Wave scattering in frequency domain

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This report shows formulation of wave scattering in frequency domain. The formulation provides an understanding of S-matrix solver which is named as SMatrAn. It is an abbreviation for ‘Scattering Matrix Analyzer’ or ‘Scattering Matrix Analysis’.

The S-matrix has the whole of amplitude and phase information for reflected and transmitted waves from a complicated scatterer. Accurate S-matrix leads to quantitative evaluation of scattering wave. SMatrAn can provide useful information to engineers and scientists.

You can understand all formulas for the SMatrAn after reading this report. The S-matrix provided by SMatrAn will give you detailed analysis on complicated scattering in optical structure. I can hardly shorten its update period, but I will respond to needs from users as much as possible. Please let me know if you have any questions and comments.
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1. Introduction

Analysis of wave scattering will start from a propagation equation (3.1) in frequency domain. The equation can be derived from any fundamental equation, e.g. Maxwell equations, Shrödinger equation or Newton equation of motion. Chapter 2, 3 and 4 define analytical formulas for coordinates, modes and S-matrix. Chapter 5 focuses on roughness scattering by using the formulas. Chapter 6, 7 and 8 give us discrete formulation for numerical calculation. Appendix A, B, C, D, E, F, G, H and I show detailed derivations of the formulas. The following section 1.1 shows notation for the SMatrAn formulas before explaining details of the formulas.

1.1. Notation for the formulas

The report consists of many formulas. This section will show notation for the formulas.

1. Three dimensional coordinates are represented as \((x, y, z)\) or \((x_0, x_1, x_2)\), because cyclic permutation of the latter is directly related to modulo 3 operation. The report will also use \((r_0, r_1, r_2)\) or \((u_0, u_1, u_2)\). The \(z\), \(x_2\), \(r_2\) or \(u_2\) is propagating axis. The report chooses the above simpler notation in order to avoid mistakes in operating and programming physical models, and it will never use the general notation \((x_1, x_2, x_3)\).

2. Partial derivative by \(u_\nu\) is represented as \(\partial \partial u_\nu\) or \(\partial u_\nu\). Derivative of function is sometimes noted as \(\text{”}^n\text{”}\).

3. The report frequently uses matrix and vector notation, and it does not distinguish between the notations. Matrix and column vector are represented by bold symbol fonts as \(A\) for example. Especially, \(\Phi_\nu\) means column vector of the \(\nu\)-th mode. Transpose and Hermite operators are notated as \(\text{”}^T\text{”}\) and \(\text{”}^\dagger\text{”}\), respectively. The \(\text{”}^{*}\text{”}\) means complex conjugate, and then \(A^{\dagger}\) is represented as \(k^T r\), where \(k\) and \(r\) are wavenumber vector and position vector, respectively.

4. \((\partial / \partial x)^n\) means differential operator to the left side as \(f \partial (\partial / \partial x)^\dagger g = (\partial f / \partial x)^\dagger g\). Integration by parts gives us a relation: \((\partial / \partial x)^\dagger = -\partial / \partial x\) when \(f^\dagger g\) satisfies a periodic boundary condition.

5. Dual basis of \(\Phi_\nu\) is represented as \(\Phi_\nu^\dagger\). The product \(\Phi_\nu^\dagger \Phi_\nu\) includes integral for cross section. We will not explicitly show \(\int \int du_0 dh_1\).

6. Imaginary unit is denoted as \(i\). The \(\text{”}^i\text{”}\) will be only used as integer parameter, and \(\text{”}^l\text{”}\), \(\text{”}^m\text{”}\), \(\text{”}^n\text{”}\) and their capital letters are also integer. As an exception, the \(\text{”}^L_m\text{”}\) has a special meaning for system length, e.g. scattering region along the \(u_2\)-axis is defined as \(-L_n/2 < u_2 < +L_n/2\). The \(\text{”}^R\text{”}\) means correlation length for other exception. The modulo operation is used only for non-negative integer in order to avoid confusion caused by several definitions, and it is represented as \(\text{”mod”}\) or \(\text{”\%”}\). A notation \(\text{”\%3”}\) is frequently omitted in the modulo 3 operation.

7. Plane wave is defined as \(\exp (ik^T r - i \omega t)\), where \(\omega\) and \(t\) are angular frequency and time, respectively. The definition is well known in physics as eq. (34) in Chapter 1 of [1] and in other scientific society [2]. However it is different from the manner of engineering [3, 4]. If you usually use \(\exp (j \omega t - j k^T r)\) as the plane wave, the \(\text{”}^i\text{”}\) has to be replaced to \(\text{”}^{-i}\text{”}\) in the report. \(\beta_n\) is also used as a propagation constant of the \(n\)-th mode instead of wavenumber \(\text{”}^k\text{”}\).

8. Fourier-transform (FT) of \(f (z)\) is defined as \(\hat{f} (k) = \int_{-\infty}^{\infty} f (z) e^{-ikz} dz\). The inverse transformation is that \(f (z) = (2\pi)^{-1} \int_{-\infty}^{\infty} \hat{f} (k) e^{ikz} dk\). Discrete Fourier transform (DFT) is also defined as \(\hat{f}_{\text{DFT}}\) in Section 1.7.

9. The \(f [l]\) represents the discretization of a continuous function \(f (x)\), which also means an array.

10. The \(\text{”}^\dagger\text{”}\) and \(\text{”}^\ast\text{”}\), which are not wide as \(\text{”}^\dagger\text{”}\) nor \(\text{”}^\ast\text{”}\), mean temporary modification of parameters.

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2. Coordinate transformation for waveguide

This chapter reports coordinate transformation which can be applied to general waveguides. The goal is that we obtain the scale factors after transforming coordinates as shown in Fig. 2.1.

Let us consider two step transformation for orthogonal curvilinear coordinates such as \( x \Rightarrow r \Rightarrow u \). Considered waveguide is laid on the \( x_0x_2 \)-plane, and then \( x_1 \Rightarrow r_1 \Rightarrow u_1 \) is identity transformation. We will ignore the \( x_1 \)-axis in the following sections. The \( r_2 \)-axis and the \( u_2 \)-axis are propagation axis, and \(|r_2|,|u_2|<L_s/2\) (see section 1.1). Note that we will introduce two curvatures \( \kappa_b \) and \( \kappa_w \) to the transformation, and the region of \( r_0 \) (and \( u_0 \)) is limited by \( \kappa_b \) and \( \kappa_w \).

2.1. Two steps of the transformation: \( x \Rightarrow r \Rightarrow u \)

The first step \((x_0, x_2) \Rightarrow (r_0, r_2)\) is that

\[
\begin{align*}
x_2(r_0, r_2) &= \int_0^{r_2} f(r) \, dr - r_0 g(r_2), \\
x_0(r_0, r_2) &= \int_0^{r_2} g(r) \, dr + r_0 f(r_2), \\
f(r_2) &= \cos \left( \int_0^{r_2} \kappa_b(r) \, dr \right), \\
g(r_2) &= \sin \left( \int_0^{r_2} \kappa_b(r) \, dr \right).
\end{align*}
\]

(2.1)

Section A.1 in Appendix A shows details of the above transformation. Equation (A.1) ensures that the coordinates \((r_0, r_2)\) are orthogonal curvilinear coordinates. Note that \( \kappa_b(r_2) \) is a signed curvature for waveguide bending as shown in Fig. 2.1, since eq. (A.4) gives us the definition of signed curvature:

\[
\kappa_b = \frac{\frac{\partial x_0}{\partial r_2} \frac{\partial^2 x_0}{\partial r_2^2} - \frac{\partial x_2}{\partial r_2} \frac{\partial^2 x_0}{\partial r_2^2}}{\left( \frac{\partial x_0}{\partial r_2} \right)^2 + \left( \frac{\partial x_2}{\partial r_2} \right)^2} \bigg|_{r_0=0}^{3/2}.
\]
The second step \((r_0, r_2) \Rightarrow (u_0, u_2)\) is defined by

\[
\begin{align*}
2.1 \quad r_2 (u_0, u_2) &= u_2 - \int_0^{u_0} F_{\text{2D}} (r_0 (u, u_2), r_2 (u, u_2)) \, du, \\
r_0 (u_0, u_2) &= u_0 \zeta (r_2 (u_0, u_2)), \\
F_{\text{2D}} (r_0, r_2) &= \frac{r_0 \kappa_w (r_2) \zeta (r_2)}{(1 - r_0 \kappa_b (r_2))^2 + (r_0 \kappa_w (r_2))^2}, \\
\zeta (r_2) &= \exp \left( \int_0^{r_2} \kappa_w (r) \, dr \right).
\end{align*}
\] (2.2)

Equations (A.5), (A.6) and (A.7) in Section A.2 ensure that the coordinates \((u_0, u_2)\) are orthogonal curvilinear coordinates. Note that \(\kappa_w (r_2 (0, u_2))\) is a signed curvature for waveguide broadening as shown in Fig. 2.1, since eq. (A.8) give us the definition of signed curvature:

\[
\kappa_w = \left. \frac{\partial^2 x_j}{\partial u_0 \partial u_2} \left( \left( \frac{\partial x_0}{\partial u_0} \right)^2 + \left( \frac{\partial x_2}{\partial u_0} \right)^2 \right)^{3/2} \right|_{u_0=0}.
\]

The region of \(u_0\) must be numerically checked by eqs. (2.1) and (2.2) after setting an initial condition:

\[
|u_0| < \min_{-L/2 < r < L/2} \left( \frac{1}{\zeta (r) \max (|\kappa_b (r)|, |\kappa_w (r)|)} \right).
\]

### 2.2. Scale factor

Let us obtain scale factor \(h_0\) and \(h_2\) from eqs. (A.9) and (A.10) in Section A.3.

\[
\begin{align*}
2.2 \quad h_0 &\triangleq \frac{2}{\sum_{j=0}^2 \left( \frac{\partial x_j}{\partial u_0} \right)^2} \sqrt{\left( \frac{\partial x_0}{\partial u_0} \right)^2 + \left( \frac{\partial x_2}{\partial u_0} \right)^2} = \frac{(1 - r_0 \kappa_b)}{\sqrt{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2}}, \\
2.2 \quad h_2 &\triangleq \frac{2}{\sum_{j=0}^2 \left( \frac{\partial x_j}{\partial u_2} \right)^2} \sqrt{\left( \frac{\partial x_0}{\partial u_2} \right)^2 + \left( \frac{\partial x_2}{\partial u_2} \right)^2} = \frac{\partial r_2}{\partial u_2} \sqrt{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2}.
\end{align*}
\] (2.3)

Note that \(\kappa_b, \kappa_w\) and \(\zeta\) are functions of \(r_2\). The \(\partial r_2/\partial u_2\) for \(h_2\) can be numerically solved by

\[
\begin{align*}
\partial r_2 (u_0, u_2) &= 1 - \int_0^{u_0} \left[ \frac{\partial}{\partial u_2} F_{\text{2D}} (r_0 (u, u_2), r_2 (u, u_2)) \right] \, du, \\
\partial F_{\text{2D}} (r_0, r_2) = \partial r_2 \frac{r_0 \zeta}{\kappa_w (1 - r_0 \kappa_b)^2 + 2 \kappa_w (1 - r_0 \kappa_b) (\kappa_w + r_0 \kappa_b') - r_0^2 \kappa_w^2 \kappa_w'}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2}.
\end{align*}
\] (2.4)

where \(\kappa' = d\kappa_b/\partial r_2\) and \(\kappa'_w = d\kappa_w/\partial r_2\). See eq. (A.11) for details of \(\partial F_{\text{2D}}/\partial u_2\).

When \(|u_0 \kappa_b|, |u_0 \kappa_w| \ll 1\) and \(|u_0^2 \kappa'_b|, |u_0^2 \kappa'_w| \ll 1\), eq. (2.3) is approximated to

\[
\begin{align*}
2.5 \quad h_0 &\simeq \zeta (u_2), \\
2.5 \quad \Delta h_2 &\triangleq h_2 - 1 \simeq -u_0 \zeta \kappa_b - \frac{u_0^2}{2} \zeta^2 \kappa'_w.
\end{align*}
\] (2.5)

Note that \(r_2\) can be replaced to \(u_2\), since \(r_2 = u_2 - O (u_0^2 \kappa_w)\) from eq. (2.2).

When a condition \(\zeta \simeq 1\), i.e. \(|\kappa_w| \ll 2/L\) is applied to eq. (2.5), \(h_0\) and \(h_2\) are furthermore approximated to

\[
\begin{align*}
2.6 \quad \Delta h_0 &\triangleq h_0 - 1 \simeq \int_0^{u_2} \kappa_w (u) \, du, \\
\Delta h_2 &\triangleq h_2 - 1 \simeq -u_0 \kappa_b - \frac{u_0^2}{2} \kappa'_w.
\end{align*}
\]

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3. Propagation equation

Fundamental equations, which are Maxwell equation, Shrödinger equation and Newton equation of motion, can be unified to an equation focused on wave propagation in frequency domain $\omega$. All analysis in the report derives from the propagation equation.

3.1. Basic relations from propagation equation

Wave-function $\Psi = (\psi_\alpha^T \psi_\beta^T)^T$ as a column vector satisfies the following propagation-equation along propagation axis $u_2$:

$$M\Psi = -i \frac{\partial}{\partial u_2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi. \quad (3.1)$$

The $2 \times 2$ matrix elements in the right hand side are square submatrices. Each submatrix is the same size as continuous (or discretized) fields in 2D cross-section of the modes. The square matrix $M$ does not have $\partial^2$, that is, $M u_2^2 = u_2 M$. We introduce generalized power-flow $P$ along the $u_2$ axis, and conservation of the power flow is derived from eq. (3.1):

$$\begin{cases} P(u_2) \triangleq \Psi^\dagger (u_2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi(u_2) , \\ \frac{\partial P}{\partial u_2} = i \Psi^\dagger (M - M^\dagger) \Psi. \end{cases} \quad (3.2)$$

The right hand side of the second in eq. (3.2) means power dissipation or power gain. When $M = M^\dagger$, the system has no power-loss for wave propagation.

We also consider the following eigen-mode equation with replacing $-i \partial_2$ to propagation constant $\beta_n$ as the $n$-th eigenvalue for eq. (3.1):

$$M \Phi_n = \beta_n \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_n. \quad (3.3)$$

The orthogonality of modes is derived from eq. (3.3) with $M = M^\dagger$.

$$\Phi_m^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_n = 0 \quad \text{for} \quad \beta_m^* \neq \beta_n. \quad (3.4)$$

Previous work has already discussed orthogonality relation of propagation modes (see equations (3.2-24) in [3] and (10.120) in [4]). We can set power-flow normalization and mode numbering for real $\beta_n$ with satisfying that

$$\Phi_n^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_n = \frac{n}{|n|} \quad \text{for} \quad n \neq 0. \quad (3.5)$$

The above numbering physically means that power flow for positive (negative) $n$ is always positive (negative). If we happen to have a mode with exactly zero power-flow and real $\beta_n$, we can number the mode as $n = 0$ and normalize it as $\Phi_0^\dagger \Phi_0 = 1$. There is a maximum number $n_{\text{max}} \triangleq \max |n|$ for real $\beta_n$. Non-real $\beta_n$ is numbered $n \gtrless \pm n_{\text{max}}$ with satisfying $n \text{Im}\beta_n > 0$, that is, the $n > n_{\text{max}}$ ($n < -n_{\text{max}}$) means evanescent (divergent) wave along the $u_2$ axis. A pair of complex conjugate $\beta_n$ is also set as $\beta_n = \beta_n^*$, and the pair is normalized as

$$\Phi_n^\dagger \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_{-n} = 1 \quad \text{for} \quad n \gtrless \pm n_{\text{max}}. \quad (3.6)$$

All of $\beta_n$ consists of real numbers and/or complex conjugate pairs when $M = M^\dagger$, because a secular equation for generalized eigenvalue problem $AX = \lambda BX$ can be deformed into $|A - \lambda B| = |A^\dagger - \lambda^* B^\dagger| = 0$. Note that the
numbering of the complex conjugate pairs except for pure imaginary \( \beta_n \) is different from one of Fig. 10.14 and eq. (10.125) in [4]. Here, we try to define dual basis \( \tilde{\Phi}_n \) for the basis \( \Phi_n \):

\[
\tilde{\Phi}_n = \begin{cases} 
\frac{1}{n} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_n & \text{for } 0 < |n| \leq n_{\text{max}}, \\
\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_{-n} & \text{for } |n| > n_{\text{max}}, \\
\Phi_0 - \sum_{m \neq 0} (\Phi_m^\dagger \Phi_0) \Phi_m & \text{for } n = 0. 
\end{cases}
\tag{3.7}
\]

Equation (3.4) and the above normalization rules give us bi-orthogonality [2, 5] and p. 285 of [6] as

\[
\Phi_m^\dagger \tilde{\Phi}_n = \delta_{mn}, \quad \text{and } \sum_n \Phi_n \tilde{\Phi}_n = 1.
\]

The \( n = 0 \) will be void below, because practical calculations can avoid it by slightly shifting the frequency \( \omega \).

The mode equation (3.3) can be extended to periodic system using the \( M_p \) of eq. (B.8) in Appendix B. Note that the representation basis with non-real eigenvalue of the \( M_p \) have to be redefined to satisfy eq. (3.5) as shown in eq. (B.6).

### 3.2. Special cases of mode equation

Appendices C, D and E show details of eq. (3.1) for the Shrödinger equation, Maxwell’s equations and Newton’s equation of motion, respectively.

This section focuses on two special cases: Shrödinger equation (C.1) when \( \varepsilon = 0 \), and Maxwell equation (D.1) when \( \varepsilon \) and \( \mu \) are diagonal hermitian and \( \alpha = \gamma = 0 \). From eqs. (C.3) and (D.13), the propagation equation (3.1) becomes that

\[
M \Psi = \begin{pmatrix} m_{aa} & 0 \\ 0 & m_{bb} \end{pmatrix} \Psi = -i \frac{\partial}{\partial u_2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi.
\]

Then,

\[
m_{aa} \psi_a = -\frac{\partial \psi_b}{\partial u_2}, \quad m_{bb} \psi_b = -\frac{\partial \psi_a}{\partial u_2}.
\]

For eq. (C.3), \( m_{aa} \) and \( m_{bb} \) are Hermite matrix and a real number, respectively. For eq. (D.13), \( m_{aa} \) and \( m_{bb} \) are real symmetric matrices. The mode equation (3.3) is also that \( m_{aa} \phi_{an} = \beta_n \phi_{an} \) and \( m_{bb} \phi_{bn} = \beta_n \phi_{bn} \) as \( \Phi_n = (\phi_n^T \phi_n^T) \). Therefore, eigenvalue problem for \( \beta_n \) is solved by

\[
m_{bb} m_{aa} \beta_n^2 = \beta_n^4 \phi_{an} \quad \text{or} \quad m_{aa} m_{bb} \beta_n^2 = \beta_n^4 \phi_{bn}.
\]

For the special case of Shrödinger equation (C.3), square of the eigenvalue \( \beta_n^2 \) is always real, since \( (m_{bb} m_{aa})^\dagger = m_{aa} m_{bb} = m_{bb} m_{aa} \). Furthermore, the \( \Phi_n \) satisfies the simpler orthogonality:

\[
\phi_{am}^\dagger \phi_{an} = \phi_{bn}^\dagger \phi_{bn} = 0 \quad \text{when } \beta_{n}^2 \neq \beta_{m}^2.
\tag{3.8}
\]

The special case (C.6) for 2D tight-binding model (C.4) has the same properties as the above.

For the special case of Maxwell equation (D.1), properties of the \( \Phi_n \) are different from them for Shrödinger equation. The \( \beta_n^2 \) is real or complex, since \( (m_{bb} m_{aa})^\dagger = m_{aa} m_{bb} \neq m_{bb} m_{aa} \) for eq. (D.13). The \( \Phi_n \) does not always satisfy eq. (3.8).

### 3.3. Perfectly matched layer (PML) method

The dominating way for treating unbounded problems in numerical simulation is with the PML method [7]. From eq. (1) with \( \zeta = 1 \) of [8] and eq. (2.7) of [9], equation (3.3) can be modified to

\[
[1 + i \tilde{\sigma}_2 (u_2)] M e^{i \beta_n \int_{-\infty}^{\infty} [1 + i \tilde{\sigma}_2(z)] dz} \Phi_n = -i \frac{\partial}{\partial u_2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} e^{i \beta_n \int_{-\infty}^{\infty} [1 + i \tilde{\sigma}_2(z)] dz} \Phi_n.
\tag{3.9}
\]

Note that \( n \tilde{\beta}_n \tilde{\sigma}_2 \geq 0 \) when \( 0 < |n| \leq n_{\text{max}} \). The theoretical reflectance \( |R_n|^2 \) of PML with thickness \( d \) and power number \( M \) is defined as eq. (3) of [10]:

\[
|R_n|^2 = \exp \left[ -4 |\beta_n| d \max (\tilde{\sigma}_2) / (M + 1) \right], \quad \text{where } d \gtrsim 2 \lambda_0 / 3 \text{ for vacuum wavelength } \lambda_0, \text{ and } M = 2, 3, \text{ or } 4 [9, 10].
\]

Details of PML formulation for Maxwell’s equations will be shown in eq. (6.6).

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4. Non-adiabatic transition in frequency domain

This chapter discusses non-adiabatic transition by using adiabatic picture. Equation (3.1) is slightly modified to

\[ [M^{(0)}(z) + M^{(1)}(z)] \Psi(z) = -i \frac{\partial}{\partial z} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi(z), \]  

(4.1)

where the \( M^{(0)} \) always satisfies that \( M^{(0)} = M^{(0)\dagger} \), but the additional term \( M^{(1)} \) has no limit of Hermitian property. Equation (4.1) has boundaries at \( a \) and \( b \) as \( -L_s/2 \leq a < b \leq L_s/2 \) (see section 1.1). The \( M^{(0)} \) and \( M^{(1)} \) satisfy the following conditions as

\[ \frac{\partial M^{(0)}}{\partial z} = 0 \text{ and } M^{(1)} = 0 \text{ when } z \leq a \text{ or } b \leq z. \]  

(4.2)

The eigen-mode equation (3.3) is rewritten as

\[ M^{(0)}(z) \Phi_m(z) = \beta_m(z) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_m(z). \]

4.1. Adiabatic picture

To discuss the \( \Psi(z) \) in eq. (4.1), we introduce adiabatic picture:

\[ \Psi_m^{(0)}(z) \triangleq \exp \left( i \int_0^z \beta_m(u) \, du \right) \Phi_m(z) \quad \text{and} \quad \Psi_m^{(0)\dagger}(z) \triangleq \Phi_m^{\dagger}(z) \exp \left( -i \int_0^z \beta_m(u) \, du \right), \]  

(4.3)

where eqs. (3.7) and (4.3) give us

\[ \tilde{\Psi}_m^{(0)\dagger}(z) \Psi_m^{(0)}(z) = \delta_{mn} \quad \text{and} \quad \sum_{m \neq 0} \Psi_m^{(0)}(z) \tilde{\Psi}_m^{(0)\dagger}(z) = 1. \]  

(4.4)

The \( \tilde{\Psi}_m^{(0)\dagger}(z) \) and \( \Psi_m^{(0)}(z) \) can also represent \( \langle \tilde{\Psi}_m^{(0)}(z) | \Psi_m^{(0)}(z) \rangle \) using the bra-ket notation, respectively. Equations (4.3) and (4.4) describe the operators \( M^{(0)}(z) \) and \( M^{(1)}(z) \) in eq. (4.1) as

\[ M^{(0)}(z) = \sum_{m \neq 0} \beta_m(z) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi_m^{(0)}(z) \tilde{\Psi}_m^{(0)\dagger}(z) \quad \text{and} \quad M^{(1)}(z) = \sum_{m,n \neq 0} M_{mn}^{(1)} \Psi_m^{(0)}(z) \tilde{\Psi}_n^{(0)\dagger}(z). \]  

(4.5)

From eqs. (4.5) and (4.3), the \( \Psi_m^{(0)}(z) \) satisfies that

\[ \left[ \frac{\partial}{\partial z} - i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} (M^{(0)} + M^{(1)}) \right] \Psi_m^{(0)}(z) = \left[ D(z) - i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} M^{(1)}(z) \right] \Psi_m^{(0)}(z) + \Psi_m^{(0)}(z) \frac{\partial}{\partial z}, \]  

(4.6)

where

\[ D(z) \triangleq \sum_{n \neq 0} \exp \left( i \int_0^z \beta_n(u) \, du \right) \frac{\partial \Phi_n}{\partial z} \tilde{\Psi}_n^{(0)\dagger}(z) = \sum_{m,n \neq 0} \Psi_m^{(0)}(z) D_{mn}(z) \tilde{\Psi}_n^{(0)\dagger}(z), \]

\[ D_{mn} = \Phi_m^{\dagger}(z) \exp \left( -i \int_0^z (\beta_m(u) - \beta_n(u)) \, du \right) \frac{\partial \Phi_n}{\partial z}. \]  

(4.7)
4.2. Lippmann-Schwinger equation

We show the following Lippmann-Schwinger equation for the $n$-th mode with outgoing “+” (incoming “−”) scattered wave:

$$
\Psi_n^{(\pm)}(z) = \Psi_n^{(0)}(z) + \int_a^b G_0^{(\pm)}(z, z') \tilde{M}(z') \Psi_n^{(\pm)}(z') \, dz'.
$$

(4.8)

Here we introduce an adiabatic Green operator $G_0^{(\pm)}(z, z')$ to eq. (4.8):

$$
G_0^{(\pm)}(z, z') \equiv \pm \sum_{m \neq 0} \Psi_m^{(0)}(z) \frac{m}{|m|} H \left( \pm \frac{m}{|m|} (z - z') \right) \tilde{\Psi}_m^{(0)}(z')
$$

(4.9)

with using the Heaviside step function

$$
H(z) = \begin{cases} 
1, & z > 0, \\
0, & z < 0.
\end{cases}
$$

The $\tilde{M}$ in eq. (4.8) is also defined by

$$
\tilde{M}(z) \equiv -D(z) + i \left( \begin{array}{cc} 0 & 1 \\
1 & 0 \end{array} \right) \left[ \sum_{m,n \neq 0} \Psi_m^{(0)}(z) \tilde{M}_{mn}(z) \Psi_n^{(0)\dagger}(z) \right],
$$

(4.10)

We can show the Dyson equation for the non-adiabatic transition.  

4.3. Dyson equation and T-matrix equation

We can show the Dyson equation for the non-adiabatic transition.

$$
G^{(\pm)}(z_0, z') \equiv G_0^{(\pm)}(z_0, z') + \sum_{N=2}^{\infty} \prod_{j=1}^{N-1} \int_a^b dz_j G_0^{(\pm)}(z_{j-1}, z_j) \tilde{M}(z_j)
$$

$$
= G_0^{(\pm)}(z_0, z') + \int_a^b dz_1 G_0^{(\pm)}(z_0, z_1) \tilde{M}(z_1) G^{(\pm)}(z_1, z').
$$

The T-matrix called as the transition matrix can be also introduced into the non-adiabatic transition as

$$
T^{(\pm)}(z_0) \equiv \tilde{M}(z_0) \left[ 1 + \sum_{N=1}^{\infty} \prod_{j=1}^{N-1} \int_a^b dz_j G_0^{(\pm)}(z_{j-1}, z_j) \tilde{M}(z_j) \right] = \tilde{M}(z_0) \left[ 1 + \int_a^b dz_1 G_0^{(\pm)}(z_0, z_1) T^{(\pm)}(z_1) \right].
$$

(4.12)
The perturbed Green operator $G^{(\pm)}$ or the T-matrix $T^{(\pm)}$ represents eq. (4.8) as

$$
\Psi_n^{(\pm)}(z_0) - \Psi_n^{(0)}(z_0) = \sum_{N=1}^{\infty} \left[ \prod_{j=1}^{N} \int_a^b dz_j G_0^{(\pm)}(z_{j-1}, z_j) \dot{M}(z_j) \right] \Psi_n^{(0)}(z_N)
= \int_a^b dz' G^{(\pm)}(z_0, z') \dot{M}(z') \Psi_n^{(0)}(z') = \int_a^b dz' G_0^{(\pm)}(z_0, z') T^{(\pm)}(z') \Psi_n^{(0)}(z') .
$$

(4.13)

Note that the T-matrix of eq. (4.12) is different from transfer matrix discussed in Section B.2.

