluate spatial and spectral representations of PGF.

When evaluating PGF for spectral or spatial representations, the cells closest to the observation point contribute the most to the magnitude of PGF. To avoid numerical roundoff, the sum should be evaluated from smallest values to largest values. However, we do not know apriori how many cells should be summed. Instead, we use a spiral sum strategy (see Figure 2.2). The sum is terminated when the magnitude of the new cell contribution over the magnitude of the current sum is small. Since the running sums for spatial and spectral PGF tend to oscillate, this evaluation method does not produce the most accurate results.
Figure 2.3: The PGF is computed using spatial, spectral, and Ewald representations using the following parameters: $r' = (0.48, -0.91, 0)$, $r = (0, 0, 0)$, $a_1 = (0.95, 0, 0)$, $a_2 = (0, 0.95, 0)$, $\theta = 45^\circ$, $\phi = 25^\circ$, $\lambda = 1$, $k = \frac{2\pi}{\lambda}(1 + i 0.1)$.

Figure 2.4: This illustrates the slow convergence of the spectral representation when the $z$-component of $r$ is zero.
Figure 2.5: The PGF is computed using spatial, spectral, and Ewald representations using the following parameters: \( \mathbf{r} = (0.48, -0.91, 0.1), \mathbf{r}' = (0, 0, 0), \mathbf{a}_1 = (0.95, 0, 0), \mathbf{a}_2 = (0, 0.95, 0), \theta = 45^\circ, \phi = 25^\circ, \lambda = 1, k = \frac{2\pi}{\lambda}(1 + i0.1) \).

Figure 2.6: The spectral and Ewald representations require few terms to converge when the \( z \)-component of \( \mathbf{r} \) is not zero.

From Figures 2.3 and 2.5, it can be observed that the spatial representation of PGF requires summing over many cells in order to converge. The conver-
gence rate is also quite slow. In contrast, the Ewald representation of PGF converges using much fewer terms and does not oscillate around the correct value of PGF. Figure 2.4 illustrates the case in which the observation point lies on the plane of the 2-D lattice. For this case, the spectral representation of PGF no longer converges at an exponential rate. Figure 2.6 illustrates the case when the observation point does not lie on the 2-D lattice plane. Both Ewald and spectral representations of PGF converge at an exponential rate for this case.

The Ewald representation of PGF produces an accurate and exponentially convergent representation of PGF. It requires the evaluation of special functions, thus making it slow compared to FGF. Furthermore, the Ewald representation shown here is used for direct interactions. This representation is used in our MOM discretization of periodic EFIE and MFIE.
3.1 Periodic EFIE and MFIE

In CEM, integral equations (IE) describe a linear relationship between surface currents and incident fields. EFIE and MFIE are two of the most common and fundamental IEs. Either equation can be used to describe the scattering by a PEC or dielectric object. The discretization of EFIE and MFIE for PEC provides fundamental building blocks from which all other IE can be derived. Knowing this, attention is given to scattering by PEC. The equations for EFIE and MFIE for a PEC object can be written as

\[
\hat{n} \times \mathbf{E}_{\text{inc}} = Z_0 \hat{n} \times \mathbf{L}(\mathbf{J}_s),
\]

\[
\hat{n} \times \mathbf{H}_{\text{inc}} = \frac{1}{2} \mathbf{J}_s + Z_0 \hat{n} \times \mathbf{K}_{PV}(\mathbf{J}_s),
\]

where \(Z_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}}\), \(\hat{n} \equiv \hat{n}(\mathbf{r})\) is the surface normal at \(\mathbf{r}\), and

\[
\mathbf{L}(\mathbf{X}) = -ik \int_S (\mathbf{X} g_0(k, \mathbf{r}, \mathbf{r}') + \frac{1}{k^2} \nabla' \cdot \mathbf{X} \nabla g_0(k, \mathbf{r}, \mathbf{r}')) \, d\mathbf{r}',
\]

\[
\mathbf{K}(\mathbf{X}) = \int_S \mathbf{X} \times \nabla g_0(k, \mathbf{r}, \mathbf{r}') \, d\mathbf{r}'.
\]

It can be seen from (3.3) and (3.4) that both EFIE and MFIE are dependent on FGF. Converting these IEs to their periodic counterparts is simply a matter of replacing \(g_0(k, \mathbf{r}, \mathbf{r}')\) with \(g_\Lambda(k, \mathbf{r}, \mathbf{r}')\) for \(\mathbf{L}\) and \(\mathbf{K}\). This converts an aperiodic surface to a periodic surface according to the lattice embedded in \(g_\Lambda(k, \mathbf{r}, \mathbf{r}')\).

Both EFIE and MFIE integrals can be converted into matrix equations by expanding and testing with Rao-Wilton-Glisson (RWG) basis functions [21]. Given an existing implementation of EFIE and MFIE using RWG basis
functions, the changes that need to be made to adapt the code for periodic geometry is to replace FGF with PGF and modify the singularity subtraction procedure. The expansion of EFIE and MFIE for FGF is widely documented in literature. We will focus on the differences with particular attention to singularity subtraction.

IE can be reduced to $\mathbf{Z} \cdot \mathbf{I} = \mathbf{V}$ where $\mathbf{Z}$ is the impedance matrix, $\mathbf{V}$ is the excitation vector, and $\mathbf{I}$ is a vector of current coefficients. For PGF, the excitation vector is a plane wave with polarization $\mathbf{E}_0$ and wavevector $\mathbf{k}$. The elements of the excitation vector are

$$[\mathbf{V}]_m = \int_{S_m} \Lambda_m(\mathbf{r}) \cdot \mathbf{E}_0 e^{i \mathbf{k} \cdot \mathbf{r}} d\mathbf{r}. \quad (3.5)$$

$S_m$ corresponds to $\mathbf{r}$ such that $\Lambda_m(\mathbf{r}) \neq 0$. The matrix elements of periodic EFIE are

$$[\mathbf{Z}]_{mn} = -i \omega \mu \int_{S_m} \int_{S_n} \left( \Lambda_m(\mathbf{r}) \cdot \Lambda_n(\mathbf{r}') - \frac{1}{k^2} \nabla \cdot \Lambda_m(\mathbf{r}) \nabla' \cdot \Lambda_n(\mathbf{r}') \right) g_{\Lambda}(k, \mathbf{k}, \mathbf{R}) d\mathbf{r}' d\mathbf{r}. \quad (3.6)$$

The matrix elements of periodic MFIE are

$$[\mathbf{Z}]_{mn} = \frac{1}{2} \int_{S_m} \Lambda_m(\mathbf{r}) \cdot \Lambda_n(\mathbf{r}) d\mathbf{r}$$

$$+ P.V. \int_{S_m} \Lambda_m(\mathbf{r}) \cdot \hat{n} \times \int_{S_n} \nabla' g_{\Lambda}(k, \mathbf{k}, \mathbf{R}) \times \Lambda_n(\mathbf{r}') d\mathbf{r}' d\mathbf{r}, \quad (3.7)$$

where $P.V.$ stands for principal value. For basis functions defined over a flat surface (such as RWG), this means that integration is performed only over areas where $S_m$ and $S_n$ do not overlap.

Green’s function is singular when $\mathbf{r} = \mathbf{r}'$, which can only occur when $S_m$ and $S_n$ overlap. Despite having a singularity, the integration over this singularity is a finite value. The impedance matrix element for the overlapping case can be determined accurately by performing singularity subtraction, by re-writing Green’s function in terms of its regular and singular parts. The regular part can be integrated using numerical techniques such as Gaussian quadrature. The singular part is chosen such that it can be integrated analytically. Both EFIE and periodic EFIE use similar singularity subtraction
procedures. That is,
\[
\lim_{R \to 0} \left( g_0(k, r, r') - \frac{1}{4\pi R} \right) = \frac{ik}{4\pi},
\]
(3.8)
\[
\lim_{R \to 0} \left( g_R(k, k, R) - \frac{1}{4\pi R} \right) = -\frac{4\eta}{\sqrt{\pi}} - 2ik \text{erf} \left( \frac{ik}{2\eta} \right),
\]
(3.9)
where (3.9) is derived using the Ewald representation.

The singular term in (3.9) comes from \( g_R(k, k, R) \), which can be expanded into
\[
g_R(k, k, R) = \frac{1}{8\pi} \sum_{R_n \in A/\Lambda_0} \frac{e^{ikR_n}}{|R - R_n|} \sum_{\pm} e^{\pm ik|R - R_n|} \text{erfc} \left( \frac{|R - R_n|}{2\eta} \right)
\]
\[
+ \sum_{\pm} \frac{e^{\pm ikR}}{8\pi R} \text{erfc} \left( \frac{iR}{2\eta} \right),
\]
(3.10)
where the second term on the RHS is the singular term. Using the fact that \( \text{erfc}(z) = 1 - \text{erf}(z) \) where \( \text{erf}''(z) = \frac{2}{\sqrt{\pi}} e^{-z^2} \), applying L’Hopital’s rule produces the following limit:
\[
\lim_{R \to 0} \sum_{\pm} \frac{e^{\pm ikR}}{8\pi R} \text{erfc} \left( \frac{R \eta}{2\eta} \right) - \frac{1}{4\pi R}
\]
(3.11)
\[
= -\frac{1}{2\pi \sqrt{\pi}} \frac{k^2}{4\eta^2} + \frac{ik}{8\pi} \left( \text{erfc} \left( \frac{ik}{2\eta} \right) - \text{erfc} \left( -\frac{ik}{2\eta} \right) \right).
\]
(3.12)
This limit can be computed before the matrix-fill routine and stored since its value does not change during matrix construction.

For periodic MFIE, one may also re-use the existing singularity subtraction technique used in aperiodic MFIE. Unlike EFIE, one does not need to determine a limit for regularized Green’s function due to \( P.V. \) integration. Expressions for the gradient of PGF may be found Appendix A. We conclude this section with some important implementation notes. For periodic EFIE, singularity subtraction is only applicable for the Green’s function attached to the reference cell source. Singularity subtraction is not applied to the image cells which are far away. Similarly for periodic MFIE, when using RWG basis functions, one normally ignores the case when observation and source facets are overlapping due to \( P.V. \) integration. This only applies to the basis function in the reference cell. The image basis functions do not overlap with
Figure 3.1: (a) and (b) are the current distributions for a single PEC sphere computed using EFIE. (c) and (d) are the current distributions for an array of PEC spheres computed with periodic EFIE with \( \mathbf{a}_1 = \hat{x}3, \mathbf{a}_2 = \hat{y}3, (\mu_r, \epsilon_r) = (1, 1) \). The excitation for both configurations is a plane wave with \( f = 3 \times 10^8, (\theta, \phi) = (0, 0), \) and \( \mathbf{E}_0 = \hat{x} \).

the observation facet and one must be careful not to neglect them. In Section 3.2, we present some calculations using periodic EFIE and MFIE.

