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Exponential Convergence Theory of the Multipole and Local Expansions for the 3-D Laplace Equation in Layered Media

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Dedicated to the memory of Professor Zhongci Shi

Abstract. In this paper, we establish the exponential convergence theory for the multipole and local expansions, shifting and translation operators for the Green's function of 3-dimensional Laplace equation in layered media. An immediate application of the theory is to ensure the exponential convergence of the FMM which has been shown by the numerical results reported in [27]. As the Green's function in layered media consists of free space and reaction field components and the theory for the free space components is well known, this paper will focus on the analysis for the reaction components. We first prove that the density functions in the integral representations of the reaction components are analytic and bounded in the right half complex wave number plane. Then, by using the Cagniard-de Hoop transform and contour deformations, estimates for the remainder terms of the truncated expansions are given, and, as a result, the exponential convergence for the expansions and translation operators is proven.

AMS subject classifications: 15A15, 15A09, 15A23

Key words: Fast multipole method, layered media, multipole expansions, local expansions, 3-D Laplace equation, Cagniard–de Hoop transform, equivalent polarization sources.

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1 Introduction

Many important computational problems in science and engineering involve solving the Laplace equation in layered media. For instance, finding the electric static potential in a layered dielectric medium has important application in semi-conductor industry, such as calculating the capacitance of interconnects (ICs) in very large-scale integrated (VLSI) circuits for microchip designs [22–24, 31]. Other applications of solving Laplace equation in layered media can be found in medical imaging of brains [30], modeling of triboelectric nanogenerators [19], elasticity of composite materials [3–5], complex scattering problem in meta-materials [8], electrostatic potential computation in ion channel simulation [20], and electrical impedance tomography for geophysical applications [6].

Due to complex geometric structure of the physical objects and the layered medium setting from aforementioned application problems, integral methods with the Green's function of layered media (cf. [22, 33]) are usually adopted, which results in a huge dense linear algebraic system to be solved by an iterative method such as GMRES [7], etc. As a result, it will incur an $\mathcal{O}(N^2)$ computational cost for computing the product of a $N\times N$ matrix with a vector (a basic operation for the GMRES iterative solver). The well-known fast multipole method (FMM) proposed by Greengard and Rohklin [13, 14] for sources in free space has been applied to accelerate the iterative solvers for dense linear system resulting from boundary integral methods [21, 25]. However, the algorithm is only applicable for problems in free space and the FMM for Green's function in layered media has been one of the important un-resolved problems in the fast algorithm research community. Since the early 1990s, many researchers have been working on this problem and proposed several fast algorithms including complex image approximation [2, 10, 12, 16, 18], inhomogeneous plane wave expansion [9, 17], etc. Nevertheless, the multipole expansion theory of the Green's function of Laplace equation in layered media has not been established, which forms the core component of the FMMs.

The free space FMM was based on low rank approximations for the far field of sources, obtained by using truncated multipole expansions (MEs) and local expansions (LEs) with a small 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. The mathematical foundation of the MEs and their shifting and translation operators is the classical addition theory for Legendre polynomials or Bessel functions (cf. [1, 11, 15, 29]).

Recently, we have derived MEs, LEs and translation operators for Green's functions in layered media and later extended the FMMs of the Helmholtz, Laplace and Poisson-Botzmann equations from free space to layered media (cf. [26–28, 32]). The numerical results showed that the new FMMs have similar efficiency and accuracy as the free space FMM while significantly enlarge the application area of the classic ones. Although the effectiveness of the new FMMs has been validated by extensive numerical results, a mathematical proof for the exponential convergence of the MEs and LEs and the corresponding translation operators is highly desirable for the development and future application of the new FMMs. Moreover, the theoretical results on the MEs for layered Green's function could be a helpful mathematical tool in many other research area.

In contrast with the cases in free space, the Green's functions in layered media do not have closed forms in the physical space, Sommerfeld-type integral representations and extended Funck-Hecke formulas were used to derive the MEs, LEs and translation operators in our work mentioned above. The distinct feature of the expansions and translation operators 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. Previously, we proved the exponential convergence for the 2-dimensional Helmholtz equation case [32] and numerically showed that the MEs in 3-dimensional cases (including Helmholtz, Laplace and Poisson Boltzmann equations) also have exponential convergence similar to their 2-dimensional counterparts. In this paper, we will continue our previous work on 2-D Helmholtz equation [32] to establish the exponential convergence theory for 3-dimensional Laplace equations in layered media. The main difficulty in the analysis of 3-dimensional problems is due to the double improper integrals in the 2-dimensional inverse Fourier transform used in the representation of the 3-dimensional layered Green's function while only 1-dimensional inverse Fourier transform is used in the 2-dimensional cases.

As the layered Green's function consists of free space and reaction components, and the theory for free space components is exactly the same as that for free space Green's function, our contribution is mainly on the analysis for the reaction components. Firstly, we prove that the density functions in the integral representation of the reaction components are analytic and bounded in the right half complex wave number plane. It will play a key role in the estimate of the Sommerfeld integrals. Secondly, we follow the idea of introducing equivalent polarization sources (cf. [26]) to reformulate the reaction components and propose a general framework to derive their MEs, LEs and translation operators. By proving delicate estimates for the truncation errors under a general framework, we then give theoretical proof for the exponential convergence of the MEs, LEs and translation operators 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 MEs, LEs and translation operators with equivalent polarization sources in the FMMs for the reaction components. The theoretical results proved in this paper show that the FMM for Laplace equation in layered media [27] is mathematically justified to have similar accuracy and error controls 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 first review the derivation and convergence analysis of MEs, LEs, shifting and translation operators for the free space Green's function. Then, proofs for the exponential convergence of the MEs, LEs and translation operators for the reaction components of the layered Green's function are presented. In Section 4, the error estimate of FMM for the 3-dimensional Laplace equation in layered media is discussed by using the theoretical results proved in Section 3. Finally, a conclusion is given in Section 5.

2 Spectral property of the Green's function of 3-dimensional Laplace equation in layered media

In this section, we will first introduce the Green's function for the Laplace equation in 3-D layer media, and then prove the analyticity and boundedness properties for its spectral form in the Fourier transform domain, which will be a key ingredient for the analysis presented in this paper.

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

$$\boldsymbol{\Delta} u_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=-\delta(\boldsymbol{r},\boldsymbol{r}'), \tag{2.1}$$

at field point $\boldsymbol{r}=(x,y,z)$ in the ℓth layer $(d_\ell<z<d_\ell-1)$, where $\delta(\boldsymbol{r},\boldsymbol{r}')$ 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

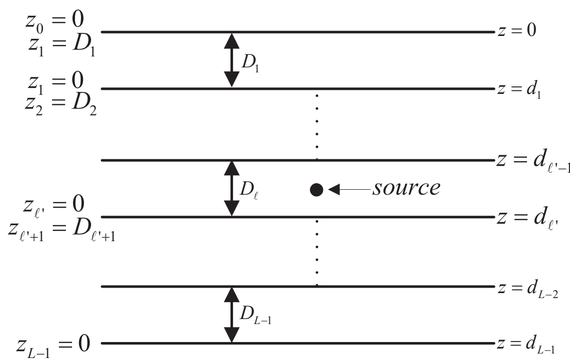


Figure 1: Sketch of the layer structure for general multi-layer media.

at the interface between ℓth and $(\ell-1)$th layer $(z=d_{\ell-1})$, i.e.,

$$u_{\ell-1,\ell'}(x,y,z)=u_{\ell\ell'}(x,y,z), \quad \varepsilon_{\ell-1}\frac{\partial u_{\ell-1,\ell'}(x,y,z)}{\partial z}=\varepsilon_\ell\frac{\partial u_{\ell\ell'}(k_x,k_y,z)}{\partial z}, \tag{2.2}$$

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 directions and solving the resulted ODE with interface conditions, we can obtain the expression of the Green's function in the physical domain as (cf. [27, Appendix B])

$$u_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=\begin{cases} u^{11}_{0\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{12}_{0\ell'}(\boldsymbol{r},\boldsymbol{r}'), \\ u^{11}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{12}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{21}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{22}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'), & \ell\neq\ell', \\ u^{11}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{12}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{21}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{22}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')+\dfrac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}, & \ell=\ell', \\ u^{21}_{L\ell'}(\boldsymbol{r},\boldsymbol{r}')+u^{22}_{L\ell'}(\boldsymbol{r},\boldsymbol{r}'), \end{cases} \tag{2.3}$$

with reaction components given by Sommerfeld-type integrals:

$$u^{\mathfrak{ab}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\tau}^{\mathfrak{ab}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')}\sigma^{\mathfrak{ab}}_{\ell\ell'}(k_\rho)dk_xdk_y, \quad \mathfrak{a},\mathfrak{b}=1,2, \tag{2.4}$$

where $\mathrm{i}=\sqrt{-1}$, $k_\rho=\sqrt{k_x^2+k_y^2}$, $\boldsymbol{k}=(k_x,k_y,\mathrm{i}k_\rho)$,

$$\boldsymbol{\tau}^{11}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=(x-x',y-y',z-d_\ell+z'-d_{\ell'}), \tag{2.5a}$$
$$\boldsymbol{\tau}^{12}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=(x-x',y-y',z-d_\ell+d_{\ell'-1}-z'), \tag{2.5b}$$
$$\boldsymbol{\tau}^{21}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=(x-x',y-y',d_{\ell-1}+z'-d_{\ell'}-z), \tag{2.5c}$$
$$\boldsymbol{\tau}^{22}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}')=(x-x',y-y',d_{\ell-1}+d_{\ell'-1}-z'-z), \tag{2.5d}$$

are coordinate mappings depending on interfaces and $\{\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)\}$ are the reaction densities in the Fourier spectral space. The expression (2.3) is a general formula for source $\boldsymbol{r}'$ in an inner layer. In the cases of the source $\boldsymbol{r}'$ in the top or bottom most layer, the reaction components $\{u_{\ell\ell'}^{\mathfrak{a}2}(\boldsymbol{r},\boldsymbol{r}')\}_{\mathfrak{a}=1}^2$ and $\{u_{\ell\ell'}^{\mathfrak{a}1}(\boldsymbol{r},\boldsymbol{r}')\}_{\mathfrak{a}=1}^2$ will vanish, respectively. It should be noted that strictly speaking, the term "reaction field", resulting from the polarization field of dissimilar dielectric materials in different layers, is only accurate in (2.3) for the case when $\ell=\ell'$ where the field of the free space (singular) part is subtracted from the total potential field there. For simplicity in notations, we will use the same term for other cases $\ell\neq\ell'$, considering that the field of the free space part from a source in the ℓ'th layer is smooth in the ℓth layer.

The reaction densities $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ only depend on the layered structure and the material parameter ε_ℓ in each layer. According to the derivation in [27, Appendix B], a stable recurrence formula is available for large number of layers with more general interface conditions

$$a_{\ell-1}u_{\ell-1,\ell'}(x,y,z)=a_\ell u_{\ell\ell'}(x,y,z),\quad b_{\ell-1}\frac{\partial u_{\ell-1,\ell'}(x,y,z)}{\partial z}=b_\ell\frac{\partial u_{\ell\ell'}(k_x,k_y,z)}{\partial z}, \tag{2.6}$$

where $\{a_\ell,b_\ell\}_{\ell=0}^L$ are given positive constants. In order to prove some key properties of the densities, we will review the recurrence formula. For this purpose, let us define

$$d_{-1}:=d_0,\quad d_{L+1}:=d_L,\quad D_\ell:=d_{\ell-1}-d_\ell,\quad e_\ell:=e^{-k_\rho D_\ell},\qquad \ell=0,1,\cdots,L, \tag{2.7a}$$

$$\gamma_\ell^+=\frac{a_\ell}{a_{\ell-1}}+\frac{b_\ell}{b_{\ell-1}},\quad \gamma_\ell^-=\frac{a_\ell}{a_{\ell-1}}-\frac{b_\ell}{b_{\ell-1}},\quad C^{(\ell)}=\prod_{j=0}^{\ell-1}\frac{1}{2e_j},\qquad \ell=1,2,\cdots,L, \tag{2.7b}$$

and matrices

$$\mathbb{T}^{\ell-1,\ell}:=\begin{pmatrix}T_{11}^{\ell-1,\ell} & T_{12}^{\ell-1,\ell}\\ T_{21}^{\ell-1,\ell} & T_{22}^{\ell-1,\ell}\end{pmatrix}=\frac{1}{2e_{\ell-1}}\begin{pmatrix}e_{\ell-1}e_\ell\gamma_\ell^+ & e_{\ell-1}\gamma_\ell^-\\ e_\ell\gamma_\ell^- & \gamma_\ell^+\end{pmatrix}:=\frac{1}{2e_{\ell-1}}\widetilde{\mathbb{T}}^{\ell-1,\ell}, \tag{2.8a}$$

$$\mathbb{A}^{(\ell)}:=\begin{pmatrix}\alpha_{11}^{(\ell)} & \alpha_{12}^{(\ell)}\\ \alpha_{21}^{(\ell)} & \alpha_{22}^{(\ell)}\end{pmatrix}=\widetilde{\mathbb{T}}^{01}\cdots\widetilde{\mathbb{T}}^{\ell-1,\ell},\quad \breve{\mathbb{S}}^{(\ell)}:=\begin{pmatrix}\breve{S}_{11}^{(\ell)} & \breve{S}_{12}^{(\ell)}\\ \breve{S}_{21}^{(\ell)} & \breve{S}_{22}^{(\ell)}\end{pmatrix}=\frac{1}{2}\begin{pmatrix}\dfrac{1}{a_\ell} & \dfrac{1}{b_\ell}\\ \dfrac{1}{a_\ell e_\ell} & -\dfrac{1}{b_\ell e_\ell}\end{pmatrix}. \tag{2.8b}$$

It is worthy to point out that, we will use $\mathbb{T}^{\ell-1,\ell}$, $\mathbb{A}^{(\ell)}$ for $\ell=1,2,\cdots,L$ and $\breve{\mathbb{S}}^{(\ell)}$ for $\ell=0,1,\cdots,L$. Then, the recursive algorithm is summarized in Algorithm 2.1.

Algorithm 2.1 Stable and efficient algorithm for reaction densities $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ in (2.4).

for $\ell'=0\to L$ **do**
if $\ell'<L$ **then**

$$\sigma_{L\ell'}^{21}(k_\rho)=-\frac{C^{(\ell'+1)}}{C^{(L)}\alpha_{22}^{(L)}}\begin{pmatrix}\alpha_{21}^{(\ell')} & \alpha_{22}^{(\ell')}\end{pmatrix}2e_{\ell'}\breve{\mathbb{S}}^{(\ell')}\begin{pmatrix}-a_{\ell'}\\ b_{\ell'}\end{pmatrix}, \tag{2.9}$$

end if
if $\ell'>0$ **then**

$$\sigma_{L\ell'}^{22}(k_\rho)=-\frac{C^{(\ell')}}{C^{(L)}\alpha_{22}^{(L)}}\begin{pmatrix}\alpha_{21}^{(\ell'-1)} & \alpha_{22}^{(\ell'-1)}\end{pmatrix}2e_{\ell'-1}\breve{\mathbb{S}}^{(\ell'-1)}\begin{pmatrix}a_{\ell'}\\ b_{\ell'}\end{pmatrix}, \tag{2.10}$$

end if
for $\ell=L-1\to 0$ **do**
if $\ell=\ell'$ **then**

$$\sigma_{\ell\ell'}^{11}(k_\rho)=T_{11}^{\ell'\ell'+1}\sigma_{\ell'+1,\ell'}^{11}+T_{12}^{\ell'\ell'+1}\sigma_{\ell'+1,\ell'}^{21}-\breve{S}_{11}^{(\ell')}a_{\ell'}+\breve{S}_{12}^{(\ell')}b_{\ell'}, \tag{2.11}$$

else

$$\sigma_{\ell\ell'}^{11}(k_\rho)=T_{11}^{\ell\ell+1}\sigma_{\ell+1,\ell'}^{11}+T_{12}^{\ell\ell+1}\sigma_{\ell+1,\ell'}^{21}, \tag{2.12}$$

end if
if $\ell=\ell'-1$ **then**

$$\sigma_{\ell\ell'}^{12}(k_\rho)=T_{11}^{\ell'-1,\ell'}\sigma_{\ell'\ell'}^{12}+T_{12}^{\ell'-1,\ell'}\sigma_{\ell'\ell'}^{22}+\breve{S}_{11}^{(\ell'-1)}a_{\ell'}+\breve{S}_{12}^{(\ell'-1)}b_{\ell'}, \tag{2.13}$$

else

$$\sigma_{\ell\ell'}^{12}(k_\rho)=T_{11}^{\ell\ell+1}\sigma_{\ell+1,\ell'}^{12}+T_{12}^{\ell\ell+1}\sigma_{\ell+1,\ell'}^{22}, \tag{2.14}$$

end if
if $\ell>0$ **then**
if $\ell>\ell'$ **then**

$$\sigma_{\ell\ell'}^{21}(k_\rho)=\frac{-1}{\alpha_{22}^{(\ell)}}\begin{pmatrix}0 & 1\end{pmatrix}\left[\frac{C^{(\ell'+1)}}{C^{(\ell)}}\mathbb{A}^{(\ell')}2e_{\ell'}\breve{\mathbb{S}}^{(\ell')}\begin{pmatrix}-a_{\ell'}\\ b_{\ell'}\end{pmatrix}+\mathbb{A}^{(\ell)}\begin{pmatrix}\sigma_{\ell\ell'}^{11}\\ 0\end{pmatrix}\right], \tag{2.15}$$

else

$$\sigma_{\ell\ell'}^{21}(k_\rho)=-\alpha_{21}^{(\ell)}\sigma_{\ell\ell'}^{11}(k_\rho)/\alpha_{22}^{(\ell)}, \tag{2.16}$$

end if
if $\ell>\ell'-1$ **then**

$$\sigma_{\ell\ell'}^{22}(k_\rho)=\frac{-1}{\alpha_{22}^{(\ell)}}\begin{pmatrix}0 & 1\end{pmatrix}\left[\frac{C^{(\ell')}}{C^{(\ell)}}\mathbb{A}^{(\ell'-1)}2e_{\ell'-1}\breve{\mathbb{S}}^{(\ell'-1)}\begin{pmatrix}a_{\ell'}\\ b_{\ell'}\end{pmatrix}+\mathbb{A}^{(\ell)}\begin{pmatrix}\sigma_{\ell\ell'}^{12}\\ 0\end{pmatrix}\right], \tag{2.17}$$

else

$$\sigma_{\ell\ell'}^{22}(k_\rho)=-\alpha_{21}^{(\ell)}\sigma_{\ell\ell'}^{12}(k_\rho)/\alpha_{22}^{(\ell)}. \tag{2.18}$$

end if
end if
end for
end for

According to the formulas used in the Algorithm 2.1, we are able to prove some important properties of the reaction densities, which will play a key role in the analysis in the rest of this paper. First, we have the following lemma for the matrices $\mathbb{A}^{(\ell)}$ defined in (2.8).

Lemma 2.1. *Suppose $a_\ell,b_\ell>0$ for all $\ell=0,1,\cdots,L$, then the entries in the second row of the matrices $\mathbb{A}^{(\ell)}$ satisfy*

$$|\alpha_{22}^{(\ell)}|^2-|\alpha_{21}^{(\ell)}|^2\geq(|\gamma_1^+|^2-|\gamma_1^-|^2)(|\gamma_2^+|^2-|\gamma_2^-|^2)\cdots(|\gamma_\ell^+|^2-|\gamma_\ell^-|^2)>0 \tag{2.19}$$

for $\ell=1,2,\cdots,L$, and any $k_\rho\in\{z\in\mathbb{C}|\mathfrak{Re}z\geq0\}$.

