EXponential Convergence for Multipole and Local Expansions and their Translations for Sources in Layered Media: Three-Dimensional Laplace Equation

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Abstract. In this paper, we prove the exponential convergence of the multipole and local expansions, shifting and translation operators used in fast multipole methods (FMMs) for 3-dimensional Laplace equations in layered media. These theoretical results ensure the exponential convergence of the FMM which has been shown by the numerical results recently reported in [9]. As the free space components are calculated by the classic FMM, this paper will focus on the analysis for the reaction components of the Green’s function for the Laplace equation in layered media. We first prove that the density functions in the integral representations of the reaction components are analytic and bounded in the right half complex plane. Then, using the Cagniard-de Hoop transform and contour deformations, estimate for the remainder terms of the truncated expansions is given, and, as a result, the exponential convergence for the expansions and translation operators is proven.

1. Introduction

The well-known fast multipole method (FMM) proposed by Greengard and Rokhlin [4, 5] for particles in free spaces has been a revolutionary development for scientific and engineering computing. The algorithm was based on low rank approximations for the far field of sources, which are obtained by using truncated multipole expansions (MEs) and local expansions (LEs) with a truncation number $p$. The capability of using a small number $p$ to achieve high accuracy is due to the exponential convergence of the MEs and LEs, as well as the shifting and translation operators for multipole to multipole (M2M), local to local (L2L), and multipole to local (M2L) conversions. Recently, we have extended the FMMs of the Helmholtz, Laplace and Poisson-Boltzmann equations from free space to layered media (cf. [10, 12, 9, 11]). The new FMMs significantly enlarge the application area of the classic ones. Many important applications, e.g. parasitic parameter extraction of very large-scale integrated (VLSI) circuits [8, 13], complex scattering problem in meta-materials [1], electrical potential computation in ion channel simulation [7], etc, can be solved more efficiently and accurately by using the FMMs for layered media.

The mathematical proof for the exponential convergence of the MEs and LEs and the corresponding translation operators is one of the key issues in developing FMMs for the aforementioned equations in layered media. As the reaction components of the Green’s functions in layered media do not have a closed form in the physical space, Sommerfeld-type integral representations and extended Funk-Hecke formula are used to derive the MEs, LEs and translation operators for the FMMs mentioned above. The distinct feature of the expansions and translation operators for reaction components is that they involve Sommerfeld-type integrals with integrands depending on the layered structure of the media. Hence, the main difficulty in the convergence analysis is how to give a delicate estimate on the Sommerfeld-type integrals. Recently, we have proved the exponential convergence for the 2-dimensional Helmholtz equation case [12] and numerically showed that the MEs in 3-dimensional cases also have exponential convergence similarly as in 2-dimensional cases. However, the theoretical...
proof for 3-dimensional cases are much more involved technically due to the double improper integrals induced by the 2-dimensional inverse Fourier transform used in the derivation of the 3-dimensional layered Green’s function while only 1-dimensional inverse Fourier transform is needed in 2-dimensional cases.

In this paper, we will continue our previous work on 2-D Helmholtz equation \[12\] and prove the exponential convergence of the MEs, LEs and corresponding translation operators for the Green’s function of 3-dimensional Laplace equation in layered media. First, we consider the direct MEs for reaction components. We prove that they have exponential convergence but with convergence rates depend on polarization distances as defined in \[10\] and then used by \[9, 11\]. Therefore, the concept of equivalent polarization sources is crucial for the development of the FMMs for reaction components. By introducing the equivalent polarization sources, the reaction components have been reformulated and the MEs, LEs and translation operators are re-derived according to the new formulations. In this paper, we further give theoretical proof for their exponential convergence and show that the convergence rates are determined by the Euclidean distance between the targets and corresponding equivalent polarization sources. As a result, we validate the idea of using the re-derived MEs, LEs and translation operators with equivalent polarization sources in the FMMs for the reaction components. All theoretical results proved in this paper show that the FMM for Laplace equation in layered media developed in \[9\] is a highly accurate and error controllable algorithm as same as the free space FMM.

The rest of the paper is organized as follows. In section 2, we review the integral representation of the Green’s function of Laplace equation in layered media and a recursive algorithm for a stable and efficient calculation of the reaction densities of general multi-layered media. Based on the recursive formulas, we prove that the reaction densities are bounded and analytic in the right half complex plane, which is important for the estimate of the Sommerfeld-type integrals. Section 3 will review the derivation of MEs, LEs, shifting and translation operators for layered Green’s function. In section 4, we first review the exponential convergence of the ME, LE, shifting and translation operators for the free space components of layered Green’s function. Then, proofs for the exponential convergence of the MEs, LEs and translation operators for the reaction components are presented. Finally, a conclusion is given in Section 5.

2. Green’s function of 3-dimensional Laplace equation in layered media

Consider a layered medium consisting of \(L\)-interfaces located at \(z = d_\ell, \ell = 0, 1, \ldots, L - 1\), see Fig. 2. The piece wise constant material parameter is described by \(\{\varepsilon_\ell\}_{\ell=0}^L\). Suppose we have a point source at \(r' = (x', y', z')\) in the \(\ell'\)th layer \((d_{\ell'} < z' < d_{\ell' - 1})\), then, the layered media Green’s function \(u_{\ell\ell'}(r, r')\) for the Laplace equation satisfies

\[
\Delta u_{\ell\ell'}(r, r') = -\delta(r, r'),
\]

at field point \(r = (x, y, z)\) in the \(\ell\)th layer \((d_{\ell} < z < d_{\ell} - 1)\) where \(\delta(r, r')\) is the Dirac delta function. By using Fourier transforms along \(x-\) and \(y-\)directions, the problem can be solved analytically for each layer in \(z\) by imposing transmission conditions at the interface between \(\ell\)th and \((\ell - 1)\)th layer \((z = d_{\ell - 1})\), i.e.,

\[
u_{\ell-1,\ell'}(x, y, z) = u_{\ell\ell'}(x, y, z), \quad \varepsilon_{\ell-1} \frac{\partial u_{\ell-1,\ell'}(x, y, z)}{\partial z} = \varepsilon_{\ell} \frac{\partial \hat{u}_{\ell\ell'}(k_x, k_y, z)}{\partial z},
\]

as well as the decaying conditions in the top and bottom-most layers as \(z \to \pm \infty\).

By applying Fourier transform in \(x, y\) direction and solving the resulted ODE with interface conditions, we can obtain the expression of the Green’s function in the physical domain as
will review the recurrence formula. For this purpose, let us define (cf. [9] Appendix B.)

\[
\begin{align*}
\rho_{\ell d} = \begin{cases} 
\rho_{\ell d}^{11}(r, r') + \rho_{\ell d}^{12}(r, r'), & \ell \neq \ell', \\
\rho_{\ell d}^{11}(r, r') + \rho_{\ell d}^{12}(r, r') + \rho_{\ell d}^{21}(r, r') + \rho_{\ell d}^{22}(r, r'), & \ell = \ell',
\end{cases}
\end{align*}
\]

with reaction components given by Sommerfeld-type integrals:

\[
u_{\ell \ell'}^{ab}(r, r') = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{\e^{ik\cdot\tau^{ab}_{\ell \ell'}(r, r')}}{k_{\rho}^2} \sigma_{\ell \ell'}^{ab}(k_{\rho}) dk_x dk_y,
\]

where \(k_{\rho} = \sqrt{k_x^2 + k_y^2}, k = (k_x, k_y, ik_{\rho}),\)

\[
\begin{align*}
\tau^{11}_{\ell \ell'}(r, r') &= (x - x', y - y', z - d_\ell + z' - d_{\ell'}), \\
\tau^{12}_{\ell \ell'}(r, r') &= (x - x', y - y', z - d_\ell + d_{\ell - 1} - z'), \\
\tau^{21}_{\ell \ell'}(r, r') &= (x - x', y - y', d_{\ell - 1} - z + z' - d_{\ell'}), \\
\tau^{22}_{\ell \ell'}(r, r') &= (x - x', y - y', d_{\ell - 1} - z + d_{\ell - 1} - z'),
\end{align*}
\]

are coordinate mappings depend on interfaces and \(\sigma_{\ell \ell'}^{ab}(k_{\rho})\) are the reaction densities in Fourier spectral space. The expression (2.3) is a general formula for source \(r'\) in the middle layer. In the cases of the source \(r'\) in the top or bottom most layer, the reaction components \(\{u_{\ell \ell'}^{a2}(r, r')\}_{a=1}^{2}\) and \(\{u_{\ell \ell'}^{1a}(r, r')\}_{a=1}^{2}\) will vanish, respectively.

The reaction densities \(\sigma_{\ell \ell'}^{ab}(k_{\rho})\) only depend on the layered structure and the material parameter \(\varepsilon_{\ell}\) in each layer. According to the derivation in [9] Appendix B], a stable recurrence formula is available for more general interface conditions

\[
\begin{align*}
a_{\ell - 1} u_{\ell - 1, \ell'}(x, y, z) = a_{\ell} u_{\ell \ell'}(x, y, z), \\
b_{\ell - 1} \frac{\partial u_{\ell - 1, \ell'}(x, y, z)}{\partial z} = b_{\ell} \frac{\partial u_{\ell \ell'}(x, y, k_z)}{\partial z},
\end{align*}
\]

where \(\{a_\ell, b_\ell\}\) are given constants. In order to prove some key properties of the densities, we will review the recurrence formula. For this purpose, let us define

\[
\begin{align*}
d_{-1} := d_0, \\
D_{L+1} := d_L, \\
D_{\ell} := d_{\ell - 1} - d_\ell, \\
\varepsilon_{\ell} := e^{-k_x D_{\ell}}, \\
\gamma_{\ell}^+ = \frac{a_{\ell}}{a_{\ell - 1}} + \frac{b_{\ell}}{b_{\ell - 1}}, \\
\gamma_{\ell}^- = \frac{a_{\ell}}{a_{\ell - 1}} - \frac{b_{\ell}}{b_{\ell - 1}}, \\
C^{(\ell)} = \prod_{j=0}^{\ell - 1} \frac{1}{2\varepsilon_j},
\end{align*}
\]

Figure 2.1. Sketch of the layer structure for general multi-layer media.
Lemma 2.1. \[ |\alpha_{21}|^2 - |\alpha_{21}|^2 \geq (|\gamma_1^+|^2 - |\gamma_1^-|^2)(|\gamma_2^+|^2 - |\gamma_2^-|^2) \cdots (|\gamma_k^+|^2 - |\gamma_k^-|^2) > 0, \] for all \( |e| \leq 1 \) and \( k = 1, 2, \ldots, L \), we obtain

\[ |\gamma_1^+|^2 = |a_{12}|^2 + |b_{12}|^2 > 0, \] for all \( k = 1, 2, \ldots, L \), and any \( k = k \in \{ z \in \mathbb{C} | Rez \geq 0 \} \).

Proof. By the definition of (2.8), the entries \( \{\alpha_{21}(\ell), \alpha_{22}(\ell)\} \) can be calculated recursively as

\[ \begin{align*}
\alpha_{21}(\ell) &= \alpha_{21}(\ell-1) \gamma_1^+ e_{\ell-1} e_1 + \alpha_{22}(\ell-1) \gamma_1^- e_\ell, \\
\alpha_{22}(\ell) &= \alpha_{21}(\ell-1) \gamma_1^- e_{\ell-1} + \alpha_{22}(\ell-1) \gamma_1^+ e_\ell, \\
&\quad \vdots
\end{align*} \]

(2.20)

Naturally, we will prove the conclusion (2.19) by induction. As \( a_\ell, b_\ell > 0 \) by assumption and \( |e| \leq 1 \) for all \( k \in \{ z \in \mathbb{C} | Rez \geq 0 \} \), we obtain

\[ |\gamma_1^+|^2 = |a_{12}|^2 + |b_{12}|^2 > 0, \] for all \( k = 1, 2, \ldots, L \), and any \( k = k \in \{ z \in \mathbb{C} | Rez \geq 0 \} \).

Therefore, (2.19) is true for \( \ell = 1 \) as

\[ |\alpha_{21}|^2 - |\alpha_{21}|^2 \geq |\gamma_1^+|^2 - |\gamma_1^-|^2 \geq |\gamma_1^+|^2 - |\gamma_1^-|^2 > 0. \] (2.22)

Assume

\[ |\alpha_{22}(s)|^2 - |\alpha_{22}(s)|^2 \geq (|\gamma_1^+|^2 - |\gamma_1^-|^2)(|\gamma_2^+|^2 - |\gamma_2^-|^2) \cdots (|\gamma_k^+|^2 - |\gamma_k^-|^2), \] (2.23)

is true for all \( s = 2, 3, \ldots, \ell - 1 \). By recursion (2.20), we have

\[ |\alpha_{21}(\ell)| = |\beta_{\ell-1} \gamma_1^+ e_{\ell-1} + \gamma_1^- |\alpha_{22}(\ell-1) e_\ell|, \quad |\alpha_{22}(\ell)| = |\beta_{\ell-1} \gamma_1^- e_{\ell-1} + \gamma_1^+ |\alpha_{22}(\ell-1)|, \] (2.24)

where \( \beta_{\ell} := \alpha_{21}(\ell) / \alpha_{22}(\ell) \). Noting that \( \gamma_\ell^\pm \) are real, then

\[ |\beta_{\ell-1} \gamma_1^+ e_{\ell-1} + \gamma_1^- |\alpha_{22}(\ell-1) e_\ell|^2 = |\beta_{\ell-1} \gamma_1^- e_{\ell-1} + \gamma_1^+ |\alpha_{22}(\ell-1)|^2, \]

\[ |\beta_{\ell-1} \gamma_1^- e_{\ell-1} + \gamma_1^+ |\alpha_{22}(\ell-1)|^2 = |\beta_{\ell-1} \gamma_1^- e_{\ell-1} + \gamma_1^+ |\alpha_{22}(\ell-1)|^2. \]

Therefore

\[ |\beta_{\ell-1} \gamma_1^- e_{\ell-1} + \gamma_1^+ |\alpha_{22}(\ell-1)|^2 = |\beta_{\ell-1} \gamma_1^- e_{\ell-1} + \gamma_1^+ |\alpha_{22}(\ell-1)|^2. \]

Together with (2.24) and the fact \( |e| \leq 1 \) for all \( k \in \{ z \in \mathbb{C} | Rez \geq 0 \} \), we obtain

\[ |\alpha_{22}(\ell)|^2 - |\alpha_{22}(\ell)|^2 \geq (|\gamma_\ell^+|^2 - |\gamma_\ell^-|^2) (1 - |\beta_{\ell-1} e_{\ell-1}|^2). \]

Then, we complete the proof by applying the assumption (2.23). \( \square \)
Algorithm 1 Stable and efficient algorithm for reaction densities $\sigma_{L\ell'}^{ab}(k_p)$ in (2.4).

