Advanced Computation:
Computational Electromagnetics

Formulation of Rigorous Coupled-Wave Analysis (RCWA)

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Outline

- Background
- Semi-analytical form of Maxwell's equations in Fourier space
- Matrix form of Maxwell's equations
- Matrix wave equation
- Solution to the matrix wave equation
- Multilayer framework: scattering matrices
- Calculate transmission and reflection

$$\text{TMM} + \text{PWEM} = \text{RCWA}$$

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Background

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Rigorous Coupled-Wave Analysis

- Developed in 1980's
  - Dr. M. G. "Jim" Moharam
  - Dr. Thomas K. Gaylord
- Alternate Names for the Method
  - Rigorous coupled-wave analysis
  - Fourier modal method
  - Transfer matrix method with a plane wave basis

Dr. M. G. "Jim" Moharam

Dr. Thomas K. Gaylord

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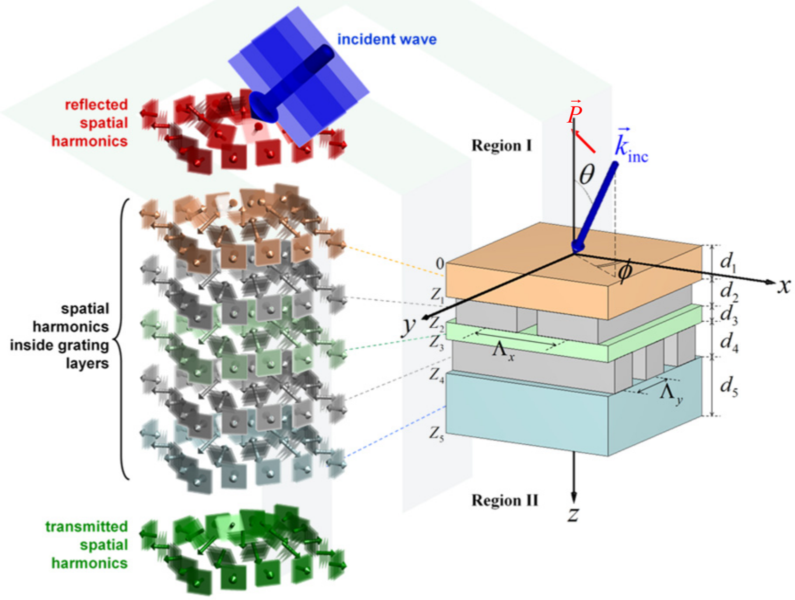
Geometry of RCWA



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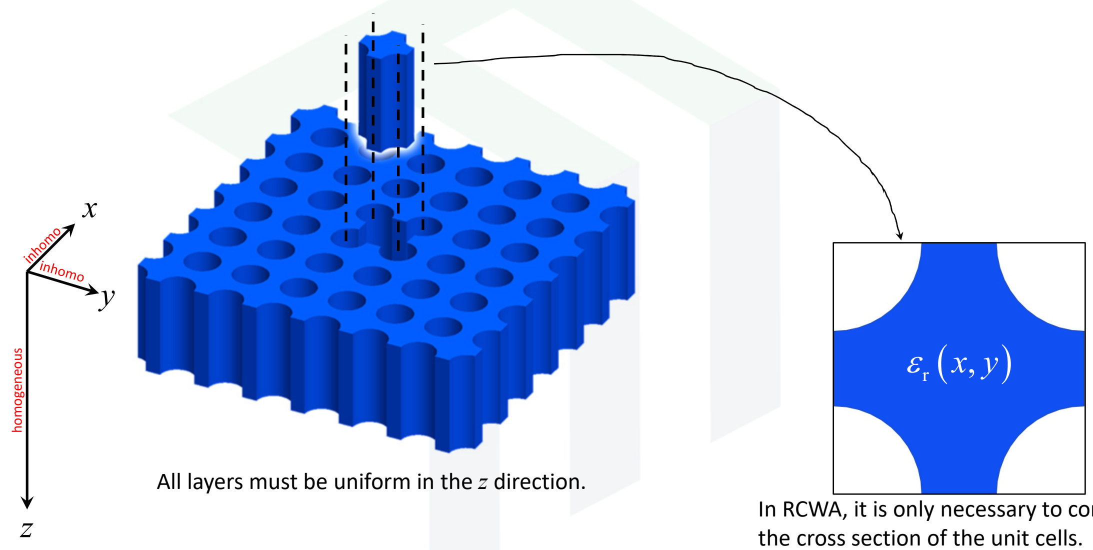
The 2D Unit Cell for Single Layer



All layers must be uniform in the z direction.

In RCWA, it is only necessary to construct the cross section of the unit cells. Thickness is conveyed elsewhere.