Proof. By the definition of $\widetilde{\mathbb{T}}^{\ell-1,\ell}$, $\mathbb{A}^{(\ell)}$ in (2.8) for $\ell=1,2,\cdots,L$, the entries $\{\alpha_{21}^{(\ell)},\alpha_{22}^{(\ell)}\}_{\ell=1}^L$ can be calculated recursively as

$$\alpha_{21}^{(1)}=e_1\gamma_1^-,\qquad \alpha_{22}^{(1)}=\gamma_1^+, \tag{2.20a}$$

$$\alpha_{21}^{(2)}=\alpha_{21}^{(1)}\gamma_2^+e_1e_2+\alpha_{22}^{(1)}\gamma_2^-e_2,\qquad \alpha_{22}^{(2)}=\alpha_{21}^{(1)}\gamma_2^-e_1+\alpha_{22}^{(1)}\gamma_2^+,\quad\cdots, \tag{2.20b}$$

$$\alpha_{21}^{(\ell)}=\alpha_{21}^{(\ell-1)}\gamma_\ell^+e_{\ell-1}e_\ell+\alpha_{22}^{(\ell-1)}\gamma_\ell^-e_\ell,\qquad \alpha_{22}^{(\ell)}=\alpha_{21}^{(\ell-1)}\gamma_\ell^-e_{\ell-1}+\alpha_{22}^{(\ell-1)}\gamma_\ell^+. \tag{2.20c}$$

Naturally, we will prove the conclusion (2.19) by induction. As we have $a_\ell,b_\ell>0$ by assumption and $|e_\ell|\leq1$ for all $k_\rho\in\{z\in\mathbb{C}|\mathfrak{Re}z\geq0\}$, then

$$|\gamma_\ell^+|=\Big|\frac{a_\ell}{a_{\ell-1}}+\frac{b_\ell}{b_{\ell-1}}\Big|>\Big|\frac{a_\ell}{a_{\ell-1}}-\frac{b_\ell}{b_{\ell-1}}\Big|=|\gamma_\ell^-|\geq|\gamma_\ell^-e_\ell|,\quad\text{if}\ \ \mathfrak{Re}k_\rho\geq0. \tag{2.21}$$

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

$$\big|\alpha_{22}^{(1)}\big|^2-\big|\alpha_{21}^{(1)}\big|^2=|\gamma_1^+|^2-|\gamma_1^-e_1|^2\geq|\gamma_1^+|^2-|\gamma_1^-|^2>0. \tag{2.22}$$

Assume

$$\big|\alpha_{22}^{(s)}\big|^2-\big|\alpha_{21}^{(s)}\big|^2\geq(|\gamma_1^+|^2-|\gamma_1^-|^2)(|\gamma_2^+|^2-|\gamma_2^-|^2)\cdots(|\gamma_s^+|^2-|\gamma_s^-|^2), \tag{2.23}$$

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

$$\big|\alpha_{21}^{(\ell)}\big|=|\beta_{\ell-1}\gamma_\ell^+e_{\ell-1}+\gamma_\ell^-|\big|\alpha_{22}^{(\ell-1)}e_\ell\big|,\quad \big|\alpha_{22}^{(\ell)}\big|=|\beta_{\ell-1}\gamma_\ell^-e_{\ell-1}+\gamma_\ell^+||\alpha_{22}^{(\ell-1)}|, \tag{2.24}$$

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

$$|\beta_{\ell-1}\gamma_\ell^+ e_{\ell-1}+\gamma_\ell^-|^2=|\beta_{\ell-1}e_{\ell-1}|^2(\gamma_\ell^+)^2+2\gamma_\ell^+\gamma_\ell^-\mathfrak{Re}\{\beta_{\ell-1}e_{\ell-1}\}+(\gamma_\ell^-)^2,$$
$$|\beta_{\ell-1}\gamma_\ell^- e_{\ell-1}+\gamma_\ell^+|^2=|\beta_{\ell-1}e_{\ell-1}|^2(\gamma_\ell^-)^2+2\gamma_\ell^+\gamma_\ell^-\mathfrak{Re}\{\beta_{\ell-1}e_{\ell-1}\}+(\gamma_\ell^+)^2.$$

Therefore

$$|\beta_{\ell-1}\gamma_\ell^- e_{\ell-1}+\gamma_\ell^+|^2-|\beta_{\ell-1}\gamma_\ell^+ e_{\ell-1}+\gamma_\ell^-|^2=[(\gamma_\ell^+)^2-(\gamma_\ell^-)^2](1-|\beta_{\ell-1}e_{\ell-1}|^2).$$

Together with (2.24) and the fact $|e_\ell|\le 1$ for all $k_\rho\in\{z\in\mathbb{C}|\mathfrak{Re}z\ge 0\}$, we obtain

$$\begin{aligned}\big|\alpha_{22}^{(\ell)}\big|^2-\big|\alpha_{21}^{(\ell)}\big|^2 &\ge[(\gamma_\ell^+)^2-(\gamma_\ell^-)^2](1-|\beta_{\ell-1}|^2)\big|\alpha_{22}^{(\ell-1)}\big|^2\\ &=[(\gamma_\ell^+)^2-(\gamma_\ell^-)^2](\big|\alpha_{22}^{(\ell-1)}\big|^2-\big|\alpha_{21}^{(\ell-1)}\big|^2).\end{aligned}$$

Then, we complete the proof by applying the assumption (2.23). □

Proposition 2.1. *Suppose $a_\ell,b_\ell>0$ for all $\ell=0,1,\cdots,L$, then all reaction densities $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ in (2.4) are continuous and bounded in $\{k_\rho|\mathfrak{Re}k_\rho\ge 0\}$. Moreover, they are analytic in the right half complex plane $\{k_\rho|\mathfrak{Re}k_\rho>0\}$.*

Proof. From the definition (2.7) and (2.8), we have

$$T_{11}^{\ell\ell+1}=\frac{a_{\ell+1}b_\ell+a_\ell b_{\ell+1}}{2a_\ell b_\ell}e_{\ell+1},\quad T_{12}^{\ell\ell+1}=\frac{a_{\ell+1}b_\ell-a_\ell b_{\ell+1}}{2a_\ell b_\ell},\quad \widetilde{\mathbb{T}}^{\ell-1,\ell}=\begin{pmatrix}\gamma_\ell^+ e_{\ell-1}e_\ell & \gamma_\ell^- e_{\ell-1}\\ \gamma_\ell^- e_\ell & \gamma_\ell^+\end{pmatrix},$$

$$2e_\ell\breve{\mathbb{S}}^{(\ell)}=\begin{pmatrix}a_\ell^{-1}e_\ell & b_\ell^{-1}e_\ell\\ a_\ell^{-1} & -b_\ell^{-1}\end{pmatrix},\quad \frac{C^{(\ell_1)}}{C^{(\ell_2)}}=\begin{cases}1, & \ell_1=\ell_2,\\ 2^{\ell_2-\ell_1}e^{-k_\rho(d_{\ell_1-1}-d_{\ell_2-1})}, & 0\le\ell_1<\ell_2.\end{cases}$$

As they consist of constants $\{a_\ell,b_\ell\}_{\ell=0}^L$ and their product with exponential functions of k_ρ, $\{T_{11}^{\ell\ell+1},T_{12}^{\ell\ell+1}\}_{\ell=0}^{L-1}$, $\{\breve{S}_{11}^{(\ell)},\breve{S}_{12}^{(\ell)}\}_{\ell=0}^L$, $\{C^{(\ell_1)}/C^{(\ell_2)}\}_{\ell_1\le\ell_2}$ and the entries of matrices $\{\widetilde{\mathbb{T}}^{\ell-1,\ell}\}_{\ell=1}^L$, $\{2e_\ell\breve{\mathbb{S}}^{(\ell)}\}_{\ell=0}^L$ and $\mathbb{A}^{(\ell)}=\widetilde{\mathbb{T}}^{01}\cdots\widetilde{\mathbb{T}}^{\ell-1,\ell}$ are all continuous and bounded in $\{k_\rho|\mathfrak{Re}k_\rho\ge 0\}$. Moreover, by Lemma 2.1, the module of the denominators $\{\alpha_{22}^{(\ell)}\}_{\ell=1}^L$ in (2.9)-(2.18) are bounded below in $\{k_\rho|\mathfrak{Re}k_\rho\ge 0\}$ by some positive constants determined by $\{a_\ell,b_\ell\}_{\ell=0}^L$. 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 $\{k_\rho|\mathfrak{Re}k_\rho\ge 0\}$ and analytic in the right half complex plane. □

3 Convergence theory for the expansions of the Green's function of 3-dimensional Laplace equation in layered media

In this section, we will establish the convergence theory of the multipole and local expansions of the Green's function of 3-dimensional Laplace equation in layered media.

According to the expression (2.3), the layered media Green's function consists of free space and reaction field components. The expansions and their convergence results for free space components are well-known and have laid the theoretical foundation of the free space FMM. The theory presented in this paper is mainly established for the reaction field components and will also include the exponential convergence of the shifting and translation operators.

3.1 Convergence theory for the expansions of the free space components

Let us first review the theoretical results for the free space components. It is mostly for the completeness of the theory and comparison with the results that we will prove for the reaction field components.

The addition theorems (cf. [11,15]) have been used to derive source/target separated ME, LE and corresponding shifting and translation operators for the free space Green's function. As in [27], we state the addition theorems (see Appendix A) using scaled spherical harmonics

$$Y_n^m(\theta,\varphi)=(-1)^m\sqrt{\frac{2n+1}{4\pi}\frac{(n-m)!}{(n+m)!}}P_n^m(\cos\theta)e^{\mathrm{i}m\varphi}:=\widehat{P}_n^m(\cos\theta)e^{\mathrm{i}m\varphi}, \tag{3.1}$$

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

$$c_n=\sqrt{\frac{2n+1}{4\pi}}, \quad A_n^m=\frac{(-1)^n c_n}{\sqrt{(n-m)!(n+m)!}}, \quad |m|\le n, \tag{3.2}$$

in the presentation of the addition theorems and the rest part of this paper.

Given source and target centers $\boldsymbol{r}_c^s$ and $\boldsymbol{r}_c^t$ close to source $\boldsymbol{r}'$ and target $\boldsymbol{r}$ such that $|\boldsymbol{r}'-\boldsymbol{r}_c^s|<|\boldsymbol{r}-\boldsymbol{r}_c^s|$ and $|\boldsymbol{r}'-\boldsymbol{r}_c^t|>|\boldsymbol{r}-\boldsymbol{r}_c^t|$, the free space Green's function has Taylor expansions

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=\frac{1}{4\pi|(\boldsymbol{r}-\boldsymbol{r}_c^s)-(\boldsymbol{r}'-\boldsymbol{r}_c^s)|}=\frac{1}{4\pi}\sum_{n=0}^{\infty}\frac{P_n(\cos\gamma_s)}{r_s}\Big(\frac{r_s'}{r_s}\Big)^n, \tag{3.3}$$

and

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=\frac{1}{4\pi|(\boldsymbol{r}-\boldsymbol{r}_c^t)-(\boldsymbol{r}'-\boldsymbol{r}_c^t)|}=\frac{1}{4\pi}\sum_{n=0}^{\infty}\frac{P_n(\cos\gamma_t)}{r_t'}\Big(\frac{r_t}{r_t'}\Big)^n, \tag{3.4}$$

where $P_n(x)$ is the n-th order Legendre polynomial. Further, applying Legendre addition Theorem A.1 to expansions (3.3) and (3.4) gives source/target separated ME

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}M_{nm}\frac{Y_n^m(\theta_s,\varphi_s)}{r_s^{n+1}},\quad M_{nm}:=\frac{1}{4\pi c_n^2}r_s'^n\overline{Y_n^m(\theta_s',\varphi_s')}, \tag{3.5}$$

and LE

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}L_{nm}r_t^nY_n^m(\theta_t,\varphi_t),\quad L_{nm}:=\frac{1}{4\pi c_n^2}r_t'^{-n-1}\overline{Y_n^m(\theta_t',\varphi_t')}. \tag{3.6}$$

In the formulas above, (r_s,θ_s,φ_s), (r_t,θ_t,φ_t) are the spherical coordinates of $\boldsymbol{r}-\boldsymbol{r}_c^s$ and $\boldsymbol{r}-\boldsymbol{r}_c^t$, i.e.,

$$\boldsymbol{r}-\boldsymbol{r}_c^s=(r_s\sin\theta_s\cos\varphi_s,r_s\sin\theta_s\sin\varphi_s,r_s\cos\theta_s), \tag{3.7a}$$
$$\boldsymbol{r}-\boldsymbol{r}_c^t=(r_t\sin\theta_t\cos\varphi_t,r_t\sin\theta_t\sin\varphi_t,r_t\cos\theta_t), \tag{3.7b}$$

$(r_s',\theta_s',\varphi_s')$, $(r_t',\theta_t',\varphi_t')$ are the spherical coordinates of $\boldsymbol{r}'-\boldsymbol{r}_c^s$ and $\boldsymbol{r}'-\boldsymbol{r}_c^t$ (see Fig. 2), i.e.,

$$\boldsymbol{r}'-\boldsymbol{r}_c^s=(r_s'\sin\theta_s'\cos\varphi_s',r_s'\sin\theta_s'\sin\varphi_s',r_s'\cos\theta_s'), \tag{3.8a}$$
$$\boldsymbol{r}'-\boldsymbol{r}_c^t=(r_t'\sin\theta_t'\cos\varphi_t',r_t'\sin\theta_t'\sin\varphi_t',r_t'\cos\theta_t'), \tag{3.8b}$$

γ_s is the angle between $\boldsymbol{r}-\boldsymbol{r}_c^s$ and $\boldsymbol{r}'-\boldsymbol{r}_c^s$ and γ_t the angle between $\boldsymbol{r}-\boldsymbol{r}_c^t$ and $\boldsymbol{r}'-\boldsymbol{r}_c^t$. It is worthy to note that the notations (r_s,θ_s,φ_s) and (r_t,θ_t,φ_t) will be used in many important formulas in the rest part of this paper.

Applying Theorem A.3 in ME (3.5) provides a translation from ME (3.5) to LE (3.6) which is given by

$$L_{nm}=\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu+|m|}A_\nu^\mu A_n^m Y_{n+\nu}^{\mu-m}(\theta_{st},\varphi_{st})}{c_\nu^2 A_{n+\nu}^{\mu-m} r_{st}^{n+\nu+1}}M_{\nu\mu}, \tag{3.9}$$

where $(r_{st},\theta_{st},\varphi_{st})$ is the spherical coordinate of $\boldsymbol{r}_c^s-\boldsymbol{r}_c^t$. On the other hand, given two new centers $\tilde{\boldsymbol{r}}_c^s$ and $\tilde{\boldsymbol{r}}_c^t$ close to $\boldsymbol{r}_c^s$ and $\boldsymbol{r}_c^t$, respectively. By using the addition Theorems A.2 and A.4 in (3.5)-(3.6) and rearranging terms in the results, we have

$$\begin{aligned}
&\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu}M_{\nu\mu}\frac{Y_\nu^\mu(\theta_s,\varphi_s)}{r_s^{\nu+1}}\\
=&\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu}\sum_{n'=0}^{\infty}\sum_{m'=-n'}^{n'}M_{\nu\mu}\frac{(-1)^{|m'+\mu|-|\mu|}A_{n'}^{m'}A_\nu^\mu r_{ss}^{n'}Y_{n'}^{-m'}(\theta_{ss},\varphi_{ss})}{c_{n'}^2A_{n'+\nu}^{m'+\mu}}\frac{Y_{n'+\nu}^{m'+\mu}(\tilde{\theta}_s,\tilde{\varphi}_s)}{\tilde{r}_s^{n'+\nu+1}}\\
=&\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\sum_{\nu=0}^{n}\sum_{\mu=-\nu}^{\nu}M_{\nu\mu}\frac{(-1)^{|m|-|\mu|}A_{n-\nu}^{m-\mu}A_\nu^\mu r_{ss}^{n-\nu}Y_{n-\nu}^{\mu-m}(\theta_{ss},\varphi_{ss})}{c_{n-\nu}^2A_n^m}\frac{Y_n^m(\tilde{\theta}_s,\tilde{\varphi}_s)}{\tilde{r}_s^{n+1}},
\end{aligned}$$

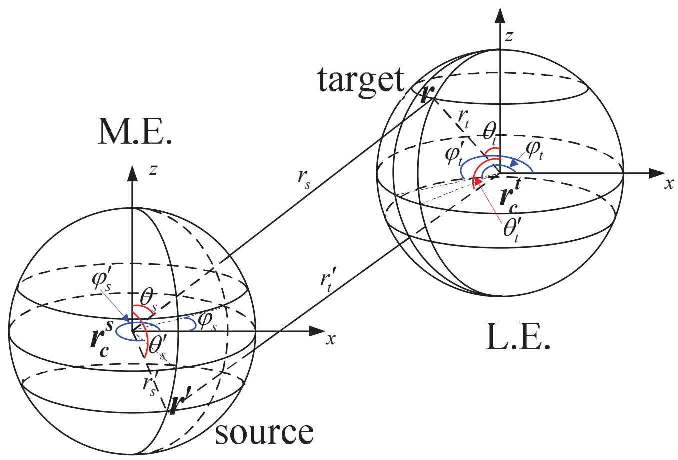


Figure 2: Spherical coordinates used in multipole and local expansions.

and

$$
\begin{aligned}
&\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu} L_{\nu\mu} r_t^{\nu} Y_{\nu}^{\mu}(\theta_t,\varphi_t)\\
=&\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu}\sum_{n'=0}^{\nu}\sum_{m'=-n'}^{n'} L_{\nu\mu}\frac{(-1)^{n'-|m'|+|\mu|-|\mu-m'|}c_{\nu}^2 A_{n'}^{m'} A_{\nu-n'}^{\mu-m'} r_{tt}^{n'} Y_{n'}^{m'}(\theta_{tt},\varphi_{tt})}{c_{n'}^2 c_{\nu-n'}^2 A_{\nu}^{\mu}\tilde{r}_t^{n'-\nu}} Y_{\nu-n'}^{\mu-m'}(\tilde{\theta}_t,\tilde{\varphi}_t)\\
=&\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\sum_{\nu=n}^{\infty}\sum_{\mu=-\nu}^{\nu} L_{\nu\mu}\frac{(-1)^{\nu-n-|\mu-m|+|\mu|-|m|}c_{\nu}^2 A_{\nu-n}^{\mu-m} A_n^m r_{tt}^{\nu-n} Y_{\nu-n}^{\mu-m}(\theta_{tt},\varphi_{tt})}{c_{\nu-n}^2 c_n^2 A_{\nu}^{\mu}}\tilde{r}_t^n Y_n^m(\tilde{\theta}_t,\tilde{\varphi}_t),
\end{aligned}
$$

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 $\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^s$, $\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^t$, $\boldsymbol{r}_c^s-\tilde{\boldsymbol{r}}_c^s$ and $\boldsymbol{r}_c^t-\tilde{\boldsymbol{r}}_c^t$, i.e.,

$$\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^s=(\tilde{r}_s\sin\tilde{\theta}_s\cos\tilde{\varphi}_s,\tilde{r}_s\sin\tilde{\theta}_s\sin\tilde{\varphi}_s,\tilde{r}_s\cos\tilde{\theta}_s), \tag{3.10a}$$
$$\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^t=(\tilde{r}_t\sin\tilde{\theta}_t\cos\tilde{\varphi}_t,\tilde{r}_t\sin\tilde{\theta}_t\sin\tilde{\varphi}_t,\tilde{r}_t\cos\tilde{\theta}_t), \tag{3.10b}$$
$$\boldsymbol{r}_c^s-\tilde{\boldsymbol{r}}_c^s=(r_{ss}\sin\theta_{ss}\cos\varphi_{ss},r_{ss}\sin\theta_{ss}\sin\varphi_{ss},r_{ss}\cos\theta_{ss}), \tag{3.10c}$$
$$\boldsymbol{r}_c^t-\tilde{\boldsymbol{r}}_c^t=(r_{tt}\sin\theta_{tt}\cos\varphi_{tt},r_{tt}\sin\theta_{tt}\sin\varphi_{tt},r_{tt}\cos\theta_{tt}). \tag{3.10d}$$

These two formulas implies that the coefficients

$$\tilde{M}_{nm}=\frac{1}{4\pi c_n^2}\tilde{r}_s'^{n}\overline{Y_n^m(\tilde{\theta}_s',\tilde{\varphi}_s')},\quad \tilde{L}_{nm}=\frac{1}{4\pi c_n^2}\tilde{r}_t'^{-n-1}\overline{Y_n^m(\tilde{\theta}_t',\tilde{\varphi}_t')}, \tag{3.11}$$

of the ME and LE at new centers $\tilde{\boldsymbol{r}}_c^t$ and $\tilde{\boldsymbol{r}}_c^s$ can be obtained via center shifting

$$\tilde{M}_{nm}=\sum_{\nu=0}^{n}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{|m|-|\mu|}A_{n-\nu}^{m-\mu}A_{\nu}^{\mu}r_{ss}^{n-\nu}Y_{n-\nu}^{\mu-m}(\theta_{ss},\varphi_{ss})}{c_{n-\nu}^2A_n^m}M_{\nu\mu}, \tag{3.12a}$$

$$\tilde{L}_{nm}=\sum_{\nu=n}^{\infty}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu-n-|\mu-m|+|\mu|-|m|}c_\nu^2A_{\nu-n}^{\mu-m}A_n^mr_{tt}^{\nu-n}Y_{\nu-n}^{\mu-m}(\theta_{tt},\varphi_{tt})}{c_{\nu-n}^2c_n^2A_\nu^\mu}L_{\nu\mu}. \tag{3.12b}$$

Apparently, the following truncation error estimates

$$\left|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\frac{1}{4\pi}\sum_{n=0}^{p}\frac{P_n(\cos\gamma_s)}{r_s}\left(\frac{r_s'}{r_s}\right)^n\right|\le\frac{1}{4\pi(r_s-r_s')}\left(\frac{r_s'}{r_s}\right)^{p+1},\quad r_s>r_s', \tag{3.13}$$

and

$$\left|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\frac{1}{4\pi}\sum_{n=0}^{p}\frac{P_n(\cos\gamma_t)}{r_t'}\left(\frac{r_t}{r_t'}\right)^n\right|\le\frac{1}{4\pi(r_t'-r_t)}\left(\frac{r_t}{r_t'}\right)^{p+1},\quad r_t<r_t', \tag{3.14}$$

for the Taylor expansions (3.3)-(3.4) can be obtained by using the fact $|P_n(x)|\le 1$ for all $x\in[-1,1]$. Recalling the derivation of the ME (3.5) and the LE (3.6), we directly obtain the convergence theory for the ME and LE.

Theorem 3.1. *Given $a>0$, $\boldsymbol{r},\boldsymbol{r}_c^s\in\mathbb{R}^3$ such that $|\boldsymbol{r}-\boldsymbol{r}_c^s|>a$, then for any $\boldsymbol{r}'$ inside the sphere $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^s|\le a\}$, the ME* (3.5) *holds and has truncation error estimate*

$$\left|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\sum_{n=0}^{p}\sum_{m=-n}^{n}M_{nm}\frac{Y_n^m(\theta_s,\varphi_s)}{r_s^{n+1}}\right|\le\frac{1}{4\pi}\frac{1}{r_s-a}\left(\frac{a}{r_s}\right)^{p+1}. \tag{3.15}$$

Theorem 3.2. *Given $a>0$, $\boldsymbol{r},\boldsymbol{r}_c^t\in\mathbb{R}^3$ such that $|\boldsymbol{r}-\boldsymbol{r}_c^t|\le a$, then for any $\boldsymbol{r}'$ outside the sphere $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^t|\le a\}$, the LE* (4.5) *holds and has truncation error estimate*

$$\left|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}r_t^nY_n^m(\theta_t,\varphi_t)\right|\le\frac{1}{4\pi}\frac{1}{a-r_t}\left(\frac{r_t}{a}\right)^{p+1}. \tag{3.16}$$

The ME to LE translation (3.9) is usually truncated to give approximate local expansion coefficients

$$L_{nm}^p=\sum_{|\nu|=0}^{p}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu+|m|}A_\nu^\mu A_n^mY_{n+\nu}^{\mu-m}(\theta_{st},\varphi_{st})}{c_\nu^2A_{n+\nu}^{\mu-m}r_{st}^{n+\nu+1}}M_{\nu\mu}. \tag{3.17}$$

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 the following theorem with the details of the proof given in the Appendix B. The geometric configuration of the ME to LE translation is demonstrated in Fig. 3 via a 2-D sketch.

