Boundary integral equation method for electromagnetic and elastic waves

Kun Chen

Iowa State University

Follow this and additional works at: http://lib.dr.iastate.edu/etd

Part of the Acoustics, Dynamics, and Controls Commons, Electrical and Electronics Commons, and the Electromagnetics and Photonics Commons

Recommended Citation

Chen, Kun, "Boundary integral equation method for electromagnetic and elastic waves" (2016). Graduate Theses and Dissertations. 15679.

http://lib.dr.iastate.edu/etd/15679
Boundary integral equation method for electromagnetic and elastic waves

by

Kun Chen

A dissertation submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of
DOCTOR OF PHILOSOPHY

Major: Electrical Engineering

Program of Study Committee:
Jiming Song, Major Professor
John R. Bowler
Nathan Neihart
Ronald A. Roberts
Timothy Bigelow

Iowa State University
Ames, Iowa
2016

Copyright © Kun Chen, 2016. All rights reserved.
DEDICATION

For their vast love and sacrifice
that have sheltered me,
for their industry and integrity constantly
maintained even in times of extreme difficulties
that have enlightened me,
I dedicate this thesis
to my beloved parents
Shirong Zou and Gensheng Chen.
TABLE OF CONTENTS

LIST OF TABLES ................................................................. vi
LIST OF FIGURES ............................................................... vii
ACKNOWLEDGEMENTS .......................................................... x
ABSTRACT .......................................................... xi

CHAPTER 1. INTRODUCTION .................................................... 1
  1.1 Boundary Integral Equation Method ........................................ 1
     1.1.1 Boundary Integral Equations for Electromagnetic Waves ......... 2
     1.1.2 Boundary Integral Equations for Elastic Waves .................... 5
     1.1.3 Solution to Boundary Integral Equations ........................... 6
  1.2 Motivation of the Thesis ................................................. 7
     1.2.1 Metal Strip Grating on Grounded Dielectric Slab and Shielded
          Interconnect .......................................................... 8
     1.2.2 Computation of Layered Medium Doubly Periodic Green’s Func-
          tion in Matrix-Friendly Formulation ............................... 9
     1.2.3 Fast High Order Nyström Method for Elastodynamic Scattering 9
  1.3 Organization of the Thesis ................................................ 10

CHAPTER 2. METAL STRIP GRATING ON GROUNDED DIELECTRIC SLAB
           AND SHIELDED INTERCONNECT .................................... 12
  2.1 Spectral Domain Approach ............................................... 12
  2.2 Relations with PEC/PMC Shielded Microstrips .......................... 15
     2.2.1 Symmetric Case .................................................. 15
     2.2.2 Non-symmetric Case .............................................. 18
  2.3 Numerical Results ..................................................... 20
  2.4 Summary .......................................................... 26
5.6 Numerical Results ........................................... 76
5.7 Summary .................................................... 83

CHAPTER 6. CONCLUDING REMARKS ......................... 86

BIBLIOGRAPHY ................................................... 88

APPENDIX A. POISSON SUMMATION FOR DOUBLY PERIODIC
STRUCTURE ....................................................... 98

APPENDIX B. SINGULARITY OF LAYERED MEDIUM DOUBLY
PERIODIC GREEN’S FUNCTION ................................. 100

APPENDIX C. EWALD TRANSFORMATION FOR DOUBLY PE-
RIODIC STRUCTURE ............................................. 104
# LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Summary of Modal Relations</td>
<td>18</td>
</tr>
<tr>
<td>2.2</td>
<td>Normalized Wavenumber in Y Direction</td>
<td>19</td>
</tr>
<tr>
<td>3.1</td>
<td>CPU time (sec) for evaluating Green’s functions for orthogonal lattice with 6 significant digits. Parameters same as those in Fig. 3.4.</td>
<td>48</td>
</tr>
<tr>
<td>3.2</td>
<td>CPU time (sec) for evaluating Green’s functions at 100 frequencies uniformly sampled between 1 GHz and 5 GHz for orthogonal lattice with 6 significant digits. Parameters same as those for Tab. 3.1 except the frequency.</td>
<td>48</td>
</tr>
<tr>
<td>5.1</td>
<td>MLFMA for sphere with $k_c a = 4\pi$</td>
<td>80</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1</td>
<td>Derivation of boundary integral equations.</td>
<td>4</td>
</tr>
<tr>
<td>1.2</td>
<td>A triangular surface mesh for a penny shape crack.</td>
<td>7</td>
</tr>
<tr>
<td>2.1</td>
<td>Metal strip grating on grounded dielectric slab.</td>
<td>13</td>
</tr>
<tr>
<td>2.2</td>
<td>Shielded microstrips.</td>
<td>16</td>
</tr>
<tr>
<td>2.3</td>
<td>Periodic extension for non-symmetric shielded microstrip.</td>
<td>18</td>
</tr>
<tr>
<td>2.4</td>
<td>Effective permittivity for the PEC/PMC shielded microstrip v.s. frequency. Parameters: $\varepsilon_r = 9.7$, $\mu_r = 1$, $\varepsilon_r = \mu_r = 1$, $w = 1.219$ mm, $h = 1.27$ mm, and $P/w = 5$.</td>
<td>19</td>
</tr>
<tr>
<td>2.5</td>
<td>Effective permittivity for the PEC/PMC shielded microstrip v.s. geometry, with parameters $\varepsilon_r = 9.7$, $\mu_r = 1$, $\varepsilon_r = \mu_r = 1$, $w = 1.219$ mm.</td>
<td>22</td>
</tr>
<tr>
<td>2.6</td>
<td>Electric field (in V/m) distributions for PEC/PMC shielded microstrips. Parameters follow the two points at $P = 1.5w$ in Fig. 2.5a.</td>
<td>23</td>
</tr>
<tr>
<td>2.7</td>
<td>Electric field (in V/m) distributions for PEC/PMC shielded microstrips. Parameters follow the two points at $h = w$ in Fig. 2.5b.</td>
<td>24</td>
</tr>
<tr>
<td>2.8</td>
<td>Magnetic field (in A/m) distributions for PEC/PMC shielded microstrips. Parameters follow the two points at $h = 10w$ in Fig. 2.5b.</td>
<td>25</td>
</tr>
<tr>
<td>3.1</td>
<td>Planarly layered medium with doubly periodic inclusions.</td>
<td>29</td>
</tr>
<tr>
<td>3.2</td>
<td>Convergence of $S_{002}$ evaluated using KET and KPT. The parameters are $r_s = (0.01, 0.01)$, $a_1 = a_2 = 1$ ($a_i =</td>
<td>a_i</td>
</tr>
</tbody>
</table>
Figure 3.3 Convergence of $S_{002}$ evaluated using Ewald transform and KPT. The parameters are the same as Fig. 3.2 except $k_0 = (0.5, 0.5), z = 0.001$. .......................................................... 46

Figure 3.4 Convergence for $g_{S}^{TE}$ for an orthogonal periodic structure in a 5-layer medium at 3 GHz with source in the central plane of the middle layer. The thicknesses of the layers are $(\infty, 0.1, 0.1, 0.1, \infty) \lambda$, $\epsilon_r = (1, 2, 10, 2, 1), \mu_r = 1$ for all layers, $a_1 = a_2 = \lambda/2, \varphi = \pi/2, \mathbf{r}_s' = (0, 0), \mathbf{r}_s = (\lambda/10, \lambda/10), k_0 = (0.2, 0.1)\lambda^{-1}$. $z = z'$ in (a), and $z - z' = 10^{-3}\lambda$ in (b). .................................................. 47

Figure 4.1 Boundary elements with mesh nodes (red) and field sampling nodes (green). ........................................... 52

Figure 4.2 Scattering of a 1 KHz planar P-wave from a unit copper sphere in aluminum. Aluminum: $\rho = 2700$ kg/m$^3$, $\lambda = 6.138 \times 10^{10}$ N/m$^2$, $\mu = 2.95 \times 10^{10}$ N/m$^2$; Copper: $\rho = 8930$ kg/m$^3$, $\lambda = 1.32 \times 10^{11}$ N/m$^2$, $\mu = 4.60 \times 10^{10}$ N/m$^2$. ......................................................... 63

Figure 4.3 Normal incidence scattering of a 1KHz planar P-wave from penny shaped cracks of radius 1 m and different aspect ratios embedded in aluminum with $\rho = 2700$ kg/m$^3$, $\lambda = 6.138 \times 10^{10}$ N/m$^2$, $\mu = 2.95 \times 10^{10}$ N/m$^2$. ......................................................... 64

Figure 4.4 Forward scattering of a plane P-wave from a penny-shaped crack of unit radius. Parameters: $\rho = 1$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$. .... 65

Figure 4.5 Convergence of Nyström method of different orders in scattering of a P-wave from a spherical cavity with $k_c a = \pi$. Parameters: $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$. ......................................................... 66

Figure 4.6 Surface displacement along the principal cut of an elastic sphere with $k_c a = 8$ upon incidence of a planar P-wave propagating in z direction. Parameters are $\rho = 1$ kg/m$^3$, $\lambda = 0.1$ N/m$^2$, $\mu = 0.4$ N/m$^2$ for host, and $\rho = 2$ kg/m$^3$, $\lambda = 0.2$ N/m$^2$, $\mu = 0.5$ N/m$^2$ for the elastic sphere. ......................................................... 68

Figure 5.1 Multipole expansion. ......................................................... 71
Figure 5.2 Multilevel interaction in MLFMA. ......................................................... 71
Figure 5.3 Multilevel grid for MLFMA. ......................................................... 74
Figure 5.4  P-wave scattering from a unit sphere with $k_c a = 2\pi$. Host: $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$; Elastic sphere: $\rho = 6$ kg/m$^3$, $\lambda = \mu = 2$ N/m$^2$.

Figure 5.5  P-wave scattering from a unit sphere with $k_c a = 4\pi$. Host: $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$; Elastic sphere: $\rho = 6$ kg/m$^3$, $\lambda = \mu = 2$ N/m$^2$.

Figure 5.6  Scattering of P-wave from a unit elastic sphere with $k_c a = 15\pi$. Parameters: $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$ for host, and $\rho = 6$ kg/m$^3$, $\lambda = \mu = 2$ N/m$^2$ for the elastic sphere.

Figure 5.7  Plane P-wave (propagating in $z$ direction) scattering from a $5 \times 5 \times 5$ cubic array of unit spherical pores ($k_c a = 0.4\pi$) centered at origin in a host with $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$.

Figure 5.8  Pulse-echo of twin sphere pores (1 mm radius, 6 mm separation, and 30 degree slant) in aluminum. The transmitted signal is the planar Gaussian pulse $\cos (2\pi f_0 (t - t_p)) \exp \left( -(t - t_p)^2 / (2\tau_s^2) \right)$ with $f_0 = 2$ MHz, $t_s = \sigma$, $t_p = 3.5\sigma$ where $\sigma = 1/(\pi f_0)$. The transducer is located 64 mm away from the center of the twin-sphere array.

Figure 5.9  Transmitted and received signals for the configuration in Fig. 5.8.
ACKNOWLEDGEMENTS

I would like to seize this opportunity to express my heartfelt gratitude to those who have helped me through the passage of my graduate studies.

First and foremost, Dr. Jiming Song, my major professor, for his patient guidance and support with great academic insights and expertise, without which the completion of this thesis is impossible. His teachings make invaluable treasures for me that will keep inspiring me in my future careers.

I'd also like to say thanks to my committee members, Dr. John Bowler, Dr. Nathan Neihart, Dr. Timothy Bigelow, and Dr. Ron Roberts, for their time and efforts in evaluating my research and providing me with valuable advice.

My thanks also go to Dr. Telesphor Kamgaing from Intel Corporation, and Dr. Ron Roberts from Center of Nondestructive Evaluation (CNDE), for their collaboration and support in my first and second research projects. Thank Intel and CNDE CRC program for funding my research.

I also appreciate the help from my officemates, particularly Hongsheng Xu and Teng Zhao, and also thank Praveen Gurrala for running some tests of my program.

Last but not least, thank all my friends in Ames, too many to name, who have made my life colorful in the past five years.
ABSTRACT

In this thesis, the boundary integral equation method (BIEM) is studied and applied to electromagnetic and elastic wave problems.

First of all, a spectral domain BIEM called the spectral domain approach is employed for full wave analysis of metal strip grating on grounded dielectric slab (MSG-GDS) and microstrips shielded with either perfect electric conductor (PEC) or perfect magnetic conductor (PMC) walls. The modal relations between these structures are revealed by exploring their symmetries. It is derived analytically and validated numerically that all the even and odd modes of the latter two (when they are mirror symmetric) find their correspondence in the modes of metal strip grating on grounded dielectric slab when the phase shift between adjacent two unit cells is 0 or $\pi$. Extension to non-symmetric case is also made. Several factors, including frequency, grating period, slab thickness and strip width, are further investigated for their impacts on the effective permittivity of the dominant mode of PEC/PMC shielded microstrips. It is found that the PMC shielded microstrip generally has a larger wave number than the PEC shielded microstrip.

Secondly, computational aspects of the layered medium doubly periodic Green’s function (LMDPGF) in matrix-friendly formulation (MFF) are investigated. The MFF for doubly periodic structures in layered medium is derived, and the singularity of the periodic Green’s function when the transverse wave number equals zero in this formulation is analytically extracted. A novel approach is proposed to calculate the LMDPGF, which makes delicate use of several techniques including factorization of the Green’s function, generalized pencil of function (GPOF) method and high order Taylor expansion to derive the high order asymptotic expressions, which are then evaluated by newly derived fast convergent series. This approach exhibits robustness, high accuracy and fast and high order convergence; it also allows fast frequency sweep for calculating Brillouin diagram in eigenvalue problem and for normal incidence in scattering problem.

Thirdly, a high order Nyström method is developed for elastodynamic scattering that features a simple local correction scheme due to a careful choice of basis functions. A novel simple and efficient singularity subtraction scheme and a new effective near singularity subtraction scheme are proposed for performing singular and nearly singular
integrals on curvilinear triangular elements. The robustness, high accuracy and high order convergence of the proposed approached are demonstrated by numerical results.

Finally, the multilevel fast multipole algorithm (MLFMA) is applied to accelerate the proposed Nyström method for solving large scale problems. A Formulation that can significantly reduce the memory requirements in MLFMA is come up with. Numerical examples in frequency domain are first given to show the accuracy and efficiency of the algorithm. By solving at multiple frequencies and performing the inverse Fourier transform, time domain results are also presented that are of interest to ultrasonic non-destructive evaluation.
CHAPTER 1. INTRODUCTION

Mathematical modeling plays a very important role in both science and technology because it provides principles of numerical reckoning for the problems of interest, which is “the first essential step in the direction of learning any subject” [1]. In the early days, researchers relied highly on their analytic skills to solve those models, which came usually in the form of differential or integral equations. However, the fast pace of scientific and technological evolution demands the solution of more and more complex problems that are beyond the capacity of pencil and ruler. As a result, the use of numerical methods implemented on computers has become a common practice nowadays.

1.1 Boundary Integral Equation Method

The boundary integral equation method (BIEM), among others like the finite element method (FEM) and the finite difference method (FDM), is one of the most popular numerical methods for solving differential equations [2]. It has a long history of development, but interests in its numerical implementation thrived only after digital computers became available in the 1960s [3]. It has been a very powerful method since then, especially for open-region problems like scattering and radiation. Compared with other approaches, the BIEM has the boundary rather than the volume of the object as the solution domain, which yields fewer unknowns (degrees of freedom) after the fields on the whole solution domain is approximated with those on a collection of small boundary elements approximating the geometry of the domain. Also, because of the employment of Green’s functions to represent the interaction between different elements, the BIEM usually delivers higher accuracy. The bottleneck, however, exists that the linear systems resulted from the BIEM are dense and very difficult to solve when the dimension goes tremendous [4]. It was not until the 1990s when fast algorithms were developed that the BIEM could truly handle very large scale problems [5,6].

In the past two decades, the pursuit of more powerful BIEM hasn’t for a moment
ceased among computational scientists. Topics such as how to solve problems accurately and efficiently from very low to very high frequencies, how to address the accuracy issue brought about by internal resonance [7], how to deal with thin cracks [8], layered medium [9] and periodic structures [10], how to seek a solution for multi-scale and multi-physics problems, and how to take advantage of parallel computing to deliver results faster [11, 12], have all attracted great interests from researchers, and many novel and advanced techniques have been or are being developed.

1.1.1 Boundary Integral Equations for Electromagnetic Waves

The time harmonic electromagnetic waves are governed by Maxwell’s equations:

\[ \nabla \times \mathbf{E} = i\omega \mathbf{B} - \mathbf{M} \]  
\[ \nabla \times \mathbf{H} = -i\omega \mathbf{D} + \mathbf{J} \]  
\[ \nabla \cdot \mathbf{D} = \rho_e \]  
\[ \nabla \cdot \mathbf{B} = \rho_m \]

where \( \mathbf{J}, \rho_e, \mathbf{M} \) and \( \rho_m \) are densities of electric current, electric charge, and (fictitious) magnetic current and charge. Maxwell’s equations are famous for its predicting power of electromagnetic phenomena, and the application of the theory has brought about revolutionary changes to human society. The science of solving Maxwell’s equations with certain boundary conditions is known as computational electromagnetics (CEM). In the community of CEM, boundary integral equations (BIEs) are more often referred as surface integral equations (SIEs) [7].

The key to the formulation of integral equations is the dyadic Green’s function [13]. From (1.1) and (1.2), one can derive the following vector wave equation for a homogeneous medium with \( \mathbf{D} = \epsilon \mathbf{E} \) and \( \mathbf{B} = \mu \mathbf{H} \):

\[ \nabla \times \nabla \times \mathbf{E}(\mathbf{r}) - k^2 \mathbf{E}(\mathbf{r}) = i\omega \mu \mathbf{J}(\mathbf{r}) - \nabla \times \mathbf{M}(\mathbf{r}) \]  

where \( \epsilon \) and \( \mu \) are the permittivity and permeability, and \( k = \omega \sqrt{\mu \epsilon} \) is the wave number in the medium. Since we have the following expansions

\[ \mathbf{J}(\mathbf{r}) = \int_V \mathbf{I} \delta(\mathbf{R}) \cdot \mathbf{J}(\mathbf{r'})d\mathbf{r'} \]  
\[ \nabla \times \mathbf{M}(\mathbf{r}) = \int_V \nabla \times \mathbf{I} \delta(\mathbf{R}) \cdot \mathbf{M}(\mathbf{r'})d\mathbf{r'} \]
where \( \bar{I} = \hat{x}\hat{x} + \hat{y}\hat{y} + \hat{z}\hat{z} \) is the unit dyad and \( \delta(R) \) with \( R = r - r' \) is the Dirac delta function, we are also justified by the principle of superposition that the electric field can be cast in the following form

\[
E(r) = i\omega\mu \int_V \bar{G}^{EJ}(r, r') \cdot J(r') dr' + \int_V \bar{G}^{EM}(r, r') \cdot M(r') dr'
\]  

(1.8)

where \( \bar{G}^{EJ}(r, r') \) and \( \bar{G}^{EM}(r, r') \) are called electric dyadic Green’s functions for electric and magnetic sources, and they satisfy the following equations

\[
\nabla \times \nabla \times \bar{G}^{EJ}(r, r') - k^2 \bar{G}^{EJ}(r, r') = \bar{I}\delta(R)
\]

(1.9)

\[
\nabla \times \nabla \times \bar{G}^{EM}(r, r') - k^2 \bar{G}^{EM}(r, r') = -\nabla \times \bar{I}\delta(r - r')
\]

(1.10)

which can be solved to yield

\[
\bar{G}^{EJ}(r, r') = (\bar{I} + \frac{1}{k^2} \nabla \nabla)g(k, R)
\]

(1.11)

\[
\bar{G}^{EM}(r, r') = -\nabla \times \bar{G}^{EJ} = -\nabla g(k, R) \times \bar{I}
\]

(1.12)

where \( R = |R| \), and

\[
g(k, R) = \frac{e^{ikR}}{4\pi R}
\]

(1.13)

is the scalar Green’s function. From duality theorem, we have

\[
H(r) = \int_V \bar{G}^{HJ}(r, r') \cdot J(r') dr' + i\omega\epsilon \int_V \bar{G}^{HM}(r, r') \cdot M(r') dr'
\]

(1.14)

where the magnetic dyadic Green’s functions are

\[
\bar{G}^{HJ}(r, r') = -\bar{G}^{EM}(r, r')
\]

(1.15)

\[
\bar{G}^{HM}(r, r') = \bar{G}^{EJ}(r, r')
\]

(1.16)

To derive the SIE, we refer to Figure 1.1, where each of the regions \( V_\pm \) is occupied by one homogeneous isotropic material, and we let the impressed sources \( X_\pm = J_\pm \). According to the equivalence principle and extinction theorem [7], the contribution to the fields external to \( S \) from the object enclosed by it can be made equal to that from a set of equivalent surface electric current \( J_s(r) = \hat{n}(r) \times H(r) \) and magnetic current \( M_s(r) = E(r) \times \hat{n}(r) \) \( r \in S, \hat{n} \) is the outward unit surface normal of \( S \) radiating in a homogeneous space composed of the material from \( V_+ \) while the total field in \( V_- \) is set null; similarly, the contribution to the fields internal to \( S \) from all sources in \( V_+ \) can also be reproduced by \(-J_s\) and \(-M_s\) radiating in a homogeneous space occupied by the
material of \( V_- \) while the total field in \( V_+ \) is set null. Hence in each region, the total fields can be expressed as the sum of the fields from internal sources and boundary equivalent sources. Mathematically, we have

\[
E(r) \cdot (r \in \overline{V}_\pm) = E_{i\pm}(r) \pm i\omega \mu \int_{\overline{V}_\pm} \overline{G}^{EJ}_{\pm}(r, r') \cdot J_s(r') dS' \pm \int_{\overline{S}} \overline{G}^{EM}_{\pm}(r, r') \cdot M_s(r') dS' \\
H(r) \cdot (r \in \overline{V}_\pm) = H_{i\pm}(r) \pm i\omega \epsilon \int_{\overline{V}_\pm} \overline{G}^{HJ}_{\pm}(r, r') \cdot J_s(r') dS' \pm \int_{\overline{S}} \overline{G}^{HM}_{\pm}(r, r') \cdot M_s(r') dS' 
\]

(1.17)  

(1.18)

where \( \overline{V}_\pm \) are the closure of \( V_\pm \), \( \overline{G}^{EJ}_{\pm}, \overline{G}^{EM}_{\pm}, \overline{G}^{HJ}_{\pm} \) and \( \overline{G}^{HM}_{\pm} \) are the dyadic Green’s functions for the two materials, and

\[
E_{i\pm}(r) = i\omega \mu \int_{V} \overline{G}^{EJ}_{\pm}(r, r') \cdot J_s(r') dr' \\
H_{i\pm}(r) = \int_{V} \overline{G}^{HJ}_{\pm}(r, r') \cdot J_s(r') dr'
\]

(1.19)  

(1.20)

For scattering problems, \( E_{i\pm} \) and \( H_{i\pm} \) can be regarded as the incident fields. The equations (1.17) and (1.18) can be evaluated on \( S \), and then the boundary conditions of the continuity of tangential fields can be applied to arrive at the famous electric field integral equation (EFIE) and magnetic field integral equation (MFIE). It is worth pointing out that when \( r \in S \), the integrals have to be interpreted as Cauchy principle integrals due to the singularity of the dyadic Green’s functions.
1.1.2 Boundary Integral Equations for Elastic Waves

The motion of particles in a solid material is governed by Newton’s second law. When time-varying forces are applied, the particles in the solid will experience small perturbations which disrupt their equilibrium. However, if the material is elastic, it will provide restoring forces for the displaced particles, the balance of which will lead to the elastic wave equation. For time-harmonic case, the elastic wave equation is [7]

\[
\gamma \nabla \nabla \cdot \mathbf{u}(\mathbf{r}) - \mu \nabla \times \nabla \times \mathbf{u}(\mathbf{r}) + \rho \omega^2 \mathbf{u}(\mathbf{r}) = -\mathbf{f}(\mathbf{r}) \tag{1.21}
\]

where \( \mathbf{u} \) is the displacement, \( \mathbf{f} \) is the applied force density, \( \gamma = \lambda + 2\mu \), \( \lambda \) and \( \mu \) here are Lamé constants (not to confuse with wavelength and permeability), and \( \rho \) the mass density, \( \omega \) the angular frequency. By the same argument as for the electromagnetic wave equation, the solution of (1.21) can also be represented via a dyadic Green’s function in the following form

\[
\mathbf{u}(\mathbf{r}) = \int_V \mathbf{G}^{uf}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{f}(\mathbf{r}')d\mathbf{r}' \tag{1.22}
\]

where the dyadic Green’s function satisfies

\[
\gamma \nabla \nabla \cdot \mathbf{G}^{uf}(\mathbf{r}, \mathbf{r}') - \mu \nabla \times \nabla \times \mathbf{G}^{uf}(\mathbf{r}, \mathbf{r}') + \rho \omega^2 \mathbf{G}^{uf}(\mathbf{r}, \mathbf{r}') = -\mathbf{I} \delta(\mathbf{r} - \mathbf{r}') \tag{1.23}
\]

the solution of which is found to be [7]

\[
\mathbf{G}^{uf}(\mathbf{r}, \mathbf{r}') = \frac{1}{\mu} \left( \mathbf{I} + \frac{\nabla \nabla}{k^2_s} \right) g(k_s, R) - \frac{\nabla \nabla}{k^2_c} g(k_c, R) \tag{1.24}
\]

with \( k_s = \frac{\omega \sqrt{\rho/\mu}}{\mu} \), \( k_c = \frac{\omega \sqrt{\rho/\gamma}}{\gamma} \) being the wave numbers for shear and compressional waves respectively.