for $\ell' = 0 \rightarrow L$ do
  if $\ell' < L$ then
    $\sigma_{L\ell'}^{21}(k_p) = -\frac{C(\ell'+1)}{C(L)\alpha_{22}^{(L)}} \left( \alpha_{21}^{(\ell')} \alpha_{22}^{(\ell')} \right) 2e_{\ell'}\bar{S}(\ell') \left(\frac{-a_{\ell'}}{b_{\ell'}}\right)$,
  end if
  if $\ell' > 0$ then
    $\sigma_{L\ell'}^{22}(k_p) = -\frac{C(\ell')}{C(L)\alpha_{22}^{(L)}} \left( \alpha_{21}^{(\ell'-1)} \alpha_{22}^{(\ell'-1)} \right) 2e_{\ell'-1}\bar{S}(\ell'-1) \left(\frac{a_{\ell'}}{b_{\ell'}}\right)$,
  end if
  for $\ell = L - 1 \rightarrow 0$ do
    if $\ell = \ell'$ then
      $\sigma_{L\ell'}^{11}(k_p) = T_{11}^{\ell'1} \sigma_{11}^{11} + T_{12}^{\ell'1} \sigma_{11}^{21} - \bar{S}_{11}(\ell') a_{\ell'} + \bar{S}_{12}(\ell') b_{\ell'}$,
    else
      $\sigma_{L\ell'}^{12}(k_p) = T_{11}^{\ell'1} \sigma_{11}^{11} + T_{12}^{\ell'1} \sigma_{11}^{21}$,
    end if
    if $\ell = \ell' - 1$ then
      $\sigma_{L\ell'}^{12}(k_p) = T_{11}^{\ell'1} \sigma_{11}^{11} + T_{12}^{\ell'1} \sigma_{11}^{22} + \bar{S}_{11}(\ell'-1) a_{\ell'} + \bar{S}_{12}(\ell'-1) b_{\ell'}$,
    else
      $\sigma_{L\ell'}^{12}(k_p) = T_{11}^{\ell'1} \sigma_{11}^{11} + T_{12}^{\ell'1} \sigma_{11}^{22}$,
    end if
    if $\ell > 0$ then
      if $\ell > \ell'$ then
        $\sigma_{L\ell'}^{21}(k_p) = \frac{-1}{\alpha_{22}^{(\ell)}} \left[ \frac{C(\ell'+1)}{C(L)} A_{12}^{(\ell')} 2e_{\ell'}\bar{S}(\ell') \left(\frac{-a_{\ell'}}{b_{\ell'}}\right) + A_{12}^{(\ell)} \left(\frac{\sigma_{11}^{11}}{0}\right) \right]$,
      else
        $\sigma_{L\ell'}^{21}(k_p) = -a_{21}^{(\ell)} \sigma_{L\ell'}^{11}(k_p) / \alpha_{22}^{(\ell)}$,
      end if
      if $\ell > \ell' - 1$ then
        $\sigma_{L\ell'}^{22}(k_p) = \frac{-1}{\alpha_{22}^{(\ell)}} \left[ \frac{C(\ell')}{C(L)} A_{12}^{(\ell'-1)} 2e_{\ell'-1}\bar{S}(\ell'-1) \left(\frac{a_{\ell'}}{b_{\ell'}}\right) + A_{12}^{(\ell)} \left(\frac{\sigma_{11}^{12}}{0}\right) \right]$,
      else
        $\sigma_{L\ell'}^{22}(k_p) = -a_{21}^{(\ell)} \sigma_{L\ell'}^{12}(k_p) / \alpha_{22}^{(\ell)}$,
      end if
    end if
  end for
end for

Proposition 2.1. Suppose $a_{\ell}, b_{\ell} > 0$ for all $\ell = 0, 1, \cdots, L$, then all reaction densities $\sigma_{L\ell'}^{ab}(k_p)$ in (2.4) are continuous and bounded in $\{k_p | \Re k_p \geq 0\}$. Moreover, they are analytic in the right half complex plane $\{k_p | \Re k_p > 0\}$.
Proof. From the definition (2.7) and (2.8), we have
\[ T_{11}^{\ell+1} = \frac{a_{\ell+1} b_{\ell} + a_{\ell} b_{\ell+1}}{2a_{\ell} b_{\ell}} e_{\ell+1}, \quad T_{12}^{\ell+1} = \frac{a_{\ell+1} b_{\ell} - a_{\ell} b_{\ell+1}}{2a_{\ell} b_{\ell}}, \quad \bar{T}_{\ell-1, \ell} = \left( \begin{array}{cc} \gamma_+ e_{\ell-1} e_{\ell} & \gamma_- e_{\ell-1} \\ \gamma_- e_{\ell} & \gamma_+ e_{\ell} \end{array} \right), \]
\[ 2\epsilon_{\ell} S(\ell) = \left( \begin{array}{cc} a_{\ell}^{-1} e_{\ell} & b_{\ell}^{-1} e_{\ell} \\ a_{\ell}^{-1} & b_{\ell}^{-1} \end{array} \right), \quad C(\ell_1) / C(\ell_2) = \begin{cases} 1 & \ell_1 = \ell_2, \\ 2^{\ell_2 - \ell_1} e^{-k_p (d_{\ell_1} - d_{\ell_2})} & 0 \leq \ell_1 < \ell_2. \end{cases} \]
As they consist of constants \( \{a_{\ell_1}, b_{\ell_1}\}_{\ell_1=0}^L \) and their product with exponential functions of \( k_p \), \( \{T_{11}^{\ell+1}, T_{12}^{\ell+1}\}_{\ell=0}^L \), \( \{C(\ell)/C(\ell_2)\}_{\ell_1 < \ell_2} \), and the entries of matrices \( \{\bar{T}_{\ell-1, \ell}\}_{\ell=0}^L \) and \( \{a_{\ell} S(\ell)\}_{\ell=0}^L \) are all continuous and bounded in \( \{k_p \mid \Re k_p \geq 0\} \). Moreover, by Lemma 2.1, the module of the denominators \( \{a_{\ell_2} S(\ell)\}_{\ell_2=1}^L \) in (2.9)-(2.18) are bounded below in \( \{k_p \mid \Re k_p \geq 0\} \) by some positive constants determined by \( \{a_{\ell_2} b_{\ell_2}\}_{\ell_2=0}^L \). Therefore, checking the formulas (2.9)-(2.18) with the discussions above, it is not difficult to conclude that all reaction densities are continuous and bounded in \( \{k_p \mid \Re k_p \geq 0\} \) and analytic in the right half complex plane.

\[ \square \]

3. MULTIPLE AND LOCAL EXPANSIONS, SHIFTING AND TRANSLATION OPERATORS FOR THE GREEN’S FUNCTION OF 3-DIMENSIONAL LAPLACE EQUATION IN LAYERED MEDIA

In this section, we review the derivation of the ME, LEs and shifting and translation operators used in the FMM for charge interaction in multi-layered media.(cf. [9]).

3.1. MULTIPOLAR AND LOCAL EXPANSIONS, SHIFTING AND TRANSLATION OPERATORS FOR FREE SPACE GREEN’S FUNCTION. According to the expression (2.3), the layered media Green’s function consists of free space and reaction field components. The FMM for Laplace equation in layered media (cf. [9]) is a combination of the classic FMM and new FMMs for the free space and reaction field components, respectively. Before we go to the expansions for the reaction field components, let us first review the classic formulas on which the classic FMM rely.

Given source and target centers \( r_s^e \) and \( r_t^e \) close to source \( r' \) and target \( r \), i.e., \( |r' - r_s^e| < |r - r_s^e| \) and \( |r' - r_t^e| > |r - r_t^e| \), the free space Green’s function has Taylor expansions
\[ \frac{1}{4\pi |r - r'|} = \frac{1}{4\pi ((r - r_s^e) - (r' - r_s^e))} = \frac{1}{4\pi} \sum_{n=0}^{\infty} P_n(\cos \gamma_s) \left( \frac{r_s^e}{r_s} \right)^n, \quad (3.1) \]
and
\[ \frac{1}{4\pi |r - r'|} = \frac{1}{4\pi ((r - r_t^e) - (r' - r_t^e))} = \frac{1}{4\pi} \sum_{n=0}^{\infty} P_n(\cos \gamma_t) \left( \frac{r_t^e}{r_t} \right)^n, \quad (3.2) \]
where \( (r_s, \theta_s, \phi_s) \), \( (r_t, \theta_t, \phi_t) \) are the spherical coordinates of \( r - r_s^e \) and \( r' - r_s^e \), \( (r_s', \theta_s', \phi_s') \), \( (r_t', \theta_t', \phi_t') \) are the spherical coordinates of \( r' - r_t^e \) and \( r' - r_t^e \) (see Fig. 3.1) and
\[ \cos \gamma_s = \cos \theta_s \cos \theta_s' + \sin \theta_s \sin \theta_s' \cos (\phi_s - \phi_s'), \]
\[ \cos \gamma_t = \cos \theta_t \cos \theta_t' + \sin \theta_t \sin \theta_t' \cos (\phi_t - \phi_t'). \]
Moreover, the following error estimates
\[ \left| \frac{1}{4\pi |r - r'|} - \frac{1}{4\pi} \sum_{n=0}^{p} P_n(\cos \gamma_s) \left( \frac{r_s^e}{r_s} \right)^n \right| \leq \frac{1}{4\pi (r_s - r_s^e)} \left( \frac{r_s^e}{r_s} \right)^{p+1}, \quad r_s > r_s', \quad (3.4) \]
and
\[ \left| \frac{1}{4\pi |r - r'|} - \frac{1}{4\pi} \sum_{n=0}^{p} P_n(\cos \gamma_t) \left( \frac{r_t^e}{r_t} \right)^n \right| \leq \frac{1}{4\pi (r_t' - r_t)} \left( \frac{r_t'}{r_t} \right)^{p+1}, \quad r_t < r_t', \quad (3.5) \]
for any \( p \geq 1 \) can be obtained by using the fact \( |P_n(x)| \leq 1 \) for all \( x \in [-1,1] \).
Figure 3.1. Spherical coordinates used in multipole and local expansions.

Note that $P_n^m(\cos \gamma_s)$, $P_n^m(\cos \gamma_t)$ still mix the source and target information ($r$ and $r'$) together. The following addition theorems (cf. [6, 3]) will be used to derive source/target separated ME, LE and corresponding shifting and translation operators. As in [9], we will re-present the theorems using scaled spherical harmonics

$$Y^m_n(\theta, \varphi) = (-1)^m \sqrt{\frac{2n+1}{4\pi}} \frac{(n-m)!}{(n+m)!} P^m_n(\cos \theta) e^{im\varphi},$$

where $P^m_n(x)$ (resp. $\hat{P}^m_n(x)$) is the associated (resp. normalized) Legendre function of degree $n$ and order $m$. We also use notations

$$c_n = \sqrt{\frac{2n+1}{4\pi}}, \quad A^m_n = \frac{(-1)^n c_n}{\sqrt{(n-m)!(n+m)!}}, \quad |m| \leq n,$$

in the rest part of this paper.

**Theorem 3.1. (Addition theorem for Legendre polynomials)** Let $P$ and $Q$ be points with spherical coordinates $(r, \theta, \varphi)$ and $(\rho, \alpha, \beta)$, respectively, and let $\gamma$ be the angle subtended between them. Then

$$P_n^m(\cos \gamma) = \frac{4\pi}{2n+1} \sum_{m=-n}^{n} Y^m_n(\alpha, \beta) Y^m_n(\theta, \varphi).$$

**Theorem 3.2.** Let $Q = (\rho, \alpha, \beta)$ be the center of expansion of an arbitrary spherical harmonic of negative degree. Let the point $P = (r, \theta, \varphi)$, with $r > \rho$, and $P - Q = (r', \theta', \varphi')$. Then

$$\frac{Y^m_n(\theta', \varphi')}{r^{m'}+1} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \frac{(-1)^{|m+m'|-|m'|} A^m_n A^{m'}_{n'} \rho^n Y^{-m}(\alpha, \beta) Y^{m'+m'}_{n+n'}(\theta, \varphi)}{c_n^2 A^{m+m'}_{n+n'}}.$$
Theorem 3.3. Let \( Q = (\rho, \alpha, \beta) \) be the center of expansion of an arbitrary spherical harmonic of negative degree. Let the point \( P = (r, \theta, \varphi) \), with \( r < \rho \), and \( P - Q = (r', \theta', \varphi') \). Then

\[
\frac{Y^m_n'(\theta', \varphi')}{r^{m'+1}} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (-1)^{n + |m| + |m'|} A^m_n A^m_{n'} \cdot \frac{Y^m_{n+m}(\alpha, \beta)}{c^2 A^m_{n+n'} r^{n+n'+1}} r^n Y^m_n(\theta, \varphi).
\]

Theorem 3.4. Let \( Q = (\rho, \alpha, \beta) \) be the center of expansion of an arbitrary spherical harmonic of negative degree. Let the point \( P = (r, \theta, \varphi) \) and \( P - Q = (r', \theta', \varphi') \). Then

\[
r^n Y^m_n'(\theta', \varphi') = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} (-1)^{n + |m| + |m'|} c^2 A^m_{n+n'} \cdot \frac{Y^m_{n+m}(\alpha, \beta)}{\rho^n Y^m_n(\alpha, \beta)} r^{n'+1} Y^m_{n'}(\theta', \varphi').
\]

In the above theorems, the definition \( A^m_n = 0 \), \( Y^m_n(\theta, \varphi) \equiv 0 \) for \( |m| > n \) is used.

Applying Legendre addition theorem to expansions (3.1) and (3.2) gives ME

\[
\frac{1}{4\pi |r - r'|} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_{nm} \frac{Y^m_n(\theta_s, \varphi_s)}{r^{n+1}} e^{-i\nu r},
\]

and LE

\[
\frac{1}{4\pi |r - r'|} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} L_{nm} r^n Y^m_n(\theta_t, \varphi_t),
\]

where

\[
M_{nm} = \frac{1}{4\pi c_n^2} \frac{r^n}{r_{s}^{n+1}} Y^m_n(\theta_s, \varphi_s), \quad L_{nm} = \frac{1}{4\pi c_n^2} \frac{r_{t}^{-n-1}}{r_{s}^{n+1}} Y^m_n(\theta_t', \varphi_t').
\]

Further, applying Theorem 3.3 in ME (3.9) provides a translation from ME (3.9) to LE (3.10) which is given by

\[
L_{nm} = \sum_{\nu=0}^{\nu} \sum_{\mu=-\nu}^{\mu} (-1)^{\nu + |\mu|} \frac{A^\mu_{\nu} A^n_{n+\nu} Y^m_{n+\nu}(\theta_{s, s}, \varphi_{s, s})}{c^2 A^n_{n+\nu} Y^m_{n+\nu}(\theta_{s, s}, \varphi_{s, s})} M_{\nu \mu},
\]

where \((r_{s, s}, \theta_{s, s}, \varphi_{s, s})\) is the spherical coordinate of \( r_{s}^c - r_{t}^c \).

Given two new centers \( r_{s}^c \) and \( r_{t}^c \) close to \( r_{s}^c \) and \( r_{t}^c \), respectively. By using the addition Theorems 3.2 and 3.4 in (3.9)-(3.10) and rearranging terms in the results, we obtain

\[
\sum_{\nu=0}^{\nu} \sum_{\mu=-\nu}^{\mu} M_{\nu \mu} \frac{Y^\mu_{\nu}(\theta_t, \varphi_t)}{r^{n+1}} = \sum_{\nu=0}^{\nu} \sum_{\mu=-\nu}^{\mu} M_{\nu \mu} \frac{Y^\mu_{\nu}(\theta_{s, s}, \varphi_{s, s})}{c^2 A^n_{n+\nu} Y^m_{n+\nu}(\theta_{s, s}, \varphi_{s, s})} M_{\nu \mu},
\]

and

\[
\sum_{\nu=0}^{\nu} \sum_{\mu=-\nu}^{\mu} L_{\nu \mu} r^n Y^\mu_{\nu}(\theta_t, \varphi_t) = \sum_{\nu=0}^{\nu} \sum_{\mu=-\nu}^{\mu} L_{\nu \mu} \frac{Y^\mu_{\nu}(\theta_{s, s}, \varphi_{s, s})}{c^2 A^n_{n+\nu} Y^m_{n+\nu}(\theta_{s, s}, \varphi_{s, s})} M_{\nu \mu},
\]
where \((\tilde{r}_s, \tilde{\theta}_s, \tilde{\varphi}_s), (\tilde{r}_t, \tilde{\theta}_t, \tilde{\varphi}_t), (r_{ss}, \theta_{ss}, \varphi_{ss})\) and \((r_{tt}, \theta_{tt}, \varphi_{tt})\) are the spherical coordinates of \(r - \tilde{r}_s^c, r - \tilde{r}_t^c, r_s^c - \tilde{r}_s^c\) and \(r_t^c - \tilde{r}_t^c, (\tilde{r}_s, \tilde{\theta}_s, \tilde{\varphi}_s)\). The above formulas imply that the coefficients

\[
\tilde{M}_{nm} = \frac{1}{4\pi c_n^2} \bar{m}_n Y_n^m (\theta_{tt}, \varphi_{tt}), \quad \tilde{L}_{nm} = \frac{1}{4\pi c_n^2} \bar{l}_{t}^{l - n - 1} Y_n^m (\theta_{tt}, \varphi_{tt}),
\]

of the shifted ME and LE at new centers \(\tilde{r}_t^c\) and \(\tilde{r}_s^c\) can be obtained via center shifting

\[
\tilde{M}_{nm} = \sum_{\nu = 0}^{n} \sum_{\mu = -\nu}^{\nu} \left(-1\right)^{\nu} c_s^{\nu - \mu} A_m^{\nu - \mu} Y_{n - \nu}^{\mu} (\theta_{ss}, \varphi_{ss}) M_{\mu \nu}, \quad \tilde{L}_{nm} = \sum_{\nu = n}^{\infty} \sum_{\mu = -n}^{-\nu} \left(-1\right)^{\nu - n} c_s^{\nu + n} A_m^{\nu} Y_{n + \nu}^{\mu} (\theta_{tt}, \varphi_{tt}) L_{\mu \nu}.
\]

Besides using the addition theorems, we have proposed a new derivation for (3.9) and (3.10) by using the integral representation of \(1/|r - r'|\). Moreover, the methodology has been further applied to derive multipole and local expansions for the reaction components of the Green’s function in layered media (cf. [9]).