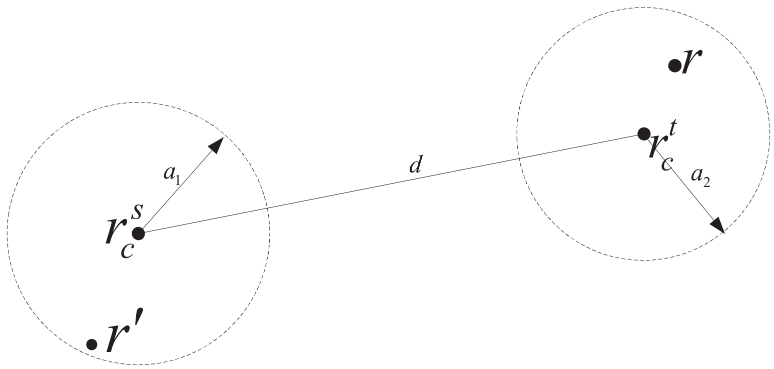
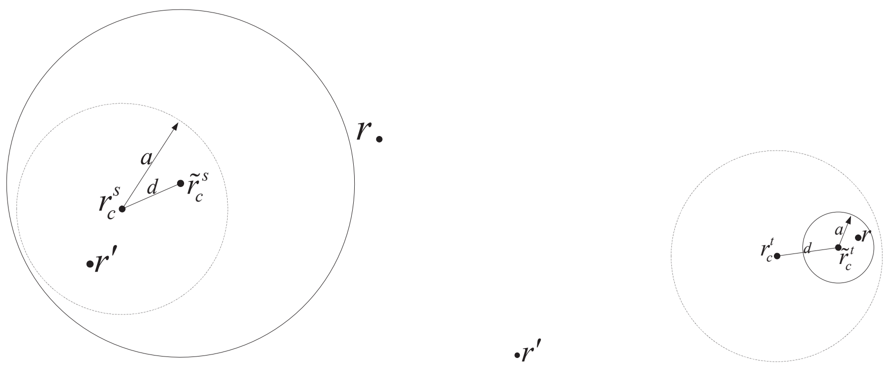


Figure 3: The geometric configuration of the M2L translation for source far away from the target point.



(a) ME to ME shifting (b) LE to LE shifting

Figure 4: The geometric configuration for the center shifting.

Theorem 3.3. *Given* $a_1>0$, $a_2>0$, $\boldsymbol{r}_c^s,\boldsymbol{r}_c^t\in\mathbb{R}^3$ *such that* $|\boldsymbol{r}_c^s-\boldsymbol{r}_c^t|>a_1+ca_2$ *with* $c>1$. *Then, for any* $\boldsymbol{r}'$ *inside the sphere* $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^s|\le a_1\}$ *and any* $\boldsymbol{r}$ *inside the sphere* $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^t|\le a_2\}$, *the truncated ME to LE translation* (3.17) *leads to approximation with error estimate*

$$\Big|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}^{p}r_t^nY_n^m(\theta_t,\varphi_t)\Big|\le\frac{1}{4\pi}\frac{1}{(c-1)a_2}\Big(\frac{a_1+a_2}{a_1+ca_2}\Big)^{p+1}. \tag{3.18}$$

Now, we consider the center shifting. The geometric configurations are demonstrated in Fig. 4. Noting that the ME center shifting formulation (3.12a) gives exactly the coefficients of the unique multipole expansion with respect to the new center $\tilde{r}_c^s$. By Theorem 3.1, we have error estimate for the shifted ME as follows.

Corollary 3.1. *Given $a>0$ and two centers $\boldsymbol{r}_c^s,\tilde{\boldsymbol{r}}_c^s\in\mathbb{R}^3$ close to each other with distance $d=|\tilde{\boldsymbol{r}}_c^s-\boldsymbol{r}_c^s|$, $\boldsymbol{r}$ is another given point far away from them such that $|\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^s|>a+d$, then for any $\boldsymbol{r}'$ inside the sphere $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^s|\le a\}$, the ME shifting formulation* (3.12a) *leads to approximation with error estimate*

$$\Big|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{M}_{nm}\frac{Y_n^m(\tilde{\theta}_s,\tilde{\varphi}_s)}{\tilde{r}_s^{n+1}}\Big|\le\frac{1}{4\pi}\frac{1}{\tilde{r}_s-a-d}\Big(\frac{a+d}{\tilde{r}_s}\Big)^{p+1}. \tag{3.19}$$

Although, the LE to LE shifting operator (3.12b) has an infinite summation, the shifting operation remains exact with finite sum when we are shifting a truncated LE to a new center. More clearly, we truncate the LE (3.6) to get approximation

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}\approx\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}r_t^nY_n^m(\theta_t,\varphi_t):=\Phi_p(\boldsymbol{r},\boldsymbol{r}'). \tag{3.20}$$

Obviously, $\Phi_p(\boldsymbol{r},\boldsymbol{r}')$ can be seen as an infinite sum

$$\Phi_p(\boldsymbol{r},\boldsymbol{r}')=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\hat{L}_{nm}r_t^nY_n^m(\theta_t,\varphi_t) \tag{3.21}$$

with coefficients defined as

$$\hat{L}_{nm}=\begin{cases}L_{nm}, & n\le p,\quad |m|\le n,\\ 0, & n>p,\quad |m|\le n.\end{cases} \tag{3.22}$$

Applying the LE center shifting (3.12b) to (3.21) leads to

$$\Phi_p(\boldsymbol{r},\boldsymbol{r}')=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\tilde{L}_{nm}\tilde{r}_t^nY_n^m(\tilde{\theta}_t,\tilde{\varphi}_t) \tag{3.23}$$

and the coefficients are given by

$$\begin{aligned}\tilde{L}_{nm}&=\sum_{\nu=n}^{\infty}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu-n-|\mu-m|+|\mu|-|m|}c_\nu^2A_{\nu-n}^{\mu-m}A_n^mr_{tt}^{\nu-n}Y_{\nu-n}^{\mu-m}(\theta_{tt},\varphi_{tt})}{c_{\nu-n}^2c_n^2A_\nu^\mu}\hat{L}_{\nu\mu}\\&=\sum_{\nu=n}^{p}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu-n-|\mu-m|+|\mu|-|m|}c_\nu^2A_{\nu-n}^{\mu-m}A_n^mr_{tt}^{\nu-n}Y_{\nu-n}^{\mu-m}(\theta_{tt},\varphi_{tt})}{c_{\nu-n}^2c_n^2A_\nu^\mu}L_{\nu\mu}.\end{aligned} \tag{3.24}$$

Here, the definition (3.22) for $\hat{L}_{nm}$ is used to reduce the infinite summation to the finite one. Moreover, we have $\tilde{L}_{nm}=0$ for all $n>p$. As a result, (3.20) and (3.23) imply

$$\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}r_t^nY_n^m(\theta_t,\varphi_t)=\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{L}_{nm}\tilde{r}_t^nY_n^m(\tilde{\theta}_t,\tilde{\varphi}_t), \tag{3.25}$$

where the coefficients $\tilde{L}_{nm}$ are calculated via (3.24). Together with convergence result in Theorem 3.2, we have error estimate for the LE center shifting as follows.

Corollary 3.2. *Given $a>0$ and two centers $\boldsymbol{r}_c^t, \tilde{\boldsymbol{r}}_c^t \in \mathbb{R}^3$ close to each other with distance $d=|\tilde{\boldsymbol{r}}_c^t-\boldsymbol{r}_c^t|$, $\boldsymbol{r}$ is another given point inside the sphere $\{\boldsymbol{x}:|\boldsymbol{x}-\tilde{\boldsymbol{r}}_c^t|\le a\}$, then for any $\boldsymbol{r}'$ outside the sphere $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^t|>a+d\}$, applying the truncated LE shifting formula* (3.12b) *to the truncated LE* (3.20) *leads to approximation with error estimate*

$$\Big|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{L}_{nm}\tilde{r}_t^n Y_n^m(\tilde{\theta}_t,\tilde{\varphi}_t)\Big|\le\frac{1}{4\pi}\frac{1}{a-\tilde{r}_t}\Big(\frac{\tilde{r}_t+d}{a+d}\Big)^{p+1}. \tag{3.26}$$

3.2 A general framework for the derivation of the expansions, shifting and translation operators for the reaction components

Besides using the addition theorems as presented above, we have proposed a different derivation (cf. [27]) for (3.5) and (3.6) using the integral representation of $1/|\boldsymbol{r}-\boldsymbol{r}'|$. Moreover, the methodology has been further applied to derive multipole and local expansions for the reaction components defined in (2.4).

Below, we will propose a general framework for the derivation and convergence analysis of the expansions and corresponding translation operators for the reaction components. For this purpose, we define a general integral

$$\mathcal{I}(\boldsymbol{r};\sigma)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\sigma(k_\rho)dk_xdk_y, \quad \forall \boldsymbol{r}=(x,y,z)\in\mathbb{R}^3, \tag{3.27}$$

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

$$\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}';\sigma)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\sum_{n=0}^{\infty}\frac{1}{k_\rho}\frac{(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}')^n}{n!}\sigma(k_\rho)dk_xdk_y, \tag{3.28a}$$

$$\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\frac{1}{k_\rho}\frac{(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}')^n(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'')^\nu}{n!\nu!}\sigma(k_\rho)dk_xdk_y, \tag{3.28b}$$

for any $\boldsymbol{r}'=(x',y',z')$, $\boldsymbol{r}''=(x'',y'',z'')$ 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 (3.27) and (3.28) are absolutely convergent as $|e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}|=e^{-k_\rho z}$. Let us first present the main conclusion that the order of the improper integral and the infinite summation in (3.28) can be exchanged and the resulting series have exponential convergence under suitable conditions. Detailed proof will be given in Section 3.4. For the sake of brevity, we will use notations

$$\mathcal{I}_n(\boldsymbol{r},\boldsymbol{r}';\sigma)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\frac{(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}')^n}{n!}\sigma(k_\rho)dk_xdk_y, \tag{3.29a}$$

$$\mathcal{I}_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\frac{(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}')^n(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}'')^\nu}{n!\nu!}\sigma(k_\rho)dk_xdk_y. \tag{3.29b}$$

These integrals are all absolutely convergent due to the exponential decaying factor $e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$.

Theorem 3.4. *Suppose the density function $\sigma(k_\rho)$ is analytic and has a bound $|\sigma(k_\rho)|\le M_\sigma$ in the right half complex plane $\{k_\rho:\mathfrak{Re}k_\rho>0\}$, $\boldsymbol{r}=(x,y,z)$, $\boldsymbol{r}'=(x',y',z')\in\mathbb{R}^3$ such that $z>0$, $z+z'>0$, and $|\boldsymbol{r}|>|\boldsymbol{r}'|$. Then, the expansion*

$$\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}';\sigma)=\sum_{n=0}^{\infty}\mathcal{I}_n(\boldsymbol{r},\boldsymbol{r}';\sigma) \tag{3.30}$$

holds while the truncation error estimate is given by

$$\Big|\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}';\sigma)-\sum_{n=0}^{p}\mathcal{I}_n(\boldsymbol{r},\boldsymbol{r}';\sigma)\Big|\le\frac{2\pi M_\sigma}{|\boldsymbol{r}|-|\boldsymbol{r}'|}\left(\frac{|\boldsymbol{r}'|}{|\boldsymbol{r}|}\right)^{p+1}. \tag{3.31}$$

In addition, suppose $\boldsymbol{r}''=(x'',y'',z'')\in\mathbb{R}^3$ such that $z+z'+z''>0$ and $|\boldsymbol{r}|>|\boldsymbol{r}'|+|\boldsymbol{r}''|$. Then, the expansion

$$\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma)=\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\mathcal{I}_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma) \tag{3.32}$$

holds and the truncation error estimate is given by

$$\begin{aligned}&\Big|\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma)-\sum_{n=0}^{p}\sum_{\nu=0}^{p}\mathcal{I}_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma)\Big|\\&\le\frac{4\pi M_\sigma}{|\boldsymbol{r}|-|\boldsymbol{r}'|-|\boldsymbol{r}''|}\left[\Big(\frac{|\boldsymbol{r}'|}{|\boldsymbol{r}|-|\boldsymbol{r}''|}\Big)^{p+1}+\Big(\frac{|\boldsymbol{r}''|}{|\boldsymbol{r}|-|\boldsymbol{r}'|}\Big)^{p+1}\right].\end{aligned} \tag{3.33}$$

The following limiting version of the extended Legendre addition theorem will also be used to derive MEs and LEs for the reaction components of the layered Green's function.

Theorem 3.5. *Let θ, φ be the azimuthal angle and polar angles of a unit vector $\hat{\boldsymbol{r}}$, $\alpha\in[0,2\pi)$ be a given angle. Define a vector $\boldsymbol{k}_0=(\cos\alpha,\sin\alpha,\mathrm{i})$ with complex entry. Then*

$$\frac{(\mathrm{i}\boldsymbol{k}_0\cdot\hat{\boldsymbol{r}})^n}{n!}=\sum_{m=-n}^{n}C_n^m\widehat{P}_n^m(\cos\theta)e^{\mathrm{i}m(\alpha-\varphi)}, \tag{3.34}$$

where

$$C_n^m=\mathrm{i}^{2n-m}\sqrt{\frac{4\pi}{(2n+1)(n+m)!(n-m)!}}. \tag{3.35}$$

Now, we are ready to present the expansions and their translation operators for reaction components. According to the expressions (2.4)-(2.5) for the reaction components $u_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}')$, it is natural to introduce notations

$$\boldsymbol{r}'_{11}:=(x',y',d_\ell-(z'-d_{\ell'})), \qquad \boldsymbol{r}'_{12}:=(x',y',d_\ell-(d_{\ell'-1}-z')), \tag{3.36a}$$

$$\boldsymbol{r}'_{21}:=(x',y',d_{\ell-1}+(z'-d_{\ell'})), \qquad \boldsymbol{r}'_{22}:=(x',y',d_{\ell-1}+(d_{\ell'-1}-z')), \tag{3.36b}$$

which will simplify the coordinates mapping in (2.5) as follows

$$\boldsymbol{\tau}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}')=\boldsymbol{r}-\boldsymbol{r}'_{1\mathfrak{b}}, \quad \boldsymbol{\tau}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}')=\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}'_{2\mathfrak{b}}), \quad \mathfrak{b}=1,2. \tag{3.37}$$

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

$$|\boldsymbol{\tau}(\boldsymbol{r})|=|\boldsymbol{r}|, \quad \boldsymbol{\tau}(\boldsymbol{r}+\boldsymbol{r}')=\boldsymbol{\tau}(\boldsymbol{r})+\boldsymbol{\tau}(\boldsymbol{r}'), \quad \boldsymbol{\tau}(a\boldsymbol{r})=a\boldsymbol{\tau}(\boldsymbol{r}), \quad \forall \boldsymbol{r},\boldsymbol{r}'\in\mathbb{R}^3, \quad \forall a\in\mathbb{R}. \tag{3.38}$$

As a result, we can get rid of the heavy notations $\boldsymbol{\tau}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}')$ in (2.4) by using the new coordinates to re-express the reaction components as follows

$$u_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}'_{1\mathfrak{b}})}\sigma_{\ell\ell'}^{1\mathfrak{b}}(k_\rho)dk_xdk_y:=\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}}), \tag{3.39a}$$

$$u_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}'_{2\mathfrak{b}})}\sigma_{\ell\ell'}^{2\mathfrak{b}}(k_\rho)dk_xdk_y:=\tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}}). \tag{3.39b}$$

By the definition (3.27), we have

$$\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\mathcal{I}(\boldsymbol{r}-\boldsymbol{r}'_{1\mathfrak{b}};\sigma_{\ell\ell'}^{1\mathfrak{b}}), \quad \tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})=\mathcal{I}(\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}'_{2\mathfrak{b}});\sigma_{\ell\ell'}^{2\mathfrak{b}}). \tag{3.40}$$

The coordinates in (3.36) are exactly the equivalent polarization sources (see Fig. 5) which we have introduced in [26, 27]. As in our previous papers, we will also use notations $(x'_{\mathfrak{ab}},y'_{\mathfrak{ab}},z'_{\mathfrak{ab}})$ for the coordinates of $\boldsymbol{r}'_{\mathfrak{ab}}$, $\mathfrak{a},\mathfrak{b}=1,2$, in this paper.

Remark 3.1. There are two special cases

$$u^{12}_{\ell\ell+1}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')}\sigma^{12}_{\ell\ell+1}(k_\rho)dk_xdk_y,$$
$$u^{21}_{\ell\ell-1}(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{1}{k_\rho}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}')}\sigma^{21}_{\ell\ell-1}(k_\rho)dk_xdk_y,$$

in which we have

$$\boldsymbol{\tau}^{12}_{\ell\ell+1}(\boldsymbol{r},\boldsymbol{r}')=\boldsymbol{r}-\boldsymbol{r}',\quad \boldsymbol{\tau}^{21}_{\ell\ell-1}(\boldsymbol{r},\boldsymbol{r}')=\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}').$$

Actually, we will have $\boldsymbol{r}'_{12}=\boldsymbol{r}'$ and $\boldsymbol{r}'_{21}=\boldsymbol{r}'$ in these two cases, respectively.

Next, we will consider the expansions for $\tilde{u}^{\mathfrak{ab}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})$ with respect to (*polarization*) source center $\boldsymbol{r}^{\mathfrak{ab}}_c=(x^{\mathfrak{ab}}_c,y^{\mathfrak{ab}}_c,z^{\mathfrak{ab}}_c)$ and target center $\boldsymbol{r}^t_c=(x^t_c,y^t_c,z^t_c)$. As we are considering targets in the ℓ-th layer and the equivalent polarized coordinates are always located either above the interface $z=d_{\ell-1}$ or below the interface $z=d_\ell$ (see Fig. 5), it is reasonable to assume that the z-coordinates of $\boldsymbol{r}^{\mathfrak{ab}}_c$ and $\boldsymbol{r}^t_c$ satisfy (see Fig. 6)

$$z^{1\mathfrak{b}}_c<d_\ell,\quad z^{2\mathfrak{b}}_c>d_{\ell-1},\quad d_\ell<z^t_c<d_{\ell-1}. \tag{3.41}$$

By the definition (3.27) and the linear features (3.38) of $\boldsymbol{\tau}(\boldsymbol{r})$, we can insert the source center $\boldsymbol{r}^{\mathfrak{ab}}_c$ and the target center $\boldsymbol{r}^t_c$ in (3.40) to give

$$\tilde{u}^{1\mathfrak{b}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\mathcal{I}(\boldsymbol{r}-\boldsymbol{r}^{1\mathfrak{b}}_c-(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}^{1\mathfrak{b}}_c);\sigma^{1\mathfrak{b}}_{\ell\ell'}), \tag{3.42a}$$
$$\tilde{u}^{2\mathfrak{b}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})=\frac{1}{8\pi^2}\mathcal{I}(\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}^{2\mathfrak{b}}_c)-\boldsymbol{\tau}(\boldsymbol{r}'_{2\mathfrak{b}}-\boldsymbol{r}^{2\mathfrak{b}}_c);\sigma^{2\mathfrak{b}}_{\ell\ell'}), \tag{3.42b}$$

and

$$\tilde{u}^{1\mathfrak{b}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\mathcal{I}(\boldsymbol{r}-\boldsymbol{r}^t_c+(\boldsymbol{r}^t_c-\boldsymbol{r}'_{1\mathfrak{b}});\sigma^{1\mathfrak{b}}_{\ell\ell'}), \tag{3.43a}$$
$$\tilde{u}^{2\mathfrak{b}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})=\frac{1}{8\pi^2}\mathcal{I}(\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}^t_c)-\boldsymbol{\tau}(\boldsymbol{r}^t_c-\boldsymbol{r}'_{2\mathfrak{b}});\sigma^{2\mathfrak{b}}_{\ell\ell'}). \tag{3.43b}$$

By definition (3.36) and assumptions in (3.41), we have

$$z-z^{1\mathfrak{b}}_c>0,\quad z^t_c-z'_{1\mathfrak{b}}>0,\quad z^{2\mathfrak{b}}_c-z>0,\quad z'_{2\mathfrak{b}}-z^t_c>0,\quad z-z'_{1\mathfrak{b}}>0,\quad z'_{2\mathfrak{b}}-z>0. \tag{3.44}$$

Assume the centers $\boldsymbol{r}^{\mathfrak{ab}}_c$ and $\boldsymbol{r}^t_c$ further satisfy $|\boldsymbol{r}-\boldsymbol{r}^{\mathfrak{ab}}_c|>|\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}^{\mathfrak{ab}}_c|$, and $|\boldsymbol{r}-\boldsymbol{r}^t_c|<|\boldsymbol{r}^t_c-\boldsymbol{r}'_{\mathfrak{ab}}|$, then (3.44) and Proposition 2.1 implies that Theorem 3.4 can be applied