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Sign Convention

The negative sign convention will be used here for a wave travelling in the $+z$ direction.

$$e^{-jkz}$$

Semi-Analytical Form of Maxwell's Equations in Fourier Space

Starting Point for RCWA

Start with Maxwell's equations in the following form…

$$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=k_0\mu_r\tilde{H}_x \qquad \frac{\partial \tilde{H}_z}{\partial y}-\frac{\partial \tilde{H}_y}{\partial z}=k_0\varepsilon_r E_x$$

$$\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=k_0\mu_r\tilde{H}_y \qquad \frac{\partial \tilde{H}_x}{\partial z}-\frac{\partial \tilde{H}_z}{\partial x}=k_0\varepsilon_r E_y$$

$$\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=k_0\mu_r\tilde{H}_z \qquad \frac{\partial \tilde{H}_y}{\partial x}-\frac{\partial \tilde{H}_x}{\partial y}=k_0\varepsilon_r E_z$$

Recall that the magnetic field was normalized according to

$$\vec{\tilde{H}}=-j\sqrt{\frac{\mu_0}{\varepsilon_0}}\vec{H}$$

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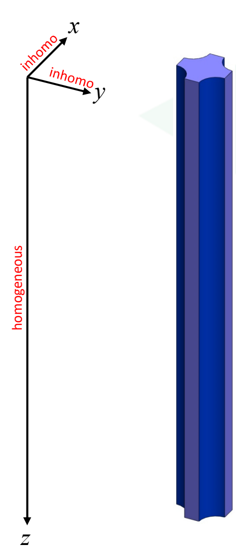
z-Uniform Media



We are going to consider Maxwell's equation inside a medium that is uniform in the z direction.

The medium may still be inhomogeneous in the x-y plane, but it must be uniform in the z direction.

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Fourier Transform in x and y Only

Unlike PWEM, RCWA only Fourier transforms along x and y. The z parameter remains analytical and unchanged. The Fourier expansion of the materials in the x-y plane are

$$\varepsilon_{\mathrm{r}}(x,y)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}a_{m,n}e^{j(m\vec{T}_1+n\vec{T}_2)\bullet\vec{r}}$$

$$a_{m,n}=\frac{1}{\Lambda_x\Lambda_y}\int_{-\Lambda_x/2}^{\Lambda_x/2}\int_{-\Lambda_y/2}^{\Lambda_y/2}\varepsilon_{\mathrm{r}}(x,y)e^{-j(m\vec{T}_1+n\vec{T}_2)\bullet\vec{r}}dxdy$$

$$\mu_{\mathrm{r}}(x,y)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}b_{m,n}e^{j(m\vec{T}_1+n\vec{T}_2)\bullet\vec{r}}$$

$$b_{m,n}=\frac{1}{\Lambda_x\Lambda_y}\int_{-\Lambda_x/2}^{\Lambda_x/2}\int_{-\Lambda_y/2}^{\Lambda_y/2}\mu_{\mathrm{r}}(x,y)e^{-j(m\vec{T}_1+n\vec{T}_2)\bullet\vec{r}}dxdy$$

It follows that the Fourier expansion of the fields are

$$E_x(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_x(m,n;z)\cdot e^{-j[k_x(m,n)x+k_y(m,n)y]}$$

$$E_y(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_y(m,n;z)\cdot e^{-j[k_x(m,n)x+k_y(m,n)y]}$$

$$E_z(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_z(m,n;z)\cdot e^{-j[k_x(m,n)x+k_y(m,n)y]}$$

$$\tilde{H}_x(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}U_x(m,n;z)\cdot e^{-j[k_x(m,n)x+k_y(m,n)y]}$$

$$\tilde{H}_y(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}U_y(m,n;z)\cdot e^{-j[k_x(m,n)x+k_y(m,n)y]}$$

$$\tilde{H}_z(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}U_z(m,n;z)\cdot e^{-j[k_x(m,n)x+k_y(m,n)y]}$$

$$\vec{k}_{xy}(m,n)=\vec{k}_{xy,\mathrm{inc}}-m\vec{T}_1-n\vec{T}_2$$

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Wave Vector Components

The transverse components of the wave vectors are equal throughout all layers of the device.

$$k_x(m,n)=k_{x,\mathrm{inc}}-mT_{1,x}-nT_{2,x}\qquad m=-\infty,\cdots,-2,-1,0,1,2,\cdots,\infty$$

$$k_y(m,n)=k_{y,\mathrm{inc}}-mT_{1,y}-nT_{2,y}\qquad n=-\infty,\cdots,-2,-1,0,1,2,\cdots,\infty$$

$$\vec{k}_{xy}(m,n)=\vec{k}_{xy,\mathrm{inc}}-m\vec{T}_1-n\vec{T}_2$$

The longitudinal components of the wave vectors are needed for:

(1) calculating diffraction efficiencies
(2) calculating the eigen-modes of a homogeneous layer analytically

These are calculated from the dispersion relation in the medium of interest.

$$k_z(m,n)=\left\{\sqrt{k_0^2\mu_{\mathrm{r}}^*\varepsilon_{\mathrm{r}}^*-k_x^2(m,n)-k_y^2(m,n)}\right\}^*$$

The conjugate operations enforce the negative sign convention.