### 3.2. Multipole expansions for general reaction component

Consider a general reaction component \(u_{\ell}^\alpha (r, r')\) given in (2.4). By inserting the source center \(r_c^s = (x_s^c, y_s^c, z_s^c)\), the exponential kernels in (2.4) have source/target separations

\[
e^{ik r_s^c(r, r')} = e^{ik r_s^c(r, r')} e^{ik r_s^c(r', r')} = e^{ik r_s^c(r, r')} e^{-ik r_s^c}, \quad a, b = 1, 2, (3.16)
\]

Here, \(r_s' = r' - r_s^c, \tau(r) = (x, y, -z)\) is the reflection of any \(r = (x, y, z)\) in \(\mathbb{R}^3\) according to \(xy\)-plane. Obviously, the reflection \(\tau(r)\) satisfies

\[
|\tau(r)| = |r|, \quad \tau(r + r') = \tau(r) + \tau(r'), \quad \tau(ar) = a\tau(r), \quad \forall a, r, r' \in \mathbb{R}^3, \forall a \in \mathbb{R}.
\]

Moreover, applying source/target separations (3.16) and the Taylor expansions

\[
e^{ik r_s^c(r, r')} = e^{ik r_s^c(r, r')} \sum_{n=0}^{\infty} \frac{[i k \cdot \tau(-r_s')]^n}{n!}, \quad e^{ik r_s^c(r, r')} = e^{ik r_s^c(r, r')} \sum_{n=0}^{\infty} \frac{[-ik \cdot r_s']^n}{n!},
\]

in (2.4) gives expansions

\[
u_{\ell}^\alpha (r, r') = \sum_{n=0}^{\infty} \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} k_{r'}^{n-1} e^{ik r_s^c(r, r')} \frac{[i k \cdot \tau(-r_s')]^n}{n!} \sigma_{\ell}^{\alpha}(k_{r'}) dk_r dk_{r'},
\]

\[
u_{\ell}^\alpha (r, r') = \sum_{n=0}^{\infty} \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} k_{r'}^{n-1} e^{ik r_s^c(r, r')} \frac{[-ik \cdot r_s']^n}{n!} \sigma_{\ell}^{\alpha}(k_{r'}) dk_r dk_{r'},
\]

for \(a = 1, 2\). Here, we have directly exchanged the order of the infinite summations and improper integrals. Rigorous theoretical proof will be presented in Theorem 4.11.

To derive ME for the general reaction component \(u_{\ell}^\alpha (r, r')\), we shall use the following limit version of the extended Legendre addition theorem (cf. [9]).

**Theorem 3.5.** Let \(k_0 = (\cos \alpha, \sin \alpha, 1)\) be a vector with complex entry, \(\theta, \varphi\) be the azimuthal angle and polar angles of a unit vector \(\hat{r}\). Then

\[
\frac{(ik_0 \cdot \hat{r})^n}{n!} = \sum_{m=-n}^{n} C_n^m \bar{P}_n^m (\cos \theta) e^{im(\alpha - \varphi)},
\]

where

\[
C_n^m = \frac{4\pi}{(2n+1)(n+m)!} \sqrt{(2m+1)(n+m)!}. (3.20)
\]
By applying Theorem 3.5 in expansions (3.18) and then using identities
\[ Y^m_n(\pi - \theta, \varphi) = (-1)^{n+m} Y^m_n(\theta, \varphi), \quad Y^m_n(\theta, \pi + \varphi) = (-1)^m Y^m_n(\theta, \varphi), \] (3.21)
we obtain MEs
\[ u_{\ell\ell'}(r, r') = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_{nm}^{ab} \Phi_{nm}(r, r') \quad \text{and} \quad M_{nm}^{ab} = \frac{1}{4\pi r_n} r_{n+1} Y_n^m(\theta_n, \varphi_n), \] (3.22)
at source centers \( r^a_c \). Here, \( \Phi_{nm}(r, r') \) are represented by Sommerfeld-type integrals
\[
\begin{align*}
\mathcal{F}_{nm}^{a1}(r, r'^c) &= \frac{(-1)^{n+1} e^{ikr^a_c(r', r')}}{2\pi r_n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(r^a_c(r, r')-r_n)} \sigma_{\ell\ell'}^{1b}(k) k_\rho^{-1} e^{i\alpha} dk_x dk_y, \\
\mathcal{F}_{nm}^{a2}(r, r'^c) &= \frac{(-1)^{n} e^{ikr^a_c(r', r')}}{2\pi r_n} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ikr^a_c(r, r')-r_n} \sigma_{\ell\ell'}^{2b}(k) k_\rho^{-1} e^{i\alpha} dk_x dk_y.
\end{align*}
\] (3.23)

4. Exponential convergence of the MEs and LEs, shifting and translation operators

In this section, we prove the exponential convergence of the approximations used in the FMM for 3-dimensional Laplace equation in layered media. Let \( \mathcal{P}_\ell = \{(Q_{j\ell}, r_{j\ell})\}, \ell = 1, 2, \ldots, N_\ell \), \( \ell = 1, 2, \ldots, L \) be \( L \) groups of source charges distributed in a multi-layer medium with \( L + 1 \) layers (see Fig. 2). The group of charges in \( \ell \)-th layer is denoted by \( \mathcal{P}_\ell \). The FMM provides a fast algorithm to compute interactions
\[
\Phi_\ell(r_{\ell t}) = \Phi_{\ell t}^{\text{free}}(r_{\ell t}) + \sum_{\ell' = 0}^{L-1} \Phi_{\ell'\ell t}^{11}(r_{\ell t}) + \Phi_{\ell'\ell t}^{21}(r_{\ell t}) + \sum_{\ell' = 1}^{L} \Phi_{\ell'\ell t}^{12}(r_{\ell t}) + \Phi_{\ell'\ell t}^{22}(r_{\ell t}),
\] (4.1)
where
\[
\Phi_{\ell t}^{\text{free}}(r_{\ell t}) := \sum_{j=1}^{N_\ell} Q_{j\ell} \frac{Q_{j\ell}}{4\pi |r_{\ell t} - r_{j\ell}|}, \quad \Phi_{\ell\ell'}^{ab}(r_{\ell t}) := \sum_{j=1}^{N_\ell} Q_{j\ell} u_{j\ell'\ell}^{ab}(r_{\ell t}, r_{j\ell}), \] (4.2)
are free space and reaction field components, respectively. Far field approximations are used for both free space and reaction field components. Below, we first review the well-known theoretical results of the FMM for the free space components. It is mostly for the integrity of the theory and comparison with the convergence results that we will prove for the approximations of the reaction field components.

4.1. Exponential convergence of ME and LE, shifting and translation operators for the free space components. Let \( \Phi_{\ell t, \text{in}}(r) \) and \( \Phi_{\ell t, \text{out}}(r) \) be the free space components of the potentials induced by all particles inside a given source box \( B_s \) centered at \( r^a_c \) and all particles far away from a given target box \( B_t \) centered at \( r^a_t \) (see Fig. 3), i.e.,
\[
\Phi_{\ell t, \text{in}}(r) = \sum_{j \in \mathcal{J}} \frac{Q_{j\ell}}{4\pi |r - r_{j\ell}|}, \quad \Phi_{\ell t, \text{out}}(r) = \sum_{j \in \mathcal{K}} \frac{Q_{j\ell}}{4\pi |r - r_{j\ell}|},
\] (4.3)
where \( \mathcal{J} \) and \( \mathcal{K} \) are the sets of indices of particles inside \( B_s \) and of particles far away from \( B_t \), respectively. The FMM for free space components use ME
\[
\Phi_{\ell t, \text{in}}(r) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_{nm}^{\text{in}} Y_n^m(\theta_n, \varphi_n),
\] (4.4)
at any target points far away from \( B_t \) and LE
\[
\Phi_{\ell t, \text{out}}(r) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} L_{nm}^{\text{out}} Y_n^m(\theta_n, \varphi_n),
\] (4.5)
inside $B_t$, where $(r_s, \theta_s, \phi_s)$ and $(r_t, \theta_t, \phi_t)$ are spherical coordinates of $r - r_c^s$ and $r - r_c^t$, respectively. The coefficients are given by

$$M_{nm}^{in} = \frac{c_n^2}{4\pi} \sum_{j \in J} Q_{\ell j} (r_{\ell j}^s)^n Y_n^m(\theta_{\ell j}, \varphi_{\ell j})$$

$$L_{nm}^{out} = \frac{c_n^2}{4\pi} \sum_{j \in K} Q_{\ell j} (r_{\ell j}^t)^{-n-1} Y_n^m(\theta_{\ell j}, \varphi_{\ell j})$$

where $(r_{\ell j}^s, \theta_{\ell j}, \phi_{\ell j})$ and $(r_{\ell j}^t, \theta_{\ell j}, \phi_{\ell j})$ are spherical coordinates of $r_{\ell j} = r_c^s$ and $r_{\ell j}^t - r_{\ell j}^t$, respectively. These expansions can be obtained by applying expansions (3.9)-(3.10) to the free space Green’s function involved in the summation (4.2). By using Legendre addition theorem and estimates (3.4) and (3.5), there holds the following error estimates (cf. [6]).

**Theorem 4.6.** Denote the radius of the circumscribed sphere of the source box $B_s$ by $a_s$. Then, the ME (4.4) has error estimate

$$\left| \Phi_{\ell, in}^{free}(r) - \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{in} \frac{Y_n^m(\theta_s, \varphi_s)}{r_s^{n+1}} \right| \leq \frac{1}{4\pi} \frac{Q_J}{r_s - a_s} \left( \frac{a_s}{r_s} \right)^{p+1}, \quad \forall p \geq 1,$$

for any $r$ outside the circumscribed sphere, i.e., $|r - r_c^s| > a_s$, where

$$Q_J = \sum_{j \in J} |Q_{\ell j}|.$$

**Theorem 4.7.** Denote the radius of the circumscribed sphere of the target box $B_t$ by $a_t$. Suppose $K$ is the set of indices of all particles $(Q_{\ell j}, r_{\ell j})$ such that $|r_{\ell j} - r_c^t| > a_t$, then the LE (4.5) has error estimate

$$\left| \Phi_{\ell, out}^{free}(r) - \sum_{n=0}^{p} \sum_{m=-n}^{n} L_{nm}^{out} \frac{Y_n^m(\theta_t, \varphi_t)}{r_t^{n+1}} \right| \leq \frac{1}{4\pi} \frac{Q_K}{a_t - r_t} \left( \frac{r_t}{a_t} \right)^{p+1}, \quad \forall p \geq 1,$$

for any $r \in B_t$, where

$$Q_K = \sum_{j \in K} |Q_{\ell j}|.$$

Let $B_{parent}^s$ be a parent box of the source box $B_s$ and $B_{child}^t$ be a child box of the target box $B_t$ in the tree structure. Denote by $\tilde{r}_c^s$ and $\tilde{r}_c^t$ the centers of $B_{parent}^s$ and $B_{child}^t$, respectively. In the FMM, the shifting operations from the ME (4.4) at $r_c^s$ to new ME at $\tilde{r}_c^s$ and from the LE (4.5) at $r_c^t$ to new LE at $\tilde{r}_c^t$ are required. Denote the ME and LE at new centers $\tilde{r}_c^s$ and $\tilde{r}_c^t$ by

$$\Phi_{\ell, in}^{free}(r) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} M_{nm}^{in} Y_n^m(\tilde{\theta}_s, \tilde{\varphi}_s), \quad \Phi_{\ell, out}^{free}(r) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} L_{nm}^{out} Y_n^m(\tilde{\theta}_t, \tilde{\varphi}_t).$$
Recall shifting operators (3.14)-(3.15), we have
\[
\tilde{M}^\text{in}_{nm} = \sum_{\nu=0}^{n-1} \sum_{\mu=-\nu}^{\nu} (-1)^{\nu-n-\mu} a_{nm}\nu^m a_{\mu \nu} n^m Y^\mu_{n-\nu} (\theta_{ss}, \varphi_{ss}) M^\text{in}_{\nu \mu}, \quad (4.12)
\]
\[
\tilde{L}^\text{out}_{nm} = \sum_{\nu=0}^{n-1} \sum_{\mu=-\nu}^{\nu} (-1)^{\nu-n-\mu} a_{\nu n}^0 a_{\mu \nu} n^m Y^\mu_{\nu-\nu} (\theta_{tt}, \varphi_{tt}) L^\text{out}_{\nu \mu}, \quad (4.13)
\]
where
\[
(r_s, \tilde{\theta}_s, \tilde{\varphi}_s), (r_{ss}, \theta_{ss}, \varphi_{ss}), (r_t, \tilde{\theta}_t, \tilde{\varphi}_t) \text{ and } (r_{tt}, \theta_{tt}, \varphi_{tt}) \text{ are the spherical coordinates of } r - \tilde{r}_s, r_s - \tilde{r}_s, r - \tilde{r}_t \text{ and } \tilde{r}_t - \tilde{r}_c, \text{ respectively.}
\]
According to the ME to ME translation (4.12), we see that any ME coefficients \( \tilde{M}^\text{in}_{nm} \) in the ME at \( \tilde{r}_c \) can be computed exactly by the ME coefficients \( \{M^\text{in}_{\nu \mu}\}_{\nu=0}^\infty \) in the ME at \( r_s \). Therefore, the ME obtained via shifting operator (4.13) is actually the the unique ME of \( \Phi^\text{free}_{\nu \mu}(r) \) at \( \tilde{r}_c \). As in Theorem 4.6, the following error estimate holds.

**Theorem 4.8.** Denote the radius of the circumscribed sphere of the source box \( B_s \) by \( a_s \). For any \( |r - \tilde{r}_s| > a_s + r_{ss} \), the first expansion in (4.11) has error estimate
\[
\left| \Phi^\text{free}_{\nu \mu}(r) - \sum_{n=0}^{p} \sum_{m=0}^{n} \tilde{M}^\text{in}_{nm} \frac{Y^m_{n \nu-\nu}(\tilde{\theta}_s, \tilde{\varphi}_s)}{r_s^{n+1}} \right| \leq \frac{Q_s}{4\pi r_s - (a_s + r_{ss})} \left( \frac{a_s + r_{ss}}{r_s} \right)^{p+1}, \quad (4.14)
\]
where \( Q_s \) is defined in (4.8).

Although, the LE to LE shifting operator (4.13) has an infinite summation, the shifting operation remains exact with finite sum when we are shifting a truncated LE to a new center. In practice, the truncated LE
\[
\tilde{\Phi}^\text{free}_{\nu \mu}(r) \approx \tilde{\Phi}^\text{free}_{\nu \mu}(r) = \sum_{n=0}^{p} \sum_{m=0}^{n} \tilde{L}^\text{out}_{nm} \frac{Y^m_{n \nu-\nu}(\tilde{\theta}_t, \tilde{\varphi}_t)}{r_t^{n+1}}, \quad (4.15)
\]
is used in the FMM. It can be seen as an infinite sum with \( L^\text{out}_{nm} = 0 \) for \( n > p \). Then by (4.13), we have \( \tilde{L}^\text{out}_{nm} = 0 \) for \( n > p \). The shifting LE in (4.11) reduce to finite summation:
\[
\tilde{\Phi}^\text{free}_{\nu \mu}(r) = \sum_{n=0}^{p} \sum_{m=0}^{n} \frac{L^\text{out}_{nm} \frac{Y^m_{n \nu-\nu}(\tilde{\theta}_t, \tilde{\varphi}_t)}{r_t^{n+1}}}{r_t^{n+1}}, \quad (4.16)
\]
where
\[
\tilde{L}^\text{out}_{nm} = \sum_{\nu=n}^{p} \sum_{\mu=-\nu}^{\nu} \frac{(-1)^{\nu-n-\mu} a_{nm}^0 a_{\mu \nu} n^m Y^\mu_{\nu-\nu} (\theta_{tt}, \varphi_{tt})}{c_{\nu \mu}^2 A_{r_{tt}}^2 A_{\nu}^2} L^\text{out}_{\nu \mu}. \quad (4.17)
\]
Therefore, the truncated LE to LE shifting (4.17) used in the FMM implementation is exact.