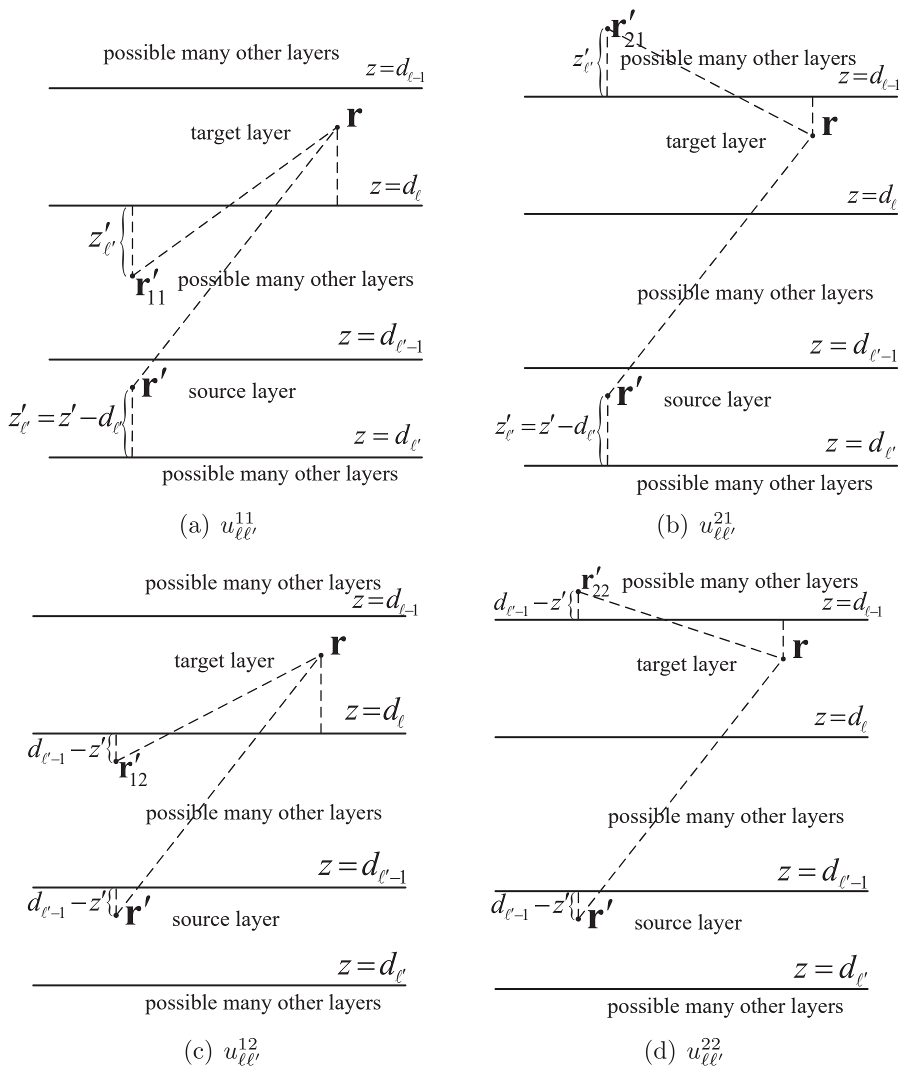


Figure 5: Location of equivalent polarization sources associated to $u^{\mathfrak{ab}}_{\ell\ell'}$.

to give expansions for the integrals in (3.42)-(3.43), i.e.,

$$\tilde{u}^{1\mathfrak{b}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_c^{1\mathfrak{b}})}\frac{[-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}})]^n}{n!k_\rho}\sigma^{1\mathfrak{b}}_{\ell\ell'}(k_\rho)dk_xdk_y, \tag{3.45a}$$

$$\tilde{u}^{2\mathfrak{b}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})=\frac{1}{8\pi^2}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}-\boldsymbol{r}_c^{2\mathfrak{b}})}\frac{[-\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}'_{2\mathfrak{b}}-\boldsymbol{r}_c^{2\mathfrak{b}})]^n}{n!k_\rho}\sigma^{2\mathfrak{b}}_{\ell\ell'}(k_\rho)dk_xdk_y, \tag{3.45b}$$

and

$$\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}_c^t-\boldsymbol{r}'_{1\mathfrak{b}})}\frac{[\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_c^t)]^n}{n!k_\rho}\sigma_{\ell\ell'}^{1\mathfrak{b}}(k_\rho)dk_xdk_y, \tag{3.46a}$$

$$\tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})=\frac{1}{8\pi^2}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}_c^t-\boldsymbol{r}'_{2\mathfrak{b}})}\frac{[\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}-\boldsymbol{r}_c^t)]^n}{n!k_\rho}\sigma_{\ell\ell'}^{2\mathfrak{b}}(k_\rho)dk_xdk_y. \tag{3.46b}$$

Further, applying Theorem 3.5 to the expansions in (3.45)-(3.46) and then using the identities

$$Y_n^m(\pi-\theta,\varphi)=(-1)^{n+m}Y_n^m(\theta,\varphi),\quad Y_n^m(\theta,\pi+\varphi)=(-1)^mY_n^m(\theta,\varphi), \tag{3.47}$$

to simplify the obtained results, we obtain MEs

$$\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}M_{nm}^{\mathfrak{ab}}\mathcal{F}_{nm}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}_c^{\mathfrak{ab}}),\quad M_{nm}^{\mathfrak{ab}}=\frac{c_n^{-2}}{4\pi}(r_c^{\mathfrak{ab}})^n\overline{Y_n^m(\theta_c^{\mathfrak{ab}},\varphi_c^{\mathfrak{ab}})}, \tag{3.48}$$

at equivalent polarization source centers $\boldsymbol{r}_c^{\mathfrak{ab}}$ and LEs

$$\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}L_{nm}^{\mathfrak{ab}}r_t^nY_n^m(\theta_t,\varphi_t) \tag{3.49}$$

at target center $\boldsymbol{r}_c^t$, respectively. Here, $(r_c^{\mathfrak{ab}},\theta_c^{\mathfrak{ab}},\varphi_c^{\mathfrak{ab}})$ and (r_t,θ_t,φ_t) are the spherical coordinates of $\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}_c^{\mathfrak{ab}}$ and $\boldsymbol{r}-\boldsymbol{r}_c^t$ (no $'$ notation is included in the spherical coordinates of $\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}_c^{\mathfrak{ab}}$ for simpler notation), the ME basis functions $\mathcal{F}_{nm}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}_c^{\mathfrak{ab}})$ are represented by Sommerfeld-type integrals

$$\mathcal{F}_{nm}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}_c^{1\mathfrak{b}})=\frac{(-1)^nc_n^2C_n^m}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_c^{1\mathfrak{b}})}\sigma_{\ell\ell'}^{1\mathfrak{b}}(k_\rho)k_\rho^{n-1}e^{\mathrm{i}m\alpha}dk_xdk_y, \tag{3.50a}$$

$$\mathcal{F}_{nm}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}_c^{2\mathfrak{b}})=\frac{(-1)^mc_n^2C_n^m}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}-\boldsymbol{r}_c^{2\mathfrak{b}})}\sigma_{\ell\ell'}^{2\mathfrak{b}}(k_\rho)k_\rho^{n-1}e^{\mathrm{i}m\alpha}dk_xdk_y, \tag{3.50b}$$

and the local expansion coefficients $L_{nm}^{\mathfrak{ab}}$ are given by

$$L_{nm}^{1\mathfrak{b}}=\frac{C_n^m}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}_c^t-\boldsymbol{r}'_{1\mathfrak{b}})}\sigma_{\ell\ell'}^{1\mathfrak{b}}(k_\rho)k_\rho^{n-1}e^{-\mathrm{i}m\alpha}dk_xdk_y, \tag{3.51a}$$

$$L_{nm}^{2\mathfrak{b}}=\frac{(-1)^{n+m}C_n^m}{8\pi^2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}_c^t-\boldsymbol{r}'_{2\mathfrak{b}})}\sigma_{\ell\ell'}^{2\mathfrak{b}}(k_\rho)k_\rho^{n-1}e^{-\mathrm{i}m\alpha}dk_xdk_y. \tag{3.51b}$$

A desirable feature of the expansions of reaction components discussed above is that the formula in (3.48) for the ME coefficients and the formula (3.49) 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 (3.12a) and (3.12b).

As in (3.42)-(3.43), the reaction components in (3.39) can also be represented as

$$\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\mathcal{I}(\boldsymbol{r}-\boldsymbol{r}_c^t+(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}})-(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}});\sigma_{\ell\ell'}^{1\mathfrak{b}}), \tag{3.52a}$$

$$\tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\mathcal{I}(\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}_c^t)+\boldsymbol{\tau}(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{2\mathfrak{b}})-\boldsymbol{\tau}(\boldsymbol{r}'_{2\mathfrak{b}}-\boldsymbol{r}_c^{2\mathfrak{b}});\sigma_{\ell\ell'}^{2\mathfrak{b}}). \tag{3.52b}$$

Apparently, from (3.41), we have

$$z_c^t-z_c^{1\mathfrak{b}}>0,\quad z_c^{2\mathfrak{b}}-z_c^t>0. \tag{3.53}$$

Assume the given centers $\boldsymbol{r}_c^{\mathfrak{ab}}$ and $\boldsymbol{r}_c^t$ satisfy $|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{\mathfrak{ab}}|>|\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}_c^{\mathfrak{ab}}|+|\boldsymbol{r}-\boldsymbol{r}_c^t|$, then (3.44), (3.53) and Proposition 2.1 implies that Theorem 3.4 can be applied to give expansions for the integrals in (3.52), i.e.,

$$\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})=\frac{1}{8\pi^2}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\mathcal{I}_{n\nu}(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}},\boldsymbol{r}-\boldsymbol{r}_c^t,-(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}});\sigma_{\ell\ell'}^{1\mathfrak{b}}), \tag{3.54a}$$

$$\tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})=\frac{1}{8\pi^2}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\mathcal{I}_{n\nu}(\boldsymbol{\tau}(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{2\mathfrak{b}}),\boldsymbol{\tau}(\boldsymbol{r}-\boldsymbol{r}_c^t),-\boldsymbol{\tau}(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}});\sigma_{\ell\ell'}^{2\mathfrak{b}}). \tag{3.54b}$$

Applying Proposition 3.5 to the integrand of $\mathcal{I}_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)$, we obtain the translation from ME (3.48) to LE (3.49), i.e.,

$$L_{nm}^{\mathfrak{ab}}=\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu}T_{nm,\nu\mu}^{\mathfrak{ab}}M_{\nu\mu}^{\mathfrak{ab}}, \tag{3.55}$$

where the translation operators are given as follows

$$T_{nm,\nu\mu}^{1\mathfrak{b}}=\frac{D_{nm\nu\mu}^1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}})}\sigma_{\ell\ell'}^{1\mathfrak{b}}(k_\rho)k_\rho^{n+\nu-1}e^{\mathrm{i}(\mu-m)\alpha}dk_xdk_y, \tag{3.56a}$$

$$T_{nm,\nu\mu}^{2\mathfrak{b}}=\frac{D_{nm\nu\mu}^2}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{2\mathfrak{b}})}\sigma_{\ell\ell'}^{2\mathfrak{b}}(k_\rho)k_\rho^{n+\nu-1}e^{\mathrm{i}(\mu-m)\alpha}dk_xdk_y, \tag{3.56b}$$

and

$$D_{nm\nu\mu}^1=(-1)^\nu c_\nu^2C_n^mC_\nu^\mu,\quad D_{nm\nu\mu}^2=(-1)^{n+m+\mu}c_\nu^2C_n^mC_\nu^\mu.$$

3.3 Convergence theory for the expansions of the reaction components

Recalling the derivation of the ME (3.5) and the LE (3.6), we have the following exponential convergence for the ME and LE.

Theorem 3.6. *Given* $a>0$, $\boldsymbol{r}=(x,y,z)$ *a target point in the* ℓ*-th layer and* $\boldsymbol{r}_c^{\mathfrak{ab}}=(x_c^{\mathfrak{ab}},y_c^{\mathfrak{ab}},z_c^{\mathfrak{ab}})$ *a (polarization) source center satisfying conditions in* (3.41)*. Suppose* $|\boldsymbol{r}-\boldsymbol{r}_c^{\mathfrak{ab}}|>a$*, then, for any equivalent polarization source* $\boldsymbol{r}'_{\mathfrak{ab}}$ *inside the sphere* $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^{\mathfrak{ab}}|\le a\}$*, the MEs in* (3.48) *hold and have truncation error estimates*

$$\Big|\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})-\sum_{n=0}^{p}\sum_{m=-n}^{n}M_{nm}^{\mathfrak{ab}}\mathcal{F}_{nm}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}_c^{\mathfrak{ab}})\Big|\le\frac{1}{4\pi}\frac{M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}}{|\boldsymbol{r}-\boldsymbol{r}_c^{\mathfrak{ab}}|-a}\Big(\frac{a}{|\boldsymbol{r}-\boldsymbol{r}_c^{\mathfrak{ab}}|}\Big)^{p+1} \tag{3.57}$$

for $\mathfrak{a},\mathfrak{b}=1,2$*, where* $M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}$ *is the bound of* $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ *in the right half complex plane.*

Proof. The MEs in (3.48) have been proved in the last subsection. Here, we only need to consider the error estimate. By assumptions in (3.41), we have

$$z-z_c^{1\mathfrak{b}}>0,\quad z_c^{2\mathfrak{b}}-z>0,\quad z-z'_{1\mathfrak{b}}>0,\quad z'_{2\mathfrak{b}}-z>0.$$

Together with the assumption $|\boldsymbol{r}-\boldsymbol{r}_c^{\mathfrak{ab}}|>a\ge|\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}_c^{\mathfrak{ab}}|$ and Proposition 2.1, we can apply the truncation error estimates (3.31) to obtain

$$\begin{aligned}&\Big|\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})-\sum_{n=0}^{p}\sum_{m=-n}^{n}M_{nm}^{1\mathfrak{b}}\mathcal{F}_{nm}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}_c^{1\mathfrak{b}})\Big|\\
=&\frac{1}{8\pi^2}\Big|\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'_{1\mathfrak{b}};\sigma_{\ell\ell'}^{1\mathfrak{b}})-\sum_{n=0}^{p}\mathcal{I}_n(\boldsymbol{r}-\boldsymbol{r}_c^{1\mathfrak{b}},-(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}});\sigma_{\ell\ell'}^{1\mathfrak{b}})\Big|,\\
\le&\frac{M_{\sigma_{\ell\ell'}^{1\mathfrak{b}}}}{4\pi(|\boldsymbol{r}-\boldsymbol{r}_c^{1\mathfrak{b}}|-|\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}}|)}\Big(\frac{|\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}}|}{|\boldsymbol{r}-\boldsymbol{r}_c^{1\mathfrak{b}}|}\Big)^{p+1},\end{aligned}$$

and similarly

$$\begin{aligned}&\Big|\tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})-\sum_{n=0}^{p}\sum_{m=-n}^{n}M_{nm}^{2\mathfrak{b}}\mathcal{F}_{nm}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}_c^{2\mathfrak{b}})\Big|\\
\le&\frac{M_{\sigma_{\ell\ell'}^{2\mathfrak{b}}}}{4\pi(|\boldsymbol{r}-\boldsymbol{r}_c^{2\mathfrak{b}}|-|\boldsymbol{r}'_{2\mathfrak{b}}-\boldsymbol{r}_c^{2\mathfrak{b}}|)}\Big(\frac{|\boldsymbol{r}'_{2\mathfrak{b}}-\boldsymbol{r}_c^{2\mathfrak{b}}|}{|\boldsymbol{r}-\boldsymbol{r}_c^{2\mathfrak{b}}|}\Big)^{p+1}.\end{aligned}$$

Consequently, the error estimate (3.57) follows by applying the assumption $|\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}_c^{\mathfrak{ab}}|\le a$ in the above estimates. □

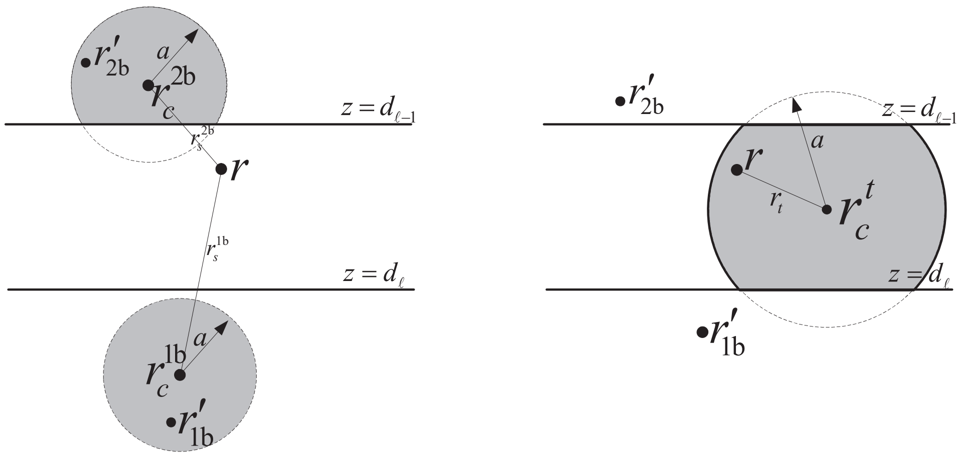


Figure 6: The geometric configuration for the ME and LE of the reaction components.

It is worthy to mention that the above theoretical results have been predicted by the numerical results in [27, Section 3.3]. Following a similar proof, we have the error estimate for the truncated LE as follows.

Theorem 3.7. *Given $a>0$, $\boldsymbol{r}=(x,y,z)$ a target point in the ℓ-th layer and $\boldsymbol{r}_c^t=(x_c^t,y_c^t,z_c^t)$ a center satisfying conditions in* (3.41)*. Suppose $|\boldsymbol{r}-\boldsymbol{r}_c^t|\le a$, then, for any equivalent polarization source $\boldsymbol{r}'_{\mathfrak{ab}}$ outside the sphere $\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^t|\le a\}$, the LEs* (3.49) *hold and have truncation error estimates*

$$\left|\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})-\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}^{\mathfrak{ab}}r_t^nY_n^m(\theta_t,\varphi_t)\right|\le\frac{1}{4\pi}\frac{M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}}{a-|\boldsymbol{r}-\boldsymbol{r}_c^t|}\left(\frac{|\boldsymbol{r}-\boldsymbol{r}_c^t|}{a}\right)^{p+1} \tag{3.58}$$

for $\mathfrak{a},\mathfrak{b}=1,2$, where $M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}$ is the bound of $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ in the right half complex plane.

It is worthy to emphasize that the equivalent polarization sources $\boldsymbol{r}'_{1\mathfrak{b}}$ and $\boldsymbol{r}'_{2\mathfrak{b}}$ are defined to be below the lower and above the upper interfaces of the target layer, respectively (see Fig. 6). The ME centers are required to be located on the same side as the corresponding equivalent polarization sources. Accordingly, the target center is required to be in the same layer as the target point $\boldsymbol{r}$. We refer to Fig. 6 for an illustration of the geometric configurations. The shadowed areas indicate the feasible zones of the equivalent polarization sources and targets such that the expansions and corresponding convergence results hold.

Now, we consider the error estimate for the ME to LE translation. Suppose the

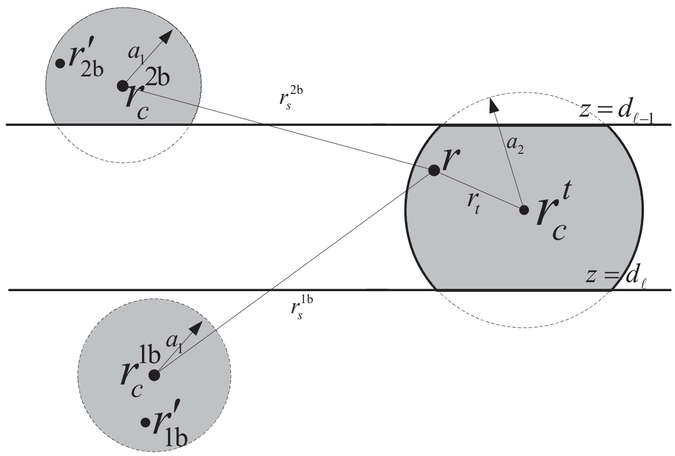


Figure 7: The geometric configuration for the center shifting.

ME to LE translations in (3.55) are truncated to give approximated LE coefficients

$$L_{nm}^{\mathfrak{ab},p} := \sum_{\nu=0}^{p} \sum_{\mu=-\nu}^{\nu} T_{nm,\nu\mu}^{\mathfrak{ab}} M_{\nu\mu}^{\mathfrak{ab},\mathrm{in}}. \tag{3.59}$$

Thus, approximate LEs

$$\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}}) \approx \tilde{u}_{\ell\ell'}^{\mathfrak{ab},p}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}}) := \sum_{n=0}^{p} \sum_{m=-n}^{n} L_{nm}^{\mathfrak{ab},p} r_t^n Y_n^m(\theta_t,\varphi_t) \tag{3.60}$$

with approximate LE coefficients defined in (3.59) are obtained after M2L translation. Recalling representation (3.52) and expansion (3.54), the approximate LEs $\tilde{u}_{\ell\ell'}^{\mathfrak{ab},p}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})$ have representations

$$\tilde{u}_{\ell\ell'}^{1\mathfrak{b},p}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}}) = \frac{1}{8\pi^2} \sum_{n=0}^{p} \sum_{\nu=0}^{p} \mathcal{I}_{n\nu}(\boldsymbol{r}_c^t - \boldsymbol{r}_c^{1\mathfrak{b}}, \boldsymbol{r} - \boldsymbol{r}_c^t, -(\boldsymbol{r}'_{1\mathfrak{b}} - \boldsymbol{r}_c^{1\mathfrak{b}}); \sigma_{\ell\ell'}^{1\mathfrak{b}}), \tag{3.61a}$$

$$\tilde{u}_{\ell\ell'}^{2\mathfrak{b},p}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}}) = \frac{1}{8\pi^2} \sum_{n=0}^{p} \sum_{\nu=0}^{p} \mathcal{I}_{n\nu}(\boldsymbol{\tau}(\boldsymbol{r}_c^t - \boldsymbol{r}_c^{2\mathfrak{b}}), \boldsymbol{\tau}(\boldsymbol{r} - \boldsymbol{r}_c^t), -\boldsymbol{\tau}(\boldsymbol{r}'_{2\mathfrak{b}} - \boldsymbol{r}_c^{2\mathfrak{b}}); \sigma_{\ell\ell'}^{2\mathfrak{b}}). \tag{3.61b}$$

Obviously, they are rectangular truncation of the double Taylor series. Hence, we have the following error estimate.