4.4. S-matrix and its Born approximation

We define elements of S-matrix which is discussed in Section B.1:

$$
S_{mn} = \begin{cases} 
\bar{\Psi}^{(0)\dagger}_m(b) \Psi_n^{(\pm)}(b) = \delta_{mn} + \int_a^b dz T^{(\pm)}_{mn}(z) & \text{for } m > 0, \\
\bar{\Psi}^{(0)\dagger}_m(a) \Psi_n^{(\pm)}(a) = \delta_{mn} - \int_a^b dz T^{(\mp)}_{mn}(z) & \text{for } m < 0.
\end{cases}
$$

(4.14)

The S-matrix shows the outgoing waves scattered in the region: $-L_s/2 \leq a < z < b \leq +L_s/2$. The SMatrAn can numerically create the S-matrix of eq. (4.14) by directly solving the propagation equation (3.1).

If we consider the $\dot{M}$ as a small perturbation term, we can apply the Born approximation to eq. (4.12):

$$
T(z) = \dot{M}(z) + O(\|\dot{M}\|^2).
$$

The $S$ of eq. (4.14) is approximated to

$$
S_{mn} \simeq \begin{cases} 
\delta_{mn} + \int_a^b \dot{M}_{mn}(z) dz & \text{for } m > 0, \\
\delta_{mn} - \int_a^b \dot{M}_{mn}(z) dz & \text{for } m < 0.
\end{cases}
$$

(4.15)

Equations (4.11) and (4.15) give us two pictures for wave-scattering. When $M^{(1)} = 0$,

$$
\|S - 1\| \propto \left\| \frac{\partial M^{(0)}}{\partial z} \right\|
$$

which shows non-adiabatic transition in adiabatic structure. When $\partial M^{(0)}/\partial z = 0$ and $\Im M^{(1)} \neq 0$,

$$
|S_{nn}|^2 = 1 - O \left( \left\| iM^{(1)} \right\|^2 \right) \quad \text{and} \quad |S_{mn}|^2 = O \left( \left\| iM^{(1)} \right\|^2 \right) \quad \text{for } m \neq n .
$$

Then, we can ignore scattered power from weak absorber as compared to absorbed power in it.

The Born approximation of eq. (4.15) is suit for not only understanding scattering process but also evaluating roughness scattering. The following section shows the roughness scattering in the framework of the Born approximation.
5. Roughness scattering

We introduce parameter diagonal matrix \( \mathbf{V} (u_0, u_1, u_2) \) into \( \mathbf{M} \) in eq. (3.1), and the \( \mathbf{V} \) consists of several scalar functions of \( u_0, u_1 \) and \( u_2 \) for the media. The \( \mathbf{M} \) consists of \( \partial_{u_0}, \partial_{u_1} \) and \( \mathbf{V} \), and it is linear with \( \mathbf{V} \), i.e. \( \mathbf{M} (\eta \mathbf{V}) = \eta \mathbf{M} (\mathbf{V}) \). We separate the \( \mathbf{V} \) into adiabatic part \( \mathbf{V}^{(0)} \) and non-adiabatic part \( \mathbf{V}^{(1)} \) to use eq. (4.1) as

\[
\mathbf{M}^{(0)} = \mathbf{M} \left( \mathbf{V}^{(0)} \right) \quad \text{and} \quad \mathbf{M}^{(1)} = \mathbf{M} \left( \mathbf{V}^{(1)} \right). \tag{5.1}
\]

5.1. Edge roughness of straight waveguide

When the \( \mathbf{M}^{(0)}(u_2) \) does not depend on \( u_2, \beta_n \) and \( \Phi_n \) are constant for \( u_2 \) (or \( z \)), and then this case simplifies eq. (4.11) for \( 0 < |m| \leq n_{\text{max}} \)

\[
\hat{\mathbf{M}}_{mn}(u_2) = i \frac{m}{|m|} \Psi_m^{(0)\dagger}(u_2) \mathbf{M}^{(1)}(u_2) \Psi_n^{(0)}(u_2) = i \frac{m}{|m|} e^{-i(\beta_m - \beta_n)u_2} \Phi_m^{\dagger} \mathbf{M}^{(1)}(u_2) \Phi_n. \tag{5.2}
\]

Fourier transform (FT) of the above \( \mathbf{M}^{(1)} \) can be used as

\[
\int_{-L_s/2}^{L_s/2} \hat{\mathbf{M}}_{mn}(u_2) du_2 = i \frac{m}{|m|} \Phi_m^{\dagger} \left[ \int_{-\infty}^{\infty} \mathbf{M}^{(1)}(u_2) e^{-i(\beta_m - \beta_n)u_2} du_2 \right] \Phi_n = i \frac{m}{|m|} \Phi_m^{\dagger} \mathbf{M}^{(1)}(\beta_m - \beta_n) \Phi_n, \tag{5.3}
\]

since \( \mathbf{M}^{(1)} = 0 \) for \( |u_2| > L_s/2 \). Then equation (4.15) can be deformed by eqs. (5.1) and (5.2):

\[
S_{mn} - \delta_{mn} \simeq i \Phi_m^{\dagger} \mathbf{M}^{(1)}(\beta_m - \beta_n) \Phi_n = i \Phi_m^{\dagger} \mathbf{M} \left( \mathbf{V}^{(1)}(\beta_m - \beta_n) \right) \Phi_n. \tag{5.3}
\]

Let us apply eqs. (5.2) and (5.3) to wave scattering by waveguide edge roughness. The straight waveguide without roughness has a constant waveguide-width \( W_{\text{wg}} \) and a constant waveguide-height \( V_{\text{wg}} \), such as the abrupt case shown in Fig. 5.1. The \( L_s \) means scattering region as mentioned in section 1.1. This section focuses on roughness by two edges at \( u_0 = \pm W_{\text{wg}}/2 \). Note that the unperturbed part \( \mathbf{V}^{(0)} \) does not depend on \( u_2 \), and it is function only of \( u_0 \) and \( u_1 \).

Here, we add two kinds of roughness functions \( A_w(z) \) and \( A_c(z) \) as shown in Fig. 5.2 to the straight waveguide in Fig. 5.1. The \( A_w \) and \( A_c \) represent line width roughness (LWR) and line center roughness (LCR)[11], respectively. We try to import the roughness functions into the perturbed part \( \mathbf{V}^{(1)} \) of eq. (5.3). There are two approaches of importing the roughness functions.

5.1.1. Approach I

The first approach describes the roughness as displacement of waveguide media, and then the \((u_0, u_1, u_2)\) coordinates are merely identity transformation of the \((x_0, x_1, x_2)\) coordinates, i.e. \( h_j = 1 \) for \( j = 0, 1, 2 \). The perturbed
Figure 5.2: Two kinds of edge roughness: (a) line width roughness (LWR) and (b) line center roughness (LCR).

part \( V^{(1)} \) can be regarded as function of \( u_2 \) via \( A_w \) and \( A_c \) from Fig. 5.2:

\[
V^{(1)} (A_w (u_2), A_c (u_2)) = V^{(0)} \left( \frac{u_2}{1 + A_w/W_{wg}} - A_c, u_1 \right) - V^{(0)} (u_0, u_1) \\
\simeq V^{(0)} (u_2 - u_0 A_w/W_{wg} - A_c, u_1) - V^{(0)} (u_0, u_1) \simeq - \left[ \frac{u_0 A_w(u_2)}{W_{wg}} + A_c(u_2) \right] \frac{\partial V^{(0)} (u_0, u_1)}{\partial u_0}.
\]

(5.4)

when \( A_w/2, A_c \ll W/2 \). In the framework of the above formulation (5.4), the \( \hat{V}^{(1)} (k) \) in eq. (5.3) is given by

\[
\hat{V}^{(1)} (k) = - \left[ \frac{u_0 A_w(k)}{W_{wg}} + \hat{A}_c(k) \right] \frac{\partial V^{(0)} (u_0, u_1)}{\partial u_0}.
\]

(5.5)

For abrupt structure of the waveguide, \( V^{(0)} \) and \( V^{(1)} \) can be set as

\[
\begin{aligned}
V^{(0)} &= V_{clad} + V_{pp} (u_1) H \left( \frac{W_{wg}}{2} - u_0 \right) H \left( \frac{W_{wg}}{2} + u_0 \right), \\
V^{(1)} &= - \left[ \frac{u_0 A_w(u_2)}{W_{wg}} + A_c(u_2) \right] V_{pp} (u_1) \left[ -\delta \left( \frac{W_{wg}}{2} - u_0 \right) + \delta \left( \frac{W_{wg}}{2} + u_0 \right) \right] \\
&= \left[ \frac{1}{2} A_w(u_2) + \frac{u_0}{W_{wg}/2} A_c(u_2) \right] V_{pp} (u_1) \delta \left( \frac{W_{wg}}{2} - |u_0| \right), \\
\hat{V}^{(1)} &= \left[ \frac{1}{2} \hat{A}_w(k) + \frac{u_0}{W_{wg}/2} \hat{A}_c(k) \right] V_{pp} (u_1) \delta \left( \frac{W_{wg}}{2} - |u_0| \right).
\end{aligned}
\]

(5.6)

The first term \( V_{clad} \) for \( V^{(0)} \) is constant. The \( H \) in the above equation is Heaviside step function used for eq. (4.9). The \( V^{(1)} \) and \( \hat{V}^{(1)} \) of eq. (5.6) are derived by using eqs. (5.4) and (5.5) respectively.

5.1.2. Approach II

The second approach describes the roughness as space curvature. In the \((u_0, u_1, u_2)\) coordinates, the waveguide with roughness becomes straight as shown in Fig. 5.1. The perturbed part \( V^{(1)} \) can be regarded as a function of \( u_2 \) via the changes of scale factors \( \Delta h_0 \) and \( \Delta h_2 \) which are defined in eq. (2.6), and then it is represented as \( V^{(1)} (\Delta h_0, \Delta h_2) \).

From Section 2.1 and Fig. 5.2, the two curvatures \( \kappa_w \) and \( \kappa_b \) are related to the two roughness \( A_w \) and \( A_c \) when \(|\kappa_w|, |\kappa_b| \ll W_{wg}^{-1}\). The \( \kappa_w \) and \( \kappa_b \) are given by

\[
\kappa_w (u_2) \simeq \frac{1}{W_{wg}} \frac{dA_w(u_2)}{du_2} \quad \text{and} \quad \kappa_b (u_2) \simeq \frac{d^2A_c(u_2)}{du_2^2}.
\]

From eq. (2.6), the \( \Delta h_0 \) and \( \Delta h_2 \) are given by the roughness functions:

\[
\Delta h_0 (u_2) \simeq \frac{A_w(u_2)}{W_{wg}} \quad \text{and} \quad \Delta h_2 (u_0, u_2) \simeq -u_0 \frac{d^2A_c}{du_2^2} - \frac{u_0^2}{2W_{wg}} \frac{d^2A_w}{du_2^2}.
\]

The \( \hat{V}^{(1)} (k) \) of eq. (5.3) is given by FT of \( \Delta h_0 \) and \( \Delta h_2 \) as

\[
\begin{aligned}
\hat{V}^{(1)} (k) &\simeq V^{(1)} \left( \Delta h_0 (k), \Delta h_2 (u_0, k) \right), \\
\hat{\Delta h}_0 (k) &\simeq \frac{1}{W_{wg}} \hat{A}_w(k) \quad \text{and} \quad \hat{\Delta h}_2 (u_0, k) \simeq u_0 k^2 \hat{A}_c (k) + \frac{u_0^2}{2W_{wg}} k^2 \hat{A}_w (k).
\end{aligned}
\]

(5.7)
The representation of eq. (5.5) is different from one of eq. (5.7), but two representations should give us the same results for roughness scattering. Cross-check by eqs. (5.5) and (5.7) will show the validity of the formulation in this chapter.

### 5.2. Auto-correlation function of roughness

Let us consider ensemble average for roughness $A_{\nu}$ as $\nu = \omega, \epsilon$. This section introduces normalized roughness $a_{\nu}$ defined by

$$a_{\nu} (u_2) = \frac{A_{\nu} (u_2)}{\sqrt{L_s}},$$

(5.8)

since we presume that the integral of $A_{\nu}^2 (u_2)$ is related to $L_s$ under randomness. Note that $A_{\nu} (u_2) = a_{\nu} (u_2) = 0$ when $|u_2| \geq L_s/2$.

We define an auto-correlation function $R_{\nu}$ for roughness $A_{\nu}$:

$$R_{\nu} (z) \triangleq \frac{1}{L_s} \int_{-\infty}^{\infty} A_{\nu} (z') A_{\nu} (z' + z) \, dz' = \int_{-\infty}^{\infty} \langle a_{\nu} (z') a_{\nu} (z' + z) \rangle \, dz',$$

(5.9)

where $\langle \cdots \rangle$ means ensemble average. A power spectral density (PSD) $G_{\nu} (k)$ can be also defined by

$$G_{\nu} (k) \triangleq \frac{1}{L_s} \langle \left| \hat{A}_{\nu} (k) \right|^2 \rangle = \langle |\hat{a}_{\nu} (k)|^2 \rangle.$$

(5.10)

Equations (5.9) and (5.10) give us the Wiener–Khinchin theorem as

$$G_{\nu} (k) = \left\langle \int_{-\infty}^{\infty} a_{\nu} (z) \exp (iku) \, dz \int_{-\infty}^{\infty} a_{\nu} (z') \exp (-iku) \, dz' \right\rangle$$

$$= \int_{-\infty}^{\infty} dz \int_{-\infty}^{\infty} du \langle a_{\nu} (z) a_{\nu} (z + u) \rangle \exp (-iku) = \int_{-\infty}^{\infty} R_{\nu} (u) \exp (-iku) \, du = \hat{R}_{\nu} (k).$$

Then

$$\lim_{L_s \to +\infty} \left| \hat{a}_{\nu} (k) \right|^2 = \left| \left\langle \hat{a}_{\nu} (k_n) \right\rangle \right|^2 = G_{\nu} (k).$$

(5.11)

when roughness is ergodic.

General discussion [12] of roughness uses a three-parameter model, and we apply it to $R_w (z)$:

$$R_w (z) = \sigma^2 \exp \left( - \left( \frac{|z|}{L_c} \right)^{2\alpha} \right)$$

(5.12)

with standard deviation $\sigma$, roughness (or Hurst) exponent $\alpha$ and correlation length $L_c$. Three parameters are given by scanning electron microscope (SEM) measurements for waveguides. From eq. (5.12),

$$\ln \left( \ln \frac{R_w (0)}{R_w (z)} \right) = 2\alpha \ln |z| - 2\alpha \ln L_c.$$

We can obtain the parameters from measurement data by using the above equation.

$$G_w (k) = \sigma^2 \int_{-\infty}^{\infty} \exp \left( - \left( \frac{|z|}{L_c} \right)^{2\alpha} - ikz \right) \, dz = \sigma^2 \int_{-\infty}^{\infty} \exp \left( - \left( \frac{|z|}{L_c} \right)^{2\alpha} \right) \cos (kz) \, dz.$$

(5.13)

Let us approximate $\hat{a}_{w} (k)$ with finite $L_s$ by using eqs. (5.11) and (5.13): $|\hat{a}_{w} (k)|^2 \simeq G_w (k)$. Then, we can numerically obtain $\hat{a}_{w} (k) = \pm \sqrt{G_w (k)} \exp (i\phi (k))$, where the real function $\phi (k)$ and “±” are randomly given, and it also satisfies $\phi (-k) = -\phi (k)$.

The waveguide has two line edges with line edge roughness (LER) $a_1 (z)$ and $a_2 (z)$. LWR $a_w$ and LCR $a_c$ can be represented by LER $a_1$ and $a_2$ as follows:

$$a_w (z) = a_1 (z) - a_2 (z),$$

$$a_c (z) = \frac{a_1 (z) + a_2 (z)}{2}.$$

If $A_1$ and $A_2$ have the same three-parameters and are not correlated, the standard deviations for LWR, LER and LCR are $\sigma$, $\sigma/\sqrt{2}$ and $\sigma/2$, respectively [13].

[Go to table of contents.] [Go to home.]
6. Numerical discretization for Maxwell equation

This chapter shows a way of numerical discretization in order to calculate wave propagation in the waveguides. As in Appendix F, we consider Maxwell equation with scalar permittivity \( \varepsilon \) and scalar magnetic-permeability \( \mu \), and then the generalized Maxwell equation (D.1) in frequency domain is simplified to

\[
\begin{bmatrix}
0 & i \nabla \times \\
-i \nabla \times & 0
\end{bmatrix}
\begin{bmatrix}
E \\
H
\end{bmatrix}
= i \omega
\begin{bmatrix}
\varepsilon & 0 \\
0 & \mu
\end{bmatrix}
\begin{bmatrix}
E \\
H
\end{bmatrix}.
\]

We should avoid to use huge or tiny value in numerical calculation, and then it is better to normalize the above equation by using normalization constants.

6.1. Normalization constants for numerical formulation

We introduce a characteristic wave-number \( k_0 \) as normalization constant, e.g. \( k_0 = 2\pi/1\mu m \) to the cases of c-band or o-band. Note that the \( 1\mu m \) is not equal to the wavelength, but it is set as close value. Then, length and wave-number (propagation constant) are normalized as

\[
\frac{u}{k_0^{-1}} \Rightarrow u, \quad \text{and} \quad \frac{\beta}{k_0} \Rightarrow \beta.
\]

The permittivity and magnetic permeability are also normalized by electric constant \( \varepsilon_0 \) and magnetic constant \( \mu_0 = 4\pi \times 10^{-7} \text{NA}^{-2} \), respectively:

\[
\frac{\varepsilon}{\varepsilon_0} \Rightarrow \varepsilon, \quad \text{and} \quad \frac{\mu}{\mu_0} \Rightarrow \varepsilon.
\]

Then, the \( \omega \) and time \( t \) are normalized to

\[
\frac{\omega}{k_0\sqrt{\varepsilon_0\mu_0}} \Rightarrow \omega, \quad \text{and} \quad \frac{t}{\sqrt{\varepsilon_0\mu_0}k_0} \Rightarrow t.
\]

Finally, we try to normalize the electromagnetic field \( E \) and \( H \):

\[
\frac{E}{\sqrt{\frac{k_0}{\varepsilon_0\mu_0}}} \Rightarrow E, \quad \text{and} \quad \frac{H}{\sqrt{\frac{k_0}{\mu_0\varepsilon_0}}} \Rightarrow H.
\]

Note that the density of electromagnetic energy derived from two normalization constants is equal to a photon energy with wave-number \( k_0 \) in a cube \( k_0^{-3} \) with vacuum.

The normalization, which uses the above seven constants, does not change the representation of eq. (6.1).

6.2. Two steps of transformation: \( u \Rightarrow \xi \Rightarrow l \)

Numerical analysis requires to discretize the dimensionless \( u \)-space: \( u_j \Rightarrow \xi_j \Rightarrow l_j \), where \( l_j \) as \( j = 0, 1, 2 \) is non-negative integer. Then, we can define positive integer \( L_j \):

\[
L_j \triangleq 1 + \max(l_j), \quad \text{then} \quad 0 \leq l_j < L_j.
\]

The \( \xi_j \) is continuous variable, and \( 0 \leq \xi_j < L_j \). The \( u_j \) is a monotonically increasing function of \( \xi_j \), i.e. \( u_j' \triangleq du_j/d\xi_j \) is always positive. The system length \( L_s \) as shown in Section 1.1 is given by \( L_s = \int_0^{L_2} u_2' d\xi_2 \). If we apply periodical (or anti-periodical) boundary condition to electromagnetic field along \( u_j \) axis, periodical boundary condition has to be applied to \( u_j \) as

\[
u_j' (\xi_j) = u_j' (\xi_j + L_j).
\]
Even in the case of bend waveguide as in Chapter 2, the above periodical condition could be applied to the case of \( j = 1 \) at least. Appendix G shows an example of non-uniform mesh, and eq. (G.4) gives us functions \( u_j(\xi) \) and \( \overline{u}_j(\xi) \).

In the same manner as Section D.1, the rotation operator \( \nabla \times \) in the coordinates \( x = (x_0, x_1, x_2) \) can be transformed to an operator in other coordinates \( \xi = (\xi_0, \xi_1, \xi_2) \) via the coordinates \( u = (u_0, u_1, u_2) \).

\[
\nabla \times = \sum_{j=0}^{2} \frac{1}{u_j h_j} f_\xi (\nabla \xi \times) f_\xi ,
\]

where
\[
f_\xi = \begin{pmatrix}
u_0' h_0 & 0 & 0 \\
0 & u_1' h_1 & 0 \\
0 & 0 & u_2' h_2
\end{pmatrix} , \quad \nabla \xi \times = \begin{pmatrix} 0 & -\partial_{\xi_2} & \partial_{\xi_1} \\
\partial_{\xi_2} & 0 & -\partial_{\xi_0} \\
-\partial_{\xi_1} & \partial_{\xi_0} & 0
\end{pmatrix} \quad \text{as} \quad \partial_{\xi_j} \triangleq \frac{\partial}{\partial \xi_j}.
\]

If we use the scheme of Chapter 2, the scale factors \( h_0 \) and \( h_2 \) are given by eq. (2.3), and \( h_1 = 1 \).

By using eq. (6.2), the Maxwell equation (6.1) could be deformed to

\[
\begin{pmatrix} 0 \\
-i \nabla \xi \times
\end{pmatrix} \begin{pmatrix} f_\xi E \\
f_\xi H
\end{pmatrix} = \omega \begin{pmatrix} \varepsilon_\xi & 0 \\
0 & \mu_\xi
\end{pmatrix} \begin{pmatrix} f_\xi E \\
f_\xi H
\end{pmatrix} ,
\]

where
\[
\begin{align*}
\varepsilon_\xi (\xi) &= \prod_{n=0}^{2} u_n' h_n f_\xi^{-1} = \xi_0 , \xi_1 , \xi_2 \\
= &\begin{pmatrix}
\xi_{00} & 0 & 0 \\
0 & \xi_{11} & 0 \\
0 & 0 & \xi_{22}
\end{pmatrix} , \quad \varepsilon_{\xi,jj} = \frac{u_{j+1}' u_{j+2}' h_{j+1} h_{j+2}}{u_j h_j} \varepsilon (\xi) , \\
\mu_\xi (\xi) &= \prod_{n=0}^{2} u_n' h_n f_\xi^{-1} = \begin{pmatrix}
\mu_{00} & 0 & 0 \\
0 & \mu_{11} & 0 \\
0 & 0 & \mu_{22}
\end{pmatrix} , \quad \mu_{\xi,jj} = \frac{u_{j+1}' u_{j+2}' h_{j+1} h_{j+2}}{u_j h_j} \mu (\xi) .
\end{align*}
\]

Let us approximate eq. (6.3) to discretized equation with transforming \( \xi = (\xi_0 , \xi_1 , \xi_2) \Rightarrow l = (l_0 , l_1 , l_2) \) in the framework of Yee’s lattice [14].

### 6.3. Discretization by Yee’s lattice

Figure 6.1 gives us an arrangement of discrete functions from the continuous functions \( f_\xi E , f_\xi H , \varepsilon_\xi \) and \( \mu_\xi \), where the discrete functions are allocated at a cell address \( [l] \). Discrete electromagnetic fields \( f_\xi E (\xi) \Rightarrow E_l [l] \) and \( f_\xi H (\xi) \Rightarrow H_l [l] \) are derived by eq. (6.4) and Fig. 6.1. The components of \( E_l [l] \) and \( H_l [l] \) are defined as

\[
\begin{align*}
E_{ij} [l] &\triangleq u_j' h_j E_j \left( l_0 + \frac{1 - \delta_{jj}}{2} , l_1 + \frac{1 - \delta_{jj}}{2} , l_2 + \frac{1 - \delta_{jj}}{2} \right) , \\
H_{ij} [l] &\triangleq u_j' h_j H_j \left( l_0 + \delta_{jj} , l_1 + \frac{\delta_{jj}}{2} , l_2 + \frac{\delta_{jj}}{2} \right) .
\end{align*}
\]

Discrete medium, which consists of \( \varepsilon_\xi (\xi) \Rightarrow \varepsilon_l [l] \) and \( \mu_\xi (\xi) \Rightarrow \mu_l [l] \), is also derived by eq. (6.4) and Fig. 6.1. The components of \( \varepsilon_l [l] \) and \( \mu_l [l] \) are defined with PML factor \( \tilde{\sigma}_j (\xi_j) \) from eq. (3.9) and correction factor \( \eta \) from eqs. (H.3) and (H.4):

\[
\begin{align*}
\varepsilon_{ljj} [l] &\triangleq \frac{u_{j+1}' u_{j+2}' h_{j+1} h_{j+2} [1 + i \tilde{\sigma}_{j+1} (l_{j+1} + 1/2)] [1 + i \tilde{\sigma}_{j+2} (l_{j+2} + 1/2)]}{1 + i \tilde{\sigma}_j (l_j)} \\
&\times \frac{\varepsilon (l_0 + (1 - \delta_{jj})/2 , l_1 + (1 - \delta_{jj})/2 , l_2 + (1 - \delta_{jj})/2)}{1 + \eta (l_0 + (1 - \delta_{jj})/2 , l_1 + (1 - \delta_{jj})/2 , l_2 + (1 - \delta_{jj})/2)} .
\end{align*}
\]

\[
\begin{align*}
\mu_{ljj} [l] &\triangleq \frac{u_{j+1}' u_{j+2}' h_{j+1} h_{j+2} [1 + i \tilde{\sigma}_{j+1} (l_{j+1})] [1 + i \tilde{\sigma}_{j+2} (l_{j+2})]}{1 + i \tilde{\sigma}_j (l_j + 1/2)} \\
&\times \frac{\mu (l_0 + \delta_{jj}/2 , l_1 + \delta_{jj}/2 , l_2 + \delta_{jj}/2)}{1 + \eta (l_0 + \delta_{jj}/2 , l_1 + \delta_{jj}/2 , l_2 + \delta_{jj}/2)} .
\end{align*}
\]
Figure 6.1: Yee cell [14]. We select the cell where $E_{i0}$ and $E_{i1}$ exist at half-integer $\xi_2$, because discussion about optics frequently focuses on properties of electric field.