Suppose target box \( B_t \) is far away from the source box \( B_s \). Recall the translation operator (3.12), the LE expansion coefficient in (4.5) can be calculated from ME coefficients via
\[
L^\text{out}_{nm} = \sum_{|\nu|=0}^{p} \sum_{\mu=-\nu}^{\nu} \frac{(-1)^{\nu+|\mu|} A_{\nu}^\mu A_{\nu} n^m Y^\mu_{n+\nu} (\theta_{st}, \varphi_{st})}{c_{\nu \mu}^2 A_{r_{tt}}^2} M^\text{in}_{\nu \mu}. \quad (4.18)
\]
Again, (4.18) can not be directly used in the FMM due to the infinite summation. In the FMM, the formulas in (4.18) for local expansion coefficients \( L^\text{out}_{nm} \) are further truncated which gives approximated local expansion coefficients
\[
L^\text{out}_{nm} = \sum_{|\nu|=0}^{p} \sum_{\mu=-\nu}^{\nu} \frac{(-1)^{\nu+|\mu|} A_{\nu}^\mu A_{\nu} n^m Y^\mu_{n+\nu} (\theta_{st}, \varphi_{st})}{c_{\nu \mu}^2 A_{r_{tt}}^2} M^\text{in}_{\nu \mu}. \quad (4.19)
\]
We find that the detailed proof of the error estimate for the truncated M2L translation has not been presented in the literature. Therefore, we present a proof as follow:
Theorem 4.9. Suppose $B_s$ and $B_t$ are well separated cubic boxes and denote the radii of their circumscribed spheres by $a_s$ and $a_t$. The well separateness of the boxes means that $|r_s^e - r_t^e| > a_s + c a_t$ with $c > 1$. Then
\[
\phi_{\ell,\text{out}}(r) - \sum_{n=0}^{p} \sum_{m=-n}^{n} L_{nm}^p r_s^m Y_{\ell m}^n(\theta_t, \varphi_t) \leq \frac{1}{4\pi} \frac{Q_J}{(c-1)a_t} \frac{(a_s + a_t)}{(a_s + c a_t)}^{p+1}, \forall r \in B_t, \tag{4.20}
\]
where $Q_J$ is defined in (4.8).

Proof. By the assumption $|r_s^e - r_t^e| > a_s + c a_t$ ($c > 1$), we have $|r' - r_s^e| + |r - r_t^e| < |r_t^e - r_s^e|$ for any $r \in B_t$, $r' \in B_s$. Then, as in (3.1)–(3.2), we have Taylor expansion
\[
\frac{1}{4\pi|r - r'|} = \frac{1}{4\pi|r_t - r_s^e - (r_s^e - r_t)|} = \frac{1}{4\pi} \sum_{n'=0}^{\infty} \frac{P_{n'}(\xi)}{|r_s^e - r_t|^n'} \left( \frac{|r_t - r_s^e|}{|r_s^e - r_t|} \right)^{n'}, \tag{4.21}
\]
where
\[
\xi = \frac{(r_s^e - r_t) \cdot (r_t - r')}{|r_s^e - r_t||r_t - r'|}, \quad r_s^e = r' - r_s^e, \quad r_t = r - r_t^e.
\]
Truncate the expansion (4.21) and denote the approximation by
\[
\psi^p(r, r') = \frac{1}{4\pi} \sum_{n'=0}^{p} \frac{P_{n'}(\xi)}{|r_s^e - r_t|^n'} \left( \frac{|r_t - r_s^e|}{|r_s^e - r_t|} \right)^{n'}. \tag{4.23}
\]
Then, we directly have error estimate
\[
\left| \frac{1}{4\pi|r - r'|} - \psi^p(r, r') \right| \leq \frac{1}{4\pi} \left( \frac{|r_t - r_s^e|}{|r_s^e - r_t|} \right)^{p+1} \leq \frac{1}{4\pi} \frac{(a_s + a_t)}{(a_s + c a_t)}^{p+1} \tag{4.24}
\]
Applying identity $P_n(-x) = (-1)^n P_n(x)$ and Legendre addition theorem in (4.23) gives
\[
\psi^p(r, r') = \sum_{n'=0}^{p} \frac{1}{2n' + 1} \sum_{m'=n'}^{n'} \sum_{m'=n'}^{n'} Y_{n'n'}^{m'}(\theta_s, \varphi_s) Y_{n'n'}^{m'}(\theta_t, \varphi_t) Y_{n'n'}^{m'}(r_s^e - r_t), \tag{4.25}
\]
where $(r_s, \theta_s, \varphi_s)$ is the spherical coordinates of $r_s^e - r_t^e$. Further, applying addition theorem (3.4) and then rearranging the resulted summation, we obtain
\[
\psi^p(r, r') = \sum_{n'=0}^{p} \sum_{m'=n'}^{n'} \sum_{m'=n'}^{n'} \sum_{n=0}^{p} \sum_{m=-n}^{n} \frac{Y_{n'n'}^{m'}(\theta_s, \varphi_s)}{4\pi r_s^{n'+1}} \sum_{n=0}^{p} \sum_{m=-n}^{n} \sum_{m'=-n}^{n'} B_{nm'm'}^{n'n'}(r_s^e)^{n'-n} Y_{n'n'}^{m'-n}(\theta_s, \varphi_s) Y_{n'n'}^{m'}(\theta_t, \varphi_t)
\]
\[
= \sum_{n=0}^{p} \sum_{m=-n}^{n} \sum_{m'=n'}^{n'} \frac{Y_{n'n'}^{m'}(\theta_s, \varphi_s)}{4\pi r_s^{n'+1}} B_{nm'm'}^{n'n'}(r_s^e)^{n'-n} Y_{n'n'}^{m'-n}(\theta_s, \varphi_s) Y_{n'n'}^{m'}(\theta_t, \varphi_t)
\]
\[
= \sum_{n=0}^{p} \sum_{m=-n}^{n} \sum_{m'=n'}^{n'} \frac{Y_{n'n'}^{m'}(\theta_s, \varphi_s)}{4\pi r_s^{n'+1}} B_{nm'm'}^{n'n'}(r_s^e)^{n'-n} Y_{n'n'}^{m'-n}(\theta_s, \varphi_s) Y_{n'n'}^{m'}(\theta_t, \varphi_t),
\]
where
\[
B_{nm'm'}^{n'n'} = (-1)^{n'+n-m'|m'|-m'|-m'|-m'} A_n A_{m'\bar{m}'} A_{n'n'}^{-n'} A_{n'n'}^{m'n'},
\]
$(r_t, \theta_t, \varphi_t)$ and $(r'_s, \theta'_s, \varphi'_s)$, are the spherical coordinates of $r - r_t^e$ and $r' - r_c^e$, respectively. Apparently, $\psi^p(r, r')$ is a truncated LE at target center $r_c^e$ with coefficients given by
\[
\tilde{L}_{nm} = \sum_{\nu=0}^{p} \sum_{\mu=-\nu}^{\nu} \frac{Y_{n'n'}^{m'+\nu}(\theta_s, \varphi_s)}{4\pi r_s^{n'+\nu+1}} B_{nm'\bar{m}'\bar{\nu}}^{n'n'}(r_s^e)^{n'-n} Y_{n'n'}^{m'-n}(\theta_s, \varphi_s) Y_{n'n'}^{m'}(\theta_t, \varphi_t). \tag{4.26}
\]
derivation in section 3.2, we only need to prove the convergence and error estimates of the smoothness of the presentation, the detailed proof will be postponed to subsection 3.4.

Here, we first present the main theorem which is the key to prove the exponential convergence error estimates for the MEs (3.22) of the reaction components of layered Green’s function.

The exponential convergence in the Theorem 4.10.

4.2. Exponential convergence of the ME for reaction components and the conception of equivalent polarization source. The exponential convergence in the Theorem 4.6 is a direct result of the error estimate (4.14). However, it is much more difficult to derive error estimates for the MEs (3.22) of the reaction components of layered Green’s function. Here, we first present the main theorem which is the key to prove the exponential convergence of the MEs, LEs and M2L translation operators in this and the next subsections. For the smoothness of the presentation, the detailed proof will be postponed to subsection 3.4.

Let us consider the convergence and error estimates of the MEs in (3.22). According to its derivation in section 3.2, we only need to prove the convergence and error estimates of the expansions in (3.18). For this purpose, define general integral

\[
\mathcal{I}(r; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{k_\rho} e^{i k \cdot r} \sigma(k_\rho) d k_x d k_y, \quad \forall r = (x, y, z) \in \mathbb{R}^3,
\]

where \( k_\rho = \sqrt{k_x^2 + k_y^2} \), \( k = (k_x, k_y, i k_\rho) \), \( \sigma(k_\rho) \) is a given density function. Applying Taylor expansion gives

\[
\mathcal{I}(r + r'; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i k \cdot r} \sum_{n=0}^{\infty} \frac{1}{n!} \left(\frac{i k \cdot r'}{n!}\right)^n \sigma(k_\rho) d k_x d k_y,
\]

\[
\mathcal{I}(r + r' + r''; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{k_\rho} e^{i k \cdot r} \sum_{n=0}^{\infty} \sum_{n'=0}^{\infty} \frac{(i k \cdot r')^n (i k \cdot r'')^{n'}}{n! n'!} \sigma(k_\rho) d k_x d k_y,
\]

for any \( r' = (x', y', z') \), \( r'' = (x'', y'', z'') \) in \( \mathbb{R}^3 \). Suppose \( z > 0, z + z' > 0, z + z' + z'' > 0 \), and the density function \( \sigma(k_\rho) \) is not increasing exponentially as \( k_\rho \to \infty \), then the integrals in (4.29) and (4.30) are convergent. We first present the conclusion that the improper integral and the infinite summation in (4.30) can exchange order and the resulted series have exponential convergence under suitable conditions. Detailed proof will be given in section 4.5. For the sake of brevity, we denote

\[
\mathcal{I}_n(r, r'; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{k_\rho} e^{i k \cdot r} \frac{(i k \cdot r')^n}{n!} \sigma(k_\rho) d k_x d k_y,
\]

\[
\mathcal{I}_{n\nu}(r, r', r''; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{k_\rho} e^{i k \cdot r} \frac{(i k \cdot r')^n (i k \cdot r'')^{n'}}{n! n'!} \sigma(k_\rho) d k_x d k_y.
\]

Theorem 4.10. Suppose the density function \( \sigma(k_\rho) \) is analytic and has a bound \( |\sigma(k_\rho)| \leq M_\sigma \) in the right half complex plane \( \{k_\rho : \Re k_\rho > 0\} \), \( r = (x, y, z) \), \( r' = (x', y', z') \), \( r'' = (x'', y'', z'') \).
Theorem 4.11. Given \((x', y', z') \in \mathbb{R}^3\) such that \(z > 0, z + z' > 0, z + z' + z'' > 0\) and \(|r| > |r'|, |r| > |r' + r''|\). Then, the following expansions

\[
\mathcal{I}(r + r'; \sigma) = \sum_{n=0}^{\infty} \mathcal{I}_n(r, r'; \sigma), \quad \mathcal{I}(r + r' + r''; \sigma) = \sum_{n=0}^{\infty} \sum_{\nu=0}^{\infty} \mathcal{I}_{n\nu}(r, r', r''; \sigma),
\]

(4.32)

hold. Moreover, the truncation error estimates are given by

\[
|\mathcal{I}(r + r'; \sigma) - \sum_{n=0}^{P} \mathcal{I}_n(r, r'; \sigma)| \leq \frac{2\pi M_{ab}}{|r| - |r'|} |r'|^{p+1},
\]

(4.33)

and

\[
|\mathcal{I}(r + r' + r''; \sigma) - \sum_{n=0}^{P} \sum_{\nu=0}^{P} \mathcal{I}_{n\nu}(r, r', r''; \sigma)| \leq \frac{4\pi M_{ab}}{|r| - |r'| - |r''|} \left( |r' - r''|^{p+1} \right).
\]

(4.34)

Applying the above theorem, we can prove the convergence of the MEs in (3.22).

**Theorem 4.11.** Given \(r = (x, y, z)\) and \(r' = (x', y', z')\) be two points in the \(l\)-th and \(l'\)-th layer, i.e., \(d_\ell < z < d_{\ell-1}, d_{l'} < z' < d_{l'-1}\), respectively. Suppose \(r_c^s\) is a source center in the \(l\)-th layer such that \(|r' - r_c^s| < |\tau_{\ell\ell}^{ab}(r, r_c^s)|\), then the expansions in (3.22) hold and have the following error estimate

\[
|u_{\ell\ell}^{ab}(r, r') - \sum_{n=0}^{P} \sum_{m=-n}^{n} M_{nm}^{ab}\tau_{nm}^{ab}(r, r_c^s)| \leq \frac{(4\pi)^{-1} M_{\ell\ell}^{ab}}{|\tau_{\ell\ell}^{ab}(r, r_c^s)|} \left| |r' - r_c^s| \right|^{p+1},
\]

(4.35)

where \(M_{\ell\ell}^{ab}\) is the bound of \(\sigma_{\ell\ell}^{ab}(k_p)\) in the right half complex plane.

**Proof.** As in the analysis presented in the last subsection, it is more convenient to prove the expansions (3.18). Recalling definition (4.29) and (4.4), we obtain

\[
u_{\ell\ell}^{ab}(r, r') = \frac{1}{8\pi^2} \mathcal{I}(\sigma_{\ell\ell}^{ab}(r, r_c^s) + \tau(-r_c^s); \sigma_{\ell\ell}^{ab}), \quad \nu_{\ell\ell}^{ab}(r, r') = \frac{1}{8\pi^2} \mathcal{I}(\tau_{\ell\ell}^{ab}(r, r_c^s) - |r' - r_c^s|; \sigma_{\ell\ell}^{ab}).
\]

(4.36)

From definition (2.5), we can see that \(\tau_{\ell\ell}^{ab}(r, r_c^s)\) always have positive \(z\)-coordinates given \(r\) in the \(l\)-th layer and \(r_c^s\) in the \(l'\)-th layer. Moreover, Proposition 2.14 shows that the density function \(\sigma_{\ell\ell}^{ab}(k_p)\) is analytic and bounded in the right half complex plane \(\{k_p : \Re k_p > 0\}\). Together with the assumption \(|r' - r_c^s| < |\tau_{\ell\ell}^{ab}(r, r_c^s)|\), theorem 4.10 with density function \(\sigma_{\ell\ell}^{ab}(k_p)\) and coordinates groups \(\{\tau_{\ell\ell}^{ab}(r, r_c^s), \tau(-r_c^s)\}, \{\tau_{\ell\ell}^{ab}(r, r_c^s), -r_c^s\}\) can be applied. Therefore, we obtain

\[
u_{\ell\ell}^{ab}(r, r') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \mathcal{I}_n(\tau_{\ell\ell}^{ab}(r, r_c^s), \tau(-r_c^s); \sigma_{\ell\ell}^{ab}),
\]

\[
u_{\ell\ell}^{ab}(r, r') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \mathcal{I}_n(\tau_{\ell\ell}^{ab}(r, r_c^s), -r_c^s; \sigma_{\ell\ell}^{ab}).
\]

(4.37)

At the mean time, the error estimate (4.35) follows by applying (4.33) in (4.37). □

The convergence results in the above indicates an important fact that the error of the truncated ME is not determined by the Euclidean distance between source center \(r_c^s\) and target \(r\) as in the free space case (see Theorem 4.6). Actually, the distances along \(z\)-direction have been replaced by summations of the distances between \(r, r_c^s\) and corresponding nearest interfaces of the layered media.