Theorem 3.8. *Given $a_1 > 0$, $a_2 > 0$, $\boldsymbol{r}$, $\boldsymbol{r}'$ are any points locate in the ℓ-th and ℓ'-th layers, respectively. Suppose $\boldsymbol{r}_c^{\mathfrak{ab}}$ and $\boldsymbol{r}_c^t$ are two points satisfy conditions in* (3.41) *and* $|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{\mathfrak{ab}}|\geq a_1+ca_2$ *with some* $c>1$ *(see Fig. 7 for configuration). Then, the truncated ME to LE translation* (3.59) *has error estimate*

$$\left|\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})-\tilde{u}_{\ell\ell'}^{\mathfrak{ab},p}(\boldsymbol{r},\boldsymbol{r}'_{\mathfrak{ab}})\right|\leq\frac{1}{2\pi}\frac{M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}}{(c-1)a_2}\left[\Big(\frac{a_1}{a_1+(c-1)a_2}\Big)^{p+1}+\Big(\frac{1}{c}\Big)^{p+1}\right], \tag{3.62}$$

where $M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}$ *is the bound of* $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ *in the right half complex plane.*

Proof. By (3.54), (3.61) and truncation error estimate (3.33), we obtain

$$\begin{aligned}
&\left|\tilde{u}_{\ell\ell'}^{1\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})-\tilde{u}_{\ell\ell'}^{1\mathfrak{b},p}(\boldsymbol{r},\boldsymbol{r}'_{1\mathfrak{b}})\right|\\
=&\frac{1}{8\pi^2}\left|\mathcal{I}(\boldsymbol{r}-\boldsymbol{r}'_{1\mathfrak{b}};\sigma_{\ell\ell'}^{1\mathfrak{b}})-\sum_{n=0}^{p}\sum_{\nu=0}^{p}\mathcal{I}_{n\nu}(\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}},\boldsymbol{r}-\boldsymbol{r}_c^t,-(\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}});\sigma_{\ell\ell'}^{1\mathfrak{b}})\right|\\
\leq&\frac{M_{\sigma_{\ell\ell'}^{1\mathfrak{b}}}}{2\pi(|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}}|-|\boldsymbol{r}-\boldsymbol{r}_c^t|-|\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}}|)}\Big(\frac{|\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}}|}{|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}}|-|\boldsymbol{r}-\boldsymbol{r}_c^t|}\Big)^{p+1}\\
&+\frac{M_{\sigma_{\ell\ell'}^{1\mathfrak{b}}}}{2\pi(|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}}|-|\boldsymbol{r}-\boldsymbol{r}_c^t|-|\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}}|)}\Big(\frac{|\boldsymbol{r}-\boldsymbol{r}_c^t|}{|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{1\mathfrak{b}}|-|\boldsymbol{r}'_{1\mathfrak{b}}-\boldsymbol{r}_c^{1\mathfrak{b}}|}\Big)^{p+1}.
\end{aligned}\tag{3.63}$$

Similar error estimate can also be obtained for the reaction component $\tilde{u}_{\ell\ell'}^{2\mathfrak{b}}(\boldsymbol{r},\boldsymbol{r}'_{2\mathfrak{b}})$ by following the same derivations. Consequently, the error estimate (3.62) follows by further applying the assumptions $|\boldsymbol{r}'_{\mathfrak{ab}}-\boldsymbol{r}_c^{\mathfrak{ab}}|<a_1$ and $|\boldsymbol{r}-\boldsymbol{r}_c^t|<a_2$ and $|\boldsymbol{r}_c^t-\boldsymbol{r}_c^{\mathfrak{ab}}|\geq a_1+ca_2$. □

Remark 3.2. The error estimates in Theorems 3.6-3.8 are almost the same as the ones in Theorems 3.1-3.3 except the dependence on the bound $M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}$ of the density $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$.

3.4 Proof for the Theorem 3.4

The proof consists of the following three steps:

Step 1: Rotation according to the azimuthal angle of $\boldsymbol{r}$. By the assumptions $z>0, z+z'>0$ and $z+z'+z''>0$, all improper integrals in the Theorem 3.4 have exponentially decaying integrands and hence are absolutely convergent. Denote by (ρ,φ) the polar coordinate of (x,y) and define a transform in the complex (k_x,k_y)-plane as follows:

$$\xi+\mathrm{i}\eta=e^{\mathrm{i}\varphi}(k_x-\mathrm{i}k_y), \tag{3.64}$$

or equivalently,

$$k_x=\xi\cos\varphi+\eta\sin\varphi,\quad k_y=\xi\sin\varphi-\eta\cos\varphi. \tag{3.65}$$

It is obvious that $k_\rho = \sqrt{\xi^2+\eta^2}$, $dk_x dk_y = -d\xi d\eta$ and

$$\begin{aligned}\frac{(\mathrm{i}\boldsymbol{k}\cdot\tilde{\boldsymbol{r}})^n}{n!} &= \frac{\mathrm{i}^n\tilde{r}^n}{n!}(\xi^2+\eta^2)^{\frac{n}{2}}\Big[\frac{\xi\cos(\varphi-\beta)+\eta\sin(\varphi-\beta)}{\sqrt{\xi^2+\eta^2}}\sin\alpha+\mathrm{i}\cos\alpha\Big]^n \\ &:= \hat{g}_n(\xi,\eta,\varphi;\tilde{\boldsymbol{r}})\end{aligned} \tag{3.66}$$

for any $\tilde{\boldsymbol{r}} = (\tilde{r}\sin\alpha\cos\beta, \tilde{r}\sin\alpha\sin\beta, \tilde{r}\cos\alpha) \in \mathbb{R}^3$. Moreover, by (3.65), we have

$$e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} = e^{\mathrm{i}(k_x x+k_y y)-k_\rho z} = e^{\mathrm{i}\xi\rho-k_\rho z}.$$

Therefore, integrals in (3.28) can be re-expressed as

$$\begin{aligned}\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}';\sigma) &= -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\hat{g}_n(\xi,\eta,\varphi;\boldsymbol{r}')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta \\ &= \int_0^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\big[\hat{g}_n(\xi,-\eta,\varphi;\boldsymbol{r}')-\hat{g}_n(\xi,\eta,\varphi;\boldsymbol{r}')\big]e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta,\end{aligned} \tag{3.67}$$

and

$$\begin{aligned}\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma) &= -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}g_{n\nu}(\xi,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta \\ &= \int_0^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\big[g_{n\nu}(\xi,-\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'') \\ &\qquad -g_{n\nu}(\xi,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\big]e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta,\end{aligned} \tag{3.68}$$

where

$$g_{n\nu}(\xi,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'') := \hat{g}_n(\xi,\eta,\varphi;\boldsymbol{r}')\hat{g}_\nu(\xi,\eta,\varphi;\boldsymbol{r}''). \tag{3.69}$$

Accordingly, the integrals in (3.29) can be re-expressed as

$$\mathcal{I}_n(\boldsymbol{r}+\boldsymbol{r}';\sigma) = \int_0^{\infty}\int_{-\infty}^{\infty}\big[\hat{g}_n(\xi,-\eta,\varphi;\boldsymbol{r}')-\hat{g}_n(\xi,\eta,\varphi;\boldsymbol{r}')\big]e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.70a}$$

$$\begin{aligned}\mathcal{I}_{n\nu}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma) &= \int_0^{\infty}\int_{-\infty}^{\infty}\big[g_{n\nu}(\xi,-\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'') \\ &\qquad -g_{n\nu}(\xi,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\big]e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta.\end{aligned} \tag{3.70b}$$

Step 2: Contour deformation. In the following analysis, we will deform the contour of the inner integrals in (3.67), (3.68) and (3.70). As the integrands involve square root function $k_\rho(\xi)=\sqrt{\xi^2+\eta^2}$, we choose branch as follows

$$\sqrt{z}=\sqrt{\frac{|z|+\mathfrak{Re}z}{2}}+\mathrm{i}\,\mathrm{sign}(\mathfrak{Im}z)\sqrt{\frac{|z|-\mathfrak{Re}z}{2}}, \quad \forall z\in\mathbb{C}. \tag{3.71}$$

Here and after, we use notations $\mathfrak{Re}z$, $\mathfrak{Im}z$ for the real and imaginary parts of any given complex number z. With this branch, $k_\rho(\xi)=\sqrt{\xi^2+\eta^2}$ for any fixed $\eta\neq 0$ has branch cut along $\{\xi|\xi=\mathrm{i}\zeta,\ \zeta>|\eta|\}$ and $\{\xi|\xi=\mathrm{i}\zeta,\ \zeta<-|\eta|\}$ (the red lines in Fig. 8) in the complex ξ-plane and is analytic with respect to ξ in the complex domain

$$\mathbb{C}\backslash(\{\xi|\xi=\mathrm{i}\zeta,\ \zeta\geq|\eta|\}\cup\{\xi|\xi=\mathrm{i}\zeta,\ \zeta\leq-|\eta|\}).$$

The contour deformation will be based on the following lemma:

Lemma 3.1. *Denote by $\Omega_\Gamma^+\subset\mathbb{C}$ the complex domain between real axis and the contour Γ defined by the parametric $\xi_\pm(t)$ in (3.74). Given real numbers $\rho\geq 0$, $z>0$ and $\eta\neq 0$, suppose $r=\sqrt{\rho^2+z^2}$, $f(\xi)$ is an analytic function in the complex domain Ω_Γ^+ and satisfies*

$$\lim_{|\xi|\rightarrow+\infty}\left|f(\xi)e^{\mathrm{i}\xi\rho-\sqrt{\eta^2+\xi^2}z}\xi\right|=0 \tag{3.72}$$

for $\xi\in\Omega_\Gamma^+$. Then, we have the following contour deformation

$$\int_{-\infty}^{\infty}f(\xi)e^{\mathrm{i}\xi\rho-\sqrt{\eta^2+\xi^2}z}d\xi=\mathrm{i}\int_1^{\infty}[f(\xi_+(t))\Lambda_+(t)+f(\xi_-(t)\Lambda_-(t)]\frac{e^{-|\eta|rt}}{\sqrt{t^2-1}}dt, \tag{3.73}$$

where $\xi_\pm(t)$, $\Lambda_\pm(t)$ are defined by the Cagniard-de Hoop transform

$$\xi_\pm(t)=\frac{|\eta|}{r}\left(\mathrm{i}\rho t\pm z\sqrt{t^2-1}\right), \quad \Lambda_\pm(t)=\frac{|\eta|}{r}(\rho\sqrt{t^2-1}\mp\mathrm{i}zt). \tag{3.74}$$

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

$$\Gamma_\pm=\{\xi_\pm(t):t\geq 1\}. \tag{3.75}$$

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. 8). Denote by $\xi_\pm(t_R)=Re^{\mathrm{i}\theta_R^\pm}$ the intersections of $O_R^\pm$ and $\Gamma^\pm$. Then, $0<\theta_R^+<\frac{\pi}{2}$, $\frac{\pi}{2}<\theta_R^-<\pi$ and

$$\left|\int_{O_R^+}f(\xi)e^{\mathrm{i}\xi\rho-\sqrt{\eta^2+\xi^2}z}d\xi\right|\leq\int_0^{\theta_R^+}\left|f(Re^{\mathrm{i}\theta})e^{\mathrm{i}Re^{\mathrm{i}\theta}\rho-\sqrt{\eta^2+R^2e^{2\mathrm{i}\theta}}z}R\right|d\theta, \tag{3.76a}$$

$$\left|\int_{O_R^-}f(\xi)e^{\mathrm{i}\xi\rho-\sqrt{\eta^2+\xi^2}z}d\xi\right|\leq\int_{\theta_R^-}^{\pi}\left|f(Re^{\mathrm{i}\theta})e^{\mathrm{i}Re^{\mathrm{i}\theta}\rho-\sqrt{\eta^2+R^2e^{2\mathrm{i}\theta}}z}R\right|d\theta. \tag{3.76b}$$

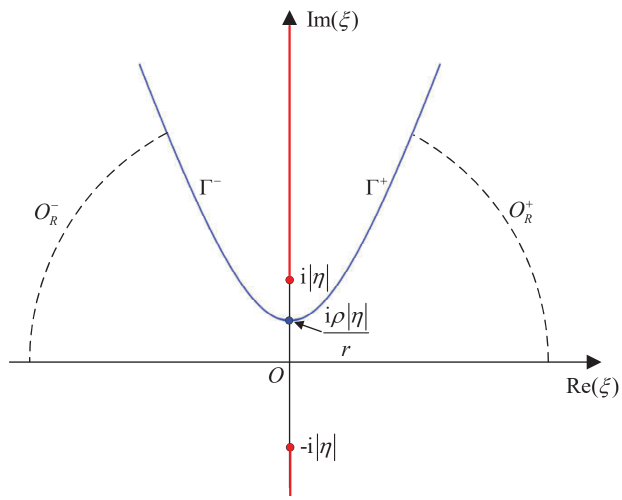


Figure 8: The Cagniard-de Hoop transform from the real axis to $\Gamma_+ \cup \Gamma_-$.

Taking limit for $R \to +\infty$ and applying the assumption (3.72) on the right hand sides gives

$$\Big|\int_{O_R^\pm} f(\xi) e^{\mathrm{i}\xi\rho - \sqrt{\eta^2+\xi^2}z} d\xi\Big| \to 0, \quad R \to +\infty. \tag{3.77}$$

Recalling the branch (3.71), the square root function $\sqrt{\eta^2+\xi^2}$ has branch cut along $\{\xi|\xi=\mathrm{i}\zeta,\ \zeta>|\eta|\}$ and $\{\xi|\xi=\mathrm{i}\zeta,\ \zeta<-|\eta|\}$ (see Fig. 8). By the assumption $z>0$, we always have $\frac{\rho|\eta|}{r}<|\eta|$ which implies that the square root function $\sqrt{\eta^2+\xi^2}$ is analytic in the domain Ω_Γ^+ for any fixed $\eta \neq 0$. Together with the assumption on $f(\xi)$, we have $f(\xi)e^{\mathrm{i}\xi\rho-\sqrt{\eta^2+\xi^2}z}$ is analytic in the domain Ω_Γ^+ for any fixed $\eta \neq 0$. Therefore, by Cauchy's theorem, (3.73) follows from the facts

$$\int_{-\infty}^{\infty} f(\xi) e^{\mathrm{i}\xi\rho - \sqrt{\eta^2+\xi^2}z} d\xi = \int_\Gamma f(\xi) e^{\mathrm{i}\xi\rho - \sqrt{\eta^2+\xi^2}z} d\xi, \quad \forall \eta \neq 0, \tag{3.78}$$

and

$$\frac{\mathrm{d}\xi_\pm(\mathrm{t})}{\mathrm{dt}} = \frac{|\eta|}{r\sqrt{t^2-1}}(\mathrm{i}\rho\sqrt{t^2-1} \pm zt) = \frac{\mathrm{i}\Lambda_\pm(t)}{\sqrt{t^2-1}}. \tag{3.79}$$

This completes the proof. □

In order to deform the contour of the inner integrals in (3.67), (3.68) and (3.70) from the real axis to the contour Γ defined in the Lemma 3.1, η is not allowed to touch 0. For this reason, we introduce sequences

$$\mathcal{E}_k^+(\boldsymbol{r},\boldsymbol{r}',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\hat{g}_n(\xi,\eta,\varphi;\boldsymbol{r}')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.80a}$$

$$\mathcal{E}_k^-(\boldsymbol{r},\boldsymbol{r}',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\hat{g}_n(\xi,-\eta,\varphi;\boldsymbol{r}')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.80b}$$

$$\mathcal{F}_k^+(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\sum_{nu=0}^{\infty}g_{n\nu}(\xi,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.80c}$$

$$\mathcal{F}_k^-(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}\sum_{n=0}^{\infty}\sum_{nu=0}^{\infty}g_{n\nu}(\xi,-\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.80d}$$

and

$$\mathcal{E}_k^{n,+}(\boldsymbol{r},\boldsymbol{r}',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}\hat{g}_n(\xi,\eta,\varphi;\boldsymbol{r}')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.81a}$$

$$\mathcal{E}_k^{n,-}(\boldsymbol{r},\boldsymbol{r}',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}\hat{g}_n(\xi,-\eta,\varphi;\boldsymbol{r}')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.81b}$$

$$\mathcal{F}_k^{n\nu,+}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}g_{n\nu}(\xi,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.81c}$$

$$\mathcal{F}_k^{n\nu,-}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_{-\infty}^{\infty}g_{n\nu}(\xi,-\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')e^{\mathrm{i}\xi\rho-k_\rho z}\frac{\sigma(k_\rho)}{k_\rho}d\xi d\eta, \tag{3.81d}$$

for $k=1,2,\cdots$. Apparently, they are all absolutely convergent integrals under the assumption $z>0$, $z+z'>0$ and $z+z'+z''>0$. Moreover, we have

$$\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}';\sigma)=\lim_{k\to\infty}\mathcal{E}_k^-(\boldsymbol{r},\boldsymbol{r}',\sigma)-\lim_{k\to\infty}\mathcal{E}_k^+(\boldsymbol{r},\boldsymbol{r}',\sigma), \tag{3.82a}$$

$$\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma)=\lim_{k\to\infty}\mathcal{F}_k^-(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)-\lim_{k\to\infty}\mathcal{F}_k^+(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma). \tag{3.82b}$$

and

$$\mathcal{I}_n(\boldsymbol{r}+\boldsymbol{r}';\sigma)=\lim_{k\to\infty}\mathcal{E}_k^{n,-}(\boldsymbol{r},\boldsymbol{r}',\sigma)-\lim_{k\to\infty}\mathcal{E}_k^{n,+}(\boldsymbol{r},\boldsymbol{r}',\sigma), \tag{3.83a}$$

$$\mathcal{I}_{n\nu}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma)=\lim_{k\to\infty}\mathcal{F}_k^{n\nu,-}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)-\lim_{k\to\infty}\mathcal{F}_k^{n\nu,+}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma). \tag{3.83b}$$

The inner integrals of the double integrals defined in (3.80)-(3.81) can change contour from real axis to Γ as proved in the following lemmas.

Lemma 3.2. *Suppose $z>0$, $z+z'>0$, $|\boldsymbol{r}'|<|\boldsymbol{r}|$ and $\sigma(k_\rho)$ is analytic and bounded in the right half complex plane, then*

$$\mathcal{E}_k^+(\boldsymbol{r},\boldsymbol{r}';\sigma)=\int_{\frac{1}{k}}^\infty\int_1^\infty\sum_{n=0}^\infty\hat{h}_n(t,\eta,\varphi;\boldsymbol{r}')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta, \tag{3.84a}$$

$$\mathcal{E}_k^-(\boldsymbol{r},\boldsymbol{r}';\sigma)=\int_{\frac{1}{k}}^\infty\int_1^\infty\sum_{n=0}^\infty\hat{h}_n(t,-\eta,\varphi;\boldsymbol{r}')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta. \tag{3.84b}$$

On the other hand, suppose $z>0$, $z+z'+z''>0$ and $|\boldsymbol{r}'+\boldsymbol{r}''|<|\boldsymbol{r}|$, then

$$\mathcal{F}_k^+(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma)=\int_{\frac{1}{k}}^\infty\int_1^\infty\sum_{n=0}^\infty\sum_{\nu=0}^\infty h_{n\nu}(t,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta, \tag{3.85a}$$

$$\mathcal{F}_k^-(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma)=\int_{\frac{1}{k}}^\infty\int_1^\infty\sum_{n=0}^\infty\sum_{\nu=0}^\infty h_{n\nu}(t,-\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta. \tag{3.85b}$$

Here, $r=|\boldsymbol{r}|$,

$$\hat{h}_n(t,\eta,\varphi;\boldsymbol{r}')=\hat{g}_n(\xi_+(t),\eta,\varphi;\boldsymbol{r}')\sigma(k_\rho^+(t))-\hat{g}_n(\xi_-(t),\eta,\varphi;\boldsymbol{r}')\sigma(k_\rho^-(t)), \tag{3.86a}$$

$$\begin{aligned}h_{n\nu}(t,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')=&\,g_{n\nu}(\xi_+(t),\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\sigma(k_\rho^+(t))\\&-g_{n\nu}(\xi_-(t),\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\sigma(k_\rho^-(t)),\end{aligned} \tag{3.86b}$$

$\xi_\pm(t)$ is defined in (3.74), and $k_\rho^\pm(t):=\sqrt{\xi_\pm(t)+\eta^2}$ is the value of k_ρ on the contour Γ introduced in Lemma 3.1.

Proof. As discussed in the proof of Lemma 3.1, the square root function $\sqrt{\eta^2+\xi^2}$ is analytic with respect to ξ in the domain Ω_Γ^+ for $z>0$ and $\eta\neq 0$. Moreover, the branch (3.71) adopted to the square root function implies

$$\mathfrak{Re}[k_\rho(\xi)]=\mathfrak{Re}[\sqrt{\xi^2+\eta^2}]>0,\quad \forall\xi\in\Omega_\Gamma^+\quad\text{and}\quad \eta\neq 0. \tag{3.87}$$

Together with the assumption $\sigma(k_\rho)$ is analytic and bounded in the right half complex plane, we obtain $\sigma(k_\rho(\xi))$ is analytic and bounded in Ω_Γ^+. On the other hand, the series

$$\sum_{n=0}^\infty\hat{g}_n(\xi,\pm\eta,\varphi;\boldsymbol{r}'),\quad \sum_{n=0}^\infty\sum_{\nu=0}^\infty g_{n\nu}(\xi,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}''), \tag{3.88}$$

are resulted from a rotation of the Taylor expansions of exponential functions. Then, the definition (3.66) and (3.69) gives

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

$$\sum_{n=0}^\infty\sum_{\nu=0}^\infty g_{n\nu}(\xi,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')=e^{\mathrm{i}\xi((x'+x'')\cos\varphi+(y'+y'')\sin\varphi)\pm\mathrm{i}\eta((x'+x'')\sin\varphi-(y'+y'')\cos\varphi)-k_\rho(z'+z'')}.$$

Together with the discussions on $k_\rho(\xi)\neq 0$ and $\sigma(k_\rho(\xi))$ in the domain Ω_Γ^+, we can conclude that

$$f_1(\xi):=\frac{\sigma(k_\rho(\xi))}{k_\rho(\xi)}\sum_{n=0}^{\infty}\hat{g}_n(\xi,\pm\eta,\varphi;\boldsymbol{r}'),$$
$$f_2(\xi):=\frac{\sigma(k_\rho(\xi))}{k_\rho(\xi)}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}g_{n\nu}(\xi,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}''),$$

are analytic in the domain Ω_Γ^+ for any $\eta\neq 0$.