Numerical calculation considers finite numbers of Yee cells as $0 \leq l_j < L_j$. Function $G[l]$, which is $H_{ij}$ for example, satisfies the following boundary conditions for $l_0$ and $l_1$.

\[
\begin{align*}
\{ G[l_0, l_1, t_2] &= B_0 G[0, l_1, l_2], \quad G[-1, l_1, l_2] = B_0 G[L_0 - 1, l_1, l_2], \\
G[l_0, L_1, l_2] &= B_1 G[l_0, 0, l_2], \quad G[l_0, -1, l_2] = B_1 G[l_0, L_1 - 1, l_2],
\end{align*}
\]  

where $|B_j| = 1$ or 0, and $G = H_{ij}$, $E_{ij}$ for example. The two parameters $B_0$ and $B_1$ are generally complex numbers, and we could choose a periodic condition $B_j = 1$ or an anti-periodic condition $B_j = -1$. We can also set $B_0 = 0$ when $\kappa_b \neq 0$, since the system does not become periodic along the $u_0$-axis.

Let us introduce forward and backward difference operators as

\[
\begin{align*}
\{ \Delta_j G[l_0, l_1, l_2] &\triangleq G[l_0 + \delta_j^0, l_1 + \delta_j^1, l_2 + \delta_j^2] - G[l_0, l_1, l_2], \\
\nabla_j G[l_0, l_1, l_2] &\triangleq G[l_0, l_1, l_2] - G[l_0 - \delta_j^0, l_1 - \delta_j^1, l_2 - \delta_j^2].
\end{align*}
\]  

From eqs. (6.7) and (6.8), the difference operators at boundaries are given by

\[
\begin{align*}
\{ \Delta_j G[l_0 - 1, l_1, l_2] &\triangleq G[l_0 - 1, l_1, l_2] - G[l_0 - 1, l_1, l_2], \quad \nabla_0 G[l_0, l_1, l_2] = G[l_0, l_1, l_2] - B_0 G[l_0 - 1, l_1, l_2], \\
\Delta_1 G[l_0, L_1 - 1, l_2] &\triangleq B_1 G[l_0, L_1 - 1, l_2] - G[l_0, L_1 - 1, l_2], \quad \nabla_1 G[l_0, 0, l_2] = G[l_0, 0, l_2] - B_1 G[l_0, L_1 - 1, l_2].
\end{align*}
\]

Therefore, discrete difference operators satisfy $\nabla_j = -\Delta_j^\dagger$, but $\Delta_j \neq -\Delta_j^\dagger$. This relation is different from the case of continuous difference operators $\partial_j = -\partial_j^\dagger$ under the boundary condition of eq. (6.7).

From eqs. (6.5), (6.6) and Fig. 6.1, the deformed Maxwell equation (6.3) could be discretized into

\[
\begin{pmatrix}
0 & iR \\
-R^\dagger & 0
\end{pmatrix}
\begin{pmatrix}
E_l \\
H_l
\end{pmatrix} = \omega
\begin{pmatrix}
\varepsilon_l & 0 \\
0 & \mu_l
\end{pmatrix}
\begin{pmatrix}
E_l \\
H_l
\end{pmatrix},
\]  

where the discrete rotation operators $R$ and $R^\dagger$ are defined by using eqs. (6.8):

\[
R \triangleq
\begin{pmatrix}
0 & -\Delta_2 & \Delta_1 \\
\Delta_2 & 0 & -\Delta_0 \\
-\Delta_1 & \Delta_0 & 0
\end{pmatrix}
\quad \text{and} \quad
R^\dagger \triangleq
\begin{pmatrix}
0 & \Delta_1^\dagger & -\Delta_0^\dagger \\
-\Delta_2^\dagger & 0 & \Delta_0^\dagger \\
\Delta_1^\dagger & -\Delta_0^\dagger & 0
\end{pmatrix}.
\]  

The $R$ and $R^\dagger$ are used in eq. (8.1).
7. Propagation equation for Yee’s lattice

This chapter shows discrete formulae derived from the discrete Maxwell-equation (6.9).

7.1. Discrete propagation-equation

Discrete formulation can be represented as similar to propagation equation (3.1) with eq. (D.13). In order to simplify mathematical notations, we only show a discrete parameter \( l \) instead of \( I \) in the following equations.

\[
M_{\pm} \Psi_{\pm} = -i \left( \begin{array}{cc} 0 & \nabla_2 \nabla_2 \\ \triangle_2 & 0 \end{array} \right) \Psi_{\pm} \quad \text{as} \quad \begin{cases} M_{+} \triangleq \left( \begin{array}{cc} m_{aa} [V_{l2}] & 0 \\ 0 & m_{bb} [V_{l2}] \end{array} \right) , \\ M_{-} \triangleq \left( \begin{array}{cc} m_{bb} [V_{l2}] & 0 \\ 0 & m_{aa} [V_{l2} + 1] \end{array} \right) . \end{cases}
\] (7.1)

The subscript \( + \) (\( - \) in eq. (7.1)) means a configuration as advanced (retarded) electric fields to magnetic fields. From eq. (I.4), the discrete \( m_{aa}, m_{bb} \) and \( \Psi_{\pm} \) are defined by

\[
\begin{align*}
& m_{aa} (V) = \begin{pmatrix} V_0 + \nabla_1 V_1 \Delta_1 - \nabla_1 V_2 \Delta_0 \\ - \nabla_0 V_2 \Delta_1 + V_1 + \nabla_0 V_2 \Delta_0 \end{pmatrix}, \\
& m_{bb} (V) = \begin{pmatrix} V_3 + \Delta_0 V_5 \nabla_0 \Delta_1 V_5 \nabla_1 \\ \Delta_0 V_5 \nabla_1 \Delta_1 V_5 \nabla_0 \\ V_4 + \Delta_1 V_3 \nabla_1 \end{pmatrix}, \\
& \Psi_+ [l2] \triangleq \begin{pmatrix} H_{2D} \lbrack l2 \rbrack \\ E_{2D} \lbrack l2 \rbrack \end{pmatrix}, \\
& \Psi_- [l2] \triangleq \begin{pmatrix} E_{2D} \lbrack l2 + 1 \rbrack \\ H_{2D} \lbrack l2 + 1 \rbrack \end{pmatrix}, \\
& H_{2D} \lbrack l2 \rbrack = \begin{pmatrix} H_{l0} \lbrack l2 \rbrack \\ H_{l1} \lbrack l2 \rbrack \end{pmatrix}, \\
& E_{2D} \lbrack l2 \rbrack = \begin{pmatrix} -E_{l1} \lbrack l2 \rbrack \\ E_{l0} \lbrack l2 \rbrack \end{pmatrix} \end{align*}
\] (7.2)

The operators \( \Delta_j \) and \( \nabla_j \) for \( j = 0, 1 \) in \( m_{aa} \) and \( m_{bb} \) of eq. (7.2) can be regarded as \( L_0L_1 \times L_0L_1 \) matrices. The \( V_0, \ldots, V_3 \) also become \( L_0L_1 \times L_0L_1 \) diagonal matrices, and then \( V \) can be set as a \( 6L_0L_1 \times 6L_0L_1 \) diagonal matrix. The \( \mu_{ij} \) and \( \varepsilon_{ij} \) in eq. (7.2) were defined by eq. (6.6). The factor \( \sqrt{\mu_0\varepsilon_0} / 2 \) of eq. (D.11) is removed from the discrete \( \Psi \) in eq. (7.2), since it does not affect the following discussion. The \( H_{ij} \) and \( E_{ij} \) for \( j = 0, 1 \) are \( L_0L_1 \times 1 \) column vectors. Note that \( M_{\pm} = M_{\pm}^\dagger \) when \( \varepsilon \) and \( \mu \) are real number.

We define two types of power flow for eq. (7.1) as similar to the first of eq. (3.2):

\[
P_{\pm} [l2] \triangleq \Psi_{\pm}^\dagger [l2] \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi_{\pm} [l2] .
\]

From the above definition and eq. (I.5), we show two relations for \( P_{\pm} \) as follows.

\[
\begin{align*}
&P_{+} [l2] - P_{-} [l2 - 1] = i H_{2D}^\dagger [l2] \left( m_{aa} [l2] - m_{aa}^\dagger [l2] \right) H_{2D} [l2] , \\
&P_{-} [l2] - P_{+} [l2 + 1] = i E_{2D}^\dagger [l2] \left( m_{bb} [l2] - m_{bb}^\dagger [l2] \right) E_{2D} [l2] .
\end{align*}
\] (7.3)

Note that \( P_{+} = P_{-} \) when \( M_{1\dagger} = M_{1} \). Equation (7.3) gives us conservation rule of \( \Psi_{\pm} \) as similar to the second of eq. (3.2):

\[
\triangle_2 P_{+} = i \Psi_{\dagger}^\dagger \left( M_{-} - M_{1\dagger} \right) \Psi_{\dagger} \quad \text{and} \quad \nabla_2 P_{-} = i \Psi_{\dagger} \left( M_{1} - M_{+} \right) \Psi_{\dagger} .
\]

In the following discussion, we only use the configuration with subscript \( + \) for eqs. (7.1) and (7.2), since it can be directly associated with \( H_{ij} \) and \( E_{ij} \) of the Yee cell in Fig. 6.1. The subscript \( + \) will be abbreviated as \( \Psi \).

From eq. (I.6), we can define transfer matrix \( T_{RL} [l2] \) as follows.

\[
\Psi [l2 + 1] = T_{RL} [l2] \Psi [l2] \quad \text{as} \quad T_{RL} [l2] \triangleq \begin{pmatrix} 1 \\ i m_{aa} [l2 + 1] \\ 1 - m_{aa} [l2 + 1] \\ m_{bb} [l2] \end{pmatrix} .
\] (7.4)
7.2. Discrete mode-equation

This section considers a scattering region and two outer regions. The scattering region is in \( 0 \leq l_2 < L_2 \), and the outer regions are in \( l_2 < 0 \) and \( l_2 \geq L_2 \), i.e. \( |L_2 - 1 - 2l_2| > L_2 - 1 \). The outer region set that the \( m_{aa} \) and \( m_{bb} \) are not depend on \( l_2 \), and \( m_{aa} = m_{aa}^* \) and \( m_{bb} = m_{bb}^* \). The definitions in eq. (7.2) derive that

\[
m_{aa}^* = m_{aa} \quad \text{and} \quad m_{bb}^* = m_{bb}.
\]  

(7.5)

By using definition of eq. (4.1), \( m_{aa}^{(0)} \) and \( m_{bb}^{(0)} \) satisfy eq. (7.5) even in the scattering region. Discrete mode-function \( \Phi_m \) as similar to eq. (3.3) could be given by solving an eigenvalue equation.

\[
\begin{pmatrix}
   m_{aa}^{(0)}(l_2) & 0 \\
   0 & m_{bb}^{(0)}(l_2)
\end{pmatrix}
\begin{pmatrix}
   \Phi_m(l_2) \\
   \Phi_{m+1}(l_2)
\end{pmatrix}
= 2\sin(\theta_m(l_2)/2)
\begin{pmatrix}
   0 & 1 \\
   1 & 0
\end{pmatrix}
\begin{pmatrix}
   \Phi_m(l_2) \\
   \Phi_{m+1}(l_2)
\end{pmatrix}
= \begin{pmatrix}
   h_{m}(l_2) \\
   e_{m}(l_2)
\end{pmatrix}
\]

(7.6)

Note that \( \sin a = -i (e^{ia} - e^{-ia})/2 \), and then \( (\sin a)^* = i (e^{-ia^*} - e^{ia^*})/2 = \sin a^* \). The cosine and the tangent are also defined in the same manner. Orthogonality and normalization for the discrete \( \Phi_m \) are given by

\[
\Phi^\dagger_n \begin{pmatrix}
   0 & 1 \\
   1 & 0
\end{pmatrix} \Phi_m = h_{m}^n e_{m} + e_{m}^n h_{m} = \begin{cases}
   \frac{\delta_{m,n}}{\cos(\theta_m/2)} & \text{for } 0 < |m| \leq n_{\max}, \\
   \frac{\delta_{m,n}}{\sin(\theta_m/2)} & \text{for } |m| > n_{\max}.
\end{cases}
\]

where the above numbering rule is the same as the rule of Section 3.1. Note that the denominator \( \cos(\theta_m/2) \) in the normalization is caused by the discretization, and it is different from the case in Section 3.2. Small \( \theta_m \) is related to the propagation constant \( \beta_m \) in eq. (3.3) by referring to Section 6.2 and eq. (6.6):

\[
\beta_m = \lim_{h_{2u_2} \to 0} \frac{2\sin(\theta_m/2)}{h_{2u_2}} \propto \frac{\theta_m}{\theta_m^2}.
\]

Equation (7.6) gives us a reduced eigenvalue-equation of \( h_{m} \) or \( e_{m} \) and a relation between \( e_{m} \) and \( h_{m} \):

\[
\begin{pmatrix}
   m_{bb}^{(0)} m_{aa}^{(0)} h_m = 4\sin^2(\theta_m/2) h_m, \\
   e_m = \frac{m_{bb}^{(0)} h_m}{2\sin(\theta_m/2)}
\end{pmatrix}
\]

\[
\left\{ \begin{array}{l}
   m_{bb}^{(0)} m_{aa}^{(0)} e_m = 4\sin^2(\theta_m/2) e_m, \\
   h_m = \frac{m_{bb}^{(0)} e_m}{2\sin(\theta_m/2)}
\end{array} \right. 
\]

(7.7)

The \( h_{m} \) and \( e_{m} \) become real vector if \( \sin(\theta_m/2) \) is real, since \( m_{aa} \) and \( m_{bb} \) are real matrix from eq. (7.5). Furthermore, \( e_{m}^\dagger h_{m} = 0 \) if \( \sin^2(\theta_m/2) \neq \sin^2(\theta_n/2) \) for real \( \sin(\theta_m/2) \) and \( \sin(\theta_n/2) \). However, we have to be careful in handling eigenvectors (i.e. modes) for other case as discussed in Section 3.2. From the definition in eq. (7.6) and the relation of \( h_{m} \) and \( e_{m} \) in eq. (7.7), the orthogonality and normalization of the \( \Phi_m \) are reduced to

\[
\begin{pmatrix}
   h_{m}^\dagger e_{m} = e_{m}^\dagger h_{m} = \frac{m_{bb}^{(0)} m_{aa}^{(0)}}{2|m| \sin(\theta_m/2)} & \text{for } 0 < |m| \leq n_{\max}, \\
   h_{m}^\dagger e_{m} = e_{m}^\dagger h_{m} = \frac{m_{bb}^{(0)} m_{aa}^{(0)}}{2|m| \cos(\theta_m/2)} & \text{for } |m| > n_{\max}.
\end{pmatrix}
\]

(7.8)

Furthermore, we can add special relations

\[
h_{-m} = h_{m} \quad \text{and} \quad e_{-m} = -e_{m} \quad \text{for } 0 < |m| \leq n_{\max}
\]

(7.9)

to eq. (7.8) without loss of generality. Discrete electromagnetic field \( \Psi_+ [l_2] \) in eq. (7.2) for \( 2l_2 + 1 - L_2 > L_2 \) can be expanded into series of modified mode function \( \Xi_m \):

\[
\Psi_+ [l_2] = \sum_{m \neq 0} c_m \exp(i\theta_m l_2) \Xi_m \quad \text{as} \quad \Xi_m \triangleq \begin{pmatrix}
   \exp(-i\theta_m/2) \\
   0
\end{pmatrix}
\begin{pmatrix}
   h_{m} \\
   e_{m}
\end{pmatrix}
\]

(7.10)

By checking eq. (1.7), we can confirm that the above expansion has consistency with the discrete propagation equation (7.1). The \( \Xi_m \) maintains the orthogonality as

\[
\Xi_n^\dagger \begin{pmatrix}
   0 & 1 \\
   1 & 0
\end{pmatrix} \Xi_m = h_{m}^\dagger \exp(i\theta_m/2) e_{m} + e_{m}^\dagger \exp(-i\theta_m/2) h_{m} = \begin{cases}
   \frac{m}{|m|} \delta_{m,n} & \text{for } 0 < |m| \leq n_{\max}, \\
   \delta_{m,n} & \text{for } |m| > n_{\max}.
\end{cases}
\]

(7.11)

The power flow \( P_+ \) is represented by \( c_m \) from eqs. (7.10) and (7.11):

\[
P_+ [l_2] = \Psi_+^\dagger [l_2] \begin{pmatrix}
   0 & 1 \\
   1 & 0
\end{pmatrix} \Psi_+ [l_2] = \sum_{0 < |m| \leq n_{\max}} \frac{m}{|m|} |c_m|^2 + \sum_{|m| > n_{\max}} c_{-m}^* c_m.
\]
7.3. Discrete scattering-matrix

Scattering matrix of eq. (4.14) can be discretized by the discrete propagation-equation (7.1) and the modified mode function (7.10).

\[
S_{mn} \equiv \exp \left(-i\Theta_n [b_m]\right) \Xi_n^\dagger [b_m] \frac{m}{|m|} \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \Psi_n [b_m]
\] (7.12)

for \(0 < |m| \leq n_{\text{max}}\) and \(0 < |n| \leq n_{\text{max}}\). The \(b_m\) in the right-hand side of eq. (7.12) is redefined as

\[
b_m = \frac{|m| + m}{2|m|} (L_2 - 1) = \begin{cases} L_2 - 1 & \text{for } m > 0, \\ 0 & \text{for } m < 0, \end{cases}
\]

and \(\Theta_n [b_m]\) is given by eq. (I.8):

\[
\frac{m}{|m|} \Theta_n [b_m] \equiv \sum_{l_2 \leq L_2 - 1} \frac{\theta_n [l_2]}{2} + \sum_{l_2 > L_2 - 1} \frac{\theta_n [l_2]}{2} = \begin{cases} \frac{\theta_n [l_2]}{2} + \sum_{l_2 \leq L_2 - 1} \frac{\theta_n [l_2]}{2} & \text{for } m = \text{even,} \\ \frac{\theta_n [l_2]}{2} + \sum_{l_2 \leq L_2 - 1} \frac{\theta_n [l_2]}{2} & \text{for } m = \text{odd,} \end{cases}
\]

The \(\Psi_n\) in eq. (7.12) is redefined as a particular solution of \(\Psi_\pm\) in eq. (7.2), which satisfies boundary conditions at outer regions:

\[
\Psi_n [b_m] = \exp \left(i\Theta_n [b_m]\right) \left( \frac{|mn| - mn}{2|mn|} \Xi_n [b_m] + \sum_{0<n < m} S_{m,n} \Xi_n' [b_m] \right).
\] (7.14)

The following discussion is based on the framework of Section I.5. Equation (I.9) at \(l_2 = b_m\) shows that

\[
\Psi_n [b_m] = \exp \left(i\Theta_n [b_m]\right) \left( \Xi_n [b_m] + \sum_{1 \leq j \leq L_2 - 1} G [b_m, j] \right),
\]

\[
G [b_m, j] = \sum_{0<n < m} g_{m,n} [j] \exp \left\{ i \left( \Theta_m [b_m] - \Theta_n [b_m] \right) - i \left( \Theta_m [j] - \Theta_n [j] \right) \right\} \Xi_n' [b_m] .
\]

By comparing the above equations and eq. (7.14), the \(S_{mn}\) is related to the \(g_{mn}\):

\[
S_{mn} = \sum_{1 \leq j \leq L_2 - 1} g_{mn} [j] \exp \left\{ i \left( \Theta_m [b_m] - \Theta_n [b_m] \right) - i \left( \Theta_m [j] - \Theta_n [j] \right) \right\} .
\] (7.15)

When \(M_+\) in eq. (I.10) is independent of \(l_2\), the \(S_{mn}\) of eq.(7.15) is simplified to

\[
S_{mn} = \sum_{0 \leq j \leq L_2} g_{mn} [j] \exp \left\{ i \left( \Theta_m [b_m] - \Theta_n [b_m] \right) \right\} \exp \left(i \frac{m}{|m|} \left( \Theta_m - \Theta_n \right) \frac{L_2 - 1}{2} \right) \Xi_n \Xi_n' DFT, \quad \text{for } m = \text{even,}
\]

where \(g_{mn} [0] = g_{mn} [L_2 - 1] = 0\), and “\(\Xi_n\)DFT” is defined by eq. (I.22). From detail of the \(\Xi_n\)DFT in eq. (I.20), the above equation is represented as

\[
|S_{mn} - \delta_{mn}|^2 = |\Xi_n^\dagger \left[ m_{ao} DFT (\theta_m - \theta_n) \right] \Xi_n |^2 = \left| \Xi_n^\dagger \left[ e^{i\theta_m} m_{ao} DFT (\theta_m - \theta_n) \right] \Xi_n \right|^2 .
\] (7.16)
7.4. Discrete edge-roughness scattering of Section F.2

This section shows $\overline{m}_{aa}^{(1)}$ DFT and $\overline{m}_{bb}^{(1)}$ DFT in eq. (7.16) by separating unperturbed part $V^{(0)}$ and perturbed part $V^{(1)}$ from the discrete $V$ in eq. (7.2). Elements of $V^{(0)}$ are given by

$$V_0^{(0)} = \omega \mu_{111}, \quad V_1^{(0)} = \omega \mu_{111}, \quad V_2^{(0)} = \frac{1}{\omega \varepsilon_{122}}, \quad V_3^{(0)} = \omega \varepsilon_{111}, \quad V_4^{(0)} = \omega \varepsilon_{111}, \quad V_5^{(0)} = \frac{1}{\omega \mu_{122}},$$

where $V^{(0)}$ is not depend on $u_2$. The DFT of $V^{(1)}$ can be approximated to the FT with care of phase shift caused by half shift in eq. (6.6).

$$\overline{V}^{(1)}_{j+3J} DFT (\phi) \simeq \frac{e^{i\phi J/2}}{u_2} V^{(1)}_{j+3J} \left( \frac{\phi}{u_2} \right) \quad \text{for} \quad \begin{cases} \quad j = 0, 1, 2, \\ \quad J = 0, 1, \end{cases}$$

when $u_2' / L_s$ is small, i.e. $L_2 \gg 1$ from eq. (1.23). Then,

$$\overline{m}_{aa}^{(1)} DFT (\phi) = \sqrt{\frac{L_s}{u_2}} m_{aa} \left( \frac{1}{\sqrt{L_s}} V^{(1)} \left( \frac{\phi}{u_2} \right) \right), \quad \overline{m}_{bb}^{(1)} DFT (\phi) = \frac{e^{i\phi / 2} \sqrt{L_s}}{u_2} m_{bb} \left( \frac{1}{\sqrt{L_s}} V^{(1)} \left( \frac{\phi}{u_2} \right) \right).$$

Note that $m_{aa}$ ($m_{bb}$) is a function of only $V_0$, $V_1$ and $V_2$ ($V_3$, $V_4$ and $V_5$). Equation (7.16) is represented as

$$\begin{aligned}
S_{mn} - \delta_{mn} \left| \frac{L_s}{u_2} \right| e^{i \theta_m} h^T_m \left[ m_{aa} \left( \frac{1}{\sqrt{L_s}} V^{(1)} (k_{mn}) \right) \right] h_n + e^{-i \theta_m} e^T_m \left[ m_{bb} \left( \frac{1}{\sqrt{L_s}} V^{(1)} (k_{mn}) \right) \right] e_n \right|^2, \\
k_{mn} = \frac{\theta_m - \theta_n}{u_2}.
\end{aligned} \tag{7.17}$$

We can estimate roughness scattering by using eq. (7.17) with the following eq. (7.19) or (7.21). Therefore, we should crosscheck numerical results against another approach.

7.4.1. Discrete representation of Approach I for F.2.1

This subsection considers that the $V$ is a function of $A_w$ and $A_c$ as shown in Fig. 5.2. Here, we use eq. (6.6) for $h_0 = h_2 = 1$ and constant $u_2'$. By using the framework of eq. (5.4), elements of $V^{(1)} (A_w, A_c)$ are given as

$$V^{(1)}_{j+3J} (A_w, A_c) = \begin{cases} V_{j+3J} \left( \Delta A_w \right) A_w \left( u_2 (l_2 + J/2) \right) & \text{for} \quad j = 0, 1, 2, \\ V_{j+3J} \left( 0, \frac{\Delta A_c}{2} \right) A_c \left( u_2 (l_2 + J/2) \right) & \text{for} \quad J = 0, 1, \end{cases} \tag{7.18}$$

where $\Delta A_w$ and $\Delta A_c$ are parameters of finite difference, and we usually set $u_2' \lesssim \Delta A_w / 2 = \Delta A_c \lesssim 2u_2'$. By using eq. (7.18), the $\overline{V}^{(1)} / \sqrt{L_s}$ in eq. (7.17) can be given as

$$\begin{aligned}
\frac{1}{\sqrt{L_s}} V^{(1)} (k_{mn}) &= V \left( \Delta A_w \right) A_w (k_{mn}) + V \left( 0, \Delta A_c \right) A_c (k_{mn}) \\
&\approx \frac{\left( j + 1 \right) \% 2}{2} \left[ \left( j + 2 \right) \% 2 \right] (1 - J) &\quad J = 0, 1. \tag{7.19}
\end{aligned}$$

7.4.2. Discrete representation of Approach II for F.2.2

This subsection uses the parameter $s_{j+3J} (u_0, u_2)$ of eq. (F.8) as

$$u_0 \left( l_0 + \left[ \left( j + 1 \right) \% 3 \right] \% 2 + \left[ \left( j + 2 \right) \% 3 \right] \% 2 \right) \left( 1 - J \right) \right), \quad u_2 \left( l_2 + \frac{J}{2} \right) = \left[ l_2 + \frac{J}{2} - \frac{L_2}{2} \right] u_2' \quad \text{for} \quad \begin{cases} \quad j = 0, 1, 2, \\ \quad J = 0, 1. \end{cases} \tag{7.20}$$

By using eq. (F.9) and the $u_0$ in eq. (7.20), elements of the $\overline{V}^{(1)} / \sqrt{L_s}$ in eq. (7.17) can be given as

$$\begin{aligned}
\frac{1}{\sqrt{L_s}} V^{(1)}_{j+3J} (k_{mn}) &= V^{(0)}_{j+3J} \left[ u_0 k_m^2 \hat{a}_c (k_{mn}) \right] + \frac{1}{W_w} \left( \frac{1}{2} u_0^2 k_m^2 - (1) \left( j + 1 \right) \% 2 \right) \hat{a}_w (k_{mn}) \right] &\quad J = 0, 1. \tag{7.21}
\end{aligned}$$
8. Finite Difference Time Domain

This chapter shows a way of Finite Difference Time Domain (FDTD). From eq. (6.9), we consider Maxwell equation in time domain, which has already been discretized for the 3D-space:

\[
\begin{pmatrix}
0 & \text{i}R \\
-\text{i}R^\dagger & 0
\end{pmatrix}
\begin{pmatrix}
E_l \\
H_l
\end{pmatrix}
= \text{i} \frac{\partial}{\partial t}
\begin{pmatrix}
\varepsilon_l & 0 \\
0 & \mu_l
\end{pmatrix}
\begin{pmatrix}
E_l \\
H_l
\end{pmatrix},
\]

where the discrete rotation operators \( R \) and \( R^\dagger \) are defined by using eq. (6.10). In order to consider \( E_l, H_l \in \mathbb{R} \), the above equation can be approximated to

\[
\begin{pmatrix}
\text{RH}_l \\
-\text{R}^\dagger E_l
\end{pmatrix}
\approx \frac{\partial}{\partial t}
\begin{pmatrix}
\text{Re} \varepsilon_l & 0 \\
0 & \text{Re} \mu_l
\end{pmatrix}
\begin{pmatrix}
E_l \\
H_l
\end{pmatrix}
+ \omega_c
\begin{pmatrix}
\text{Im} \varepsilon_l & 0 \\
0 & \text{Im} \mu_l
\end{pmatrix}
\begin{pmatrix}
E_l \\
H_l
\end{pmatrix},
\]

with introducing the center frequency \( \omega_c \).