Nevertheless, there are two special cases, i.e., \(|\tau_{\ell\ell+1}^{ab}(r, r_c^s)| = |r - r_c^s|\) if \(r\) and \(r_c^s\) are in the \(l\)-th and \((l+1)\)-th layer and \(|\tau_{\ell\ell-1}^{ab}(r, r_c^s)| = |r - r_c^s|\) if \(r\) and \(r_c^s\) are in the \(l\)-th and \((l-1)\)-th layer. Therefore, the MEs of \(u_{\ell\ell+1}^{ab}(r', r'')\) and \(u_{\ell\ell-1}^{ab}(r', r'')\) have the same convergence behavior as that of free space components.
On the other hand, the key idea of using hierarchical tree structure in FMM relies on using the Euclidean distance between source and target to determine either direct calculation or truncated ME is used for the computation of the interactions. In applying the free space FMM framework to handle the reaction field components of the layered Green’s function, the main problem is the MEs given in (3.22) are generally not compatible with the hierarchical tree structure design. In our previous work [9, 10], we have introduced the conception of equivalent polarization sources to overcome this problem. The idea was inspired by our
theoretical analysis for 2-dimensional Helmholtz equation (cf. [12]) and numerical tests for 3-dimensional Helmholtz/Laplace equations in layered media (cf. [9] [10]). Here, the theoretical results in [4.35] further verify the necessity of using the equivalent polarization sources.

According to the convergence results for MEs in Theorem 4.11, we introduce equivalent polarization sources for the four types of reaction fields (see, Fig. 4.2)

\[
\begin{align*}
\mathbf{r}'_{11} & := (x', y', d_\ell - (z' - d_\ell)), \\
\mathbf{r}'_{12} & := (x', y', d_\ell - (d_{\ell-1} - z')), \\
\mathbf{r}'_{21} & := (x', y', d_{\ell-1} + (z' - d_\ell)), \\
\mathbf{r}'_{22} & := (x', y', d_{\ell-1} + (d_{\ell-1} - z')).
\end{align*}
\]

(4.38)

With the equivalent polarization sources, we define reaction potentials

\[
\begin{align*}
\tilde{u}^{1b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}'_{1b}) & = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{k_{\rho}} e^{ik_r (\mathbf{r} - \mathbf{r}'_{1b})} \sigma^{1b}_{\ell}\ell' (k_{\rho}) dk_{x} dk_{y}, \\
\tilde{u}^{2b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}'_{2b}) & = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{1}{k_{\rho}} e^{ik_r (\mathbf{r} - \mathbf{r}'_{2b})} \sigma^{2b}_{\ell}\ell' (k_{\rho}) dk_{x} dk_{y},
\end{align*}
\]

(4.39)

where \(z_{ab}'\) denotes the \(z\)-coordinate of \(\mathbf{r}'_{ab}\), i.e.,

\[
\begin{align*}
z_{11}' & = d_\ell - (z' - d_\ell), \\
z_{12}' & = d_\ell - (d_{\ell-1} - z'), \\
z_{21}' & = d_{\ell-1} + (z' - d_\ell), \\
z_{22}' & = d_{\ell-1} + (d_{\ell-1} - z').
\end{align*}
\]

(4.40)

Apparently, we can verify that

\[
\tau^{1b}_{\ell}\ell' (\mathbf{r}, \mathbf{r}') = \mathbf{r} - \mathbf{r}'_{1b}, \\
\tau^{2b}_{\ell}\ell' (\mathbf{r}, \mathbf{r}') = \mathbf{r} - \mathbf{r}'_{2b}, \quad b = 1, 2.
\]

(4.41)

Therefore, the reaction components of layered Green’s function defined in (2.4) is equal to the introduced reaction potentials associated to equivalent polarization sources, i.e.,

\[
\begin{align*}
u^{1b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}') = \tilde{u}^{1b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}'_{1b}), \\
u^{2b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}') = \tilde{u}^{2b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}'_{2b}), \quad b = 1, 2.
\end{align*}
\]

(4.42)

In the FMM for reaction components (cf. [9]), the expressions (4.39) with equivalent polarization sources (4.38) are actually used. MEs, LEs and M2L translations for re-expressed reaction field components (4.39) are adopted in the FMM and we have verified numerically that the convergence of the MEs, LEs and M2L translations of (4.39) are determined by the Euclidean distance between targets and equivalent polarization source. In the next two subsections, we first review the MEs, LEs and M2Ls for the re-expressed reaction field components (4.39) and then prove that all of them have exponential convergence with rates depends on the Euclidean distance between targets and equivalent polarization sources.

4.3. MEs, LEs, and M2L translations for reaction field components using new expressions with equivalent polarization sources. By the definition (4.29) and the linear features (3.17) of \(\tau (\mathbf{r})\), the reaction components in (4.39) can be represented as

\[
\begin{align*}
\tilde{u}^{1b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}'_{1b}) & = \frac{1}{8\pi^2} \mathcal{I}(\mathbf{r} - \mathbf{r}'_{1b} - (\mathbf{r}'_{1b} - \mathbf{r}'_{1b})); \sigma^{1b}_{\ell}\ell' (k_{\rho}) \\
\tilde{u}^{2b}_{\ell}\ell'(\mathbf{r}, \mathbf{r}'_{2b}) & = \frac{1}{8\pi^2} \mathcal{I}(\mathbf{r} - \mathbf{r}'_{2b} - \mathbf{r}'_{2b}); \sigma^{2b}_{\ell}\ell' (k_{\rho}),
\end{align*}
\]

(4.43)

where \(\mathbf{r}'_{ab} = (x_{ab}', y_{ab}', z_{ab}')\) and \(\mathbf{r}'_{c} = (x_{c}', y_{c}', z_{c}')\) are given equivalent polarization source and target centers such that

\[
\begin{align*}
z_{1b} & < d_\ell, \\
z_{2b} & > d_{\ell-1}, \\
d_\ell & < z_{c} < d_{\ell-1}.
\end{align*}
\]

(4.44)

These restriction can be met in practice, as we are considering targets in the \(\ell\)-th layer and the equivalent polarized coordinates are always located either above the interface \(z = d_{\ell-1}\) or below the interface \(z = d_\ell\).

By (4.40) and conditions in (4.44), we have

\[
\begin{align*}
z - z_{1b} & > 0, \\
z_{c} - z_{1b} & > 0, \\
z_{2b} - z & > 0, \\
z_{2b} - z_{c} & > 0, \\
z - z_{1b} & > 0, \\
z_{2b} - z & > 0.
\end{align*}
\]

(4.45)
Assume the centers $r_{c}^{a}b$ and $r_{b}^{a}$ satisfy $|r - r_{b}^{a}| > |r_{c}^{a} - r_{c}^{b}|$, and $|r - r_{c}^{a}| < |r_{c}^{a} - r_{b}^{a}|$, then \[ (4.45) \] and Proposition 2.1 implies that theorem \[ (4.10) \] can be applied to give expansions for the integrals in \[ (4.43) \], i.e.,

\[
\hat{u}_{\ell^2}^{1b}(r, r_{1b}') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r - r_{1b}')} \left[ -\frac{i k \cdot (r_{1b}' - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{1b}(k) dk_x dk_y,
\]

\[
\hat{u}_{\ell^2}^{2b}(r, r_{2b}') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r - r_{2b}')} \left[ -\frac{i k \cdot \tau(r_{2b}' - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{2b}(k) dk_x dk_y,
\]

and

\[
\hat{u}_{\ell^2}^{1b}(r, r_{1b}') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r_{1b}' - r_{c}^{b})} \left[ \frac{i k \cdot \tau(r_{1b}' - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{1b}(k) dk_x dk_y,
\]

\[
\hat{u}_{\ell^2}^{2b}(r, r_{2b}') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot \tau(r_{2b}' - r_{c}^{b})} \left[ \frac{i k \cdot \tau(r_{2b}' - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{2b}(k) dk_x dk_y.
\]

Further, applying Proposition 3.5 in expansions \[ (4.46) \] and using identities \[ (3.21) \] again to simplify the obtained results, we obtain MEs

\[
\hat{u}_{\ell^2}^{1b}(r, r_{1b}') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot \tau(r_{c}^{a} - r_{c}^{b})} \left[ \frac{i k \cdot \tau(r_{c}^{a} - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{1b}(k) dk_x dk_y,
\]

and

\[
\hat{u}_{\ell^2}^{2b}(r, r_{2b}') = \frac{1}{8\pi^2} \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot \tau(r_{c}^{a} - r_{c}^{b})} \left[ \frac{i k \cdot \tau(r_{c}^{a} - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{2b}(k) dk_x dk_y.
\]

at target center $r_{c}^{a}$, respectively. Here, \[ \hat{F}_{nm}(r, r_{c}^{a}) \] are represented by Sommerfeld-type integrals

\[
\hat{F}_{nm}^{1b}(r, r_{c}^{a}) = \frac{\omega_{n}}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r - r_{c}^{a})} k^{n-1} e^{-i\omega_{n} \alpha} dk_x dk_y,
\]

\[
\hat{F}_{nm}^{2b}(r, r_{c}^{a}) = \frac{\omega_{n}}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r - r_{c}^{a})} k^{n-1} e^{-i\omega_{n} \alpha} dk_x dk_y,
\]

and the expansion coefficients are given by

\[
I_{nm}^{1b} = \frac{\omega_{n}}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r_{c}^{a} - r_{c}^{b})} k^{n-1} e^{-i\omega_{n} \alpha} dk_x dk_y,
\]

\[
I_{nm}^{2b} = \frac{\omega_{n}}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r_{c}^{a} - r_{c}^{b})} k^{n-1} e^{-i\omega_{n} \alpha} dk_x dk_y,
\]

Next, we discuss the center shifting and translation operators for ME \[ (4.48) \] and LE \[ (4.49) \]. A desirable feature of the expansions of reaction components discussed above is that the formula \[ (4.48) \] for the ME coefficients and the formula \[ (4.49) \] for the LE have exactly the same form as the formulas of ME coefficients and LE for free space Green’s function. Therefore, we can see that center shifting for multipole and local expansions are exactly the same as free space case given in \[ (3.14) \].

We only need to derive the translation operator from ME \[ (4.48) \] to LE \[ (4.49) \]. As in \[ (4.39) \], the reaction components in \[ (4.39) \] can be represented as

\[
\hat{u}_{\ell^2}^{1b}(r, r_{1b}') = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r - r_{c}^{a})} \left[ \frac{i k \cdot \tau(r_{1b}' - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{1b}(k) dk_x dk_y,
\]

\[
\hat{u}_{\ell^2}^{2b}(r, r_{2b}') = \frac{1}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik \cdot (r - r_{c}^{a})} \left[ \frac{i k \cdot \tau(r_{2b}' - r_{c}^{b})}{n! k^2} \right] \sigma_{\ell^2}^{2b}(k) dk_x dk_y.
\]
Apparently, from (4.44), we have
\[ z_c^I - z_c^{1b} > 0, \quad z_c^{2b} - z_c^I > 0. \]
Assume the given centers \( r_{ab} \) and \( r_c^I \) satisfy \( |r_c^I - r_{2b}^c| > |r_{ab}^c - r_c^{1b}| + |r - r_c^I| \), then (4.45), (4.53) and Proposition 2.1 implies that Theorem 4.10 can be applied to give expansions for the integrals in (4.52), i.e.,
\[ \hat{u}_{\ell\ell'}^{1b}(r, r_{1b}') = \frac{1}{8\pi^2} \sum_{m=0}^{\infty} \sum_{\nu=0}^{\infty} \mathcal{I}_{n\nu}(r_c^I - r_{1b}^c, r - r_c^I, -r_{1b}' - r_c^{1b}); \sigma_{\ell\ell'}^{1b}, \]
\[ \hat{u}_{\ell\ell'}^{2b}(r, r_{2b}') = \frac{1}{8\pi^2} \sum_{m=0}^{\infty} \sum_{\nu=0}^{\infty} \mathcal{I}_{n\nu}(r_c^I - r_{2b}^c, r - r_c^I, -r_{2b}' - r_c^{1b}); \sigma_{\ell\ell'}^{2b}. \]
Applying Proposition 3.5 to the integrand of \( \mathcal{I}_{n\nu}(r, r', \rho, \sigma) \), we obtain the translation from \( \text{ME} \) (4.48) to \( \text{LE} \) (4.49), i.e.,
\[ L_{nm}^{ab} = \sum_{n'=0}^{\infty} \sum_{|m'|=0}^{n'} T_{nm, nm'}^{ab} M_{n'm'}^{ab}, \]
where the translation operators are given as follows
\[ T_{nm, nm'}^{1b} = \frac{D_1^{nmn'm'}}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(r_c^I - r_{1b}^c)} \sigma_{\ell\ell'}^{1b}(k_p) k^{n+n'-1} e^{i(m'-m)\alpha} dk_xdk_y, \]
\[ T_{nm, nm'}^{2b} = \frac{D_2^{nmn'm'}}{2\pi} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(r_c^I - r_{2b}^c)} \sigma_{\ell\ell'}^{2b}(k_p) k^{n+n'-1} e^{i(m'-m)\alpha} dk_xdk_y, \]
where
\[ D_1^{nmn'm'} = (-1)^n c_n^2 C_{n'}^{m} C_{m'}^{n'}, \quad D_2^{nmn'm'} = (-1)^{n+m+m'} c_{n'}^2 C_{n'}^{m} C_{n}^{m'}. \]

4.4. Exponential convergence of MEs, LEs and corresponding translation operators for reaction components. Let \( \Phi_{\ell\ell', \text{in}}^{ab}(r) \) and \( \Phi_{\ell\ell', \text{out}}^{ab}(r) \) be general reaction components of potentials induced by all equivalent polarization sources inside a given source box \( B_{ab} \) centered at \( r_{ab} \) and far away from a given target box \( B_t \), i.e.,
\[ \Phi_{\ell\ell', \text{in}}^{ab}(r) = \sum_{j \in \mathcal{J}} Q_{\ell j} \hat{u}_{\ell\ell'}^{ab}(r, r_{\ell j}), \quad \Phi_{\ell\ell', \text{out}}^{ab}(r) = \sum_{j \in \mathcal{K}} Q_{\ell j} \hat{u}_{\ell\ell'}^{ab}(r, r_{\ell j}), \]
where \( \mathcal{J} \) and \( \mathcal{K} \) are the sets of indices of equivalent polarization sources inside \( B_{ab} \) and far away from \( B_t \), respectively. The FMM for the reaction component \( \Phi_{\ell\ell'}^{ab}(r) \) use ME
\[ \Phi_{\ell\ell', \text{in}}^{ab}(r) = \sum_{m=0}^{n} \sum_{m'=0}^{n} M_{nm, nm'}^{ab, \text{in}} F_{nm}^{ab}(r, r_{ab}), \]
\[ \Phi_{\ell\ell', \text{out}}^{ab}(r) = \sum_{m=0}^{n} \sum_{m'=0}^{n} L_{nm, nm'}^{ab, \text{out}} r_{\ell}^n Y_{m}^n(\theta, \varphi), \]
inside \( B_t \), where the coefficients are given by
\[ M_{nm}^{ab, \text{in}} = \frac{c_n^{-2}}{4\pi} \sum_{j \in \mathcal{J}} Q_{\ell j} (r_{\ell j})^{n} Y_{m}^n(\theta_{\ell j}, \varphi_{\ell j}), \]
\[ L_{nm}^{1b, \text{out}} = \frac{C_{nm}}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(r_r^I - r_{2b}^c)} \sigma_{\ell\ell'}^{1b}(k_p) k^{n-1} e^{-i\alpha} dk_xdk_y, \]
\[ L_{nm}^{2b, \text{out}} = \frac{(-1)^{n+m+m'}}{8\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{ik(r_r^I - r_{1b}^c)} \sigma_{\ell\ell'}^{2b}(k_p) k^{n-1} e^{-i\alpha} dk_xdk_y, \]
(r_t, \theta_t, \phi_t) and (r_{c_t}, \theta_{c_t}, \phi_{c_t}) are the spherical coordinates of \( r - r_c \) and \( r_{c_t} - r_{c} \). These expansions can be obtained by applying expansions (4.48)-(4.49) to each \( \tilde{u}_{c_t}^\ell(r, r_{c_t}) \) involved in the summations in (4.57).