Refer again to Figure 1.1, and let \( \mathbf{X}_{\pm} = \mathbf{f}_{\pm} \) be the excitation body forces in each region. The equivalence principle and extinction theorem for elastic wave are expressed as the following BIE:

\[
\mathbf{u}(\mathbf{r}) \cdot (\mathbf{r} \in \tilde{V}_{\pm}) = \mathbf{u}_{\pm}(\mathbf{r}) \pm \int_S [\mathbf{G}^{ut}_{\pm}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{t}(\mathbf{r}') - \mathbf{G}^{uu}_{\pm}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{u}(\mathbf{r}')]d\mathbf{S}' \tag{1.25}
\]

where

\[
\mathbf{u}_{\pm}(\mathbf{r}) = \int_V \mathbf{G}^{uf}_{\pm}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{f}_{\pm}(\mathbf{r}')d\mathbf{r}' \tag{1.26}
\]
and $\mathbf{G}^{\text{ut}} = \mathbf{G}^{\text{uf}}$ is the Stokes’ displacement tensor, $\mathbf{G}^{\text{uu}} = \mathbf{\bar{\Sigma}}^T$ with $\mathbf{\bar{\Sigma}}$ being the Stokes’ traction tensor. The traction vector $\mathbf{t}$ and the Stokes’ traction tensor $\mathbf{\bar{\Sigma}}$ are defined as [14]

$$
\mathbf{t}(\mathbf{r}) = -\hat{\mathbf{n}}(\mathbf{r}) \cdot \{\lambda \mathbf{\bar{\nabla}} \cdot \mathbf{u}(\mathbf{r}) + \mu [\nabla \mathbf{u}(\mathbf{r}) + \mathbf{u}(\mathbf{r}) \nabla]\}
$$

$$
\mathbf{\bar{\Sigma}}(\mathbf{r}, \mathbf{r}') = \hat{\mathbf{n}}'(\mathbf{r}') \cdot \{\lambda \mathbf{\bar{\nabla}} \cdot \mathbf{G}^{\text{uf}}(\mathbf{r}, \mathbf{r}') + \mu [\nabla \mathbf{G}^{\text{uf}}(\mathbf{r}, \mathbf{r}') + \mathbf{G}^{\text{uf}}(\mathbf{r}, \mathbf{r}') \nabla]\}
$$

The equations in (1.25) are called the conventional boundary integral equations (CBIEs) for elastodynamics. Compared with (1.17) and (1.18) where the equivalent surface sources are tangential, those in (1.25), namely $\mathbf{t}$ and $\mathbf{u}$, have both tangential and normal components, and the boundary condition requires all the components to be continuous across the surface.

### 1.1.3 Solution to Boundary Integral Equations

To solve the BIE is to find the equivalent surface sources, with which all the fields can be derived. The solution process can be described as follows. A mesh is first generated, as illustrated in Figure 1.2 for a penny shape crack, where the geometry is approximated with a set of boundary elements (triangles in the example). Sub-domain basis functions relating to a node, an edge, or an element can be defined, the linear combination (with coefficients to be determined) of which can be used to represent the fields in each boundary element. Take, for instance, the scattering from a perfect electric conductor (PEC). The EFIE is written as

$$
\mathbf{E}_i(\mathbf{r}) = -i \omega \mu \int_S \mathbf{G}^{\text{EJ}}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{J}_s(\mathbf{r}') dS', \; \mathbf{r} \in S
$$

Let $\mathbf{B}_n(\mathbf{r})$ be the $n$-th ($\mathbb{N}_+ \ni n \leq N$) basis functions relating to the $n$-th subdomain $S_n$, we have

$$
\mathbf{E}_i(\mathbf{r}) = -i \omega \mu \sum_{n=1}^{N} J_{sn} \int_{S_n} \mathbf{G}^{\text{EJ}}(\mathbf{r}, \mathbf{r}') \cdot \mathbf{B}_n(\mathbf{r}') dS', \; \mathbf{r} \in S
$$

where $J_{sn}$ are the unknown coefficients. The above BIE can then be weighted by $N$ subdomain testing functions $\mathbf{T}_m(\mathbf{r})$, and integrated over $S_m$ ($\mathbb{N}_+ \ni m \leq N$), to give the following numerically solvable linear system

$$
V_m = \sum_{n=1}^{N} Z_{mn} J_{sn}
$$
where

\[ Z_{mn} = -i\omega \mu \int_{s_m} \int_{s_n} \mathbf{T}_m(r) \cdot \mathbf{G}^{EJ}(r, r') \cdot \mathbf{B}_n(r') dS' dS \]  

(1.32)

\[ V_m = \int_{s_m} \mathbf{T}_m(r) \cdot \mathbf{E}^i(r) dS \]  

(1.33)

Figure 1.2: A triangular surface mesh for a penny shape crack.

In electromagnetics, the method of moments (MoM) [7] is the most popular solver for SIEs. And for elastodynamics, the boundary element method (BEM) is usually adopted [10]. The Nyström method (NM) is another promising approach that finds applications in both electromagnetics and elastodynamics [15,16]. The major difference between the three approaches, apart from the choice of basis and testing functions, lies in the way to treat the singular integrals in \( Z_{mn} \) when \( R \) is very small: the MoM evaluates the singular integrals directly by transferring the singularity of the Green’s functions to the basis and testing functions; the NM applies a local correction to the interaction matrix in the vicinity of the singularity; the BEM regularizes the integral equation using some global identities of the static Green’s functions.

## 1.2 Motivation of the Thesis

While the BIEM has applications in many fields, this thesis is confined to electromagnetic and elastic problems. Employing the BIEM to tackle engineering problems, and contributing to the advancement of the method itself, constitute the major motivation to the author. The specific interests of this work focus on the following subjects: the metal strip grating on grounded dielectric slab and its modal relationship with shielded interconnects; doubly periodic structure in layered medium and the computation of the
Green’s function; fast and high order Nyström method for elastodynamic scattering, with applications to ultrasonic non-destructive evaluation.

1.2.1 Metal Strip Grating on Grounded Dielectric Slab and Shielded Interconnect

In modern integrated circuits, interconnects play such an important role that accurate and efficient modeling of them is a must. For example, COMS circuits see the responsibility of interconnects for more than half of the on-chip capacitance and dynamic power dissipation, significant delay to critical paths, and noise and jitter to signals [17].

Microstrip transmission lines, as we know, are key building blocks for interconnects. Microstrips shielded with perfect electric conductors (PECs) draw attention in that they can model the effect of packaging such as providing isolation between different elements as well as mechanic support for the integrated circuit [18]. As a dual of the PEC shielded case, the perfect magnetic conductor (PMC) shielded microstrip is also worth investigation.

Metal strip grating on grounded dielectric slab (MSG-GDS), which is a grounded dielectric slab loaded with one-dimensional periodic metal strips, is another classic structure which has seen various applications in electric engineering. For instance, the behaviors of the waves travelling in the direction perpendicular to the strips are utilized to design leaky wave antennas [19]. Strip-element phased arrays [20] and polarizers with low cross-polarization [21] also account for some important applications of MSG-GDS.

In fact, we can treat the three structures mentioned above as only one: a microstrip, but with different boundary conditions. It is not unfamiliar to us that the PEC and PMC boundary conditions are used to truncate the simulation domain or analyze periodic structures in high frequency electromagnetic field solvers. But what exactly is the relationships between the PEC, the PMC and the periodic boundary conditions? Though for each of these structures, there exists an abundance of literatures, it is hardly seen in the literature an explicit elaboration of this relation. As far as we are concerned, only the literature [22] bears a short discussion about the relationships between the modes of the PEC/PMC shielded microstrips and the MSG-GDS, but it is restricted to the case in the absence of phase shift between adjacent periods. We aim in this work to reveal more comprehensively the modal relationships between MSG-GDS and the PEC/PMC shielded microstrips.
1.2.2 Computation of Layered Medium Doubly Periodic Green’s Function in Matrix-Friendly Formulation

Periodic structures in layered medium find many engineering applications such as frequency selective surfaces [23], photonic crystal slabs [24], metamaterials [25], and reflectarray antennas [26]. The MSG-GDS mentioned above is also a particular case of this type of structures. To have a good understanding of their properties, and hence good designs, it is essential to perform scattering or eigenvalue analysis for these structures.

Among various approaches, the method of moments (MoM) solution to integral equations is very appealing for its high accuracy and capability to solve large and complex problems. Quite a few researchers have adopted the renowned mixed potential integral equation (MPIE) [9] for layered medium, to name a few, [27–33]. Recently, an alternative and elegant matrix-friendly formulation [34] has also been proposed, which is comparable with Michalski-Zheng’s formulation C [9] in terms of absence of line integrals and convergence rate, and also amenable for incorporating fast algorithms [35]. For both formulations, the implementation of MoM to multilayered periodic structures involves the computation of periodic Green’s functions.

Unfortunately, the Green’s functions for doubly periodic structures in layered medium are in the form of double infinite spectral sums, which can be very slowly convergent [36], especially when the source and observation points are in the same horizontal plane or very close to each other. This poses a challenging problem which draws great interests from researchers [37].

The Kummer-Poisson transformation [38, 39], the discrete complex image method (DCIM) [40], the Ewald transformation [41, 42] and the generalized pencil of function (GPOF) method [33] have been proposed or employed to evaluate the layered medium doubly periodic Green’s function (LMDPGF). These approaches involve lots of approximations, and the accuracy, convergence, and robustness are not satisfactory and need to be improved.

1.2.3 Fast High Order Nyström Method for Elastodynamic Scattering

Non-destructive evaluation (NDE) allows people monitor the quality of dear equipments, parts and materials without doing damage to them, which plays a very important role in failure prevention and cost saving [43]. One of the fundamental problems of NDE is how to obtain the interior properties of a solid material so that we can tell if there
are some defects inside. Ultrasonic waves serve as a very popular choice for this purpose due to their cheap generation and detection, deep penetration and good resolution [44]. However, the modeling of ultrasonic wave propagation and scattering in a solid is challenging, especially when it contains complex flaws. A variety of methods exist to tackle this problem. Approximate methods such as Kirchhoff [45] and Born [46] approximations can deliver results fast, making it much welcome in NDE practitioners, but are prone to inaccuracies since it is hard to track the validity of the approximation used. Numerical methods provide another alternative, with the advantages of higher accuracy and wider scope of application than approximate methods, but are generally slower. It is hence of great value to seek a fast and accurate numerical solver for elastic wave scattering.

The Nyström method, a relatively simpler approach to solve boundary integral equations compared with the boundary element method (BEM), has been introduced to elastic wave scattering [47]. A more accurate high order Nyström method is developed for elastodynamics in [48], which utilizes singularity subtraction [16, 49] for singular integrals and evaluates nearly singular integral by recursive subdivision. The singularity subtraction approach is accurate yet laborious, while the recursive subdivision can be slowly convergent for extremely nearly singular integrals. A simpler singularity treatment and a more efficient near singularity scheme are desired. In addition, the local correction of NM can also be made simpler.

When it comes to large and complex problems, the NM becomes impractical due to high computational and memory costs. To eliminate this difficulty, one can incorporate into it fast algorithms such as the multi-level fast multipole algorithm (MLFMA) [50], the pre-corrected fast Fourier transform (pFFT) [51], the $\mathcal{H}$-matrix method [52], the $\mathcal{H}^2$-matrix method [53], the adaptive cross approximation (ACA) [54], etc. Among these, the MLFMA is believed to be one of the most efficient fast algorithms for problems involving homogeneous media. So far the MLFMA has been implemented to accelerate low order boundary integral equation method [55–57], and it is appealing to develop a fast high order one.

1.3 Organization of the Thesis

The thesis is organized as follows: Chapter 1 gives an introduction to the boundary integral equation method, as well as the problems we are going to investigate using this approach; Chapter 2 studies the MSD-GDS and its relationship with the shielded
microstrip lines; Chapter 3 presents a novel accurate and efficient computation scheme for layered medium doubly periodic Green’s function in matrix-friendly formulation; Chapter 4 develops the high order Nyström method, followed by the its acceleration using the MLFMA in Chapter 5; Chapter 6 concludes the thesis.
CHAPTER 2. METAL STRIP GRATING ON GROUNDED DIELECTRIC SLAB AND SHIELDED INTERCONNECT

The metal strip grating on grounded dielectric slab (MSG-GDS) is a planar singly periodic structure that has various applications in microwave engineering. A fundamental understanding of this structure requires an analysis of the modes supportable by it, which can be achieved by solving the eigenvalue problem. In this chapter, a spectral domain boundary integral equation method titled the spectral domain approach (SDA) [58] will be used to this end. With SDA, we also analyze the PEC/PMC shielded microstrips. Since the MSG-GDS and PEC/PMC shielded microstrips are geometrically similar, one would ask the question whether their modes are closely related, the answer to which will be reached by a theoretical derivation and verified by numerical examples [59].

2.1 Spectral Domain Approach

The MSG-GDS is drawn in Fig. 2.1a. The structure obtained by adding a top PEC shield, illustrated in Fig. 2.1b, will be considered together. A coordinate system is created in Fig. 2.1c, added with some assisting dash lines locating symmetry planes. As shown in the figure, a dielectric slab of thickness $h$ is grounded by an infinite PEC plane, and topped by a grating (with period $P$) of perfect conducting strips of widths $w$. We assume that the thickness of the metal strips is zero for convenience, but later we will discuss the generalization of our analysis to the case with finite thickness. The permittivity and permeability for the slab are $\epsilon_1$ and $\mu_1$, and for the region above the slab are $\epsilon_2$ and $\mu_2$. If there is a top shield, the distance to the top slab surface is $d$. The shielded microstrips can be obtained by placing PEC (or PMC) walls at $x = \pm P/2$, so we save their illustrations for book-keeping. For the MSG-GDS, the waves can be guided in arbitrary horizontal directions, but we focus on the case when the wave propagates along the strips.

The spectral domain approach [58] is a very accurate and efficient method to solve
the eigenproblem for microstrip structures, hence it will be adopted in this work. Given
the periodicity of the structure, the Floquet theorem enables us to confine our scope to
the first unit cell (between $x = \pm P/2$). The tangent electric fields at the top surface of
the slab can be determined by the current on the metal strip and expressed in the form
of a Fourier series as

$$\sum_{n=-\infty}^{\infty} \sum_s \tilde{G}_{rs}(k_{xn}, k_y; h) \tilde{J}_s(k_{xn}) e^{ik_{xn} x} = E_r(x, h)$$  \hspace{1cm} (2.1)$$

where $k_{xn}$ and $k_y$ are the wave numbers $x$ in and $y$ directions, with the Bloch wave
number $k_{xn} = (\phi_0 + 2n\pi)/P$ ($n \in \mathbb{Z}$), where $\phi_0$ is the phase shift between adjacent
periods, $r, s \in \{x, y\}$, $\tilde{J}_s$ is the Fourier transform of the current in the unit cell, $\tilde{G}_{rs}$ is
the spectral dyadic Green’s function available in simple analytic form [58]:

\[
\tilde{G}_{xx}(k_{xn}, k_{yn}) = -i\eta_2(k_2\Delta)^{-1} \left[ \mu_r \gamma_1 (k_{xn}^2 - k_{yn}^2) \tanh(\gamma_1 h) + \gamma_2 (k_{xn}^2 - k_{yn}^2) \Theta \right] 
\]

\[
\tilde{G}_{xy}(k_{xn}, k_{yn}) = \tilde{G}_{yx}(k_{xn}, k_{yn}) = -i\eta_2 k_{xn} k_{yn}(k_2\Delta)^{-1} \left[ \mu_r \gamma_1 (k_{yn}^2 - k_{xn}^2) \tanh(\gamma_1 h) + \gamma_2 (k_{yn}^2 - k_{xn}^2) \Theta \right] 
\]

\[
\tilde{G}_{yy}(k_{xn}, k_{yn}) = -i\eta_2(k_2\Delta)^{-1} \left[ \gamma_1 \mu_r (k_{yn}^2 - k_{yn}^2) \tanh(\gamma_1 h) + \gamma_2 (k_{yn}^2 - k_{yn}^2) \Theta \right] 
\]

with

\[
\Delta = \left[ \gamma_1 \coth(\gamma_1 h) + \mu_r \gamma_2 \Theta^{-1} \right] \left[ \gamma_1 \tanh(\gamma_1 h) + \varepsilon_r \gamma_2 \Theta \right] 
\]

where we have \( \varepsilon_r = \varepsilon_1/\varepsilon_2, \mu_r = \mu_1/\mu_2, \eta_i = \sqrt{\mu_i/\varepsilon_i}, k_i = \omega \sqrt{\mu_i \varepsilon_i} \) and \( \gamma_i = \sqrt{k_{xn}^2 + k_{yn}^2 - k_i^2} \), \( \Theta = 1 \) for Fig. 2.1a and \( \Theta = \tanh(\gamma_2 d) \) for Fig. 2.1b. When \( \gamma_2 d > 9 \), which is approximately guaranteed when \( d > 3P/2 \), the two Green’s functions has little difference if single precision is used. Since the Green’s functions for the two cases are so close, they can be handled together.

Then we apply the Galerkin’s method, where the basis and testing functions are chosen the same, to solve (2.1). Specifically, the currents are expanded as

\[
J_s(x) = \sum_{q=0}^{N_s-1} C_{sq} J_{sq}(x) 
\]

where \( C_{sq} \) are expansion coefficients, \( N_s \) are the number of basis used in the expansion, and the current basis functions are chosen to be

\[
J_{xq}(x) = -i U_q(2x/w) \sqrt{1 - (2x/w)^2} \] (2.7)

\[
J_{yq}(x) = T_q(2x/w) / \sqrt{1 - (2x/w)^2} \] (2.8)

with \( U_q \) and \( T_q \) being the Chebyshev polynomials of the first and second kind, correspondingly. The Fourier transforms of the basis functions are

\[
\tilde{J}_{xq}(k_x) = (-i)^{q+1} \frac{\pi}{k_x} J_{q+1}(wk_x/2) \] (2.9)

\[
\tilde{J}_{yq}(k_x) = (-i)^q \frac{\pi w}{2} J_q(wk_x/2) \] (2.10)

where \( J_q \) is the Bessel function of the first kind of order \( q \). Then we have

\[
\tilde{J}_s(k_x) = \sum_{q=0}^{N_s-1} C_{sq} \tilde{J}_{sq}(k_x) \] (2.11)
Substituting (2.11) into (2.1), we obtain
\[ \sum_{n=\infty}^{\infty} \sum_{s} \sum_{q} C_{sq} \tilde{G}_{rs}(k_{xn}, k_{y}; h) \tilde{J}_{sq}(k_{xn}) e^{ik_{xn}x} = E_r(x, h) \] (2.12)

Then we test both sides of the equation above by \( J_{rp}(x) \) \( (r \in \{x, y\}, N \ni p < N_r) \), to have
\[ \int_{-P/2}^{P/2} dx J_{rp}(x) \sum_{n=\infty}^{\infty} \sum_{s} \sum_{q} C_{sq} \tilde{G}_{rs}(k_{xn}, k_{y}; h) \tilde{J}_{sq}(k_{xn}) e^{ik_{xn}x} = \int_{-P/2}^{P/2} dx J_{rp}(x) E_r(x, h) \] (2.13)

which, after performing the integral over \( x \), leads us eventually to the following homogeneous linear system
\[ \begin{bmatrix} K_{xx} & K_{xy} \\ K_{yx} & K_{yy} \end{bmatrix} \begin{bmatrix} C_x \\ C_y \end{bmatrix} = 0 \] (2.14)

where \( C_x \) and \( C_y \) are vectors of the coefficients \( C_{sq}, K_{rs}(r, s \in \{x, y\}) \) is a matrix with elements given by
\[ K_{rspq} = \sum_{n=\infty}^{\infty} \tilde{J}_{rp}(-k_{xn}) \tilde{J}_{sq}(k_{xn}) \tilde{G}_{rs}(k_{xn}, k_{y}) \] (2.15)

And the right hand side vanishes due to the fact that on the metal there is no tangential field, while in dielectric the current is null.

To solve the eigenvalue problem, we require the vanishing of the determinant of the matrix in (2.14). In general, we need to find both \( \phi_0 \) and \( k_y \), but in this paper we would fix \( \phi_0 \), and just find \( k_y \) using a root-finding procedure. The series in (2.15) can be slowly convergent, so the leading asymptotic terms are extracted and summed with some fast convergent series, while the remaining part is summed directly, which, after this process, exhibits good convergence [60]. Notice that, when \( k_y = 0 \), we have \( K_{xy} = K_{yx} = 0 \), so the modes decouple into TE and TM waves, and \( k_{x0} \) is the eigenvalue to be found.

### 2.2 Relations with PEC/PMC Shielded Microstrips

#### 2.2.1 Symmetric Case

Figure 2.2 shows the symmetric and non-symmetric shielded microstrips. On the two sides, the shields can be PEC walls, or PMC walls. The top shield may be absent
when we consider their relationships with the MSG-GDS in Fig. 2.1a. Let’s first consider the symmetric case. In the periodic structure, we place phase shift walls (PSWs) at the boundary of the first unit cell and obtain a shielded structure as well. The electric and magnetic fields for this structure can be expressed in Fourier series as

$$F(x, z) = \sum_{n=-\infty}^{\infty} \tilde{F}(k_x n, z) e^{i k_x x}$$  \hspace{1cm} (2.16)

where $F \in \{E, H\}$ and $\exp(i k_y y)$ variation has been suppressed. In fact, the expressions for the fields in Fig. 2.2 are in the same form as (2.16), but the values of $k_x n$ are different. Considering the mirror symmetry of the structure with respect to the $yoz$ plane, one can classify the modes into two categories: even and odd [61]. To better understand the parity of the modal fields, we first express the components of the spectral currents using the magnetic and electric vector potentials $\Phi_i^{(e)}$ and $\Phi_i^{(h)}$ ($i$ indicates the $i^{th}$ region) as follows [62]:

$$\tilde{J}_x(k_{xn}) = -i k_y^{-1} \left[ (k_x^2 - k_y^2) \Phi_2^{(h)}(k_{xn}, h) - (k_1^2 - k_y^2) \Phi_1^{(h)}(k_{xn}, h) \right]$$ \hspace{1cm} (2.17)

$$\tilde{J}_y(k_{xn}) = i k_{xn} \left[ \Phi_2^{(h)}(k_{xn}, h) - \Phi_1^{(h)}(k_{xn}, h) \right]$$

$$- \frac{\omega}{k_y} \frac{\partial}{\partial z} \left[ \varepsilon_2 \Phi_2^{(e)}(k_{xn}, z) - \varepsilon_1 \Phi_1^{(e)}(k_{xn}, z) \right]_{z=h}$$ \hspace{1cm} (2.18)

where $\omega$ is the angular frequency. The above equations inform us that for a given mode, either even or odd, the currents in $x$ and $y$ directions have different parities in terms of $k_x$. Given the parity of a mode, parity of the current is specified, and then we can determine the parities of the potentials at the upper surface of the dielectric slab, which should be identical for all constant $z$ planes. This would in turn allow us to identify the parities of all the components of the electric and magnetic fields. If we separately
consider the two types of modes, and check the expressions for the electric and magnetic
fields, we find that $\tilde{E}_y$ and $\tilde{E}_z$ have the same parity in terms of $k_x$, which differs from
that of $\tilde{E}_x$; $\tilde{H}_y$ and $\tilde{H}_z$ have the same parity, but different from that of $\tilde{H}_x$. The parity
of the fields in spectral domain, according to the properties of Fourier transform, is the
same as that in spatial domain. With these in mind, we are ready to distinguish two
types of modes, and define the modes as even modes if $J_y, E_y, E_z, H_x$ are even and $J_x,$
$E_x, H_y, H_z$ are odd; the modes are odd modes if the converse is true. Now let’s make
use of (2.16), and examine the tangential fields at the PSWs $(x = \pm P/2)$. For $\phi_0 = 0$,
indicating the absence of phase shift between adjacent periods, we yield

$$F_{y/z}(\pm P/2, z) = \tilde{F}_{y/z}(0, z) + \sum_{n=1}^{\infty} (-1)^n \left[ \tilde{F}_{y/z}(2n\pi/P, z) + \tilde{F}_{y/z}(-2n\pi/P, z) \right]$$

(2.19)

where $F \in \{E, H\}$. Obviously it vanishes if $F_{y/z}$ is an odd function of $x$. While for
$\phi_0 = \pi$, we acquire

$$F_{y/z}(\pm P/2, z) = \pm i \sum_{n=0}^{\infty} (-1)^n \left[ \tilde{F}_{y/z}((2n + 1)\pi/P, z) - \tilde{F}_{y/z}(-(2n + 1)\pi/P, z) \right]$$

(2.20)

which again vanishes if $F_{y/z}$ is even. The implication of the vanishing of tangential fields
is that we can place PEC or PMC walls at the boundary and the modal profiles would
remain unperturbed. Now if we take into account the parities of the modal fields as have
been defined above, we conclude that the periodic boundary condition (PBC) reduces
to PEC boundary condition for the odd modes if $\phi_0 = 0$, for even modes if $\phi_0 = \pi$; it
reduces to PMC boundary condition for odd modes if $\phi_0 = \pi$, for even modes if $\phi_0 = 0$.
Think the other way around: Are all the modes of the PEC or PMC shielded microstrips
included in the modes of the MSG-GDS with phase shift $\phi_0 = 0, \pi$? The answer is yes,
because we can extend the domain of the PEC or PMC shielded structures to periodic
ones by introducing infinite number of images according to the image theory. Then we
are assured that the PEC and PMC boundary conditions are indeed special cases of the
PBC for the symmetric structure under consideration. It should be noted that the above
conclusions are not limited to the case when the strip thickness is 0, but also apply when
the strips are of finite thickness, since our derivation only assumes mirror symmetry of
the structure in this section and is independent of the zero-thickness assumption.

Since the structure is also mirror symmetric with respect to the plane $x = P/2$, we
can also place PSWs at $x = 0$ and $x = P$. Thus a corresponding PEC or PMC shielded
microstrip is obtained if PEC or PMC walls are placed. In this circumstance, the parity of a mode is defined in the same way as in the case for symmetry about $x = 0$, but referred with respect to the central plane of the shielded microstrip at $x = P/2$. The modal relations between the three structures can be analyzed similarly. We tabulate the relations for both cases in Table 2.1. For the modes in the same row, they have the same propagation constant along the longitudinal direction. We can see that when $\phi_0 = 0$, the same walls are placed and the parities are the same for both symmetric cases, while when $\phi_0 = \pi$, different walls are placed and the parities are opposite.