8.1. Discretization for time domain

Figure 8.1 shows the discretized \( E_l[l, l_t] \) and \( H_l[l, l_t] \) for time \( t \) using the same rule as shown in Fig. 6.1. We simplify the cell address \([l, l_t]\) into \([l_t]\) or \([l_2, l_t]\) in the following equations. Time step \( \Delta t \) discretizes the \( t \) to time cells.

\[
\begin{align*}
E_l[l_t-1] & \quad H_l[l_t] & \quad E_l[l_t] & \quad H_l[l_t+1] \\
(l_t-1/2)\Delta t & \quad l_t\Delta t & \quad (l_t+1/2)\Delta t & \quad (l_t+1)\Delta t
\end{align*}
\]

Figure 8.1.: We consider discretized cells of \( t \).

Equation (8.1) is discretized as follows.

\[
\begin{pmatrix}
\text{Re} \varepsilon_l \left[ l_t \right] & \text{Im} \varepsilon_l \left[ l_t \right] \\
\tau_R & \tau_I
\end{pmatrix}
\begin{pmatrix}
E_l \left[ l_t \right] \\
H_l \left[ l_t \right]
\end{pmatrix}
= \text{RH}_l \left[ l_t \right] + \left( \frac{\text{Re} \varepsilon_l \left[ l_t-1 \right]}{\tau_R} - \frac{\text{Im} \varepsilon_l \left[ l_t-1 \right]}{\tau_I} \right) E_l \left[ l_t - 1 \right],
\]

\[
\begin{pmatrix}
\text{Re} \mu_l \left[ l_t + 1 \right] & \text{Im} \mu_l \left[ l_t + 1 \right] \\
\tau_R & \tau_I
\end{pmatrix}
\begin{pmatrix}
H_l \left[ l_t + 1 \right] \\
E_l \left[ l_t \right]
\end{pmatrix}
= -\text{R}^\dagger \left[ l_t \right] + \left( \frac{\text{Re} \mu_l \left[ l_t \right]}{\tau_R} - \frac{\text{Im} \mu_l \left[ l_t \right]}{\tau_I} \right) H_l \left[ l_t \right],
\]

where \( \tau_R^{-1} \) and \( \tau_I^{-1} \) are modified from \( \Delta t^{-1} \) and \( \omega_c/2 \) for correcting discretization errors:

\[
\frac{1}{\tau_R} = \frac{1}{\Delta t} \frac{\omega_c \Delta t/2}{\sin (\omega_c \Delta t/2)} \quad \text{and} \quad \frac{1}{\tau_I} = \frac{\omega_c}{2} \frac{1}{\cos (\omega_c \Delta t/2)}.
\]

The time step \( \Delta t \) has to satisfy the Courant-Friedrichs-Lewy (CFL) condition, and eqs. (H.2) and (6.6) without \( \bar{\sigma}_j \) are applied to the CFL condition:

\[
\tau_R^2 < (\Delta t)^2 \leq \min_l \frac{\varepsilon (\xi) \mu (\xi)}{\sum_{j=0}^{2} \left( \bar{u}_j (\xi_j) h_{j} (u (\xi)) \right)^2} \approx \sqrt{\min_l \frac{\prod_{j=0}^{2} \varepsilon_{lj} [l] \mu_{lj} [l]}{\left( \sum_{j=0}^{2} \varepsilon_{lj} [l] \right) \left( \sum_{j=0}^{2} \mu_{lj} [l] \right)}}.
\]
8.2. Mode source

Equations (7.2) and (7.10) give us the $m$-th mode fields in frequency domain:

$$
\begin{pmatrix}
H_{l0}^{(m)}(\omega_c) & H_{l1}^{(m)}(\omega_c) & -E_{l1}^{(m)}(\omega_c) & E_{l0}^{(m)}(\omega_c)
\end{pmatrix}^T = \Xi_m(\omega_c) .
$$

The $m$-th mode fields in time domain can be defined by using the above mode fields.

$$
\begin{align*}
H_{lj}^{(m)}[l_t] &\equiv f_{\text{env}}(l_t \Delta t) \text{Re} \left( e^{-i\omega_c l \Delta t} H_{lj}^{(m)}(\omega_c) \right), \\
E_{lj}^{(m)}[l_t] &\equiv f_{\text{env}}((l_t + 1/2) \Delta t) \text{Re} \left( e^{-i\omega_c (l_t+1/2) \Delta t} E_{lj}^{(m)}(\omega_c) \right),
\end{align*}
$$

as $j = 0, 1$, (8.4)

where $f_{\text{env}}(t)$ is non-negative function, and $f_{\text{env}}(0) = 0$ and $|df_{\text{env}}/dt| \ll \omega_c$.

Let us induce the $m$-th mode fields of eq. (8.4) from an incidence plane at $\xi_2 = l_2 + 1/4$ into the discretized $H_l$ and $E_l$. The first terms in the right hand sides of eqs. (8.2), which are $R H_l[l_2, l_t]$ and $R^l E_l[l_2, l_t]$, are modified into

$$
\begin{align*}
R H_l[l_2, l_t] &= \begin{pmatrix} 0 & -\triangle_2 & \triangle_1 \\
\triangle_2 & 0 & -\triangle_1 \\
-\triangle_1 & \triangle_0 & 0 \end{pmatrix} \begin{pmatrix} H_{l0}[l_2, l_t] \\
H_{l1}[l_2, l_t] \\
H_{l2}[l_2, l_t] \end{pmatrix} \\
&\Rightarrow \begin{pmatrix} -H_{l1}[l_2 + 1, l_t] + H_{l1}[l_2, l_t] + \frac{m}{|m|} H_{l1}^{(m)}[l_t] + \triangle_1 H_{l2}[l_2, l_t] \\
H_{l0}[l_2 + 1, l_t] - H_{l0}[l_2, l_t] - \frac{m}{|m|} H_{l0}^{(m)}[l_t] - \triangle_0 H_{l2}[l_2, l_t] \\
-\triangle_1 H_{l0}[l_2, l_t] + \triangle_0 H_{l1}[l_2, l_t] \end{pmatrix}, \\
R^l E_l[l_2, l_t] &= \begin{pmatrix} 0 & -\triangledown_2 & \triangledown_1 \\
\triangledown_2 & 0 & -\triangledown_0 \\
-\triangledown_1 & \triangledown_0 & 0 \end{pmatrix} \begin{pmatrix} E_{l0}[l_2, l_t] \\
E_{l1}[l_2, l_t] \\
E_{l2}[l_2, l_t] \end{pmatrix} \\
&\Rightarrow \begin{pmatrix} -E_{l1}[l_2, l_t] + \frac{m}{|m|} E_{l1}^{(m)}[l_t] + E_{l1}[l_2 - 1, l_t] + \triangledown_1 E_{l2}[l_2, l_t] \\
E_{l0}[l_2, l_t] - \frac{m}{|m|} E_{l0}^{(m)}[l_t] - E_{l0}[l_2 - 1, l_t] - \triangledown_0 E_{l2}[l_2, l_t] \\
-\triangledown_1 E_{l0} + \triangledown_0 E_{l1}[l_2, l_t] \end{pmatrix} .
\end{align*}
$$

(8.5)

Figure 8.2 shows calculation manner of eq. (8.5) with the discretized $H_l$ and $E_l$ near the incidence plane.

Figure 8.2: Calculation manner of eqs. (8.2) and (8.5) near the incidence plane for the $m$-th mode. See also Fig. 2(b) in [15].

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A. Two steps of coordinate transformation

This chapter shows details of the transformation in Chapter 2.

A.1. \((x_0, x_2) \Rightarrow (r_0, r_2)\)

From eq. (2.1), partial derivatives of \(x_0\) and \(x_2\) by \(r_0\) and \(r_2\) are that

\[
\frac{\partial x_0}{\partial r_0} = f(r_2), \quad \frac{\partial x_2}{\partial r_0} = -g(r_2), \\
\frac{\partial x_0}{\partial r_2} = (1 - r_0\kappa_b(r_2))g(r_2), \quad \frac{\partial x_2}{\partial r_2} = (1 - r_0\kappa_b(r_2))f(r_2).
\]

Obviously,

\[
\frac{\partial x_0}{\partial r_2} \frac{\partial x_0}{\partial r_0} + \frac{\partial x_2}{\partial r_2} \frac{\partial x_2}{\partial r_0} = 0, 
(A.1)
\]

\[
\left(\frac{\partial x_0}{\partial r_0}\right)^2 + \left(\frac{\partial x_2}{\partial r_0}\right)^2 = 1, 
(A.2)
\]

\[
\left(\frac{\partial x_0}{\partial r_2}\right)^2 + \left(\frac{\partial x_2}{\partial r_2}\right)^2 = (1 - r_0\kappa_b(r_2))^2. 
(A.3)
\]

For \(r_0 = 0\), the partial derivatives are that

\[
\frac{\partial x_0}{\partial r_2} = g, \quad \frac{\partial x_2}{\partial r_2} = f, \\
\frac{\partial^2 x_0}{\partial r_2^2} = \kappa_b f, \quad \frac{\partial^2 x_2}{\partial r_2^2} = -\kappa_b g.
\]

Then

\[
\begin{cases}
\frac{\partial x_2}{\partial r_2} \frac{\partial^2 x_0}{\partial r_2 \partial r_0} - \frac{\partial^2 x_2}{\partial r_2^2} \frac{\partial x_0}{\partial r_2} = \kappa_b f^2 + \kappa_b g^2 = \kappa_b, \\
\left(\frac{\partial x_0}{\partial r_2}\right)^2 + \left(\frac{\partial x_2}{\partial r_2}\right)^2 = f^2 + g^2 = 1
\end{cases} 
(A.4)
\]

at \(r_0 = 0\).

A.2. \((r_0, r_2) \Rightarrow (u_0, u_2)\)

We focus on orthogonal condition for the second step \((r_0, r_2) \Rightarrow (u_0, u_2)\). Orthogonal condition \((x_0, x_2) \Rightarrow (u_0, u_2)\) is that

\[
\frac{\partial x_0}{\partial u_0} \frac{\partial x_0}{\partial u_2} + \frac{\partial x_2}{\partial u_0} \frac{\partial x_2}{\partial u_2} = 0.
\]

Here,

\[
\frac{\partial x_0}{\partial u_0} \frac{\partial x_0}{\partial u_2} = \left(\frac{\partial x_0}{\partial r_0} \frac{\partial r_0}{\partial u_0} + \frac{\partial x_0}{\partial r_2} \frac{\partial r_2}{\partial u_0}\right) \left(\frac{\partial x_0}{\partial r_0} \frac{\partial r_0}{\partial u_2} + \frac{\partial x_0}{\partial r_2} \frac{\partial r_2}{\partial u_2}\right) \\
= \left(\frac{\partial x_0}{\partial r_0}\right)^2 \frac{\partial r_0}{\partial u_0} \frac{\partial r_0}{\partial u_2} + \left(\frac{\partial x_0}{\partial r_2}\right)^2 \frac{\partial r_2}{\partial u_2} + \frac{\partial x_0}{\partial r_0} \frac{\partial x_0}{\partial r_2} \left(\frac{\partial r_2}{\partial u_0} \frac{\partial r_0}{\partial u_2} + \frac{\partial r_0}{\partial u_0} \frac{\partial r_2}{\partial u_2}\right),
\]

25
From equation (A.1),

\[
\frac{\partial x_0}{\partial u_0} \frac{\partial x_0}{\partial u_2} + \frac{\partial x_2}{\partial u_0} \frac{\partial x_2}{\partial u_2} = \left( \frac{\partial x_0}{\partial r_0} \right)^2 \frac{\partial r_0}{\partial u_0} \frac{\partial r_0}{\partial u_2} + \left( \frac{\partial x_2}{\partial r_0} \right)^2 \frac{\partial r_0}{\partial u_0} \frac{\partial r_0}{\partial u_2} + \left( \frac{\partial x_0}{\partial r_2} \right)^2 \frac{\partial r_2}{\partial u_0} \frac{\partial r_2}{\partial u_2} + \left( \frac{\partial x_2}{\partial r_2} \right)^2 \frac{\partial r_2}{\partial u_0} \frac{\partial r_2}{\partial u_2}.
\]

From equations (A.2) and (A.3), the orthogonal condition can be modified as

\[
\frac{\partial r_0}{\partial u_0} \frac{\partial r_0}{\partial u_2} + (1 - r_0 \kappa_b (r_2))^2 \frac{\partial r_2}{\partial u_0} \frac{\partial r_2}{\partial u_2} = 0.
\]

The partial derivatives for eq. (2.2) are that

\[
\left\{ \begin{array}{l}
\frac{\partial r_0}{\partial u_0} = -F_{2D} (r_0 (u_0, u_2), r_2 (u_0, u_2)), \\
\frac{\partial r_0}{\partial u_0} = \zeta (r_2) + u_0 \zeta' (r_2) \frac{\partial r_0}{\partial u_0} = \zeta (r_2) - r_0 \kappa_w (r_2) F_{2D} (r_0, r_2), \\
\frac{\partial r_0}{\partial u_2} = u_0 \zeta' (r_2) \frac{\partial r_0}{\partial u_2} = r_0 \kappa_w (r_2) \frac{\partial r_2}{\partial u_2}.
\end{array} \right.
\]

where \( \zeta' (r_2) = \kappa_w (r_2) \zeta (r_2) \). From eqs. (A.5) and (A.6),

\[
0 = \frac{\partial r_0}{\partial u_0} \frac{\partial r_0}{\partial u_2} + (1 - r_0 \kappa_b (r_2))^2 \frac{\partial r_2}{\partial u_0} \frac{\partial r_2}{\partial u_2}
= \left\{ r_0 \kappa_w (r_2) \zeta (r_2) - \left[ (1 - r_0 \kappa_b (r_2))^2 + (r_0 \kappa_w (r_2))^2 \right] F_{2D} (r_0, r_2) \right\} \frac{\partial r_2}{\partial u_2}.
\]

The definition of \( F_{2D} \) in eq. (2.2) always satisfies the above eq. (A.7). For \( u_0 = 0 \),

\[
\left. \frac{\partial^2 r_2}{\partial u_0^2} \right|_{u_0=0} = \zeta, \quad \left. \frac{\partial r_2}{\partial u_0} \right|_{u_0=0} = 0,
\]

Then

\[
\left\{ \begin{array}{l}
\frac{\partial r_2}{\partial u_0} \frac{\partial^2 r_0}{\partial u_0^2} - \frac{\partial^2 r_2}{\partial u_0^2} \frac{\partial r_0}{\partial u_0} = \kappa_w \zeta^2, \\
\left( \frac{\partial r_0}{\partial u_0} \right)^2 + \left( \frac{\partial r_2}{\partial u_0} \right)^2 = \zeta^2
\end{array} \right.
\]

at \( u_0 = 0 \).

### A.3. Partial derivatives and scale factors

Let us obtain scale factor \( h_0 \) and \( h_2 \). The partial derivatives by \( u_0 \) are that

\[
\frac{\partial x_0}{\partial u_0} = \frac{\partial x_0}{\partial r_0} \frac{\partial r_0}{\partial u_0} + \frac{\partial x_0}{\partial r_2} \frac{\partial r_2}{\partial u_0} = f \frac{(1 - u_0 \zeta \kappa_b)^2 \zeta}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2} - \frac{(1 - u_0 \zeta \kappa_b) g u_0 \zeta'}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2}
= \frac{(1 - u_0 \zeta \kappa_b) \zeta \left( f \frac{(1 - u_0 \zeta \kappa_b) - g u_0 \zeta'}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2} \right)}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2}
\]
and
\[
\frac{\partial x_2}{\partial u_0} = \frac{\partial x_2}{\partial r_0} \frac{\partial r_0}{\partial u_0} + \frac{\partial x_2}{\partial r_2} \frac{\partial r_2}{\partial u_0} = \frac{g (1 - u_0 \zeta \kappa_b)^2 \zeta}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2} - \frac{(1 - u_0 \zeta \kappa_b) f u_0 \zeta'}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2}
\]
\[
(1 - u_0 \zeta \kappa_b) \zeta \left( g (1 - u_0 \zeta \kappa_b) + f u_0 \zeta' \right)
\]
\[
(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2.
\]

Then,
\[
h_0 = \sqrt{\left( \frac{\partial x_0}{\partial u_0} \right)^2 + \left( \frac{\partial x_2}{\partial u_0} \right)^2} = \frac{(1 - u_0 \zeta \kappa_b) \zeta}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2} \sqrt{\left( f (1 - u_0 \zeta \kappa_b) - g u_0 \zeta' \right)^2 + \left( g (1 - u_0 \zeta \kappa_b) + f u_0 \zeta' \right)^2}
\]
\[
= \frac{\sqrt{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2}}{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2}.
\]

The partial derivatives by \( u_2 \) are that
\[
\frac{\partial x_0}{\partial u_2} = \frac{\partial x_0}{\partial r_0} \frac{\partial r_0}{\partial u_2} + \frac{\partial x_0}{\partial r_2} \frac{\partial r_2}{\partial u_2} = \left( f u_0 \zeta' + (1 - u_0 \zeta \kappa_b) g \right) \frac{\partial r_2}{\partial u_2}.
\]
\[
\frac{\partial x_2}{\partial u_2} = \frac{\partial x_2}{\partial r_0} \frac{\partial r_0}{\partial u_2} + \frac{\partial x_2}{\partial r_2} \frac{\partial r_2}{\partial u_2} = \left(-g u_0 \zeta' + (1 - u_0 \zeta \kappa_b) f \right) \frac{\partial r_2}{\partial u_2}.
\]

Then,
\[
h_2 = \sqrt{\left( \frac{\partial x_0}{\partial u_2} \right)^2 + \left( \frac{\partial x_2}{\partial u_2} \right)^2} = \frac{\partial r_2}{\partial u_2} \sqrt{\left( f u_0 \zeta' + (1 - u_0 \zeta \kappa_b) g \right)^2 + \left(-g u_0 \zeta' + (1 - u_0 \zeta \kappa_b) f \right)^2}
\]
\[
= \frac{\partial r_2}{\partial u_2} \sqrt{(1 - u_0 \zeta \kappa_b)^2 + (u_0 \zeta')^2}.
\]

The \( \partial r_2/\partial u_2 \) in the right side of eq. (A.10) can be numerically solved by using eq. (2.4). This section shows details of \( \partial F_{2D}/\partial u_2 \). From eq. (A.6),
\[
\frac{\partial F_{2D}}{\partial u_2} = \frac{\partial r_0}{\partial u_2} \frac{\partial F_{2D}}{\partial r_0} + \frac{\partial r_2}{\partial u_2} \frac{\partial F_{2D}}{\partial r_2} = \frac{\partial r_2}{\partial u_2} \left( r_0 \kappa_w \frac{\partial F_{2D}}{\partial r_0} + \frac{\partial F_{2D}}{\partial r_2} \right).
\]

From eq. (2.2),
\[
\frac{\partial F_{2D}}{\partial r_0} = \frac{\kappa_w \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} - \frac{r_0 \kappa_w \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} \left[2 (1 - r_0 \kappa_b) (\kappa_b) + 2 r_0 \kappa_w^2 \right]
\]
\[
\frac{\partial F_{2D}}{\partial r_2} = \frac{r_0 (\kappa_w^2 + \kappa_w^2) \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} - \frac{r_0 \kappa_w \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} \left[2 (1 - r_0 \kappa_b) (\kappa_b) + 2 r_0 \kappa_w^2 \kappa_w \right]
\]

Then
\[
\frac{\partial F_{2D}}{\partial u_2} = \frac{\partial r_2}{\partial u_2} \left\{ \frac{r_0 (\kappa_w^2 + \kappa_w^2) \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} - \frac{r_0 \kappa_w \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} \left[2 (1 - r_0 \kappa_b) (\kappa_b) + 2 r_0 \kappa_w^2 \kappa_w \right] \right\}
\]
\[
= \frac{\partial r_2}{\partial u_2} \left\{ \frac{\kappa_w^2 + \kappa_w^2}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} - \frac{r_0 \kappa_w \zeta}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} \left[2 (1 - r_0 \kappa_b) (\kappa_b) + 2 r_0 \kappa_w^2 \kappa_w \right] \right\}
\]
\[
= \frac{\partial r_2}{\partial u_2} \left\{ \frac{\kappa_w^2 (1 - r_0 \kappa_b) - \kappa_w (r_0 \kappa_w)^2 + 2 \kappa_w (1 - r_0 \kappa_b) (\kappa_w + r_0 \kappa_b)}{(1 - r_0 \kappa_b)^2 + (r_0 \kappa_w)^2} \right\}.
\]
B. S-matrix, Transfer matrix and Periodic system

This chapter shows S-matrix character, derivation of Transfer matrix and mode equation of periodic system.

B.1. S-matrix

The S-matrix was first introduced by J. A. Wheeler in the 1937 paper [16] for nuclear physics. It described the scattering between quantum states indexed by spin and angular momentum of nuclei, and its unitarity had been already discussed. In the framework of circuit theory, the concept of scattering matrix was introduced by V. Belevitch in the 1945 thesis [17]. The S-matrix “S” was independently introduced by R. H. Dicke [18] as the work of The Radiation Laboratory [19]. The “S” is defined between multi-terminals which are connected to a waveguide junction, and then it can also be represented as eq. (4.14). The S-matrix symmetry (reciprocity) was discussed in Sec. II of Ref. [20] and for Eq. (92) in Chap. 5 of Ref. [19]. Its unitarity was also given by Eq. (101) in Chap. 5 of Ref. [19]. The S-matrix of multichannel system was also studied for quantum transport, its unitarity and symmetry were shown by eqs. (3.1) and (3.2) of Ref. [21].

This section will try to show the unitarity for no-loss system and the symmetry for no-loss and time-reversal invariant system without using any specific model. Unitarity of S-matrix directly derives from flow conservation of the no-loss system. Flow conservation in case of mode “m” incident is represented by \( \sum_j |S_{jm}|^2 = 1 \). In case of incident for two modes “m” and “n”, flow conservation of a linear system gives us

\[
\sum_j |S_{jm} + S_{jn}|^2 = \sum_j |S_{jm} + iS_{jn}|^2 = 2 \quad \text{for} \quad m \neq n.
\]

Then,

\[
\sum S_{jm}^*S_{jn} + S_{jn}^*S_{jm} = i \sum S_{jm}^*S_{jn} - S_{jn}^*S_{jm} = 0 \quad \text{for} \quad m \neq n.
\]

Therefore \( \sum_j S_{jm}^*S_{jn} = \sum_j S_{mj}^{}S_{jn} = \delta_{mn} \), that is

\[
S^\dagger S = SS^\dagger = 1. \tag{B.1}
\]

Additional symmetry of S-matrix derives from time-reversal invariance. Reversed propagation for mode “m” incident (exit) is equivalent to complex conjugate of propagation for mode “m” exit (incident) only if the system remains time-reversal invariance: \( \sum_j S_{nj}S_{jm}^* = \delta_{mn} \), that is

\[
S^*S = SS^* = 1.
\]

When the linear system satisfies both of flow conservation and time-reversal invariance, S-matrix satisfies the symmetry (reciprocity) \( S^T = S \) from Eqs. (B.1) and the above relation.

B.2. Transfer Matrix

Let us consider a scattering matrix which consists of 4 submatrices for the left-hand and right-hand sides.

\[
S = \begin{pmatrix}
S_{LL} & S_{LR} \\
S_{RL} & S_{RR}
\end{pmatrix}, \tag{B.2}
\]

where we set \( S_{LR} \) and \( S_{RL} \) as regular matrices. We also consider 4 column vectors for forward and backward modes in the left-hand and right-hand sides as \( f_L, b_L, f_R \) and \( b_R \). They are related to each other by Eq. (B.2):

\[
\begin{align}
\begin{pmatrix}
f_R \\
b_L
\end{pmatrix} &= \begin{pmatrix}
S_{RL} & S_{RR}
\end{pmatrix} \begin{pmatrix}
f_L \\
b_R
\end{pmatrix}, \\
\begin{pmatrix}
f_L \\
b_R
\end{pmatrix} &= \begin{pmatrix}
S_{LL} & S_{LR}
\end{pmatrix} \begin{pmatrix}
f_R \\
b_L
\end{pmatrix}. \tag{B.3}
\end{align}
\]
A transfer matrix $T_{RL}$ is defined as
\[
\begin{pmatrix}
    f_R \\
    b_R
\end{pmatrix} = T_{RL} \begin{pmatrix}
    f_L \\
    b_L
\end{pmatrix}.
\] (B.4)

The above and Eq. (B.3) give us the following relation.
\[
T_{RL} = \begin{pmatrix}
    t_{ff} & t_{fb} \\
    b_{ff} & b_{fb}
\end{pmatrix} = \begin{pmatrix}
    s_{RL} - s_{RR}s_{LL}^{-1}s_{LR} & s_{RR}s_{LL}^{-1} \\
    -\frac{1}{s_{LR}}s_{LL}^{-1} & \frac{1}{s_{LR}}
\end{pmatrix} = \begin{pmatrix}
    \frac{1}{s_{RL}} & -\frac{1}{s_{RR}}s_{LL}^{-1}s_{LR} \\
    \frac{1}{s_{LL}}s_{RL}^{-1} & s_{LR} - s_{LL}^{-1}s_{RL}s_{RR}
\end{pmatrix}^{-1}. \tag{B.5}
\]

The S-matrix can also be represented by the 4 submatrices of the $T_{RL}$.
\[
S = \begin{pmatrix}
    s_{LL} & s_{LR} \\
    s_{RL} & s_{RR}
\end{pmatrix} = \begin{pmatrix}
    \frac{1}{s_{LR}} & \frac{1}{s_{LL}} \\
    t_{ff} - \frac{1}{s_{LR}}t_{fb} & \frac{1}{s_{LL}}t_{fb}
\end{pmatrix} = \begin{pmatrix}
    \frac{1}{s_{LR}} & \frac{1}{s_{LL}} \\
    t_{bb} - \frac{1}{s_{LR}}t_{fb} & \frac{1}{s_{LL}}t_{fb}
\end{pmatrix}^{-1}.
\]

Note that the transfer matrix $T_{RL}$ of eq. (B.4) is different from the T-matrix $T^{(\pm)}$ of eq. (4.12).

### B.3. Periodic waveguide

Both sides of a block of periodic system are connected to two hypothetical waveguides which have the same structure. First, let us redefine evanescent modes $\Phi_{\pm m}$ ($m > n_{\text{max}}$) for the hypothetical waveguide. Redefined mode $\Phi'_{\pm m}$ is given by
\[
\Phi'_{\pm m} = \frac{\Phi_m \pm \Phi_{-m}}{\sqrt{2}} \quad \text{for} \quad m > n_{\text{max}}, \tag{B.6}
\]
where original evanescent and divergent modes satisfy the normalization rule of Eq. (3.6). Then, the $\Phi'_n$ is applied to the same orthogonality as Eq. (3.5):
\[
\Phi'^{\dagger}_n \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi'_m = \frac{n}{|n|} \delta_{nm}.
\]

Accordingly, we will use the redefined mode $\Phi'_n$ as one of propagating modes in the following discussion. Note that the $\Phi'_n$ is not eigenvector of eq. (3.3) for the hypothetical waveguide, but it is still a solution of eq.(3.1).