Source box B^3

\[ \Phi_{\ell'}(r) = \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{s\ell'} \tilde{F}_{nm}(r, r_{c_t}) \]

Target box B

The \( \ell \)-th layer

Source box B^3

\[ \Phi_{\ell'}(r) = \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{s\ell'} \tilde{F}_{nm}(r, r_{c_t}) \]

\[ Q_{J} = \sum_{j \in J} |Q_{\ell'}| \]

**Theorem 4.12.** Suppose \( a_{s}^{ab} \) is the radius of the circumscribed sphere of the source box \( B_{s}^{ab} \), \( r \) is a point outside the circumscribed sphere of \( B_{s}^{ab} \), i.e., \( r_{s}^{ab} := |r - r_{c}^{ab}| > a_{s}^{ab} \), then ME (4.58) has error estimate

\[ \left| \Phi_{\ell'}(r) - \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{s\ell'} \tilde{F}_{nm}(r, r_{c_t}) \right| \leq \frac{1}{4\pi} \frac{Q_{J} M_{s\ell'}(a_{s}^{ab})}{r_{s}^{ab} - a_{s}^{ab}} (\frac{a_{s}^{ab}}{r_{s}^{ab}})^{p+1}, \]

where \( M_{s\ell'} \) is the bound of \( \sigma_{s\ell'}(k_{\mu}) \) in the right half complex plane.

**Proof.** As the MEs (4.48) are obtained by directly applying Proposition 3.5 to the Taylor expansions (4.46), we have

\[ \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{1b\ell'} \tilde{F}_{nm}(r, r_{c_t}^{1b}) = \frac{1}{8\pi^2} \sum_{j \in J} Q_{\ell'} j \sum_{n=0}^{p} \tilde{I}_{n}(r - r_{c_t}^{1b}, -(r_{c_t}^{1b} - r_{c_t}^{1b}); \sigma_{1b\ell'})(r_{c_t}^{1b}), \]

\[ \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{2b\ell'} \tilde{F}_{nm}(r, r_{c_t}^{2b}) = \frac{1}{8\pi^2} \sum_{j \in J} Q_{\ell'} j \sum_{n=0}^{p} \tilde{I}_{n}(r - r_{c_t}^{2b}, -(r_{c_t}^{2b} - r_{c_t}^{2b}); \sigma_{2b\ell'})(r_{c_t}^{2b}). \]
By conditions in (4.45), we have \( z - z_c^{1b} > 0 \) and \( z_c^{2b} - z > 0 \). Together with the assumption \(|r - r_c^{ab}| > a_t^{ab} \geq |r_{c_{ij}}^{ab} - r_{c_{ij}}^{ab}|\), we can apply the truncation error estimates (4.33) to obtain

\[
\left| \Phi_{t',in}^{ab}(r) - \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{1b} \bar{J}_{nm}(r, r_c^{1b}) \right|
\leq \frac{1}{8\pi^2} \sum_{j \in J} |Q_{t'}| \left| I(r, r_{t'}^{1b}; \sigma_{t'}^{1b}) - \sum_{n=0}^{p} T_{n}(r - r_c^{1b}, -(r_{t'}^{1b} - r_c^{1b}); \sigma_{t'}^{1b}) \right|,
\]

and similarly

\[
\left| \Phi_{t',in}^{2b}(r) - \sum_{n=0}^{p} \sum_{m=-n}^{n} M_{nm}^{2b} \bar{J}_{nm}(r, r_c^{2b}) \right| \leq \sum_{j \in J} \left| Q_{t'} \right| (4\pi)^{-1} |M_{\sigma_{t'}^{2ab}}| \frac{|r_{t'}^{2b} - r_c^{2b}|}{|r - r_c^{2b}|}^{p+1}.
\]

Consequently, the error estimate (4.61) follows by applying the above estimates in (4.63) with the assumption \(|r_{c_{ij}}^{ab} - r_{c_{ij}}^{ab}| < a_t^{ab} < r_{c_{ij}}^{ab}\).

Following a similar proof, we have the error estimate for the truncated LE as follows:

**Theorem 4.13.** Suppose \( a_t \) is the radius of the circumscribed sphere of the target box \( B_t \), \( r \) is a point inside \( B_t \), \( K \) is the set of indices of all charges \((Q_{t'}, r_{t'}^{ab})\) such that \(|r_{t'}^{ab} - r_c^{ab}| > a_t\), then the LE (4.59) has error estimate

\[
\left| \Phi_{t',in}^{ab}(r) - \sum_{n=0}^{P} \sum_{m=-n}^{n} L_{nm}^{ab} \bar{J}_{nm}(r, r_c^{ab}) \right| \leq \frac{|Q_K| M_{\sigma_{t'}^{ab}}}{a_t |r_c^{ab}|} \frac{|r_{c_i}^{ab} - r_c^{ab}| |r - r_c^{ab}|^{p+1}},
\]

where \( M_{\sigma_{t'}^{ab}} \) is the bound of \( \sigma_{t'}^{ab}(k_t) \) in the right half complex plane,

\[
Q_K = \sum_{j \in K} |Q_{t'}|.
\]

Now we consider the error estimate for the ME to LE translation. Suppose the target box \( B_t \) is far away from the source box \( B_{t'}^{ab} \). Recall (4.49), the LE of the potential \( \Phi_{t',in}^{ab} \) in \( B_t \) is given by

\[
\Phi_{t',in}^{ab}(r) = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} L_{nm}^{ab} \bar{J}_{nm}(r, r_c^{ab}), \quad \forall r \in B_t,
\]

while the LE coefficients \( L_{nm}^{ab} \) can be calculated from ME coefficients via the ME to LE translation operator (4.55) as follows

\[
L_{nm}^{ab} = \sum_{\nu=0}^{\infty} \sum_{\mu=-\nu}^{\nu} T_{nm,\nu\mu} M_{\nu\mu}^{ab}.
\]

As in the FMM for free space components, (4.66) is not the approximation used in the implementation. In fact, the formulas (4.67) for LE coefficients \( L_{nm}^{ab} \) are truncated which gives approximated LE coefficients

\[
L_{nm}^{ab} = \sum_{\nu=0}^{P} \sum_{\mu=-\nu}^{\nu} T_{nm,\nu\mu} M_{\nu\mu}^{ab}.
\]
Thus, approximate LEs
\[ \Phi_{\ell',\ell}^{ab,p}(\mathbf{r}) \approx \Phi_{\ell',\ell}^{ab,p}(\mathbf{r}) := \sum_{n=-m}^{p} \sum_{m=-n}^{n} T_{nm}^{ab,p} r^{n} y^{m}(\theta_{t}, \varphi_{t}) \quad (4.69) \]
with approximate LE coefficients defined in (4.68) are obtained after M2L translation. Recalling representation (4.52) and expansion (4.54), the approximate LEs \( \Phi_{\ell',\ell}^{ab,p}(\mathbf{r}) \) have representations
\[ \Phi_{\ell',\ell}^{ab,p}(\mathbf{r}) = \frac{1}{8\pi^{2}} \sum_{j \in \mathcal{J}} Q_{\ell'} J_{\ell'}^{ab} r^{p} \sum_{\nu=0}^{p} \mathcal{I}_{\nu\nu}(r_{c}^{t} - r_{c}^{1b}, r - r_{c}^{t} - (r_{c}^{1b} - r_{c}^{1b}); \sigma_{\ell'}^{ab}), \]
\[ \Phi_{\ell',\ell}^{2b,p}(\mathbf{r}) = \frac{1}{8\pi^{2}} \sum_{j \in \mathcal{J}} Q_{\ell'} J_{\ell'}^{2b} r^{p} \sum_{\nu=0}^{p} \mathcal{I}_{\nu\nu}(r_{c}^{t} - r_{c}^{2b}, \tau(r - r_{c}^{t}), \tau(r_{c}^{2b} - r_{c}^{2b}); \sigma_{\ell'}^{2b}). \]

(4.70)

Obviously, they are rectangular truncation of the double Taylor series.

**Theorem 4.14.** Suppose \( a_{s}^{ab} \) and \( a_{t} \) are the radii of the circumscribed spheres of two well separated boxes \( B_{a}^{s} \) and \( B_{t} \), respectively. The well separateness of the boxes means that \( |r_{c}^{p} - r_{c}^{ab}| > a_{s}^{ab} + c a_{t} \) with some \( c > 1 \). Then, the ME to LE translation has error estimate
\[ \left| \Phi_{\ell',\ell}^{ab}(\mathbf{r}) - \Phi_{\ell',\ell}^{ab,p}(\mathbf{r}) \right| \leq \frac{1}{2\pi} Q_{\mathcal{J}} M_{\sigma_{\ell'}^{ab}} \left( \frac{a_{s} + a_{t}}{a_{s} + c a_{t}} \right)^{p+1}, \forall \mathbf{r} \in B_{t}, \quad (4.71) \]
where \( M_{\sigma_{\ell'}^{ab}} \) is the bound of \( \sigma_{\ell'}^{ab}(k_{\mu}) \) in the right half complex plane, \( Q_{\mathcal{J}} \) is defined in (4.62).

**Proof.** By expression (4.70) and truncation error estimate (4.34), we obtain
\[ \left| \Phi_{\ell',\ell}^{ab}(\mathbf{r}) - \Phi_{\ell',\ell}^{ab,p}(\mathbf{r}) \right| \leq \frac{1}{8\pi^{2}} \sum_{j \in \mathcal{J}} Q_{\ell'} \left| I(r - r_{c}^{1b}; \sigma_{\ell'}^{ab}) - \sum_{n=0}^{p} \sum_{\nu=0}^{p} \mathcal{I}_{\nu\nu}(r_{c}^{t} - r_{c}^{1b}, r - r_{c}^{t} - (r_{c}^{1b} - r_{c}^{1b}); \sigma_{\ell'}^{ab}) \right| \]
\[ \leq \sum_{j \in \mathcal{J}} \frac{1}{2\pi} Q_{\ell'} M_{\sigma_{\ell'}^{ab}} \left( \frac{|r - r_{c}^{1b}| + |r_{c}^{1b} - r_{c}^{1b}|}{|r - r_{c}^{1b}|} \right)^{p+1}. \quad (4.72) \]

Similar error estimate can also be obtained for the reaction component \( \Phi_{\ell',\ell}^{ab}(\mathbf{r}) \) by following the same derivations. Consequently, the error estimate (4.71) follows by further applying the assumptions \( |r_{c}^{ab} - r_{c}^{ab}| < a_{s}^{ab} \) and \( |r_{c}^{1b} - r_{c}^{1b}| < a_{t} \) and \( |r_{c}^{1b} - r_{c}^{1b}| > a_{s}^{ab} + c a_{t} \). \( \square \)

**Remark 4.1.** The error estimates in Theorems 4.12, 4.14 are almost the same as the ones in Theorems 4.6, 4.7 and 4.9 except the bound \( M_{\sigma_{\ell'}^{ab}} \) of \( \sigma_{\ell'}^{ab} \).

**4.5. Detailed proof for the Theorem 4.10.** The proof consists of the following three steps:

**Step 1:** Rotation according to the azimuthal angle of \( \mathbf{r} \). By the assumptions \( z > 0, z' > 0 \) and \( z + z' + z'' > 0 \), all improper integrals used in the Theorem 4.10 are convergent. Denote by \((\rho, \phi)\) the polar coordinate of \((x, y)\) and define rotational transform \( \xi = k_{x} \cos \phi + k_{y} \sin \phi, \eta = k_{x} \sin \phi - k_{y} \cos \phi \), i.e., \( \xi + i \eta = e^{i\phi}(k_{x} - ik_{y}) \). It is obvious that \( k_{x}^{2} = \xi^{2} + \eta^{2} \) and
\[ \frac{(ik \cdot \hat{r})^{q}}{q!} = \frac{\hat{g}_{q}(\xi, \eta, \phi; \hat{r})}{q!} \left[ \xi \cos(\phi - \beta) + \eta \sin(\phi - \beta) \right]^{q} \sin \alpha \cos \alpha : \right. \quad (4.73)
for any $\vec{r} = (\hat{r} \sin \alpha \cos \beta, \hat{r} \sin \alpha \sin \beta, \hat{r} \cos \alpha) \in \mathbb{R}^3$. Therefore, (4.30) can be re-expressed as

$$I(r + r'; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \hat{g}_n(\xi, \eta, \phi; r') e^{i \xi \rho - \zeta z} \sigma(\zeta) d\xi d\eta$$

(4.74)

and

$$I(r + r' + r''; \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \sum_{\nu=0}^{\infty} g_{\nu n}(\xi, \eta, \phi; r', r'') e^{i \xi \rho - \zeta z} \sigma(\zeta) d\xi d\eta$$

(4.75)

where

$$\zeta = \sqrt{\xi^2 + \eta^2}, \quad g_{\nu n}(\xi, \eta, \phi; r', r'') := \frac{1}{\zeta} \hat{g}_n(\xi, \eta, \phi; r') \hat{g}_n(\xi, \eta, \phi; r'')$$

(4.76)

Define

$$\mathcal{E}_n(r, r', \sigma) = \int_{-\infty}^{\infty} \hat{g}_n(\xi, \eta, \phi; r') e^{i \xi \rho - \zeta z} \sigma(\zeta) d\xi d\eta,$$

$$\mathcal{E}_n(r, r', \sigma) = \int_{-\infty}^{\infty} \hat{g}_n(\xi, -\eta, \phi; r') e^{i \xi \rho - \zeta z} \sigma(\zeta) d\xi d\eta,$$

(4.77)

and

$$\mathcal{F}_{\nu n}(r, r', r'', \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g_{\nu n}(\xi, \eta, \phi; r', r'') e^{i \xi \rho - \zeta z} \sigma(\zeta) d\xi d\eta,$$

$$\mathcal{F}_{\nu n}(r, r', r'', \sigma) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g_{\nu n}(\xi, -\eta, \phi; r', r'') e^{i \xi \rho - \zeta z} \sigma(\zeta) d\xi d\eta.$$  

(4.78)

Then, the integrals in (4.31) have representations

$$\mathcal{I}_n(r + r'; \sigma) = \mathcal{E}_n(r, r', \sigma) + \mathcal{E}_n(r, r', \sigma),$$

$$\mathcal{I}_{\nu n}(r + r' + r''; \sigma) = \mathcal{F}_{\nu n}(r, r', r'', \sigma) + \mathcal{F}_{\nu n}(r, r', r'', \sigma).$$

(4.79)

**Step 2: Contour deformation.** In the following analysis, we will deform the contour of the inner integral in (4.74)-(4.75). As the integrands involve square root function $\zeta(\xi) = \sqrt{\xi^2 + \eta^2}$, we choose branch as follow

$$\sqrt{z} = \sqrt{\frac{|z| + z_1}{2}} + i \text{sign}(z_2) \sqrt{\frac{|z| - z_1}{2}}, \quad \forall z = z_1 + iz_2 \in \mathbb{C}.$$  

(4.80)

With this branch, $\zeta(\xi) = \sqrt{\xi^2 + \eta^2}$ for any fixed $\eta \geq 0$ has branch cut along $\{i \xi : \xi > \eta\}$ and $\{i \xi : \xi < \eta\}$ (the red lines in Fig. 4.5) in the complex $\xi$-plane and is analytic with respect to $\xi$ in the complex domain $\mathbb{C} \setminus (\{i \xi : \xi \geq \eta\} \cup \{i \xi : \xi \leq \eta\})$. The contour deformation will be based on the following lemma:

**Lemma 4.2.** Denote by $\Omega_1^+ \subset \mathbb{C}$ the complex domain between real axis and the contour $\Gamma$ defined by the parametric $\xi(t)$ in (4.82). Let $f(\xi)$ be an analytic function in $\Omega_1^+$ and satisfy $|f(\xi)| \leq C|\xi|^m$ for some integer $m$ and some constant $C > 0$. Then for any $\rho \geq 0, z > 0$ and $\eta > 0$, there holds

$$\int_{-\infty}^{\infty} f(\xi)e^{i \xi \rho - \sqrt{\eta^2 + \xi^2}} d\xi = i \int_1^{\infty} [f(\xi_+(t))\Lambda_+(t) + f(\xi_-(t))\Lambda_-(t)] \frac{e^{-\eta t}}{\sqrt{t^2 - 1}} dt,$$  