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Substitute Expansions into Maxwell's Equations

$$E_z(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_z(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}$$

$$\mu_{\mathrm{r}}(x,y)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}b_{m,n}e^{j\left(m\vec{T}_1+n\vec{T}_2\right)\bullet\vec{r}}$$

$$E_y(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_y(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}$$

$$\tilde{H}_x(x,y,z)=\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}U_x(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}$$

$$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=k_0\mu_{\mathrm{r}}\tilde{H}_x$$

$$\frac{\partial}{\partial y}\left[\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_z(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}\right]-\frac{\partial}{\partial z}\left[\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}S_y(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}\right]=k_0\left[\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}b_{m,n}e^{j\left(m\vec{T}_1+n\vec{T}_2\right)\bullet\vec{r}}\right]\left[\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}U_x(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}\right]$$

$$\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}-jk_y(m,n)S_z(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}-\left[\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\frac{\partial S_y(m,n;z)}{\partial z}\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}\right]=k_0\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\left[\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}e^{j\left[(m-q)\vec{T}_1+(n-r)\vec{T}_2\right]\bullet\vec{r}}e^{j\left[\frac{2\pi(m-q)x}{\Lambda_x}+\frac{2\pi(n-r)y}{\Lambda_y}\right]}U_x(q,r;z)e^{-j\left[k_x(q,r)x+k_y(q,r)y\right]}\right]$$

$$\sum_{m=-\infty}^{\infty}\sum_{n=-\infty}^{\infty}\left\{-jk_y(m,n)S_z(m,n;z)\cdot e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}-\frac{\partial S_y(m,n;z)}{\partial z}e^{-j\left[k_x(m,n)x+k_y(m,n)y\right]}=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}e^{j\left[(m-q)\vec{T}_1+(n-r)\vec{T}_2\right]\bullet\vec{r}}U_x(q,r;z)e^{-j\left[k_x(q,r)x+k_y(q,r)y\right]}\right\}$$

$$-jk_y(m,n)S_z(m,n;z)-\frac{dS_y(m,n;z)}{dz}=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}U_x(q,r;z)$$

The derivative is ordinary because z is the only independent variable left.

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Semi-Analytical Form of Maxwell's Equations in Fourier Space

If this is done for all of Maxwell's equations, we get…

Real-Space	Semi-Analytical Fourier-Space
$\frac{\partial\tilde{H}_z}{\partial y}-\frac{\partial\tilde{H}_y}{\partial z}=k_0\varepsilon_{\mathrm{r}}E_x$	$-jk_y(m,n)U_z(m,n;z)-\frac{dU_y(m,n;z)}{dz}=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a_{m-q,n-r}S_x(q,r;z)$
$\frac{\partial\tilde{H}_x}{\partial z}-\frac{\partial\tilde{H}_z}{\partial x}=k_0\varepsilon_{\mathrm{r}}E_y$	$\frac{dU_x(m,n;z)}{dz}+jk_x(m,n)U_z(m,n;z)=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a_{m-q,n-r}S_y(q,r;z)$
$\frac{\partial\tilde{H}_y}{\partial x}-\frac{\partial\tilde{H}_x}{\partial y}=k_0\varepsilon_{\mathrm{r}}E_z$	$-jk_x(m,n)U_y(m,n;z)+jk_y(m,n)U_x(m,n;z)=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a_{m-q,n-r}S_z(q,r;z)$
$\frac{\partial E_z}{\partial y}-\frac{\partial E_y}{\partial z}=k_0\mu_{\mathrm{r}}\tilde{H}_x$	$-jk_y(m,n)S_z(m,n;z)-\frac{dS_y(m,n;z)}{dz}=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}U_x(q,r;z)$
$\frac{\partial E_x}{\partial z}-\frac{\partial E_z}{\partial x}=k_0\mu_{\mathrm{r}}\tilde{H}_y$	$\frac{dS_x(m,n;z)}{dz}+jk_x(m,n)S_z(m,n;z)=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}U_y(q,r;z)$
$\frac{\partial E_y}{\partial x}-\frac{\partial E_x}{\partial y}=k_0\mu_{\mathrm{r}}\tilde{H}_z$	$-jk_x(m,n)S_y(m,n;z)+jk_y(m,n)S_x(m,n;z)=k_0\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}U_z(q,r;z)$

Note: $U(m,n;z)$ and $S(m,n;z)$ are functions of z. μ, ε, a, and b are not.

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Matrix Form of Maxwell's Equations

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Normalize the Fourier-Space Equations

Define normalized wave vectors.

$$\tilde{k}_x = \frac{k_x}{k_0} \qquad \tilde{k}_y = \frac{k_y}{k_0} \qquad \tilde{k}_z = \frac{k_z}{k_0}$$

Normalize the z coordinate.

$$\tilde{z} = k_0 z$$

$$\begin{aligned}
-j\tilde{k}_y(m,n)U_z(m,n;\tilde{z}) - \frac{dU_y(m,n;\tilde{z})}{d\tilde{z}} &= \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a_{m-q,n-r} S_x(q,r;\tilde{z}) \\
\frac{dU_x(m,n;\tilde{z})}{d\tilde{z}} + j\tilde{k}_x(m,n)U_z(m,n;\tilde{z}) &= \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a_{m-q,n-r} S_y(q,r;\tilde{z}) \\
-j\tilde{k}_x(m,n)U_y(m,n;\tilde{z}) + j\tilde{k}_y(m,n)U_x(m,n;\tilde{z}) &= \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a_{m-q,n-r} S_z(q,r;\tilde{z})
\end{aligned}$$

$$\begin{aligned}
-j\tilde{k}_y(m,n)S_z(m,n;\tilde{z}) - \frac{dS_y(m,n;\tilde{z})}{d\tilde{z}} &= \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} b_{m-q,n-r} U_x(q,r;\tilde{z}) \\
\frac{dS_x(m,n;\tilde{z})}{d\tilde{z}} + j\tilde{k}_x(m,n)S_z(m,n;\tilde{z}) &= \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} b_{m-q,n-r} U_y(q,r;\tilde{z}) \\
-j\tilde{k}_x(m,n)S_y(m,n;\tilde{z}) + j\tilde{k}_y(m,n)S_x(m,n;\tilde{z}) &= \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} b_{m-q,n-r} U_z(q,r;\tilde{z})
\end{aligned}$$

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Matrix Form of Maxwell's Equations (1 of 2)

Start with the first equation.

$$-j\tilde{k}_y(m,n)U_z(m,n;\tilde{z}) - \frac{dU_y(m,n;\tilde{z})}{d\tilde{z}} = \sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty} a_{m-q,n-r}S_x(q,r;\tilde{z})$$

This equation is written once for every combination of m and n.