Column vector in forward-mode (backward-mode) space of the hypothetical waveguides is shown as $f$ ($b$). Bloch function of periodic system is given by Eqs. (B.4):
\[
T_{RL} \begin{pmatrix} f \\ b \end{pmatrix} = e^{i\theta} \begin{pmatrix} f \\ b \end{pmatrix}, \quad \text{and} \quad T_{RL}^{-1} \begin{pmatrix} f \\ b \end{pmatrix} = e^{-i\theta} \begin{pmatrix} f \\ b \end{pmatrix}.
\]

Then we obtain an eigenvalue equation:
\[
\frac{1}{2i} (T_{RL} - T_{RL}^{-1}) \begin{pmatrix} f \\ b \end{pmatrix} = \sin \theta \begin{pmatrix} f \\ b \end{pmatrix}. \tag{B.7}
\]

From Eqs. (B.1) and (B.2), no-loss system satisfies that
\[
-s_{LL} \frac{1}{s_{RL}} = \frac{1}{s_{LR}}s_{RR}^{\dagger}, \quad -\frac{1}{s_{LR}}s_{LL} = \frac{1}{s_{RL}}s_{RR}^{\dagger}, \quad s_{RL} - s_{RR} \frac{1}{s_{LR}}s_{LL} = \frac{1}{s_{RL}}, \quad \text{and} \quad s_{LR} - s_{LL} \frac{1}{s_{RL}}s_{RR} = \frac{1}{s_{LR}}.
\]

From Eq. (B.5) and the above, $(T_{RL} - T_{RL}^{-1}) / (2i)$ can be deformed to
\[
\frac{1}{2i} (T_{RL} - T_{RL}^{-1}) = \frac{1}{2i} \begin{pmatrix}
    s_{RL} - s_{RR} \frac{1}{s_{LR}}s_{LL} - \frac{1}{s_{RL}} & \frac{1}{s_{RL}}s_{RR} \frac{1}{s_{LR}} + \frac{1}{s_{RL}}s_{RR} \\
    \frac{1}{s_{LR}}s_{LL} - s_{RR} - \frac{1}{s_{LR}}s_{RL}s_{RR} & s_{LR} - s_{LL} \frac{1}{s_{LR}}s_{RR}
\end{pmatrix} = \frac{1}{2i} \begin{pmatrix}
    \frac{1}{s_{RL}} & \frac{1}{s_{RL}}s_{RR} \\
    \frac{1}{s_{LR}} - \frac{1}{s_{LR}}s_{RL}s_{RR} & \frac{1}{s_{LR}} - \frac{1}{s_{LR}}s_{RL}s_{RR}
\end{pmatrix}.
\]

Then, Eq. (B.7) is deformed to
\[
\frac{1}{2i} \begin{pmatrix}
    -\frac{1}{s_{RL}} & \frac{1}{s_{RL}}s_{RR} \\
    \frac{1}{s_{LR}} & \frac{1}{s_{LR}}s_{RR}
\end{pmatrix} \begin{pmatrix}
    f \\ b
\end{pmatrix} = \sin \theta \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} f \\ b \end{pmatrix}.
\]
Finally, we can obtain the mode equation (3.3) for the periodic system as

$$M_p \left( \begin{array}{c} f + b \\ \frac{1}{\sqrt{2}} \\ f - b \end{array} \right) = \sin \theta \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \left( \begin{array}{c} f + b \\ \frac{1}{\sqrt{2}} \\ f - b \end{array} \right),$$

(B.8)

where $M_p = M_p^\dagger$, because

$$M_p = \left( \begin{array}{cc} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{array} \right) \frac{1}{2i} \left( \begin{array}{cc} \frac{1}{s_{RL}} & -\frac{1}{s_{RL}} \\ -\frac{1}{s_{LR}} & \frac{1}{s_{LR}} \end{array} \right) \left( \begin{array}{cc} \frac{1}{s_{RR}} & \frac{1}{s_{RR}} \\ \frac{1}{s_{RR}} & -\frac{1}{s_{RR}} \end{array} \right) \left( \begin{array}{cc} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{array} \right).$$

The power flow of Eq. (B.8) is given by

$$\left( \begin{array}{c} f^\dagger + b^\dagger \\ \frac{1}{\sqrt{2}} \\ f^\dagger \end{array} \right) \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \left( \begin{array}{c} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{array} \right) = \left( \begin{array}{c} f^\dagger \\ b^\dagger \end{array} \right) \left( \begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \left( \begin{array}{c} f \\ b \end{array} \right) = f^\dagger f - b^\dagger b.$$

Note that the redefined mode $\Phi'_m$ ( $\Phi'_m$ ) of Eq. (B.6) are included in $f$ ( $b$ ).
C. Shrödinger equation

We will show two cases of quantum mechanics.

C.1. Equation for an electron in static electromagnetic field

Within Pauli approximation, the Shrödinger equation of an electron shows that

\[
E \psi = \left[ \frac{1}{2m_e} \left( \frac{\hbar}{i} \nabla + eA \right)^2 + V + \frac{e\hbar}{2m_e} \sigma \cdot B \right] \psi, \tag{C.1}
\]

where \( B = \nabla \times A \) and wave function

\[
\psi = \begin{pmatrix} \psi_\uparrow (r) \\ \psi_\downarrow (r) \end{pmatrix}.
\]

We will introduce \( H_{xy} \) as \( x \) and \( y \) components of eq. (C.1) as follows.

\[
H_{xy} = \frac{1}{2m_e} \left( \frac{\hbar}{i} \frac{\partial}{\partial x} + eA_x \right)^2 + \frac{1}{2m_e} \left( \frac{\hbar}{i} \frac{\partial}{\partial y} + eA_y \right)^2 + V + \frac{e\hbar}{2m_e} \sigma \cdot B.
\]

Note that \( zH_{xy} = \mathcal{H}_{xyz} \). Equation (C.1) can be modified to

\[
(E - \mathcal{H}_{xy}) \psi = \frac{m_e}{2} \left( \frac{\hbar}{im_e} \frac{\partial}{\partial z} + \frac{e}{m_e} A_z \right)^2 \psi.
\]

Then, we obtain a propagation equation:

\[
\left( \frac{2}{\hbar} (E - \mathcal{H}_{xy}) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right) \psi = -i \frac{\partial}{\partial z} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \psi,
\]

and \( \Psi \) is given by

\[
\Psi = \sqrt{dx \, dy} \left( \begin{pmatrix} \psi \\ \psi \frac{\hbar}{im_e} \frac{\partial}{\partial z} + \frac{e}{m_e} A_z \end{pmatrix} \psi \right).
\]

The \( \sqrt{dx \, dy} \) is formally added to the \( \Psi \) for integral of the cross section, and then numerical discrete formulation does not have it. The author is grateful to Dr. Motomu Takatsu for his suggestions to eq. (C.2).

When \( A_z = 0 \), eq. (C.2) can be reduced to

\[
\left( \frac{2}{\hbar} (E - \mathcal{H}_{xy}) \begin{pmatrix} 0 & 1 \\ 0 & \frac{e}{m_e} A_z \end{pmatrix} \right) \psi = -i \frac{\partial}{\partial z} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \psi.
\]

C.2. Ando model for 2D system

Equation (2.6) in [22] shows a vector \( C_j \) that satisfies

\[
(E - \mathcal{H}_0) C_j + t PC_{j-1} + t P^* C_{j+1} = 0,
\]

where \( P \) is a diagonal matrix and \( PP^* = 1 \). Note that \( \mathcal{H}_j = \mathcal{H}_0 \), and we can set that \( C_j = e^{i\theta} C_0 \). Equation (C.4) can be modified to

\[
e^{i\theta} C_j = P \frac{\mathcal{H}_0 - E}{t} C_j - P^2 C_{j-1}
\]

with \( e^{i\theta} C_{j-1} = C_j \). The above leads to the following eigenvalue problem:

\[
e^{i\theta} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix} = \begin{pmatrix} P \frac{\mathcal{H}_0 - E}{t} & -P^2 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix}.
\]
Furthermore, we can show mode equation for \( \sin \theta \). Equation (C.4) can also be modified to

\[
e^{-i\theta} C_j = P^* \frac{\mathcal{H}_0 - E}{t} C_j - (P^*)^2 C_{j+1}
\]

with \( e^{-i\theta} C_{j+1} = C_j \). Then the above leads to another eigenvalue problem:

\[
e^{-i\theta} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\left( P^* \right)^2 & \frac{P^* \mathcal{H}_0 - E}{t} \end{pmatrix} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix}.
\]

From both eigenvalue problems,

\[
e^{i\theta} - e^{-i\theta} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix} = \begin{pmatrix} P^2 \mathcal{H}_0 - E & \frac{1}{2} - P^2 \\ P^2 \mathcal{H}_0 - E & \frac{1}{2} - P^2 \end{pmatrix} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix}.
\]

Let us introduce a diagonal matrix \( Q \): \( i P = Q^2 \) and \( QQ^* = 1 \). We obtain a mode equation of the Ando model:

\[
\begin{pmatrix} -\text{Re} P & Q^* \frac{E - \mathcal{H}_0}{2t} \\ Q \frac{E - \mathcal{H}_0}{2t} & -\text{Re} P \end{pmatrix} \Phi_n = \sin \theta_n \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_n,
\]

where

\[
\Phi_n = \begin{pmatrix} \phi_{an} \\ \phi_{bn} \end{pmatrix} = \begin{pmatrix} Q^* C_j(n) \\ -QC_{j-1}(n) \end{pmatrix}.
\]

Let us consider a special case that \( P = 1 \), i.e. \( Q = \exp(i\pi/4) \). Equation (C.5) becomes that

\[
\begin{pmatrix} -1 & -im \\ im & -1 \end{pmatrix} \Phi_n = \sin \theta_n \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Phi_n,
\]

where \( m = (E - \mathcal{H}_0) / (2t) \). Furthermore,

\[
\begin{pmatrix} 1 - mm & 0 \\ 0 & 1 - mm \end{pmatrix} \Phi_n = \sin^2 \theta_n \Phi_n.
\]

Then, we can obtain \( \Phi_n \) by solving

\[
(1 - mm) \phi_{an} = \sin^2 \theta_n \phi_{an}, \quad \phi_{bn} = (im - \sin \theta_n) \phi_{an}
\]

or

\[
(1 - mm) \phi_{bn} = \sin^2 \theta_n \phi_{bn}, \quad \phi_{an} = -(im + \sin \theta_n) \phi_{bn}.
\]

The eigenvalue \( \sin^2 \theta_n \) is always real, since \( m = m^\dagger \).

[Go to table of contents.] [Go to home.]
D. Generalized Maxwell equation

This chapter derives propagation equation (3.1) for Maxwell equation. The Maxwell equation in frequency domain is generalized into a matrix representation:

\[
\begin{pmatrix}
0 & i \nabla \times \\
-i \nabla \times & 0
\end{pmatrix}
\begin{pmatrix}
E \\
H
\end{pmatrix} = \omega
\begin{pmatrix}
\varepsilon & \alpha \\
\gamma & \mu
\end{pmatrix}
\begin{pmatrix}
E \\
H
\end{pmatrix}.
\]

We added small matrices \( \alpha \) and \( \gamma \) for multiferroics to the right hand of eq. (D.1). The following section will focus on coordinate transformations for rotation operator in the left hand of eq. (D.1).

D.1. Rotation for arbitrary orthogonal curvilinear coordinates

We consider Cartesian coordinate \((x_0, x_1, x_2)\) and orthogonal curvilinear coordinate \((u_0, u_1, u_2)\) as shown in Fig. D.1. Note that we use non-negative integers 0, 1 and 2 for the coordinate numbers, because modulo operation can be directly applicable to the numbers.

Rotation \( \nabla \times \) in an orthogonal curvilinear coordinates is defined by

\[
\nabla \times X = \sum_{j=0}^{2} \frac{1}{h_j h_k h_l} \left( h_j \frac{\partial}{\partial u_k} (h_l X_l) - h_j \frac{\partial}{\partial u_l} (h_k X_k) \right) u_j,
\]

where \( u_j \) is a unit vector in the \((u_0, u_1, u_2)\) space, \( k = j + 1 \mod 3 \) and \( l = j + 2 \mod 3 \), and \( h_k \) are scale factors:

\[
h_k = \sqrt{\sum_{j=0}^{2} \left( \frac{\partial x_j}{\partial u_k} \right)^2} \quad \text{for} \quad k = 0, 1, 2.
\]

Matrix representation of \( \nabla \times \) as in eq. (4) of [23] is that

\[
\nabla \times = \frac{1}{\prod_{j=0}^{2} h_j} f_u (\nabla_{u}\times) f_u,
\]

where

\[
f_u \triangleq \begin{pmatrix}
h_0 & 0 & 0 \\
0 & h_1 & 0 \\
0 & 0 & h_2
\end{pmatrix}, \quad \nabla_{u}\times \triangleq \begin{pmatrix}
0 & -\partial_{u_2} & \partial_{u_1} \\
\partial_{u_2} & 0 & -\partial_{u_0} \\
-\partial_{u_1} & \partial_{u_0} & 0
\end{pmatrix} \quad \text{as} \quad \partial_{u_j} = \frac{\partial}{\partial u_j}.
\]

Figure D.1.: Cartesian coordinate \((x_0, x_1, x_2)\) and orthogonal curvilinear coordinate \((u_0, u_1, u_2)\).
Maxwell equation of eq. (D.1) is deformed by eq. (D.3) into

\[
\left( \begin{array}{c} 0 \\ -i \nabla u \times \\ 0 \end{array} \right) \left( \begin{array}{c} f_u E \\ f_u H \end{array} \right) = \omega \left( \begin{array}{c} \varepsilon \\ \tilde{l} \\ \gamma \end{array} \right) \left( \begin{array}{c} \tilde{\alpha} \\ \tilde{\mu} \end{array} \right) \left( \begin{array}{c} f_u E \\ f_u H \end{array} \right),
\]

where

\[
\tilde{\varepsilon}_{jk} \triangleq \hat{h}_0 h_1 h_2 \frac{\varepsilon_{jk}}{h_j h_k}, \quad \tilde{\alpha}_{jk} \triangleq \hat{h}_0 h_1 h_2 \frac{\alpha_{jk}}{h_j h_k}, \quad \tilde{\gamma}_{jk} \triangleq \hat{h}_0 h_1 h_2 \frac{\gamma_{jk}}{h_j h_k}, \quad \tilde{\mu}_{jk} \triangleq \hat{h}_0 h_1 h_2 \frac{\mu_{jk}}{h_j h_k}.
\]

D.2. Details of deformed Maxwell equation

We will focus on a case: \( \tilde{\varepsilon}_{22} \tilde{\mu}_{22} \neq \tilde{\alpha}_{22} \tilde{\gamma}_{22} \). As shown in Section D.5, transformed \( \tilde{\varepsilon}, \tilde{\alpha}, \tilde{\gamma} \) and \( \tilde{\mu} \) can be defined as

\[
\left( \begin{array}{c} \tilde{\varepsilon} \\ \tilde{\alpha} \\ \tilde{\gamma} \\ \tilde{\mu} \end{array} \right) = (1 - u_{\varepsilon} - u_{\mu}) \left( \begin{array}{c} \varepsilon \\ \alpha \\ \gamma \\ \mu \end{array} \right) (1 - l_{\varepsilon} - l_{\mu}),
\]

where

\[
1 - l_{\varepsilon} - l_{\mu} = \left( \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -l_{\mu 0} & -l_{\mu 1} & 0 & -l_{\mu 3} \end{array} \right),
\]

as

\[
\left\{ \begin{array}{l}
 l_{\varepsilon n} = \frac{\tilde{\mu}_{22} \tilde{\varepsilon}_{22} - \tilde{\alpha}_{22} \tilde{\gamma}_{22}}{\epsilon}, \\
 l_{\mu n} = \frac{\tilde{\varepsilon}_{22} \tilde{\gamma}_{22} - \tilde{\alpha}_{22} \tilde{\mu}_{22}}{\epsilon}, \\
 l_{\varepsilon n+3} = \frac{\tilde{\mu}_{22} \tilde{\varepsilon}_{22} - \tilde{\alpha}_{22} \tilde{\gamma}_{22}}{\epsilon}, \\
 l_{\mu n+3} = \frac{\tilde{\varepsilon}_{22} \tilde{\gamma}_{22} - \tilde{\alpha}_{22} \tilde{\mu}_{22}}{\epsilon}.
\end{array} \right.
\]  

and

\[
1 - u_{\varepsilon} - u_{\mu} = \left( \begin{array}{cccc} 1 & 0 & -u_{\varepsilon 0} & 0 \\ 0 & 1 & -u_{\varepsilon 1} & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & -u_{\varepsilon 3} & 1 \end{array} \right),
\]

as

\[
\left\{ \begin{array}{l}
 u_{\varepsilon n} = \frac{\tilde{\mu}_{22} \tilde{\varepsilon}_{22} - \tilde{\gamma}_{22} \tilde{\alpha}_{n 2}}{\epsilon}, \\
 u_{\mu n} = \frac{\tilde{\varepsilon}_{22} \tilde{\alpha}_{n 2} - \tilde{\gamma}_{22} \tilde{\mu}_{n 2}}{\epsilon}, \\
 u_{\varepsilon n+3} = \frac{\tilde{\mu}_{22} \tilde{\varepsilon}_{22} - \tilde{\gamma}_{22} \tilde{\alpha}_{n 2}}{\epsilon}, \\
 u_{\mu n+3} = \frac{\tilde{\varepsilon}_{22} \tilde{\alpha}_{n 2} - \tilde{\gamma}_{22} \tilde{\mu}_{n 2}}{\epsilon}.
\end{array} \right.
\]

The \( \tilde{\varepsilon}, \tilde{\alpha}, \tilde{\gamma} \) and \( \tilde{\mu} \) are that

\[
\tilde{\varepsilon} = \left( \begin{array}{ccc} \tilde{\varepsilon}_{00} & \tilde{\varepsilon}_{01} & 0 \\ \tilde{\varepsilon}_{10} & \tilde{\varepsilon}_{11} & 0 \\ 0 & 0 & \tilde{\varepsilon}_{22} \end{array} \right), \quad \tilde{\alpha} = \left( \begin{array}{ccc} \tilde{\alpha}_{00} & \tilde{\alpha}_{01} & 0 \\ \tilde{\alpha}_{10} & \tilde{\alpha}_{11} & 0 \\ 0 & 0 & \tilde{\alpha}_{22} \end{array} \right), \quad \tilde{\gamma} = \left( \begin{array}{ccc} \tilde{\gamma}_{00} & \tilde{\gamma}_{01} & 0 \\ \tilde{\gamma}_{10} & \tilde{\gamma}_{11} & 0 \\ 0 & 0 & \tilde{\gamma}_{22} \end{array} \right), \quad \tilde{\mu} = \left( \begin{array}{ccc} \tilde{\mu}_{00} & \tilde{\mu}_{01} & 0 \\ \tilde{\mu}_{10} & \tilde{\mu}_{11} & 0 \\ 0 & 0 & \tilde{\mu}_{22} \end{array} \right),
\]

where

\[
\left\{ \begin{array}{l}
 \tilde{\varepsilon}_{mn} = \tilde{\varepsilon}_{mn} - \tilde{\varepsilon}_{m 2} l_{\varepsilon n} - \tilde{\alpha}_{m 2} l_{\mu n}, \\
 \tilde{\alpha}_{mn} = \tilde{\alpha}_{mn} - \tilde{\varepsilon}_{m 2} l_{\varepsilon n+3} - \tilde{\alpha}_{m 2} l_{\mu n+3}, \\
 \tilde{\gamma}_{mn} = \tilde{\gamma}_{mn} - \tilde{\varepsilon}_{m 2} l_{\varepsilon n+3} - \tilde{\mu}_{m 2} l_{\mu n+3}, \\
 \tilde{\mu}_{mn} = \tilde{\mu}_{mn} - \tilde{\varepsilon}_{m 2} l_{\varepsilon n+3} - \tilde{\mu}_{m 2} l_{\mu n+3}.
\end{array} \right.
\]  

for \( m, n = 0, 1 \). The \( 1 - l_{\varepsilon} - l_{\mu} \) and \( 1 + l_{\varepsilon} + l_{\mu} \) have the following relation by eq. (D.14):

\[
(1 - l_{\varepsilon} - l_{\mu}) (1 + l_{\varepsilon} + l_{\mu}) = 1.
\]  

Then, equation (D.4) is transformed to

\[
(1 - u_{\varepsilon} - u_{\mu}) \left( \begin{array}{c} 0 \\ -i \nabla u \times \\ 0 \end{array} \right) (1 - l_{\varepsilon} - l_{\mu}) \left( \begin{array}{c} \tilde{E} \\ \tilde{H} \end{array} \right) = \omega \left( \begin{array}{c} \tilde{\varepsilon} \\ \tilde{\alpha} \\ \tilde{\gamma} \\ \tilde{\mu} \end{array} \right) \left( \begin{array}{c} \tilde{E} \\ \tilde{H} \end{array} \right),
\]  

\[
(D.8)
\]
\[
\begin{align*}
\left( \begin{array}{c}
\hat{E} \\
\hat{H}
\end{array} \right) & \triangleq \left( 1 + l_\varepsilon + l_\mu \right) \left( \begin{array}{c}
f_aE \\
f_aH
\end{array} \right) = \left( h_0 E_0 \ h_1 E_1 \ \hat{E}_2 \ h_0 H_0 \ h_1 H_1 \ \hat{H}_2 \right)^T, \\
\hat{E}_2 & \triangleq h_2 E_2 + \sum_{n=0}^1 \left( l_{0n} h_n E_n + l_{1n} h_n H_n \right), \\
\hat{H}_2 & \triangleq h_2 H_2 + \sum_{n=0}^1 \left( l_{0n} h_n E_n + l_{1n} h_n H_n \right).
\end{align*}
\]

From eq. (D.16) and the above definitions of \(\hat{E}_2\) and \(\hat{H}_2\), the component of \(u_2\) can be represented by other components:
\[
\begin{align*}
\left( \begin{array}{c}
h_2 E_2 \\
h_2 H_2
\end{array} \right) & = \left[ \begin{array}{c}
\frac{i c_{22}^2}{\omega} \\
\frac{i c_{22}^2}{\omega}
\end{array} \right] \left( \begin{array}{c}
\hat{E}_2 \\
\hat{H}_2
\end{array} \right) \pm \left( \begin{array}{c}
l_{\ell 0} l_{\ell 1} \\
l_{\ell 0} l_{\ell 1}
\end{array} \right) \left( \begin{array}{c}
h_0 E_0 \\
h_1 E_1
\end{array} \right), \\
\text{with } c_{22}^{-2} & \triangleq \hat{\varepsilon}_{22} \hat{\mu}_{22} - \hat{\alpha}_{22} \hat{\gamma}_{22}.
\end{align*}
\]

Let us introduce column vector \(\Psi\) of four components:
\[
\Psi = \frac{\sqrt{du_0 d u_1}}{2} \left( \begin{array}{c}
\n h_0 H_0 \\
\n h_1 H_1 \\
\n -h_1 E_1 \\
\n -h_0 E_0
\end{array} \right)^T.
\]

The \(\sqrt{du_0 du_1}/2\) is formally added to the \(\Psi\), and then numerical discrete formulation in eq. (7.2) does not have it. By using the \(\Psi\) of eq. (D.11), we can simplify the generalized Maxwell equation (D.1) into the propagation equation (3.1). As shown in eqs. (D.17) and (D.18), the \(M\) of eq. (3.1) is given by
\[
M = \left( \begin{array}{cc}
m_{aa} & m_{ab} \\
m_{ba} & m_{bb}
\end{array} \right),
\]
\[
\begin{align*}
m_{aa} & = \left( \begin{array}{c}
\omega \mu_{00} + \partial_{u_1} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_0} - i \partial_{u_1} \varepsilon_{22} \partial_{u_0} - i \partial_{u_1} l_{\ell 4} + i u_{\ell 3} \partial_{u_0} \\
\omega \mu_{10} - \partial_{u_0} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_1} + i \partial_{u_0} \varepsilon_{22} \partial_{u_1} + i \partial_{u_0} l_{\ell 4} + i u_{\ell 3} \partial_{u_1}
\end{array} \right), \\
m_{ab} & = \left( \begin{array}{c}
\omega \mu_{01} - \partial_{u_0} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_1} + i \partial_{u_0} \varepsilon_{22} \partial_{u_1} - i \partial_{u_0} l_{\ell 4} - i u_{\ell 3} \partial_{u_1} \\
\omega \mu_{11} + \partial_{u_1} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_0} - i \partial_{u_1} \varepsilon_{22} \partial_{u_0} + i \partial_{u_1} l_{\ell 4} - i u_{\ell 3} \partial_{u_0}
\end{array} \right), \\
m_{ba} & = \left( \begin{array}{c}
\omega \mu_{00} + \partial_{u_1} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_0} - i \partial_{u_1} \varepsilon_{22} \partial_{u_0} - i \partial_{u_1} l_{\ell 4} - i u_{\ell 3} \partial_{u_0} \\
\omega \mu_{11} + \partial_{u_0} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_1} - i \partial_{u_0} \varepsilon_{22} \partial_{u_1} + i \partial_{u_0} l_{\ell 4} - i u_{\ell 3} \partial_{u_1}
\end{array} \right), \\
m_{bb} & = \left( \begin{array}{c}
\omega \mu_{01} + \partial_{u_0} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_1} + i \partial_{u_0} \varepsilon_{22} \partial_{u_1} + i \partial_{u_0} l_{\ell 4} + i u_{\ell 3} \partial_{u_1} \\
\omega \mu_{11} - \partial_{u_1} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_0} + i \partial_{u_1} \varepsilon_{22} \partial_{u_0} - i \partial_{u_1} l_{\ell 4} + i u_{\ell 3} \partial_{u_0}
\end{array} \right),
\end{align*}
\]
with \(c_{22}^{-2} = (\hat{\varepsilon}_{22} \hat{\mu}_{22} - \hat{\alpha}_{22} \hat{\gamma}_{22})^{-1}\). Note that \(M = M^\dagger\) when \(\varepsilon = \varepsilon^\dagger\), \(\mu = \mu^\dagger\), \(\gamma = \alpha^\dagger\) and \(\partial_{u_j} = -\partial_{u_j}^\dagger\) as the system satisfies boundary condition as eq. (6.7).

### D.3. Special case

This section consider a case that \(\varepsilon\) and \(\mu\) are diagonal hermitian, and \(\alpha = \gamma = 0\). Note that \(l_{\mu n} = u_{\mu n} = \ell_{\varepsilon n} = u_{\varepsilon n} = 0\) as \(n = 0, 1, 3, 4\) from eqs. (D.5) and (D.6). Therefore \(m_{ab} = m_{ba} = 0\) in eq. (D.12), and the \(M\) in eq. (3.1) can be reduced to
\[
M = \left( \begin{array}{cc}
m_{aa} & 0 \\
0 & m_{bb}
\end{array} \right)
\]

\[
\begin{align*}
m_{aa} & = \left( \begin{array}{c}
\omega \mu_{00} + \partial_{u_1} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_0} - \partial_{u_1} l_{\ell 4} - i u_{\ell 3} \partial_{u_0} \\
\omega \mu_{10} - \partial_{u_0} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_1} + i \partial_{u_0} l_{\ell 4} + i u_{\ell 3} \partial_{u_1}
\end{array} \right), \\
m_{bb} & = \left( \begin{array}{c}
\omega \mu_{01} - \partial_{u_0} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_1} + i \partial_{u_0} l_{\ell 4} - i u_{\ell 3} \partial_{u_1} \\
\omega \mu_{11} + \partial_{u_1} \frac{\varepsilon_{22} \varepsilon_{22}}{\omega} \partial_{u_0} - i \partial_{u_1} l_{\ell 4} + i u_{\ell 3} \partial_{u_0}
\end{array} \right),
\end{align*}
\]
Equation (D.13) becomes the same as eqs. (3.2-9) and (3.2-10) of [3] when \( h_0 = h_1 = h_2 = 1, \varepsilon = \varepsilon_0 \) and \( \mu = \mu_0 \).