(4.81)
where \( r = \sqrt{\rho^2 + z^2} \), and \( \xi_{\pm}(t), \Lambda_{\pm}(t) \) are defined by the Cagniard-de Hoop transform

\[
\xi_{\pm}(t) = \frac{\eta}{r} (ipt \pm z \sqrt{t^2 - 1}), \quad \Lambda_{\pm}(t) = \frac{\eta}{r} (\rho \sqrt{t^2 - 1} \mp izt).
\]

(4.82)

**Proof.** Define a hyperbolic integral path \( \Gamma = \Gamma_+ \cup \Gamma_- \), where

\[
\Gamma_\pm = \{ \xi_{\pm}(t) : t \geq 1 \}.
\]

For any \( R > 0 \), let \( O_R^+ \) and \( O_R^- \) be the parts of the circle \( \{ \xi : |\xi| = R \} \) that are bounded by the real axis and \( \Gamma_\pm \), respectively (see Fig. 4.5). Denote by \( \xi(t_R^\pm) = Re^{i\theta_R} \) the intersections of \( O_R^+ \) and \( \Gamma_\pm \). Then, \( 0 < \theta_R^+ < \frac{\pi}{2}, \frac{\pi}{2} < \theta_R^- < \pi \) and

\[
\int_{O_R^+} f(\xi)e^{i\xi - \sqrt{\eta^2 + \xi^2}z}d\xi = i \int_0^{\theta_R^+} f(Re^{i\theta})e^{-R\rho \sin \theta - \Re \zeta(\theta)z} e^{i(R\rho \cos \theta - 3m(\theta)z)} R e^{i\theta} d\theta,
\]

\[
\int_{O_R^-} f(\xi)e^{i\xi - \sqrt{\eta^2 + \xi^2}z}d\xi = i \int_{\theta_R^-}^{\pi} f(Re^{i\theta})e^{-R\rho \sin \theta - \Re \zeta(\theta)z} e^{i(R\rho \cos \theta - 3m(\theta)z)} R e^{i\theta} d\theta,
\]

(4.83)

where \( \zeta(\theta) = \sqrt{\eta^2 + R^2 e^{2i\theta}} \). Choosing the branch according to (4.80) gives a lower bound

\[
\Re \zeta(\theta) = \sqrt{\frac{(\eta^2 + R^2 \cos 2\theta)^2 + R^4 \sin^2 2\theta + \eta^2 + R^2 \cos 2\theta}{2}} \geq R|\cos \theta|.
\]

(4.84)

Noting that \( 0 < \theta_R^+ < \frac{\pi}{2}, \frac{\pi}{2} < \theta_R^- < \pi \) and \( z > 0 \), we have

\[
\cos \theta_R^+ = \frac{z \sqrt{t_R^+ - 1}}{\sqrt{\rho^2 t_R^+ + z^2(t_R^+ - 1)}} > \frac{z}{r} \sqrt{1 - \frac{1}{t_R^+}} \geq \frac{\sqrt{3}}{2} \frac{z}{r},
\]

(4.85)
for all $R$ such that $t_R \geq 2$. Thus
\begin{align}
\Re \zeta(t) & = R \cos \theta_R^+ > \frac{\sqrt{3}}{2} \frac{R^\frac{3}{2}}{r}, \quad 0 \leq \theta \leq \theta_R^+, \\
\Re \zeta(t) & = -R \cos \theta_R^- > \frac{\sqrt{3}}{2} \frac{R^\frac{3}{2}}{r}, \quad \theta_R^- \leq \theta \leq \pi,
\end{align} \tag{4.86}
if $t_R \geq 2$. Applying the above estimates in (4.83) and then using the assumption $z > 0$, we obtain
\begin{align}
\left| \int_{O_R^+} f(\xi)e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} d\xi \right| \leq CR^{m+1} e^{-\frac{\sqrt{3}}{2} R} \to 0, \quad R \to \infty. \tag{4.87}
\end{align}

By choosing the branch (4.80), the square root function $\sqrt{\eta^2 + \xi^2}$ have branch cut along $\{i\xi > \eta\}$ and $\{i\xi < -\eta\}$ (see Fig. 4.5). Therefore, $f(\xi)e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z}$ is analytic in the domain $\Omega_R^+$ for any fixed $\eta > 0$. By Cauchy’s theorem, (4.81) follows from the facts
\begin{align}
&\int_{-\infty}^{\infty} f(\xi)e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} d\xi = \int_{\Gamma} f(\xi)e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} d\xi, \quad \forall \eta > 0, \tag{4.88}
\end{align}
and
\begin{align}
\frac{d\xi(t)}{dt} = \frac{\eta}{r\sqrt{t^2 - 1}} (i\rho \sqrt{t^2 - 1} \pm z t) = \frac{i\Lambda(t)}{\sqrt{t^2 - 1}}. \tag{4.89}
\end{align}

In order to deform the contour of the inner integrals from the real axis to the contour $\Gamma$ defined in lemma 4.2, $\eta$ is not allowed to touch 0. Therefore, we define sequences
\begin{align}
\mathcal{E}^k(r, r'; \sigma) = & \int_{\tau}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} g_n(\xi, \eta, \phi; r') e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} \sigma(\xi) d\xi d\eta, \\
\mathcal{E}^k(r, r'; \sigma) = & \int_{\tau}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} g_n(\xi, -\eta, \phi; r') e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} \sigma(\xi) d\xi d\eta, \tag{4.90}
\end{align}
and
\begin{align}
\mathcal{F}^k(r, r', r''; \sigma) = & \int_{\tau}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \sum_{\nu=0}^{\infty} g_{n\nu}(\xi, \eta, \phi; r', r'') e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} \sigma(\xi) d\xi d\eta, \\
\mathcal{F}^k(r, r', r''; \sigma) = & \int_{\tau}^{\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \sum_{\nu=0}^{\infty} g_{n\nu}(\xi, -\eta, \phi; r', r'') e^{i\xi \rho - \sqrt{\eta^2 + \xi^2} z} \sigma(\xi) d\xi d\eta, \tag{4.91}
\end{align}
for $k = 1, 2, \ldots$. Further, their limit values are denoted by
\begin{align}
\mathcal{E}(r, r'; \sigma) := & \lim_{k \to \infty} \mathcal{E}^k(r, r'; \sigma), \quad \mathcal{F}(r, r', r''; \sigma) := \lim_{k \to \infty} \mathcal{F}^k(r, r', r''; \sigma), \\
\mathcal{E}(r, r'; \sigma) := & \lim_{k \to \infty} \mathcal{E}^k(r, r'; \sigma), \quad \mathcal{F}(r, r', r''; \sigma) := \lim_{k \to \infty} \mathcal{F}^k(r, r', r''; \sigma). \tag{4.92}
\end{align}

Then,
\begin{align}
\mathcal{I}(r + r'; \sigma) = & \mathcal{E}(r, r', \sigma) + \mathcal{E}(r, r'; \sigma), \\
\mathcal{I}(r + r' + r''; \sigma) = & \mathcal{F}(r, r', r''; \sigma) + \mathcal{F}(r, r', r''; \sigma). \tag{4.93}
\end{align}
Accordingly, we also define

\[
\begin{align*}
\mathcal{E}^k_n(r, r', \sigma) &= \int_{\frac{1}{2}}^{\infty} \int_{-\infty}^{\infty} \hat{g}_n(\xi, \eta, \phi; r') e^{i\xi r - \zeta \eta} \sigma(\xi) d\xi d\eta, \\
\widetilde{\mathcal{E}}^k_n(r, r', \sigma) &= \int_{\frac{1}{2}}^{\infty} \int_{-\infty}^{\infty} \hat{g}_n(\xi, -\eta, \phi; r') e^{i\xi r - \zeta \eta} \sigma(\xi) d\xi d\eta, \\
\mathcal{F}^k_{\nu\nu}(r, r', r'', \sigma) &= \int_{\frac{1}{2}}^{\infty} \int_{-\infty}^{\infty} g_{\nu\nu}(\xi, \eta, \phi; r', r'') e^{i\xi r - \zeta \eta} \sigma(\xi) d\xi d\eta, \\
\widetilde{\mathcal{F}}^k_{\nu\nu}(r, r', r'', \sigma) &= \int_{\frac{1}{2}}^{\infty} \int_{-\infty}^{\infty} g_{\nu\nu}(\xi, -\eta, \phi; r', r'') e^{i\xi r - \zeta \eta} \sigma(\xi) d\xi d\eta,
\end{align*}
\]

(4.94)

while the integrals in (4.77)-(4.78) are their limit values, i.e.,

\[
\begin{align*}
\mathcal{E}_n(r, r', \sigma) &= \lim_{k \to \infty} \mathcal{E}^k_n(r, r', \sigma), \quad \mathcal{F}_{\nu\nu}(r, r', r'', \sigma) = \lim_{k \to \infty} \mathcal{F}^k_{\nu\nu}(r, r', r'', \sigma), \\
\widetilde{\mathcal{E}}_n(r, r', \sigma) &= \lim_{k \to \infty} \widetilde{\mathcal{E}}^k_n(r, r', \sigma), \quad \widetilde{\mathcal{F}}_{\nu\nu}(r, r', r'', \sigma) = \lim_{k \to \infty} \widetilde{\mathcal{F}}^k_{\nu\nu}(r, r', r'', \sigma).
\end{align*}
\]

(4.95)

Lemma 4.3. Suppose \( z > 0 \), and \( \sigma(k_\rho) \) is analytic and bounded in the right half complex plane, then

\[
\begin{align*}
\mathcal{E}^k_n(r, r', \sigma) &= i \int_{\frac{1}{2}}^{\infty} \int_{1}^{\infty} \hat{h}_n(t, \eta, \phi; r') \sigma(\xi(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta, \\
\widetilde{\mathcal{E}}^k_n(r, r', \sigma) &= i \int_{\frac{1}{2}}^{\infty} \int_{1}^{\infty} \hat{h}_n(t, -\eta, \phi; r') \sigma(\xi(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta,
\end{align*}
\]

(4.96)

\[
\begin{align*}
\mathcal{F}^k_{\nu\nu}(r, r', r'', \sigma) &= i \int_{\frac{1}{2}}^{\infty} \int_{1}^{\infty} \hat{h}_{\nu\nu}(t, \eta, \phi; r', r'') \sigma(\xi(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta, \\
\widetilde{\mathcal{F}}^k_{\nu\nu}(r, r', r'', \sigma) &= i \int_{\frac{1}{2}}^{\infty} \int_{1}^{\infty} \hat{h}_{\nu\nu}(t, -\eta, \phi; r', r'') \sigma(\xi(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta,
\end{align*}
\]

(4.97)

where

\[
\begin{align*}
\hat{h}_n(t, \eta, \phi; r') &= \hat{g}_n(\xi_+(t), \eta, \phi; r') \Lambda_+(t) + \hat{g}_n(\xi_-(t), \eta, \phi; r') \Lambda_-(t), \\
\hat{h}_{\nu\nu}(t, \eta, \phi; r', r'') &= \hat{g}_{\nu\nu}(\xi_+(t), \eta, \phi; r') \Lambda_+(t) + \hat{g}_{\nu\nu}(\xi_-(t), \eta, \phi; r') \Lambda_-(t).
\end{align*}
\]

(4.98)

Proof. According to the branch (4.80), we choose for the square root function, given any \( \eta > 0 \), we have

\[
\text{Re}[\xi(t)] = \text{Re}[\sqrt{\xi^2 + \eta^2}] > 0, \quad \forall \xi \in \Omega_1^+.
\]

(4.99)

Together with the assumption \( \sigma(k_\rho) \) is analytic and bounded in the right half complex plane, we obtain \( \sigma(\xi(t)) \) is analytic and bounded in \( \Omega_1^+ \).

On the other hand, the branch (4.80) implies that \( \hat{g}_n(\xi, \pm \eta, \phi; r') \) defined in (4.73) only have branch cut along \( \{ \xi : \xi > \eta \} \) and \( \{ \xi : \xi < -\eta \} \) (see, Fig. 4.5) which has no intersection with \( \Omega_1^+ \) for any \( \eta \geq \frac{1}{2} > 0 \). As (4.99) has already shown that \( \sqrt{\xi^2 + \eta^2} \neq 0 \) for any given \( \eta > 0 \) and \( \xi \in \Omega_1^+ \), we can conclude from the expression (4.73) that \( \hat{g}_n(\xi, \pm \eta, \phi; r') \) is analytic and satisfies \( |\hat{g}_n(\xi, \pm \eta, \phi; r')| \leq C|\xi|^q \) in the domain \( \Omega_1^+ \). As a result, we can apply lemma 4.2 to change the contour of the inner integrals in (4.90)-(4.91) from real axis to \( \Gamma \).

\[\square\]
Lemma 4.4. Suppose $z > 0$, $z + z' > 0$, and $\sigma(k_\rho)$ is analytic and bounded in the right half complex plane, then

$$
\mathcal{E}^k(r, r'; \sigma) = i \int_1^\infty \int_1^\infty \sum_{n=0}^\infty \tilde{h}_n(t, \eta, \phi; r') \sigma(\zeta(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta,
$$

$$
\tilde{\mathcal{E}}^k(r, r'; \sigma) = i \int_1^\infty \int_1^\infty \sum_{n=0}^\infty \tilde{h}_n(t, -\eta, \phi; r') \sigma(\zeta(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta.
$$

Further, if have $z + z' + z'' > 0$, then

$$
\mathcal{F}^k(r, r', r''; \sigma) = i \int_1^\infty \int_1^\infty \sum_{n=0}^\infty \sum_{\nu=0}^\infty h_{n\nu}(t, \eta, \phi; r', r'') \sigma(\zeta(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta,
$$

$$
\tilde{\mathcal{F}}^k(r, r', r''; \sigma) = i \int_1^\infty \int_1^\infty \sum_{n=0}^\infty \sum_{\nu=0}^\infty h_{n\nu}(t, -\eta, \phi; r', r'') \sigma(\zeta(t)) \frac{e^{-\eta rt}}{\sqrt{t^2 - 1}} dt d\eta,
$$

where $\tilde{h}_n(t, \eta, \phi; r')$ and $h_{n\nu}(t, \eta, \phi; r', r'')$ are defined in (4.98).

Proof. As we have proved that $\sigma(\zeta(t))$ is analytic and bounded in $\Omega_+^+$, we will focus on the analysis for functions

$$
\sum_{n=0}^\infty \hat{g}_n(\xi, \pm \eta, \phi; r'), \sum_{n=0}^\infty \sum_{\nu=0}^\infty g_{n\nu}(\xi, \pm \eta, \phi; r', r'').
$$

Noting that they are resulted from a rotation of the Taylor expansions of exponential functions, we have

$$
\sum_{n=0}^\infty \hat{g}_n(\xi, \pm \eta, \phi; r') = e^{i\xi(x' \cos \phi + y' \sin \phi) \pm i\eta(x' \sin \phi - y' \cos \phi) - \sqrt{\xi^2 + \eta^2} z'}.
$$

(4.103)

Apparently,

$$
|e^{i\xi(x' \cos \phi + y' \sin \phi) \pm i\eta(x' \sin \phi - y' \cos \phi)}| \leq 1, \quad \forall \xi \in \Omega_+^+, \quad \eta \in \mathbb{R},
$$

(4.104)

and

$$
\sum_{n=0}^\infty \hat{g}_n(\xi, \pm \eta, \phi; r') e^{i\xi \rho - \xi^2 z'} = e^{i\xi(x' \cos \phi + y' \sin \phi) \pm i\eta(x' \sin \phi - y' \cos \phi)} e^{i\xi \rho - \xi^2 (z + z')}.
$$

(4.105)

Together with the assumptions $\rho \geq 0$, $z + z' > 0$ and the fact $\sigma(\zeta(t))$ is analytic and bounded in the domain $\Omega_+^+$ for any $\eta > 0$, we can apply lemma 4.2 to (4.90) to obtain (4.100).