3.2 Results

Here, we compute the scattering by periodic arrays of various objects using periodic EFIE and MFIE. The currents found are vectors of complex phasors. The colors for each patch are chosen as \( \|\text{Re}\{\mathbf{J}(\mathbf{r})\}\| \) to correspond with the magnitude of the currents at time \( t = 0 \). The scattering from various structures are examined using periodic EFIE.

The PEC spheres in Figure 3.1 have a radius of 1 m and the number of edge unknowns is 2,352. The same simulation is repeated in Figure 3.2 using
Figure 3.2: (a) and (b) are the current distributions for a single PEC sphere computed using MFIE. (c) and (d) are the current distributions for an array of PEC spheres computed with periodic MFIE with \( \mathbf{a}_1 = \hat{x} 3, \mathbf{a}_2 = \hat{y} 3, (\mu_r, \epsilon_r) = (1, 1) \). The excitation for both configurations is a plane wave with \( f = 3 \times 10^8, (\theta, \phi) = (0, 0) \), and \( \mathbf{H}_0 = \hat{y} Z_0^{-1} \).

MFIE and periodic MFIE. The computation time is 47 minutes.
Figure 3.3: (a) and (b) are the current distributions for a periodic array of PEC spheres computed using periodic EFIE and MFIE, respectively, where $a_1 = \hat{x}3$, $a_2 = \hat{y}3$, $(\mu_r, \epsilon_r) = (1, 1)$. The excitation for both configurations is a plane wave with $f = 1.5 \times 10^8$, $(\theta, \phi) = (0, 0)$, and $\mathbf{H}_0 = \hat{y}Z_0^{-1}$. 
FMA is a method for solving MOM problems fast and efficiently. It does this by leveraging the addition theorems for spherical harmonics to factorize the field, reducing storage cost from $O(N^2)$ to $O(N)$. Since FMA is inherently tied to iterative matrix solvers, it is also important to mention that FMA reduces the cost of matrix-vector products from $O(N^2)$ to $O(N \log N)$. There are two important steps in the FMA: pre-computation and matrix-vector product. An oct-tree is used to facilitate the operation of a matrix-vector product. The construction and initialization of the oct-tree contributes to overhead which only affects the pre-computation step of the FMA.

The matrix-vector product step comprises four phases: (1) aggregation, (2) translation, (3) disaggregation, and (4) nearfield. Multilevel, periodic FMA (MLP-FMA) affects both pre-computation and the matrix-vector product steps. It does not affect the computational complexity of storage and matrix-vector product. First, the addition theorems are illustrated pictorially to provide a visual aid for the discussion oct-tree traversal strategies. Second, the factorization of PGF using spherical multipoles is shown for both plane waves and multipoles, culminating in the conception of a lattice translator. Third, changes in the oct-tree are outlined and the concept of near-lattice neighbors (NLN) and far-lattice neighbors (FLN) are introduced. Lastly, various tree-traversal methods are outlined.

4.1 Addition Theorem

The addition theorem is what permits factorization of Green’s function. It lets us represent a field using a superposition of functions in a manner reminiscent of the Laurent series expansion. For different Green’s function, there is a different set of addition theorems. For example, $\frac{1}{R}$ can be expanded
using spherical harmonics while $\frac{e^{ikR}}{R}$ can be represented using plane waves.

We skip over the mathematical details for each addition theorem, as they are discussed extensively in [2]. Instead, we cover the general rules each addition theorem abides by. More specifically, we provide figures that illustrate the regions of validity applicable to each addition theorem. This will aid the discussion on tree traversal strategies.

For a given expansion (where expansion usually refers to plane waves or multipoles), there are three addition theorems. Each theorem corresponds to outgoing and incoming waves. The first addition theorem represents outgoing waves as outgoing waves (i.e. Hankel waves). The second addition theorem represents outgoing waves as incoming waves (i.e. Bessel waves). The third addition theorem represents incoming waves as incoming waves. Like Laurent series, each addition theorem has a region of convergence that depends on the location. For PGF, a singularity exists at the point where the observation point and source point are the same. The addition theorems mimic the field due to one source using a superposition of sources located at a new expansion center. We will refer to these sources as equivalent sources.

The region of convergence for the first addition theorem is illustrated in Figure 4.1a. This addition theorem enables what is known as the aggregation phase in FMA. The region of validity for the second addition theorem is illustrated in Figure 4.1b. This addition theorem facilitates the translation phase in FMA. The third addition theorem is valid everywhere. Figure 4.2 depicts full FMA sequence.

Figure 4.1: The red dots denote sources. (a) illustrates the region of convergence for the first addition theorem. (b) illustrates the region of convergence for the second addition theorem.
In the aggregation phase, the source is represented by equivalent sources located at the center of the white circle. In Figure 4.2, only one source is aggregated, but many more can be as long as they are within the radius of the white circle. Only the field outside the white circle is valid. By valid, we mean the equivalent sources and the original sources produce the same field within a certain region. The next step is the translation phase. The field due to the equivalent sources in the center of the white circle are represented by equivalent sources at the center of the dark green circle. These equivalent sources have the same field as the original source in the dark green region excluding the white circle. We can safely disaggregate the field from the center of the dark green circle to anywhere within the red box since the source box is sufficiently far away from the observation box.

The box in Figure 4.2 is a typical construct in an oct-tree. The circle that circumscribes this box is the boundary for the region of validity of the source furthest away from the box center (i.e. sources located at the corners). Buffer boxes are used to ensure that validity of the addition theorems. An example of what happens when buffer boxes are not used is shown in Figure 4.3. The white region in the observation box indicates points where the received field may not match the field from sources in the source box. With a geometrical
framework of the validity of addition theorem, we proceed to examine the factorization of PGF.

Figure 4.3: A reference box is normally surrounded by buffer boxes to avoid the case shown in the figure. The addition theorem is satisfied for receiver R1 but not R2.

4.2 Lattice Translator

PGF can be readily factorized using the known factorizations of FGF. For simplicity, we illustrate this concept with the plane wave factorization of FGF [22]:

\[
e^{ik|D+d|} \frac{1}{|D + d|} = \frac{i k}{4 \pi} \oint_{\hat{k}} e^{i\hat{k} \cdot d} \sum_{l=0}^{L} i^l (2l + 1) h_l^{(1)}(kD) P_l(\hat{k} \cdot \hat{D}) d^2 \hat{k}, \tag{4.1}
\]

where \( h_l^{(1)}(x) \) is the spherical Hankel function of the first kind and \( P_l(x) \) is the associated Legendre polynomial. The integral \( \oint_{\hat{k}} d^2 \hat{k} \) indicates a surface integral over a unit sphere where \( \hat{k} \) are the plane wave propagation directions (not to be confused with the incident plane wave) and \( L \) is the plane wave truncation number. While \( L \) does not have a closed form, researchers have made good approximations. We use the formula suggested by [2], which is also valid for PGF. From hereon, we denote the incident plane wave propa-
gation vector as $k_i$, only when it is necessary to make this distinction, as is the case for plane wave factorization. For the multipole case, $k$ can be used.

From Equation (2.16) in Chapter 2, PGF can be expressed as a sum of shifted and phased FGF. We can therefore write PGF as:

$$g_\Lambda(k, k_i, R) = g_0(k, r, r') + \frac{ik}{(4\pi)^2} \oint_1 e^{ik \cdot R} \sum_{l=0}^L l^2(2l + 1) \left( \sum_{R_n \in \Lambda/\Lambda_0} h_1^{(1)}(kR_n) P_l(-\hat{k} \cdot \hat{R}_n) e^{ik \cdot R_n} \right) \, d^2k, \quad (4.2)$$

where $R < R_n \forall n_1, n_2 \in \mathbb{Z}$. The reference cell contribution $g_0(k, r, r')$, which can be factorized using techniques found in [2], is separated from the rest of the lattice contributions. The reason this is done is because the lattice translator is designed such that it is only valid for $R < R_n$ for $n_1, n_2 \in \mathbb{Z}$. To understand (4.2), it is useful to refer back to the factorization of FGF. This factorization is typically expressed as

$$g(k, r_{ji}) = \frac{1}{4\pi} \oint_1 e^{ik \cdot r_m} \alpha_{mm'}(k, r_{mm'}) e^{-ik \cdot r_{m'}} \, d^2k, \quad (4.3)$$

$$\alpha_{mm'}(k, r_{mm'}) = \frac{ik}{4\pi} \sum_{l=0}^L l^2(2l + 1) h_1^{(1)}(kr_{mm'}) P_l(\hat{k} \cdot \hat{r}_{mm'}) \, d^2k, \quad (4.4)$$

where $r_i$ and $r_j$ are source and observation vectors and $r_m$ and $r_{m'}$ are expansion centers. The translation direction is denoted by $r_{mm'}$. If we compare (4.4) to (4.2), they are nearly identical. If we set the expansion centers to $r_m = r_{m'} = 0$, then we have

$$g(k, r_{ji}) = \frac{1}{4\pi} \oint_1 e^{ik \cdot r} \alpha_{mm'}(k, 0) e^{-ik \cdot r} \, d^2k. \quad (4.5)$$

The translator $\alpha_{mm'}(k, 0)$ is not meaningful and becomes infinite due to the singularity of $h_1^{(1)}(x)$ at $x = 0$. What we want to take away from (4.5) is that it appears that the expansion centers for factorized PGF are at the origin. One can also say that $r_m = r_{m'}$. This is a better interpretation, as it allows for the center of the oct-tree bounding box to be in any arbitrary location. The bounding box does not have to conform with the shape of the unit cell.
It can be smaller, but not larger. In general, we want to lean toward a smaller bounding box to minimize the size of $L$, which is dependent on box size.

Consider the illustration in Figure 4.4 where we have a parallelogram-shaped unit cell enclosing a circular scatterer. The circular scatter is enclosed within a bounding box denoted by the blue dashed square. The green arrow represents the observation location and the red arrow indicates the source location. Relative to the box center \( r_c \), the black arrow points from the observation point to the source.

![Diagram](image)

Figure 4.4: This figure depicts a circular scatterer enclosed in a bounding box whose center is denoted by \( r_c \). An arbitrary pair of observation and source locations are denoted by \( r \) and \( r' \), respectively.

Now, to observe the effect of the lattice translation, we choose an arbitrary \( R_n \) (see Figure 4.5). At \( R_n \), we have an image scatterer (the red-tinted circle) with lattice phase \( e^{ik \cdot R_n} \). The red arrow in the image scatterer points to the image source and has the same magnitude and direction as the source in the reference cell. While the red arrow points to the image source location, the aggregation direction is actually \(-r'\), as shown by the dashed red arrow in Figure 4.6. Similarly, the translation direction of the image source is \(-R_n\). The disaggregation vector is just \( r \).