**D.4. Permittivity with damping**

Permittivity with damping becomes complex number. Then we will check it by considering response of polarization. Orientation polarization is represented by \( P_o(t) = \chi_o E(t) - \gamma \frac{dP_o}{dt} \). Then,

\[
P_o(\omega) = \chi_o E(\omega) \frac{1 + i\omega\tau}{1 + \omega^2\tau^2} \chi_o E(\omega) .
\]

Displacement polarization: \( m^2 \frac{d^2 \varphi}{dt^2} = -m\omega_0^2 x(t) - m\omega_1 \frac{dx}{dt} + qE(t) \). Then,

\[
x(\omega) = \frac{q}{m} \frac{\omega_0^2 - \omega^2 + i\omega_1 \omega}{(\omega_0^2 - \omega^2)^2 + \omega_1^2 \omega^2} E(\omega) .
\]

Electron polarization is a special case of the displacement polarization: \( \omega_0^2 = 0 \).

Therefore, imaginary part of permittivity becomes positive for damped case. Note that time dependence \( \exp(-i\omega t) \) is assumed.

**D.5. Check of eqs. (D.5), (D.6), (D.7) and (D.8)**

\[
\left( \begin{array}{c} \varepsilon_1 \\ \hat{\gamma} \\ \hat{\mu} \end{array} \right) = (1 - u_e - u_\mu) \left( \begin{array}{c} \varepsilon_1 \\ \hat{\gamma} \\ \hat{\mu} \end{array} \right) (1 - \lambda_e - \lambda_\mu)
\]

\[
= (1 - u_e - u_\mu) \left( \begin{array}{cccc} \bar{\varepsilon}_{10} & \bar{\varepsilon}_{11} & \bar{\varepsilon}_{12} & \bar{\varepsilon}_{13} \\ \bar{\varepsilon}_{21} & \bar{\varepsilon}_{22} & \bar{\varepsilon}_{23} & \bar{\varepsilon}_{24} \\ \bar{\varepsilon}_{31} & \bar{\varepsilon}_{32} & \bar{\varepsilon}_{33} & \bar{\varepsilon}_{34} \\ \bar{\varepsilon}_{41} & \bar{\varepsilon}_{42} & \bar{\varepsilon}_{43} & \bar{\varepsilon}_{44} \end{array} \right) \right)
\times \left( \begin{array}{cccc} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -\lambda_{1e} & -\lambda_{1e} & -\lambda_{1e} & -\lambda_{1e} \\ -\lambda_{1e} & -\lambda_{1e} & -\lambda_{1e} & -\lambda_{1e} \end{array} \right)
\]

From eq. (D.5),

\[
\left\{ \begin{array}{l}
\bar{\varepsilon}_{2n} - \bar{\varepsilon}_{22l_{e-}} - \bar{\varepsilon}_{22l_{\mu-}} = \bar{\varepsilon}_{2n} - \bar{\varepsilon}_{22l_{e-}} - \bar{\varepsilon}_{22l_{\mu-}} \\
\bar{\gamma}_{2n} - \bar{\gamma}_{22l_{e-}} - \bar{\gamma}_{22l_{\mu-}} = \bar{\gamma}_{2n} - \bar{\gamma}_{22l_{e-}} - \bar{\gamma}_{22l_{\mu-}} \\
\bar{\alpha}_{2n} - \bar{\alpha}_{22l_{e-}} - \bar{\alpha}_{22l_{\mu-}} = \bar{\alpha}_{2n} - \bar{\alpha}_{22l_{e-}} - \bar{\alpha}_{22l_{\mu-}} \\
\bar{\mu}_{2n} - \bar{\mu}_{22l_{e-}} - \bar{\mu}_{22l_{\mu-}} = \bar{\mu}_{2n} - \bar{\mu}_{22l_{e-}} - \bar{\mu}_{22l_{\mu-}} \end{array} \right. = 0 .
\]
From the above relations and eq. (D.7),
\[
\begin{pmatrix}
\dot{\varepsilon} & \dot{\alpha} \\
\dot{\gamma} & \dot{\mu}
\end{pmatrix}
= \begin{pmatrix}
1 & 0 & -u_{e0} & 0 & 0 & -u_{\mu0} \\
0 & 1 & -u_{e1} & 0 & 0 & -u_{\mu1} \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & -u_{e3} & 1 & 0 & -u_{\mu3} \\
0 & 0 & -u_{e4} & 0 & 1 & -u_{\mu4} \\
0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
\tilde{\varepsilon}_{00} & \tilde{\varepsilon}_{01} & \tilde{\varepsilon}_{02} & \tilde{\alpha}_{00} & \tilde{\alpha}_{01} & \tilde{\alpha}_{02} \\
\tilde{\varepsilon}_{10} & \tilde{\varepsilon}_{11} & \tilde{\varepsilon}_{12} & \tilde{\alpha}_{10} & \tilde{\alpha}_{11} & \tilde{\alpha}_{12} \\
\tilde{\gamma}_{00} & \tilde{\gamma}_{01} & \tilde{\gamma}_{02} & \tilde{\mu}_{00} & \tilde{\mu}_{01} & \tilde{\mu}_{02} \\
\tilde{\gamma}_{10} & \tilde{\gamma}_{11} & \tilde{\gamma}_{12} & \tilde{\mu}_{10} & \tilde{\mu}_{11} & \tilde{\mu}_{12} \\
0 & 0 & \tilde{\gamma}_{22} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \tilde{\mu}_{22} & 0
\end{pmatrix}
\]

From eq. (D.6),
\[
\begin{align*}
\tilde{\varepsilon}_{n2} - u_{e n} \tilde{\varepsilon}_{22} - u_{\mu m} \tilde{\gamma}_{22} &= \tilde{\varepsilon}_{n2} - \frac{\tilde{\mu}_{22} \tilde{\varepsilon}_{n2} - \tilde{\gamma}_{22} \tilde{\alpha}_{n2} - \tilde{\alpha}_{22} \tilde{\varepsilon}_{n2}}{\tilde{\varepsilon}_{22} \tilde{\mu}_{22} - \tilde{\alpha}_{22} \tilde{\gamma}_{22}} = 0, \\
\tilde{\alpha}_{n2} - u_{e n} \tilde{\alpha}_{22} - u_{\mu m} \tilde{\mu}_{22} &= \tilde{\alpha}_{n2} - \frac{\tilde{\mu}_{22} \tilde{\alpha}_{n2} - \tilde{\gamma}_{22} \tilde{\alpha}_{n2} - \tilde{\alpha}_{22} \tilde{\alpha}_{n2}}{\tilde{\varepsilon}_{22} \tilde{\mu}_{22} - \tilde{\alpha}_{22} \tilde{\gamma}_{22}} = 0, \\
\tilde{\gamma}_{n2} - u_{e 3+n} \tilde{\varepsilon}_{22} - u_{\mu 3+n} \tilde{\gamma}_{22} &= \tilde{\gamma}_{n2} - \frac{\tilde{\mu}_{22} \tilde{\gamma}_{n2} - \tilde{\gamma}_{22} \tilde{\mu}_{n2} - \tilde{\alpha}_{22} \tilde{\gamma}_{n2}}{\tilde{\varepsilon}_{22} \tilde{\mu}_{22} - \tilde{\alpha}_{22} \tilde{\gamma}_{22}} = 0, \\
\tilde{\mu}_{n2} - u_{e 3+n} \tilde{\alpha}_{22} - u_{\mu 3+n} \tilde{\mu}_{22} &= \tilde{\mu}_{n2} - \frac{\tilde{\mu}_{22} \tilde{\mu}_{n2} - \tilde{\gamma}_{22} \tilde{\mu}_{n2} - \tilde{\alpha}_{22} \tilde{\mu}_{n2}}{\tilde{\varepsilon}_{22} \tilde{\mu}_{22} - \tilde{\alpha}_{22} \tilde{\gamma}_{22}} = 0.
\end{align*}
\]

Then,
\[
\begin{pmatrix}
\dot{\varepsilon} & \dot{\alpha} \\
\dot{\gamma} & \dot{\mu}
\end{pmatrix}
= \begin{pmatrix}
\tilde{\varepsilon}_{00} & \tilde{\varepsilon}_{01} & 0 & \tilde{\alpha}_{00} & \tilde{\alpha}_{01} & 0 \\
\tilde{\varepsilon}_{10} & \tilde{\varepsilon}_{11} & 0 & \tilde{\alpha}_{10} & \tilde{\alpha}_{11} & 0 \\
0 & 0 & \tilde{\varepsilon}_{22} & 0 & 0 & \tilde{\alpha}_{22} \\
\tilde{\gamma}_{00} & \tilde{\gamma}_{01} & \tilde{\gamma}_{02} & \tilde{\mu}_{00} & \tilde{\mu}_{01} & 0 \\
\tilde{\gamma}_{10} & \tilde{\gamma}_{11} & \tilde{\gamma}_{12} & \tilde{\mu}_{10} & \tilde{\mu}_{11} & 0 \\
0 & 0 & \tilde{\gamma}_{22} & 0 & 0 & \tilde{\mu}_{22}
\end{pmatrix}
\]

We checked the consistency of eqs. (D.5), (D.6) and (D.7). Furthermore, we can confirm eq. (D.8), since square of \(L_e + L_\mu\) is equal to zero:
\[
(L_e + L_\mu)^2 = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
\end{pmatrix}
= 0.
\]
D.6. Check of eqs. (D.10) and (D.12)

Details of eq. (D.9) are represented as

\[
(1 - \mathbf{u}_c - \mathbf{u}_\mu) \begin{pmatrix}
0 \\
-i\nabla_u \times \\
0
\end{pmatrix}
(1 - \mathbf{E}_c - \mathbf{E}_\mu)
\]

\[
\begin{pmatrix}
1 & 0 & -u_{c1} & 0 & 0 & 0 & -u_{\mu 0} \\
0 & 1 & -u_{c1} & 0 & 0 & 0 & -u_{\mu 1} \\
0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & -u_{c3} & 1 & 0 & -u_{\mu 3} & 0 \\
0 & 0 & -u_{c4} & 1 & -u_{\mu 4} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}
\begin{pmatrix}
-i\partial_{c1} \\
iu_{\mu 0}\partial_{c0} \\
0 \\
i\partial_{c2} \\
i\partial_{c3} \\
i\partial_{c4}
\end{pmatrix}
\begin{pmatrix}
-i\partial_{\mu 2} \\
i\partial_{c0} \\
i\partial_{c1} \\
i\partial_{c2} \\
i\partial_{c3} \\
i\partial_{c4}
\end{pmatrix}
\begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}
\begin{pmatrix}
-i\partial_{0} \\
i\partial_{0} \\
i\partial_{0} \\
i\partial_{0} \\
i\partial_{0} \\
i\partial_{0}
\end{pmatrix}
\begin{pmatrix}
h_0 E_0 \\
h_1 E_1 \\
\hat{E}_2 \\
h_0 H_0 \\
h_1 H_1 \\
H_2
\end{pmatrix}
\]

\[
(1 - \mathbf{E}_c - \mathbf{E}_\mu)
\]

\[
\begin{pmatrix}
0 \\
0 \\
0 \\
0 \\
0 \\
0
\end{pmatrix}
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 \\
-\mu_0 -\mu_1 -\mu_3 -\mu_4 1
\end{pmatrix}
\begin{pmatrix}
\hat{E}_2 \\
h_0 E_1 \\
h_0 H_0 \\
h_1 H_1 \\
H_2
\end{pmatrix}
\]

\[
(\omega)
\begin{pmatrix}
\tilde{\xi}_{00} & \tilde{\xi}_{01} & 0 & \hat{\alpha}_{00} & \hat{\alpha}_{01} & 0 \\
\tilde{\xi}_{10} & \tilde{\xi}_{11} & 0 & \hat{\alpha}_{10} & \hat{\alpha}_{11} & 0 \\
0 & 0 & \bar{\xi}_{22} & 0 & 0 & \bar{\alpha}_{22} \\
\bar{\gamma}_{00} & \bar{\gamma}_{01} & 0 & \hat{\mu}_{00} & \hat{\mu}_{01} & 0 \\
\bar{\gamma}_{10} & \bar{\gamma}_{11} & 0 & \hat{\mu}_{10} & \hat{\mu}_{11} & 0 \\
0 & 0 & \bar{\gamma}_{22} & 0 & 0 & \bar{\mu}_{22}
\end{pmatrix}
\begin{pmatrix}
h_0 E_0 \\
h_1 E_1 \\
\hat{E}_2 \\
h_0 H_0 \\
h_1 H_1 \\
H_2
\end{pmatrix}
\]

\[
(\omega)
\begin{pmatrix}
\tilde{\xi}_{22} & \tilde{\alpha}_{22} \\
\tilde{\gamma}_{22} & \tilde{\mu}_{22}
\end{pmatrix}
\begin{pmatrix}
\hat{E}_2 \\
H_2
\end{pmatrix}
\]

From eq. (D.15),

\[
\omega \begin{pmatrix}
\tilde{\xi}_{22} & \tilde{\alpha}_{22} \\
\tilde{\gamma}_{22} & \tilde{\mu}_{22}
\end{pmatrix}
\begin{pmatrix}
\hat{E}_2 \\
H_2
\end{pmatrix}
= \begin{pmatrix}
0 & 0 \\
i\partial_{a1} & -i\partial_{a0}
\end{pmatrix}
\begin{pmatrix}
h_0 E_0 \\
h_1 E_1
\end{pmatrix}
+ \begin{pmatrix}
i\partial_{a1} & i\partial_{a0}
\end{pmatrix}
\begin{pmatrix}
h_0 H_0 \\
h_1 H_1
\end{pmatrix}.
\]

Note that

\[
\begin{pmatrix}
\tilde{\mu}_{22} & -\tilde{\alpha}_{22} \\
-\tilde{\gamma}_{22} & \tilde{\xi}_{22}
\end{pmatrix}
= \tilde{\xi}_{22}\tilde{\mu}_{22} - \tilde{\alpha}_{22}\tilde{\gamma}_{22} = c_{22}^2.
\]

Then,

\[
\begin{pmatrix}
\hat{E}_2 \\
\hat{H}_2
\end{pmatrix}
= \frac{c_{22}^2}{\omega} \begin{pmatrix}
-i\tilde{\gamma}_{22}\partial_{a1} & i\tilde{\alpha}_{22}\partial_{a0} \\
i\tilde{\xi}_{22}\partial_{a1} & -i\tilde{\xi}_{22}\partial_{a0}
\end{pmatrix}
\begin{pmatrix}
h_0 E_0 \\
h_1 E_1
\end{pmatrix}
+ \frac{c_{22}^2}{\omega} \begin{pmatrix}
-i\tilde{\gamma}_{22}\partial_{a1} & i\tilde{\gamma}_{22}\partial_{a0} \\
i\tilde{\xi}_{22}\partial_{a1} & -i\tilde{\xi}_{22}\partial_{a0}
\end{pmatrix}
\begin{pmatrix}
h_0 H_0 \\
h_1 H_1
\end{pmatrix}.
\]
From eq. (D.15),

\[
\begin{pmatrix}
-i\nu_{\mu 0}\partial_{\alpha 1} - i\partial_{\alpha 1}\mu_0 & i\nu_{\mu 0}\partial_{\alpha 0} - i\partial_{\alpha 1}\mu_1 \\
-i\nu_{\alpha 1}\partial_{\alpha 1} + i\partial_{\alpha 0}\mu_0 & i\nu_{\alpha 1}\partial_{\alpha 0} + i\partial_{\alpha 0}\mu_1
\end{pmatrix}
\begin{pmatrix}
\h_0E_0 \\
\h_1E_1
\end{pmatrix}
+ \begin{pmatrix}
\partial_{\alpha 2} & i\partial_{\alpha 2} & i\partial_{\alpha 1}\mu_0 - i\partial_{\alpha 1}\mu_3 \\
-i\nu_{\alpha 2} - i\nu_{\alpha 0}\partial_{\alpha 0} - i\partial_{\alpha 1}\mu_4
\end{pmatrix}
\begin{pmatrix}
\h_0H_0 \\
\h_1H_1
\end{pmatrix}
+ \begin{pmatrix}
-i\partial_{\alpha 1} \\
\partial_{\alpha 2} + i\nu_{\alpha 1}\partial_{\alpha 0} + i\partial_{\alpha 0}\mu_3
\end{pmatrix}
\hat{H}_2
\]

\[
= \omega\begin{pmatrix}
\bar{\varepsilon}_{10} & \bar{\varepsilon}_{11}
\end{pmatrix}
\begin{pmatrix}
\h_0E_0 \\
\h_1E_1
\end{pmatrix}
+ \omega\begin{pmatrix}
\bar{\alpha}_{10} & \bar{\alpha}_{11}
\end{pmatrix}
\begin{pmatrix}
\h_0H_0 \\
\h_1H_1
\end{pmatrix}.
\]

We can check the \( m_{bb} \) and \( m_{ba} \) in eq. (D.12) with using the right side of eq. (D.17) and the \( \Psi \) definition of eq. (D.11).

From eq. (D.15),

\[
\begin{pmatrix}
-i\nu_{\mu 3}\partial_{\alpha 1} + i\partial_{\alpha 1}\mu_3 & i\partial_{\alpha 2} + i\nu_{\mu 3}\partial_{\alpha 0} + i\partial_{\alpha 1}\mu_1 \\
-i\partial_{\alpha 2} - i\nu_{\mu 3}\partial_{\alpha 1} - i\partial_{\alpha 0}\mu_0 & i\nu_{\mu 3}\partial_{\alpha 0} - i\partial_{\alpha 0}\mu_1
\end{pmatrix}
\begin{pmatrix}
\h_0E_0 \\
\h_1E_1
\end{pmatrix}
+ \begin{pmatrix}
-i\partial_{\alpha 1} \\
\partial_{\alpha 2} + i\nu_{\alpha 1}\partial_{\alpha 0} + i\partial_{\alpha 0}\mu_3
\end{pmatrix}
\hat{E}_2
\]

\[
= \omega\begin{pmatrix}
\bar{\gamma}_{10} & \bar{\gamma}_{11}
\end{pmatrix}
\begin{pmatrix}
\h_0E_0 \\
\h_1E_1
\end{pmatrix}
+ \omega\begin{pmatrix}
\bar{\mu}_{10} & \bar{\mu}_{11}
\end{pmatrix}
\begin{pmatrix}
\h_0H_0 \\
\h_1H_1
\end{pmatrix}.
\]

We can check the \( m_{ab} \) and \( m_{aa} \) in eq. (D.12) with using the right side of eq. (D.18) and the \( \Psi \) definition of eq. (D.11).

[Go to table of contents.] [Go to home.]
E. Newton’s equation of motion

This chapter derives propagation equation (3.1) for elastic waves based on the Newtonian equation of motion. We use two variables which are displacement \( \mathbf{u}(\mathbf{x}) \) and stress \( \mathbf{\tau}(\mathbf{x}) \) by Voigt notation.

\[
\mathbf{u}^T = ( u_0 \ u_1 \ u_2 )^T \quad \text{and} \quad \mathbf{\tau}^T = ( \tau_{00} \ \tau_{11} \ \tau_{22} \ \tau_{01} \ \tau_{12} \ \tau_{02} )^T .
\]

Hooke’s law connects the \( \mathbf{u} \) and \( \mathbf{\tau} \) as

\[
\mathbf{\tau} = \begin{pmatrix} (\Lambda + 2\mu) D_a \mu D_b \end{pmatrix} \mathbf{u} , \quad (E.1)
\]

where

\[
\Lambda = \begin{pmatrix} \lambda & \lambda & \lambda \\ \lambda & \lambda & \lambda \\ \lambda & \lambda & \lambda \end{pmatrix}, \quad D_a = \begin{pmatrix} \frac{\partial}{\partial x_0} & 0 & 0 \\ 0 & \frac{\partial}{\partial x_1} & 0 \\ 0 & 0 & \frac{\partial}{\partial x_2} \end{pmatrix} \quad \text{and} \quad D_b = \begin{pmatrix} 0 & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} & 0 & \frac{\partial}{\partial x_0} \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_0} & 0 \end{pmatrix} .
\]

Here note that the parameters \( \lambda(\mathbf{x}) \) and \( \mu(\mathbf{x}) \) are Lamé’s constants. From Eq. (E.1), Newtonian equation of motion is shown as

\[
\frac{\partial \mathbf{\tau}}{\partial t} = \left( (\Lambda + 2\mu) D_a \right) \mu D_b \mathbf{v} \quad \text{and} \quad \frac{\partial \mathbf{v}}{\partial t} = - \left( D_a^\dagger D_b^\dagger \right) \mathbf{\tau} , \quad (E.2)
\]

where \( \mathbf{v} = \frac{\partial \mathbf{u}}{\partial t} \), and \( \rho(\mathbf{x}) \) is density of media. In the frequency domain, Eq. (E.2) can be deformed to Eq. (3.1), i.e. \( M\Psi = -i (\partial/\partial x_2) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Psi \) by using

\[
M = \begin{pmatrix} m_{vv} & m_{v\tau} \\ m_{\tau v} & m_{\tau\tau} \end{pmatrix} \quad \text{and} \quad \Psi = \begin{pmatrix} \mathbf{v} \\ \mathbf{\tau}_2 \end{pmatrix} = \begin{pmatrix} -i\omega \mathbf{u} \\ \mathbf{\tau}_2 \end{pmatrix} ,
\]

where

\[
\begin{align*}
m_{vv} &= \frac{1}{\omega} \begin{pmatrix} \frac{\partial}{\partial x_0} & 4(\lambda+\mu) \frac{\partial}{\partial x_0} + \mu \frac{\partial}{\partial x_1} & \frac{2\lambda \mu}{\lambda+2\mu} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_1} & \mu \frac{\partial}{\partial x_1} & \frac{\lambda+\mu}{\lambda+2\mu} \frac{\partial}{\partial x_1} \\ \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_2} & 0 \end{pmatrix} - \omega \rho , \\
m_{v\tau} &= -i \begin{pmatrix} 0 & 0 & \frac{\partial}{\partial x_2} \\ 0 & 0 & \frac{\partial}{\partial x_2} \\ \frac{\partial}{\partial x_0} & \frac{\partial}{\partial x_0} & 0 \end{pmatrix} , \\
m_{\tau v} &= i \begin{pmatrix} 0 & 0 & \frac{\partial}{\partial x_0} \\ 0 & 0 & \frac{\partial}{\partial x_0} \\ \frac{\lambda}{\lambda+2\mu} \frac{\partial}{\partial x_0} & \frac{\lambda}{\lambda+2\mu} \frac{\partial}{\partial x_0} & 0 \end{pmatrix} , \\
m_{\tau\tau} &= - \begin{pmatrix} \omega & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & \omega \end{pmatrix} ,
\end{align*}
\]

The matrix \( M \) satisfies \( M = M^\dagger \) when three parameters \( \lambda, \mu \) and \( \omega \rho \) are real functions.
F. Optical scattering

Wave scattering is formally discussed in Chapter 4 and 5. This chapter shows more detailed formulas for optical scattering. We consider Maxwell equation with scalar permittivity $\varepsilon$ and scalar magnetic-permeability $\mu$, and we use the coordinate transform discussed in Chapter 2. From eq. (D.13), the propagation equation (3.1) can be reduced to

$$
M\Psi = -i\frac{\partial}{\partial u_2} \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \Psi \quad \text{as} \quad M(V) = \left( \begin{array}{cc} m_{aa} & 0 \\ 0 & m_{bb} \end{array} \right),
$$

where $V_j$ are elements of the $V$ of eq. (5.1). Note that $h_1$ is always equal to 1. The wave function $\Psi$ in eq. (F.1) is represented by electromagnetic fields and scale factors as eq. (D.11).

F.1. Optical scattering except for edge roughness

We apply the coordinate transformation in chapter 2 and the Born approximation in section 4.4 to scattering of optical guided waves. The $\varepsilon$ and $\mu$ in eq. (F.1) are split to unperturbed terms and perturbed terms:

$$
\varepsilon = \varepsilon^{(0)}(u_0, u_1) + \varepsilon^{(1)}(u_0, u_1, u_2) \quad \text{and} \quad \mu = \mu^{(0)}(u_0, u_1) + \mu^{(1)}(u_0, u_1, u_2).
$$

From eqs. (2.5) and (F.1), we can set the diagonal matrices $V^{(0)}$ and $V^{(1)}$ of eq. (5.1) as

$$
V^{(0)} = \frac{\omega \mu^{(0)}}{\zeta}, \quad V_1^{(0)} = \frac{\varepsilon^{(0)}}{\varepsilon^{(0)}}, \quad V_2^{(0)} = \frac{1}{\zeta \varepsilon^{(0)}}, \quad V_3^{(0)} = \frac{1}{\zeta \varepsilon^{(0)}}, \quad V_4^{(0)} = \frac{1}{\zeta \varepsilon^{(0)}}, \quad V_5^{(0)} = \frac{1}{\zeta \varepsilon^{(0)}}.
$$

Function of $u_2$ in eq. (F.2) is only $\zeta$, and then

$$
\begin{align*}
\partial_{u_2} m_{aa}^{(0)} &= -\kappa_w m_{aa}^{(0)} + 2\kappa_w \left( \begin{array}{cc} 0 & 0 \\ 0 & \zeta \mu^{(0)} \end{array} \right), \\
\partial_{u_2} m_{bb}^{(0)} &= -\kappa_w m_{bb}^{(0)} + 2\kappa_w \left( \begin{array}{cc} \zeta \mu^{(0)} & 0 \\ 0 & 0 \end{array} \right).
\end{align*}
$$

From eqs. (F.2) and (F.3), we obtain detail of $\tilde{M}_{mn}$ of eq. (4.11) for $|m| \leq n_{\text{max}}$:

$$
\tilde{M}_{mn}(u_2) = \frac{m}{|m|} \Psi_m^{(0)\dagger} \left[ \frac{2\kappa_w (1 - \delta_{mn})}{\beta_m - \beta_n + 0} \left( \begin{array}{cc} 0 & 0 \\ 0 & \zeta \mu^{(0)} \end{array} \right) + i \left( \begin{array}{cc} m_{aa}^{(1)} & 0 \\ 0 & m_{bb}^{(1)} \end{array} \right) \right] \Psi_m^{(0)}.
$$

From eqs. (4.15) and (F.4), we can analyze optical scattering caused by the adiabatic tapered waveguide as shown in Fig. 5.1, but we have to add edge-roughness scattering discussed in Section 5.1 to the scattering properties of optical waveguide.
F.2. Edge-roughness scattering of Section 5.1 for optical waveguide

This section shows details of two approaches in Section 5.1 by using eq. (F.1). We consider the straight waveguide, i.e. the case that $\zeta = 1$. The $V^{(0)}$ of eq. (F.2) becomes constant for $u_2$, and its components can be reduced to

$$V^{(0)}_0 = V^{(0)}_1 = \omega \mu (u_0, u_1), \quad V^{(0)}_2 = \frac{1}{\omega \varepsilon (u_0, u_1)}, \quad V^{(0)}_3 = V^{(0)}_4 = \omega \varepsilon (u_0, u_1), \quad V^{(0)}_5 = \frac{1}{\omega \mu (u_0, u_1)}. \quad (F.5)$$

F.2.1. Details of Approach I for 5.1.1

Equations (5.4) and (F.5) give us the $V^{(1)}$ of Approach I. Especially for the abrupt structure in Fig. 5.1, the $V_{clad}$ and $V_{pp}$ in eq. (5.6) are given by

$$V_{0clad} = V_{1clad} = \omega \mu_{clad}, \quad V_{2clad} = \frac{1}{\omega \varepsilon_{clad}}, \quad V_{3clad} = V_{4clad} = \omega \varepsilon_{clad}, \quad V_{5clad} = \frac{1}{\omega \mu_{clad}}, \quad (F.6)$$

where $\varepsilon_{wg}$ and $\mu_{wg}$ ($\varepsilon_{clad}$ and $\mu_{clad}$) are waveguide (clad) parameters, and $V_{wg}$ is height of the waveguide as shown in Fig. 5.1(b). By using the normalized roughness parameters of eq. (5.8), we can represent the $V^{(1)}$ in eq. (5.6):

$$\tilde{V}^{(1)} = V^{(1)} \left[ A_w (k), A_c (k) \right] = \sqrt{L_s} \left[ \frac{1}{2} \tilde{a}_w (k) + \frac{u_0}{W_{wg}/2} \tilde{a}_c (k) \right] V_{pp} (u_1) \delta (W_{wg}/2 - |u_0|). \quad (F.7)$$

Next subsection shows another approach for boundary-roughness scattering.