Denoting $\xi=Re^{\mathrm{i}\theta}$, the branch defined in (3.71) gives a lower bound

$$\mathfrak{Re}\,k_\rho(\xi)=\sqrt{\frac{\sqrt{(\eta^2+R^2\cos 2\theta)^2+R^4\sin^2 2\theta}+\eta^2+R^2\cos 2\theta}{2}}\geq R|\cos\theta|=|\mathfrak{Re}\xi|. \quad (3.89)$$

Suppose $\xi\in\Omega_\Gamma^+\cap(O_R^+\cup O_R^-)$, we have $\theta\in[0,\theta_R^+]\cup[\theta_R^-,\pi]$, where $\theta_R^\pm$ is defined as in the proof of Lemma 3.1. Then, the definition of $\theta_R^\pm$ gives

$$\frac{\sin\theta}{|\cos\theta|}\leq|\tan\theta_R^\pm|=\frac{\rho t_R}{z\sqrt{t_R^2-1}},\quad \forall\theta\in[0,\theta_R^+]\cup[\theta_R^-,\pi]. \quad (3.90)$$

Noting that $t_R\to+\infty$ as $R\to+\infty$, we obtain

$$\lim_{|\xi|\to+\infty}\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}\leq\lim_{t_R\to+\infty}\frac{\rho t_R}{z\sqrt{t_R^2-1}}=\frac{\rho}{z} \quad (3.91)$$

for $\xi\in\Omega_\Gamma^+$. By the assumption $z+z'>0$, inequality (3.89) and exponential expression for the series in (3.88), we have

$$\left|e^{\mathrm{i}\xi\rho-k_\rho z}\sum_{n=0}^{\infty}\hat{g}_n(\xi,\pm\eta,\varphi;\boldsymbol{r}')\right|\leq e^{(\rho'-\rho)\mathfrak{Im}\xi-(z+z')|\mathfrak{Re}\xi|}, \quad (3.92)$$

where $\rho':=\sqrt{x'^2+y'^2}$. Similarly, the assumption $z+z'+z''>0$ leads to

$$\left|e^{\mathrm{i}\xi\rho-k_\rho z}\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}g_{n\nu}(\xi,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\right|\leq e^{(\breve{\rho}-\rho)\mathfrak{Im}\xi-(z+z'+z'')|\mathfrak{Re}\xi|}, \quad (3.93)$$

where $\breve{\rho}:=\sqrt{(x'+x'')^2+(y'+y'')^2}$. Substituting into the definition of $f_1(\xi)$, $f_2(\xi)$ and applying the boundedness of $\sigma(k_\rho(\xi))$, we obtain

$$\lim_{|\xi|\to+\infty}\left|f_1(\xi)e^{\mathrm{i}\xi\rho-k_\rho z}\xi\right|\leq C\lim_{|\xi|\to+\infty}\exp\left\{|\mathfrak{Re}\xi|\left[(\rho'-\rho)\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}-(z+z')\right]\right\}\left|\frac{\xi}{k_\rho(\xi)}\right|,$$
$$\lim_{|\xi|+\to\infty}\left|f_2(\xi)e^{\mathrm{i}\xi\rho-k_\rho z}\xi\right|\leq C\lim_{|\xi|\to+\infty}\exp\left\{|\mathfrak{Re}\xi|\left[(\breve{\rho}-\rho)\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}-(z+z'+z'')\right]\right\}\left|\frac{\xi}{k_\rho(\xi)}\right|,$$

for $\xi\in\Omega_\Gamma^+$. If $\rho'<\rho$, then

$$|\mathfrak{Re}\xi|\Big[(\rho'-\rho)\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}-(z+z')\Big]=(\rho'-\rho)\mathfrak{Im}\xi-(z+z')|\mathfrak{Re}\xi|\to-\infty,$$

as $\xi\in\Omega_\Gamma^+$ and $|\xi|\to+\infty$. On the other hand, if $\rho'\geq\rho$, by (3.91) and the assumptions $|\boldsymbol{r}|>|\boldsymbol{r}'|$, we obtain

$$\lim_{|\xi|\to+\infty}\Big[(\rho'-\rho)\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}-(z+z')\Big]\leq\frac{\rho\rho'-\rho^2-z^2-zz'}{z}\leq\frac{|\boldsymbol{r}'|^2-|\boldsymbol{r}|^2}{2z}<0,\quad \xi\in\Omega_\Gamma^+. \tag{3.94}$$

Therefore, we always have

$$\lim_{|\xi|\to+\infty}\exp\Big\{|\mathfrak{Re}\xi|\Big[(\rho'-\rho)\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}-(z+z')\Big]\Big\}\Big|\frac{\xi}{k_\rho(\xi)}\Big|=0,\quad \xi\in\Omega_\Gamma^+, \tag{3.95}$$

which implies

$$\lim_{|\xi|\to+\infty}\Big|f_1(\xi)e^{\mathrm{i}\xi\rho-k_\rho z}\xi\Big|=0,\quad \xi\in\Omega_\Gamma^+. \tag{3.96}$$

Noting that the assumption $|\boldsymbol{r}'+\boldsymbol{r}''|<|\boldsymbol{r}|$ and the inequality (3.91) lead to

$$\begin{aligned}&\lim_{|\xi|\to+\infty}\Big[(\breve{\rho}-\rho)\frac{\mathfrak{Im}\xi}{|\mathfrak{Re}\xi|}-(z+z'+z'')\Big]\\ \leq&\frac{\rho\breve{\rho}-\rho^2-z^2-z(z'+z'')}{z}\leq\frac{|\boldsymbol{r}'+\boldsymbol{r}''|^2-|\boldsymbol{r}|^2}{2z}<0,\quad \xi\in\Omega_\Gamma^+,\end{aligned} \tag{3.97}$$

in the case $\breve{\rho}\geq\rho$. A similar derivation gives

$$\lim_{|\xi|\to+m\infty}\Big|f_2(\xi)e^{\mathrm{i}\xi\rho-k_\rho z}\xi\Big|=0,\quad \xi\in\Omega_\Gamma^+. \tag{3.98}$$

In summary, we can apply Lemma 3.1 to change the contour of integrals in (3.80). Noting that the branch (3.71) for the square root function and the definitions in (3.74) gives

$$k_\rho^\pm(t)=\sqrt{\xi_\pm(t)+\eta^2}=\pm\mathrm{i}\Lambda_\pm(t), \tag{3.99}$$

we then obtain the desired formulas in (3.84)-(3.85) by canceling $\Lambda_\pm(t)$ from $k_\rho^\pm(t)$. This completes the proof. □

Lemma 3.3. *Suppose* $z>0$*, and* $\sigma(k_\rho)$ *is analytic and bounded in the right half complex plane, then*

$$\mathcal{E}_k^{n,+}(\boldsymbol{r},\boldsymbol{r}',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}\hat{h}_n(t,\eta,\varphi;\boldsymbol{r}')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta, \tag{3.100a}$$

$$\mathcal{E}_k^{n,-}(\boldsymbol{r},\boldsymbol{r}',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}\hat{h}_n(t,-\eta,\varphi;\boldsymbol{r}')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta, \tag{3.100b}$$

$$\mathcal{F}_k^{n\nu,+}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}h_{n\nu}(t,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta, \tag{3.100c}$$

$$\mathcal{F}_k^{n\nu,-}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}h_{n\nu}(t,-\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}dtd\eta, \tag{3.100d}$$

where $r=|\boldsymbol{r}|$*,* $\hat{h}_n(t,\eta,\varphi;\boldsymbol{r}')$ *and* $h_{n\nu}(t,\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')$ *are defined in* (3.86)*.*

Proof. The proof is very similar with Lemma 3.2 except that the definition (3.66) and (3.69) lead polynomial bounds

$$\left|\hat{g}_n(\xi,\pm\eta,\varphi;\tilde{\boldsymbol{r}})\frac{\sigma(k_\rho(\xi))}{k_\rho(\xi)}\right|\le C|\xi|^{n-1}, \tag{3.101a}$$

$$\left|g_{n\nu}(\xi,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{\sigma(k_\rho(\xi))}{k_\rho(\xi)}\right|\le C|\xi|^{n+\nu-1}, \tag{3.101b}$$

as $|\xi|\to+\infty$ and $\xi\in\Omega_\Gamma^+$. Consequently, the exponential decay in $|e^{\mathrm{i}\xi\rho-k_\rho z}|$ for $|\xi|\to+\infty$ and $\xi\in\Omega_\Gamma^+$ directly ensures the contour deformation. □

Step 3: Convergence and error estimate. Recalling the equalities in (3.82)-(3.83), the order exchanging of the improper integrals and the infinite summations in (3.30)-(3.32) can be implemented by first exchanging order in (3.84)-(3.85) to obtain the following equalities

$$\mathcal{E}_k^{\pm}(\boldsymbol{r},\boldsymbol{r}',\sigma)=\sum_{n=0}^{\infty}\mathcal{E}_k^{n,\pm}(\boldsymbol{r},\boldsymbol{r}',\sigma),\quad \mathcal{F}_k^{\pm}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\mathcal{F}_k^{n\nu,\pm}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma), \tag{3.102}$$

and then taking limits for $k\to\infty$. The key ingredients to accomplish this goal are the estimates proved in Lemma 3.5.

Lemma 3.4. *Let* $\xi_\pm(t)$ *be the contour defined in* (3.74)*,* $\tilde{\boldsymbol{r}}=(\tilde{r}\sin\alpha\cos\beta,\tilde{r}\sin\alpha\sin\beta,\tilde{r}\cos\alpha)\in\mathbb{R}^3$ *is any given vector. Then,*

$$|\hat{g}_n(\xi_\pm(t),\eta,\varphi;\tilde{\boldsymbol{r}})|\le\frac{\tilde{r}^n|\Lambda_\pm(t)|^n}{n!}\left(\frac{r^2t^2}{r^2t^2-\rho^2}\right)^{\frac{n}{2}}, \tag{3.103a}$$

$$|\hat{g}_n(\xi_\pm(t),-\eta,\varphi;\tilde{\boldsymbol{r}})|\le\frac{\tilde{r}^n|\Lambda_\pm(t)|^n}{n!}\left(\frac{r^2t^2}{r^2t^2-\rho^2}\right)^{\frac{n}{2}}, \tag{3.103b}$$

hold for any $t\geq 1$ *and integer* $n\geq 0$.

Proof. Note that

$$\begin{aligned}\frac{\xi_\pm(t)\cos(\varphi-\beta)+\eta\sin(\varphi-\beta)}{\sqrt{\xi_\pm(t)^2+\eta^2}}&=\frac{1}{2}\Big[\frac{\xi_\pm(t)+\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}e^{-\mathrm{i}(\varphi-\beta)}+\frac{\xi_\pm(t)-\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}e^{\mathrm{i}(\varphi-\beta)}\Big],\\ \frac{\xi_\pm(t)\cos(\varphi-\beta)-\eta\sin(\varphi-\beta)}{\sqrt{\xi_\pm(t)^2+\eta^2}}&=\frac{1}{2}\Big[\frac{\xi_\pm(t)+\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}e^{\mathrm{i}(\varphi-\beta)}+\frac{\xi_\pm(t)-\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}e^{-\mathrm{i}(\varphi-\beta)}\Big].\end{aligned}$$

From the definitions in (3.74) and equality (3.99), we have

$$k_\rho(\xi_\pm(t))^2=\xi_\pm(t)^2+\eta^2=-\Lambda_\pm(t)^2, \tag{3.104}$$

and

$$\begin{aligned}\Big|\frac{\xi_\pm(t)+\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}\Big|&=\frac{1}{|\Lambda_\pm(t)|}\frac{\eta}{r}|\mathrm{i}(\rho t+r)\pm z\sqrt{t^2-1}|=\sqrt{\frac{rt+\rho}{rt-\rho}},\\ \Big|\frac{\xi_\pm(t)-\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}\Big|&=\frac{1}{|\Lambda_\pm(t)|}\frac{\eta}{r}|\mathrm{i}(\rho t-r)\pm z\sqrt{t^2-1}|=\sqrt{\frac{rt-\rho}{rt+\rho}}.\end{aligned}$$

Therefore, we have the following formulas

$$\frac{\xi_\pm(t)\cos(\varphi-\beta)+\eta\sin(\varphi-\beta)}{\sqrt{\xi_\pm(t)^2+\eta^2}}=\frac{(rt+\rho)e^{\mathrm{i}(\gamma_\pm-\varphi+\beta)}+(rt-\rho)e^{-\mathrm{i}(\gamma_\pm-\varphi+\beta)}}{2(r^2t^2-\rho^2)}, \tag{3.105a}$$

$$\frac{\xi_\pm(t)\cos(\varphi-\beta)-\eta\sin(\varphi-\beta)}{\sqrt{\xi_\pm(t)^2+\eta^2}}=\frac{(rt+\rho)e^{\mathrm{i}(\gamma_\pm+\varphi-\beta)}+(rt-\rho)e^{-\mathrm{i}(\gamma_\pm+\varphi-\beta)}}{2(r^2t^2-\rho^2)}, \tag{3.105b}$$

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

$$\frac{\xi_\pm(t)+\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}=\sqrt{\frac{rt+\rho}{rt-\rho}}e^{\mathrm{i}\gamma_\pm},\quad \frac{\xi_\pm(t)-\mathrm{i}\eta}{\sqrt{\xi_\pm(t)^2+\eta^2}}=\frac{\sqrt{\xi_\pm(t)^2+\eta^2}}{\xi_\pm(t)+\mathrm{i}\eta}=\sqrt{\frac{rt-\rho}{rt+\rho}}e^{-\mathrm{i}\gamma_\pm}. \tag{3.106}$$

By formulations in (3.105), we calculate that

$$\begin{aligned}&\Big|\frac{\xi_\pm(t)\cos(\varphi-\beta)+\eta\sin(\varphi-\beta)}{\sqrt{\xi_\pm(t)^2+\eta^2}}\sin\alpha+\mathrm{i}\cos\alpha\Big|^2\\ =&\frac{1}{r^2t^2-\rho^2}\Big|\Big((rt+\rho)e^{\mathrm{i}\psi_\pm}+(rt-\rho)e^{-\mathrm{i}\psi_\pm}\Big)\frac{\sin\alpha}{2}+\mathrm{i}\sqrt{r^2t^2-\rho^2}\cos\alpha\Big|^2\\ =&\frac{1}{r^2t^2-\rho^2}\Big|rt\cos(\psi_\pm)\sin\alpha+\mathrm{i}\rho\sin(\psi_\pm)\sin\alpha+\mathrm{i}\sqrt{r^2t^2-\rho^2}\cos\alpha\Big|^2\end{aligned}$$

$$
\begin{aligned}
&=\frac{1}{r^2t^2-\rho^2}\big((\rho\sin\alpha+\sqrt{r^2t^2-\rho^2}\sin\psi_\pm\cos\alpha)^2+(r^2t^2-\rho^2)\cos^2\psi_\pm\big)\\
&\le\frac{1}{r^2t^2-\rho^2}\big(\rho^2+(r^2t^2-\rho^2)\sin^2\psi_\pm+(r^2t^2-\rho^2)\cos^2\psi_\pm\big)\\
&=\frac{r^2t^2}{r^2t^2-\rho^2},
\end{aligned}
\tag{3.107}
$$

where $\psi_\pm=\gamma_\pm-\varphi+\beta$. Similarly, the following estimate

$$
\Big|\frac{\xi_\pm(t)\cos(\varphi-\beta)-\eta\sin(\varphi-\beta)}{\sqrt{\xi_\pm(t)^2+\eta^2}}\sin\alpha+\mathrm{i}\cos\alpha\Big|^2\le\frac{r^2t^2}{r^2t^2-\rho^2}
\tag{3.108}
$$

can also be obtained. Then, (3.103) follows by applying estimate (3.108) and identity (3.104) to the definition in (3.66). □

Lemma 3.5. *Let $\hat{h}_n(t,\pm\eta,\varphi;\boldsymbol{r}')$ and $h_{n\nu}(t,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')$ be the functions defined in* (3.86) *with $\xi_\pm(t)$ defined in* (3.74)*. Suppose $\rho\ge0$, $z>0$, $r=\sqrt{\rho^2+z^2}$, the density function $\sigma(k_\rho^\pm(t))$ has a uniform bound $|\sigma(k_\rho^\pm(t))|\le M_\sigma$ along the contour Γ defined in Lemma* 3.1*. Then, the following estimates*

$$
\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}\Big|\hat{h}_n(t,\pm\eta,\varphi;\boldsymbol{r}')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}\Big|dtd\eta\le\pi M_\sigma\frac{|\boldsymbol{r}'|^n}{r^{n+1}},
\tag{3.109}
$$

and

$$
\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}\Big|h_{n\nu}(t,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}\Big|dtd\eta\le\pi M_\sigma\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{r^{n+\nu+1}n!\nu!},
\tag{3.110}
$$

hold for any integers $n,\nu\ge0$.

Proof. By the definitions in (3.69), (3.74), (3.86), the estimates in Lemma 3.4 and the bound of $\sigma(k_\rho^\pm(t))$, we have

$$
\begin{aligned}
\big|h_{n\nu}(t,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\big|&\le\frac{M_\sigma|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu}{n!\nu!}\left[\left(\frac{|\Lambda_+(t)|rt}{\sqrt{r^2t^2-\rho^2}}\right)^{n+\nu}+\left(\frac{|\Lambda_-(t)|rt}{\sqrt{r^2t^2-\rho^2}}\right)^{n+\nu}\right]\\
&=\frac{2M_\sigma|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu}{n!\nu!}(\eta t)^{n+\nu}
\end{aligned}
$$

for any $\eta>0$. Direct calculation leads to estimate

$$
\begin{aligned}
&\int_{\frac{1}{k}}^{\infty}\int_1^{\infty}\Big|h_{n\nu}(t,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta rt}}{\sqrt{t^2-1}}\Big|dtd\eta\\
\le&\frac{2M_\sigma|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu}{n!\nu!}\int_1^{\infty}\frac{t^{n+\nu}}{\sqrt{t^2-1}}\int_0^{\infty}\eta^{n+\nu}e^{-\eta rt}dtd\eta\\
=&\pi M_\sigma\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{r^{n+\nu+1}n!\nu!}
\end{aligned}
\tag{3.111}
$$

for any integers $n,\nu \geq 0$. Another estimate in (3.109) can be proved similarly. $\square$

Lemma 3.6. *Suppose $|\boldsymbol{r}|>|\boldsymbol{r}'|+|\boldsymbol{r}''|$, $z>0$, $z+z'+z''>0$, and the density function $\sigma(k_\rho)$ is analytic and has a bound $|\sigma(k_\rho)|\leq M_\sigma$ in the right half complex plane. Then,*

$$\lim_{k\to\infty}\mathcal{F}_k^{\pm}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)=\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\lim_{k\to\infty}\mathcal{F}_k^{n\nu,\pm}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma), \tag{3.112}$$

where the integrals are defined in (3.80) *and* (3.81).

Proof. By the estimate (3.110), we have

$$\begin{aligned}
&\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\int_{\frac{1}{k}}^{\infty}\int_{1}^{\infty}\left|h_{n\nu}(t,\pm\eta,\varphi;\boldsymbol{r}',\boldsymbol{r}'')\frac{e^{-\eta r t}}{\sqrt{t^2-1}}\right|dtd\eta\\
\leq&\pi M_\sigma\sum_{n=0}^{\infty}\sum_{\nu=0}^{\infty}\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{|\boldsymbol{r}|^{n+\nu+1}n!\nu!}\\
=&\frac{\pi M_\sigma}{|\boldsymbol{r}|}\sum_{n=0}^{\infty}\Big(\frac{|\boldsymbol{r}'|+|\boldsymbol{r}''|}{|\boldsymbol{r}|}\Big)^n=\frac{\pi M_\sigma}{|\boldsymbol{r}|-|\boldsymbol{r}'|-|\boldsymbol{r}''|}
\end{aligned} \tag{3.113}$$

for any $|\boldsymbol{r}|>|\boldsymbol{r}'|+|\boldsymbol{r}''|$. Therefore, we can apply the Fubini theorem to exchange the order of the improper integrals and the infinite summations in (3.85). Together with Lemma 3.3, we obtain the second equality in (3.102). Note that (3.113) holds uniformly with respect to parameter k. Therefore, the series in the second equality of (3.102) are also uniform convergent with respect to parameter k. Taking limit for $k\to\infty$ in (3.102) and exchanging order of the limit and summations gives the conclusion. $\square$

Mimicking the analysis above, we obtain similar conclusion for $\mathcal{E}_k^{\pm}(\boldsymbol{r},\boldsymbol{r}',\sigma)$.

Lemma 3.7. *Suppose $|\boldsymbol{r}|>|\boldsymbol{r}'|$, $z>0$, $z+z'>0$, and the density function $\sigma(k_\rho)$ is analytic and has a bound $|\sigma(k_\rho)|\leq M_\sigma$ in the right half complex plane. Then,*

$$\lim_{k\to\infty}\mathcal{E}_k^{\pm}(\boldsymbol{r},\boldsymbol{r}',\sigma)=\sum_{n=0}^{\infty}\lim_{k\to\infty}\mathcal{E}_k^{n,\pm}(\boldsymbol{r},\boldsymbol{r}',\sigma), \tag{3.114}$$

where the integrals are defined in (3.80) *and* (3.81).