![Figure 2.3: Periodic extension for non-symmetric shielded microstrip.](image)

<table>
<thead>
<tr>
<th>$\phi_0$</th>
<th>$x = 0$ symmetry</th>
<th>$x = P/2$ symmetry</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>PEC Odd</td>
<td>PEC Odd</td>
</tr>
<tr>
<td></td>
<td>PMC Even</td>
<td>PMC Even</td>
</tr>
<tr>
<td>$\pi$</td>
<td>PEC Even</td>
<td>PMC Odd</td>
</tr>
<tr>
<td></td>
<td>PMC Odd</td>
<td>PEC Even</td>
</tr>
</tbody>
</table>

### 2.2.2 Non-symmetric Case

For non-symmetric case, the modes of the PEC/PMC shielded microstrips can no longer be divided into even and odd modes. But we can perform periodic extension in this case. As shown in Fig. 2.3, where we have supplemented the original non-symmetric shielded structure with its mirror image. We perform an odd extension for the modes of PEC shielded microstrip, and all the modes of the original non-symmetric structure now correspond to the odd modes of the extended symmetric PEC shielded structure whose width has doubled. For the PMC shielded microstrip, we conduct an even extension,
and all the modes of the original structure has correspondence to the even modes of the extended structure. Now we make up a MSG-GDS with the extended structure in Fig. 2.3 (taking away the vertical PEC or PMC walls) as the unit cell. Based on our previous discussions, we know the odd modes of the extended PEC shielded microstrip correspond to the modes with $\phi_0 = 0$ in the MSG-GDS (with extended unit cell), which means all the modes of the original non-symmetric PEC shielded microstrip correspond to the modes of MSG-GDS with $\phi_0 = 0$. Similarly, we have the correspondence between the modes of the non-symmetric PMC shielded microstrip and those of the MSG-GDS.

Table 2.2: Normalized Wavenumber in Y Direction

<table>
<thead>
<tr>
<th>Mode</th>
<th>Reference</th>
<th>Calculated</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 (even)</td>
<td>2.7102057109</td>
<td>2.7102057101</td>
</tr>
<tr>
<td>2 (odd)</td>
<td>1.2894527450</td>
<td>1.2894527434</td>
</tr>
<tr>
<td>3 (even)</td>
<td>1.1026365889</td>
<td>1.1026365888</td>
</tr>
<tr>
<td>4 (odd)</td>
<td>0.9223133480</td>
<td>0.9223133479</td>
</tr>
<tr>
<td>5 (even)</td>
<td>0.7250996002</td>
<td>0.7250996009</td>
</tr>
</tbody>
</table>

Figure 2.4: Effective permittivity for the PEC/PMC shielded microstrip v.s. frequency. Parameters: $\epsilon_r^1 = 9.7$, $\mu_r^1 = 1$, $\epsilon_r^2 = \mu_r^2 = 1$, $w = 1.219$ mm, $h = 1.27$ mm, and $P/w = 5$. 


2.3 Numerical Results

The first numerical experiment is about the PEC shielded microstrip as illustrated by Fig. 2.2a. Following the reference [63], we set the parameters as follows: \( \varepsilon_{r1} = 8.875, \mu_{r1} = 1, \varepsilon_{r2} = \mu_{r2} = 1, f = 20 \text{ GHz}, h = 1.27 \text{ mm}, w = h, d = 11.43 \text{ mm} \) and \( P = 10h \). The first 5 modes are calculated and tabulated in Table 2.2, where the normalized wavenumbers are \( k_y/k_2 \). We can see that agreement of 8-10 digits is achieved, and we only use 4 terms in the expansion of the currents in \( x \) and \( y \) directions. It is to be noted that our results are obtained not by solving the eigenproblem of the shielded microstrip directly, but by solving that for the MSG-GDS. We pick up the modes of the shielded microstrip from the set of modes of MSG-GDS by letting \( \phi_0 = 0 \) or \( \pi \) and using basis functions with proper parities according to our previous conclusions. The good agreement achieved confirms our claims about the relationships between the MSG-GDS and shielded microstrip.

In practice, the shield for the microstrips may be used to model the packaging effect. Then one question arises: Which one captures the physics better, the PEC shielded microstrip, or the PMC shielded? So it is beneficial for us to compare the behavior of the two structures. Again, we do this by finding their eigen modes from a calculation of the MSG-GDS. Fig. 2.4 shows the dispersion curves for the dominant modes of the PEC and PMC shielded microstrips in the range from 1 GHz to 25 GHz, where the effective permittivity is defined as the square of the normalized wave number. The parameters are \( \varepsilon_{r1} = 9.7, \mu_{r1} = 1, \varepsilon_{r2} = \mu_{r2} = 1, w = 1.219 \text{ mm}, h = 1.27 \text{ mm} \) and \( P/w = 5 \). Here we assume there is no top shield. As indicated by the legend, both modes are even modes. It can be seen first that both effective permittivities increase with the frequency. Also notice that the PMC shielded microstrip has a larger effective permittivity than the PEC shielded microstrip, and the difference between the two permittivities decreases with frequency and eventually almost vanishes at high frequency. The reason for this is that the electromagnetic fields aggregate more in the vicinity of the metal strip, whose width is just \( 1/5 \) of the period. Therefore we are grounded to treat the shields on both sides as far from the region where most energy rests, and it makes little difference whether we put a PEC or PMC wall.
(a) $h = 1.27 \text{ mm and } f = 10 \text{ GHz}$

(b) $f = 10 \text{ GHz and } P/w = 5$
In Fig. 2.5, the geometric parameters $P, h, w$ are explored. Parameters common to Fig. 2.5 (a-c) are $\epsilon_r = 9.7$, $\mu_r = 1$, $\epsilon_r = \mu_r = 1$, $w = 1.219$ mm. In Fig. 2.5a, $w$ is very close to $h$, and the effective permittivities are plotted against the ratio $P/w$ at 10 GHz. It is observed that the PMC shielded microstrip still has a larger effective dielectric constant than the PEC shielded microstrip, and the two permittivities approach each other when frequency is increased. At $P = 1.5w$, the electric field distributions in the two structures are drawn in Fig. 2.6. The fields are calculated by convoluting the dyadic Green’s function with the eigen-current, which can be found by solving (2.14) with the normalization that the $l_2$-norm of the expansion coefficients equals unity. The arrows in the graphs represent a snapshot of the vector fields, and color plot conveys the amplitude of the fields. It is very clear that the PEC shielded microstrip has the fields mostly confined around the two edges of the metal strip, and decays very quickly into the dielectric region and air region. Nevertheless, the PMC shielded microstrip drives most of the electric fields into the high dielectric region, and the distribution is also rather uniform. This implies that the PMC shielded microstrip in this configuration has a larger capacitance for storing electric energy, which is equivalently interpreted as a
larger effective permittivity. But when $P/w$ goes high, the PEC/PMC walls on both sides play a lesser role, which leads to very close effective permittivities.

The influence of the slab thickness is more complicated, as illustrated in Fig. 2.5b. For the PEC shielded microstrip, the effective permittivity keeps going down when the slab becomes thicker, while that for the PMC shielded microstrip descends to a valley before its rise. When $h$ is very small, the two have almost the same effective permittivity. In this situation, we can think of a very thin parallel capacitor formed between the metal strip and the metal ground, and this capacitor has a large capacitance to store the energy in the small region near the metal strip. As a result, the fields can hardly reach the boundary on the two sides, shedding light on why the two permittivities are very close. For this point, we are confirmed by the field distribution in Fig. 2.7, where the field distributions for the two structures at $h = w$ are close to each other, and most of the fields are in the slab region. Besides, the fields decay to a very weak level at the
Figure 2.7: Electric field (in V/m) distributions for PEC/PMC shielded microstrips. Parameters follow the two points at $h = w$ in Fig. 2.5b.
Figure 2.8: Magnetic field (in A/m) distributions for PEC/PMC shielded microstrips. Parameters follow the two points at $h = 10w$ in Fig. 2.5b.
PEC/PMC walls. When $h$ is very large, the PMC shielded microstrip has a much larger effective permittivity than the PEC shielded microstrip. To make sense of this, we look at the (magnetic) field distributions at $h = 10w$ in Fig. 2.8. We can see that for the PEC shielded microstrip, the fields decay away from the metal strip, but for the PMC shielded, things are different: there are peaks and valleys in the high dielectric region. The PMC shields influence the field distribution such that the mode is very close to a TEM wave in the slab region, and much more energy is stored in the slab. That is why it exhibits a larger dielectric constant. In Fig. 2.5c, the dispersion curves of the PEC and PMC shielded microstrip are plotted against $P/h$, where $h = 5w$ and $f = 5$ GHz. Similar phenomena are observed as in Fig. 2.5a. From the above discussions, we are led to claim that the PMC shielded microstrip in general has a larger effective dielectric constant than the PEC shielded microstrip, given that the frequency is not too high, the slab not too thin, and the width $P$ is not significantly larger than the slab thickness $h$ and strip width $w$.

2.4 Summary

As a summary, this chapter has investigated the eigenvalue problems of the metal strip grating on grounded dielectric slab and the PEC/PMC shielded microstrips by virtue of a spectral domain boundary integral equation method known as the spectral domain approach, with an emphasis on the modal relationships between these structures. By exploring the symmetry of these structures and examining the tangential fields at the boundary, we have found that the PEC and PMC boundary conditions are special cases for the periodic boundary conditions. To be specific, it has been revealed and verified that all the even and odd modes of the mirror symmetric PEC/PMC shielded microstrip find their correspondence in the modes of metal strip grating on grounded dielectric slab when the phase shift between adjacent two unit cells is 0 or $\pi$. By performing a periodic extention for the non-symmetric shielded structures and making up a new MSG-GDS, all the modes for the original non-symmetric shielded structures also correspond to those of the MSG-GDS with 0 or $\pi$ phase shift between adjacent unit cells. Through a calculation for the MSG-GDS and the use of the relations between the PEC/PMC shielded microstrips and MSG-GDS, we conduct a comparison of the PEC and PMC shielded microstrips. The effect of frequency and geometric parameters on the dominant modes for the PEC and PMC shielded microstrips have been studied. We found that the
dominant (even) mode of the PMC shielded microstrip has in general a larger effective
dielectric constant than the dominant (even) mode of the PEC shielded microstrip due to
a stronger capacity to drive more electromagnetic energy into the high dielectric region.
CHAPTER 3. COMPUTATION OF LAYERED MEDIUM
DOUBLY PERIODIC GREEN’S FUNCTION IN
MATRIX-FRIENDLY FORMULATION

Layered medium doubly periodic structure (LMDPS) is a much more complicated periodic structure than MSG-GDS. As for the boundary integral equation for LMDPS, the mixed potential integral equation (MPIE) [9] and the matrix-friendly formulation (MFF) [34] make use of the dyadic Green’s function for LMDPS, which can reduce the number of unknowns and improve the accuracy compared with the equivalence principle algorithm [64], but have to confront the challenge of accurate and efficient evaluation of the layered medium doubly periodic Green’s function (LMDPGF).

Researchers have carried out lots of analytic and numerical studies on evaluating the LMDPGF [37]. The Kummer-Poisson transformation (KPT) [38], initially proposed to promote the convergence of free space periodic Green’s function, can also be extended to the multilayered case [39]. The discrete complex image method (DCIM) is widely used, either to obtain approximate closed-form spatial Green’s functions [40], or the asymptotic expressions [41]. However, this procedure may necessitate formidable task to take care of the spatial and lateral waves for layered medium [65], and the computation of complementary error function (Erfc) with complex arguments is also of large computational costs [66]. In [42], the spectral Green’s function is approximated with real exponentials for certain ranges of transverse wave number. Then the Kummer’s transformation and Ewald transformation are applied and the argument for Erfc is always real since only static images are involved. Recently, a new method based on generalized pencil of function (GPOF) method and the Kummer-Poisson transformation with asymptotic expansion of arbitrarily large order has been reported [33]. Though it can yield accurate result for all range of distances between sources and observation points, the accuracy is limited to roughly four significant digits. For approximations have to be made for each pair of $z$ and $z'$, and/or each frequency in the approaches mentioned above, they are also inefficient and unstable.
Figure 3.1: Planarly layered medium with doubly periodic inclusions.

In this chapter, the MFF is adopted due to its succinctness and elegance. The LMDPGF is first derived, which is used to formulate the MFF for LMDPS. Then an accurate and efficient algorithm for evaluating the LMDPGF will be developed [67].

3.1 Layered Medium Doubly Periodic Green’s Functions

Figure 3.1 shows the configuration of an N-region layered medium with doubly periodic inclusions. With TE and TM decomposition, the dyadic Green’s functions for
homogeneous layered medium can be derived using vector wave functions as \[68\]

\[
\begin{align*}
\mathbf{G}^{TE}(r, r') &= (\nabla \times \hat{z})(\nabla' \times \hat{z})g^{TE}(r, r') \\
&+ \frac{1}{k_{nm}^2}(\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TM}(r, r') - \frac{\hat{z} \hat{z}}{k_m^2} \delta(r - r') \\
\mathbf{G}^{TM}(r, r') &= (\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TE}(r, r') \\
&+ \frac{\mu_n}{\mu_m}(\nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TM}(r, r')
\end{align*}
\] (3.1)

\[
\begin{align*}
\mathbf{G}^{TE}(r, r') &= (\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TE}(r, r') \\
&+ \frac{1}{k_{nm}^2}(\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TM}(r, r') - \frac{\hat{z} \hat{z}}{k_m^2} \delta(r - r') \\
\mathbf{G}^{TM}(r, r') &= (\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TE}(r, r') \\
&+ \frac{\mu_n}{\mu_m}(\nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z})g^{TM}(r, r')
\end{align*}
\] (3.2)

where \(k_{nm}^2 = \omega^2 \varepsilon_n \mu_m\), \(r\) is in Region \(n\), and \(r'\) in Region \(m\), \(g^{TE}\) and \(g^{TM}\) are scalar Green’s functions, which are in form of Sommerfeld integral \[7\]:

\[
g^{TE/TM}(r, r') = \frac{i}{8\pi^2} \int_0^{\infty} \int_{k_m^2 k_{nm}^2} \mathcal{E}^{TE/TM}(k_s; z, z') e^{ik_s(r_s - r_s')} \] (3.3)

The Dirac delta singularity due to \(\partial_s \partial_{z'} e^{ik_{nm}|z-z'|}\) at \(z = z'\) for \(\mathbf{G}^{TE}\) should be ignored \[68\] since it has already been extracted in the last term for \(\mathbf{G}^{TE}\). In the following, we will drop the \(\frac{\hat{z} \hat{z}}{k_m^2} \delta(r - r')\) term since its contribution can be easily retrieved. We also choose not to separate the primary and secondary fields, firstly because we still need special techniques to evaluate the contribution from the primary fields—periodic Green’s function in homogeneous media—if it is separated out, and the second reason is that both fields can be conveniently handled together in our proposed method. For doubly periodic structures with direct lattice vectors \(\mathbf{a}_1\) and \(\mathbf{a}_2\) (\(\varphi\) is the angle between \(\mathbf{a}_1\) and \(\mathbf{a}_2\)), with the help of Poisson summation formula (Appendix A), we just need to replace \(g^{TE}\) and \(g^{TM}\) for homogeneous media with the following expressions

\[
g^{TE/TM}(r, r') = \hat{S} \mathcal{F}^{TE/TM}(k_s; z, z')
\] (3.4)

where the operator \(\hat{S}\) is defined as

\[
\hat{S} f(k_s; z, z') = \frac{i}{2A_{cell}} \sum_I \frac{f(k_s; z, z')}{k_{s1} k_{m1}} e^{ik_s(r_s - r_s')}
\] (3.5)

where \(A_{cell} = |\mathbf{a}_1 \times \mathbf{a}_2|\), \(k_{s1} = k_0 + \mathbf{k}_{s1}\), \(k_{m1} = i_1 \mathbf{b}_1 + i_2 \mathbf{b}_2\), \(I = (i_1, i_2) \in \mathbb{Z} \times \mathbb{Z}\), \(k_{s1} = |k_{s1}|\) are discrete samples of transverse wave number \(k_s\), \(k_{m1} = \sqrt{k_m^2 - k_{s1}^2}\). \(r_s = (x, y)\) and \(r_s' = (x', y')\). \(k_0\) is the Bloch wave vector in the horizontal plane, which depends on frequency and incident angle in scattering problem, while in eigenvalue problem, to calculate the Brillouin diagram, eigenfrequency is sought for a fixed \(k_0\). \(\mathbf{b}_1\) and \(\mathbf{b}_2\) are reciprocal lattice vectors satisfying \(\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij}\), where \(\delta_{ij}\) is the Kronecker delta.
function. The propagation factors \( F^{TE/TM}(k_s; z, z') \) can be found as [68]

\[
F_+ (k_s; z, z') = \left[ e^{iknz}(z+d_n) + \tilde{R}_{n,n-1} e^{-iknz(z+2d_n-1-d_n)} \right] \\
\times \left[ e^{-iknz(z'+d_m-1)} + \tilde{R}_{m,m+1} e^{iknz(z'+2d_m-d_m-1)} \right] \tilde{M}_m \tilde{S}^+_mn
\]

(3.6)

\[
F_- (k_s; z, z') = \left[ e^{-iknz(z+d_n-1)} + \tilde{R}_{n,n+1} e^{iknz(z+2d_n-d_n-1)} \right] \\
\times \left[ e^{iknz(z'+d_m)} + \tilde{R}_{m,m-1} e^{-iknz(z'+2d_m-1-d_m)} \right] \tilde{M}_m \tilde{S}^-mn
\]

(3.7)

where “+” is chosen when \( z > z' \), and “−” is chosen when \( z < z' \). In above, we have

\[
\tilde{M}_m = \left[ 1 - \tilde{R}_{m,m-1} \tilde{R}_{m,m+1} e^{2iknz(d_m-d_m-1)} \right]^{-1}
\]

(3.8)

and the generalized reflection and transmission coefficients are given as

\[
\tilde{R}_{i,i+1} = \frac{R_{i,i+1} + \tilde{R}_{i+1,i+1} e^{2ik_{i+1,i}(d_{i+1}-d_i)}}{1 + R_{i,i+1} \tilde{R}_{i+1,i+1} e^{2ik_{i+1,i}(d_{i+1}-d_i)}}, \quad \tilde{R}_{N,N+1} = 0
\]

(3.9)

\[
\tilde{R}_{i,i-1} = \frac{R_{i,i-1} + \tilde{R}_{i-1,i-1} e^{-2ik_{i-1,i}(d_{i-1}-d_{i-2})}}{1 + R_{i,i-1} \tilde{R}_{i-1,i-1} e^{-2ik_{i-1,i}(d_{i-1}-d_{i-2})}}, \quad \tilde{R}_{1,0} = 0
\]

(3.10)

and

\[
\tilde{S}^+_mn = \tilde{S}^+_m,n-1 \prod_{i=n+1}^{m-1} e_i \tilde{S}^+_i,i-1, \quad m > n
\]

(3.11)

\[
\tilde{S}^\pm mn = e^{-iknz(d_m-d_m-1)}, \quad m = n
\]

(3.12)

\[
\tilde{S}^-mn = \tilde{S}^-m,m+1 \prod_{i=m+1}^{n-1} e_i \tilde{S}^-i,i+1, \quad m < n
\]

(3.13)

where \( e_i = e^{ik_{i}(d_{i}-d_{i-1})} \) and

\[
\tilde{S}^+_i,i+1 = \frac{T_{i+1,i}}{1 - R_{i,i+1} \tilde{R}_{i+1,i} e^{2ik_{i+1,i}(d_{i+1}-d_{i-1})}}
\]

(3.14)

\[
\tilde{S}^-i,i+1 = \frac{T_{i-1,i}}{1 - R_{i,i-1} \tilde{R}_{i-1,i} e^{-2ik_{i-1,i}(d_{i-1}-d_{i-2})}}
\]

(3.15)

The Fresnel reflection and transmission coefficients are

\[
P_{ij}^\vartheta = \frac{p_j k_{iz} - p_i k_{jz}}{p_j k_{iz} + p_i k_{jz}}, \quad T_{ij}^\vartheta = \frac{2p_j k_{iz}}{p_j k_{iz} + p_i k_{jz}}, \quad |i - j| = 1
\]

(3.16)

where \( p = \mu \) if \( \vartheta = \text{TE} \) and \( p = \varepsilon \) if \( \vartheta = \text{TM} \).
3.2 Matrix-Friendly Formulation

The matrix-friendly formulation can be derived with the following decomposition [7]

\[(\nabla \times \hat{z})(\nabla' \times \hat{z}) = k_s^2 \hat{I}_s - \nabla \nabla' + \nabla_z \nabla' - \nabla^\prime \nabla_z\]

(3.17)

\[(\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) = \nabla \nabla' \partial_z \partial_z' + k_m^2 \nabla \nabla_z + k_n^2 \nabla' \nabla' + k_m^2 k_n^2 \hat{z} \hat{z}\]

(3.18)

for \(\tilde{G}^{EJ}\), and

\[(\nabla \times \nabla \times \hat{z})(\nabla' \times \hat{z}) = (\nabla' \nabla' + k_n^2 \hat{z})(\nabla' \times \hat{z})\]

(3.19)

\[(\nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) = (\nabla \times \hat{z})(\nabla' \nabla' + k_m^2 \hat{z})\]

(3.20)

for \(\tilde{G}^{HJ}\), where \(\nabla_z = \partial_z \hat{z}, \nabla'_z = \partial_{z'} \hat{z}\), and \(\hat{I}_s = \hat{x}\hat{x} + \hat{y}\hat{y}\) is 2-D unit dyad. Then integration by parts is used as much as possible to transfer the differential operators to the basis and testing functions. One problem with the periodic Green’s function is that it blows up when \(k_s = 0\), therefore ways have to be found to extract this singularity. For \(\tilde{G}^{EJ}\), it can be easily observed that the singularity disappears for the term involving \(k_s^2 \hat{I}_s\), and it can be shown that for other terms this singularity would also disappear or cancel each other in the final expression of the dyadic Green’s function. Therefore, when infinity occurs due to \(k_s = 0\) in the denominator, that term can be safely discarded. However, the decomposition of (3.19) and (3.20) fails to provide such convenience. To overcome this difficulty, we suggest modifying (3.20) as

\[(\nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) = \partial_{z'} k_s^2 \hat{I}_s + \nabla' (\nabla' \times \hat{z}) \partial_{z'} + \partial_{z''} \hat{z} (\nabla \times \hat{z}) + k_s^2 (\nabla \times \hat{z}) \hat{z}\]

(3.21)

to extract the contribution from \(k_s = 0\), where we have \(\hat{I}_s = \hat{x}\hat{y} - \hat{y}\hat{x}\) (see Appendix B). With (3.19) and (3.21), the singularity disappears for terms concerning \(\partial_{z'} k_s^2 \hat{I}_s\), and would disappear or cancel each other for all the rest parts when it is substituted into the final expression for the dyadic Green’s function. Then we can ignore the contribution from the terms that go to infinity due to \(k_s = 0\) in the denominator. Notice that the above differential operators on the left-hand-side in (3.17)-(3.21) operate on \(g^{TE/TM}\), which is in series form, but in the calculation, since we can exchange the order of summation and differentiation, \(k_s^2\) is to be understood as an operator on the general term of the series.
In the MoM implementation, we can write the moment matrix elements involving $\bar{G}^{EJ}$ as

$$\langle T_i, \bar{G}^{EJ}, B_j \rangle = \langle T_{Si}, g_{s}^{TE}, B_{Sj} \rangle + \left( \nabla \cdot T_i, \frac{\partial_{zz'} g_{s}^{TM}}{k_{mn}^{2}} - g_{s}^{TE}, \nabla' \cdot B_j \right)$$

$$- \langle T_{Zi}, \frac{\mu_n}{\mu_m} \partial_{z} g_{s}^{TM} + \partial_{zz'} g_{s}^{TE}, \nabla' \cdot B_j \rangle$$

$$- \langle \nabla \cdot T_i, \frac{\varepsilon_m}{\varepsilon_n} \partial_{z} g_{s}^{TM} + \partial_{zz'} g_{s}^{TE}, B_{Zj} \rangle$$

$$+ \langle T_{Zi}, k_{mn}^{2} g_{s}^{TM} - \partial_{zz'} g_{s}^{TE}, B_{Zj} \rangle$$

(3.22)

For those involving $\bar{G}^{HJ}$, we have

$$\langle T_i, \bar{G}^{HJ}, B_j \rangle = \frac{k_{n}^{2}}{2} \langle T_{Zi}, (\nabla' \times \hat{z}) g_{s}^{TE}, B_j \rangle$$

$$- \langle \nabla \cdot T_i, (\nabla' \times \hat{z}) \partial_{z} g_{s}^{TE}, B_j \rangle$$

$$- \frac{\mu_n}{\mu_m} \langle T_i, (\nabla \times \hat{z}) \partial_{z'} g_{s}^{TM}, \nabla' \cdot B_j \rangle$$

$$+ \langle T_{Zi}, k_{mn} g_{s}^{TM} - \partial_{zz'} g_{s}^{TE}, B_{Zj} \rangle$$

$$+ \sigma_0 \langle T_i, I_s, B_j \rangle$$

(3.23)

if we use (3.19) and (3.20), where $\sigma_0$ is defined as

$$\sigma_0 = \frac{i \mu_n \partial_{z} F_{TM}^{s}(0; z, z')}{2 \mu_m k_{m} A_{cell}} \cdot (0 \in \{k_\ell \})$$

(3.24)

which accounts for the contribution from $k_\ell = 0$; or we can adopt (3.19) and (3.21) to obtain

$$\langle T_i, \bar{G}^{HJ}, B_j \rangle = \langle T_{Zi}, \partial_{z} g_{s}^{TM} \hat{z}, B_j \rangle$$

$$+ \langle T_{Zi}, (\nabla \times \hat{z}) g_{s}^{TM}, B_{Zj} \rangle$$

$$+ \langle T_{Zi}, (\nabla' \times \hat{z}) \left( k_{mn} g_{s}^{TE} - \partial_{zz'} g_{s}^{TM} \right), B_{Zj} \rangle$$

$$- \langle \nabla \cdot T_i, (\nabla' \times \hat{z}) \left( \partial_{z} g_{s}^{TE} + \partial_{zz'} g_{s}^{TM} \right), B_{Zj} \rangle$$

(3.25)

In above, $T_i$ and $B_j$ are testing and basis functions, which are RWG basis functions, and $T_{Zi} = T_i \cdot \hat{z}$, $B_{Zj} = B_j \cdot \hat{z}$, and $T_{Si} = T_i - T_{Zi}$, $B_{Sj} = B_j - B_{Zj}$, and

$$g_{s}^{TE/TM} = \hat{S}(k_{s}^{2} F_{TE/TM})$$

(3.26)

Comparing (3.23) and (3.25), we observe that in the former the Green’s functions required to be calculated have better convergence rate, while the latter handles the singularity intrinsically. In the following, we just consider (3.23).
As a short summary, to get the moment matrix, we need to calculate

\[ g^{TE}, (\partial_z, \partial_{\nu'}, \partial_{\nu'}^z) g^{TE}, g^{TE}_S, g^{TM}, (\partial_{z'}, \partial_{\nu}, \partial_{\nu'} z) g^{TM} \]  \hspace{1cm} (3.27)

for electric current sources, where \( \nu \in \{x, y, z\} \). Among them, those involving \( g^{TE}_S \), \( \partial_{zz'} g^{TE/TM} \) have the poorest convergence since the general term of the series decays as \( k^{-1}_s \). For magnetic sources, the duality theorem can be used to derive the matrix-friendly formulation, which is omitted here.