F.2.2. Details of Approach II for 5.1.2

By using $\Delta h_0$ and $\Delta h_1$ of eq. (2.6), $h_2/h_0$ and $h_0 h_2$ in the $V$ of eq. (F.1) are approximated to

$$\begin{cases} \frac{h_2}{h_0} = (1 + \Delta h_2) / (1 + \Delta h_0) \approx 1 + \Delta h_2 - \Delta h_0, \\ h_0 h_2 = (1 + \Delta h_0) (1 + \Delta h_2) \approx 1 + \Delta h_2 + \Delta h_0. \end{cases}$$

From the above equations, let us introduce parameter vector $s$ to Approach II. Elements of $s$ are defined by

$$s_{j+3j} = \Delta h_2 (u_0, u_2) - (-1)^{(j+J)/2} \Delta h_0 (u_2) \quad \text{for} \quad \begin{cases} j = 0, 1, 2, \\ J = 0, 1. \end{cases} \quad (F.8)$$

The $V^{(1)}$ in Subsection 5.1.2 can be given as product between the $V^{(0)}$ of eq. (F.5) and the $s$ of eq. (F.8):

$$V^{(1)} = V^{(0)} s = \text{diag} \left[ V^{(0)}_0 s_0, \ldots, V^{(0)}_5 s_5 \right].$$

The $V^{(1)} (k)$ of eq. (5.7) is also given as $\tilde{V}^{(1)} (k) = V^{(0)} \tilde{s} (k)$. By using eqs. (5.7), (5.8) and (F.8), elements of $\tilde{s}$ is that

$$\frac{s_{j+3j} (k)}{\sqrt{L_s}} = u_0 k^2 \tilde{a}_c (k) + \frac{1}{W_{wg}} \left( \frac{1}{2} u_0^2 k^2 - (-1)^{(j+J)/2} \right) \tilde{a}_w (k) \quad \text{for} \quad \begin{cases} j = 0, 1, 2, \\ J = 0, 1. \end{cases} \quad (F.9)$$

When $\tilde{a}_w$ and $\tilde{a}_c$ are not correlated as mentioned in the end of Section 5.2, we have to use independently each term for $\tilde{a}_w$ and $\tilde{a}_c$ in eqs. (F.7) and (F.9).

[Go to table of contents.]  [Go to home.]
This chapter shows an example of non-uniform mesh techniques discussed in Section 6.2. Then we define a periodic function \( F(\xi, K) \), and \( F(\xi_j/L_j, K_j) \) is introduced into \( du_j/d\xi_j \).

\[
F(\xi, K) = 2^{2K-1} \cos^2(\pi K) \prod_{I=1}^{K-1} \frac{I}{K+I}.
\]  

Figure G.1 (a) plots the function \( F(\xi, K) \) for \( K = 1, 5, 20 \) and \( 80 \), and it shows that \( F(\xi, 80) \approx 0 \) when \( 0.1 < \xi < 0.9 \).

By using a formula

\[
\cos^{2n} \theta = \frac{1}{2^{2n-1}} \left[ \sum_{r=0}^{n-1} \binom{2n}{r} \cos(2n-2r) \theta + \frac{1}{2} \binom{2n}{n} \right]
\]

from Iwanami Formulae II p. 190, eq. (G.1) is deformed into

\[
F(\xi, K) = \left[ \frac{1}{2} \binom{2K}{K} + \sum_{r=0}^{K-1} \binom{2K}{r} \cos(2(K-r)\pi \xi) \right] \prod_{I=1}^{K-1} \frac{I}{K+I}
\]

\[
= 1 + \sum_{r=0}^{K-1} \frac{(2K)!}{r!(2K-r)!} \frac{(K-1)!K!}{(2K-1)!} \cos(2(K-r)\pi \xi)
\]

\[
= 1 + \sum_{r=0}^{K-1} \frac{2K}{(K-r)!} \frac{K!}{(2K-1)!} \cos(2(K-r)\pi \xi)
\]

\[
= 1 + \sum_{J=1}^{K} 2 \frac{K!}{(K+J)!} \frac{K!}{(K-J)!} \cos(2\pi J \xi) = 1 + \sum_{J=1}^{K} 2 \left( \prod_{I=1}^{J} \frac{K+1-I}{K+I} \right) \cos(2\pi J \xi)
\]

\[
= 1 + \sum_{J=1}^{K} 2 \left( \prod_{I=1}^{J} \frac{K-J+I}{K+I} \right) \cos(2\pi J \xi)
\]

where

\[
\frac{1}{2} \binom{2K}{K} \prod_{I=1}^{K-1} \frac{I}{K+I} = \frac{1}{2} \frac{(2K)!}{K!K!(2K-1)!} = 1.
\]

Equations (G.1) and (G.2) for \( K = 1, 2 \) could be checked as

\[
\left\{
\begin{array}{l}
F(\xi, 1) = 2^{2-1} \cos^2(\pi \xi) = 1 + \cos(2\pi \xi), \\
F(\xi, 2) = 2^{4-1} \cos^4(\pi \xi) \prod_{I=1}^{2-1} \frac{I}{2+I} = \frac{8}{3} \left[ 1 + 2 \cos(2\pi \xi) + \frac{1+\cos(4\pi \xi)}{2} \right]
\end{array}
\right.
\]

\[
= 1 + \frac{2-1}{2+1} \cos(2\pi \xi) + 2 \left( \prod_{I=2}^{2} \frac{I}{2+I} \right) \cos(4\pi \xi) = 1 + \frac{4}{3} \cos(2\pi \xi) + \frac{1}{3} \cos(4\pi \xi).
\]

From eq. (G.2), we obtain a formula for the integral of \( F(\xi, K) \).

\[
\int_{0}^{\xi} F(x, K) \, dx = \xi + \sum_{J=1}^{K} 2 \left( \prod_{I=1}^{J} \frac{K-J+I}{K+I} \right) \frac{\sin(2\pi J \xi)}{2\pi J}.
\]  

Figure G.1(b) shows eq. (G.3) for \( K = 1, 5, 20 \) and \( 80 \). The integral of \( F \) has staircase shape.
The functions (G.1) and (G.3) have the following properties:

\[
\begin{align*}
F(\xi + 1, K) &= F(-\xi, K) = F(\xi, K), \\
\max F(\xi, K) &= F(0, K) = 2^{2K-1} \prod_{I=1}^{K-1} \frac{I}{K+I}, \\
\min F(\xi, K) &= F\left(\frac{1}{2}, K\right) = 0, \\
\int_0^1 F(\xi, K) d\xi &= 1, \\
\lim_{K \to \infty} F(\xi, K) &= \sum_{I=-\infty}^{\infty} \delta(\xi-I),
\end{align*}
\]

where \(\delta(\xi)\) is the Dirac delta function.

When ten parameters \(L_j, u_j(0), u_j(L_j), \min (du_j/d\xi_j)\) and \(K_j\) for \(j = 0, 1\) are given, we can derive the \(u_j\) by using eq. (G.3).

\[
\begin{align*}
\frac{du_j}{d\xi_j}(\xi_j) &= \frac{du_j}{d\xi_j}(0) + \xi_j \min \left(\frac{du_j}{d\xi_j}\right) + C_j \int_0^{\xi_j/L_j} F(x, K_j) dx, \\
\frac{du_j}{d\xi_j}(\xi_j) &= \min \left(\frac{du_j}{d\xi_j}\right) + \frac{C_j}{L_j} F(\xi_j/L_j, K_j), \\
C_j &= u_j(L_j) - u_j(0) - L_j \min \left(\frac{du_j}{d\xi_j}\right).
\end{align*}
\]

The maximum of \(du_j/d\xi_j\) is given by

\[
\max \left(\frac{du_j}{d\xi_j}\right) = \min \left(\frac{du_j}{d\xi_j}\right) + \left(2^{2K_j-1} \prod_{I=1}^{K_j-1} \frac{I}{K_j+I}\right) \frac{C_j}{L_j}.
\]
H. Relaxation of discretization dependency

This chapter shows correction parameter in order to reduce discretization dependency.

H.1. Correction factor

The discretization of differential operator reduces the wavenumber of plane-wave \( \exp (kx) \), because

\[
k > \frac{2}{\Delta x} \sin \left( \frac{k \Delta x}{2} \right) \quad \text{where} \quad k > 0 \quad \text{and} \quad 0 < k \Delta x < \pi.
\]

Let us introduce a correction factor \( \eta \) to emphasis the finite difference as

\[
\frac{2}{\Delta x} \sin \left( \frac{k \Delta x}{2} \right) \Rightarrow \frac{2 (1 + \eta)}{\Delta x} \sin \left( \frac{k \Delta x}{2} \right).
\]

We consider \( U \) that surface integral on sphere for squared norm of difference between the \( k_j \) and the discretized one:

\[
U = \frac{1}{4 \pi} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( \sum_{j=0}^2 \left( \frac{2 (1 + \eta)}{\Delta x_j} \sin \left( \frac{k_j \Delta x_j}{2} \right) - k_j \right)^2 \right),
\]

where

\[
k_0 = k_r \sin \theta \cos \phi, \quad k_1 = k_r \sin \theta \sin \phi, \quad k_2 = k_r \cos \theta.
\]

Note that \( \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( \frac{k_j \Delta x_j}{2} \right)^2 = \frac{4 \pi}{3} \). Variation of the \( U \) is given by

\[
\frac{\partial U}{\partial \eta} = \sum_{j=0}^2 \frac{1}{\pi (\Delta x_j)^2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( 2 (1 + \eta) \sin \left( \frac{k_j \Delta x_j}{2} \right) - k_j \Delta x_j \right) \sin \left( \frac{k_j \Delta x_j}{2} \right).
\]

Then we can obtain \( \eta \) at \( \partial U/\partial \eta = 0 \) as follows.

\[
\eta = \frac{\sum_{j=0}^2 (\Delta x_j)^{-2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( \sin \left( \frac{k_j \Delta x_j}{2} \right) - \frac{k_j \Delta x_j}{2} \right)}{\sum_{j=0}^2 (\Delta x_j)^{-2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \sin^2 \left( \frac{k_j \Delta x_j}{2} \right)}
\]

\[
\approx \frac{3! \sum_{j=0}^2 (\Delta x_j)^{-2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( \frac{k_j \Delta x_j}{2} \right)^4}{\sum_{j=0}^2 (\Delta x_j)^{-2} \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( \frac{k_j \Delta x_j}{2} \right)^2},
\]

where

\[
\int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi \left( \frac{k_j \Delta x_j}{2} \right)^2 = \left( \frac{k_r \Delta x_j}{2} \right)^2 \frac{4 \pi}{2n + 1}.
\]

When \( k_j \Delta x_j/2 \ll 1 \), we set

\[
\eta = \frac{\sum_{j=0}^2 (\Delta x_j)^{-2} \left( \frac{k_j \Delta x_j}{2} \right)^4}{3! \sum_{j=0}^2 (\Delta x_j)^{-2} \left( \frac{k_j \Delta x_j}{2} \right)^2} = \frac{\sum_{j=0}^2 (\Delta x_j)^{-2} \left( \frac{k_j \Delta x_j}{2} \right)^4}{10 \sum_{j=0}^2 (\Delta x_j)^{-2} \left( \frac{k_j \Delta x_j}{2} \right)^2}.
\]

\[
(\text{H.1})
\]
H.2. Definitions of $\Delta x_j$ and $k_r$

From section 6.2, $\Delta x_j$ for $j = 0, 1, 2$ and $k_r$ in eq. (H.1) are defined as

$$\Delta x_j (\xi) = \frac{du_j}{d\xi_j} h_j = u'_j (\xi_j) h_j (u_0 (\xi_0), u_1 (\xi_1), u_2 (\xi_2)),$$

$$k_r (\xi) = \omega \sqrt{\varepsilon (\xi)} \mu (\xi). \tag{H.2}$$

Note that eq. (H.2) is referenced in the CFL condition of eq. (8.3). From eqs. (H.1) and (H.2), correction factor $\eta$ is given by

$$\eta (\xi) = \frac{\omega^2}{120} \varepsilon (\xi) \mu (\xi) \sum_{j=0}^{2} \left( u'_j (\xi_j) h_j (u (\xi)) \right)^2. \tag{H.3}$$

Note that each point in a Yee cell only has $\varepsilon$ or $\mu$ as shown in Fig. 6.1, and then $\mu$ and $\varepsilon$ in (H.3) have to be approximated as

$$\mu \left( l_0 + \frac{1 - \delta_{0j}}{2}, l_1 + \frac{1 - \delta_{1j}}{2}, l_2 + \frac{1 - \delta_{2j}}{2} \right) \approx \frac{1}{4} \sum_{m=0}^{1} \sum_{n=0}^{1} \mu \left( l_0 + \frac{\delta_{2j+m}}{2} + n\delta_{2j1-m}, l_1 + \frac{\delta_{0j+m}}{2} + n\delta_{0j1-m}, l_2 + \frac{\delta_{1j+m}}{2} + n\delta_{1j1-m} \right),$$

$$\varepsilon \left( l_0 + \frac{\delta_{0j}}{2}, l_1 + \frac{\delta_{1j}}{2}, l_2 + \frac{\delta_{2j}}{2} \right) \approx \frac{1}{4} \sum_{m=0}^{1} \sum_{n=0}^{1} \varepsilon \left( l_0 + \frac{1 - \delta_{2j+m}}{2} - n\delta_{2j1-m}, l_1 + \frac{1 - \delta_{0j+m}}{2} - n\delta_{0j1-m}, l_2 + \frac{1 - \delta_{1j+m}}{2} - n\delta_{1j1-m} \right), \tag{H.4}$$

where $j = 0, 1, 2$. Equations (H.3) and (H.4) give us the $\eta$ in eq. (6.6).

Here, we can check eq. (H.4) as follows.

$$\mu \left( l_0, l_1 + \frac{1}{2}, l_2 + \frac{1}{2} \right) \approx \frac{\mu \left( l_0, l_1 + \frac{1}{2}, l_2 + \frac{1}{2} \right) + \mu \left( l_0, l_1, l_2 + \frac{1}{2} \right) + \mu \left( l_0, l_1 + 1, l_2 + 1 \right) + \mu \left( l_0, l_1, l_2 + 1 \right)}{4}$$

and

$$\varepsilon \left( l_0, l_1 + \frac{1}{2}, l_2 \right) \approx \frac{\varepsilon \left( l_0, l_1 + \frac{1}{2}, l_2 \right) + \varepsilon \left( l_0, l_1, l_2 + \frac{1}{2} \right) + \varepsilon \left( l_0, l_1 + 1, l_2 \right) + \varepsilon \left( l_0, l_1, l_2 + 1 \right)}{4}$$

[Go to table of contents.] [Go to home.]
I. Details of discrete equations

This chapter shows detailed derivation of discrete equations.

I.1. Derivation of propagation equation (7.1)

Details of the discrete Maxwell equation (6.9) are given as follows.

\[
\begin{pmatrix}
0 & -\Delta_2 & \Delta_1 \\
\Delta_2 & 0 & -\Delta_0 \\
-\nabla_1 & \nabla_0 & 0
\end{pmatrix}
\begin{pmatrix}
H_{i0} \\
H_{i1} \\
H_{i2}
\end{pmatrix}
= -i\omega
\begin{pmatrix}
\varepsilon_{i00} & 0 & 0 \\
0 & \varepsilon_{i11} & 0 \\
0 & 0 & \varepsilon_{i22}
\end{pmatrix}
\begin{pmatrix}
E_{i0} \\
E_{i1} \\
E_{i2}
\end{pmatrix},
\]

(I.1)

The four equations in eq. (I.1) are

\[
\begin{align*}
-\Delta_2 H_{i1} + \Delta_1 H_{i2} &= -i\omega\varepsilon_{i00} E_{i0}, \\
\Delta_2 H_{i0} - \Delta_0 H_{i2} &= -i\omega\varepsilon_{i11} E_{i1}, \\
-\nabla_2 E_{i1} + \nabla_1 E_{i2} &= i\omega\mu_{i00} H_{i0}, \\
\nabla_2 E_{i0} - \nabla_0 E_{i2} &= i\omega\mu_{i11} H_{i1}.
\end{align*}
\]

(I.2)

From eq. (I.1), the \(E_{i2}\) and \(H_{i2}\) can be represented by other components:

\[
E_{i2} = \frac{i}{\omega\varepsilon_{i22}} (-\nabla_1 H_{i0} + \Delta_0 H_{i1}), \quad \text{and} \quad H_{i2} = \frac{-i}{\omega\mu_{i22}} (-\nabla_1 E_{i0} + \nabla_0 E_{i1}).
\]

(I.3)

The above \(E_{i2}\) and \(H_{i2}\) of (I.3) can be substituted into eqs. (I.2), and then

\[
\begin{align*}
-\Delta_2 H_{i1} + \Delta_1 \left[ -\frac{i}{\omega\mu_{i22}} (-\nabla_1 E_{i0} + \nabla_0 E_{i1}) \right] &= -i\omega\varepsilon_{i00} E_{i0}, \\
\Delta_2 H_{i0} - \Delta_0 \left[ -\frac{i}{\omega\mu_{i22}} (-\nabla_1 E_{i0} + \nabla_0 E_{i1}) \right] &= -i\omega\varepsilon_{i11} E_{i1}, \\
-\nabla_2 E_{i1} + \nabla_1 \left[ \frac{i}{\omega\varepsilon_{i22}} (-\nabla_1 H_{i0} + \Delta_0 H_{i1}) \right] &= i\omega\mu_{i00} H_{i0}, \\
\nabla_2 E_{i0} - \nabla_0 \left[ \frac{i}{\omega\varepsilon_{i22}} (-\nabla_1 H_{i0} + \Delta_0 H_{i1}) \right] &= i\omega\mu_{i11} H_{i1}.
\end{align*}
\]

Therefore, the above four equations are deformed into

\[
\begin{align*}
-i \Delta_2 H_{i0} &= \Delta_0 \left[ \frac{1}{\omega\mu_{i22}} (-\nabla_1 E_{i0} - \nabla_0 E_{i1}) \right] - \omega\varepsilon_{i11} E_{i1}, \\
-i \Delta_2 H_{i1} &= \Delta_1 \left[ \frac{1}{\omega\mu_{i22}} (-\nabla_1 E_{i0} - \nabla_0 E_{i1}) \right] + \omega\varepsilon_{i00} E_{i0}, \\
i \nabla_2 E_{i1} &= \nabla_1 \left[ \frac{1}{\omega\varepsilon_{i22}} (\nabla_1 H_{i0} - \Delta_0 H_{i1}) \right] + \omega\mu_{i00} H_{i0}, \\
-i \nabla_2 E_{i0} &= \nabla_0 \left[ \frac{1}{\omega\varepsilon_{i22}} (-\nabla_1 H_{i0} + \Delta_0 H_{i1}) \right] + \omega\mu_{i11} H_{i1}.
\end{align*}
\]

(I.4)

The four left sides in the above equations are obviously equal to the right side of eq. (7.1), and the four right sides give us matrix elements of \(m_{bb}\) and \(m_{aa}\) in eq. (7.2).
I.2. Details of power flow relations in eq. (7.3)

From eq. (7.1),

\[ H_{2D}^\dagger m_{aa} H_{2D} = -i H_{2D}^\dagger \nabla_2 E_{2D} = -i H_{2D}^\dagger [l_2] E_{2D} [l_2] + i H_{2D}^\dagger [l_2] E_{2D} [l_2 - 1] \]

and

\[ E_{2D}^\dagger m_{bb} E_{2D} = -i E_{2D}^\dagger \Delta_2 H_{2D} = -i E_{2D}^\dagger [l_2] H_{2D} [l_2 + 1] + i E_{2D}^\dagger [l_2] H_{2D} [l_2] \]

By using the definition \( \Psi \) in eq. (7.2), the above equations are deformed to

\[
\begin{cases}
  i H_{2D}^\dagger [l_2] \left( m_{aa} [l_2] - m_{aa}^\dagger [l_2] \right) H_{2D} [l_2] \\
  = H_{2D}^\dagger [l_2] E_{2D} [l_2] - H_{2D}^\dagger [l_2] E_{2D} [l_2 - 1] + E_{2D}^\dagger [l_2] H_{2D} [l_2] - E_{2D}^\dagger [l_2 - 1] H_{2D} [l_2] \\
  = \Psi_+ [l_2] \left( \begin{array}{c} 0 \\
  1 \end{array} \right) \Psi_+ [l_2] - \Psi_- [l_2 - 1] \left( \begin{array}{c} 0 \\
  1 \end{array} \right) \Psi_- [l_2 - 1],
\end{cases}
\]

\( (I.5) \)

\[
\begin{cases}
  i E_{2D}^\dagger [l_2] \left( m_{bb} [l_2] - m_{bb}^\dagger [l_2] \right) E_{2D} [l_2] \\
  = E_{2D}^\dagger [l_2] H_{2D} [l_2 + 1] - E_{2D}^\dagger [l_2] H_{2D} [l_2] + H_{2D}^\dagger [l_2] E_{2D} [l_2] - H_{2D}^\dagger [l_2] E_{2D} [l_2] \\
  = \Psi_+ [l_2] \left( \begin{array}{c} 0 \\
  1 \end{array} \right) \Psi_+ [l_2] - \Psi_- [l_2] \left( \begin{array}{c} 0 \\
  1 \end{array} \right) \Psi_- [l_2].
\end{cases}
\]

I.3. Derivation of transfer matrix of eq. (7.4)

From eqs. (7.1) and (7.2),

\[
\begin{cases}
  im_{aa} [l_2] H_{2D} [l_2] = E_{2D} [l_2] - E_{2D} [l_2 - 1], \\
  im_{bb} [l_2] E_{2D} [l_2] = H_{2D} [l_2 + 1] - H_{2D} [l_2].
\end{cases}
\]

The above two equations are deformed to

\[
\begin{cases}
  H_{2D} [l_2 + 1] = H_{2D} [l_2] + im_{bb} [l_2] E_{2D} [l_2], \\
  E_{2D} [l_2 + 1] = im_{aa} [l_2 + 1] H_{2D} [l_2 + 1] + E_{2D} [l_2] \\
  = im_{aa} [l_2 + 1] (H_{2D} [l_2] + im_{bb} [l_2] E_{2D} [l_2]) + E_{2D} [l_2] \\
  = im_{aa} [l_2 + 1] H_{2D} [l_2] + (1 - m_{aa} [l_2 + 1] m_{bb} [l_2]) E_{2D} [l_2].
\end{cases}
\]

Then, we obtain the transfer matrix of eq. (7.4).