In Figure 4.7, the full transfer of the field from the image cell to the reference cell is shown.
Figure 4.5: This figure shows an arbitrary lattice vector $\mathbf{R}_n$ (dashed yellow arrow) with respect to a coordinate system centered on the bounding box inside the reference cell.

Figure 4.6: This figure shows the aggregation vector (dashed red arrow) with respect to a coordinate system centered on the bounding box inside the image cell.
Figure 4.7: This figure shows the transfer of the field from the image cell source to the reference cell through translation by $-\mathbf{R}_n$ (yellow arrow) and disaggregation by $\mathbf{r}$ (green arrow).

The field from all image sources can be transferred by repeating the steps shown in Figures 4.5, 4.6, and 4.7 for all $\mathbf{R}_n$ except $\mathbf{R}_n = 0$.

The lattice sum in (4.2) is difficult to evaluate using fast methods due to the term $P_l(\hat{k} \cdot \hat{R}_n)$ when $\hat{k}$ is not in the $\hat{z}$ direction. To alleviate this, we can expand $P_l(\hat{k} \cdot \hat{R}_n)$ as a sum of spherical harmonics to effectively separate $\hat{k}$ and $\hat{R}_n$:

$$P_l(\hat{k} \cdot \hat{R}_n) = (-1)^l P_l(\hat{k} \cdot \hat{R}_n) = \frac{4\pi(-1)^l}{2l + 1} \sum_{m=-l}^{l} Y^*_{lm}(\hat{R}_n)Y_{lm}(\hat{k}). \quad (4.6)$$

Doing so allows us to re-write (4.2) as

$$g_\Lambda(k, k_i, \mathbf{R}) = g_0(k, \mathbf{r}, \mathbf{r}')$$

$$+ \frac{ik}{4\pi} \int_{1} e^{i\mathbf{k} \cdot \mathbf{R}} \sum_{l=0}^{L} \sum_{m=-l}^{l} Y_{lm}(\hat{k}) \left( \sum_{\mathbf{R}_n \in \Lambda / \Lambda_0} h_t^{(1)}(k\mathbf{R}_n)Y^*_{lm}(\hat{R}_n)e^{i\mathbf{k} \cdot \mathbf{R}_n} \right) d^2\hat{k} \quad (4.7)$$

$$R < R_n \forall n_1, n_2 \in \mathbb{Z}.$$
The result is similar to plane wave factorization for mixed-form FMA [23].
The primary difference is the translation operation in parenthesis. A visual interpretation of (4.7) is provided in Figure 4.8.

Figure 4.8: An illustration of the lattice translator. The reference cell is shaded in green. The lattice cells are shaded in red.

The lattice sum in (4.7) can be accelerated using Ewald summation. This can be seen by expanding the field emanated by sources outside the reference cell. Let us denote this field as

\[
D_\Lambda(k, \mathbf{k}, \mathbf{R}) = g_\Lambda(k, \mathbf{k}, \mathbf{R}) - g_0(k, \mathbf{R}).
\]

Within the reference cell, the field produced by \(D_\Lambda(k, \mathbf{k}, \mathbf{R})\) is free of singularities. Therefore, \(D_\Lambda(k, \mathbf{k}, \mathbf{R})\) can be written as a multipole expansion which is valid within the reference cell. From the second addition theorem, it can be shown that

\[
\frac{e^{i\mathbf{k} \cdot (\mathbf{R} - \mathbf{R}_n)}}{4\pi |\mathbf{R} - \mathbf{R}_n|} = i k \sum_L h_l^{(1)}(k \mathbf{R}_n) Y_{lm}^*(\hat{\mathbf{R}}_n) Y_l^m(\hat{\mathbf{R}}) j_l(k \mathbf{R}), \quad \mathbf{R} < \mathbf{R}_n,
\]

from which one can deduce that

\[
D_\Lambda(k, \mathbf{k}, \mathbf{R}) = i k \sum_{l=0} L \sum_{m=-l}^l \sigma_l^m(k, \mathbf{k}) Y_{lm}(\hat{\mathbf{R}}) j_l(k \mathbf{R}) \quad (4.10)
\]

\[
\sigma_l^m(k, \mathbf{k}) = \sum_{\mathbf{R}_n \in \Lambda/\Lambda_0} h_l^{(1)}(k \mathbf{R}_n) Y_{lm}^*(\hat{\mathbf{R}}_n) e^{i\mathbf{k} \cdot \mathbf{R}_n}. \quad (4.11)
\]

The term \(\sigma_l^m(k, \mathbf{k})\) are known as lattice constants. Determining these constants requires evaluating a slowly convergent lattice sum similar to the
spatial representation of PGF. Equating (4.8) to (4.10) and replacing \( g_0(k, R) \) with the Ewald representation in (2.34), one arrives at

\[
g_K(k, k, R) + g_R(k, k, R) - g_0(k, R) = ik \sum_{l=0}^{L} \sum_{m=-l}^{l} \sigma_l^m(k, k) Y_{lm}(\hat{R}) j_l(kR). \tag{4.12}
\]

Using the orthogonality of spherical harmonics,

\[
\sigma_l^m(k, k) = \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint D_\Lambda(k, k, R) Y_{lm}^*(\hat{R}) d\Omega,
\tag{4.13}
\]

where \( \oint d\Omega \equiv \int_0^{2\pi} \int_0^{\pi} \sin \theta d\theta d\phi \) and \( \hat{R} = \hat{x} \sin \theta \cos \phi + \hat{y} \sin \theta \sin \phi + \hat{z} \cos \theta \).

Since \( D_\Lambda(k, k, R) \) is singularity-free, there exists a term in \( g_\Lambda(k, k, R) \) which cancels out the singularity in \( g_0(k, R) \). This term is found in \( g_R(k, k, R) \).

Let us denote \( \tilde{g}_R(k, k, R) \) as

\[
\tilde{g}_R(k, k, R) = \frac{1}{2\pi \sqrt{\pi}} \sum_{R_n \in \Lambda/\Lambda_0} e^{ikR_n} \int_{\eta}^{\infty} e^{-|R-R_n|^2 + \frac{k^2}{4\xi^2}} d\xi,
\tag{4.14}
\]

where \( R_n \in \Lambda/\Lambda_0 \) indicates the exclusion of \( \Lambda_0 \) from \( \Lambda \). The \( \Lambda_0 \) term is paired with \( g_0(k, R) \) to cancel out the singularity. Having established this, \( \sigma_l^m(k, k) \) can be expressed as

\[
\sigma_l^m(k, k) = \sigma_l^m(0)(k) + \sigma_l^m(1)(k, k) + \sigma_l^m(2)(k, k),
\tag{4.15}
\]

where

\[
\sigma_l^m(0)(k) = \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint \left( \frac{1}{2\pi \sqrt{\pi}} \int_{\eta}^{\infty} e^{-R^2\xi^2 + \frac{k^2}{4\xi^2}} d\xi - g_0(k, R) \right) Y_{L}^*(\hat{R}) d\Omega,
\tag{4.16}
\]

\[
\sigma_l^m(1)(k, k) = \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint g_K(k, k, R) Y_{L}^*(\hat{R}) d\Omega,
\tag{4.17}
\]

\[
\sigma_l^m(2)(k, k) = \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint \tilde{g}_R(k, k, R) Y_{L}^*(\hat{R}) d\Omega.
\tag{4.18}
\]

Evaluation of (4.16)–(4.18) is quite tedious and can be found in Appendix
B. The results are presented below:

\[
\sigma_{l}^{m(0)}(k) = \delta_{l,0} \left( -\frac{1}{2\sqrt{\pi}} + \frac{i}{2\pi} \sum_{j=0}^{\infty} \frac{1}{j!(1-2j)} \left( \frac{k}{2\eta} \right)^{2j-1} \right), \quad (4.19)
\]

\[
\sigma_{l}^{m(1)}(k, \mathbf{k}) = \frac{i^{m-2|m|}}{2\pi} \sqrt{\pi} (2l + 1)(l + m)!(l - m)! \sum_{n=0}^{l-|m|} e^{-i\frac{m}{2}(\mathbf{k} + \mathbf{K}_{l} \cdot \mathbf{R}_{n})} \frac{e^{-i\frac{m}{2}(\mathbf{k} + \mathbf{K}_{l} \cdot \mathbf{R}_{n})}}{2\eta} e^{-i\frac{m}{2}(\mathbf{k} + \mathbf{K}_{l} \cdot \mathbf{R}_{n})}, \quad (4.20)
\]

\[
\sigma_{l}^{m(2)}(k, \mathbf{k}) = \frac{2l-1}{i2l+1} \sum_{\mathbf{R}_{n} \in \Lambda / \Lambda_{0}} R_{n}^{l-1} Y_{l}^{m}(\hat{R}_{n}) e^{ik \cdot \mathbf{R}_{n} + i\frac{k}{2\eta}}, \quad (4.21)
\]

Up until this point, we have derived the spatial, spectral, and Ewald representations of PGF. For the purposes of debugging, it is useful to implement each of these representations to cross-check with one another. A good order to implement these equations is to start with the spatial representation and debug it against the spectral representation. Once their results agree, we implement the Ewald representation and debug this against the spectral representation. Errors in the Ewald representation arise when \( \eta \) is chosen poorly or the number of terms used in spatial or spectral sums are insufficient. Once these direct forms of PGF have been implemented, they can be used to debug the plane wave or multipole factorizations of PGF.