### 3.3 Computation Scheme with High Order Convergence

In the following, we will use \( g^{TE/TM}_S \) for \( z \geq z' \) as an example to develop the novel fast and efficient algorithm for the evaluation of the doubly periodic Green’s functions. The procedure includes a delicate extraction of high order asymptotic terms, and the application of the Kummer’s transformation. The derivation applies to all the other Green’s functions in (3.27). Without confusion, we suppress the superscript and simply denote it as \( g_S \).

We start with casting the propagation factor into

\[ F_+(k_s; z, z') = \sum_{p=1}^{4} F_{mn}^p \tilde{Q}_{mnp} \]  \hspace{1cm} (3.28)

where for \( m > n \)

\[ F_{mn}^1 = \tilde{S}_{mn}^a e^{ik_{mz}(z+d_n)} e^{-ik_{mz}(z'+d_m-1)} \]
\[ F_{mn}^2 = R_{m,m+1} \tilde{S}_{mn}^a e^{ik_{mz}(z+d_n)} e^{ik_{mz}(z'+2d_m-d_m-1)} \]
\[ F_{mn}^3 = R_{n,n-1} \tilde{S}_{mn}^a e^{-ik_{mz}(z+2d_n-1-d_n)} e^{-ik_{mz}(z'+d_m-1)} \]
\[ F_{mn}^4 = R_{m,m+1} R_{n,n-1} \tilde{S}_{mn}^a e^{-ik_{mz}(z+2d_n-1-d_n)} e^{ik_{mz}(z'+2d_m-d_m-1)} \]  \hspace{1cm} (3.29)

with \( \tilde{S}_{mn}^a = T_{m,m-1} \prod_{i=n+1}^{m-1} e_i T_{i,i-1} \), and for \( m = n \)

\[ F_{mn}^1 = e^{ik_{mz}|z-z'|} \]
\[ F_{mn}^2 = R_{m,m+1} e^{ik_{mz}|z+z'+2d_m|} \]
\[ F_{mn}^3 = R_{m,m-1} e^{ik_{mz}|z+2d_m-1+z'|} \]
\[ F_{mn}^4 = R_{m,m-1} R_{m,m+1} e^{ik_{mz}|z-z'+2d_m-1-2d_n|} \]  \hspace{1cm} (3.30)
The $\tilde{Q}$ terms are easily identified for $m \geq n$ to be

$$
\tilde{Q}_{mn1} = \tilde{Q}_m^M \tilde{Q}_{mn}^S \\
\tilde{Q}_{mn2} = \tilde{Q}_{m,m+1}^R \tilde{Q}_m^M \tilde{Q}_{mn}^S \\
\tilde{Q}_{mn3} = \tilde{Q}_{n,n-1}^R \tilde{Q}_m^M \tilde{Q}_{mn}^S \\
\tilde{Q}_{mn4} = \tilde{Q}_{m,m+1}^R \tilde{Q}_{n,n-1}^R \tilde{Q}_m^M \tilde{Q}_{mn}^S
$$

(3.31)

where

$$
\tilde{Q}_{i,i \pm 1}^R = \tilde{R}_{i,i \pm 1} R_{i,i \pm 1}^{-1} \\
\tilde{Q}_m^M = \tilde{M}_m \\
\tilde{Q}_{mn}^S = \prod_{i=n+1}^{m} (1 - Q_{i,i-1})^{-1} \\
\tilde{Q}_{mn}^S = 1
$$

(3.32)

with $Q_{i+1,i} = R_{i,i+1} \tilde{R}_{i,i-1} e^{2ik_{x}z(d_{i}-d_{i-1})}$. $\tilde{Q}_{mn}^r$ can be regarded as an infinite geometric series with the asymptotic form $\sum_{i=0}^{\infty} (ae^{-k_{x}b})^i (a$ and $b$ are constants, and $b$ is related to the thickness of the layers) for $k_{s} \to \infty$. We can approximate $\tilde{Q}_{mn}^r$ with a few real exponentials to high accuracy when $k_{s}$ is large enough (e.g. $k_{s} > 1.2k_{max}$ [33], where $k_{max}$ is the maximum wave number for all layers), because we have spared no effort to put as many terms to $F_{mn}^p$ as possible, which makes $\tilde{Q}_{mn}^r$ much smoother. In detail, we have

$$
\tilde{Q}_{mn}^r \approx \sum_{r=1}^{N_r} C_{mnpr} \tilde{E}_{mnpr}^r
$$

(3.33)

where $\tilde{E}_{mnpr}^r = e^{-k_{x}t_{mnpr}}, C_{mnpr}$ and $t_{mnpr}$ can be got via the generalized pencil of function (GPOF) method [69]. The number of exponentials $N_r$ is very small because $\tilde{Q}_{mn}^r$ is very smooth, and usually $N_r = 2$ to 5 can make the relative error between the approximate and exact values decrease very quickly to $10^{-8}$ with the increase of $k_{s}$. It should be emphasized that we just approximate $\tilde{Q}_{mn}^r$ once, and the result can be used for all combinations of source and observation points because $\tilde{Q}_{mn}^r$ is independent of $z$ or $z'$. Also, for a given frequency band, since $\tilde{Q}_{mn}^r$ has the same asymptotic behavior when $k_{s} \to \infty$, we can approximate it only at the central frequency using GPOF, and the exponentials $\tilde{E}_{mnpr}^r$ thus obtained for this frequency are used as a basis to fit other frequencies using least square method. Namely, for other frequencies, we just need to find the coefficients $C_{mnpr}$ via least square method. In so doing, lots of efforts are saved and robustness is improved if we want to analyze a wide frequency band.
Using Taylor series expansion, one can express $F_{mn}^p$ as

$$F_{mn}^p = \tilde{F}_{mn}^p E_{mn}^p \quad (3.34)$$

where $E_{mn}^p = e^{-k_s t_{mn}}$, with

$$t_{mn1} = |z - z'|$$
$$t_{mn2} = |z + z' + 2d_m|$$
$$t_{mn3} = |z + z' + 2d_{n-1}|$$
$$t_{mn4} = |z - z' - 2d_m + 2d_{n-1}| \quad (3.35)$$

and

$$\tilde{F}_{mn}^1 = \tilde{S}_{mn}^a \tau_n (|z + d_n|) \tau_m (|z' + d_{m-1}|)$$
$$\tilde{F}_{mn}^2 = R_{m,m+1} \tilde{S}_{mn}^a \tau_n (|z + d_n|) \tau_m (|z' + 2d_m - d_{m-1}|)$$
$$\tilde{F}_{mn}^3 = R_{n,n-1} \tilde{S}_{mn}^a \tau_n (|z + 2d_{n-1} - d_n|) \tau_m (|z' + d_{m-1}|)$$
$$\tilde{F}_{mn}^4 = R_{m,m+1} R_{n,n-1} \tilde{S}_{mn}^a \tau_n (|z + 2d_{n-1} - d_n|) \tau_m (|z' + 2d_m - d_{m-1}|) \quad (3.36)$$

for $m > n$, and

$$\tilde{F}_{mn}^1 = \tau_m (|z - z'|)$$
$$\tilde{F}_{mn}^2 = R_{m,m+1} \tau_m (|z + z' + 2d_m|)$$
$$\tilde{F}_{mn}^3 = R_{m,m-1} \tau_m (|z + z' + 2d_{m-1}|)$$
$$\tilde{F}_{mn}^4 = R_{m,m-1} R_{m,m+1} \tau_m (|z - z' + 2d_{m-1} - 2d_m|) \quad (3.37)$$

for $m = n$, where

$$\tilde{S}_{mn}^a = \prod_{i=n+1}^{m-1} T_{i,i-1} T_i (d_i - d_{i-1}) T_{m,m-1} \quad (3.38)$$

and $\tau_m(z) (z \geq 0)$ is defined by the following

$$e^{ik_m z} = e^{-k_s z} \left[ 1 + \frac{z k_m^2}{2 k_s^2} + \frac{z^2 k_m^4}{8 k_s^4} + O (k_s^{-3}) \right]$$
$$= e^{-k_s z} \tau_m(z) \quad (3.39)$$

where Taylor expansions of both square root function and exponential function are applied. The Taylor series representation of the Fresnel reflection and transmission coefficients are

$$R_{ij}^\sigma = R_{ij}^{\sigma 0} + \frac{R_{ij}^{\sigma 2}}{k_s^2} + O (k_s^{-4}) \quad , \quad T_{ij}^\sigma = 1 + R_{ij}^\sigma \quad (3.40)$$
where
\[ R_{ij}^{(0)} = \frac{p_j - p_i}{p_i + p_j}, \quad R_{ij}^{(2)} = \frac{p_i p_j (k_j^2 - k_i^2)}{(p_i + p_j)^2} \] (3.41)

Then we have
\[ F_+(k_s; z, z') \approx \sum_{p=1}^{4} \sum_{r=1}^{N_r} C_{mnpr} \tilde{F}_p^{mn} \tilde{E}_r^{mnpr} \] (3.42)

where \( \tilde{E}_r^{mnpr} = e^{-k_s(t_{mnpr} + t_{mnpr})} \). Substituting (3.42) into (3.4), we yield
\[ g_S \approx i 2 A_{cell} \sum_{p=1}^{N_r} \sum_{r=1}^{N_r} C_{mnpr} \left[ \sum_{u=1}^{N_u} \xi_{mu} A_{mn}^{pu} k_s^{1-u} \tilde{E}_r^{mnpr} e^{i k_s (r_s - r'_s)} \right] \] (3.43)

The Taylor series for \( k_{mz}^{-1} \) is
\[ k_{mz}^{-1} = -\frac{i}{k_s} \left[ 1 + \frac{k_m^2}{2k_s^2} + O(k_s^{-4}) \right] = -\frac{i}{k_s} \xi_m \] (3.44)

which leads to
\[ g_S \approx \frac{1}{2A_{cell}} \sum_{p=1}^{4} \sum_{r=1}^{N_r} C_{mnpr} \left[ \sum_{u=1}^{N_u} \xi_{mu} \tilde{F}_p^{mn} \tilde{E}_r^{mnpr} e^{i k_s (r_s - r'_s)} \right] \] (3.45)

Keeping the first \( N_u (\leq 3) \) terms for \( \xi_{mu} \tilde{F}_p^{mn} \), namely,
\[ \xi_{mu} \tilde{F}_p^{mn} \approx \sum_{u=1}^{N_u} A_{mn}^{pu} k_s^{1-u} \] (3.46)

where the coefficients \( A_{mn}^{pu} \) can be easily specified, we further write
\[ g_S \approx \frac{1}{2A_{cell}} \sum_{p=1}^{4} \sum_{r=1}^{N_r} \sum_{u=1}^{N_u} C_{mnpr} A_{mn}^{pu} \left[ \sum_{u=1}^{N_u} k_s^{-u} \tilde{E}_r^{mnpr} e^{i k_s (r_s - r'_s)} \right] \] (3.47)

By invoking the Kummer’s transformation, we have
\[ g_S = (g_S - \tilde{g}_S) + \tilde{g}_S \] (3.48)

where \( \tilde{g}_S \) is the asymptotic expression in (3.45). The general term for \( g_S - \tilde{g}_S \) decays as \( k_s^{-N_u-1} \) when \( k_s \) increases, indicating that the series would converge very fast if \( N_u = 3 \); \( \tilde{g}_S \) can be efficiently evaluated using novel fast convergent series derived from Ewald transformation. We stop at \( N_u = 3 \) because we only have the fast convergent series for these cases; also, we are satisfied with the convergence rate offered by it. It should be pointed out that the inner-most double infinite series in (3.45) needs to be calculated only
once and can then be used for all frequencies if \( k_0 \) is fixed, which is the case for normal incidence (\( k_0 = 0 \)) in scattering problem, and for the calculation of Brillouin diagram in eigenproblem. Therefore, fast frequency sweep is allowed in these circumstances. The proposed method is able to deliver higher accuracy and higher order convergence than that in [33], where the “high order asymptotic extraction” is only applied to the asymptotic series, but the asymptotic series itself is not a high order asymptotic expression for the original periodic Green’s function.

### 3.4 Derivation of Fast Convergent Series

#### 3.4.1 General Considerations

From (3.27) and (3.47), we can see that the asymptotic series are of the form

\[
S_{\alpha\beta\gamma} = \sum_I \frac{k_I^\alpha k_y^\beta}{k_s^\gamma} e^{-k_s z_I} e^{i k_s \cdot r_s} \tag{3.49}
\]

where \((\alpha, \beta) \in \{(0,0), (0,1), (1,0)\}\), \(\gamma \in \{1,2,3\}\), and the transverse wave vector \(k_s \equiv k_0 + i_1 b_1 + i_2 b_2\) is defined the same as before, which can be equivalently expressed as \(k_s \equiv k_{s1} \hat{x} + k_{s2} \hat{y}\). \(\alpha = 1 (\beta = 1)\) is found for components of the dyadic Green’s function which are obtained by taking \(x (y)\) derivative of \(g^{TE/TM}\), and a larger \(\gamma\) results in for higher order terms in the Taylor expansion. Here we assume \(r_s\) and \(z\) are merely used as parameters rather than actual coordinates without confusion. But when \(0 \in \{k_{s1}\}\) (e.g. normal incidence), \(S_{\alpha\beta\gamma}\) blows up, making it inappropriate to calculate the Green’s function. However, considering the fact that we just need its asymptotic behavior instead of its absolute final sum, the difficulty is eradicated by replacing it with

\[
\tilde{S}_{\alpha\beta\gamma} = \sum_{i=1}^{M} w_i S^{i}_{\alpha\beta\gamma}, \quad S^{i}_{\alpha\beta\gamma} = \sum_I \frac{k_I^\alpha k_y^\beta}{k_s^\gamma} e^{-k_s z_I} e^{i k_s \cdot r_s} \tag{3.50}
\]

in the asymptotic expression of the Green’s function when \(k_{s1} = 0\) is possible, where \(k_{s1} = \sqrt{k_{s1}^2 + \kappa_i^2}\), \(i = 1, \cdots, M \in \mathbb{N}\). The parameters \(\kappa_i (> 0)\), \(M\) and the weights \(w_i\) are determined such that the general term of the series \(|S_{\alpha\beta\gamma} - \tilde{S}_{\alpha\beta\gamma}|\) behaves like \(e^{-k_s z} O(k_s^{-\theta})\) (\(\theta\) is an integer large enough) when \(k_s \to \infty\), plus the computational cost for \(S_{\alpha\beta\gamma}\) is optimally small. As for the given ranges of \(\alpha, \beta\) and \(\gamma\), the following holds

\[
X_{\alpha\beta\gamma} = (-i)^{\alpha + \beta} (-1)^{1-\gamma} \partial_x^\alpha \partial_y^\beta \partial_z^{\gamma-1} X_{001} \tag{3.51}
\]
where $X \in \{S, \tilde{S}\}$, $\partial_x^\alpha$ and $\partial_y^\beta$ mean differentiation of order with respect to $x$ and $y$ respectively, and $i_z^{-1}$ stands for integration for $\gamma - 1$ times from $\infty$ to $z$. Then we just need to determine $M$, $\kappa_i$ and $w_i$ for $\alpha = \beta = 0, \gamma = 1$.

In detail, let

$$\Gamma_{001} = \sum_i \Gamma_{001i}$$

where

$$\Gamma_{001i} = \frac{e^{-k_s z}}{k_s I} - \sum_{i=1}^M w_i e^{-\sqrt{k_s^2 + \kappa_i^2 z}}$$

$$= \frac{e^{-k_s z}}{k_s I} \left\{ 1 - \sum_{i=1}^M \sum_{j=1}^M w_i \phi_j^{i,j-1} + O(k_s^{-M}) \right\}$$

with the understanding that the term blowing up shall be removed, and the coefficients $\phi_j^{i,j}$ can be easily sought by Taylor expansion. When $z = 0$, the coefficients have closed form solution \[33\]

$$w_i = \begin{cases} 1, & i = M = 1 \\ \prod_{j=1, j \neq i}^M \kappa_j^2 / (\kappa_j^2 - \kappa_i^2), & i = 1, \ldots, M, \; M > 1 \end{cases}$$

that makes $\Gamma_{001} \sim e^{-k_s z} O(k_s^{-2M-1})$ when $k_s \to \infty$. When $z \neq 0$, $w_i$ can be sought by forcing the coefficients for $k_s^{1-j} (j = 1, \ldots, M)$ to vanish, which leads to the linear system

$$\sum_{i=1}^M w_i \phi_j^{i,j} = \delta_{j1}.$$  

These weights would give $\Gamma_{001}$ the asymptotic behavior $\sim e^{-k_s z} O(k_s^{-M-1})$. In view of that the general term for $g_S - \tilde{g}_S$ decays as $e^{-k_s z} O(k_s^{-4})$ at best ($N_u = 3$), the value of $M$ is at most 2 for $z = 0$, and 3 for $z \neq 0$, although a smaller $M$ may also perform quite well if the absolute value of $\Gamma_{001}$ decays fast enough. Fortunately, for $z \neq 0$, $w_i$ happens to have the same closed form solution as (3.54) for $M = 1, 2, 3$.

If $\gamma = 2$, $M = 1$ for $z = 0$, and $M \leq 2$ for $z \neq 0$. If $\gamma = 3$, $M = 1$ for both cases. The parameters $\kappa_i$ has to be properly chosen to ensure both convergence and accuracy, whose treatment is delayed to the next two parts because the choice depends on the way we derive the fast convergent series.
### 3.4.2 Fast Convergent Series from Ewald Transformation

The Ewald transformation (Appendix C) is a very powerful analytic tool for evaluating the doubly periodic Green’s function. Though it has been very successful in treating the periodic Green’s function in free space, the use of it for layered medium is not that satisfactory, mostly due to the lack of a high order asymptotic extraction in the literature. Now that we have managed to find the high order asymptotic terms, we are ready to fulfill the potential of this transformation.

From Ewald transformation [70, 71], we have

\[ S_{001}^{i} = 2A_{\text{cel}l} (\Psi_{1} + \Psi_{2}) \tag{3.56} \]

where

\[ \Psi_{1} = \frac{1}{4A_{\text{cel}l}} \sum_{I} \Psi_{1} e^{i{k_{s1}} r_{s}} \tag{3.57} \]

\[ \Psi_{1} = \sum_{\pm} e^{\pm {k_{s1}} z} \text{Erfc} \left( \frac{k_{s1} z}{2E} \pm Ez \right) \tag{3.58} \]

and

\[ \Psi_{2} = \frac{1}{8\pi} \sum_{L} e^{i{k_{0} - r_{L}}} \sum_{\pm} \frac{e^{\pm {k_{s1}} R_{L}}}{R_{L}} \text{Erfc} \left( R_{L} E \pm \frac{\kappa_{i}}{2E} \right) \tag{3.59} \]

In above expressions, we have \( r = (x, y, z) \), \( R_{L} = |r - r_{L}| = \sqrt{r_{L}^{2} + z^{2}} \), \( r_{L} = l_{1}a_{1} + l_{2}a_{2} = (x_{L}, y_{L}) \), \( L = (l_{1}, l_{2}) \in \mathbb{Z} \times \mathbb{Z} \), and the splitting parameter \( E = \sqrt{\pi/A_{\text{cel}l}} \). It has to be mentioned that we have used the Ewald transformation with the wave number being purely imaginary \((i{\kappa_{i}})\), in which case the arguments of the complimentary error function \((\text{Erfc})\) are always real, and the trouble from \(\text{Erfc}\) with complex arguments is avoided. Then we obtain

\[ S_{001}^{i} = 2(-i)^{\alpha+\beta}(-1)^{1-\gamma}A_{\text{cel}l}\partial_{x}^{\alpha}\partial_{y}^{\beta}\partial_{z}^{\gamma-1} (\Psi_{1} + \Psi_{2}) \tag{3.60} \]

It can be shown that

\[ i_{2}^{1}\Psi_{1} = \frac{1}{4A_{\text{cel}l}} \sum_{I} i_{2}^{1}\tilde{\Psi}_{1} e^{i{k_{s1}} r_{s}} \tag{3.61} \]

where

\[ i_{2}^{1}\tilde{\Psi}_{1} = \frac{1}{k_{s1}^{2}} \left[ -2e^{-\frac{i z^{2}}{4E^{2}}} \text{Erfc} (Ez) + \sum_{\pm} e^{\pm {k_{s1}} z} \text{Erfc} \left( \frac{k_{s1} z}{2E} \pm Ez \right) \right] \tag{3.62} \]

and

\[ i_{2}^{2}\Psi_{1} = \frac{1}{4A_{\text{cel}l}} \sum_{I} i_{2}^{2}\tilde{\Psi}_{1} e^{i{k_{s1}} r_{s}} \tag{3.63} \]
where
\[ i_z^2 \tilde{\Psi}_1 = \frac{2}{k_{sl}^2} e^{-\frac{i^2 \Delta}{4E}} \left[ e^{-E^2 z^2} - z \cdot \text{Erfc} (E z) \right] + \frac{1}{k_{sl}^3} \sum_{\pm} e^{\pm k_{sl} z} \text{Erfc} \left( \frac{k_{sl} I}{2E} \pm E z \right) \] (3.64)

To integrate \( \Psi_2 \), we use an alternative expression \[ \Psi_2 = \frac{1}{2\pi} \sum_L e^{i k_0 \cdot r_L} \int_E^\infty \int_E^\infty e^{-\rho_L^2 \xi^2 - \frac{\kappa_i^2}{4\pi}} d\xi d\rho \] (3.65)

Then we have, after exchanging the order of integration,
\[ i_z^1 \Psi_2 = \frac{1}{2\pi} \sum_L e^{i k_0 \cdot r_L} \left[ 2e^{-\kappa_i R_L} - \sum_{\pm} e^{\pm k_{sl} R_L} \text{Erfc} \left( \frac{K_i}{2E} \pm R_L E \right) \right] + z i_z^1 \Psi_2 \] (3.66)

The last infinite integral has a smooth integrand and converges extremely fast, and truncation to
\[ \xi_{\text{max}} = \min \left\{ E + \frac{10}{z}, \max \left\{ E, \sqrt{\frac{\kappa_i}{2R_L}} \right\} + \frac{10}{R_L} \right\} \] (3.67)

would be enough to yield machine accuracy with Gaussian quadrature. One more operation of integration for \( i_z^1 \Psi_2 \), we acquire
\[ i_z^2 \Psi_2 = \frac{1}{8\pi \kappa_i} \sum_L e^{i k_0 \cdot r_L} \left[ 2e^{-\kappa_i R_L} - \sum_{\pm} e^{\pm k_{sl} R_L} \text{Erfc} \left( \frac{K_i}{2E} \pm R_L E \right) \right] + z i_z^1 \Psi_2 \] (3.68)

Now let’s look at the derivatives with respect to \( x \) and \( y \). It is easy to see that
\[ \partial_{\zeta} \tilde{\Psi}_1 = \frac{i}{4A} \sum_I k_{\zeta} I I \Psi_1 e^{i k_{\zeta} \cdot r_s} \] (3.69)

where \( I \in \{ 1, i_z^1, i_z^2 \}, \zeta \in \{ x, y \} \). For the derivatives of \( \Psi_2 \), we have
\[ \partial_{\zeta} \Psi_2 = \frac{1}{8\pi} \sum_L e^{i k_0 \cdot r_L} \frac{\zeta - \zeta_L}{R_L^2} \left[ -\frac{4E}{\sqrt{\pi}} e^{-\left( \frac{\zeta}{R_L} \right)^2 - (R_L E)^2} \right. \]
\[ + \sum_{\pm} \left( \pm k - \frac{1}{R_L} \right) e^{\pm k_{sl} R_L} \text{Erfc} \left( R_L E \pm \frac{K_i}{2E} \right) \] (3.70)

Furthermore, we obtain
\[ \partial_{\zeta} i_z^1 \Psi_2 = \frac{1}{2\pi} \sum_L e^{i k_0 \cdot r_L} (\zeta - \zeta_L) \int_E^\infty \xi \text{Erfc} (\xi z) e^{-\rho_L^2 \xi^2 - \frac{\kappa_i^2}{4\pi}} d\xi \] (3.71)
and
\[ \partial_{\xi}^2 z \Psi_2 = z \partial_{\xi}^1 z \Psi_2 + \frac{1}{8\pi} \sum_{L} e^{i k_0 r_L} \frac{\zeta - \zeta_L}{R_L} \times \left\{ -2e^{-\kappa_i r_L} + \sum_{s=1}^{2} (-1)^{s+1} e^{(-1)^s \kappa_i r_L} \text{Erfc} \left[ \frac{K_i}{2E} + (-1)^s R_L E \right] \right\} \tag{3.72} \]

It is beneficial if we let \( \kappa_i = 0 \) since this will give the expression for \( S_{\alpha\beta\gamma} \), which will be of great use when \( 0 \notin \{k_{si}\} \), as is for most cases. We find that integrals in \( \partial_{\xi} \hat{I} \Psi_2 \) are integrable:
\[ \partial_{\xi}^1 z \Psi_2 = \sum_{L} e^{i k_0 r_L} \frac{\zeta - \zeta_L}{4\pi \rho_L^2} \text{Erfc} \left( E z \right) - \frac{z}{R_L} \text{Erfc} \left( R_L E \right) \tag{3.73} \]
\[ \partial_{\xi}^2 z \Psi_2 = z \partial_{\xi}^1 z \psi_2 - \sum_{L} e^{i k_0 r_L} \frac{\zeta - \zeta_L}{4\pi R_L} \text{Erfc} \left( R_L E \right) \tag{3.74} \]

The limit exists for (3.73) when \( \rho_L \to 0 \). In the special case of \( z = 0 \) and \( \rho_L \neq 0 \),
\[ \partial_{\xi}^1 z \psi_2 = -\frac{1}{8\pi} \sum_{L} e^{i k_0 r_L} E_1 \left( (\rho_L E)^2 \right) \tag{3.75} \]
where
\[ E_1(z) = \int_{z}^{\infty} \frac{t e^{-t} dt}{t} \tag{3.76} \]
is the exponential integral. Hence \( \partial_{\xi}^1 z \psi_2, \partial_{\xi}^2 z \psi_2 \) are also free from the need to perform integrals by us. The series derived above have Gaussian convergence.