By (3.82), (3.83) and Lemmas 3.6-3.7, we finish the proof of (3.30)-(3.32).

Next, let us prove the truncation error estimate (3.33). Another error estimate (3.31) can be proved similarly. By (3.100) and estimates (3.110), we have

$$\lim_{k\to\infty}|\mathcal{F}_{n\nu}^{k,\pm}(\boldsymbol{r},\varphi,\boldsymbol{r}',\boldsymbol{r}'';\sigma)|\leq\pi M_\sigma\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{|\boldsymbol{r}|^{n+\nu+1}n!\nu!}. \tag{3.115}$$

Therefore, (3.83) implies

$$\begin{aligned}|\mathcal{I}_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma)| &= |\lim_{k\to\infty}\mathcal{F}^-_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)-\lim_{k\to\infty}\mathcal{F}^+_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)| \\ &\le \lim_{k\to\infty}|\mathcal{F}^+_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)|+\lim_{k\to\infty}|\mathcal{F}^-_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'',\sigma)| \\ &\le 2\pi M_\sigma\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{|\boldsymbol{r}|^{n+\nu+1}n!\nu!}. \end{aligned} \tag{3.116}$$

Together with (3.32) and the assumption $|\boldsymbol{r}'|+|\boldsymbol{r}''|<|\boldsymbol{r}|$, we obtain

$$\begin{aligned}&\Big|\mathcal{I}(\boldsymbol{r}+\boldsymbol{r}'+\boldsymbol{r}'';\sigma)-\sum_{n=0}^{p}\sum_{\nu=0}^{p}\mathcal{I}_{n\nu}(\boldsymbol{r},\boldsymbol{r}',\boldsymbol{r}'';\sigma)\Big| \\ \le& 2\pi M_\sigma\left[\sum_{n=0}^{\infty}\sum_{\nu=p+1}^{\infty}\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{|\boldsymbol{r}|^{n+\nu+1}n!\nu!}+\sum_{n=p+1}^{\infty}\sum_{\nu=0}^{\infty}\frac{|\boldsymbol{r}'|^n|\boldsymbol{r}''|^\nu(n+\nu)!}{|\boldsymbol{r}|^{n+\nu+1}n!\nu!}\right] \\ =& 2\pi M_\sigma\left[\sum_{\nu=p+1}^{\infty}\frac{|\boldsymbol{r}''|^\nu}{|\boldsymbol{r}|^{\nu+1}}\sum_{n=0}^{\infty}\frac{|\boldsymbol{r}'|^n(n+\nu)!}{|\boldsymbol{r}|^n n!\nu!}+\sum_{n=p+1}^{\infty}\frac{|\boldsymbol{r}'|^n}{|\boldsymbol{r}|^{n+1}}\sum_{\nu=0}^{\infty}\frac{|\boldsymbol{r}''|^\nu(n+\nu)!}{|\boldsymbol{r}|^\nu n!\nu!}\right] \\ =& 2\pi M_\sigma\left[\sum_{\nu=p+1}^{\infty}\frac{|\boldsymbol{r}''|^\nu}{|\boldsymbol{r}|^{\nu+1}}\frac{|\boldsymbol{r}|^{\nu+1}}{(|\boldsymbol{r}|-|\boldsymbol{r}'|)^{\nu+1}}+\sum_{n=p+1}^{\infty}\frac{|\boldsymbol{r}'|^n}{|\boldsymbol{r}|^{n+1}}\frac{|\boldsymbol{r}|^{n+1}}{(|\boldsymbol{r}|-|\boldsymbol{r}''|)^{n+1}}\right] \\ =& \frac{4\pi M_\sigma}{|\boldsymbol{r}|-|\boldsymbol{r}'|-|\boldsymbol{r}''|}\left[\Big(\frac{|\boldsymbol{r}''|}{|\boldsymbol{r}|-|\boldsymbol{r}'|}\Big)^{p+1}+\Big(\frac{|\boldsymbol{r}'|}{|\boldsymbol{r}|-|\boldsymbol{r}''|}\Big)^{p+1}\right]. \end{aligned} \tag{3.117}$$

4 Application of the convergence analysis to the FMM for 3-dimensional Laplace equation in layered media

In this section, we will employ the convergence theory established in the last section to give error estimates for the approximations used in the FMM for 3-dimensional Laplace equation in layered media.

Let $\mathscr{P}_\ell=\{(Q_{\ell j},\boldsymbol{r}_{\ell j}),\ j=1,2,\cdots,N_\ell\}$, $\ell=0,1,\cdots,L$ be L groups of source charges distributed in a multi-layer medium with $L+1$ layers (see Fig. 1). The group of charges in ℓ-th layer is denoted by $\mathscr{P}_\ell$. The FMM proposed in [27] provides a fast algorithm to compute interactions

$$\Phi_\ell(\boldsymbol{r}_{\ell i})=\Phi^{\rm free}_\ell(\boldsymbol{r}_{\ell i})+\sum_{\ell'=0}^{L-1}[\Phi^{11}_{\ell\ell'}(\boldsymbol{r}_{\ell i})+\Phi^{21}_{\ell\ell'}(\boldsymbol{r}_{\ell i})]+\sum_{\ell'=1}^{L}[\Phi^{12}_{\ell\ell'}(\boldsymbol{r}_{\ell i})+\Phi^{22}_{\ell\ell'}(\boldsymbol{r}_{\ell i})], \tag{4.1}$$

where

$$\Phi_\ell^{\rm free}(\boldsymbol{r}_{\ell i}) := \sum_{j=1,j\neq i}^{N_\ell} \frac{Q_{\ell j}}{4\pi|\boldsymbol{r}_{\ell i}-\boldsymbol{r}_{\ell j}|}, \quad \Phi_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r}_{\ell i}) := \sum_{j=1}^{N_{\ell'}} Q_{\ell' j} u_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r}_{\ell i},\boldsymbol{r}_{\ell' j}), \quad \mathfrak{a},\mathfrak{b}=1,2, \tag{4.2}$$

are free space and reaction field components, respectively. Far field approximations are used for both free space and reaction field components.

4.1 A review of the error estimates for the approximations used in the FMM for free space components

Let $\Phi_{\ell,\rm in}^{\rm free}(\boldsymbol{r})$ and $\Phi_{\ell,\rm out}^{\rm free}(\boldsymbol{r})$ be the free space components of the potentials induced by all particles inside a given source box B_s centered at $\boldsymbol{r}_c^s$ and all particles far away from a given target box B_t centered at $\boldsymbol{r}_c^t$ (see. Fig. 9), i.e.,

$$\Phi_{\ell,\rm in}^{\rm free}(\boldsymbol{r}) = \sum_{j\in\mathcal{J}} \frac{Q_{\ell j}}{4\pi|\boldsymbol{r}-\boldsymbol{r}_{\ell j}|}, \quad \Phi_{\ell,\rm out}^{\rm free}(\boldsymbol{r}) = \sum_{j\in\mathcal{K}} \frac{Q_{\ell j}}{4\pi|\boldsymbol{r}-\boldsymbol{r}_{\ell j}|}, \tag{4.3}$$

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

$$\Phi_{\ell,\rm in}^{\rm free}(\boldsymbol{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} M_{nm}^{\rm in} \frac{Y_n^m(\theta_s,\varphi_s)}{r_s^{n+1}}, \tag{4.4}$$

at any target points far away from B_s and LE

$$\Phi_{\ell,\rm out}^{\rm free}(\boldsymbol{r}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} L_{nm}^{\rm out} r_t^n Y_n^m(\theta_t,\varphi_t), \tag{4.5}$$

inside B_t, where (r_s,θ_s,φ_s) and (r_t,θ_t,φ_t) are spherical coordinates of $\boldsymbol{r}-\boldsymbol{r}_c^s$ and $\boldsymbol{r}-\boldsymbol{r}_c^t$, respectively. The coefficients are given by

$$M_{nm}^{\rm in} = \frac{c_n^{-2}}{4\pi} \sum_{j\in\mathcal{J}} Q_{\ell j} (r_{\ell j}^s)^n \overline{Y_n^m(\theta_{\ell j}^s,\varphi_{\ell j}^s)}, \quad L_{nm}^{\rm out} = \frac{c_n^{-2}}{4\pi} \sum_{j\in\mathcal{K}} Q_{\ell j} (r_{\ell j}^t)^{-n-1} \overline{Y_n^m(\theta_{\ell j}^t,\varphi_{\ell j}^t)}, \tag{4.6}$$

where $(r_{\ell j}^s,\theta_{\ell j}^s,\varphi_{\ell j}^s)$ and $(r_{\ell j}^t,\theta_{\ell j}^t,\varphi_{\ell j}^t)$ are spherical coordinates of $\boldsymbol{r}_{\ell j}-\boldsymbol{r}_c^s$ and $\boldsymbol{r}_{\ell j}-\boldsymbol{r}_c^t$, respectively. These expansions can be obtained by applying expansions (3.5)-(3.6) to each term in the summations given by (4.3). Moreover, applying Theorem 3.1 and Theorem 3.2 to the expansion of each term immediately leads to the following error estimates (cf. [15]).

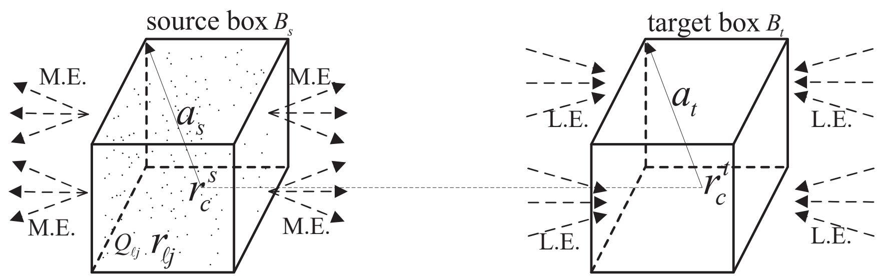


Figure 9: An illustration of the source and target box for the free space component in the ℓ-th layer.

Theorem 4.1. *Denote the radius of the circumscribed sphere of the source box* B_s *by* a_s*. Suppose* $\mathcal{J}$ *is the set of indices of all particles in* B_s*, then the ME* (4.4) *has truncation error estimate*

$$\Big|\varphi^{\rm free}_{\ell,{\rm in}}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}M^{\rm in}_{nm}\frac{Y_n^m(\theta_s,\varphi_s)}{r_s^{n+1}}\Big|\le\frac{1}{4\pi}\frac{Q_{\mathcal{J}}}{r_s-a_s}\Big(\frac{a_s}{r_s}\Big)^{p+1} \tag{4.7}$$

for any $\boldsymbol{r}$ *outside the circumscribed sphere, i.e.,* $|\boldsymbol{r}-\boldsymbol{r}_c^s|>a_s$*, where*

$$Q_{\mathcal{J}}=\sum_{j\in\mathcal{J}}|Q_{\ell j}|. \tag{4.8}$$

Theorem 4.2. *Denote the radius of the circumscribed sphere of the target box* B_t *by* a_t*. Suppose* $\mathcal{K}$ *is the set of indices of all particles* $(Q_{\ell j},\boldsymbol{r}_{\ell j})$ *such that* $|\boldsymbol{r}_{\ell j}-\boldsymbol{r}_c^t|>a_t$*, then the LE* (4.5) *has truncation error estimate*

$$\Big|\varphi^{\rm free}_{\ell,{\rm out}}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}L^{\rm out}_{nm}r_t^nY_n^m(\theta_t,\varphi_t)\Big|\le\frac{1}{4\pi}\frac{Q_{\mathcal{K}}}{a_t-r_t}\Big(\frac{r_t}{a_t}\Big)^{p+1} \tag{4.9}$$

for any $\boldsymbol{r}\in B_t$*, where*

$$Q_{\mathcal{K}}=\sum_{j\in\mathcal{K}}|Q_{\ell j}|. \tag{4.10}$$

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

$$\varphi^{\rm free}_{\ell,{\rm in}}(\boldsymbol{r})\approx\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{M}^{\rm in}_{nm}\frac{Y_n^m(\tilde{\theta}_s,\tilde{\varphi}_s)}{\tilde{r}_s^{n+1}},\quad \varphi^{\rm free}_{\ell,{\rm out}}(\boldsymbol{r})\approx\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{L}^{\rm out}_{nm}\tilde{r}_t^nY_n^m(\tilde{\theta}_t,\tilde{\varphi}_t), \tag{4.11}$$

where the coefficients are calculated via center shifting

$$\tilde{M}_{nm}^{\rm in}=\sum_{\nu=0}^{n}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{|m|-|\mu|}A_{n-\nu}^{m-\mu}A_{\nu}^{\mu}r_{ss}^{n-\nu}Y_{n-\nu}^{\mu-m}(\theta_{ss},\varphi_{ss})}{c_{n-\nu}^2A_n^m}M_{\nu\mu}^{\rm in}, \tag{4.12a}$$

$$\tilde{L}_{nm}^{\rm out}=\sum_{\nu=n}^{p}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu-n-|\mu-m|+|\mu|-|m|}c_{\nu}^2A_{\nu-n}^{\mu-m}A_n^m r_{tt}^{\nu-n}Y_{\nu-n}^{\mu-m}(\theta_{tt},\varphi_{tt})}{c_{\nu-n}^2c_n^2A_{\nu}^{\mu}}L_{\nu\mu}^{\rm out}, \tag{4.12b}$$

$(\tilde{r}_s,\tilde{\theta}_s,\tilde{\varphi}_s)$, $(r_{ss},\theta_{ss},\varphi_{ss})$, $(\tilde{r}_t,\tilde{\theta}_t,\tilde{\varphi}_t)$ and $(r_{tt},\theta_{tt},\varphi_{tt})$ are the spherical coordinates of $\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^s$, $\boldsymbol{r}_c^s-\tilde{\boldsymbol{r}}_c^s$, $\boldsymbol{r}-\tilde{\boldsymbol{r}}_t^s$ and $\tilde{\boldsymbol{r}}_c^t-\boldsymbol{r}_c^t$, respectively. By Corollary 3.1 and Corollary 3.2, we obtain the following error estimates.

Theorem 4.3. *Denote the radius of the circumscribed sphere of the source box B_s by a_s. Suppose $\mathcal{J}$ is the set of indices of all particles in B_s. For any $|\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^s|>a_s+r_{ss}$, the first expansion in* (4.11) *has error estimate*

$$\Big|\Phi_{\ell,\rm in}^{\rm free}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{M}_{nm}^{\rm in}\frac{Y_n^m(\tilde{\theta}_s,\tilde{\varphi}_s)}{\tilde{r}_s^{n+1}}\Big|\leq\frac{1}{4\pi}\frac{Q_{\mathcal{J}}}{\tilde{r}_s-(a_s+r_{ss})}\Big(\frac{a_s+r_{ss}}{\tilde{r}_s}\Big)^{p+1}, \tag{4.13}$$

where $Q_{\mathcal{J}}$ is defined in (4.8).

Theorem 4.4. *Denote the radius of the circumscribed sphere of the source box B_t by a_t. Suppose $\mathcal{K}$ is the set of indices of all particles $(Q_{\ell j},\boldsymbol{r}_{\ell j})$ such that $|\boldsymbol{r}_{\ell j}-\boldsymbol{r}_c^t|>a_t$. For any $|\boldsymbol{r}-\tilde{\boldsymbol{r}}_c^t|\leq a_t-r_{tt}$, the second approximation in* (4.11) *has error estimate*

$$\Big|\Phi_{\ell,\rm out}^{\rm free}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}\tilde{L}_{nm}^{\rm out}\tilde{r}_t^nY_n^m(\tilde{\theta}_t,\tilde{\varphi}_t)\Big|\leq\frac{1}{4\pi}\frac{Q_{\mathcal{K}}}{a_t-r_{tt}-\tilde{r}_t}\Big(\frac{\tilde{r}_t+r_{tt}}{a_t}\Big)^{p+1}, \tag{4.14}$$

where $Q_{\mathcal{K}}$ is defined in (4.10).

Suppose target box B_t is far away from the source box B_s. Recall the translation operator (3.9), the ME (4.4) can be translated to an LE with respect to center $\boldsymbol{r}_c^t$ where the LE expansion coefficients are calculated from ME coefficients via

$$L_{nm}^{\rm in}=\sum_{\nu=0}^{\infty}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu+|m|}A_{\nu}^{\mu}A_n^mY_{n+\nu}^{\mu-m}(\theta_{st},\varphi_{st})}{c_{\nu}^2A_{n+\nu}^{\mu-m}r_{st}^{n+\nu+1}}M_{\nu\mu}^{\rm in}. \tag{4.15}$$

In the FMM, the translation in (4.15) is further truncated which gives approximated local expansion coefficients

$$L_{nm}^{p}=\sum_{\nu=0}^{p}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu+|m|}A_{\nu}^{\mu}A_n^mY_{n+\nu}^{\mu-m}(\theta_{st},\varphi_{st})}{c_{\nu}^2A_{n+\nu}^{\mu-m}r_{st}^{n+\nu+1}}M_{\nu\mu}^{\rm in}. \tag{4.16}$$

Applying Theorem 3.3, we have error estimate:

Theorem 4.5. *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, $\mathcal{J}$ is the set of indices of all particles in B_s. The well separateness of the boxes means that $|\boldsymbol{r}_c^s-\boldsymbol{r}_c^t|>a_s+ca_t$ with $c>1$. Then*

$$\Big|\varphi_{\ell,\rm in}^{\rm free}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}^{p}r_t^nY_n^m(\theta_t,\varphi_t)\Big|\le\frac{1}{4\pi}\frac{Q_{\mathcal{J}}}{(c-1)a_t}\Big(\frac{a_s+a_t}{a_s+ca_t}\Big)^{p+1},\quad\forall\boldsymbol{r}\in B_t,\tag{4.17}$$

where $Q_{\mathcal{J}}$ is defined in (4.8).

4.2 Error estimates for the approximations used in the FMMs for reaction components

Let $\Phi_{\ell\ell',\rm in}^{\mathfrak{ab}}(\boldsymbol{r})$ and $\Phi_{\ell\ell',\rm out}^{\mathfrak{ab}}(\boldsymbol{r})$ be general reaction components of potentials induced by all equivalent polarizaion sources inside a given polarization source box $B_s^{\mathfrak{ab}}$ centered at $\boldsymbol{r}_c^{\mathfrak{ab}}$ and far away from a given target box B_t centered at $\boldsymbol{r}_c^t$, i.e.,

$$\Phi_{\ell\ell',\rm in}^{\mathfrak{ab}}(\boldsymbol{r})=\sum_{j\in\mathcal{J}}Q_{\ell'j}\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}_{\ell'j}^{\mathfrak{ab}}),\quad \Phi_{\ell\ell',\rm out}^{\mathfrak{ab}}(\boldsymbol{r})=\sum_{j\in\mathcal{K}}Q_{\ell'j}\tilde{u}_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}_{\ell'j}^{\mathfrak{ab}}),\tag{4.18}$$

where $\mathcal{J}$ and $\mathcal{K}$ are the sets of indices of equivalent polarization sources inside $B_s^{\mathfrak{ab}}$ and far away from B_t, respectively (see Fig. 10). The FMM for the reaction component $\Phi_{\ell\ell'}^{\mathfrak{ab}}(\boldsymbol{r})$ use ME

$$\Phi_{\ell\ell',\rm in}^{\mathfrak{ab}}(\boldsymbol{r})=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}M_{nm}^{\mathfrak{ab},\rm in}\mathcal{F}_{nm}^{\mathfrak{ab}}(\boldsymbol{r},\boldsymbol{r}_c^{\mathfrak{ab}})\tag{4.19}$$

at any target points far away from $B_s^{\mathfrak{ab}}$ and LE

$$\Phi_{\ell\ell',\rm out}^{\mathfrak{ab}}(\boldsymbol{r})=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}L_{nm}^{\mathfrak{ab},\rm out}r_t^nY_n^m(\theta_t,\varphi_t)\tag{4.20}$$

for all targets inside B_t, where the coefficients are given by

$$M_{nm}^{\mathfrak{ab},\rm in}=\frac{c_n^{-2}}{4\pi}\sum_{j\in\mathcal{J}}Q_{\ell'j}(r_{\ell'j}^{\mathfrak{ab}})^n\overline{Y_n^m(\theta_{\ell'j}^{\mathfrak{ab}},\varphi_{\ell'j}^{\mathfrak{ab}})},\tag{4.21a}$$

$$L_{nm}^{1\mathfrak{b},\rm out}=\frac{C_n^m}{8\pi^2}\sum_{j\in\mathcal{K}}Q_{\ell'j}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}_c^t-\boldsymbol{r}_{\ell'j}^{1\mathfrak{b}})}\sigma_{\ell\ell'}^{1\mathfrak{b}}(k_\rho)k_\rho^{n-1}e^{-\mathrm{i}m\alpha}dk_xdk_y,\tag{4.21b}$$

$$L_{nm}^{2\mathfrak{b},\rm out}=\frac{(-1)^{n+m}C_n^m}{8\pi^2}\sum_{j\in\mathcal{K}}Q_{\ell'j}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}e^{\mathrm{i}\boldsymbol{k}\cdot\tau(\boldsymbol{r}_c^t-\boldsymbol{r}_{\ell'j}^{2\mathfrak{b}})}\sigma_{\ell\ell'}^{2\mathfrak{b}}(k_\rho)k_\rho^{n-1}e^{-\mathrm{i}m\alpha}dk_xdk_y,\tag{4.21c}$$

$\mathcal{F}^{\mathfrak{ab}}_{nm}(\boldsymbol{r},\boldsymbol{r}^{\mathfrak{ab}}_c)$ are defined in (3.50), (r_t,θ_t,φ_t) and $(r^{\mathfrak{ab}}_{\ell'j},\theta^{\mathfrak{ab}}_{\ell'j},\varphi^{\mathfrak{ab}}_{\ell'j})$ are the spherical coordinates of $\boldsymbol{r}-\boldsymbol{r}^t_c$ and $\boldsymbol{r}^{\mathfrak{ab}}_{\ell'j}-\boldsymbol{r}^{\mathfrak{ab}}_c$, respectively. Apparently, these expansions can be obtained by applying expansions (3.48)-(3.49) to each term in the summations given by (4.18). Moreover, applying Theorems 3.6 and 3.7 term by term gives the following error estimates.