The plane wave factorization in (4.7) can be expressed in terms of the lattice constants as

\[
g_{\Lambda}(k, \mathbf{k}, \mathbf{R}) = g_{0}(k, \mathbf{r}, \mathbf{r}') + \frac{ik}{4\pi} \int e^{ik \cdot \mathbf{R}} T_{\Lambda,pw}(k, \mathbf{k}) d^{2}\hat{k}, \quad (4.25)
\]

\[
T_{\Lambda,pw}(k, \mathbf{k}) = \sum_{l=0}^{L} \sum_{m=-l}^{l} Y_{lm}(\hat{k}) \sigma_{l}^{m}(k, \mathbf{k}), \quad (4.26)
\]
where $T_{\Lambda, pw}(k, k_i)$ is the lattice translator for plane waves. For completeness, we also provide the factorization for PGF using spherical multipoles. The multipole factorization of PGF can be written as

$$g_\Lambda(k, k, R) = g_0(k, r, r') + ik \sum_{l_1} \sum_{l_2} \beta_{0, L_1}(r) T_{\Lambda, mp}(k, k) \beta_{L_2, 0}(-r'),$$  \hspace{1cm} (4.27)$$

$$T_{\Lambda, mp}(k, k) = 4\pi i^{l_2-l_1}(-1)^{m_3} \sum_{l_3=|l_2-l_1|} \sum_{l_3} i^{l_3} A_{L_1, L_2, L_3} \sigma_{l_3}^{m_3}(k, k),$$  \hspace{1cm} (4.28)$$

$$\beta_{L_2, L_1}(R) = \sum_{l_3=|l_2-l_1|} 4\pi i^{l_3+l_2-l_1} Y_{l_3}^{m_3}(\hat{R}) j_{l_3}(kR) A_{L_1, L_2, L_3},$$  \hspace{1cm} (4.29)$$

where $m_3 = m_1 - m_2$, $T_{\Lambda, mp}(k, k)$ is the lattice translator for multipoles, $\sum_{L_n} = \sum_{l_n=0}^{l_n=0} \sum_{m_n=-l_n}$, $\beta_{L_2, L_1}(R)$ is multipole aggregation/disaggregation, and $A_{L_1, L_2, L_3}$ is the Gaunt coefficient related to the Wigner-3j symbols (see Appendix D of [17]):

$$A_{L_1, L_2, L_3} \equiv A(l_1, m_1, l_2, m_2, l_3, m_3)$$

$$= (-1)^{m_1} \sqrt{(2l_1+1)(2l_2+1)(2l_3+1)} \times \left( \begin{array}{ccc} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{array} \right) \left( \begin{array}{ccc} l_1 & l_2 & l_3 \\ -m_1 & m_2 & m_3 \end{array} \right).$$  \hspace{1cm} (4.30)$$

The periodic mixed-form translator is equal to the periodic plane wave translator multiplied by $4\pi$.

With plane wave, mixed-form, and multipole factorizations, a mixed-form MLP-FMA can be implemented which is stable when box sizes in the oct-tree are fractions of a wavelength [23]. In our code, we choose $0.2\Lambda$ to be the switching point between plane waves and multipoles, as is done in [23]. This gives us the freedom to use more levels in the oct-tree without the subwavelength box limitation. In both factorizations, the lattice translator only accounts for the cells where $R_n \neq 0$. The term $g_0(k, r, r')$ can be factorized using the ordinary ML-FMA discussed in [2].

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4.3 Matrix-Vector Product

4.3.1 Oct-Tree

The oct-tree is used to facilitate the operation of a matrix-vector product, enforce the validity of the addition theorems, and separate near and far interactions. An oct-tree is constructed by enclosing the scatterer inside a box and recursively dividing that box into sub-boxes \( L \) times so that there are \( L + 1 \) levels in the tree. If we consider \( l = 0 \) to be the box which bounds the entire scatterer, then the finest level or leafy level of the tree is \( l = L - 1 \). If a box is not empty, then it has exactly one parent and at most eight children. Each box contains two interaction lists that identify which boxes are its touching near-neighbors (TNN) and non-touching near-neighbors (NTNN).

For a given reference box, its TNN are the non-empty boxes which are touching it, including itself. Its NTNN are the children of its parent’s TNN, excluding its own TNN. Any box in the leaf level is able to communicate with any other box. This is achieved through upward and downward traversal of the tree from levels \( l = 2, \ldots, L - 1 \). The introduction of PBC produces image image cells which must be accounted for by the interaction lists. While our actual algorithm uses oct-tree, a quad-tree will be used to illustrate concepts in this section. The ideas are analogous.

The oct-tree for MLP-FMA builds on top of the existing oct-tree used for ML-FMA. The primary differences are the use of levels \( l = 0 \) and \( l = 1 \) in the tree, which traditionally do not have NTNN, to communicate with image cells in the lattice. In our illustrations, the bounding box is used as the reference cell though it may be smaller than the reference cell.

Next, we introduce the concept of near-lattice neighbors (NLN) and far-lattice neighbors (FLN). The use of NLN and FLN are implicit. That is, no actual memory is used to store NLN or FLN interaction lists (there would be an infinite number of FLN). Fields due to NLN are computed using one method and fields due to FLN are computed using a different method. In Otani and Nishimura’s approach, the translators used on level \( l = 1 \) correspond to NLN while the translator used on level \( l = 0 \) corresponds to FLN. In our approach, we also use \( l = 0 \) to handle FLN interactions but NLN interactions are handled on \( l = 2, \ldots, L - 1 \). First, we will discuss changes to TNN and NTNN when PBC are considered.
Figure 4.9: The TNN (orange) and NTNN (blue) of a corner reference box (green) for a scatterer without PBC.

For \( l = 2 \), Figure 4.9 depicts a reference box (shaded in green) for a given structure has the following TNN (shaded in orange) and NTNN (shaded in blue). When PBC are applied, image cells appear which introduce image sources that are close to the reference box. These sources are included in the reference box’s TNN list. In Figure 4.10, the boxes outlined in red are a subset of the image cells introduced by PBC and the boxes in yellow are the additional TNN. Image cells are implied by the equations and are not a required part of the mesh. In ordinary ML-FMA, we only have information about geometry inside the reference cell. For MLP-FMA, re-use and build on top of this information. To do this, we address the new TNN using existing boxes in the reference cell. This can be done by changing some of the NTNN boxes into TNN boxes, as shown in Figure 4.11. This approach requires more plane waves and a slight increase in MVP time. This can be a hinderance when the bandwidth is large since lattice constants are difficult to compute accurately for large \( L \).

4.3.2 The Lattice Translator

The lattice translator we devised is similar to the standard translator. The standard translator converts outgoing waves to incoming waves between reference and NTNN boxes in the reference cell. The lattice translator converts
Figure 4.10: The image cells (outlined in red) introduce new TNN boxes (yellow) which must be treated using nearfield techniques such as MOM.

Figure 4.11: The TNN (orange) and NTNN (blue) of a corner reference box (green) for a scatterer with PBC.
outgoing waves to incoming waves from all cells except the reference cell. The difference between these two translators is shown in Figure 4.12.

Figure 4.12: In (a), the standard translation vector transfers the field directly from NTNN to a reference box. In (b), the lattice translator can only perform translations with respect to the lattice vector, so an additional disaggregation is required to transfer the field after it arrives at the reference cell to the reference box.

The lattice translator can only perform translations with respect to the lattice vector $R_n$. In order to transfer the field from the lattice cells to the reference box, the lattice translation operation is followed by disaggregation. Using this approach requires construction of aggregation/disaggregation vectors for NTNN. An alternative method is to aggregate the fields to $l = 0$ of the oct-tree. This is illustrated in Figure 4.13.

Figure 4.13: A method of using the lattice translator that uses aggregation to $l = 0$ instead of aggregation/disaggregation to NTNN at $l = 2$. 
4.3.3 Near and Far Lattice Neighbors

Near and far lattice neighbors is a new concept introduced in MLP-FMA. Like, TNN and NTNN, it separates cells which are near and far from the reference cell using similar criteria. This avoids violation of the first addition theorem, which is illustrated in Figure 4.14.

Figure 4.14: Image sources from adjacent cells can violate the first addition theorem. A simple example is shown in this figure. The circle around the image cell denotes the boundary of the region of convergence. The red arrow points to the source and the dotted red arrow points to its image. The green arrow indicates the observation point.

For a 2-D lattice, a reference cell has nine NLN (including itself). Since the lattice occupies the $x - y$ plane, one must take care not to include image cells in the $\hat{z}$ direction. In the ideal scenario, the NTNN of the NLN are chosen according to Figure 4.15. The NTNN of the NLN are shaded in blue and the TNN of the NLN are boxes shaded in orange.

Figure 4.15: For the given reference cell (green), the blue boxes represent NTNN boxes for the ideal case.

In practice, the boxes shaded in blue in Figure 4.15 are not the boxes we choose as NTNN because, for boxes that border the reference cell, we have
to account for special cases where some NTNN interactions apply to all nine NLN while some NTNN only apply to eight. An example of this is shown in Figure 4.16.

Figure 4.16: The white and red boxes are a set of NTNN whose centers all have the same vector offsets relative to the origin of their parent cell. There are nine red NTNN and only eight white NTNN. The number of NTNN depends on where the TNN of the reference cell are.

In our approach, NLN are treated at \( l = 2, \ldots, L - 1 \) of the tree using a combination of MOM and the ordinary ML-FMA translator. The ordinary ML-FMA translator is augmented by summing eight additional directions corresponding to the NLN surrounding the reference cell. The MOM interactions undergo similar modification. This is illustrated in Figure 4.17. By making this choice, we can always be certain that any interaction (TNN or NTNN) are applied to all nine lattice cells, which the algorithm from a coding perspective. This also requires that the Green’s function used for TNN be augmented by the eight additional lattice directions.
Figure 4.17: This figure shows which boxes among NLN are chosen as TNN and NTNN. The orange boxes denote TNN and the blue boxes denote NTNN. The green boxes are the reference box and its images, which are also classified as TNN.

Our approach for handling NLN differs from [4], [5]. In [4], aggregation/disaggregation is performed to $l = 0$. Level $l = 1$ facilitates communication between the reference cell and its NLN. This can be done by applying the rules for TNN and NTNN to $l = 1$, as shown in Figure 4.18.

Figure 4.18: TNN (orange) and NTNN (blue) at $l = 1$ corresponding to a particular reference box (green).

Shanker does not use the concept of NLN. Instead, both nearfield and farfield interactions are computed using Ewald summation. Following this
approach, the top level in the tree remains $l = 2$. Direct interactions using
MOM and far interactions using ACE are replicated over the entire lattice
through Ewald summation. This can be seen from Figure 4.19. The only
drawback to this method is that it uses Ewald summation for TNN interac-
tions, which we have noted to be extremely slow. While this method should
produce greater accuracy, it comes at the cost of evaluating many farfield
interactions directly.

Field contributions from FLN are accounted for using the lattice translator.
In our method, the lattice translator accounts for all image cells excluding
the reference cell. We have already accounted for eight of these cells in our
treatment of NLN. Therefore, we must explicitly subtract these directions
from the lattice translator to avoid repetition. The FLN are shown as purple
boxes in Figure 4.20.

Figure 4.19: Ewald summation for both TNN (orange) and NTNN (blue)
interactions.
4.4 Results

To demonstrate the accuracy of MLP-FMA, we compare matrices generated by MOM and MLP-FMA. The MOM matrix is generated using Ewald summation for all $N^2$ interactions and is considered the exact solution. Since MLP-FMA does not store the full matrix, the MLP-FMA matrix is generated column-by-column using the matrix-vector product operation of MLP-FMA. The entries of these two matrices are compared for both EFIE and MFIE for the PEC case.