The parameters \( \kappa_i \), just like the splitting parameter \( E \), has to be properly chosen to guarantee convergence and avoid cancellation error or overflow. When too large, its presence as an exponent can lead to cancellation error and overflow. Smaller \( \kappa_i \) would make \( \Gamma_{001} \) decay faster. But when they are too small, it will also lead to cancellation error because in the worst case we have \( \kappa_i^3 \) in the denominator. We suggest the following:
\[ \kappa_i = 0.01(9 + i) \times \min \{ \{k_{si}\} \setminus 0 \}, i = 1, \cdots, M \tag{3.77} \]

It is in the order of one tenth of the minimum value of \( k_{si} \) excluding 0, and numerical results show that it will neither be too small nor too large, ensuring both convergence and accuracy. It should be noted that the series \( S_{\alpha\beta\gamma} \) with \( \gamma = 2, 3 \) are used, to our knowledge, for the first time to accelerate the convergence for evaluating doubly periodic Green’s function in layered medium, which allows us to achieve high order convergence.
3.4.3 Fast Convergent Series from Poisson Transformation

For comparative studies, we mention that an alternative way to derive fast convergent series is to use the Poisson transformation [37], which will lead to exponentially convergent series. The difference is that we can only use $\tilde{S}_{\alpha\beta\gamma}$ as the asymptotic series because in this method, the fast decay rate of the series stems from the proper choice of $\kappa_i$, which is less critical in Ewald transformation since the decay rate is mostly dominated by the splitting parameter $E$. The derivation procedure is similar with that using Ewald transformation, and we just give the final result here:

$$ S_{\alpha\beta\gamma}^i = 2(-i)^{\alpha+\beta}(-1)^{1-\gamma}A_{cell}\partial_x^\alpha\partial_y^\beta\xi_z^{-1}\Psi $$

(3.78)

where

$$ \Psi = \sum_L e^{-\kappa_i R_L} e^{i k_0 \cdot r_L} $$

(3.79)

We also have

$$ i_z^1 \Psi = -\frac{1}{4\pi} \sum_L e^{i k_0 \cdot r_L} \int_0^\infty \text{Erfc} \left( \frac{\xi z}{\xi} \right) e^{-\xi^2 \xi^2 - \kappa_i^2} d\xi $$

(3.80)

where the integral can be evaluated numerically. When $z = 0$, by referring to the identity in [72], we obtain

$$ i_z^1 \Psi = -\frac{1}{4\pi} \sum_L K_0(\kappa_i \rho_L) e^{i k_0 \cdot r_L} $$

(3.81)

where $K_0$ is the modified Bessel function of order 0 of the second kind. An equivalent equation of $i_z^1 \Psi$ and its derivatives with respect to $x$ and $y$ when $z = 0$, also appear in [12, 32]. We further write

$$ i_z^2 \Psi = \frac{1}{4\pi} \sum_L \frac{e^{-\kappa_i r_L}}{\kappa_i} e^{i k_0 \cdot r_L} + z i_z^1 \Psi $$

(3.82)

The derivatives of $i \Psi$ can be trivially derived, which we omit here.

The parameters $\kappa_i$ have to be chosen so that convergence is achieved and cancellation error is avoided, and for a general lattice, whether rectangular or skew, it is suggested [73]

$$ \kappa_i = |\text{Im}(k_0)| + 1.5 M (0.9 + 0.1 i)|/|a_1 + a_2|, i = 1, \cdots , M $$

(3.83)

It should be mentioned that the Poisson method is more sensitive to the choice of $\kappa_i$ since from (3.79) we see that the fast convergence rate is highly dependent on $\kappa_i$, while in Ewald method, this dependence is pretty weak.
3.5 Numerical Results

We first conduct a comparison of the fast convergent series derived from Ewald and Poisson transformations. Fig. 3.2 shows the convergence of the two approaches in the calculation of $S_{002}$. $k_0 = (0, 0)$ indicates $k_s I$ could equal 0, and we can only calculate $S_{002}$ by applying Kummer’s transformation first, namely $S_{002} = (S_{002} - \tilde{S}_{002}) + \tilde{S}_{002}$, then $(S_{002} - \tilde{S}_{002})$ is computed by direct summation, and $\tilde{S}_{002}$ by Ewald or Poisson transformation. We call these two approaches the Kummer-Ewald transformation (KET) and Kummer-Poisson transformation (KPT), respectively.

When $z = 0$ in Fig. 3.2a, with closed form for the general term, the fast convergent series derived from Poisson transformation would see its best performance, but Ewald transformation would show its worst since it is involved with integration and also has to be combined with Kummer’s transformation, which increases its computational burden. The observation can be made from Fig. 3.2a that direct summation converges very slowly for this case, and the KET and KPT show much better performance. As for the CPU time, it is found that, for moderate accuracy (4-6 digits), the KET takes slightly longer (a few percent), but for high accuracy (10-12 digits), the KET takes less time (All calculations in this paper are performed on a Dell Inspiron N4110 laptop with Intel i3-2310M CPU and 4GB RAM memory).

In Fig. 3.2b, $z \neq 0$, so integrals are involved in Ewald method; $k_s I$ could equal 0, thus KET has to be used for the approach involving Ewald transformation. It is found that for the same number of terms, both methods take roughly the same time, but the KET yields much more accurate result than KPT for the same $M$. Fig. 3.3 depicts the case when $z \neq 0$ and $k_s I \neq 0$, which is most common. In this case, the fast convergent series derived from Ewald transformation can be used directly without resorting to Kummer’s transformation. Fig. 3.3 clearly informs us of the advantage of Ewald method in terms of convergence.

We also checked the CPU times, and found that for the same number of terms, the Ewald method yields much more accurate result yet consumes much shorter time. Further numerical simulations also convince us that, for moderate accuracy, the KPT is comparable with Ewald method only in the case when $z = 0$ as well as $0 \in \{k_s I\}$, and in other cases the Ewald method is superior. For highly accurate evaluation of $S_{\alpha\beta\gamma}$, the Ewald method outweighs the KPT significantly, especially when $k_s \neq 0$ and $\alpha = 1$ or $\beta = 1$ because in these cases the Ewald method is free from integration and
<table>
<thead>
<tr>
<th>NO. of Terms</th>
<th>Relative Error</th>
<th>Direct</th>
<th>KET (M=1)</th>
<th>KET (M=3)</th>
<th>KET (M=5)</th>
<th>KPT (M=1)</th>
<th>KPT (M=3)</th>
<th>KPT (M=5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$10^{-14}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>$10^{-12}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$10^{-10}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>$10^{-8}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>20</td>
<td>$10^{-6}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>50</td>
<td>$10^{-4}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>100</td>
<td>$10^{-2}$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>200</td>
<td>$10^0$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>500</td>
<td>$10^2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1000</td>
<td>$10^4$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2000</td>
<td>$10^6$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 3.2: Convergence of $S_{002}$ evaluated using KET and KPT. The parameters are $r_1 = (0.01, 0.01)$, $a_1 = a_2 = 1$ ($a_i = |a_i|$), $\varphi = \frac{\pi}{2}$. (a) $k_0 = (0, 0), z = 0$; (b) $k_0 = (0, 0), z = 0.001$. 
Figure 3.3: Convergence of $S_{002}$ evaluated using Ewald transform and KPT. The parameters are the same as Fig. 3.2 except $k_0 = (0.5, 0.5)$, $z = 0.001$.

there is not need to invoke the Kummer transformation. For example, when $k_0 = (0.5, 0.5)$, $r_s = (0.01, 0.01)$, $z = 0$, $a_1 = a_2 = 1$, $\varphi = \pi/2$, evaluation of $S_{102}$ takes the Ewald method averagely 0.012s and 0.028s to get 6 and 12 digits respectively, while the time for same accuracy for the KPT with optimal $M$ is 0.035s and 0.63s, and to compute $S_{001}$ with 6 and 12 digits, the CPU times for Ewald method are 0.0023s and 0.0052s, while those for the KPT are 0.0080s and 0.16s. In above simulations, we limit $M$ to 5 due to the fact that no improvement is observed for larger value of $M$ with both convergence and CPU time in mind. In addition, as we have previously argued in Sec. 3.4.1, there is no necessity in using $M$ larger than 3 for the evaluation of the periodic Green’s function.

Fig. 3.4 shows the convergence in the evaluation of the scalar periodic Green’s function $g_{5TE}^T$ for a 5-layer medium. The periods in both directions are chosen as $a_1 = a_2 = \lambda/2$ based on practical considerations. For example, photonic crystal slabs have a unit size in the order of wavelength, while the unit size of metamaterial is much smaller than the wavelength. Since the smaller the periods, the faster the convergence for the periodic Green’s functions, we won’t show results for structures with electrically small unit cells. The reference values for Fig. 3.4a is $-10.254346 - i1.99661543$, and for Fig. 3.4b $-10.253512 - i1.9964767$, both of which are calculated using time consuming direct
<table>
<thead>
<tr>
<th>NO. of Terms</th>
<th>Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct</td>
<td>1st Lead</td>
</tr>
<tr>
<td></td>
<td>2nd Lead</td>
</tr>
<tr>
<td></td>
<td>3rd Lead</td>
</tr>
</tbody>
</table>

Figure 3.4: Convergence for $g_{SE}^{TE}$ for an orthogonal periodic structure in a 5-layer medium at 3 GHz with source in the central plane of the middle layer. The thicknesses of the layers are $(\infty, 0.1, 0.1, 0.1, \infty)\lambda$, $\epsilon_r = (1, 2, 10, 2, 1)$, $\mu_r = 1$ for all layers, $a_1 = a_2 = \lambda/2$, $\varphi = \pi/2$, $r'_s = (0, 0)$, $r_s = (\lambda/10, \lambda/10)$, $k_0 = (0.2, 0.1)\lambda^{-1}$. $z = z'$ in (a), and $z - z' = 10^{-3}\lambda$ in (b).
Table 3.1: CPU time (sec) for evaluating Green’s functions for orthogonal lattice with 6 significant digits. Parameters same as those in Fig. 3.4.

<table>
<thead>
<tr>
<th>PGF</th>
<th>Ewald</th>
<th>Poisson</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\partial_z g^{TM}$</td>
<td>1.81</td>
<td>14.3</td>
</tr>
<tr>
<td>$\partial_{z'} g^{TM}$</td>
<td>0.81</td>
<td>18.9</td>
</tr>
<tr>
<td>$\partial_z g^{TE}$</td>
<td>1.45</td>
<td>12.0</td>
</tr>
<tr>
<td>$g_S^{TE}$</td>
<td>1.43</td>
<td>13.2</td>
</tr>
</tbody>
</table>

Table 3.2: CPU time (sec) for evaluating Green’s functions at 100 frequencies uniformly sampled between 1 GHz and 5 GHz for orthogonal lattice with 6 significant digits. Parameters same as those for Tab. 3.1 except the frequency.

<table>
<thead>
<tr>
<th>PGF</th>
<th>$z = z'$</th>
<th>$z \neq z'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\partial_z g^{TM}$</td>
<td>2.55</td>
<td>2.48</td>
</tr>
<tr>
<td>$\partial_{z'} g^{TM}$</td>
<td>1.90</td>
<td>1.86</td>
</tr>
<tr>
<td>$\partial_z g^{TE}$</td>
<td>2.37</td>
<td>2.31</td>
</tr>
<tr>
<td>$g_S^{TE}$</td>
<td>2.47</td>
<td>2.48</td>
</tr>
</tbody>
</table>

As shown in Fig. 3.4, it will be very difficult to get an accurate result using direct summation since the convergence is so slow. We see improvement of convergence when the leading terms are extracted. The convergence for the case with first ($N_u = 1$) and second ($N_u = 2$) order leading term extraction almost overlap with each other, because the coefficients for the second leading term is very small when $|z - z'|$ is small. In Fig. 3.4, to achieve 6 digits of accuracy, around 10,000 terms are needed for 1st and 2nd leading term extraction, while only about 200-300 terms are required if the third asymptotic term is extracted ($N_u = 3$). Thus significant improvement of convergence is achieved if the 3rd leading term extraction is performed.

Table 3.1 gives a comparison of the CPU time for computing the Green’s functions with 6 digits of accuracy using the proposed method and the Kummer-Poisson transformation [33] for an orthogonal lattice. We use “Ewald” and “Poisson” to represent the two approaches, since they are related to the two transformations. The structure parameters and source and observation points are the same as those in Fig. 3.4. For $\partial_z g^{TE}$, $\partial_z g^{TM}$ and $g_S^{TE}$, the method using Ewald transformation is about 8 times faster than that exploiting Poisson transformation. For $\partial_{z'} g^{TM}$, the Ewald method performs
even better, more than 20 times faster. The advantages of Ewald method over Poisson method lies in that the fast convergent series from it is of Gaussian convergence. And in our implementation, we have also made the arguments of the Error functions involved real so that efficiency is improved.

In Table 3.2, the CPU times are shown for calculating the Green’s functions with 6 digits of accuracy for 100 frequencies uniformly sampled from 1 GHz to 5 GHz. We have fixed $k_0$ to be the value at 3 GHz. Due to the extraction of high order leading terms, the remaining series converge very fast, and we just need a few hundred terms to achieve the desired accuracy even for those Green’s functions decaying as $\sim k_s^{-1}$. Comparing Table 3.2 with Table 3.1, we can see that the overhead of CPU time for calculating 100 frequencies over that for a single frequency is very small.

3.6 Summary

The matrix friendly formulation for doubly periodic structure in layered medium is derived, and the singularity at $k_s = 0$ is analytically addressed in the formulation. A novel accurate and efficient approach has been proposed for computing the doubly periodic Green’s function for layered medium in the context of matrix-friendly formulation, which features the extraction of high order asymptotic expressions for the periodic Green’s functions, and the derivation of novel fast convergent series using Ewald transformations. The proposed method minimizes the uses of approximations and is hence robust. It delivers highly accurate results with fast and high order convergence, and also allows fast frequency sweep for calculating Brillouin diagram in eigenvalue problem and for normal incidence in scattering problem.
CHAPTER 4. HIGH ORDER NYSTRÖM METHOD FOR ELASTODYNAMIC SCATTERING

Elastodynamic scattering finds important applications in ultrasonic non-destructive evaluation, where the far field scattering amplitude of the flaw is a key parameter to look for in the Thompson ultrasonic measurement model [74]. Potentially it may also be used in seismology and dynamic soil-structure interaction. To solve elastodynamic scattering problems, the Nyström method is a relatively simple approach since it approximates the integral operator with quadrature and evaluates the field also at the quadrature nodes, which makes the far field interaction integration free [47]. But to fully realize the capacity of this approach, a high order Nyström method with curvilinear elements and high order interpolation is desired. This chapter presents a new implementation of the high order Nyström method for solving elastodynamic scattering accurately and efficiently [75, 76].

4.1 Boundary Integral Equations

In Chapter 1, the conventional boundary integral equation (CBIE) for elastic wave scattering has been introduced. For convenience, we replicate it here

\[
\frac{1}{2} u(r) - \int_S \left[ \bar{G}_u^u(r, r') \cdot t(r') - \bar{G}_u^u(r, r') \cdot u(r') \right] dS' = u_{inc}(r) \quad (4.1)
\]

\[
\frac{1}{2} u(r) + \int_S \left[ \bar{G}_u^u(r, r') \cdot t(r') - \bar{G}_u^u(r, r') \cdot u(r') \right] dS' = 0 \quad (4.2)
\]

where \( r \in S \), \( X_+ = u_{inc} \) (the incident displacement field), \( X_- = 0 \) in Fig. 1.1, and the 1/2 arises from explicitly extracting the contribution from the singular point in the surface integrals. Let the material parameters for the two regions be denoted as \( \rho_\pm, \lambda_\pm, \) and \( \mu_\pm \).

Adopting the dyadic convention, we cast the Green’s functions in the following
\[ \vec{G}^{\text{ut}} = \frac{C \hat{\mathbf{R}} \mathbf{R} + D \mathbf{I}}{4\pi \rho \omega^2 R^4} \]

\[ \vec{G}^{\text{uu}} = \frac{(\lambda \psi_c + 2\mu C) \hat{\mathbf{R}} \mathbf{n}' + \mu (\psi_s + 2C) \left( \mathbf{n}' \hat{\mathbf{R}} + \mathbf{n}' \cdot \hat{\mathbf{R}} \mathbf{I} \right) + 2\mu F \left( \mathbf{n}' \cdot \hat{\mathbf{R}} \right) \hat{\mathbf{R}} \mathbf{R}}{4\pi \rho \omega^2 R^4} \]

where \( \hat{\mathbf{R}} = \mathbf{R}/R \), \( \mathbf{n}' \) is the unit surface normal at \( \mathbf{r}' \), and

\[ C = \Omega_\alpha e^{ik_s R} - \Omega_c e^{ik_c R} \]
\[ D = \left( (k_s R)^2 + ik_s R - 1 \right) e^{ik_s R} - (ik_c R - 1) e^{ik_c R} \]
\[ F = H_c e^{ik_c R} - H_s e^{ik_s R} \]
\[ \Omega_\alpha = -k_\alpha R^2 - 3ik_\alpha R + 3 \]
\[ H_\alpha = ik_\alpha R^3 - 6k_\alpha R^2 - 15ik_\alpha R + 15 \]
\[ \psi_\alpha = (k_\alpha R)^2 (ik_\alpha R - 1) e^{ik_\alpha R} \]

with \( \alpha \in \{s, c\} \).

Asymptotically, namely when \( R \to 0 \), we have

\[ C = \frac{1}{2} \left( k_s^2 - k_c^2 \right) R^2 + O(R^4) \]
\[ D = \frac{1}{2} \left( k_c^2 + k_s^2 \right) R^2 + O(R^3) \]
\[ F = \frac{3}{2} \left( k_c^2 - k_s^2 \right) R^2 + O(R^4) \]
\[ \lambda \psi_c + 2\mu C = \mu k_c^2 R^2 + O(R^4) \]
\[ \psi_s + 2C = -k_c^2 R^2 + O(R^4) \]

It is clear that \( \vec{G}^{\text{ut}} \) has \( 1/R \) (weak) singularity, while \( \vec{G}^{\text{uu}} \) has \( 1/R^2 \) (strong) singularity.

### 4.2 Nyström Discretization

#### 4.2.1 Curved Triangular Elements

To describe the object surface, we use triangular elements, which are popular due to its flexibility. Other elements can also be fit into our approach easily, like the quadrilateral elements, which can help improve the efficiency for some situations [77]. Each element
can be interpolated from a set of chosen nodes, illustrated in Fig. 4.1 for linear and quadratic elements, as follows:

\[ \mathbf{r} = L^{ijk}(\xi)\mathbf{r}_{ijk}, \text{ no sum on } k \]  

(4.16)

where \( L^{ijk} \) is the interpolation polynomial for the node \( \mathbf{r}_{ijk} \). The simplex coordinates of the nodes, for \( M^{th} \) order interpolation, are

\[ \xi_{ijk} = \{\frac{i}{M}, \frac{j}{M}, \frac{k}{M}\} \]  

(4.17)

where \( i, j, k = 0, 1, \cdots M, i+j+k = M \). The interpolation polynomial can be constructed as a product of the Silvester and Ferrari polynomials [78]

\[ L^{ijk}(\xi^1, \xi^2, \xi^3) = L^i(M, \xi^1)L^j(M, \xi^2)L^k(M, \xi^3) \]  

(4.18)

with

\[ L^s(M, \xi) = \frac{1}{s!} \prod_{k=0}^{s-1} (M\xi - k), \quad L^0(M, \xi) = 1 \]  

(4.19)

### 4.2.2 Curvilinear Basis Functions

High order Nyström method employs basis functions defined on curvilinear elements. For a given element \( p \), we can write the fields on it in the following form [79]

\[ \mathbf{f}_p(\mathbf{r}) = \sum_{i=1}^{N_p} \mathbf{L}_{pi}(\mathbf{r}) \cdot \mathbf{f}_{pi} \]  

(4.20)
where \( f_{pi} = f_{pi}^\alpha e_\alpha(\xi_i) \) is the field (\( t \) or \( u \)) at the \( i^{th} \) field sampling node \( r_i(\xi_i) \) in \( p \) (green dots in Fig. 4.1), and \( \tilde{L}_{pi}(r) \) is the interpolation dyad that satisfies the condition

\[
\tilde{L}_{pi}(r_j) = I \delta_{ij}, \quad N \ni i, j \leq N_n
\]

with \( N_n \) being the number of nodes. Now let’s define the tangent and normal basis vectors in the parametric \( \xi \) space as the following:

\[
e_i(\xi) = \frac{\partial r}{\partial \xi^i}, \quad i \in \{1, 2\} \tag{4.22}
\]

\[
e_3(\xi) = n(\xi) = e_1(\xi) \times e_2(\xi) \tag{4.23}
\]

The dual basis vectors are defined by

\[
e^\alpha(\xi) \cdot e_\beta(\xi) = \delta^\alpha_\beta \tag{4.24}
\]

with \( \alpha, \beta \in \{1, 2, 3\} \). Also, we have the metric tensor and its dual

\[
g_{\alpha\beta}(\xi) = e_\alpha(\xi) \cdot e_\beta(\xi) \tag{4.25}
\]

\[
g^{\alpha\beta}(\xi) = e^\alpha(\xi) \cdot e^\beta(\xi) \tag{4.26}
\]

And the Jacobian can be found as

\[
J(\xi) = \left| e_3(\xi) \right| = \left| n(\xi) \right| = \sqrt{g_{11}(\xi)g_{22}(\xi) - g_{12}(\xi)g_{21}(\xi)} \tag{4.27}
\]

Then we can adopt the following representation using a scalar interpolation function \( L_{pi}(\xi) \):

\[
f_p(r) = \sum_{i=1}^{N_n} L_{pi}(\xi) [e_\alpha(\xi)e^\alpha(\xi_i) \cdot f_p(r_i)]
\]

\[
= \sum_{i=1}^{N_n} L_{pi}(\xi) e_\alpha(\xi) g^{\alpha\beta}(\xi_i) e_\beta(\xi_i) \cdot f_p(r_i) \tag{4.28}
\]

From the above, we can see that

\[
\tilde{L}_{pi}(\xi) = L_{pi}(\xi) g^{\alpha\beta}(\xi_i) e_\alpha(\xi) e_\beta(\xi_i) \tag{4.29}
\]

where \( i \) indicates evaluation at the \( i^{th} \) node. From (4.21), we require that

\[
L_{pi}(\xi_j) = \delta_{ij} \tag{4.30}
\]

In the above, a subscript of a factor is assumed to be summed if it is also a superscript of another factor in the same product expression.
4.2.3 Field Interpolation

Now let’s define the interpolation polynomial for the \(i^{th}\) node, denoted as \(L_{pi}(\xi^1, \xi^2)\), from the space of \(n^{th}\) order polynomials [79]

\[
P_n^2 := \text{span}\{(\xi^1)^a(\xi^2)^b | a, b \geq 0, a + b \leq n\} \tag{4.31}
\]

The degrees of freedom of the space is

\[
\text{dof } P_n^2 = \frac{(n+2)(n+1)}{2} \tag{4.32}
\]

And we have the first few spaces as

\[
\begin{align*}
n = 0, \ \text{dof} = 1 & \quad P_n^2 = \text{span}\{1\} \tag{4.33} \\
n = 1, \ \text{dof} = 3 & \quad P_n^2 = \text{span}\{1, \xi^1, \xi^2\} \tag{4.34} \\
n = 2, \ \text{dof} = 6 & \quad P_n^2 = \text{span}\{1, \xi^1, \xi^2, (\xi^1)^2, (\xi^2)^2, \xi^1\xi^2\} \tag{4.35} \\
n = 3, \ \text{dof} = 10 & \quad P_n^2 = \text{span}\{1, \xi^1, \xi^2, (\xi^1)^2, (\xi^2)^2, \xi^1\xi^2, (\xi^1)^3, (\xi^2)^3, (\xi^1)^2\xi^2, \xi^1(\xi^2)^2\} \tag{4.36}
\end{align*}
\]

Then we can define the interpolation functions as follows:

\[
L_{pi}(\xi^1, \xi^2) = \sum_{k=1}^{N_n} A_{ik} P^k(\xi^1, \xi^2) \tag{4.37}
\]

\[
L_{pij} = L_{pi}(\xi^1_j, \xi^2_j) = \delta_{ij} \tag{4.38}
\]

where \(P^k(\xi^1, \xi^2)\) are the monomials making up the functional space. We have, for a given \(i\), \(N_n\) unknowns, so we need \(N_n\) equations, to define \(L_{pi}(\xi^1, \xi^2)\). We just sample over \(N_n\) points in the \((\xi^1, \xi^2)\) space. As a result, we have

\[
L_{pij} = A_{ik} P^k_j = \delta_{ij} \tag{4.39}
\]

from which we can solve for the coefficients \(A_{ik}\).

When \(n = 3\), for reasons to be revealed, we can add two degrees of freedom to form the following space:

\[
P_n^2 = \text{span}\{1, \xi^1, \xi^2, (\xi^1)^2, \xi^1\xi^2, (\xi^2)^2, (\xi^1)^2\xi^2, \xi^1(\xi^2)^2, (\xi^2)^3, (\xi^1)^2\xi^2, \xi^1(\xi^2)^2\} \tag{4.40}
\]
4.2.4 Discretization

To illustrate the Nyström method, consider the integral over the element \( p \):

\[
h_p(r) = \sum_{i=1}^{N_n} \int_{S_p} \bar{G}(r, r') \cdot \bar{L}_{pi}(r') \cdot f_{pi} dS'
\]

(4.41)

where \( \bar{G} \) is the appropriate Green’s function. For the far field interaction, the kernel is smooth and can be evaluated using Gaussian quadrature as

\[
h_p(r) = \sum_{i=1}^{N_n} \sum_{j=1}^{N_q} W_j \bar{G}(r, r_j) \cdot \bar{L}_{pi}(r_j) \cdot f_{pi}
\]

(4.42)

where \( N_q \) is the number of quadrature samples, and \( W_j = w^j J(\xi_j)/2 \), with \( w^j \) being the weights for the quadrature rule. However, if we choose the nodes the same as the quadrature nodes, it simplifies to

\[
h_p(r) = \sum_{i=1}^{N_n} W_i \bar{G}(r, r_i) \cdot f_{pi}
\]

(4.43)

by using (4.21), which involves only one evaluation of the Green’s function for each node. This simplicity brought by the coincidence of the interpolating and integrating nodes makes an appealing point for the implementation of the Nyström method. Since we don’t have a good 10 point quadrature rule, two degrees of freedoms are added in (4.40) considering the existence of a good 12 point quadrature rule [79].