I.4. Check of \( \Xi \) definition in eq. (7.10)

From eq. (7.6), the expansion in eq. (7.10) satisfies the discrete propagation equation (7.1) as

\[
M_+ \Phi_+ [l_2] = \left( \begin{array}{cc}
  m_{aa} & 0 \\
  0 & m_{bb}
\end{array} \right) \sum_{m \neq 0} c_m \exp (i \theta_m l_2) \Xi_m = \sum_{m \neq 0} c_m \exp (i \theta_m l_2) \left( \begin{array}{cc}
  \exp (-i \theta_m / 2) & 0 \\
  0 & \exp (i \theta_m / 2)
\end{array} \right) 2 \sin (\theta_m / 2) \left( \begin{array}{cc}
  0 & 1 \\
  1 & 0
\end{array} \right) \Phi_m
\]

\( (I.7) \)

\[
= \sum_{m \neq 0} -ic_m \exp (i \theta_m l_2) \left( \begin{array}{cc}
  0 & \exp (-i \theta_m / 2) \\
  \exp (i \theta_m / 2) & 0
\end{array} \right) \left( \begin{array}{cc}
  \exp (i \theta_m / 2) - \exp (-i \theta_m / 2) & 1 - \exp (-i \theta_m) \\
  1 - \exp (-i \theta_m) & \exp (i \theta_m / 2) - \exp (-i \theta_m / 2)
\end{array} \right) \Phi_m
\]

\[
= \sum_{m \neq 0} -i \left( \begin{array}{cc}
  0 & 1 - \exp (-i \theta_m) \\
  \exp (i \theta_m) - 1 & 0
\end{array} \right) c_m \exp (i \theta_m l_2) \Xi_m = -i \left( \begin{array}{cc}
  0 & \nabla_2 \\
  \Delta_2 & 0
\end{array} \right) \Phi_+ [l_2].
\]

\[
= \sum_{m \neq 0} -i \left( \begin{array}{cc}
  0 & 1 - \exp (-i \theta_m) \\
  \exp (i \theta_m) - 1 & 0
\end{array} \right) c_m \exp (i \theta_m l_2) \Xi_m = -i \left( \begin{array}{cc}
  0 & \nabla_2 \\
  \Delta_2 & 0
\end{array} \right) \Phi_+ [l_2].
\]
1.5. Born approximation for discrete Green’s function in eq. (7.12)

Phase shift $\Theta_n[l_2]$ from a center of the system is defined by

$$\Theta_n[l_2] = \begin{cases} \sum_{\frac{l_2-1}{2} < j < l_2} \frac{\theta_n[j]}{2} + \sum_{\frac{l_2-1}{2} < j < l_2} \frac{\theta_n[j]}{2} & \text{for } l_2 > \frac{l_2-1}{2}, \\ 0 & \text{if } l_2 = \frac{l_2-1}{2}, \\ -\sum_{l_2 < j < \frac{l_2-1}{2}} \frac{\theta_n[j]}{2} - \sum_{l_2 < j < \frac{l_2-1}{2}} \frac{\theta_n[j]}{2} & \text{for } l_2 < \frac{l_2-1}{2}. \end{cases} \tag{I.8}$$

The above equation is equal to eq. (7.13) when $l_2 = b_m$. Equation (7.14) can be represented by Green’s function which is defined as

$$\Psi_n[l_2] = \exp(i\Theta_n[l_2]) \left( \Xi_n[l_2] + \sum_{1 \leq j \neq l_2 < L-1} G[l_2, j] \right), \tag{I.9}$$

$$G[l_2 \geq j, j] \triangleq \sum_{m \geq 0} g_{mn} \exp \left\{ i (\Theta_m[l_2] - \Theta_n[l_2]) - i (\Theta_m[j] - \Theta_n[j]) \right\} \Xi_m[l_2].$$

This section considers only propagative modes (i.e., $0 < |m| \leq n_{\text{max}}$), and it shows derivation of the $G[l_2, j]$ from eq. (7.1). We try to separate the $M_+$ of eq. (7.1) into unperturbed term $M_+^{(0)}$ and perturbed term $M_+^{(1)}$.

$$i \left( M_+^{(0)}[l_2] + M_+^{(1)}[l_2] \right) \Psi_n[l_2] = \begin{pmatrix} 0 & \nabla_2 \\ \Delta_2 & 0 \end{pmatrix} \Psi_n[l_2], \tag{I.10}$$

where the $M_+^{(j)}$ for $j = 0, 1$ and function of $l_2$ are commutative, e.g. $\exp(i\Theta_n[l_2]) M_+^{(j)}[l_2] = M_+^{(j)}[l_2] \exp(i\Theta_n[l_2])$. Note that the coefficient $g_{mn}$ in eq. (I.9) is set as small value: $g_{mn}[j] = O \left( \left\| M_+^{(1)} \right\| \right)$. By using the formula of eq. (I.21), the right side of eq. (I.10) is deformed to

$$\begin{pmatrix} 0 & \nabla_2 \\ \Delta_2 & 0 \end{pmatrix} \exp(i\Theta_n[l_2]) \Xi_n[l_2] = \begin{pmatrix} 0 & 1 - \exp \left[ -i \left( \frac{\theta_n[l_2]}{2} + \frac{\theta_n[l_2-1]}{2} \right) \right] \\ \exp \left[ i \left( \frac{\theta_n[l_2+1]}{2} + \frac{\theta_n[l_2]}{2} \right) \right] - 1 & 0 \end{pmatrix} \exp(i\Theta_n[l_2]) \begin{pmatrix} 1 + \frac{\Delta_2}{2} & 0 \\ 0 & 1 - \frac{\nabla_2}{2} \end{pmatrix} \Xi_n[l_2]$$

$$+ \begin{pmatrix} 0 & 1 - \exp \left[ -i \left( \frac{\theta_n[l_2]}{2} + \frac{\theta_n[l_2-1]}{2} \right) \right] \\ \exp \left[ i \left( \frac{\theta_n[l_2+1]}{2} + \frac{\theta_n[l_2]}{2} \right) \right] - 1 & 0 \end{pmatrix} \exp(i\Theta_n[l_2]) \Xi_n[l_2]$$

$$= \begin{pmatrix} 0 & 1 - \exp \left[ i \Theta_n[l_2 - 1] \right] \\ \exp(i\Theta_n[l_2+1]) \Delta_2 \Xi_n[l_2] - 1 & 0 \end{pmatrix} \exp(i\Theta_n[l_2]) \Xi_n[l_2].$$

Furthermore, equation (I.7) gives us

$$iM_+^{(0)}[l_2] \Xi_n[l_2] = \begin{pmatrix} \Delta_2 & 0 \\ 0 & \nabla_2 \end{pmatrix} \Xi_n[l_2].$$

From the above two relations, a part of the right side in eq. (I.10) is deformed to

$$\begin{pmatrix} 0 & \nabla_2 \\ \Delta_2 & 0 \end{pmatrix} \exp(i\Theta_n[l_2]) \Xi_n[l_2] = iM_+^{(0)}[l_2] \exp(i\Theta_n[l_2]) \Xi_n[l_2]$$

$$+ \begin{pmatrix} \exp \left[ i \frac{\theta_n[l_2+1]}{2} \right] - \exp \left[ i \frac{\theta_n[l_2]}{2} \right] \\ \exp \left[ i \frac{\theta_n[l_2]}{2} \right] \right) \exp(i\Theta_n[l_2]) \Xi_n[l_2]$$

$$\times \begin{pmatrix} 0 & \exp \left[ -i \frac{\theta_n[l_2]}{2} \right] \\ \exp \left[ -i \frac{\theta_n[l_2]}{2} \right] \right) \exp(i\Theta_n[l_2]) \Xi_n[l_2]$$

$$+ \begin{pmatrix} 0 \\ \exp(i\Theta_n[l_2+1]) \Delta_2 \Xi_n[l_2] \right) \exp(i\Theta_n[l_2 - 1]) \nabla_2 \Xi_n[l_2].$$

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Then,
\[ i\hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \Xi_n \begin{bmatrix} l_2 \end{bmatrix} + i\hat{M}^{(0)}_+ \begin{bmatrix} l_2 \end{bmatrix} \sum_{1 \leq j \neq l_2 < L_2 - 1} G \begin{bmatrix} l_2, j \end{bmatrix} \]
\[ = \sum_{1 \leq j \neq l_2 < L_2 - 1} \exp(-i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \left( \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) G \begin{bmatrix} l_2, j \end{bmatrix} + o \left( \left\| \hat{M}^{(1)}_+ \right\| \right), \] (I.11)
where
\[ i\hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \Xi_n \begin{bmatrix} l_2 \end{bmatrix} \triangleq i\hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \Xi_n \begin{bmatrix} l_2 \end{bmatrix} \]
\[ = \left( \begin{array}{cc} \nabla_2 \exp\left(i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}\right) \exp\left(i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}\right) & \nabla_2 \exp\left(-i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}\right) \exp\left(-i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}\right) \end{array} \right) \Xi_n \begin{bmatrix} l_2 \end{bmatrix} \] (I.12)
\[ - \left( \begin{array}{cc} 0 & \nabla_2 \exp\left(i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}\right) \end{array} \right) \exp\left(-i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}\right) \Xi_n \begin{bmatrix} l_2 \end{bmatrix}. \]

It is assumed that \( O \left( \left\| \hat{M}^{(1)}_+ \right\| \right) = O \left( \left\| M^{(1)}_+ \right\| \right). \) The third term in the right-hand side of eq. (I.12) causes that \( \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \neq \hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \) even though \( \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) M^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} = M^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \). We consider the first term in the right-hand side of eq. (I.11), and we can deform it to
\[ \exp(-i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \left( \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) G \begin{bmatrix} l_2, j \end{bmatrix} \]
\[ = \left( \exp\left(i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix} + \theta_n \begin{bmatrix} l_2 + 1 \end{bmatrix}}{2}\right) \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(-i\frac{\theta_n \begin{bmatrix} l_2 - 1 \end{bmatrix} + \theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}) G \begin{bmatrix} l_2, j \end{bmatrix}. \] (I.13)

The above equation (I.13) can be deformed to the following equation by using the definition of \( G \) in eq. (I.9):
\[ \exp(-i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \left( \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) G \begin{bmatrix} l_2, j \end{bmatrix} = i\hat{M}^{(0)}_+ \begin{bmatrix} l_2 \end{bmatrix} G \begin{bmatrix} l_2, j \end{bmatrix} + o \left( \left\| \hat{M}^{(1)}_+ \right\| \right) \text{ for } j \leq l_2 + 1. \] (I.14)

Here, we can approximate \( \theta_m \begin{bmatrix} l_2 \end{bmatrix} \approx \theta_m \begin{bmatrix} l_2 \end{bmatrix} \) and \( \Xi_m \begin{bmatrix} l_2 \end{bmatrix} \approx \Xi_m \begin{bmatrix} l_2 \end{bmatrix} \) for the \( G \) in the left-hand side of the above equation. Equation (I.11) can be simplified by eq. (I.14), and its right-hand side can be expanded by using (I.13):
\[ i\hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \Xi_n \begin{bmatrix} l_2 \end{bmatrix} + i\hat{M}^{(0)}_+ \begin{bmatrix} l_2 \end{bmatrix} \begin{bmatrix} G \begin{bmatrix} l_2, l_2 - 1 \end{bmatrix} + G \begin{bmatrix} l_2, l_2 + 1 \end{bmatrix} \end{bmatrix} + o \left( \left\| \hat{M}^{(1)}_+ \right\| \right) \]
\[ = \sum_{j=l_2-1, l_2+1} \exp(-i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) \left( \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(i\theta_n \begin{bmatrix} l_2 \end{bmatrix}) G \begin{bmatrix} l_2, j \end{bmatrix} \]
\[ = \left( \exp\left(i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix} + \theta_n \begin{bmatrix} l_2 + 1 \end{bmatrix}}{2}\right) \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(-i\frac{\theta_n \begin{bmatrix} l_2 - 1 \end{bmatrix} + \theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}) \begin{bmatrix} G \begin{bmatrix} l_2, 1, l_2 - 1 \end{bmatrix} + G \begin{bmatrix} l_2 + 1, l_2 + 1 \end{bmatrix} \end{bmatrix} \]
\[ + \left( \begin{array}{cc} 0 & \nabla_2 \nabla_2 \end{array} \right) \exp(-i\frac{\theta_n \begin{bmatrix} l_2 - 1 \end{bmatrix} + \theta_n \begin{bmatrix} l_2 \end{bmatrix}}{2}) \begin{bmatrix} G \begin{bmatrix} l_2 - 1, l_2 - 1 \end{bmatrix} + G \begin{bmatrix} l_2 - 1, l_2 + 1 \end{bmatrix} \end{bmatrix}. \]

We can apply the same deformation as eqs. (I.13) and (I.14) only to \( \Delta_2 (\nabla_2) \) operation when \( j = l_2 - 1 \) \( (j = l_2 + 1) \). Then, terms for \( G \begin{bmatrix} l_2, l_2 - 1 \end{bmatrix} \) and \( G \begin{bmatrix} l_2, l_2 + 1 \end{bmatrix} \) can be partially canceled in the above equation:
\[ i\hat{M}^{(1)}_+ \begin{bmatrix} l_2 \end{bmatrix} \Xi_n \begin{bmatrix} l_2 \end{bmatrix} + \begin{bmatrix} i \begin{bmatrix} 1 \end{bmatrix} \end{bmatrix} M^{(0)}_+ \begin{bmatrix} l_2 \end{bmatrix} - \begin{bmatrix} 0 \end{bmatrix} 1 \begin{bmatrix} l_2 - 1 \end{bmatrix} \end{bmatrix} G \begin{bmatrix} l_2, l_2 - 1 \end{bmatrix} \]
\[ + \begin{bmatrix} 0 \begin{bmatrix} 1 \end{bmatrix} \end{bmatrix} M^{(0)}_+ \begin{bmatrix} l_2 \end{bmatrix} + \begin{bmatrix} 0 \end{bmatrix} 1 \begin{bmatrix} l_2 + 1 \end{bmatrix} \end{bmatrix} G \begin{bmatrix} l_2, l_2 + 1 \end{bmatrix} + o \left( \left\| \hat{M}^{(1)}_+ \right\| \right) \] (I.15)
\[ = \begin{bmatrix} \exp\left(i\frac{\theta_n \begin{bmatrix} l_2 \end{bmatrix} + \theta_n \begin{bmatrix} l_2 + 1 \end{bmatrix}}{2}\right) \begin{bmatrix} 0 \end{bmatrix} \end{bmatrix} 1 \begin{bmatrix} l_2 - 1 \end{bmatrix} \end{bmatrix} G \begin{bmatrix} l_2 - 1, l_2 - 1 \end{bmatrix}. \]
The second and third terms in the left-hand side of eq. (I.15) are expanded by $\Xi_m$:

$$
\begin{align*}
&\left[ \left( \begin{array}{cc} i & 0 \\ 0 & 0 \end{array} \right) M_+^{(0)} [l_2] - \left( \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right) \right] G [l_2, l_2 - 1] + \left[ \left( \begin{array}{cc} 0 & 0 \\ 0 & i \end{array} \right) M_+^{(0)} [l_2] + \left( \begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array} \right) \right] G [l_2, l_2 + 1] \\
= \sum_{m>0} \left[ \left( \begin{array}{cc} i & 0 \\ 0 & 0 \end{array} \right) M_+^{(0)} [l_2] - \left( \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right) \right] g_{mn} [l_2 - 1] \exp \left( \frac{i \theta_n [l_2 - 1] + \theta_m [l_2] - i \theta_n [l_2 - 1] + \theta_n [l_2]}{2} \right) \Xi_m [l_2] \\
&+ \sum_{m<0} \left[ \left( \begin{array}{cc} 0 & 0 \\ 0 & i \end{array} \right) M_+^{(0)} [l_2] + \left( \begin{array}{cc} 0 & 0 \\ 1 & 0 \end{array} \right) \right] g_{mn} [l_2 + 1] \exp \left( -i \frac{\theta_m [l_2] + \theta_m [l_2 + 1] + i \theta_n [l_2] + \theta_n [l_2 + 1]}{2} \right) \Xi_m [l_2],
\end{align*}
$$

By using the above relation, equation (I.15) is deformed to

$$
\begin{align*}
iM_+^{(1)} [l_2] \Xi_n [l_2] + \sum_{m>0} g_{mn} [l_2 - 1] \exp (-i \theta_n [l_2]) \left( \begin{array}{cc} 0 & -1 \\ 0 & 0 \end{array} \right) \Xi_m [l_2] \\
&+ \sum_{m<0} g_{mn} [l_2 + 1] \exp (+i \theta_n [l_2]) \left( \begin{array}{cc} 0 & 0 \\ 1 & 0 \end{array} \right) \Xi_m [l_2] + o \left( \| \tilde{M}_+^{(1)} \| \right) \\
= \begin{pmatrix}
\exp \left( i \frac{\theta_n [l_2] + \theta_n [l_2 + 1]}{2} \right) & 0 \\
0 & 0
\end{pmatrix} G [l_2 + 1, l_2 + 1] - \begin{pmatrix}
0 & \exp \left( -i \frac{\theta_n [l_2 - 1] + \theta_n [l_2]}{2} \right) \\
0 & 0
\end{pmatrix} G [l_2 - 1, l_2 - 1].
\end{align*}
$$

We try to introduce $G [l_2, l_2]$ into the above equation as

$$
G [l_2, l_2] \triangleq \begin{pmatrix}
g_{mn} [l_2] & 0 \\
0 & 0
\end{pmatrix} \Xi_m [l_2] + \sum_{m<0} \begin{pmatrix}
0 & 0 \\
0 & g_{mn} [l_2]
\end{pmatrix} \Xi_m [l_2].
$$

If we define other formulation, e.g. inverting positive and negative of $m$ instead of eq. (I.17), there is no consistency with electric and magnetic perturbation-terms and forward and backward scattering-waves. From eqs. (I.16) and (I.17),

$$
\begin{align*}
&i\tilde{M}_+^{(1)} \Xi_n + \sum_{m>0} g_{mn} [l_2 - 1] e^{-i \theta_n} \left( \begin{array}{cc} 0 & -1 \\ 0 & 0 \end{array} \right) \Xi_m + \sum_{m<0} g_{mn} [l_2 + 1] e^{i \theta_n} \left( \begin{array}{cc} 0 & 1 \\ 0 & 0 \end{array} \right) \Xi_m + o \left( \| \tilde{M}_+^{(1)} \| \right) \\
= \sum_{m>0} g_{mn} [l_2 + 1] \left( \begin{array}{cc} 0 & 0 \\ e^{i \theta_n} & 0 \end{array} \right) \Xi_m - \sum_{m<0} g_{mn} [l_2 - 1] \left( \begin{array}{cc} 0 & e^{-i \theta_n} \\ 0 & 0 \end{array} \right) \Xi_m,
\end{align*}
$$

where we omit “$[l_2]$” from the above notation. Furthermore, $o \left( \| \tilde{M}_+^{(1)} \| \right)$ is omitted from the above equation:

$$
\begin{align*}
i\tilde{M}_+^{(1)} [l_2] \Xi_n = & \sum_{m>0} \left( e^{i \theta_n} g_{mn} [l_2 + 1] e^{-i \theta_n} g_{mn} [l_2 - 1] \right) \Xi_m \\
&- \sum_{m<0} \left( e^{i \theta_n} g_{mn} [l_2 + 1] e^{-i \theta_n} g_{mn} [l_2 - 1] \right) \Xi_m.
\end{align*}
$$

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From the special setting of eq. (7.9) and the definition of eq. (7.10),

\[
\begin{align*}
    i\tilde{M}^{(1)}_+ \Xi_n &= \sum_{m=0}^{\infty} \left( \begin{array}{cc} 0 & e^{-i\theta_n}g_{mn} [l_2 + 1] \\ e^{i\theta_n}g_{mn} [l_2 - 1] & 0 \end{array} \right) \left( \begin{array}{c} e^{-i\theta_m/2} h_m \\ e^{i\theta_m/2} h_m \end{array} \right) \\
    &= \sum_{m=0}^{\infty} \left( e^{-i\theta_n}g_{mn} [l_2 - 1] e_m - e^{-i\theta_n}g_{mn} [l_2 + 1] e^{-i\theta_m/2} h_m \right) - \left( e^{i\theta_n}g_{mn} [l_2 - 1] e_m - e^{i\theta_n}g_{mn} [l_2 + 1] e^{i\theta_m/2} h_m \right) \\
    &= \sum_{m=0}^{\infty} \left( e^{-i\theta_n}g_{mn} [l_2 - 1] e_m + g_{mn} [l_2 - 1] e_m \right) \\
    &= \sum_{m=0}^{\infty} \left( e^{-i\theta_n}g_{mn} [l_2 - 1] + e^{-i\theta_m/2} g_{mn} [l_2 + 1] - e^{i\theta_m/2} g_{mn} [l_2 + 1] \right) h_m,
\end{align*}
\]

where \( \theta_m = -\theta_n \). From the orthogonality of \( h_m \) and \( e_m \) in eq. (7.8), the above equation gives us the following two equations.

\[
\left\{ \begin{array}{l}
    (h_m^T \, 0) \, i\tilde{M}^{(1)}_+ [l_2 + 1] \Xi_n = \frac{e^{-i\theta_n}}{2 \cos (\theta_m/2)} [g_{mn} + g_{mn}], \\
    (0 \, e_m^T) \, i\tilde{M}^{(1)}_+ [l_2 - 1] \Xi_n = \frac{e^{i\theta_n}}{2 \cos (\theta_m/2)} [e^{-i\theta_m/2} g_{mn} - e^{i\theta_m/2} g_{mn}]
\end{array} \right. \quad \text{for } m > 0.
\]

Then, we can solve the above equations for \( g_{mn} \) as

\[
g_{mn} [l_2] = \left( \begin{array}{cc} e^{i\theta_m/2} h_m^T & 0 \end{array} \right) i\tilde{M}^{(1)}_+ [l_2 + 1] \Xi_n + \left( \begin{array}{c} e^{i\theta_n} \tilde{M}^{(1)}_+ [l_2 - 1] \Xi_n \end{array} \right) \mu + o \left( \| \tilde{M}^{(1)}_+ \| \right). \quad (1.18)
\]

Note that \( g_{mn} [l_2 \leq 0] = g_{mn} [l_2 \geq L_2 - 1] = 0 \) from eq. (1.9). Two terms in the right-hand side of eq. (1.18) then satisfy that

\[
\left\{ \begin{array}{l}
    (h_m^T \, 0) \, i\tilde{M}^{(1)}_+ [l_2 \leq 1] \Xi_n = 0 \quad \text{for } g_{mn} [l_2 \leq 0] = 0, \\
    (0 \, e_m^T) \, i\tilde{M}^{(1)}_+ [l_2 \geq L_2 - 2] \Xi_n = 0 \quad \text{for } g_{mn} [l_2 \geq L_2 - 1] = 0.
\end{array} \right.
\]

From the above conditions and the definitions of eqs. (1.12), (7.1) and (7.2), the \( \varepsilon_{ljj} \) and \( \mu_{ljj} \) satisfy that

\[
\begin{align*}
    \nabla_2 \varepsilon_{l00} [l_2 \leq 0] &= \nabla_2 \varepsilon_{l11} [l_2 \leq 0] = \nabla_2 \mu_{l22} [l_2 \leq 0] = 0, \\
    \nabla_2 \mu_{l00} [l_2 \leq 1] &= \nabla_2 \mu_{l11} [l_2 \leq 1] = \nabla_2 \varepsilon_{l22} [l_2 \leq 1] = 0, \\
    \Delta_2 \varepsilon_{l00} [l_2 \geq L_2 - 2] &= \Delta_2 \varepsilon_{l11} [l_2 \geq L_2 - 2] = \Delta_2 \mu_{l22} [l_2 \geq L_2 - 2] = 0, \\
    \Delta_2 \mu_{l00} [l_2 \geq L_2 - 1] &= \Delta_2 \mu_{l11} [l_2 \geq L_2 - 1] = \Delta_2 \varepsilon_{l22} [l_2 \geq L_2 - 1] = 0.
\end{align*}
\]

If we consider the symmetry for forward and backward directions, we should change the first equation in the above into

\[
\begin{align*}
    \nabla_2 \varepsilon_{l00} [l_2 \leq 1] &= \nabla_2 \varepsilon_{l11} [l_2 \leq 1] = \nabla_2 \mu_{l22} [l_2 \leq 1] = 0.
\end{align*}
\]

When \( M^{(0)}_+ \) is independent of \( l_2 \), the \( \theta_n \) and \( \Xi_m \) are also independent of \( l_2 \). Equations (1.12) and (1.18) can be then simplified to

\[
\begin{align*}
    \tilde{M}^{(1)}_+ [l_2] &= M^{(1)}_+ [l_2] = \left( \begin{array}{cc} m_{aa}^{(1)} [l_2] & 0 \\ 0 & m_{bb}^{(1)} [l_2] \end{array} \right), \\
    g_{mn} [l_2] &= i\Xi_m^\dagger \left( \begin{array}{cc} e^{i\theta_n}m_{aa}^{(1)} [l_2 + 1] & 0 \\ 0 & e^{-i\theta_n}m_{bb}^{(1)} [l_2 - 1] \end{array} \right) \Xi_n, \\
    &\quad \text{if } \Delta_2 M^{(0)}_+ = \nabla_2 M^{(0)}_+ = 0. \\
\end{align*}
\]

Let us apply discrete Fourier transform (DFT) in subsection I.7 to \( g_{mn} \). By using the formula of eq. (1.22), equation (1.19) is transformed to

\[
\begin{align*}
    \tilde{g}_{mn}^{\text{DFT}} (\phi) = i\Xi_m^\dagger \left( \begin{array}{cc} e^{(i\theta_n+\phi)}m_{aa}^{(1)} \text{DFT} (\phi) & 0 \\ 0 & e^{-i(\theta_n+\phi)}m_{bb}^{(1)} \text{DFT} (\phi) \end{array} \right) \Xi_n + o \left( \| \tilde{M}^{(1)}_+ \| \right).
\end{align*}
\]

The above \( \tilde{g}_{mn}^{\text{DFT}} \) can be applied to the discrete \( S_{mn} \) of eq. (7.16).
1.6. Formulas of discrete difference operators

Note that

\[
\begin{align*}
\Delta A[j] B[j] &= A[j + 1] B[j + 1] - A[j] B[j] \\
&= (A[j + 1] - A[j]) \left( \frac{B[j + 1] + B[j]}{2} + \frac{A[j + 1] + A[j]}{2} \right) \left( B[j + 1] - B[j] \right) \\
&= (\Delta A[j]) \left( 1 + \frac{\Delta }{2} \right) B[j] + \left( \left( 1 + \frac{\Delta }{2} \right) A[j] \right) \Delta B[j], \\
\n\n|A[j] B[j] &= A[j] B[j] - A[j - 1] B[j - 1] \\
&= (A[j] - A[j - 1]) \left( \frac{B[j] + B[j - 1]}{2} + \frac{A[j] + A[j - 1]}{2} \right) \left( B[j] - B[j - 1] \right) \\
&= (\nabla A[j]) \left( 1 - \frac{\nabla }{2} \right) B[j] + \left( \left( 1 - \frac{\nabla }{2} \right) A[j] \right) \nabla B[j].
\end{align*}
\]

(1.21)

1.7. Notation and formulas of discrete Fourier transform (DFT)

Notation of DFT keeps consistency to one of Fourier transform (FT) in Section 1.1. We consider a discrete function \( f_d[l_2] \) for \( 0 \leq l_2 < L_2 \). The \( f_d[l_2] \) is discreted from the continuous function \( f_c(u_2) \) as follows.

\[ f_d[l_2] = f_c(u_2[l_2]) = f_c \left( \left( l_2 - \frac{L_2 - 1}{2} \right) u_2 \right) , \]

where we use the notation in Section 6.2, and we assume that \( u_2' \) is constant.

DFT of \( f_d[l_2] \) is given by

\[ \tilde{f}_{DFT}(\phi) \triangleq \sum_{l_2=0}^{L_2-1} f_d[l_2] \exp \left[ -i \phi \left( l_2 - \frac{L_2 - 1}{2} \right) \right] \text{ for } -\pi < \phi < \pi . \] (1.22)

We can approximate the above summation to integration:

\[ \tilde{f}_{DFT}(\phi) \approx \frac{1}{u_2} \int_{-\frac{L_2 - 1}{2}u_2}^{\frac{L_2 - 1}{2}u_2} f_c(u_2) \exp \left( -i \frac{\phi u_2}{u_2} \right) du_2 < O \left( \max \left| \frac{df_c}{du_2} u_2 - i\phi f_c \right| L_2 \right). \]

Therefore, DFT for \( l_2 \) is related to FT for \( u_2 \):

\[ \lim_{u_2 \to 0} u_2 \tilde{f}_{DFT}(\phi) = \hat{f}_c(k) \text{ as } k = \lim_{u_2 \to 0} \frac{\phi}{u_2}, \] (1.23)

when we assume that \( \lim_{u_2' \to 0} L_2 u_2' = L_s \), and \( f_c(u_2 < -L_s/2) = f_c(u_2 > L_s/2) = 0 \).

If \( \phi \) becomes discrete as \( \phi_n = 2\pi [n - (L_2 - 1)/2] / L_2 \), we can define inverse discrete Fourier transform (IDFT) as

\[ f_d[l] = \frac{1}{L_2} \sum_{n=0}^{L_2-1} \tilde{f}_{DFT}(\phi_n) \exp \left( i \phi_n \left( l - \frac{L_2 - 1}{2} \right) \right) \]

\[ = \frac{1}{L_2} \sum_{n=0}^{L_2-1} \sum_{l' = 0}^{L_2-1} f_d[l'] \exp \left( -i \phi_n \left( l' - \frac{L_2 - 1}{2} \right) \right) \exp \left( i \phi_n \left( l - \frac{L_2 - 1}{2} \right) \right) \]

\[ = \frac{1}{L_2} \sum_{l' = 0}^{L_2-1} f_d[l'] \sum_{n=0}^{L_2-1} \exp \left( -i \phi_n \left( l' - l \right) \right) = \sum_{l' = 0}^{L_2-1} f_d[l'] \frac{e^{-\pi i (l'-l)/L_2} \left( e^{\pi i (l'-l)} - e^{-\pi i (l'-l)} \right)}{L_2 \left( 1 - e^{-2\pi i (l'-l)/L_2} \right)} \]

\[ = \sum_{l' = 0}^{L_2-1} f_d[l'] \delta_{l,l} = f_d[l] . \]
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