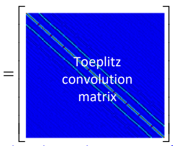
This large set of equations can be written in matrix form as

$$-j\tilde{\mathbf{K}}_y\mathbf{u}_z - \frac{d}{d\tilde{z}}\mathbf{u}_y = [\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_x$$

$$\tilde{\mathbf{K}}_y = \begin{bmatrix} \tilde{k}_y(1,1) & & & 0 \\ & \tilde{k}_y(1,2) & & \\ & & \ddots & \\ 0 & & & \tilde{k}_y(M,N) \end{bmatrix}$$

$$\mathbf{u}_z = \begin{bmatrix} U_z(1,1) \\ U_z(1,2) \\ \vdots \\ U_z(M,N) \end{bmatrix} \quad \mathbf{u}_y = \begin{bmatrix} U_y(1,1) \\ U_y(1,2) \\ \vdots \\ U_y(M,N) \end{bmatrix} \quad \mathbf{s}_x = \begin{bmatrix} S_x(1,1) \\ S_x(1,2) \\ \vdots \\ S_x(M,N) \end{bmatrix}$$

$[\![\varepsilon_\mathrm{r}]\!] =$



Note: only truly Toeplitz symmetry for 1D gratings.

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Matrix Form of Maxwell's Equations (2 of 2)

$$-j\tilde{k}_y(m,n)U_z(m,n;\tilde{z}) - \frac{dU_y(m,n;\tilde{z})}{d\tilde{z}} = \sum_{q=-M/2}^{M/2}\sum_{r=-N/2}^{N/2} a_{m-q,n-r}S_x(q,r;\tilde{z})$$
$$\frac{dU_x(m,n;\tilde{z})}{d\tilde{z}} + j\tilde{k}_x(m,n)U_z(m,n;\tilde{z}) = \sum_{q=-M/2}^{M/2}\sum_{r=-N/2}^{N/2} a_{m-q,n-r}S_y(q,r;\tilde{z})$$
$$-j\tilde{k}_x(m,n)U_y(m,n;\tilde{z}) + j\tilde{k}_y(m,n)U_x(m,n;\tilde{z}) = \sum_{q=-M/2}^{M/2}\sum_{r=-N/2}^{N/2} a_{m-q,n-r}S_z(q,r;\tilde{z})$$

$$\Rightarrow \boxed{\begin{aligned} -j\tilde{\mathbf{K}}_y\mathbf{u}_z - \frac{d}{d\tilde{z}}\mathbf{u}_y &= [\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_x \\ \frac{d}{d\tilde{z}}\mathbf{u}_x + j\tilde{\mathbf{K}}_x\mathbf{u}_z &= [\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_y \\ \tilde{\mathbf{K}}_x\mathbf{u}_y - \tilde{\mathbf{K}}_y\mathbf{u}_x &= j[\![\varepsilon_\mathrm{r}]\!]\mathbf{s}_z \end{aligned}}$$

$$-jk_y(m,n)S_z(m,n;z) - \frac{dS_y(m,n;z)}{dz} = k_0\sum_{q=-M/2}^{M/2}\sum_{r=-N/2}^{N/2} b_{m-q,n-r}U_x(q,r;z)$$
$$\frac{dS_x(m,n;z)}{dz} + jk_x(m,n)S_z(m,n;z) = k_0\sum_{q=-M/2}^{M/2}\sum_{r=-N/2}^{N/2} b_{m-q,n-r}U_y(q,r;z)$$
$$-jk_x(m,n)S_y(m,n;z) + jk_y(m,n)S_x(m,n;z) = k_0\sum_{q=-M/2}^{M/2}\sum_{r=-N/2}^{N/2} b_{m-q,n-r}U_z(q,r;z)$$

$$\Rightarrow \boxed{\begin{aligned} -j\tilde{\mathbf{K}}_y\mathbf{s}_z - \frac{d}{d\tilde{z}}\mathbf{s}_y &= [\![\mu_\mathrm{r}]\!]\mathbf{u}_x \\ \frac{d}{d\tilde{z}}\mathbf{s}_x + j\tilde{\mathbf{K}}_x\mathbf{s}_z &= [\![\mu_\mathrm{r}]\!]\mathbf{u}_y \\ \tilde{\mathbf{K}}_x\mathbf{s}_y - \tilde{\mathbf{K}}_y\mathbf{s}_x &= j[\![\mu_\mathrm{r}]\!]\mathbf{u}_z \end{aligned}}$$

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Matrix Wave Equation

Solve for Longitudinal Field Components

To eliminate the longitudinal field components $\mathbf{s}_z$ and $\mathbf{u}_z$, start by solving the third and sixth equation for these terms.