For the near interaction, we cannot do this since the kernel is usually singular. In this case, we can perform the integration in the parameter space:

\[
h_p(r) = \sum_{i=1}^{N_n} \int_{S_p} \bar{G}(r, \xi') \cdot \bar{L}_{pi}(\xi') \cdot f_{pi} \cdot J(\xi') d\xi'
\]

(4.44)

We can see that, due to the proper choice of the basis functions, the local correction becomes simply a surface integral.

Summing up the contribution from all the elements, and evaluate the fields at each interpolation (quadrature) node \( r_j \), we obtain

\[
h(r_j) = \sum_{p=1}^{N_p} h_p(r_j)
\]

(4.45)

where \( N_p \) is the number of element patches.
Applying the above procedure to (4.1) and (4.2), we are led to the following linear system

\[
\begin{bmatrix}
-\bar{U}_+ & \bar{T}_+ + I/2 \\
-\bar{U}_- & \bar{T}_- - I/2
\end{bmatrix}
\begin{bmatrix}
\mathbf{t} \\
\mathbf{u}
\end{bmatrix}
= 
\begin{bmatrix}
\mathbf{u}_{inc} \\
0
\end{bmatrix}
\]

(4.46)

where

\[
U^\beta_{mm'\alpha\pm} = \int_{S_p} dS' \left[ e^\beta_q(\xi_j) \cdot \bar{\mathbf{G}}_{\pm}^{ut}(\mathbf{r}_{qj}, \mathbf{r'}) \cdot \mathbf{e}_{\pm\alpha}(\xi'_i) \right] \mathbf{L}_{pi}(\xi')
\]

(4.47)

\[
T^\beta_{mm'\alpha\pm} = \int_{S_p} dS' \left[ e^\beta_q(\xi_j) \cdot \bar{\mathbf{G}}_{\pm}^{uu}(\mathbf{r}_{qj}, \mathbf{r'}) \cdot \mathbf{e}_{\pm\alpha}(\xi'_i) \right] \mathbf{L}_{pi}(\xi')
\]

(4.48)

and

\[
u^\beta_{inc,m} = u^\beta_{inc,qj}, \quad \nu^\alpha_{m'} = u^\alpha_{pi}, \quad t^\alpha_{m'} = t^\alpha_{pi}
\]

(4.49)

In the above, \(m\) and \(m'\) are global indices for the nodes corresponding to the element and node indices \((q, j)\) and \((p, i)\) respectively, and \(v^\alpha = \mathbf{v} \cdot \mathbf{e}^\alpha\) with \(\mathbf{v}\) being an arbitrary vector. And the interpolation polynomial \(\tilde{L}_{pi}(\xi')\) in (4.47) is defined as

\[
\tilde{L}_{pi}(\xi') = \frac{J(\xi'_i)}{J(\xi')} L_{pi}(\xi')
\]

(4.50)

which can be used to cancel the undesirable behavior of the Jacobian in the numerical integral.

For far field interaction, the matrix elements are simply

\[
U^\beta_{mm'\alpha\pm} = W_q e^\beta_q(\xi_j) \cdot \bar{\mathbf{G}}_{\pm}^{ut}(\mathbf{r}_{qj}, \mathbf{r'}) \cdot \mathbf{e}_{\pm\alpha}(\xi'_i)
\]

(4.51)

\[
T^\beta_{mm'\alpha\pm} = W_q e^\beta_q(\xi_j) \cdot \bar{\mathbf{G}}_{\pm}^{uu}(\mathbf{r}_{qj}, \mathbf{r'}) \cdot \mathbf{e}_{\pm\alpha}(\xi'_i)
\]

(4.52)

where no integration is required. It should be pointed out that this simple form of far field interaction makes it easy for us to incorporate fast algorithms.

For scattering from traction free objects, we have

\[
(\bar{T}_+ + I/2) \mathbf{u} = \mathbf{u}_{inc}
\]

(4.53)

While in the case of a rigid scatterer, the equation becomes

\[
\bar{U}_+ \mathbf{t} = -\mathbf{u}_{inc}
\]

(4.54)
4.3 Singular Integrals

The integrals in (4.47) and (4.48) are called singular integrals when \( p = q \). For (4.47), we have

\[
U_{mm'\alpha}^\beta = \frac{1}{4\pi \rho \omega^2} \int_{S_p} dS' \left[ \mathbf{e}_q^\beta(\xi_j) \cdot \left( C\hat{R}\hat{R} + D\hat{I} \right) \cdot e_{\rho\alpha}(\xi') \right] \frac{L_{pi}(\xi')}{R^3} \quad (4.55)
\]

Since it is only weakly singular, the polar transformation technique can be directly used for its evaluation. For (4.47), strong singularity exists, and singularity extraction is usually performed to reduce to weak singularity so that it can be handled by polar transformation directly. The general algorithms by [16, 49] are very popular, but the extraction procedure is laborious. Here we propose a simpler extraction approach.

We can first split (4.48) into two parts, as follows

\[
T_{mm'\alpha}^\beta = T_{mm'\alpha_1}^\beta + T_{mm'\alpha_2}^\beta \quad (4.56)
\]

where

\[
T_{mm'\alpha_1}^\beta = \int_{S_p} dS' \left\{ \mathbf{e}_q^\beta(\xi_j) \cdot \left[ \mu(\psi_s + 2C)\hat{n}' \cdot \hat{R}\hat{I} + 2\mu F\left( \hat{n}' \cdot \hat{R} \right) \hat{R}\hat{R} \right] \cdot e_{\rho\alpha}(\xi') \right\} \frac{L_{pi}(\xi')}{4\pi \rho \omega^2 R^4} \quad (4.57)
\]

\[
T_{mm'\alpha_2}^\beta = \int_{S_p} dS' \left\{ \mathbf{e}_q^\beta(\xi_j) \cdot \left[ (\lambda\psi_c + 2C)\hat{R}\hat{n}' + \mu(\psi_s + 2C)\left( \hat{n}' \cdot \hat{R} \right) \right] \cdot e_{\rho\alpha}(\xi') \right\} \frac{L_{pi}(\xi')}{4\pi \rho \omega^2 R^4} \quad (4.58)
\]

\( T_{mm'\alpha_1}^\beta \) is weakly singular from the observation that \( \hat{n}' \cdot \hat{R} \sim R \) when \( R \to 0 \). \( T_{mm'\alpha_2}^\beta \) is at most weakly singular if \( i \neq j \) since \( L_{pi}(\xi') \to 0 \) when \( \xi' \to \xi_j \). When \( i = j \), \( T_{mm'\alpha_2}^\beta \) is strongly singular only when 1) \( \alpha = 3, \beta \neq 3 \); 2) \( \alpha \neq 3, \beta = 3 \). So we only need to carry out singularity extraction for these cases.

By using the identity that \( \nabla g(0, R) = -\hat{R}/(4\pi R^2) \), we can put \( T_{mm'\alpha_2}^\beta \) in this form

\[
T_{mm'\alpha_2}^\beta = \frac{-1}{\rho \omega^2} \int_{S_p} dS' \nabla g(0, R) \cdot \mathbf{P}(\xi_j, \xi') \quad (4.59)
\]

where

\[
\mathbf{P}(\xi_j, \xi') = \left[ \left( \frac{\lambda\psi_c + 2C}{r^2} \right) \mathbf{e}_q^\beta(\xi_j) \hat{n}' \cdot e_{\rho\alpha}(\xi') + \frac{\mu(\psi_s + 2C)}{r^2} e_{\rho\alpha}(\xi') e_q^\beta(\xi_j) \cdot \hat{n}' \right] L_{pi}(\xi') \quad (4.60)
\]
Now if we subtract the tangential components of $\mathbf{P}$ at the neighborhood of $r_j$ in (4.59), it will become weakly singular. To this end, a good choice is [15]

$$
\int_{S_p} dS' \nabla g(0, R) \cdot \mathbf{P}(\xi, \xi') = \int_{S_p} dS' \nabla g(0, R) \cdot \left[ \mathbf{P}(\xi, \xi') - \tilde{P}_\gamma \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] 
+ \bar{P}_\gamma \int_{S_p} dS' \nabla g(0, R) \cdot \left[ \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] \tag{4.61}
$$

where $\tilde{P}_\gamma, \gamma \in \{1, 2\}$ are coefficients defined by

$$
\tilde{P}_\gamma = \mathcal{J}(\xi_j) P_\gamma(\xi_j, \xi_j) = \mathcal{J}(\xi_j) \mathbf{P}(\xi_j, \xi_j) \cdot e_\gamma(\xi_j) \tag{4.62}
$$

The first integral in (4.61) now is only weakly singular in the neighborhood of $r_j$. For the second integral, we have

$$
\int_{S_p} dS' \nabla g(0, R) \cdot \left[ \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] = - \int_{S_p} dS' \nabla g(0, R) \cdot \left[ \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] 
+ \int_{S_p} dS' g(0, R) \nabla' \cdot \left[ \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] \tag{4.63}
$$

Since the divergence of a vector in a curvilinear coordinate is calculated as

$$
\nabla \cdot \mathbf{V}(x) = \frac{1}{\mathcal{J}(x)} \frac{\partial}{\partial x^\alpha} [V^\alpha(x) \mathcal{J}(x)] \tag{4.64}
$$

the last integral in (4.63) vanishes. Invoking the surface divergence theorem for a tangent vector $\mathbf{V}$ that

$$
\int_S \nabla \cdot \mathbf{V}(x) dS = \int_{C_p} (dl \times \hat{n}) \cdot \mathbf{V}(x) \tag{4.65}
$$

we yield

$$
\int_{S_p} dS' \nabla g(0, R) \cdot \left[ \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] = - \int_{C_p} dl' (\hat{l} \times \hat{n}') \cdot g(0, R) \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \tag{4.66}
$$

Finally, we have the expression suitable for numerically integrating $T_{mm'\alpha 2}^3$ as

$$
T_{mm'\alpha 2}^3 = - \frac{1}{\rho \omega^2} \int_{S_p} dS' \nabla g(0, R) \cdot \left[ \mathbf{P}(\xi, \xi') - \tilde{P}_\gamma \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \right] 
+ \frac{\bar{P}_\gamma}{\rho \omega^2} \int_{C_p} dl' (\hat{l} \times \hat{n}') \cdot g(0, R) \frac{e_\gamma(\xi')}{\mathcal{J}(\xi')} \tag{4.67}
$$

where $C_p$ is the boundary contour of $S_p$. The first integral can be performed using the polar transformation, while the second line integral can be directly integrated using Gaussian quadrature.
4.4 Nearly Singular Integrals

Nearly singular integrals arise when the observation point is very close to, but not on the source element, such as when the observation point lies in the adjacent element and approaches the common edge, or when the scatterer has a thin crack-like shape. It is very important, yet challenging, to evaluate these nearly singular integrals accurately and efficiently.

Near singularity cancellation (SC) schemes are very popular among the literature, but most of them intended for flat elements [80–83]. In [81,83], a SC scheme with a disc region treated separately is proposed to enhance the efficiency of SC for strongly nearly singular kernels. Recently efforts are made in [84] and [85] to extend the singularity cancellation to treat weakly and strongly nearly singular integrals on curvilinear triangular elements, and [86] gives a detailed analysis of SC methods on curvilinear elements.

Another approach to deal with singular and nearly singular integrals is the singularity subtraction technique [87], but the approach is case specific and the remaining integrals are still nearly weakly singular. Here, a general and efficient singularity subtraction scheme applicable to various orders of singularity is proposed to calculate nearly singular 2D integrals on curvilinear triangular elements.

From (4.55) and (4.56), we have, when $R \to 0$,

$$U_{mm',\alpha}^\beta \sim \frac{k_z^2 + k_c^2}{8\pi \rho \omega^2} \int_{\Delta \xi} d \xi' e_q^\beta(\xi_j) \cdot e_{pa}(\xi') \frac{L_{pi}(\xi')}{R}$$

$$+ \frac{k_z^2 - k_c^2}{8\pi \rho \omega^2} \int_{\Delta \xi} d \xi' e_q^\beta(\xi_j) \cdot RR \cdot e_{pa}(\xi') \frac{L_{pi}(\xi')}{R^3}$$

$$T_{mm',\alpha}^\beta \sim \frac{\mu k_c^2}{4\pi \rho \omega^2} \int_{\Delta \xi} d \xi' [e_q^\beta(\xi_j) \cdot R n' \cdot e_{pa}(\xi') - e_q^\beta(\xi_j) \cdot n' R \cdot e_{pa}(\xi')]$$

$$- n' \cdot Re_q^\beta(\xi_j) \cdot e_{pa}(\xi') \frac{L_{pi}(\xi')}{R^3}$$

$$+ \frac{3\mu (k_z^2 - k_c^2)}{4\pi \rho \omega^2} \int_{\Delta \xi} d \xi' (n' \cdot R) e_q^\beta(\xi_j) \cdot RR \cdot e_{pa}(\xi') \frac{L_{pi}(\xi')}{R^5}$$

where $\Delta \xi$ is the intrinsic triangular space specified by $(\xi^1, \xi^2) = (0,0), (1,0), (0,1)$. In the above, the Jacobian is canceled by properly choosing the basis functions in (4.47) and (4.48). In general, the asymptotic integrals can be put in the following form

$$\mathcal{I} = \int_{\Delta \xi} d \xi' \frac{L(\xi)}{R^s}$$
where $L(\xi)$ is made a polynomial of $\xi^\alpha$, $\alpha \in \{1, 2\}$, and $s \in \{1, 3, 5\}$.

For a given $r$, one can find a projection point $r_0$ on the curved element with simplex coordinate $\xi_0$ using Newton method [84]. As suggested by [16], it is more advantageous to consider the above integral in another parametric space $\eta$ with

$$
\eta^1 = \xi^1 + [g_{12}(\xi_0)/g_{11}(\xi_0)] \xi^2 \\
\eta^2 = [J(\xi_0)/g_{11}(\xi_0)] \xi^2
$$

The advantage of using $\eta$ lies in that the map from it to $r$ is conformal at $r_0$. At $\eta_0$ (image of $\xi_0$), setting up the polar coordinate system

$$
\eta^1 = \eta^1_0 + \rho \cos \theta \\
\eta^2 = \eta^2_0 + \rho \sin \theta
$$

we can put (4.70) as

$$
I = \frac{g_{11}(\xi_0)}{J(\xi_0)} \int_{\Delta \eta} \frac{L(\rho, \theta)}{R^s} \rho d\rho d\theta
$$

where

$$
L(\rho, \theta) = \sum_{k=1}^{K} \rho^k f_k(\theta)
$$

with $K \in \mathcal{N}_+$, and $f_k(\theta)$ are simple trigonometric functions which can be easily found.

For $R$, keeping terms up to second order, we have

$$
R \sim R_a = \sqrt{d^2 + 2d \cdot A(\theta) \rho + [A^2 + 2d \cdot B(\theta)] \rho^2}
$$

where $d = r - r_0$, $d = |d|$, and

$$
A(\theta) = - \sum_{\alpha} e_{\alpha}(\eta_0) h^\alpha \\
B(\theta) = -\frac{1}{2} \sum_{\alpha, \beta} e_{\alpha \beta}(\eta_0) h^\alpha h^\beta
$$

where $h^1 = \cos \theta, h^2 = \sin \theta, e_{\alpha}(\eta) = r, e_{\alpha}(\eta)$ is the tangent vector in $\eta$ space, and $e_{\alpha \beta}(\eta) = r, e_{\alpha \beta}(\eta)$ is the derivative of the tangent vector. Notice first that if the projection point $r_0$ is accurate enough, which is the case in most cases, $2d \cdot A \ll d$; Also, because of the choice of $\eta$ parameter, $A = |A|$ is pleasingly a constant. When $d$ is small, we have $2d \cdot B \ll A^2$. Therefore, the dependence of $R_a$ on $\theta$ is very weak, which observation will later allow us derive a more efficient integration scheme.
Then we propose the following singularity subtraction scheme:

\[ \mathcal{I} = \mathcal{I}_R + \mathcal{I}_S \]  

(4.80)

where

\[ \mathcal{I}_R = \sum_{i=1}^{3} \int_{\theta_i^-}^{\theta_i^+} \int_{0}^{\tilde{\rho}(\theta)} F_R(\rho, \theta) d\rho d\theta \]  

(4.81)

\[ \mathcal{I}_S = \sum_{i=1}^{3} \int_{\theta_i^-}^{\theta_i^+} \int_{0}^{\tilde{\rho}(\theta)} \frac{L(\rho, \theta)}{R_s} d\rho d\theta \]  

(4.82)

with

\[ F_R(\rho, \theta) = L(\rho, \theta) \left[ \frac{1}{R_s} - \frac{1}{R_a} \right] \]  

(4.83)

and the integral split into three, each over a sub-triangle formed by \( \eta_0 \) and one pair of vertices from \( \Delta \eta \), no matter where \( \eta_0 \) locates relative to \( \Delta \eta \). \( \theta_i^\pm \) are the upper and lower limits of \( \theta \) for the \( i \)th subtriangle, and \( \tilde{\rho}(\theta) \) is the maximum radial distance at \( \theta \). It can be shown that \( F_R(\rho, \theta) \sim O(1) \) is non-singular when \( R \to 0 \), hence is amenable for numerical quadrature.

Let us denote

\[ \mathcal{I}_j^i(\theta) = \int_{0}^{\tilde{\rho}(\theta)} \frac{\rho^j}{R_a} d\rho, \quad j \text{ odd} \]  

(4.84)

which can be evaluated analytically in a recursive manner for \( i = 0, 1, 2, ... \) \[88\]. Then, combining \( \mathcal{I}_R \) and \( \mathcal{I}_S \), we arrive at

\[ \mathcal{I} = \sum_{i=1}^{3} \int_{\theta_i^-}^{\theta_i^+} \left[ F_S(\theta) + \int_{0}^{\tilde{\rho}(\theta)} F_R(\rho, \theta) d\rho \right] d\theta \]  

(4.85)

where \( F_S(\theta) = \sum_k I_k^s(\theta) f_k(\theta) \). The integral in each dimension is performed using Gaussian quadrature. Notice that, instead of evaluating the integral of \( F_S \) separately, we have merged it with the integral of \( F_R \), in consideration firstly that \( I_k^s \) only weakly depends on \( \theta \) and \( f_k \) is smooth in \( \theta \), promising fast convergence, and secondly that \( F_S \) shares most of the calculations with \( F_R \). This tactic will lower the computational cost. When the observation point is very close to the element boundary, it is suggested in \[16\] the Sigmoid transformation be incorporated for the integral over \( \theta \) to enhance the efficiency further. Another important feature of (4.85) is that when \( r = r_0 \notin S_r \), implying \( d = 0 \), one can simply drop the singular term from \( \rho = 0 \) in the \( \rho \) integral and the formula still holds \[49\]. Furthermore, this approach can also be used to handle truly singular...
integrals, which is just the special case that $r = r_0 \in S_p$. Numerical results show that the proposed singularity subtraction is very accurate and efficient [89].

With the above approach, we can now efficiently evaluate the asymptotic integrals. For the difference of the original kernel and its asymptotic terms is no longer singular, it can be evaluated using ordinary quadrature.

4.5 Numerical Results

Figure 4.2 shows the scattering of a copper sphere inside an aluminum host medium. The material parameters for aluminum are $\rho = 2700 \text{ kg/m}^3$, $\lambda = 6.138 \times 10^{10} \text{ N/m}^2$, $\mu = 2.95 \times 10^{10} \text{ N/m}^2$ and for copper $\rho = 8930 \text{ kg/m}^3$, $\lambda = 1.32 \times 10^{11} \text{ N/m}^2$, $\mu = 4.60 \times 10^{10} \text{ N/m}^2$. This example is considered referring to the aluminum alloy 2000 series having about 4% of copper. We set $k_c a = 0.97869$ and $k_s a = 2.0669$ for the host medium, corresponding to a frequency of 1 KHz, where $a = 1 \text{ m}$ is the radius of the sphere. The incident plane wave has a unit amplitude and propagates in the $z$ direction. A mesh of 80 quadratic elements is used, where in each element we have 36 unknowns, so in total we have 2880 unknowns. The result is compared with analytical solution. We can see that the result has very high accuracy, with relative error below 0.3%.

In Fig. 4.3, the scattering of a plane wave by penny shaped cracks of different aspect ratios situated in aluminum host is studied. The parameters are again $k_c a = 0.97869$ and $k_s a = 2.0669$, where $a = 1 \text{ m}$ is the largest radius of the cross section of the crack in the $xoy$ plane. The incident field is propagating along the axis of the crack. For very thin shapes, we use a systematic near singularity treatment scheme that yields very accurate results for the matrix elements in the linear system. As a result, we can handle this geometry with very high aspect ratios without resorting to a more complex integral equation formulation. As shown in Fig. 4.3, as we increase the aspect ratio of the crack, the results tend to converge to some level that corresponds to the case with infinite aspect ratio, namely the disc situation. However, one has to use more complicated formulations [90] to address the ill-conditioning of the integral equations for thin geometries.

Figure 4.4 compares the numerical solution of the forward scattering of a penny shaped crack of unit radius and different aspect ratios with the analytic solution [91] for the limiting case of a disc. In the figure, $\rho = 1 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$, and $\Sigma_p$ is the normalized scattering cross-section. We can observe better and better agreement with
Figure 4.2: Scattering of a 1 KHz planar P-wave from a unit copper sphere in aluminum. Aluminum: $\rho = 2700$ kg/m$^3$, $\lambda = 6.138 \times 10^{10}$ N/m$^2$, $\mu = 2.95 \times 10^{10}$ N/m$^2$; Copper: $\rho = 8930$ kg/m$^3$, $\lambda = 1.32 \times 10^{11}$ N/m$^2$, $\mu = 4.60 \times 10^{10}$ N/m$^2$. 
Figure 4.3: Normal incidence scattering of a 1KHz planar P-wave from penny shaped cracks of radius 1 m and different aspect ratios embedded in aluminum with \( \rho = 2700 \) kg/m\(^3\), \( \lambda = 6.138 \times 10^{10} \) N/m\(^2\), \( \mu = 2.95 \times 10^{10} \) N/m\(^2\).
Figure 4.4: Forward scattering of a plane P-wave from a penny-shaped crack of unit radius. Parameters: $\rho = 1 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$. 
Figure 4.5: Convergence of Nyström method of different orders in scattering of a P-wave from a spherical cavity with $k_c a = \pi$. Parameters: $\rho = 3 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$. 
the analytic solution when we increase the aspect ratio up to 500, except at $k_s a = 2$ where relatively larger error occurs probably due to the tip singularity of the crack [90]. For the CBIE, it should be pointed out that our nearly singular integral treatment enables us to get very accurate result for cracks with aspect ratios even up to 1000, as opposed to only 20 in [90].

A convergence study is carried out in Fig. 4.5, where the RMS error of the shear wave scattering amplitude (pressure wave behavior is similar, hence not shown) is plotted against the number of nodes per shear wavelength. The host medium parameters are $\rho = 3 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$, and the scatterer is a unit spherical cavity with origin as its center. The incident wave is a plane P-wave propagating in the positive $z$ direction with $k_c = \pi$. The scattering amplitude has $N = 181$ uniform samples from $\theta = 0$ to $\theta = \pi$, and the RMS error is calculated as the $\|a - a^*\|_2/\|a^*\|_2$, where $a$ and $a^*$ are the numerical and analytic solution vectors of size $N$ respectively. In this figure, flat elements are used for the $0^{th}$ and $1^{st}$ order basis functions, and quadratic elements for the $2^{nd}$ and $3^{rd}$ orders. Fig. 4.5a shows the overlay of the numerical solution using 80 quadratic elements with $2^{nd}$ order basis against the analytic solution, where very good agreement is observed. From Fig. 4.5b, we can see that higher order generally behaves with faster convergence rate, allowing us to solve problems more accurately with even fewer unknowns. The $3^{rd}$ order doesn’t show significant advantage over the $2^{nd}$ order, probably due to the geometric error.

To further demonstrate the advantage of the high order method, the example of an elastic sphere of normalized size $k_c a = 8$ in Fig. 6 of [56] is solved here as well, with the surface displacement along the principle cut shown in Fig. 4.6. Analytic solution is used as the reference. The material parameters for host are $\rho = 1 \text{ kg/m}^3$, $\lambda = 0.1 \text{ N/m}^2$, $\mu = 0.4 \text{ N/m}^2$ and for the sphere $\rho = 2 \text{ kg/m}^3$, $\lambda = 0.2 \text{ N/m}^2$, $\mu = 0.5 \text{ N/m}^2$. We only use 320 isoparametric quadratic elements (11520 unknowns in total, 6.3 nodes per sphere $\lambda_s$) to obtain a result more accurate than that obtained using 237600 unknowns in [56].

4.6 Summary

This chapter presents a higher order Nyström method for solving elastodynamic scattering problems with high accuracy. The local correction is greatly simplified by carefully chosen basis functions. Novel simple and efficient singularity and near singular-
Figure 4.6: Surface displacement along the principal cut of an elastic sphere with $k_c \alpha = 8$ upon incidence of a planar P-wave propagating in z direction. Parameters are $\rho = 1$ kg/m$^3$, $\lambda = 0.1$ N/m$^2$, $\mu = 0.4$ N/m$^2$ for host, and $\rho = 2$ kg/m$^3$, $\lambda = 0.2$ N/m$^2$, $\mu = 0.5$ N/m$^2$ for the elastic sphere.