Theorem 4.6. *Suppose $a^{\mathfrak{ab}}_s$ is the radius of the circumscribed sphere of the box $B^{\mathfrak{ab}}_s$, $\mathcal{J}$ is the set of indices of all equivalent polarization sources in $B^{\mathfrak{ab}}_s$, then ME (4.19) has truncation error estimate*

$$\left|\Phi^{\mathfrak{ab}}_{\ell\ell',\mathrm{in}}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}M^{\mathfrak{ab},\mathrm{in}}_{nm}\mathcal{F}^{\mathfrak{ab}}_{nm}(\boldsymbol{r},\boldsymbol{r}^{\mathfrak{ab}}_c)\right|\le\frac{1}{4\pi}\frac{Q_{\mathcal{J}}M_{\sigma^{\mathfrak{ab}}_{\ell\ell'}}}{|\boldsymbol{r}-\boldsymbol{r}^{\mathfrak{ab}}_c|-a^{\mathfrak{ab}}_s}\left(\frac{a^{\mathfrak{ab}}_s}{|\boldsymbol{r}-\boldsymbol{r}^{\mathfrak{ab}}_c|}\right)^{p+1} \tag{4.22}$$

for any $\boldsymbol{r}$ such that $|\boldsymbol{r}-\boldsymbol{r}^{\mathfrak{ab}}_c|>a^{ab}_s$, where $M_{\sigma^{\mathfrak{ab}}_{\ell\ell'}}$ is the bound of $\sigma^{\mathfrak{ab}}_{\ell\ell'}(k_\rho)$ in the right half complex plane,

$$Q_{\mathcal{J}}=\sum_{j\in\mathcal{J}}|Q_{\ell'j}|. \tag{4.23}$$

Proof. By Theorem 3.6 and triangle inequality, we have

$$\begin{aligned}&\left|\Phi^{\mathfrak{ab}}_{\ell\ell',\mathrm{in}}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}M^{\mathfrak{ab},\mathrm{in}}_{nm}\mathcal{F}^{\mathfrak{ab}}_{nm}(\boldsymbol{r},\boldsymbol{r}^{\mathfrak{ab}}_c)\right|\\ \le&\sum_{j\in\mathcal{J}}|Q_{\ell'j}|\left|\tilde{u}^{\mathfrak{ab}}_{\ell\ell'}(\boldsymbol{r},\boldsymbol{r}^{\mathfrak{ab}}_{\ell'j})-\frac{c_n^{-2}}{4\pi}(r^{\mathfrak{ab}}_{\ell'j})^n\overline{Y_n^m(\theta^{\mathfrak{ab}}_{\ell'j},\varphi^{\mathfrak{ab}}_{\ell'j})}\mathcal{F}^{\mathfrak{ab}}_{nm}(\boldsymbol{r},\boldsymbol{r}^{\mathfrak{ab}}_c)\right|\\ \le&\frac{1}{4\pi}\frac{Q_{\mathcal{J}}M_{\sigma^{\mathfrak{ab}}_{\ell\ell'}}}{|\boldsymbol{r}-\boldsymbol{r}^{\mathfrak{ab}}_c|-a^{\mathfrak{ab}}_s}\left(\frac{a^{\mathfrak{ab}}_s}{|\boldsymbol{r}-\boldsymbol{r}^{\mathfrak{ab}}_c|}\right)^{p+1}.\end{aligned}$$

This completes the proof. □

Theorem 4.7. *Suppose a_t is the radius of the circumscribed sphere of the target box B_t, $\boldsymbol{r}$ is a point inside B_t, $\mathcal{K}$ is the set of indices of all charges $(Q_{\ell'j},\boldsymbol{r}^{\mathfrak{ab}}_{\ell'j})$ such that $|\boldsymbol{r}^{\mathfrak{ab}}_{\ell'j}-\boldsymbol{r}^t_c|>a_t$, then the LE (4.20) has truncation error estimate*

$$\left|\Phi^{\mathfrak{ab}}_{\ell\ell',\mathrm{out}}(\boldsymbol{r})-\sum_{n=0}^{p}\sum_{m=-n}^{n}L^{\mathfrak{ab},\mathrm{out}}_{nm}r_t^nY_n^m(\theta_t,\varphi_t)\right|\le\frac{1}{4\pi}\frac{Q_{\mathcal{K}}M_{\sigma^{\mathfrak{ab}}_{\ell\ell'}}}{a_t-|\boldsymbol{r}-\boldsymbol{r}^t_c|}\left(\frac{|\boldsymbol{r}-\boldsymbol{r}^t_c|}{a_t}\right)^{p+1}, \tag{4.24}$$

where $M_{\sigma^{\mathfrak{ab}}_{\ell\ell'}}$ is the bound of $\sigma^{\mathfrak{ab}}_{\ell\ell'}(k_\rho)$ in the right half complex plane,

$$Q_{\mathcal{K}}=\sum_{j\in\mathcal{K}}|Q_{\ell'j}|. \tag{4.25}$$

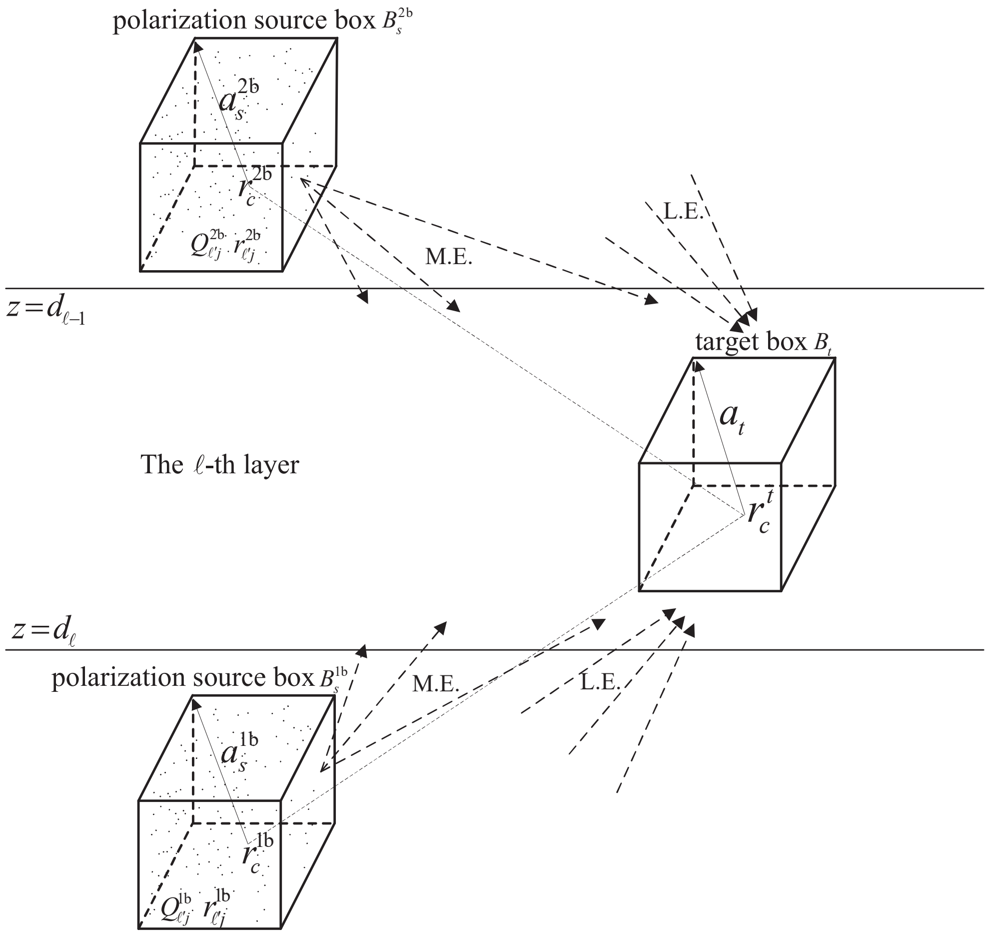


Figure 10: An illustration of equivalent polarization source and target box for the reaction components in the ℓ-th layer due to sources in ℓ'-th layer.

As reported in the last section, the center shifting operators in the FMMs for reaction components are exactly the same as in the free space FMM. Therefore, we will only consider the error estimate for the ME to LE translation here. Suppose the target box B_t is far away from the polarization source box $B_s^{\mathfrak{ab}}$, see Fig. 10. Recalling the truncated translation (3.59), an approximated LE of the potential $\Phi_{\ell\ell',\text{in}}^{\mathfrak{ab}}$ in the target box B_t is obtained, i.e.,

$$\Phi_{\ell\ell',\text{in}}^{\mathfrak{ab},p}(\boldsymbol{r}) := \sum_{n=0}^{p} \sum_{m=-n}^{n} L_{nm}^{\mathfrak{ab},p} r_t^n Y_n^m(\theta_t, \varphi_t), \tag{4.26}$$

where the coefficients are given by

$$L_{nm}^{\mathfrak{ab},p} = \sum_{\nu=0}^{p} \sum_{\mu=-\nu}^{\nu} T_{nm,\nu\mu}^{\mathfrak{ab}} M_{\nu\mu}^{\mathfrak{ab},\mathrm{in}}. \tag{4.27}$$

These are the M2L translations which actually used in the FMMs for reaction components. By applying Theorem 3.8 term by term, we obtain the following estimate.

Theorem 4.8. *Suppose $a_s^{\mathfrak{ab}}$ and a_t are the radii of the circumscribed spheres of two well separated boxes $B_s^{\mathfrak{ab}}$ (polarization source box) and B_t (target box), respectively. The well separateness of the boxes means that $|\boldsymbol{r}_c^t - \boldsymbol{r}_c^{\mathfrak{ab}}| > a_s^{\mathfrak{ab}} + ca_t$ with some $c>1$. Denoted by $\mathcal{J}$ the set of indices of all equivalent polarization sources in $B_s^{\mathfrak{ab}}$, then the truncated ME to LE translation* (4.27) *leads to approximation with truncation error estimate*

$$\left|\Phi_{\ell\ell',\mathrm{in}}^{\mathfrak{ab}}(\boldsymbol{r}) - \Phi_{\ell\ell',\mathrm{in}}^{\mathfrak{ab},p}(\boldsymbol{r})\right| \le \frac{1}{2\pi} \frac{Q_{\mathcal{J}} M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}}{(c-1)a_t} \left(\frac{a_s^{\mathfrak{ab}} + a_t}{a_s^{\mathfrak{ab}} + ca_t}\right)^{p+1}, \quad \forall \boldsymbol{r} \in B_t, \tag{4.28}$$

where $M_{\sigma_{\ell\ell'}^{\mathfrak{ab}}}$ is the bound of $\sigma_{\ell\ell'}^{\mathfrak{ab}}(k_\rho)$ in the right half complex plane, $Q_{\mathcal{J}}$ is defined in (4.23).

5 Conclusions

In this paper, we established the convergence theory for the multipole and local expansions of the Green's function of a 3-dimensional Laplace equation in layered media. We first showed that the reaction density functions involved in the integral representation of the layered Green's function are analytic and bounded in the right half complex wave number plane. Then, we proved that the MEs, LEs and corresponding shifting and translation operators for the Green's function of the 3-dimensional Laplace equation in layered media have exponential convergence similar to the classic theory for the Green's function in free space. As in the analysis for the FMM in free space, the theory presented in this paper proves that the FMM developed for the 3-D Laplace equations in layered media (cf. [27]) has an exponential convergence.

In a future work, we will carry out the error estimate for the expansions, shifting and translation operators of the Green's function of 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, LEs and M2L translation operators.

Appendix A: Addition theorems

Theorem A.1 (Addition theorem for Legendre polynomials)**.** *Let P and Q be points with spherical coordinates (r,θ,φ) and (ρ,α,β), respectively, and let γ be the angle subtended between them. Then*

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

Theorem A.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*

$$\frac{Y_{n'}^{m'}(\theta',\varphi')}{r'^{n'+1}}=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{(-1)^{|m+m'|-|m'|}A_n^mA_{n'}^{m'}\rho^nY_n^{-m}(\alpha,\beta)}{c_n^2A_{n+n'}^{m+m'}}\frac{Y_{n+n'}^{m+m'}(\theta,\varphi)}{r^{n+n'+1}}.$$

Theorem A.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*

$$\frac{Y_{n'}^{m'}(\theta',\varphi')}{r'^{n'+1}}=\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{(-1)^{n'+|m|}A_n^mA_{n'}^{m'}\cdot Y_{n+n'}^{m'-m}(\alpha,\beta)}{c_n^2A_{n+n'}^{m'-m}\rho^{n+n'+1}}r^nY_n^m(\theta,\varphi).$$

Theorem A.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*

$$\begin{aligned}&r'^{n'}Y_{n'}^{m'}(\theta',\varphi')\\=&\sum_{n=0}^{n'}\sum_{m=-n}^{n}\frac{(-1)^{n-|m|+|m'|-|m'-m|}c_{n'}^2A_n^mA_{n'-n}^{m'-m}\cdot\rho^nY_n^m(\alpha,\beta)}{c_n^2c_{n'-n}^2A_{n'}^{m'}r^{n-n'}}Y_{n'-n}^{m'-m}(\theta,\varphi).\end{aligned}$$

In the above theorems, the definition $A_n^m=0$, $Y_n^m(\theta,\varphi)\equiv 0$ for $|m|>n$ is used.

Appendix B: The proof of Theorem 3.3

Proof. By the assumption $|\boldsymbol{r}_c^s-\boldsymbol{r}_c^t|>a_1+ca_2$ $(c>1)$, we have $|\boldsymbol{r}'-\boldsymbol{r}_c^s|+|\boldsymbol{r}-\boldsymbol{r}_c^t|<|\boldsymbol{r}_c^t-\boldsymbol{r}_c^s|$ for any $\boldsymbol{r}\in\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^t|\le a_2\}$, $\boldsymbol{r}'\in\{\boldsymbol{x}:|\boldsymbol{x}-\boldsymbol{r}_c^s|\le a_1\}$. Then, as in (3.3)-(3.4), we have Taylor expansion

$$\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}=\frac{1}{4\pi|\boldsymbol{r}_t-\boldsymbol{r}'_s-(\boldsymbol{r}_c^s-\boldsymbol{r}_c^t)|}=\frac{1}{4\pi}\sum_{n'=0}^{\infty}\frac{P_{n'}(\xi)}{|\boldsymbol{r}_c^t-\boldsymbol{r}_c^s|}\left(\frac{|\boldsymbol{r}_t-\boldsymbol{r}'_s|}{|\boldsymbol{r}_c^t-\boldsymbol{r}_c^s|}\right)^{n'}, \tag{B.1}$$

where

$$\xi=-\frac{(\boldsymbol{r}'_s-\boldsymbol{r}_t)\cdot(\boldsymbol{r}^s_c-\boldsymbol{r}^t_c)}{|\boldsymbol{r}'_s-\boldsymbol{r}_t||\boldsymbol{r}^s_c-\boldsymbol{r}^t_c|},\quad \boldsymbol{r}'_s=\boldsymbol{r}'-\boldsymbol{r}^s_c,\quad \boldsymbol{r}_t=\boldsymbol{r}-\boldsymbol{r}^t_c. \tag{B.2}$$

Truncate the expansion (B.1) and denote the approximation by

$$\psi^p(\boldsymbol{r},\boldsymbol{r}')=\frac{1}{4\pi}\sum_{n'=0}^{p}\frac{P_{n'}(\xi)}{|\boldsymbol{r}^t_c-\boldsymbol{r}^s_c|}\Big(\frac{|\boldsymbol{r}_t-\boldsymbol{r}'_s|}{|\boldsymbol{r}^t_c-\boldsymbol{r}^s_c|}\Big)^{n'}. \tag{B.3}$$

Then, we directly have error estimate

$$\begin{aligned}\Big|\frac{1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|}-\psi^p(\boldsymbol{r},\boldsymbol{r}')\Big|&\le\frac{1}{4\pi(|\boldsymbol{r}^s_c-\boldsymbol{r}^t_c|-|\boldsymbol{r}_t-\boldsymbol{r}'_s|)}\left(\frac{|\boldsymbol{r}_t-\boldsymbol{r}'_s|}{|\boldsymbol{r}^s_c-\boldsymbol{r}^t_c|}\right)^{p+1}\\&\le\frac{1}{4\pi(c-1)a_2}\Big(\frac{a_1+a_2}{a_1+ca_2}\Big)^{p+1}.\end{aligned} \tag{B.4}$$

Applying identity $P_n(-x)=(-1)^nP_n(x)$ and Legendre addition theorem in (B.3) gives

$$\psi^p(\boldsymbol{r},\boldsymbol{r}')=\sum_{n'=0}^{p}\frac{1}{2n'+1}\frac{(-1)^{n'}}{r_{st}^{n'+1}}\sum_{m'=-n'}^{n'}\overline{Y_{n'}^{m'}(\theta_{st},\varphi_{st})}|\boldsymbol{r}'_s-\boldsymbol{r}_t|^{n'}Y_{n'}^{m'}(\widehat{\boldsymbol{r}'_s-\boldsymbol{r}_t}), \tag{B.5}$$

where $(r_{st},\theta_{st},\varphi_{st})$ is the spherical coordinates of $\boldsymbol{r}^s_c-\boldsymbol{r}^t_c$. Further, applying addition Theorem A.4 and then rearranging the resulted summation, we obtain

$$\begin{aligned}\psi^p(\boldsymbol{r},\boldsymbol{r}')&=\sum_{n'=0}^{p}\sum_{m'=-n'}^{n'}\frac{\overline{Y_{n'}^{m'}(\theta_{st},\varphi_{st})}}{4\pi r_{st}^{n'+1}}\sum_{n=0}^{n'}\sum_{m=-n}^{n}B_{n'm'}^{nm}(r'_s)^{n'-n}Y_{n'-n}^{m'-m}(\theta'_s,\varphi'_s)r_t^nY_n^m(\theta_t,\varphi_t)\\&=\sum_{n=0}^{p}\sum_{m=-n}^{n}\sum_{n'=n}^{p}\sum_{m'=-n'}^{n'}\frac{\overline{Y_{n'}^{m'}(\theta_{st},\varphi_{st})}}{4\pi r_{st}^{n'+1}}B_{n'm'}^{nm}(r'_s)^{n'-n}Y_{n'-n}^{m'-m}(\theta'_s,\varphi'_s)r_t^nY_n^m(\theta_t,\varphi_t)\\&=\sum_{n=0}^{p}\sum_{m=-n}^{n}\Big[\sum_{\nu=0}^{p}\sum_{\mu=-\nu}^{\nu}\frac{\overline{Y_{n+\nu}^{m+\mu}(\theta_{st},\varphi_{st})}}{4\pi r_{st}^{n+\nu+1}}B_{n+\nu,m+\mu}^{nm}(r'_s)^{\nu}Y_{\nu}^{\mu}(\theta'_s,\varphi'_s)\Big]r_t^nY_n^m(\theta_t,\varphi_t),\end{aligned}$$

where

$$B_{n'm'}^{nm}=\frac{(-1)^{n'+n-|m|+|m'|-|m'-m|}A_n^mA_{n'-n}^{m'-m}}{c_n^2c_{n'-n}^2A_{n'}^{m'}},$$

(r_t,θ_t,φ_t) and $(r'_s,\theta'_s,\varphi'_s)$, are the spherical coordinates of $\boldsymbol{r}-\boldsymbol{r}^t_c$ and $\boldsymbol{r}'-\boldsymbol{r}^s_c$, respectively. Apparently, $\psi^p(\boldsymbol{r},\boldsymbol{r}')$ is a truncated LE at target center $\boldsymbol{r}^t_c$ with coefficients given by

$$\hat{L}_{nm}^p=\sum_{\nu=0}^{p}\sum_{\mu=-\nu}^{\nu}\frac{\overline{Y_{n+\nu}^{m+\mu}(\theta_{st},\varphi_{st})}}{4\pi r_{st}^{n+\nu+1}}B_{n+\nu,m+\mu}^{nm}(r'_s)^{\nu}Y_{\nu}^{\mu}(\theta'_s,\varphi'_s). \tag{B.6}$$

By identity $Y_\nu^\mu(\theta,\varphi)=(-1)^\mu\overline{Y_\nu^{-\mu}(\theta,\varphi)}$, the coefficients $\hat{L}_{nm}^p$ can be re-expressed as

$$\begin{aligned}\hat{L}_{nm}^p=&\sum_{\nu=0}^{p}\sum_{\mu=-\nu}^{\nu}\frac{\overline{Y_{n+\nu}^{m-\mu}(\theta_{st},\varphi_{st})}}{r_{st}^{n+\nu+1}}B_{n+\nu,m-\mu}^{nm}(r_s')^\nu(-1)^\mu\overline{Y_\nu^\mu(\theta_s',\varphi_s')}\\=&\sum_{\nu=0}^{p}\sum_{\mu=-\nu}^{\nu}\frac{(-1)^{\nu-|m|}A_n^mA_\nu^{-\mu}Y_{n+\nu}^{\mu-m}(\theta_{st},\varphi_{st})}{c_n^2A_{n+\nu}^{m-\mu}r_{st}^{n+\nu+1}}M_{\nu\mu}.\end{aligned} \tag{B.7}$$

Noting that $A_n^m=A_n^{-m}$, the above coefficients is exactly the truncated M2L coefficients given in (3.17). As a result, we have

$$\sum_{n=0}^{p}\sum_{m=-n}^{n}L_{nm}^p r_t^n Y_n^m(\theta_t,\varphi_t)=\psi^p(\boldsymbol{r},\boldsymbol{r}'), \tag{B.8}$$

and the error estimate (3.18) follows by applying (B.4). □

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