$$-j\tilde{\mathbf{K}}_y\mathbf{u}_z - \frac{d}{d\tilde{z}}\mathbf{u}_y = [\![\varepsilon_r]\!]\mathbf{s}_x$$

$$\frac{d}{d\tilde{z}}\mathbf{u}_x + j\tilde{\mathbf{K}}_x\mathbf{u}_z = [\![\varepsilon_r]\!]\mathbf{s}_y$$

$$\tilde{\mathbf{K}}_x\mathbf{u}_y - \tilde{\mathbf{K}}_y\mathbf{u}_x = j[\![\varepsilon_r]\!]\mathbf{s}_z \longrightarrow \mathbf{s}_z = -j[\![\varepsilon_r]\!]^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{u}_y - \tilde{\mathbf{K}}_y\mathbf{u}_x\right)$$

$$-j\tilde{\mathbf{K}}_y\mathbf{s}_z - \frac{d}{d\tilde{z}}\mathbf{s}_y = [\![\mu_r]\!]\mathbf{u}_x$$

$$\frac{d}{d\tilde{z}}\mathbf{s}_x + j\tilde{\mathbf{K}}_x\mathbf{s}_z = [\![\mu_r]\!]\mathbf{u}_y$$

$$\tilde{\mathbf{K}}_x\mathbf{s}_y - \tilde{\mathbf{K}}_y\mathbf{s}_x = j[\![\mu_r]\!]\mathbf{u}_z \longrightarrow \mathbf{u}_z = -j[\![\mu_r]\!]^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{s}_y - \tilde{\mathbf{K}}_y\mathbf{s}_x\right)$$

Eliminate Longitudinal Field Components

Substitute $\mathbf{s}_z$ and $\mathbf{u}_z$ back into the remaining four equations.

$$-j\tilde{\mathbf{K}}_y\mathbf{u}_z-\frac{d}{d\tilde{z}}\mathbf{u}_y=\llbracket\varepsilon_{\mathrm{r}}\rrbracket\mathbf{s}_x$$
$$\frac{d}{d\tilde{z}}\mathbf{u}_x+j\tilde{\mathbf{K}}_x\mathbf{u}_z=\llbracket\varepsilon_{\mathrm{r}}\rrbracket\mathbf{s}_y$$
$$\mathbf{s}_z=-j\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{u}_y-\tilde{\mathbf{K}}_y\mathbf{u}_x\right)$$

$$-\tilde{\mathbf{K}}_y\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{s}_y-\tilde{\mathbf{K}}_y\mathbf{s}_x\right)-\frac{d}{d\tilde{z}}\mathbf{u}_y=\llbracket\varepsilon_{\mathrm{r}}\rrbracket\mathbf{s}_x$$
$$\frac{d}{d\tilde{z}}\mathbf{u}_x+\tilde{\mathbf{K}}_x\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{s}_y-\tilde{\mathbf{K}}_y\mathbf{s}_x\right)=\llbracket\varepsilon_{\mathrm{r}}\rrbracket\mathbf{s}_y$$

$$-j\tilde{\mathbf{K}}_y\mathbf{s}_z-\frac{d}{d\tilde{z}}\mathbf{s}_y=\llbracket\mu_{\mathrm{r}}\rrbracket\mathbf{u}_x$$
$$\frac{d}{d\tilde{z}}\mathbf{s}_x+j\tilde{\mathbf{K}}_x\mathbf{s}_z=\llbracket\mu_{\mathrm{r}}\rrbracket\mathbf{u}_y$$
$$\mathbf{u}_z=-j\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{s}_y-\tilde{\mathbf{K}}_y\mathbf{s}_x\right)$$

$$-\tilde{\mathbf{K}}_y\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{u}_y-\tilde{\mathbf{K}}_y\mathbf{u}_x\right)-\frac{d}{d\tilde{z}}\mathbf{s}_y=\llbracket\mu_{\mathrm{r}}\rrbracket\mathbf{u}_x$$
$$\frac{d}{d\tilde{z}}\mathbf{s}_x+\tilde{\mathbf{K}}_x\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{u}_y-\tilde{\mathbf{K}}_y\mathbf{u}_x\right)=\llbracket\mu_{\mathrm{r}}\rrbracket\mathbf{u}_y$$

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Rearrange the Terms

Next, expand the equations and rearrange the terms.

$$-\tilde{\mathbf{K}}_y\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{s}_y-\tilde{\mathbf{K}}_y\mathbf{s}_x\right)-\frac{d}{d\tilde{z}}\mathbf{u}_y=\llbracket\varepsilon_{\mathrm{r}}\rrbracket\mathbf{s}_x$$
$$\frac{d}{d\tilde{z}}\mathbf{u}_x+\tilde{\mathbf{K}}_x\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{s}_y-\tilde{\mathbf{K}}_y\mathbf{s}_x\right)=\llbracket\varepsilon_{\mathrm{r}}\rrbracket\mathbf{s}_y$$

$$\frac{d}{d\tilde{z}}\mathbf{u}_x=\tilde{\mathbf{K}}_x\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_y\mathbf{s}_x+\left(\llbracket\varepsilon_{\mathrm{r}}\rrbracket-\tilde{\mathbf{K}}_x\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_x\right)\mathbf{s}_y$$
$$\frac{d}{d\tilde{z}}\mathbf{u}_y=\left(\tilde{\mathbf{K}}_y\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_y-\llbracket\varepsilon_{\mathrm{r}}\rrbracket\right)\mathbf{s}_x-\tilde{\mathbf{K}}_y\llbracket\mu_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_x\mathbf{s}_y$$