...density treatment schemes are proposed, and the developed approach is capable of handling thin crack-like shapes of high aspect ratios with just the conventional boundary integral equations. Numerical results have demonstrated the high accuracy and high order convergence of the proposed method.
CHAPTER 5. FAST MULTIPOLe NYSTRÖM METHOD FOR ELASTODYNAMIC SCATTERING

The high order Nyström method developed in Chapter 4 is able to solve elastic scattering problems accurately and efficiently, but the linear system is solved with a direct LU decomposition, which has $O(N^2)$ memory and $O(N^3)$ computational complexity. In practice, more often than not one will encounter problems discretized with a large number of unknowns. As a result, such high memory and computational complexity become prohibitive. To enable the Nyström method to solve large scale problems, one can enhance it by fast algorithms based on iterative solvers. The multi-level fast multipole algorithm [5], which delivers a computational and memory complexity of $O(N\log N)$ by efficiently calculating the matrix vector multiplication in the iterative solver, serves as the accelerator of the Nyström method in this chapter.

5.1 Factorization of Green’s Functions

5.1.1 Scalar Green’s Function

Figure 5.1 shows two ways of interaction between a source point $r_{m'}$ and an observation point $r_m$: direct and indirect. For $N$-point direct mutual interaction, there will be $N^2$ direct links. To reduce the complexity, one can consider the indirect interaction, which process can be divided as three steps: aggregation of multiple sources to a local group center; translation between group centers; dis-aggregation from local group centers to destination. Mathematically, this requires a factorization of the interaction function into three factors, each containing $R_{m_L,m'} = r_{m'} - r_{m'}$, $R_{m_L,m_L'} = r_{m_L} - r_{m_L'}$, and $R_{m,m_L} = r_m - r_{m_L}$, respectively. As for Nyström method, the interaction functions in (4.51) and (4.52) are nothing but Green’s functions contracted by the basis and dual basis vectors.

For the scalar Green’s function, we have the plane wave expansion [5], which can be
where $k = k\hat{k} = k (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, $d^2 \hat{k} = \sin^2 \theta d\theta d\phi$ and the integral domain $\Omega$ is the surface of the unit sphere. In above,

$$\alpha_{m L_m l'} (\hat{k} \cdot \hat{R}_{m L m'_l}, k R_{m L m'_l}) = \frac{i k}{(4\pi)^2} \sum_{l=0}^{L} l^l (2l + 1) h_l^{(1)} (k r_{m L m'_l}) P_l (\hat{k} \cdot \hat{R}_{m L m'_l})$$

is the translation operator, with $h_l^{(1)}$ being the spherical Hankel function of the first kind of order $l$, and $P_l$ is the Legendre polynomial of order $l$, and $L$ is the number of modes retained in the infinite series. Formulas exist for determining the number of modes, with the following being widely used [92]:

$$L = kd + \beta (kd)^{1/3}$$

where $d = |R_{mm L} + R_{m'_l m'}| < R_{m L m'_l}$, and $\beta$ is a constant related to the accuracy of the truncation. For convenience, let’s denote $\beta_{m_1 m_2} (k) = \exp (i k \cdot R_{m_1 m_2})$, then we have

$$g(k, R_{mm'}) \approx \int_{\Omega} d^2 \hat{k} e^{i k (R_{m m L} + R_{m'_l m'})} \alpha_{m L m'_l}$$

(5.1)

where $\alpha_{m L m'_l} (\hat{k} \cdot \hat{R}_{m L m'_l}, k R_{m L m'_l})$ is the translation operator, with $h_l^{(1)}$ being the spherical Hankel function of the first kind of order $l$, and $P_l$ is the Legendre polynomial of order $l$, and $L$ is the number of modes retained in the infinite series. Formulas exist for determining the number of modes, with the following being widely used [92]:

$$L = kd + \beta (kd)^{1/3}$$

(5.3)

It is straightforward to generalize this factorization to a multilevel version as illustrated by Fig. 5.2:

$$\tilde{g}_{mm'} (k) = \beta_{mm L} (k) \cdot \alpha_{m L m'_l} \cdot \beta_{m'_l m'} (k)$$

(5.5)

where the sub-sub-script $L$ is for the bottom level, and $l \leq L$ indexes upper levels.

Without confusion, we have neglected the arguments of the functions, which practice will be followed thereafter when necessary.

### 5.1.2 Stokes’ Tensors

The Stokes’ tensors for elastic waves are given in Chapter 1. Without confusion, let us use $\mathbf{G}$ and $\mathbf{\Sigma}^T$ to denote $\mathbf{G}^{uu}$ and $\mathbf{G}^{ut}$. For the spectrum of $\mathbf{G}$, using the identity $\nabla = i k$, we have

$$\tilde{G} = \frac{1}{\mu} (\mathbf{I} - \hat{k}_s \hat{k}_s) \tilde{g}_s + \frac{1}{\gamma} \hat{k}_c \hat{k}_c \tilde{g}_c$$

(5.7)
where the subscript $s$ and $c$ are for shear and compressional waves, and $\tilde{g}_\sigma$, $\sigma \in \{s, c\}$ are the spectrum of $g(k_\sigma, R)$ following the definition in (5.4) and (5.5). Then we can write

$$\nabla \cdot \tilde{G} = \frac{ik_c}{\gamma} \hat{k}_c \tilde{g}_c$$  \hfill (5.8)$$

$$\nabla \tilde{G} = \frac{ik_s}{\mu} \hat{k}_s \left( \hat{I} - \hat{k}_s \hat{k}_s \right) \tilde{g}_s + \frac{ik_c}{\gamma} \hat{k}_c \hat{k}_c \tilde{g}_c$$  \hfill (5.9)$$

$$\tilde{G} \nabla = \frac{ik_s}{\mu} \left( x^\alpha \hat{k}_s x_\alpha - \hat{k}_s \hat{k}_s \hat{k}_s \right) \tilde{g}_s + \frac{ik_c}{\gamma} \hat{k}_c \hat{k}_c \tilde{g}_c$$  \hfill (5.10)$$

where $x_\alpha$ and $x^\alpha$ are the basis and dual basis vectors with $\alpha \in \{1, 2, 3\}$ and they satisfy $x^\alpha x_\alpha = \hat{I}$. Then we obtain

$$\tilde{\boldsymbol{\Sigma}} = \frac{ik_c}{\gamma} \left( \lambda \hat{n}' + 2\mu \hat{n}' \cdot \hat{k}_s \hat{k}_c \right) \hat{k}_c \tilde{g}_c + ik_s \left( \hat{n}' \cdot \hat{k}_s x^\alpha x_\alpha + \hat{n}' \cdot x^\alpha \hat{k}_s x_\alpha - 2\hat{n}' \cdot \hat{k}_s \hat{k}_s \hat{k}_s \right) \tilde{g}_s$$  \hfill (5.11)$$
which can be more favorably put as
\[
\tilde{\Sigma}^T = \frac{i k_c}{\gamma} \hat{k}_c \left( \lambda \hat{n}' + 2 \mu \hat{n}' \cdot \hat{k}_s \hat{k}_s \right) \tilde{g}_c + i k_s \left[ \tilde{n}' \cdot \hat{k}_s \left( \tilde{I} - \hat{k}_s \hat{k}_s \right) + \left( \tilde{I} - \hat{k}_s \hat{k}_s \right) \cdot \tilde{n}' \hat{k}_s \right] \tilde{g}_s
\]  
(5.12)

### 5.2 Factorization of Far Field Interaction

The far field interactions, as given by (4.51) and (4.52), are contracted versions of the Stokes’ tensors. By using the above factorization of the Stokes’ tensors, we get the spectrum of \( U^\beta_{m'm'\alpha} \) as
\[
U^\beta_{m'm'\alpha} = W_i e^\beta_{qj} \cdot \tilde{\Theta}_{m'm'} e_{pia} = \tilde{U}^\beta_{smm'\alpha} + \tilde{U}^\beta_{cmm'\alpha}
\]  
(5.13)

where
\[
\tilde{U}^\beta_{smm'\alpha} = \frac{1}{\mu} e^\beta_{qj} \cdot \beta_{smm'\alpha} \left( \tilde{I} - \hat{k}_s \hat{k}_s \right) \cdot e_{pia} W_i
\]  
(5.14)
\[
\tilde{U}^\beta_{cmm'\alpha} = \frac{1}{\gamma} e^\beta_{qj} \cdot \beta_{cmm'\alpha} \left( \hat{k}_s \hat{k}_s \cdot e_{pia} W_i \right)
\]  
(5.15)

where \( e^\beta_{qj} = e^\beta_q (\zeta_j), e_{pia} = e_{pia} (\xi'_i), \alpha_s \) and \( \alpha_c \) are the translation operators for the s- and c-waves respectively. It is suggested in [50, 56] that we use the identity that \( \tilde{I} - \hat{k}_s \hat{k}_s = \hat{\theta}_s \hat{\theta}_s + \hat{\phi}_s \hat{\phi}_s \) in (5.14) to have
\[
\tilde{U}^\beta_{smm'\alpha} = \frac{1}{\mu} e^\beta_{qj} \cdot \beta_{smm'\alpha} \left( \hat{\theta}_s \hat{\theta}_s \cdot e_{pia} + \hat{\phi}_s \hat{\phi}_s \cdot e_{pia} \right) W_i
\]  
(5.16)

In the above, with the use of the spherical coordinate, (5.15) and (5.16) involve only one and two components for the radiation patterns as appear in the square brackets. However, if we use the Cartesian coordinate, each will have three components. Being able to reduce the number of radiation patterns is very beneficial in the implementation of the MLFMA, since it helps reduce the memory requirement significantly.

We can apply this idea to \( \tilde{T}^\beta_{m'm'\alpha} \) as well based on our formulation. To be specific, we have
\[
\tilde{T}^\beta_{m'm'\alpha} = W_i e^\beta_{qj} \cdot \tilde{\Sigma}^T \cdot e_{pia} = \tilde{T}^\beta_{smm'\alpha} + \tilde{T}^\beta_{cmm'\alpha}
\]  
(5.17)

where
\[
\tilde{T}^\beta_{smm'\alpha} = i k_s e^\beta_{qj} \cdot \beta_{smm'\alpha} \left\{ \left[ \hat{\theta}_s \left( \tilde{n}' \cdot \hat{k}_s \hat{\theta}_s \cdot e_{pia} + \hat{\theta}_s \cdot \tilde{n}' \hat{k}_s \cdot e_{pia} \right) \right] W_i \right\}
\]  
(5.18)
and
\[ \tilde{T}_\alpha^{\beta m'm' \alpha} = i k_c e^{\beta}_{qj} \cdot \beta_{cm'm'L} \alpha_{cm'Lm'} \left( \hat{k}_c \left( \frac{\lambda}{\gamma} \hat{n}' \cdot e_{pia} + \frac{2\mu}{\gamma} \hat{n}' \cdot \hat{k}_c \cdot e_{pia} \right) \beta_{cm'Lm'} W_i \right) \]
(5.19)

Again, we only have one and two components for the radiating shear and compressional patterns.

With the spectrum of the far field interaction, we can integrate all the modes to obtain
\[ Z_{\beta mm'\alpha} = \int_\Omega \tilde{\Z}_{\beta smm'\alpha}(k_s) d^2 \hat{k}_s + \int_\Omega \tilde{\Z}_{\beta cmm'\alpha}(k_c) d^2 \hat{k}_c, \quad Z \in \{U, T\} \]
(5.20)

### 5.3 Further Pattern Reduction

When there are two media, we can further reduce the number of radiation patterns that are required to store in MLFMA. In detail, we write
\[ \tilde{U}_{\beta smm'\alpha} = \frac{1}{\mu} V_{smm'\alpha} \cdot \alpha_{sm'Lm'} V_{sm'Lm'\alpha} \]
(5.21)
\[ \tilde{U}_{\beta cmm'\alpha} = \frac{1}{\gamma} V_{cmm'\alpha} \alpha_{cm'Lm'} V_{cm'Lm'\alpha} \]
(5.22)

where
\[ V_{smm'\alpha} = \beta_{smm'\alpha} e^{\beta}_{qj} \]
(5.23)
\[ V_{sm'Lm'\alpha} = W_{i \beta_{sm'Lm'}(\hat{\theta}_s \hat{\phi}_s + \hat{\phi}_s \hat{\theta}_s)} \cdot e_{pia} \]
(5.24)
\[ V_{cmm'\alpha} = \beta_{cmm'\alpha} e^{\beta}_{qj} \cdot \hat{k}_c \]
(5.25)
\[ V_{cm'Lm'\alpha} = W_{i \beta_{cm'Lm'} \hat{k}_c} \cdot e_{pia} \]
(5.26)

And for \( T_{mm'\alpha} \), we have
\[ \tilde{T}_{\alpha smm'\alpha} = i k_s V_{smm'\alpha} \cdot \alpha_{sm'Lm'} \left( e_{sm'Lm'} + e_{sm'Lm'} V_{sm'Lm'} \right) \]
(5.27)
\[ \tilde{T}_{\alpha cmm'\alpha} = i k_c V_{cmm'\alpha} \alpha_{cm'Lm'} V_{cm'Lm'\alpha} \]
(5.28)

where
\[ e_{sm'\alpha} = \mathcal{J}_{m'}^{-1} \hat{k}_s \cdot e_{pia} \]
(5.29)
\[ V_{cm'Lm'\alpha} = \left( \frac{\lambda}{\gamma} \mathcal{J}_{m'} \delta_{3a} W_{i \beta_{cm'Lm'} \hat{k}_c} + \frac{2\mu}{\gamma} \mathcal{J}_{m'}^{-1} \hat{k}_c \cdot e_{pia} V_{cm'Lm'\alpha} \right) \]
(5.30)
with $J_m'$ being the Jacobian at $m'$. Suppose there are $N_p$ element patches, each patch has $N_n$ nodes, and each node pertains $M$ unknowns. Suppose also that the number of modes needed are $K_s$ and $K_c$ for the s- and c- wave respectively. Then for the radiation patterns, the above formulation consumes a memory of $(9K_s + 6K_c)N_nN_p$ units, while the strategy in the previous section takes up a memory of $(12K_s + 6K_c)N_nN_p$ units. Typically, $k_s \approx 2k_c$, and $K_s \approx 4K_c$, so the memory saving for the radiation patterns is more than 20 percent.

![Figure 5.3: Multilevel grid for MLFMA.](image)

### 5.4 Notes on Implementation

The MLFMA solves (4.46) using iterative solvers, like the generalized minimal residue (GMRES) method, and it relies on a multilevel grouping scheme as such [5]: A cube containing the scatterer is regarded as level 0; a recursive subdivision of all the
cubes in level $l$ into 8 identical subcubes in level $l + 1$ is carried out, until level $L$ that has cubes of about $0.3 \sim 0.6\lambda_s$ ($\lambda_s$ is the shear wavelength). The elements in the mesh belong to the groups that contain them in each level. Fig. 5.3 is an illustrative example of the grouping strategy in MLFMA.

The interaction matrix is split into two parts: near (adjacent groups in level $L$) and far (non-adjacent groups in level $L$) interactions. The former is calculated and stored, and can be used for matrix-vector multiplication (MVP) for all iterations; while the contribution to the MVP from the latter is calculated using a multilevel scheme invoked by the multilevel factorization of the interaction function. In so doing, the overall computational and memory complexities are both $O(N\log N)$, allowing the solution of large scale problems.

To increase the convergence of the iterative solver, a block diagonal pre-conditioner is used. And interpolation and anterpolation between different levels have to be employed since the number of modes required for upper levels is larger than that for lower levels. The literature [55, 56] provide a good reference on the implementation of the MLFMA to elastodynamics.

This work has implemented the MLFMA for elastodynamic scattering using C++, and double precision is used.

5.5 Frequency Domain to Time Domain

Although we are solving in frequency domain, time domain results can be obtained by virtue of Fourier transform. To this end, one can first Fourier transform the time domain input signal $s_i(t)$ to get its frequency spectrum $\tilde{s}_i(\omega)$; then find the spectrum of the response $s_r(\omega)$ using the frequency domain solver; then inverse Fourier transform $\tilde{s}_r(\omega)$ to obtain the time domain response $s_r(t)$. Since it is very difficult to evaluate the highly oscillatory Fourier integrals, the discrete Fourier transform can be used. One can show that

$$s_r = \frac{N\Omega_s}{\pi} \text{Re} \{\text{IDFT} \circ \tilde{s}_r\} - \frac{\Omega_s}{2\pi} \tilde{s}_r(0)$$

(5.31)

where $s_r$ and $\tilde{s}_r$ are vectors of samples for $s_r(t)$ at $t = \frac{2\pi n}{\Omega_s} \frac{N}{N}$ and $\tilde{s}_r(\omega)$ at $\omega = n\Omega_s$ respectively, with $\Omega_s$ being the sampling period in the (angular) frequency domain, $N$ the total number of samples, and $N \geq n < N$. To satisfy the Nyquist sampling rate, one has to make sure $\Omega_s \leq \pi/t_{max}$, where $t_{max}$ is the maximum time considered for a transient
process. To get good time domain signals, one also needs to guarantee that \( |\tilde{s}_r(\omega)| \) is negligible for \( \omega > N\Omega_s \). It is worth mentioning that the inverse fast Fourier transform (IFFT) is the fast algorithm for performing the inverse discrete Fourier transform (IDFT).

5.6 Numerical Results

The first example in Fig. 5.4 is the P-wave (propagating in \( z \) direction) scattering from a unit sphere. The medium is with \( \rho = 3 \text{ kg/m}^3, \lambda = \mu = 1 \text{ N/m}^2 \), and the elastic sphere has parameters \( \rho = 6 \text{ kg/m}^3, \lambda = \mu = 2 \text{ N/m}^2 \). The frequency is chosen as 1 Hz so \( k_c a = 2\pi \). The results in Fig. 5.4 are calculated using the analytic solution (Ref.) and the MLFMA accelerated Nyström method (NM) with \( 10^{-3} \) residue error in GMRES. We use only 320 iso-parametric quadratic elements (equivalently 7 nodes per \( \lambda_s \)), corresponding to 5760, 5760 and 11520 unknowns for the three cases respectively. In the simulation, 4-level MLFMA is used, and the size of the finest cubes in the grid is \( 0.4\lambda_s \). The RMS error for P-wave for the 3 cases are 0.02, 0.001, and 0.002 respectively, which is very satisfactory given the node density. For the elastic sphere, the direct solver would take 448 seconds to build up the matrix, and 2740 seconds to perform LUD, with 4.5 GB memory occupation; while for MLFMA, 450 seconds is used to precompute the near interaction, radiation/receiving patterns and translation operators, and 2160 seconds (300 GMRES iterations, each 7.2 seconds), and the total memory is 900 MB. This example indicates that the MLFMA solver starts to excel the direct solver for our program when the number of unknowns exceeds 10,000. Computations, unless otherwise specified, are done on a Dell Precision T7500 workstation with 4 CPUs of 2.13 GHz and 24 GB memory and no parallel computing is involved.
(a) Void

(b) Rigid
Figure 5.4: P-wave scattering from a unit sphere with $k_c a = 2\pi$. Host: $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$; Elastic sphere: $\rho = 6$ kg/m$^3$, $\lambda = \mu = 2$ N/m$^2$.

In Fig. 5.5, the scattering from the sphere in Fig. 5.4 is considered again, but with the frequency doubled to 2 Hz. The statistics for the solution using 5-level MLFMA is presented in Table 5.1. Again, we see that for this larger problem, very accurate result can be obtained with a low mesh density (7 nodes/$\lambda_s$). It can also be observed that the elastic case takes more iterations to converge.
(a) Void

(b) Rigid
Figure 5.5: P-wave scattering from a unit sphere with $k_{c}a = 4\pi$. Host: $\rho = 3$ kg/m$^3$, $\lambda = \mu = 1$ N/m$^2$; Elastic sphere: $\rho = 6$ kg/m$^3$, $\lambda = \mu = 2$ N/m$^2$.

Table 5.1: MLFMA for sphere with $k_{c}a = 4\pi$

<table>
<thead>
<tr>
<th>BC</th>
<th>N</th>
<th>Mem/GB</th>
<th>Time/s</th>
<th>No. Itr.</th>
<th>Error P</th>
<th>Error S</th>
</tr>
</thead>
<tbody>
<tr>
<td>Void</td>
<td>23040</td>
<td>2.3</td>
<td>13</td>
<td>245</td>
<td>9e$^{-4}$</td>
<td>1e$^{-3}$</td>
</tr>
<tr>
<td>Rigid</td>
<td>23040</td>
<td>2.3</td>
<td>10</td>
<td>167</td>
<td>3e$^{-4}$</td>
<td>2e$^{-3}$</td>
</tr>
<tr>
<td>Elastic</td>
<td>46080</td>
<td>5.1</td>
<td>46</td>
<td>398</td>
<td>7e$^{-3}$</td>
<td>7e$^{-3}$</td>
</tr>
</tbody>
</table>

In Fig. 5.6, we increase the frequency further to 7.5Hz for the elastic sphere in the previous example, making it of $k_{c}a = 15\pi$, or $26\lambda_s$ in diameter, which is very large and very challenging to solve. In our simulation, the sphere is discretized into 5120 isoparametric quadratic elements (184320 unknowns), with a node density of only $3.8/\lambda_s$. The number of levels in MLFMA is 5, and 1000 GMRES iterations are used, with each consuming 175 sec. The memory usage is 19GB. From the plot, we see that the numerical solution agrees very well with the analytic solution, although the node density is so small. We also note that the number of iterations is large, which indicates a slow convergence nature of the conventional boundary integral equation for very large problems.
Figure 5.6: Scattering of P-wave from a unit elastic sphere with $k_c a = 15\pi$. Parameters: $\rho = 3 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$ for host, and $\rho = 6 \text{ kg/m}^3$, $\lambda = \mu = 2 \text{ N/m}^2$ for the elastic sphere.

As another example, the scattering of a plane P-wave propagating in $z$ direction from a $5 \times 5 \times 5$ cubic array of unit spherical pores is solved in Fig. 5.7. The center of the array is at the coordinate origin, and the coordinate axes are parallel to the lattice vectors which are of magnitude 3. The frequency is set to be 0.2 Hz so $k_c a = 0.4\pi$ in the host which is chosen to have $\rho = 3 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$. The surface displacement is plotted in (a), and (b) gives the scattering amplitude in the $xoz$ plane. A 5-level MLFMA is used to solve the problem, which is discretized to pose 180,000 degrees of freedom. It takes 3286 seconds to build the solver, and 80 GMRES iterations each of which consumes 20 seconds, while the memory used is 14 GB.

Finally, let’s look at the time domain simulation. Shown in Fig. 5.8 is the pulse-echo scattering of an incident Gaussian pulse of a plane wave by twin spheres of radius 1 mm with 6 mm separation between the two sphere centers. The host material is set as aluminum, and we don’t consider interfaces for simplicity. A slant angle of 30 degree is formed from the horizontal plane. The transducer is placed at a position 64 mm away from the center of the two spheres, and the transmitted displacement signal (see Fig.
Figure 5.7: Plane P-wave (propagating in $z$ direction) scattering from a $5 \times 5 \times 5$ cubic array of unit spherical pores ($k_c a = 0.4\pi$) centered at origin in a host with $\rho = 3 \text{ kg/m}^3$, $\lambda = \mu = 1 \text{ N/m}^2$. 
Figure 5.8: Pulse-echo of twin sphere pores (1 mm radius, 6 mm separation, and 30 degree slant) in aluminum. The transmitted signal is the planar Gaussian pulse $\cos(2\pi f_0(t - t_p)) \exp\left(-\frac{(t - t_p)^2}{(2\tau_s^2)}\right)$ with $f_0 = 2$ MHz, $\tau_s = \sigma$, $t_p = 3.5\sigma$ where $\sigma = 1/(\pi f_0)$. The transducer is located 64 mm away from the center of the twin-sphere array.

5.9a) is assumed to be

$$s_i(t) = \cos(2\pi f_0(t - t_p)) \exp\left(-\frac{(t - t_p)^2}{(2\tau_s^2)}\right)$$  \hspace{1cm} (5.32)

with $f_0 = 2$ MHz, $\tau_s = \sigma$, $t_p = 3.5\sigma$ where $\sigma = 1/(\pi f_0)$. The simulated received displacement signal is shown in Fig. 5.9b, where MLFMA accelerated Nyström method (NM) is compared with the Kirchhoff approximation (KA). Good agreement is observed between KA and NM for the first several peaks which represent the leading response from the two spheres. The difference of the two results arises from the fact that the KA fails to capture the contribution from the creeping wave and multiple scattering.

5.7 Summary

The MLFMA has been successfully applied to accelerate the high order Nyström method for solving large scale elastodynamic scattering problems accurately and efficiently. A formulation is also proposed that can significantly reduce the memory re-
Figure 5.9: Transmitted and received signals for the configuration in Fig. 5.8
quirements in the implementation. We have demonstrated the efficiency of our solver in scattering problems with scatterers sized up to tens of wavelength. By solving in the frequency domain and performing the inverse Fourier transform, time domain applications are also demonstrated.
CHAPTER 6. CONCLUDING REMARKS

This thesis has made contributions in the following aspects:

1. By utilizing the spectral domain approach to the metal strip grating on grounded dielectric slab and the shielded microstrips, this thesis has revealed the modal relationship between these structures, as tabulated in Table 2.1. It is also shown numerically that the PMC shielded microtrips has a stronger capacity to drive electromagnetic energy into the high dielectric region than the PEC shielded microstrips, which indicates that the former exhibits a larger capacitance.

2. The matrix-friendly formulation for doubly periodic structure is presented, with the singularity at $k_s = 0$ extracted analytically. A novel approach has been developed for the computation of the doubly periodic Green’s function for layered medium in the context of matrix-friendly formulation, which delivers highly accurate results with higher order convergence, more robustness and less CPU time, and it also allows fast frequency sweep for calculating Brillouin diagram in eigenvalue problem and for normal incidence in scattering problem.

3. A high order Nyström method for elastic wave scattering is developed. The approach differs from ordinary Nyström method by its careful choice of basis functions that makes a very simple local correction scheme. This thesis also proposes a simple and efficient singularity treatment for the conventional boundary integral equation (CBIE) for elastodynamics. Furthermore, a novel general singularity subtraction technique for evaluating nearly singular integrals is first reported that enables us to solve cracks with very high aspect ratios. The high order convergence of the high order Nyström method is demonstrated, which allows the solution of problems with fewer degrees of freedom yet higher accuracy.

4. The multi-level fast multipole algorithm is applied to the high order Nyström method to solve large scale problems. The formulation proposed here can save the memory significantly.