The geometry being modeled is a sphere with radius $r = 1$ m and $N = 924$ unknowns. The incident field is a plane wave with $\lambda = 2$, $k = \hat{z}2\pi/\lambda$, and $\mathbf{E}_0 = \hat{x}$. The number of levels used in MLP-FMA is three with the number of active levels being zero and two, inclusive. Figure 4.21 shows the relative error of a MVP. Given that vector resulting from MVP by MOM and MLP-FMA are $\mathbf{v}$ and $\tilde{\mathbf{v}}$ respectively, relative error (per element) is defined as

$$[E]_n = \frac{|[v]_n - [\tilde{v}]_n|}{\max_n\{|[v]_n|\}}.$$  

(4.31)

A similar definition can be used for matrices. Let $\mathbf{Z}$ represent the MOM
matrix and \( \bar{Z} \). The relative error matrix can be expressed as

\[
[E]_{i,j} = \frac{|[Z]_{i,j} - [\bar{Z}]_{i,j}|}{\max_{i,j} \{|[Z]_{i,j}|\}}.
\] (4.32)

Figure 4.21 shows the relative error for EFIE using MLP-FMA. A histogram of the elements in the error matrix is used to show the number of elements that fall within a certain relative error. As one can see, a majority of the matrix elements have a relative error less than \( 1 \times 10^{-4} \) which is very good.

To gauge the difference in computation time between ML-FMA and MLP-FMA, we present simulation times for a sphere with \( N = 2,352 \) for ML-FMA and MLP-FMA to show where the added costs are reflected. We expect MLP-FMA to spend more time in the pre-computation phase. The MLP-FMA should take roughly nine times as long to compute nearfield and O2I operators for NLN interactions. We did not use any interpolation methods to reduce the computation time of O2I translators [24]. Doing so would definitely reduce the pre-computation time. Additionally, no parallelization is enabled. The code is not written for speed so timing may be higher than what one may expect.

Table 4.1 compares the computation time between ML-FMA and MLP-FMA using the same mesh. The time required to compute the translation operators for MLP-FMA is more than 45 times more compared to ML-FMA. In this code, all possible translation directions are initialized per level. This means for ML-FMA, 316 directions are computed. For MLP-FMA, this number increases to 1,156. Additionally, each translator requires summing nine
Table 4.1: A comparison of timings between ML-FMA and MLP-FMA for $N = 2,352$.

<table>
<thead>
<tr>
<th></th>
<th>ML-FMA</th>
<th>MLP-FMA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Agg/Disaggregation</td>
<td>0.78s</td>
<td>0.76s</td>
</tr>
<tr>
<td>Translation</td>
<td>2.03s</td>
<td>89.8s</td>
</tr>
<tr>
<td>Nearfield</td>
<td>21.3s</td>
<td>116s</td>
</tr>
<tr>
<td>Matrix-Vector Product</td>
<td>0.0255s</td>
<td>0.0411s</td>
</tr>
</tbody>
</table>

translation directions. Therefore, the total number of translators that MLP-FMA needs to compute is 10,404 which is 33 times the number of translators required by ML-FMA. Some of the overhead is contributed by the computation of the lattice translator. In this simulation, the time taken to compute the lattice translator is ten seconds.
CHAPTER 5
CONCLUSION

Periodic structures have many uses in engineering applications but their design is often guided by intuition rather than precise engineering. This was also the case during the early days of antenna design. With the development of advanced electromagnetic solvers, antenna designs have not only improved but use of EM solvers has become an integral part of the design process. The same sort of impact can be had on the design of periodic structures.

In this thesis, we develop a fast multipole based method for computing scattering by 2-D periodic arrays. We call this method MLP-FMA, and it is used to accelerate the MOM solution for periodic structures, which uses PGF. Both periodic and aperiodic MOM have $O(N^2)$ storage complexity and require $O(N^3)$ to invert. However, the evaluation of PGF is much longer than FGF, leading to long matrix fill times. ML-FMA can reduce the storage complexity of an aperiodic problem to $O(N)$ and the cost of inversion to $O(\kappa N \log N)$ where $\kappa$ depends on the conditioning and number of unknowns. We show that ML-FMA can also be adapted to solve periodic MOM problems.

The main difference between MOM for aperiodic and periodic structures is the evaluation of PGF. The PGF can be thought of as the field due to a periodic distribution of sources. There exist numerous ways to express PGF mathematically. For numerical simulation, we try to find a representation for PGF which has a balance of speed, accuracy, and ease of implementation. We evaluate three representations for PGF (spatial, spectral, and Ewald) to get an idea of the convergence rate of each representation. Of these three, the Ewald representation performs the best. The Ewald representation converges exponentially and is much more accurate than spatial or spectral representations, making it the representation of choice for developing a fast method. Researchers have looked into other ways of factorizing PGF. Compared to [4], [5], our factorization is unique in that it uses spherical multipoles com-
combined with Ewald summation. The use of spherical multipoles aligns better with what researchers have done in the past. This enables existing ML-FMA codes to be easily augmented to solve periodic structures.

A computational bottleneck in the factorized form of PGF is the lattice constant, which arises naturally from performing a lattice sum over existing factorizations of FGF. Using Ewald summation, the lattice constant can be divided into three terms and evaluated with exponential convergence. The factorization of PGF and exponential evaluation of lattice constants brought us closer to a fast method. The remaining step was to determine how to perform MVP using the oct-tree. Like factorization, there is more than one way to perform the matrix-vector product. To handle image cells in the lattice, NLN and FLN are introduced. In our method, field contributions from NLN are determined using conventional ML-FMA while field contributions from FLN are accounted for using a lattice translator on level \( l = 0 \) of the tree. This approach ensures that every NTNN in the reference cell has eight mirror NTNN as opposed to other approaches that allow the number of mirror NTNN to vary, thereby requiring indexing of mirror NTNN. By using ML-FMA for NLN, our method never uses Ewald summation for direct interactions. This is one of the main differences between our method and that in [5]. Ewald summation is only used to compute the lattice translator, which affects the pre-computation phase. The cost to perform an MVP is still \( O(N \log N) \) and comparable to ML-FMA.

Aperiodic problems with thousands of unknowns can be solved in minutes using MOM. Periodic problems using the same geometry and number of unknowns extend the solution time to hours if not days. A problem with thousands of unknowns is usually considered a small problem. Therefore, the need for MLP-FMA is even greater when considering the amount of time spent to solve problems with a few thousand unknowns. In this thesis, we presented the factorizations for plane wave and multipole factorization of PGF using spherical harmonics. The key difference between factorization of FGF and PGF is the translation operator. The name lattice translator is used to distinguish between the two kinds of translation operators. For future work, we want to study periodic nanoparticle arrays using MLP-FMA. We also want to explore methods for coupling periodic structures with aperiodic structures.
REFERENCES


A.1 Spatial and Spectral Representations

From Section 2.2, the spatial PGF is

$$g_\Lambda(k, k, R) = \sum_{R_n \in \Lambda} \frac{e^{i k |R - R_n|}}{4 \pi |R - R_n|} e^{i k R_n}.$$  (A.1)

Using Equation (A.2)

$$\nabla \frac{e^{i k |R - R_n|}}{|R - R_n|} = (R_n - R)(1 - i k |R - R_n|) \frac{e^{i k |R - R_n|}}{|R - R_n|^3},$$  (A.2)

it can be shown that the spatial representation of $\nabla g_\Lambda(k, k, R)$ is

$$\nabla g_\Lambda(k, k, R) = -\frac{1}{4 \pi} \sum_{R_n \in \Lambda} e^{i k R_n} (R_n - R)(1 - i k |R - R_n|) \frac{e^{i k |R - R_n|}}{|R - R_n|^3}.$$  (A.3)

Similarly, the spectral representation of $\nabla g_\Lambda(k, k, R)$ can be found by direct application of $\nabla$ to (2.23). The spectral representation of $\nabla g_\Lambda(k, k, R)$ is

$$\nabla g_\Lambda(k, k, R) = -\frac{1}{8 \pi^2} \sum_{\mathbf{K} \in \Lambda^*} (\mathbf{k} + \mathbf{K}) \hat{\mathbf{z}} \text{sgn}(z - z') K_{\perp, l} e^{i (k_x + K_l) R_x + i K_{\perp, l} |z - z'|} \frac{e^{i (k_x + K_l) R_x + i K_{\perp, l} |z - z'|}}{K_{\perp, l}}.$$  (A.4)
A.2 Ewald Representation

From Section 2.4, the PGF can be expressed as

\[
g_{\Lambda}(k, k, R) = g_K(k, k, R) + g_R(k, k, R)
\]

where

\[
g_K(k, k, R) = \frac{i}{4A} \sum_{K_l \in \Lambda^*} \frac{e^{i(k_s + K_l) \cdot R_s}}{K_{\perp,l}} \sum_{\pm} e^{\pm iK_{\perp,l}|z - z'|} \text{erfc} \left( \frac{-iK_{\perp,l}}{2\eta} \mp |z - z'| \eta \right),
\]

\[
g_R(k, k, R) = \frac{1}{8\pi} \sum_{R_n \in \Lambda} \frac{e^{ikR_n}}{|R - R_n|} \sum_{\pm} e^{\pm i|k| |R - R_n|} \text{erfc} \left( |R - R_n| \eta \pm \frac{i k}{2\eta} \right).
\]

The gradient of PGF, \( \nabla g_{\Lambda}(k, k, R) \), can be found by direct application of the \( \nabla \) operator. To find \( \nabla g_K(k, k, R) \), let

\[
A^\pm = e^{i(k_s + K_l) \cdot R_s} \pm iK_{\perp,l} |z - z'| |z - z'| \eta,
\]

\[
B^\pm = \text{erfc} \left( -\frac{iK_{\perp,l}}{2\eta} \mp |z - z'| \eta \right),
\]

such that

\[
g_K(k, k, R) = \frac{i}{4A} \sum_{K_l \in \Lambda^*} \sum_{\pm} B^\pm A^\pm.
\]

Then, using the identity \( \nabla (AB) = A \nabla B + B \nabla A \), it can be shown that

\[
g_K(k, k, R) = \frac{i}{4A} \sum_{K_l \in \Lambda^*} \sum_{\pm} A^\pm \nabla B^\pm + B^\pm \nabla A^\pm,
\]

where

\[
\nabla A^\pm = i(k_s + K_l \pm \hat{z} K_{\perp,l}) A^\pm,
\]

\[
\nabla B^\pm = \pm \hat{z} \frac{2\eta}{\sqrt{\pi}} e^{-\left( \frac{-iK_{\perp,l} \mp (z - z') \eta}{2\eta} \right)^2}.
\]
Similarly, to find $\nabla g_R(k, k, R)$, let

$$C^\pm = \frac{e^{\pm ik|R-R_n|}}{|R-R_n|}, \quad (A.13)$$

$$D^\pm = \operatorname{erfc} \left( |R-R_n| \eta \pm \frac{i k}{2 \eta} \right), \quad (A.14)$$

such that

$$g_R(k, k, R) = \frac{1}{8\pi} \sum_{R_n \in \Lambda} e^{ikR_n} \sum_\pm C^\pm D^\pm. \quad (A.15)$$