$$-\tilde{\mathbf{K}}_y\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{u}_y-\tilde{\mathbf{K}}_y\mathbf{u}_x\right)-\frac{d}{d\tilde{z}}\mathbf{s}_y=\llbracket\mu_{\mathrm{r}}\rrbracket\mathbf{u}_x$$
$$\frac{d}{d\tilde{z}}\mathbf{s}_x+\tilde{\mathbf{K}}_x\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\left(\tilde{\mathbf{K}}_x\mathbf{u}_y-\tilde{\mathbf{K}}_y\mathbf{u}_x\right)=\llbracket\mu_{\mathrm{r}}\rrbracket\mathbf{u}_y$$

$$\frac{d}{d\tilde{z}}\mathbf{s}_x=\tilde{\mathbf{K}}_x\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_y\mathbf{u}_x+\left(\llbracket\mu_{\mathrm{r}}\rrbracket-\tilde{\mathbf{K}}_x\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_x\right)\mathbf{u}_y$$
$$\frac{d}{d\tilde{z}}\mathbf{s}_y=\left(\tilde{\mathbf{K}}_y\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_y-\llbracket\mu_{\mathrm{r}}\rrbracket\right)\mathbf{u}_x-\tilde{\mathbf{K}}_y\llbracket\varepsilon_{\mathrm{r}}\rrbracket^{-1}\tilde{\mathbf{K}}_x\mathbf{u}_y$$

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Block Matrix Form

Just as was done for the transfer matrix method using scattering matrices, write the matrix equations in block matrix form.

$$\frac{d}{d\tilde{z}}\mathbf{u}_x = \tilde{\mathbf{K}}_x [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_y \mathbf{s}_x + \left([\![\varepsilon_r]\!] - \tilde{\mathbf{K}}_x [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_x\right)\mathbf{s}_y$$

$$\frac{d}{d\tilde{z}}\mathbf{u}_y = \left(\tilde{\mathbf{K}}_y [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\varepsilon_r]\!]\right)\mathbf{s}_x - \tilde{\mathbf{K}}_y [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_x \mathbf{s}_y$$

$$\Rightarrow \quad \frac{d}{d\tilde{z}}\begin{bmatrix}\mathbf{u}_x\\ \mathbf{u}_y\end{bmatrix} = \mathbf{Q}\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} \tilde{\mathbf{K}}_x [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\varepsilon_r]\!] - \tilde{\mathbf{K}}_x [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\varepsilon_r]\!] & -\tilde{\mathbf{K}}_y [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\frac{d}{d\tilde{z}}\mathbf{s}_x = \tilde{\mathbf{K}}_x [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_y \mathbf{u}_x + \left([\![\mu_r]\!] - \tilde{\mathbf{K}}_x [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_x\right)\mathbf{u}_y$$

$$\frac{d}{d\tilde{z}}\mathbf{s}_y = \left(\tilde{\mathbf{K}}_y [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\mu_r]\!]\right)\mathbf{u}_x - \tilde{\mathbf{K}}_y [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_x \mathbf{u}_y$$

$$\Rightarrow \quad \frac{d}{d\tilde{z}}\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix} = \mathbf{P}\begin{bmatrix}\mathbf{u}_x\\ \mathbf{u}_y\end{bmatrix}$$

$$\mathbf{P} = \begin{bmatrix} \tilde{\mathbf{K}}_x [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\mu_r]\!] - \tilde{\mathbf{K}}_x [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\mu_r]\!] & -\tilde{\mathbf{K}}_y [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

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TMM vs. RCWA

TMM

$$\mathbf{P} = \frac{1}{\varepsilon_r}\begin{bmatrix} \tilde{k}_x\tilde{k}_y & \mu_r\varepsilon_r - \tilde{k}_x^2 \\ \tilde{k}_y^2 - \mu_r\varepsilon_r & -\tilde{k}_x\tilde{k}_y \end{bmatrix}$$

$$\mathbf{Q} = \frac{1}{\mu_r}\begin{bmatrix} \tilde{k}_x\tilde{k}_y & \mu_r\varepsilon_r - \tilde{k}_x^2 \\ \tilde{k}_y^2 - \mu_r\varepsilon_r & -\tilde{k}_x\tilde{k}_y \end{bmatrix}$$

RCWA

$$\mathbf{P} = \begin{bmatrix} \tilde{\mathbf{K}}_x [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\mu_r]\!] - \tilde{\mathbf{K}}_x [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\mu_r]\!] & -\tilde{\mathbf{K}}_y [\![\varepsilon_r]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\mathbf{Q} = \begin{bmatrix} \tilde{\mathbf{K}}_x [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\varepsilon_r]\!] - \tilde{\mathbf{K}}_x [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\varepsilon_r]\!] & -\tilde{\mathbf{K}}_y [\![\mu_r]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

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P and Q in Homogeneous Layers