The field of BIEM is broad and deep, and the need for more accurate and efficient
boundary integral equation solvers will continue to grow. Future endeavors can be di-
rected towards developing efficient parallel algorithms for existing fast algorithms so that
the advantages of both software and hardware are embodied [93]. For large and complex
structures, the iterative solver can be very slowly convergent, which indicates the need
for well-conditioned integral equation formulations or good preconditioners [94, 95]. For
problems involving multiple excitations, the iterative solver has to solve for each excita-
tion, which is very time consuming. Consequently an efficient direct solver that has low
complexity is being sought by researchers with rising interests [96]. From engineering
point of view, accurate full wave BIEM can be used to solve large numbers of problems
and acquire voluminous empirical data which can be used to train neural networks and
develop artificial intelligence that can be useful in inverse problems like oil finding and
non-destructive evaluation [97, 98].
BIBLIOGRAPHY


APPENDIX A. POISSON SUMMATION FOR DOUBLY PERIODIC STRUCTURE

The Poisson summation formula enables us to relate the summation in the spatial domain to the summation in the spectrum domain. Consider a doubly periodic lattice with direct and reciprocal lattice vectors \( \mathbf{a}_i \) and \( \mathbf{b}_i, \ i \in \{1, 2\} \). For a general scalar doubly periodic Green’s function for layered medium, the Poisson summation formula states that

\[
g(u_s; z, z') = \sum_L f(u_{sL}; z, z')e^{i k_0 \cdot \rho_L}
= \frac{1}{A_{cell}} \sum I \tilde{f}(k_{sI}; z, z')e^{i k_{sI} \cdot u_s}
\]

where

\[
\tilde{f}(k_s; z, z') = \mathcal{F}\{f(u_s; z, z')\}
\]

is the Fourier transform of \( f(u_s; z, z') \), \( A_{cell} = |a_1 \times a_2| \) is the area of the unit cell in the lattice plane, and \( u_s = r_s - r'_s, u_{sL} = u_s - \rho_L, \rho_L = l_1 a_1 + l_2 a_2, k_{sI} = k_0 + i_1 b_1 + i_2 b_2 = k_0 + k_{sI}, \) with \( L(l_1, l_2) \) and \( I(i_1, i_2) \) being the double indices for the spatial and spectral domains respectively.

**Proof.** According to Floquet theorem, the periodic Green’s function must satisfy the following:

\[
g(u_s; z, z') = h(u_s; z, z')e^{i k_0 \cdot u_s}
\]
\[
h(u_s; z, z') = h(u_s - \rho_L; z, z')
\]

where \( h \) is periodic on the lattice with lattice vectors \( a_1 \) and \( a_2 \). Then we have

\[
h(u_s; z, z') = g(u_s; z, z')e^{-i k_0 \cdot u_s}
\]

Because of its periodicity, we can express \( h \) as a Fourier series

\[
h(u_s; z, z') = \sum I \bar{h}_I e^{i k_{sI} \cdot u_s}
\]
where \( \tilde{h}_I \) are the coefficients. To find the coefficients, we multiply both sides of (A.6) by \( e^{-i k_0 \cdot u} \) (\( J(j_1, j_2) \) is a double index), and integrate in the unit cell, to have

\[
\sum_I \tilde{h}_I \int_{cell} du_s e^{i(k_\rho-I \cdot k_\omega) \cdot u_s} = A_{cell} \tilde{h}_J \tag{A.7}
\]

where we have used the following fact

\[
\int_{cell} du_s e^{i(\beta_1 b_1 + \beta_2 b_2) \cdot u_s} = a_1 a_2 \sin \varphi \int_0^1 \int_0^1 e^{2\pi i(\alpha_1 \beta_1 + \alpha_2 \beta_2)} d\alpha_1 d\alpha_2
\]

with \( \beta_i \in \mathbb{Z} \) and \( \varphi \) is the angle between \( \mathbf{a}_1 \) and \( \mathbf{a}_2 \). Therefore, we arrive at

\[
\tilde{h}_I = \frac{1}{A_{cell}} \int_{cell} du_s \left[ g(u_s) e^{-i k_0 \cdot u_s} \right] e^{-i k_\rho \cdot u_s}
\]

\[
= \frac{1}{A_{cell}} \int_{cell} du_s \left[ \sum_L f(u_{sL}; z, z') e^{-i k_0 \cdot u_{sL}} \right] e^{-i k_\rho \cdot u_s} \tag{A.9}
\]

where we have invoked the spatial summation form of the Green’s function in (A.1). Since \( e^{-i k_\rho \cdot u_{sL}} = 1 \) holds true for all \( I, J \), we can rewrite the above to yield

\[
\tilde{h}_I = \frac{1}{A_{cell}} \int_{cell} du_s \left[ \sum_L f(u_{sL}; z, z') e^{-i k_0 \cdot u_{sL}} e^{-i k_\rho \cdot u_{sL}} \right] \tag{A.10}
\]

\[
= \frac{1}{A_{cell}} \int_{cell} du_s \left[ f(u_s; z, z') e^{-i k_0 \cdot u_s} \right] e^{-i k_\rho \cdot u_s}
\]

\[
= \frac{1}{A_{cell}} \int_{\infty} du_s \left[ f(u_s; z, z') e^{-i k_0 \cdot u_s} \right] e^{-i k_\rho \cdot u_s}
\]

\[
= \frac{1}{A_{cell}} \tilde{f}(k_s; z, z') |_{k_s = k_{s+1}}
\]

where the integral domain “\( \infty \)” in (A.11) and (A.12) refers to the whole plane. Then we have

\[
h(u_s; z, z') = \frac{1}{A_{cell}} \sum_I \tilde{f}(k_{sI}; z, z') e^{i k_{sI} \cdot u_s} \tag{A.14}
\]

\[
g(u_s; z, z') = \frac{1}{A_{cell}} \sum_I \tilde{f}(k_{sI}; z, z') e^{i k_{sI} \cdot u_s}
\]

which gives us the spectrum sum of the periodic Green’s function. \( \square \)
APPENDIX B. SINGULARITY OF LAYERED MEDIUM 
DOUBLY PERIODIC GREEN’S FUNCTION

From Chapter 3, the scalar Green’s functions $g^{TE/TM}$ for doubly periodic structure in layered media have expressions

$$g^{TE/TM}(\mathbf{r}, \mathbf{r}') = \hat{S}F^{TE/TM}(k_{sI}; z, z')$$

where the operator $\hat{S}$ is defined in (3.5). For convenience, define

$$F^{TE/TM}(k_{sI}; \mathbf{r}, \mathbf{r}') = \frac{iF^{TE/TM}(k_{sI}; z, z')}{2A_{cell}k_{sI}^2k_{mI}}e^{ik_{sI}(\mathbf{r}_s - \mathbf{r}_s')}$$

hence we have

$$g^{TE/TM}(\mathbf{r}, \mathbf{r}') = \sum_I F^{TE/TM}(k_{sI}; \mathbf{r}, \mathbf{r}')$$

It is observed that when $k_s = 0$, the Green’s function blows up, which is non-physical. This difficulty arises due to the decomposition of the dyadic Green’s function, and we can eliminate it by examining the dyadic Green’s function as a whole:

$$\bar{G}^{EJ} = (\nabla \times \hat{z})(\nabla' \times \hat{z}) g^{TE} + \frac{1}{k_{nm}^2} (\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) g^{TM}$$
$$\bar{G}^{HJ} = (\nabla \times \nabla \times \hat{z})(\nabla' \times \hat{z}) g^{TE} + \frac{\mu_n}{\mu_m} (\nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) g^{TM}$$

where we have neglected the delta function for convenience. Exchanging the order of summation and differentiation and suppressing the arguments for $F^{TE/TM}(k_{sI}; \mathbf{r}, \mathbf{r}')$, we obtain

$$\bar{G}^{EJ} = \sum_I \left[ (\nabla \times \hat{z})(\nabla' \times \hat{z}) F^{TE} + \frac{1}{k_{nm}^2} (\nabla \times \nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) F^{TM} \right]$$
$$\bar{G}^{HJ} = \sum_I \left[ (\nabla \times \nabla \times \hat{z})(\nabla' \times \hat{z}) F^{TE} + \frac{\mu_n}{\mu_m} (\nabla \times \hat{z})(\nabla' \times \nabla' \times \hat{z}) F^{TM} \right]$$

where $\partial_\zeta = ik_\zeta$, $\partial_{\zeta'} = -ik_\zeta$ with $\zeta \in \{x, y\}$. Denote the general terms as $\tilde{G}^{EJ}$ and $\tilde{G}^{HJ}$ for (B.6) and (B.7) respectively.
From above, with $e^{i \mathbf{k}_s \cdot (r_x - r_x')}$ suppressed, we have

$$
\tilde{G}_{xx}^{EJ} = \frac{i}{2A_{cell} k_z^2 k_{mz1}} \left[ \partial_{yy'} F^{TE}(k_z; z, z') + \frac{1}{k_{nm}^2} \partial_{xx'} \partial_{zz'} F^{TM}(k_z; z, z') \right]
$$

(B.8)

Let’s consider the case when $k_s \to 0$. It is easy to see that and $k_{iz} \to k_i$ when $k_s \to 0$. Further, from the definition of the Fresnel reflection coefficients (3.16), we have

$$
R_{ij}^{TE} = -R_{ij}^{TM} + O \left( k_s^2 \right)
$$

(B.9)

which suggests that

$$
\tilde{R}_{ij}^{TE} = -\tilde{R}_{ij}^{TM} + O \left( k_s^2 \right), |i - j| = 1
$$

(B.10)

Then we obtain

$$
\tilde{M}^{TE}_m = \tilde{M}^{TM}_m + O \left( k_s^2 \right)
$$

(B.11)

$$
\tilde{S}^{TE}_{i \pm 1, i} = \tilde{S}^{TM}_{i \pm 1, i} + O \left( k_s^2 \right) = \frac{\eta_i}{\eta_{i \pm 1}} + O \left( k_s^2 \right)
$$

(B.12)

which allows us to find

$$
\frac{\tilde{S}^{TE}_{mn}}{S^{TM}_{mn}} = \frac{\eta_m}{\eta_n} + O \left( k_s^2 \right)
$$

(B.13)

with $\eta_i = \sqrt{\mu_i / \epsilon_i}$.

The propagation factor, assuming Einstein’s summation convention, can be written as (3.28):

$$
F(k_z; z, z') = F_{mn}^p \tilde{Q}_{mnp}
$$

(B.14)

The $z$ derivatives can be put as

$$
\partial_z F = (\partial_z F_{mn}^p) \tilde{Q}_{mnp} = ik_n \left[ 1 + O \left( k_s^2 \right) \right] \Upsilon_{z}^p F_{mn}^p \tilde{Q}_{mnp}
$$

(B.15)

$$
\partial_{z'} F = (\partial_{z'} F_{mn}^p) \tilde{Q}_{mnp} = -ik_m \left[ 1 + O \left( k_s^2 \right) \right] \Upsilon_{z'}^p F_{mn}^p \tilde{Q}_{mnp}
$$

(B.16)

$$
\partial_{zz'} F = (\partial_{zz'} F_{mn}^p) \tilde{Q}_{mnp} = k_m k_n \left[ 1 + O \left( k_s^2 \right) \right] \Upsilon_{zz'}^p F_{mn}^p \tilde{Q}_{mnp}
$$

(B.17)

where $\Upsilon_{z}^p$, $\Upsilon_{z'}^p$ and $\Upsilon_{zz'}^p$ are components of the following vectors

$$
\Upsilon_{z} = (1, 1, -1, -1)
$$

(B.18)

$$
\Upsilon_{z'} = (1, -1, 1, -1)
$$

(B.19)

$$
\Upsilon_{zz'} = (1, -1, -1, 1)
$$

(B.20)
Also one can show that

\[
F_{mn}^{TEp} = \frac{\eta_n}{\eta_m} \gamma_p^{TM} F_{mn}^{TM} + O\left(k_s^2\right) \tag{B.21}
\]

\[
\tilde{Q}_{mp}^{TE} = \tilde{Q}_{mp}^{TM} + O\left(k_s^3\right) \tag{B.22}
\]

where \(\gamma_p = \gamma_{zz}^p\). Substituting these relations in (B.8), we yield

\[
\lim_{k_s \to 0} \tilde{G}_{zz}^{E_J} = \lim_{k_s \to 0} \frac{i}{2 A_{cell} k_s^2 k_m z m I} \left[ k_y^2 \frac{\eta_n}{\eta_m} \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} + \frac{k_s^2}{k_m} k_m k_n \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} \right] \tag{B.23}
\]

\[
= \lim_{k_s \to 0} \frac{i}{2 A_{cell} k_s^2 k_m z m I} \left[ \left( k_y^2 \frac{\eta_n}{\eta_m} + \frac{k_s^2}{k_m} k_m k_n \right) \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} \right] \tag{B.24}
\]

Since we have \(k_m k_n = k_m k_m, k_m/k_m = \eta_n/\eta_m\), the above simplifies to

\[
\lim_{k_s \to 0} \tilde{G}_{zz}^{E_J} = \frac{i \eta_n}{2 \eta_m k_m A_{cell}} \gamma_p^{TM} \tilde{Q}_{mp}^{TM}(0; z, z') = \frac{i \eta_n \partial_{zz'} F^{TM}(0; z, z')}{2 \eta_m k_m k_n A_{cell}} \tag{B.25}
\]

which is a finite quantity with each factor evaluated at \(k_s = 0\). Following the same procedure, one can show that \(\lim_{k_s \to 0} \tilde{G}_{zz}^{E_J} = \lim_{k_s \to 0} \tilde{G}_{zz}^{E_J}\). But for other components of \(\tilde{G}_{zz}^{E_J}\), the contribution is nil when \(k_s \to 0\), which means that we can safely drop the term with \(k_s = 0\) for these components. If we adopt the decomposition

\[
(\nabla \times \hat{z}) (\nabla' \times \hat{z}) = k_s^2 \hat{I}_s - \nabla \nabla' + \nabla z \nabla' + \nabla \nabla' z - \nabla z \nabla \tag{B.26}
\]

\[
(\nabla \times \nabla \times \hat{z}) (\nabla' \times \nabla' \times \hat{z}) = \nabla \nabla' \partial_z \partial_{z'} + k_s^2 \nabla \nabla z + k_s^2 \nabla' \nabla' z + \frac{k_s^2}{k_m} \nabla \nabla' \zeta \tag{B.27}
\]

the finite contributions from \(\tilde{G}_{zz}^{E_J}\) and \(\tilde{G}_{zz}^{E_J}\) are effectively extracted, and the singularity at \(k_s = 0\) becomes a false one which can be discarded.

For \(\tilde{G}_{zz}^{H_J}(r, r')\), one can show that \(\tilde{G}_{zz}^{H_J}\) and \(\tilde{G}_{zz}^{H_J}\) would not vanish when \(k_s \to 0\). To be more detailed, we have

\[
\tilde{G}_{zz}^{H_J} = \frac{i}{2 A_{cell} k_s^2 k_m z m I} \left[ -\partial_{xx'} \partial_z F^{TE}(k_s I; z, z') + \frac{\mu_n}{\mu_m} \partial_{yy'} \partial_{z'} F^{TM}(k_s I; z, z') \right] \tag{B.28}
\]

\[
\tilde{G}_{zz}^{H_J} = \frac{i}{2 A_{cell} k_s^2 k_m z m I} \left[ -\partial_{xx'} \partial_z F^{TE}(k_s I; z, z') - \frac{\mu_n}{\mu_m} \partial_{yy'} \partial_{z'} F^{TM}(k_s I; z, z') \right] \tag{B.29}
\]

from which we get

\[
\lim_{k_s \to 0} \tilde{G}_{zz}^{H_J} = \lim_{k_s \to 0} \frac{-i}{2 A_{cell} k_s^2 k_m z m I} \left( ik_s^2 k_m \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} + i \frac{\mu_n}{\mu_m} k_s^2 k_m \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} \right) \tag{B.30}
\]

\[
\lim_{k_s \to 0} \tilde{G}_{zz}^{H_J} = \lim_{k_s \to 0} \frac{i}{2 A_{cell} k_s^2 k_m z m I} \left( ik_s^2 k_m \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} + i \frac{\mu_n}{\mu_m} k_s^2 k_m \gamma_p^{TM} F_{mn}^{TM} \tilde{Q}_{mp}^{TM} \right) \tag{B.31}
\]
Simplifying the above, one writes

\[
\lim_{k_s \to 0} \tilde{G}^{HJ}_{xy} = - \lim_{k_s \to 0} \tilde{G}^{HJ}_{yx} = \frac{i \mu_n \partial \tilde{z} F^{TM}(0; z, z')}{2 \mu_m k_m A_{cell}} \tag{B.32}
\]

which is the result given in (3.24). After going through the algebra, one finds that the rest of the components of \( \tilde{G}^{HJ} \) vanishes. This is why we propose the decomposition

\[
(\nabla \times \nabla \times \dot{z'}) (\nabla' \times \dot{z}) = (\nabla \partial \tilde{z} + k_n^2 \dot{z}) (\nabla' \times \dot{z}) \tag{B.33}
\]

\[
(\nabla \times \dot{z}) (\nabla' \times \nabla' \times \dot{z}) = \partial \tilde{z} k_s^2 \vec{I}_s + \nabla' (\nabla \times \dot{z}) \partial \tilde{z'} + k_{mz}^2 \dot{z} (\nabla \times \dot{z}) + k_s^2 (\nabla \times \dot{z}) \dot{z} \tag{B.34}
\]

with \( \vec{I}_s = \hat{x} \hat{y} - \hat{y} \hat{x} \), to account properly for the singularity at \( k_s = 0 \).
APPENDIX C. EWALD TRANSFORMATION FOR
DOUBLY PERIODIC STRUCTURE

The Ewald transformation is a very important theorem for the fast computation of periodic Green’s functions. It permits fast convergence of the series for the periodic Green’s function by splitting it into two parts, one is summed in spatial domain, while the other in spectral domain. This theorem can be expressed as [71]

\[ \sum_{L} \frac{e^{ikR_L}}{4\pi R_L} e^{ik_0 \cdot \rho_L} = \frac{1}{A_{cell}} \sum_{I} \frac{e^{-\gamma_{zI} |z-z'|}}{2\gamma_{zI}} e^{ik_{zI} \cdot (r_s-r_s')} = \Psi_1 + \Psi_2 \quad (C.1) \]

where

\[ \Psi_1 = \frac{1}{4A} \sum_{I} e^{ik_{zI} \cdot u} \sum_{\pm} \frac{e^{\pm \gamma_{zI} (z-z')}}{\gamma_{zI}} \text{Erfc} \left( \frac{\gamma_{zI}}{2E} \pm (z-z')E \right) \quad (C.2) \]

\[ \Psi_2 = \frac{1}{8\pi} \sum_{L} \frac{e^{\pm ikR_L}}{R_L} \sum_{\pm} \frac{e^{\pm ikR_L}}{R_L} \text{Erfc} \left( R_L E \pm \frac{i k}{2E} \right) \quad (C.3) \]

with \( R_L = |R - r_L| = \sqrt{p_L^2 + (z-z')^2} \), \( r_L = l_1a_1 + l_2a_2 = (x_L, y_L) \), \( L = (l_1, l_2) \in \mathbb{Z} \times \mathbb{Z} \), \( \gamma_{zI} = \sqrt{k_{zI}^2 - k^2} \), \( \text{Erfc} \) being the complementary error function, and \( E \) is a parameter properly chosen to ensure optimal convergence.

**Proof.** Firstly, we have the identity [70]

\[ \frac{e^{ikR}}{R} = \frac{2}{\sqrt{\pi}} \int_{0}^{\infty} e^{-R^2 \xi^2 + \frac{k^2}{4 \xi^2}} d\xi \quad (C.4) \]

where \( \xi \) is a complex variable and the integration path has to be chosen such that the integrand is finite when \( \xi \to 0 \) and decays when \( \xi \to \infty \). Splitting the integral into two parts, we obtain

\[ \frac{e^{ikR}}{R} = \frac{2}{\sqrt{\pi}} \left[ \left( \int_{0}^{E} + \int_{E}^{\infty} \right) e^{-R^2 \xi^2 + \frac{k^2}{4 \xi^2}} d\xi \right] \quad (C.5) \]
Then the spatial domain periodic Green’s function can be put as the sum of the following two parts:

\[ \Psi_1 = \frac{1}{2\pi\sqrt{\pi}} \sum_L \left[ \int_0^E e^{-R_L^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi \right] e^{ik_0 \cdot \rho_L} \] (C.6)

\[ \Psi_2 = \frac{1}{2\pi\sqrt{\pi}} \sum_L \left[ \int_E^\infty e^{-R_L^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi \right] e^{ik_0 \cdot \rho_L} \] (C.7)

For \( \Psi_2 \), using the identity that [99]

\[ \int_r^\infty e^{-p^2\xi^2 + \frac{q^2}{4\xi^2}} d\xi = \frac{\sqrt{\pi}}{4p} \sum_{\pm} e^{\pm ipq} \text{Erfc} \left( pr \pm \frac{iq}{2r} \right) \] (C.8)

we acquire

\[ \Psi_2 = \frac{1}{8\pi} \sum_L \left[ \frac{1}{R_L} \sum_{\pm} e^{\pm ikR_L \text{Erfc} \left( R_L E \pm \frac{i\xi}{2E} \right) } \right] e^{ik_0 \cdot \rho_L} \] (C.9)

where \( \rho_L = l_1 a_1 + l_2 a_2, \ u_s = r_s - r'_s, \ k_{s\downarrow} = k_0 + i_1 b_1 + i_2 b_2 = k_0 + k_{s\downarrow}, \ a_i \cdot b_j = 2\pi \delta_{ij} \).

For \( \Psi_1 \), we first use the Poisson summation formula to convert it to a spectral sum as

\[ \Psi_1 = \frac{1}{2\pi\sqrt{\pi}A_{cell}} \sum_L \left[ \tilde{f}(k_{s\downarrow}; z, z') \right] e^{ik_{s\downarrow} \cdot u} \] (C.10)

where \( \tilde{f}(k_{s\downarrow}; z, z') \) is the Fourier transform of the following

\[ f(u; z, z') = \int_0^E e^{-R^2 \xi^2 + \frac{k^2}{4\xi^2}} d\xi \]

\[ = \int_0^E e^{-(u^2 + \Delta z^2)\xi^2 + \frac{k^2}{4\xi^2}} d\xi \] (C.11)

\[ = \int_0^E e^{-u^2\xi^2 - \Delta z^2\xi^2 + \frac{k^2}{4\xi^2}} d\xi \]

with \( u = \rho - \rho', \ u = |u| \) and \( \Delta z = z - z' \). Then we have

\[ \tilde{f}(k_{s\downarrow}; z, z') = \int_0^E d\xi e^{-\Delta z^2\xi^2 + \frac{k^2}{4\xi^2}} \int_{\infty}^\infty e^{-u^2\xi^2} e^{-ik_{s\downarrow} \cdot u} du \] (C.12)

By using the Fourier transform pair

\[ e^{-\xi^2u^2} \leftrightarrow \pi \xi^{-2} e^{-k^2/(4\xi^2)} \] (C.13)
we yield

\[
\tilde{f}(k_s; z, z') = 2\pi \int_0^E \frac{1}{2s^2} e^{-\frac{k^2}{4s^2}} e^{-\Delta z^2 \xi^2 + \frac{k^2}{4s^2}} d\xi
\]

\[
= \pi \int_{E^{-1}}^{\infty} e^{-\frac{\Delta z^2}{s^2} + \frac{k^2 + \Delta s^2}{4s^2}} dx
\]

\[
= \pi \frac{\sqrt{\pi}}{2\gamma_s} \sum_\pm e^{\pm \gamma_s \Delta z} \text{Erfc} \left( \frac{\gamma_s}{2E} \pm \frac{\Delta z}{E} \right)
\]

which leads to

\[
\Psi_1 = \frac{1}{4A_{cell}} \sum_L \left[ \frac{1}{\gamma_s} \sum_\pm e^{\pm \gamma_s \Delta z} \text{Erfc} \left( \frac{\gamma_s}{2E} \pm \Delta z \right) \right] e^{ik_L \cdot u}
\]

Asymptotically, we have

\[
\tilde{\Psi}_1 = \sum_\pm e^{\pm \gamma_1 (z-z')} \gamma_1 \text{Erfc} \left[ \frac{\gamma_1}{2E} \pm (z-z')E \right] \sim c_{11} e^{-(k_1/E)^2}
\]

\[
\tilde{\Psi}_2 = \sum_\pm e^{\pm ikR_L} \frac{1}{R_L} \text{Erfc} \left( R_L E \pm \frac{ik}{2E} \right) \sim c_{2L} e^{-(\rho_L/E)^2}
\]

where \(c_{11}\) and \(c_{2L}\) are factors that are non-dominant for the decay. In the special case of a rectangular lattice, the above becomes

\[
\tilde{\Psi}_1 \sim c_{11} e^{-\frac{\pi^2}{E^2} \left( \frac{1}{a_1^2} + \frac{1}{a_2^2} \right)}
\]

\[
\tilde{\Psi}_2 \sim c_{2L} e^{-E^2 \left( \frac{1}{a_1^2} + \frac{1}{a_2^2} \right)}
\]

By requiring that the two series have the same rate of decay and use the same number of terms, we have an estimate of the parameter \(E\) as follows:

\[
\frac{\pi^2}{E^2 a_i^2} = E^2 a_i^2 \Rightarrow E = \frac{\sqrt{\pi} a_i}{a_i}
\]

Taking the geometric mean, we get

\[
E = \sqrt{\pi / A_{cell}}
\]

When the frequency is high, or the unit cell is large (meaning small value of \(E\)), the first few terms may have large imaginary arguments for the complementary error function in both \(\Psi_1\) and \(\Psi_2\),

\[
\text{Erfc} \left( \frac{\gamma_1}{2E} \pm \Delta z \right) \sim \frac{2iE}{\sqrt{\pi} k} e^{k^2/(4E^2)}
\]

\[
\text{Erfc} \left( R_L E \pm \frac{ik}{2E} \right) \sim \frac{2iE}{\sqrt{\pi} k} e^{k^2/(4E^2)}
\]
These terms are large and close to each other, which leads to cancellation error and loss of accuracy. A remedy is to give a lower bound to $E$, hence the following criteria can be adopted:

$$E = \max \left( \sqrt{\frac{\pi}{A_{cell}}}, \frac{k}{2H} \right)$$

where $H^2$ is a maximum permitted exponent. Notice that in our work, we have used the Ewald transformation with $k = i\kappa$ being purely imaginary. □