Then,

$$\nabla g_R(k, k, R) = \frac{1}{8\pi} \sum_{R_n \in \Lambda} e^{ikR_n} \sum_\pm C^\pm \nabla D^\pm + D^\pm \nabla C^\pm, \quad (A.16)$$

where

$$\nabla C^\pm = - (R-R_n) \left( 1 \mp ik|R-R_n| \right) \frac{e^{\pm ik|R-R_n|}}{|R-R_n|^3}, \quad (A.17)$$

$$\nabla D^\pm = - \frac{R-R_n}{|R-R_n|} \frac{2\eta}{\sqrt{\pi}} e^{-\left( |R-R_n| \eta \pm \frac{i k}{2 \eta} \right)^2}. \quad (A.18)$$
APPENDIX B

EVALUATION OF LATTICE CONSTANTS WITH EWALD SUMMATION

B.1 Derivation of $\sigma_{l}^{m(0)}(k)$

$\sigma_{l}^{m(0)}(k)$ can be thought of as the regular contribution of the $\Lambda_{0}$ term. It is not a function of $k$ because it has no lattice phase. Using

$$\int Y_{L}(\hat{R}) \, d\Omega = \sqrt{4\pi} \delta_{L0}, \quad (B.1)$$

along with the fact that $g_{0}(k, R)$ and the integral term are independent of $\Omega$, $\sigma_{l}^{m(0)}(k)$ can be expressed as

$$\sigma_{l}^{m(0)}(k) = \lim_{R \to 0} \frac{(ik)^{-1}}{j_{l}(kR)} \int Y_{L}^{*}(\hat{R}) \times \left( \frac{1}{2\pi \sqrt{\pi}} \int_{\eta}^{\infty} e^{-R^{2}\xi^{2} + \frac{k^{2}}{4\xi^{2}}} \, d\xi - g_{0}(k, R) \right) \, d\Omega, \quad (B.2)$$

$$= \lim_{R \to 0} \frac{\delta_{L0} \sqrt{4\pi}}{ik j_{l}(kR)} \left( \frac{1}{2\pi \sqrt{\pi}} \int_{\eta}^{\infty} e^{-R^{2}\xi^{2} + \frac{k^{2}}{4\xi^{2}}} \, d\xi - g_{0}(k, R) \right). \quad (B.3)$$

The integral term can be evaluated using a Taylor series expansion. Let

$$e^{\frac{k^{2}}{4\xi^{2}}} = \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{k}{2} \right)^{2j} \xi^{-2j}, \quad (B.4)$$
such that

$$\frac{1}{2\pi \sqrt{\pi}} \int_{\eta}^{\infty} e^{-R^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi, \quad (B.5)$$

$$= \frac{1}{2\pi \sqrt{\pi}} \int_{\eta}^{\infty} e^{-R^2 \xi^2} \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{k}{2} \right)^{2j} \xi^{-2j} d\xi, \quad (B.6)$$

$$= \frac{1}{2\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{k}{2} \right)^{2j} \int_{\eta}^{\infty} e^{-R^2 \xi^2} \xi^{-2j} d\xi. \quad (B.7)$$

Let \( t = R^2 \xi^2 \) and \( dt = 2R^2 \xi d\xi \). Equation (B.7) becomes

$$\frac{k}{8\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{kR^2}{2} \right)^{2j-1} \int_{R^2 \eta^2}^{\infty} e^{-t} t^{-j-\frac{1}{2}} dt. \quad (B.8)$$

Using integration by parts,

$$u = e^{-t}, \quad v = \frac{2t^{-j+\frac{1}{2}}}{1-2j}, \quad du = -e^{-t} dt, \quad dv = t^{-j-\frac{1}{2}} dt \quad (B.9)$$

$$\int_{R^2 \eta^2}^{\infty} e^{-t} t^{-j-\frac{1}{2}} dt = \left. \frac{2t^{-j+\frac{1}{2}} e^{-t}}{1-2j} \right|_{R^2 \eta^2}^{\infty} + \frac{2}{1-2j} \int_{R^2 \eta^2}^{\infty} t^{-j+\frac{1}{2}} e^{-t} dt, \quad (B.10)$$

$$= -\frac{2(R\eta)^{-2j+1} e^{-R^2 \eta^2}}{1-2j} + \frac{2}{1-2j} \int_{R^2 \eta^2}^{\infty} t^{-j+\frac{1}{2}} e^{-t} dt, \quad (B.11)$$

we obtain two terms. The first term is the one we want to keep. This term can be written as

$$-\lim_{R \to 0} \frac{k}{8\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{kR^2}{2} \right)^{2j-1} \frac{2(R\eta)^{-2j+1} e^{-R^2 \eta^2}}{1-2j}, \quad (B.12)$$

which simplifies to

$$= -\lim_{R \to 0} \frac{k}{4\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!} \left( \frac{k}{2\eta} \right)^{2j-1} e^{-R^2 \eta^2} \frac{1}{1-2j}, \quad (B.13)$$

$$= -\frac{k}{4\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!(1-2j)} \left( \frac{k}{2\eta} \right)^{2j-1}. \quad (B.14)$$
The second term cancels out with the singularity in $g_0(k, R)$. The second term is

\[
\lim_{R \to 0} \frac{k}{4\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!(1 - 2j)} \left( \frac{kR}{2} \right)^{2j-1} \int_{R^2 \eta^2}^{\infty} t^{-j + \frac{1}{2}} e^{-t} dt. \quad (B.15)
\]

For $j > 0$, the summand is zero when $R \to 0$. Hence, we only need to consider the $j = 0$ term. This term can be reduced to an upper incomplete gamma function, as shown below:

\[
\lim_{R \to 0} \frac{k}{4\pi \sqrt{\pi}} \left( \frac{kR}{2} \right)^{-1} \int_{R^2 \eta^2}^{\infty} t^{\frac{1}{2}} e^{-t} dt, \quad (B.16)
\]

\[
= \lim_{R \to 0} \frac{1}{2R \pi \sqrt{\pi}} \int_{R^2 \eta^2}^{\infty} t^{\frac{1}{2}} e^{-t} dt, \quad (B.17)
\]

\[
= \lim_{R \to 0} \frac{1}{2R \pi \sqrt{\pi}} \Gamma \left( \frac{3}{2}, R^2 \eta^2 \right). \quad (B.18)
\]

Using the identity

\[
b\Gamma(b, x) = \Gamma(b + 1, x) - x^b e^{-x}, \quad (B.19)
\]

equation (B.18) can be written as

\[
\lim_{R \to 0} \frac{1}{4R \pi \sqrt{\pi}} \left( \frac{1}{2} \Gamma \left( \frac{1}{2}, R^2 \eta^2 \right) + \left( \frac{1}{2} R^2 \eta^2 \right)^{\frac{1}{2}} e^{-R^2 \eta^2} \right), \quad (B.20)
\]

\[
= \frac{\eta}{2\pi \sqrt{\pi}} + \frac{1}{4R \pi \sqrt{\pi}} \lim_{R \to 0} \int_{R^2 \eta^2}^{\infty} t^{-\frac{1}{2}} e^{-t} dt. \quad (B.21)
\]

Let $dx = t^{-1/2} dt$ such that

\[
\frac{\eta}{2\pi \sqrt{\pi}} + \lim_{R \to 0} \frac{1}{4\pi \sqrt{\pi}} \int_{2R \eta}^{\infty} e^{-\frac{x^2}{4}} dx, \quad (B.22)
\]

followed by another change of variables, $y^2 = x^2/4$ and $dy = dx/2$. Then,

\[
\frac{\eta}{2\pi \sqrt{\pi}} + \lim_{R \to 0} \frac{1}{2\pi \sqrt{\pi}} \int_{R \eta}^{\infty} e^{-y^2} dy. \quad (B.23)
\]
Equation (B.23) can be written as a complementary error function

\[
\frac{\eta}{2\pi \sqrt{\pi}} + \lim_{R \to 0} \frac{1}{4\pi R} \text{erfc}(R\eta), \quad (B.24)
\]

which has a Taylor series expansion of the form

\[
\text{erfc}(z) = 1 - \frac{2z}{\sqrt{\pi}} + \mathcal{O}(z^2). \quad (B.25)
\]

Replacing the complementary error function with its Taylor series expansion, (B.24) becomes

\[
\frac{\eta}{2\pi \sqrt{\pi}} + \lim_{R \to 0} \frac{1}{4\pi R} \left( 1 - \frac{2R\eta}{\sqrt{\pi}} + \mathcal{O}(R^2\eta^2) \right), \quad (B.26)
\]

\[
= \frac{\eta}{2\pi \sqrt{\pi}} + \lim_{R \to 0} \frac{1}{4\pi R} - \frac{\eta}{2\pi \sqrt{\pi}}. \quad (B.27)
\]

\[
= \lim_{R \to 0} \frac{1}{4\pi R}. \quad (B.28)
\]

The remaining term given by (B.28) is the singularity term we are looking for to cancel out the singularity in \(g_0(k, R)\). That is,

\[
- \lim_{R \to 0} \left( \frac{e^{ikR} - 1}{4\pi R} \right) = - \frac{ik}{4\pi}. \quad (B.29)
\]

Gathering the results from (B.18) and (B.29), we obtain

\[
\sigma_{l}^{m(0)}(k) = \delta_{L0} \frac{\sqrt{4\pi}}{ik} \left( - \frac{ik}{4\pi} - \frac{k}{4\pi \sqrt{\pi}} \sum_{j=0}^{\infty} \frac{1}{j!(1-2j)} \left( \frac{k}{2\eta} \right)^{2j-1} \right), \quad (B.30)
\]

where we have used the fact that \(\delta_{L0} \lim_{R \to 0} j_l(kR) = \delta_{L0}\). Finally, we can write

\[
\sigma_{l}^{m(0)}(k) = \delta_{L0} \left( - \frac{1}{2\sqrt{\pi}} + \frac{i}{2\pi} \sum_{j=0}^{\infty} \frac{1}{j!(1-2j)} \left( \frac{k}{2\eta} \right)^{2j-1} \right), \quad (B.31)
\]

which is the desired form of \(\sigma_{l}^{m(0)}(k)\).
B.2 Derivation of $\sigma_m^{(1)}(k, k)$