When a layer is homogeneous, the $\mathbf{P}$ and $\mathbf{Q}$ matrices reduce to

$$\mathbf{P} = \varepsilon_{\mathrm{r}}^{-1}\begin{bmatrix} \tilde{\mathbf{K}}_x\tilde{\mathbf{K}}_y & \mu_{\mathrm{r}}\varepsilon_{\mathrm{r}}\mathbf{I} - \tilde{\mathbf{K}}_x^2 \\ \tilde{\mathbf{K}}_y^2 - \mu_{\mathrm{r}}\varepsilon_{\mathrm{r}}\mathbf{I} & -\tilde{\mathbf{K}}_y\tilde{\mathbf{K}}_x \end{bmatrix} \qquad \mathbf{Q} = \mu_{\mathrm{r}}^{-1}\begin{bmatrix} \tilde{\mathbf{K}}_x\tilde{\mathbf{K}}_y & \mu_{\mathrm{r}}\varepsilon_{\mathrm{r}}\mathbf{I} - \tilde{\mathbf{K}}_x^2 \\ \tilde{\mathbf{K}}_y^2 - \mu_{\mathrm{r}}\varepsilon_{\mathrm{r}}\mathbf{I} & -\tilde{\mathbf{K}}_y\tilde{\mathbf{K}}_x \end{bmatrix}$$

$$= \frac{\varepsilon_{\mathrm{r}}}{\mu_{\mathrm{r}}}\mathbf{P}$$

Notice that these matrices do not contain computationally intensive convolution matrices.

Therefore, they are very fast and efficient to calculate for this special case.

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Matrix Wave Equation

From here, derive a wave equation just as was done for TMM.

$$\frac{d}{d\tilde{z}}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} = \mathbf{P}\begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y\end{bmatrix} \quad \text{Eq. (1)} \qquad \frac{d}{d\tilde{z}}\begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y\end{bmatrix} = \mathbf{Q}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} \quad \text{Eq. (2)}$$

First, differentiate Eq. (1) with respect to z.

$$\frac{d^2}{d\tilde{z}^2}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} = \mathbf{P}\cdot\frac{d}{d\tilde{z}}\begin{bmatrix}\mathbf{u}_x \\ \mathbf{u}_y\end{bmatrix} \quad \text{Eq. (3)}$$

Second, substitute Eq. (2) into Eq. (3) to eliminate the magnetic fields.

$$\frac{d^2}{d\tilde{z}^2}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} = \mathbf{PQ}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix}$$

Third, the final matrix wave equation is

$$\frac{d^2}{d\tilde{z}^2}\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} - \mathbf{\Omega}^2\begin{bmatrix}\mathbf{s}_x \\ \mathbf{s}_y\end{bmatrix} = \mathbf{0} \qquad \mathbf{\Omega}^2 = \mathbf{PQ}$$

This is the standard "PQ" form!

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Solution to the Matrix Wave Equation

Analytical Solution in the z Direction

The matrix wave equation is

$$\frac{d^2}{d\tilde{z}^2}\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix}-\mathbf{\Omega}^2\begin{bmatrix}\mathbf{s}_x\\ \mathbf{s}_y\end{bmatrix}=\mathbf{0}$$

This is really a large set of ordinary differential equations that can each be solved analytically. This set of solutions is

$$\begin{bmatrix}\mathbf{s}_x(\tilde{z})\\ \mathbf{s}_y(\tilde{z})\end{bmatrix}=e^{-\mathbf{\Omega}\tilde{z}}\mathbf{s}^+(0)+e^{\mathbf{\Omega}\tilde{z}}\mathbf{s}^-(0)$$

The terms $\mathbf{s}^+(0)$ and $\mathbf{s}^-(0)$ are the initial values for this differential equation.

The ± superscripts indicate whether they pertain to forward propagating waves (+) or backward propagating waves (-).

Computation of $e^{\pm\Omega z}$

Recall from TMM…

$$f(\mathbf{A}) = \mathbf{W}\cdot f(\boldsymbol{\lambda})\cdot\mathbf{W}^{-1}$$

$\mathbf{A} \equiv$ Arbitrary square matrix (full rank)
$\mathbf{W} \equiv$ Eigen-vector matrix calculated from $\mathbf{A}$
$\boldsymbol{\lambda} \equiv$ Diagonal eigen-value matrix calculated from $\mathbf{A}$

Use this relation to compute the matrix exponentials.

$$e^{-\boldsymbol{\Omega}z'} = \mathbf{W}e^{-\boldsymbol{\lambda}z'}\mathbf{W}^{-1} \qquad e^{\boldsymbol{\Omega}z'} = \mathbf{W}e^{\boldsymbol{\lambda}z'}\mathbf{W}^{-1}$$

$\mathbf{W} \equiv$ Eigen-vector matrix of $\boldsymbol{\Omega}^2$
$\boldsymbol{\lambda}^2 \equiv$ Eigen-value matrix of $\boldsymbol{\Omega}^2$

$$e^{\lambda z'} = \begin{bmatrix} e^{\sqrt{\lambda_1^2}z'} & & & \\ & e^{\sqrt{\lambda_2^2}z'} & & \\ & & \ddots & \\ & & & e^{\sqrt{\lambda_N^2}z'} \end{bmatrix}$$

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Revised Solution

Start with the following solution.

$$\begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{bmatrix} = e^{-\boldsymbol{\Omega}\tilde{z}}\mathbf{s}^+(0) + e^{\boldsymbol{\Omega}\tilde{z}}\mathbf{s}^-(0) \quad \text{Eq. (1)}$$

$$\begin{aligned} e^{-\boldsymbol{\Omega}\tilde{z}} &= \mathbf{W}\cdot\exp(-\boldsymbol{\lambda}\tilde{z})\cdot\mathbf{W}^{-1} \\ e^{\boldsymbol{\Omega}\tilde{z}} &= \mathbf{W}\cdot\exp(\boldsymbol{\lambda}\tilde{z})\cdot\mathbf{W}^{-1} \end{aligned} \quad \text{Eq. (2)}$$