The proof for (4.101) can be obtained similarly as $g_{n\nu}(\xi, \pm \eta, \phi; r', r'')$ are just the product of $\hat{g}_n(\xi, \pm \eta, \phi; r')$ and $\tilde{g}_\nu(\xi, \pm \eta, \phi; r'')$ as defined in (4.76).

\[\square\]

Step 3: Convergence and error estimate. In order to exchange the order of the improper integrals and infinite summations in (4.100)-(4.101), estimates for the following integrals

$$
\mathcal{E}^k_{n;}(r, \rho, \phi; r'; \sigma) = \int_1^\infty \int_1^\infty \left| \hat{g}_n(\xi_{\pm}(t), \eta, \phi; r') \frac{\Lambda_{\pm}(t) e^{-\eta rt}}{\sqrt{t^2 - 1}} \sigma(\zeta(t)) \right| dt d\eta,
$$

$$
\tilde{\mathcal{E}}^k_{n;}(r, \rho, \phi; r'; \sigma) = \int_1^\infty \int_1^\infty \left| \hat{g}_n(\xi_{\pm}(t), -\eta, \phi; r') \frac{\Lambda_{\pm}(t) e^{-\eta rt}}{\sqrt{t^2 - 1}} \sigma(\zeta(t)) \right| dt d\eta,
$$

$$
\mathcal{F}^k_{n\nu}(r, \rho, \phi; r', r''; \sigma) = \int_1^\infty \int_1^\infty \left| g_{n\nu}(\xi_{\pm}(t), \eta, \phi; r', r'') \frac{\Lambda_{\pm}(t) e^{-\eta rt}}{\sqrt{t^2 - 1}} \sigma(\zeta(t)) \right| dt d\eta,
$$

$$
\tilde{\mathcal{F}}^k_{n\nu}(r, \rho, \phi; r', r''; \sigma) = \int_1^\infty \int_1^\infty \left| g_{n\nu}(\xi_{\pm}(t), -\eta, \phi; r', r'') \frac{\Lambda_{\pm}(t) e^{-\eta rt}}{\sqrt{t^2 - 1}} \sigma(\zeta(t)) \right| dt d\eta,
$$

(4.106)
are needed for any integer \( k > 0 \). Let us first prove estimate for their integrands.

**Lemma 4.5.** Let \( \xi_{\pm}(t) \) be the contour defined in (4.8.2), \( \mathbf{\hat{r}} = (\hat{r} \sin \alpha \cos \beta, \hat{r} \sin \alpha \sin \beta, \hat{r} \cos \alpha) \in \mathbb{R}^3 \) is any given vector. Then,

\[
|\hat{g}_q(\xi_{\pm}(t), \eta, \phi; \mathbf{\hat{r}})| \leq \frac{\tilde{r}^q |\Lambda_{\pm}(t)|^q}{q!} \left( \frac{r^2 t^2}{r^2 t^2 - \rho^2} \right)^{\frac{q}{2}}, \quad \forall t > 1,
\]

\[
|\hat{g}_q(\xi_{\pm}(t), -\eta, \phi; \mathbf{\hat{r}})| \leq \frac{\tilde{r}^q |\Lambda_{\pm}(t)|^q}{q!} \left( \frac{r^2 t^2}{r^2 t^2 - \rho^2} \right)^{\frac{q}{2}}, \quad \forall t > 1,
\]

hold for any integer \( q \geq 0 \).

**Proof.** Note that

\[
\frac{\xi_{\pm}(t) \cos(\phi - \beta) + \eta \sin(\phi - \beta)}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \frac{1}{2} \left[ \frac{\xi_{\pm}(t) + i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} e^{-i(\phi - \beta)} + \frac{\xi_{\pm}(t) - i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} e^{i(\phi - \beta)} \right],
\]

\[
\frac{\xi_{\pm}(t) \cos(\phi - \beta) - \eta \sin(\phi - \beta)}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \frac{1}{2} \left[ \frac{\xi_{\pm}(t) + i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} e^{i(\phi - \beta)} + \frac{\xi_{\pm}(t) - i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} e^{-i(\phi - \beta)} \right].
\]

From the definitions in (4.8.2), we have

\[
\xi_{\pm}(t)^2 + \eta^2 = -\Lambda_{\pm}(t)^2, \quad \xi_{\pm}(t)^2 + \eta^2 = \Lambda_{\pm}(t)^2,
\]

and

\[
\frac{\xi_{\pm}(t) + i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \frac{1}{|\Lambda_{\pm}(t)|} \frac{\eta}{r} \left[ (\rho t + r)e^{-i(\gamma_{\pm} + \phi - \beta)} + (\rho t - r)e^{-i(\gamma_{\pm} - \phi - \beta)} \right],
\]

\[
\frac{\xi_{\pm}(t) - i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \frac{1}{|\Lambda_{\pm}(t)|} \frac{\eta}{r} \left[ (\rho t + r)e^{i(\gamma_{\pm} + \phi - \beta)} + (\rho t - r)e^{i(\gamma_{\pm} - \phi - \beta)} \right].
\]

Therefore, we have the following concise formulas

\[
\frac{\xi_{\pm}(t) \cos(\phi - \beta) + \eta \sin(\phi - \beta)}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \frac{2(r^2 t^2 - \rho^2)}{(r^2 t^2)^2 - \rho^2},
\]

\[
\frac{\xi_{\pm}(t) \cos(\phi - \beta) - \eta \sin(\phi - \beta)}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \frac{2(r^2 t^2 - \rho^2)}{(r^2 t^2)^2 - \rho^2},
\]

where \( \gamma_{\pm} \) denote the phases of the complex numbers \((\xi_{\pm}(t) + i\eta)/\sqrt{\xi_{\pm}(t)^2 + \eta^2}, \) i.e.,

\[
\frac{\xi_{\pm}(t) + i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \sqrt{\frac{rt + \rho}{rt - \rho}} e^{i\gamma_{\pm}}, \quad \frac{\xi_{\pm}(t) - i\eta}{\sqrt{\xi_{\pm}(t)^2 + \eta^2}} = \sqrt{\frac{rt - \rho}{rt + \rho}} e^{-i\gamma_{\pm}}.
\]

By formulations in (4.109), we calculate that

\[
|\xi_{\pm}(t) \cos(\phi - \beta) + \eta \sin(\phi - \beta)|^2 = \frac{1}{r^2 t^2 - \rho^2} \left| \left( (rt + \rho) e^{i\psi_{\pm}} + (rt - \rho) e^{-i\psi_{\pm}} \right) \sin \alpha + i \sqrt{r^2 t^2 - \rho^2} \cos \alpha \right|^2 \leq \frac{1}{r^2 t^2 - \rho^2} \left( \rho^2 + (r^2 t^2 - \rho^2) \sin^2 \psi_{\pm} + (r^2 t^2 - \rho^2) \cos^2 \psi_{\pm} \right) \leq \frac{r^2 t^2}{r^2 t^2 - \rho^2},
\]

where \( \psi_{\pm} = \gamma_{\pm} - \phi + \beta \). The inequality is due to the fact

\[
(a \sin \theta + b \cos \theta)^2 = a^2 + b^2 - (a \cos \theta - b \sin \theta)^2.
\]
for any a, b and θ in R. Similarly, the following estimate
\[ |ξ_±(t)\cos(\phi - \beta) - \eta\sin(\phi - \beta)| \leq \frac{r^2t^2}{\sqrt{\xi_±(t)^2 + \eta^2}} \sin \alpha + i \cos \alpha \leq \frac{r^2t^2}{r^2t^2 - \rho^2}, \] (4.113)
can also be obtained. Then, (4.107) follows by applying estimate (4.113) and identity (4.108) to the definition in (4.73).

**Lemma 4.6.** Suppose for any \( r > \rho \geq 0 \), the density function \( \sigma(\zeta(t)) \) has a uniform bound \( |\sigma(\zeta(t))| \leq M_σ \) along the contour \( \Gamma \) defined in lemma 4.2. Then, the following estimates
\[ F^k_ν(r, \phi, \rho'; r''; \sigma) \leq \frac{\pi M_σ |r''|^n |r''|^{n+\nu} \Lambda(\zeta(t))}{n\nu!}, \] (4.114)
and
\[ E^k_ν(r, \phi, \rho'; \sigma) \leq \frac{\pi M_σ |r''|^n |r''|^{n+\nu}}{n\nu!}, \] (4.115)
hold for any integers \( n, \nu \geq 0 \).

**Proof.** By (4.76), (4.82), identity (4.108) and estimates in lemma 4.5, we have
\[ |g_{νr}(\zeta(t), \pm \eta; \phi', \rho''; \zeta(t))\Lambda(\zeta(t))| \leq \frac{|r''|^n |r''|^{n+\nu} \Lambda(\zeta(t))}{\sqrt{r'^2t^2 - \rho^2}} \leq \frac{|r''|^n |r''|^{n+\nu} \Lambda(\zeta(t))}{\sqrt{r'^2t^2 - \rho^2}^n \nu!}. \]
With the above estimates and the bound of \( \sigma(\zeta(t)) \), we derive from expressions (4.106) that
\[ F^k_ν(r, \phi, \rho'; r''; \sigma) \leq \frac{M_σ |r''|^n |r''|^{n+\nu}}{n\nu!} \int_1^∞ \frac{t^{n+\nu}}{\sqrt{t^2 - 1}} \int_0^∞ \eta^{n+\nu} e^{-\eta t} d\eta d\theta \]
\[ = \frac{M_σ |r''|^n |r''|^{n+\nu} \Lambda(\zeta(t))}{n\nu!} \int_1^∞ \frac{1}{t^{\nu+1}} dt = \frac{\pi M_σ |r''|^n |r''|^{n+\nu} \Lambda(\zeta(t))}{n\nu!}, \] (4.116)
for any integers \( n, \nu \geq 0 \). The other estimates in (4.114) and (4.115) can be proved similarly. \( \square \)

**Theorem 4.15.** Suppose \( |r| > |r'| + |r''|, \ z > 0, \ z + z' + z'' > 0 \), and the density function \( \sigma(\zeta) \) is analytic and has a bound \( |\sigma(\zeta)| \leq M_σ \) in the right half complex plane. Then,
\[ F(r, r', r''; \sigma) = \sum_{n=0}^∞ \sum_{\nu=0}^∞ F^k_ν(r, r', r''; \sigma), \] (4.117)
\[ \bar{F}(r, r', r''; \sigma) = \sum_{n=0}^∞ \sum_{\nu=0}^∞ \bar{F}^k_ν(r, r', r''; \sigma), \]
where the integrals are defined in (4.92) and (4.95).

**Proof.** We only present the proof for the first summation in (4.117). Similar analysis can be done for the second one.

By the estimate (4.114), we have
\[ \sum_{n=0}^∞ \sum_{\nu=0}^∞ F^k_ν(r, \phi, r', r''; \sigma) \leq \frac{\pi M_σ}{2} \sum_{n=0}^∞ \sum_{\nu=0}^∞ \frac{|r'| |r''|^{n+\nu} \Lambda(\zeta(t))}{n\nu!} \]
\[ = \frac{\pi M_σ}{2} \sum_{n=0}^∞ \left( \frac{|r'| + |r''|}{r} \right)^n \leq \frac{\pi M_σ}{2(r - |r'| - |r''|)}. \] (4.118)
for any \( r > |r'| + |r''| \). Therefore, we can apply the Fubini theorem to exchange the order of the improper integrals and infinite summations in (4.111). Together with the expressions in (4.97), we obtain

\[
\mathcal{F}^k(r, r', r'', \sigma) = \sum_{n=0}^{\infty} \sum_{\nu=0}^{\infty} \mathcal{F}_{n\nu}^k(r, r', r'', \sigma). \tag{4.119}
\]

Note that (4.118) holds uniformly with respect to parameter \( k \). Therefore, the series in (4.119) is also uniformly convergent with respect to parameter \( k \). Taking limit for \( k \to \infty \) in (4.119) and exchanging order of the limit and summations, we obtain the first equality in (4.117). \( \square \)

By following the same analysis above, we have similar conclusions for the simpler cases.

**Theorem 4.16.** Suppose \(|r| > |r'|, z > 0, z + z' > 0, \) and the density function \( \sigma(\zeta) \) is analytic and has a bound \(|\sigma(\zeta)| \leq M_\sigma \) in the right half complex plane. Then,

\[
\mathcal{E}(r, r'; \sigma) = \sum_{n=0}^{\infty} \mathcal{E}_n(r, r'; \sigma), \quad \tilde{\mathcal{E}}(r, r'; \sigma) = \sum_{n=0}^{\infty} \tilde{\mathcal{E}}_n(r, r'; \sigma), \tag{4.120}
\]

where the integrals are defined in (4.92) and (4.95).

Summing up expansions in (4.117) and (4.120), respectively, and recalling identities (4.79) and (4.93), we complete the proof for (4.32).

Next, let us prove the truncation error estimate (4.34). Another error estimate (4.33) can be proved similarly. By the definition (4.94), lemma 4.2 and estimates (4.111), we have

\[
|\mathcal{F}_{n\nu}(r, r', r'', \sigma)| \leq \lim_{k \to \infty} |\mathcal{F}_{n\nu}^k(r, r', r'', \sigma)| = \lim_{k \to \infty} |\mathcal{F}_{n\nu}^{k+}(r, r', r'', \sigma) + \mathcal{F}_{n\nu}^{k-}(r, r', r'', \sigma)| \leq \pi M_\sigma \left| r \right|^n |r''|^{\nu}(n+\nu)! \left| r \right|^{n+\nu+1} n! \nu! \tag{4.121}
\]

Therefore

\[
|\mathcal{I}_{n\nu}(r, r', r'', \sigma)| = |\mathcal{F}_{n\nu}(r, r', r'', \sigma) + \mathcal{F}_{n\nu}(r, r', r'', \sigma)| \leq 2\pi M_\sigma \left| r \right|^n |r''|^{\nu}(n+\nu)! \left| r \right|^{n+\nu+1} n! \nu! \] \tag{4.122}
\]

and

\[
\left| \tilde{\mathcal{I}}(r, r', r'', \sigma) - \sum_{n=0}^{p} \sum_{\nu=0}^{p} \mathcal{I}_{n\nu}(r, r', r'', \sigma) \right| \leq 2\pi M_\sigma \left[ \sum_{n=0}^{p} \sum_{\nu=p+1}^{\infty} \frac{|r'|^{n} |r''|^{\nu}(n+\nu)!}{|r|^{n+\nu+1} n! \nu!} + \sum_{n=p+1}^{\infty} \sum_{\nu=0}^{\infty} \frac{|r'|^{n} |r''|^{\nu}(n+\nu)!}{|r|^{n+\nu+1} n! \nu!} \right] \tag{4.123}
\]

\[
\leq 4\pi M_\sigma \sum_{n=p+1}^{\infty} \left( \frac{|r'| + |r''|}{|r|} \right)^n \left( \frac{1}{|r|} \right) \tag{4.124}
\]

5. Conclusion

In this paper, we have shown that the reaction density functions involved in the Green’s function of 3-dimensional Laplace equation in multi-layered media are analytic and bounded in the right half complex plane. Based on this theoretical result, we are able to show that the ME and LE and M2L, M2M, and L2L translation operators for the Green’s functions of
a 3-dimensional Laplace equation in layered media have exponential convergence similar to the classic FMM for free space problem.

The detailed analysis and estimates done here for the 3-D Laplace equation in layered media will allow us to tackle more challenging tasks in establishing the mathematical foundation for the FMMs we developed for the 3-D Poisson-Boltzmann and Helmholtz equations, and moreover, the Maxwell’s equations. As an immediate future work, we will carry out the error estimate for the FMMs for the 3-dimensional Helmholtz equation in layered media, which will require new techniques to address the effect of the surface waves (poles of density function close to the real axis) on the exponential convergence property of the MEs and LEs and M2L translation operators.

ACKNOWLEDGEMENT

The research of the first author is partially supported by NSFC (grant 11771137), the Construct Program of the Key Discipline in Hunan Province and a Scientific Research Fund of Hunan Provincial Education Department (No. 16B154).

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