$\sigma_m^{(1)}(k, k)$ is the term which contains the reciprocal lattice contribution to the field. It can be expressed as

$$\sigma_m^{(1)}(k, k) = \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint g_K(k, k) R Y_L^*(\hat{R}) \, d\Omega$$

(B.32)

$$= \frac{A^{-1}}{2\sqrt{\pi}} \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint \sum_{K_l \in \Lambda^*} e^{i(k_s + K_l) \cdot R_s} Y_L^*(\hat{R}),$$

$$\times \int_{1/\eta}^{\infty} e^{-s^2 \left( \frac{(k_s + K_l) \cdot (k_s + K_l)}{4} - \frac{k^2}{4} \right) - \frac{|z - z'|^2}{s^2}} \, ds \, d\Omega. \quad \text{(B.33)}$$

Similar to the derivation of $\sigma_m^{(0)}(k)$, Taylor series is used to expand

$$e^{-|z - z'|^2 / s^2} = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \left( \frac{|z - z'|}{s} \right)^{2n}, \quad \text{(B.34)}$$

which permits us to write

$$\sigma_m^{(1)}(k, k) = \frac{A^{-1}}{2\sqrt{\pi}} \lim_{R \to 0} \frac{(ik)^{-1}}{j_l(kR)} \oint \sum_{K_l \in \Lambda^*} e^{i(k_s + K_l) \cdot R_s} Y_L^*(\hat{R})$$

$$\times \int_{1/\eta}^{\infty} e^{-s^2 \left( \frac{(k_s + K_l) \cdot (k_s + K_l)}{4} - \frac{k^2}{4} \right) - \frac{|z - z'|^2}{s^2}} \, ds \, d\Omega. \quad \text{(B.35)}$$

Expanding $Y_L^*(\hat{R})$ as

$$Y_L^*(\hat{R}) = i^{m - |m|} N_l^{m|} P_l^{m|} (\cos \theta) e^{-im\phi}, \quad \text{(B.36)}$$

$$N_l^{m|} = \sqrt{\frac{2|l| + 1 (l - m)!}{4\pi (l + m)!}}, \quad \text{(B.37)}$$

and letting $|z - z'| = R|\cos \theta|$, $R_s = \hat{x}R \sin \theta \cos \phi + \hat{y}R \sin \theta \sin \phi$, and $k_s + K_l = |k_s + K_l|((\hat{x} \cos \phi_{k_s + K_l} + \hat{y} \sin \phi_{k_s + K_l})$ such that

$$(k_s + K_l) \cdot R_s = R|k_s + K_l| \sin \theta \cos(\phi_{k_s + K_l} - \phi), \quad \text{(B.38)}$$

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gives us
\[
\sigma_{l}^{m(1)}(k, k) = \frac{i^{m-|m|}}{2^{\pm}} \frac{N_{l}^{|m|}}{2 \sqrt{\pi}} \sum_{K \in A^{*}} \sum_{n=0}^{\infty} \frac{(-1)^{n}}{n!} \sum_{l=1}^{A} \frac{R^{2n}}{j_{l}(kR)}
\]
\[
\times \left\{ \int e^{iR|k_{s} + K|} \sin \theta \cos(\phi_{k_{s} + K} - \phi) - i m \phi P_{l}^{m}(\cos \theta)(\cos \theta)^{2n} d\Omega \right. \\
\times \left. \int_{1/\eta}^{\infty} s^{-2n} e^{-s^{2} \left( \frac{(k_{s} + K_{2})(k_{s} + K_{2})}{4} - \frac{\ell^{2}}{\pi} \right)} ds \right\}.
\]  

Denoting the integrals with respect to \(s\) and \(\Omega\) as
\[
I_{\Omega, n} = \int e^{iR|k_{s} + K|} \sin \theta \cos(\phi_{k_{s} + K} - \phi) - i m \phi P_{l}^{m}(\cos \theta)(\cos \theta)^{2n} d\Omega, 
\]
\[
I_{s, n} = \int_{1/\eta}^{\infty} s^{-2n} e^{-s^{2} \left( \frac{(k_{s} + K_{2})(k_{s} + K_{2})}{4} - \frac{\ell^{2}}{\pi} \right)} ds, 
\]

such that
\[
\sigma_{l}^{m(1)}(k, k) = \frac{i^{m-|m|}}{2^{\pm}} \frac{N_{l}^{|m|}}{2 \sqrt{\pi}} \sum_{K \in A^{*}} \sum_{n=0}^{\infty} \frac{(-1)^{n}}{n!} I_{s, n} \lim_{R \to 0} \frac{R^{2n}}{j_{l}(kR)} I_{\Omega, n}, 
\]

it can be seen that \(I_{s, n}\) has the form of a Gaussian which is exponentially convergent and can be converted into a sum of upper incomplete gamma functions. An upper incomplete gamma function is defined as
\[
\Gamma(s, z) = \int_{z}^{\infty} t^{s-1} e^{-t} dt, \quad \text{(Upper Incomplete Gamma)}.
\]

Equation (B.41) can be written as
\[
I_{s, n} = \int_{1/\eta}^{\infty} s^{-2n} e^{-s^{2} \left( \frac{(k_{s} + K_{2})(k_{s} + K_{2})}{4} \right)} ds. 
\]
Let \( t = s^2(iK_{\perp,l})^2/4 \) and \( dt = s(iK_{\perp,l})^2/2 \, ds \). Equation (B.44) becomes

\[
I_{s,n} = \frac{1}{iK_{\perp,l}} \int_{-\infty}^{-\infty} \left( \frac{2t^{1/2}}{iK_{\perp,l}} \right)^{-2n} e^{-t - 1/2} \, dt, \quad (B.45)
\]

\[
= \frac{1}{iK_{\perp,l}} \left( \frac{2}{iK_{\perp,l}} \right)^{-2n} \int_{-\infty}^{-\infty} e^{-t - 1/2 - n} \, dt, \quad (B.46)
\]

\[
= \frac{1}{iK_{\perp,l}} \left( \frac{iK_{\perp,l}}{2} \right)^{2n} \Gamma \left( -n + 1/2, -\frac{K_{\perp,l}^2}{4\eta^2} \right). \quad (B.47)
\]

Alternatively, let

\[
I_{s,n} = \int_{1/\eta}^{\infty} s^{-2n} e^{s^2 K_{\perp,l}^2/4} \, ds \quad (B.48)
\]

and let \( t = -\frac{s^2 K_{\perp,l}^2}{4} \) and \( dt = -\frac{s K_{\perp,l}^2}{2} \, ds \). Then,

\[
I_{s,n} = -\int_{\frac{-\kappa_{\perp,l}^2}{\eta^2}}^{\infty} s^{-2n} e^{-4t K_{\perp,l}^2} \frac{2}{s K_{\perp,l}^2} \, dt, \quad (B.49)
\]

\[
= -\int_{\frac{-\kappa_{\perp,l}^2}{\eta^2}}^{\infty} \left( -4t K_{\perp,l}^2 \right)^{-n} e^{-t} \frac{2}{s K_{\perp,l}^2} \, dt, \quad (B.50)
\]

\[
= -\int_{\frac{-\kappa_{\perp,l}^2}{\eta^2}}^{\infty} \left( -4t K_{\perp,l}^2 \right)^{-n} \frac{1}{s K_{\perp,l}^2} \, dt, \quad (B.51)
\]

\[
= -\frac{2}{K_{\perp,l}^2} \left( -4 K_{\perp,l}^2 \right)^{-n} \sqrt{-K_{\perp,l}^2/4} \int_{\frac{-\kappa_{\perp,l}^2}{\eta^2}}^{\infty} t^{-n-1/2} e^{-t} \, dt, \quad (B.52)
\]

\[
= -i \left( \frac{-1}{2^{2n}} \right) (K_{\perp,l}^2)^{n-1/2} \int_{\frac{-\kappa_{\perp,l}^2}{\eta^2}}^{\infty} t^{-n-1/2} e^{-t} \, dt. \quad (B.53)
\]

Equations (B.47) and (B.53) both contain gamma functions which depend on \( n \). One can also express \( I_{s,n} \) in terms of a complementary error function that is independent of \( n \). This reduces the number of special function evaluations from \( (l - |m|)/2 \) to 1. In addition, finding a software library that computes \( \text{erfc}(z) \) for complex arguments is easier than finding a library that computes \( \Gamma(s, z) \) for complex \( s \) and \( z \). The representation we choose for \( I_{s,n} \) is

\[
I_{s,n} = \frac{i\sqrt{\pi}}{K_{\perp,l}} \text{erfc} \left( \frac{-iK_{\perp,l}}{2\eta} \right). \quad (B.54)
\]
To evaluate $I_{\Omega,n}$ in closed form, $I_{\Omega,n}$ can be written as

$$I_{\Omega,n} = \int e^{iR|k_s + K_l| \sin \theta \cos (\phi_{k_s + K_l} - \phi) - im\phi} P^{|m|}_l(\cos \theta)(\cos \theta)^{2n} d\Omega. \quad (B.55)$$

Letting $d\Omega = \sin \theta d\theta d\phi$, equation (B.55) becomes

$$I_{\Omega,n} = \int_0^{2\pi} \int_0^\pi e^{iR|k_s + K_l| \sin \theta \cos (\phi_{k_s + K_l} - \phi) - im\phi} P^{|m|}_l(\cos \theta)(\cos \theta)^{2n} \sin \theta d\theta d\phi, \quad (B.56)$$

$$= \int_0^\pi P^{|m|}_l(\cos \theta)(\cos \theta)^{2n} \sin \theta \int_0^{2\pi} e^{iR|k_s + K_l| \sin \theta \cos (\phi_{k_s + K_l} - \phi) - im\phi} d\phi \, d\theta, \quad (B.57)$$

$$= 2\pi i^{|m|} e^{-im\phi_{k_s + K_l}} \int_0^\pi P^{|m|}_l(\cos \theta)(\cos \theta)^{2n} \sin \theta J^{|m|}_m(R|k_s + K_l| \sin \theta) \, d\theta, \quad (B.58)$$

where (B.58) uses the integral representation of cylindrical Bessel function:

$$\int_0^{2\pi} e^{-im\phi + iz \cos (\phi_0 - \phi)} \, d\phi = 2\pi i^{|m|} e^{-im\phi_0} J^{|m|}_m(z). \quad (B.59)$$

Using the Taylor series expansion of Bessel function,

$$J^{|m|}_m(z) = \left(\frac{z}{2}\right)^{|m|} \sum_{j=0}^{\infty} \frac{(-z^2/4)^j}{j!(|m| + j)!}, \quad (B.60)$$

equation (B.58) becomes

$$I_{\Omega,n} = 2\pi i^{|m|} e^{-im\phi_{k_s + K_l}} \int_0^\pi P^{|m|}_l(\cos \theta)(\cos \theta)^{2n} \sin \theta \left(\frac{R|k_s + K_l| \sin \theta}{2}\right)^{|m|}$$

$$\times \sum_{j=0}^{\infty} \frac{(-R|k_s + K_l| \sin \theta)^2/4)^j}{j!(|m| + j)!} \, d\theta, \quad (B.61)$$

which can be re-arranged into

$$I_{\Omega,n} = 2\pi i^{|m|} e^{-im\phi_{k_s + K_l}} \sum_{j=0}^{\infty} \frac{(-1)^j(R|k_s + K_l|)^{2j+|m|}}{2^{|m|+2j}j!(|m| + j)!} I_{\theta,j}, \quad (B.62)$$

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where
\[
I_{\theta,j} = \int_0^\pi P_l^{|m|}(\cos \theta)(\cos \theta)^{2n} \sin \theta^{2j+|m|+1} d\theta, \quad \text{(B.63)}
\]
\[
= \int_{-1}^1 x^{2n}(1-x^2)^{j+|m|/2} P_l^{|m|}(x) dx. \quad \text{(B.64)}
\]

Using integration by parts, it can be shown that \(I_{\theta,j} = 0\) for odd \(l - |m|\). For even \(l - |m|\), it can be shown that
\[
\lim_{R \to 0} \frac{R^{2n} I_{\Omega,n}}{j_l(kR)} = 0, \quad j + n > \frac{l - |m|}{2}. \quad \text{(B.65)}
\]

That is, non-zero contributions to the sum occur when
\[
j + n \leq \frac{l - |m|}{2}. \quad \text{(B.66)}
\]

Additionally, using the binomial theorem to expand the term
\[
(1 - x^2)^j = \sum_{s=0}^{j} (-1)^s \binom{j}{s} x^{2s}, \quad \text{(B.67)}
\]
in (B.64) results in
\[
I_{\theta,j} = \sum_{s=0}^{j} (-1)^s \binom{j}{s} \int_{-1}^1 x^{2n+2s}(1-x^2)^{|m|/2} P_l^{|m|}(x) dx, \quad \text{(B.68)}
\]
from which it can be shown that non-zero contributions occur when
\[
n + s \geq \frac{l - |m|}{2}. \quad \text{(B.69)}
\]

From (B.67), \(s \in [0, j]\). Therefore, the only way to satisfy (B.66) and (B.69) simultaneously is when
\[
s = j, \quad \text{(B.70)}
\]
\[
n + j = \frac{l - |m|}{2}. \quad \text{(B.71)}
\]
The condition in (B.70) lets us evaluate $I_{\theta,j}$ in closed form. The resultant expression is

$$I_{\theta,j} = (-1)^{j+|m|} \frac{2^{l+1}!(l+|m|)!}{(2l+1)!}. \quad (B.72)$$

The condition in (B.71) implies that $n \leq \frac{l-|m|}{2}$. This is due to the fact that $j, n \geq 0$. The minimum value of $j$ is zero, which means the maximum value of $n$ is $\frac{l-|m|}{2}$. By letting $j = \frac{l-|m|}{2} - n$, the sum over $n$ and $j$ can now be written as just a sum over $n$. Equation (B.62) reduces to

$$I_{\Omega,n} = 2\pi i^{l-|m|} e^{-im\phi_{k_s+k_l}} (R|k_s + K_l|/2)^{l-2n} \frac{2^{l+1}!(l+|m|)!}{(2l+1)!}. \quad (B.73)$$

In the limiting case as $R \to 0$,

$$j_l(kR) = \frac{2l!}{(2l+1)!} (kR)^l \quad (R \to 0). \quad (B.74)$$

Using this fact, it can be shown that

$$\lim_{R \to 0} \frac{R^{2n}}{j_l(kR)} I_{\Omega,n} = \frac{4\pi i^{l-|m|} e^{-im\phi_{k_s+k_l}(l+|m|)!(|k_s + K_l|/2)^{l-2n}}}{k^l ((l-|m|)/2 - n)!((l+|m|)/2 - n)!}. \quad (B.75)$$

Inserting (B.54) and (B.75) into (B.42), $\sigma^{m(1)}_t$ can be expressed as

$$\sigma^{m(1)}_t(k, k) = \frac{i^{m-|m|}}{ik} N_l^{m+1} A^{-1} 2\sqrt{\pi} \sum_{K_l \in \Lambda^*} \sum_{n=0}^{l-|m|} i\sqrt{\pi} \frac{K_{\perp,l}}{2\eta} \text{erfc} \left( \frac{-iK_{\perp,l}}{2\eta} \right)$$

$$\times 4\pi \frac{i^{-|m|}}{k^l} e^{-im\phi_{k_s+k_l}} \frac{(-1)^n (l+|m|)!(|k_s + K_l|/2)^{l-2n}}{n!((l-|m|)/2 - n)!((l+|m|)/2 - n)!}, \quad (B.76)$$

which can be reduced to

$$\sigma^{m(1)}_t(k, k) = \frac{i^{m-2|m|}}{Ak^{l+1}} \sqrt{\pi} (2l+1)(l+|m|)! (l-|m|)!$$

$$\times \sum_{K_l \in \Lambda^*} \frac{e^{-im\phi_{k_s+k_l}}}{K_{\perp,l}} \text{erfc} \left( \frac{-iK_{\perp,l}}{2\eta} \right)$$

$$\times \sum_{n=0}^{l-|m|} \frac{(-1)^n (|k_s + K_l|/2)^{l-2n}}{n!((l-|m|)/2 - n)!((l+|m|)/2 - n)!}. \quad (B.77)$$
B.3 Derivation of $\sigma^m_\ell (2)(k, k)$

$\sigma^m_\ell (2)(k, k)$ encapsulates the field contribution from the regular spatial lattice term $\tilde{g}_R(k, k, R)$. Starting from

$$
\sigma^m_\ell (2)(k, k) = \frac{(ik)^{-1}}{2\pi \sqrt{\pi}} \lim_{R \to 0} \frac{1}{j_1(kR)} \int_\Lambda \sum_{R_n \in \Lambda} e^{i\mathbf{k} \cdot \mathbf{R}_n} 
\times \int_\eta e^{-|\mathbf{R} - \mathbf{R}_n|^2 + \frac{k^2}{4\xi^2} Y_L^*(\hat{R})} d\Omega, \quad (B.78)
$$

spherical harmonics can be used to expand the exponential term. Given that

$$
e^{i \mathbf{k} \cdot \mathbf{r}} = 4\pi \sum_L i^L j_1(kr) Y_L(\theta_r, \phi_r) Y_L^*(\theta_k, \phi_k), \quad (B.79)
$$

we can write

$$
e^{-|\mathbf{R} - \mathbf{R}_n|^2 \xi^2} = e^{-(R^2 + R_n^2)\xi^2} e^{2\xi^2 \mathbf{R} \cdot \mathbf{R}_n}, \quad (B.80)
$$

$$
= 4\pi e^{-(R^2 + R_n^2)\xi^2} \sum_L i^L j_1(-i2\xi^2 R_n R) Y_L^*(\hat{R}_n) Y_L(\hat{R}). \quad (B.81)
$$

This results in

$$
\sigma^m_\ell (2)(k, k) = \frac{2}{ik \sqrt{\pi}} \lim_{R \to 0} \frac{1}{j_1(kR)} 
\times \sum_{R_n \in \Lambda/\Lambda_0} e^{i\mathbf{k} \cdot \mathbf{R}_n} \int_\eta e^{-(R^2 + R_n^2)\xi^2 + \frac{k^2}{4\xi^2} j_1(-i2\xi^2 R_n R)} 
\times \sum_L i^L Y_L^*(\hat{R}_n) \int Y_{L'}(\hat{R}) Y_L^*(\hat{R}) d\Omega d\xi, \quad (B.82)
$$

$$
= \frac{2}{\sqrt{\pi}} \lim_{R \to 0} \sum_{R_n \in \Lambda/\Lambda_0} i^L Y_L^*(\hat{R}_n) e^{i\mathbf{k} \cdot \mathbf{R}_n} 
\times \int_\eta e^{-(R^2 + R_n^2)\xi^2 + \frac{k^2}{4\xi^2} j_1(-i2\xi^2 R_n R)} j_1(kR) d\xi. \quad (B.83)
$$

Taking the limit as $R \to 0$ and using

$$
\lim_{R \to 0} \frac{j_1(aR)}{j_1(bR)} = \frac{a^l}{b^l}, \quad (B.84)
$$

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equation (B.83) becomes

\[
\sigma_{l}^{m(2)}(k, k) = \frac{2^{l+1}(-1)^{l}i^{2l-1}}{k^{l+1} \sqrt{\pi}} \sum_{\hat{R}_{n} \in \Lambda / \Lambda_{0}} R_{n}^{l} Y_{L}^{*}(\hat{R}_{n}) e^{ik \hat{R}_{n}} \int_{\eta}^{\infty} e^{-R_{n}^{2} \xi^{2} + \frac{k^{2}}{4\eta^{2}} \xi^{2l}} d\xi.
\]  

(B.85)

Which can be re-written as

\[
\sigma_{l}^{m(2)}(k, k) = \frac{2^{l+1}}{ik^{l+1} \sqrt{\pi}} \sum_{\hat{R}_{n} \in \Lambda / \Lambda_{0}} R_{n}^{l} Y_{L}^{*}(\hat{R}_{n}) e^{ik \hat{R}_{n}} \int_{\eta}^{\infty} e^{-R_{n}^{2} \xi^{2} + \frac{k^{2}}{4\eta^{2}} \xi^{2l}} d\xi. \quad (B.86)
\]

Using the fact that

\[
\int_{\eta}^{\infty} e^{-R_{n}^{2} \xi^{2} + \frac{k^{2}}{4\eta^{2}} \xi^{2l}} d\xi = \frac{\sqrt{\pi}}{4R_{n}} \sum_{\pm} e^{\pm ikR_{n}} \text{erfc} \left( R_{n} \eta \pm \frac{iK}{2\eta} \right), \quad (B.87)
\]

equation (B.86) simplifies to

\[
\sigma_{l}^{m(2)}(k, k) = \frac{2^{l-1}}{ik^{l+1}} \sum_{\hat{R}_{n} \in \Lambda / \Lambda_{0}} R_{n}^{l-1} Y_{L}^{*}(\hat{R}_{n}) e^{ik \hat{R}_{n}} \sum_{\pm} e^{\pm ikR_{n}} \text{erfc} \left( R_{n} \eta \pm \frac{iK}{2\eta} \right). \quad (B.88)
\]

Alternatively, the integral in (B.86) can be evaluated directly using Gaussian quadrature or by converting the integral into a sum of upper incomplete gamma functions.