Substituting Eq. (2) into Eq. (1) yields

$$\begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{bmatrix} = \mathbf{W}e^{-\boldsymbol{\lambda}\tilde{z}}\underbrace{\mathbf{W}^{-1}\mathbf{s}^+(0)}_{\mathbf{c}^+} + \mathbf{W}e^{\boldsymbol{\lambda}\tilde{z}}\underbrace{\mathbf{W}^{-1}\mathbf{s}^-(0)}_{\mathbf{c}^-}$$

The terms $\mathbf{s}^+(0)$ and $\mathbf{s}^-(0)$ are initial values that have yet to be calculated. Therefore $\mathbf{W}^{-1}$ can be combined with these terms to produce column vectors of proportionality constants $\mathbf{c}^+$ and $\mathbf{c}^-$.

$$\begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{bmatrix} = \mathbf{W}e^{-\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^+ + \mathbf{W}e^{\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^-$$

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Solution for the Magnetic Fields (1 of 2)

A similar solution can be written for the magnetic fields.

$$\begin{bmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = -\mathbf{V}e^{-\lambda\tilde{z}}\mathbf{c}^+ + \mathbf{V}e^{\lambda\tilde{z}}\mathbf{c}^-$$

$\mathbf{V}$ must be calculated from the eigen-value solution of $\mathbf{\Omega}^2$. To put this equation in terms of the electric field, differentiate with respect to z.

$$\frac{d}{d\tilde{z}}\begin{bmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = \mathbf{V}\boldsymbol{\lambda}e^{-\lambda\tilde{z}}\mathbf{c}^+ + \mathbf{V}\boldsymbol{\lambda}e^{\lambda\tilde{z}}\mathbf{c}^-$$

The negative sign is needed so both terms will be positive after differentiation.

Solution for the Magnetic Fields (2 of 2)

Recall,

$$\frac{d}{d\tilde{z}}\begin{bmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = \mathbf{Q}\begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{bmatrix} \quad \text{Eq. (1)}$$

$$\begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{bmatrix} = \mathbf{W}e^{-\lambda\tilde{z}}\mathbf{c}^+ + \mathbf{W}e^{\lambda\tilde{z}}\mathbf{c}^- \quad \text{Eq. (2)}$$

$$\frac{d}{d\tilde{z}}\begin{bmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = \mathbf{V}\boldsymbol{\lambda}e^{-\lambda\tilde{z}}\mathbf{c}^+ + \mathbf{V}\boldsymbol{\lambda}e^{\lambda\tilde{z}}\mathbf{c}^- \quad \text{Eq. (3)}$$

Substitute Eq. (2) into Eq. (1) to eliminate $\mathbf{s}_x$ and $\mathbf{s}_y$.

$$\frac{d}{d\tilde{z}}\begin{bmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = \mathbf{QW}e^{-\lambda\tilde{z}}\mathbf{c}^+ + \mathbf{QW}e^{\lambda\tilde{z}}\mathbf{c}^-$$

Compare this expression to Eq. (3).

$$\mathbf{V}\boldsymbol{\lambda} = \mathbf{QW} \longrightarrow \boxed{\mathbf{V} = \mathbf{QW}\boldsymbol{\lambda}^{-1}}$$

Overall Field Solution

The field solutions for both the electric and magnetic fields were

$$\begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{bmatrix} = \mathbf{W}e^{-\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{+} + \mathbf{W}e^{\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{-}$$

$$\begin{bmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = -\mathbf{V}e^{-\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{+} + \mathbf{V}e^{\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{-}$$

Combining these into a single matrix equation yields

$$\boldsymbol{\psi}(\tilde{z}) = \begin{bmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \\ \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{bmatrix} = \begin{bmatrix} \mathbf{W} & \mathbf{W} \\ -\mathbf{V} & \mathbf{V} \end{bmatrix} \begin{bmatrix} e^{-\boldsymbol{\lambda}\tilde{z}} & \mathbf{0} \\ \mathbf{0} & e^{\boldsymbol{\lambda}\tilde{z}} \end{bmatrix} \begin{bmatrix} \mathbf{c}^{+} \\ \mathbf{c}^{-} \end{bmatrix} \qquad \text{where } \mathbf{V} = \mathbf{Q}\mathbf{W}\boldsymbol{\lambda}^{-1}$$

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Interpretation of the Solution

$$\boldsymbol{\psi}(\tilde{z}) = \mathbf{W}e^{\boldsymbol{\lambda}\tilde{z}}\mathbf{c}$$

$\boldsymbol{\psi}(z)$ – Overall solution which is the sum of all the modes at plane z'.

c – Column vector containing the amplitude coefficient of each of the modes. This quantities how much energy is in each mode.

W – Square matrix who's column vectors describe the "modes" that can exist in the material. These are essentially pictures of the modes which quantify the relative amplitudes of E_x, E_y, H_x, and H_y.

$e^{\lambda z'}$ – Diagonal matrix describing how the modes propagate. This includes accumulation of phase as well as decaying (loss) or growing (gain) amplitude.

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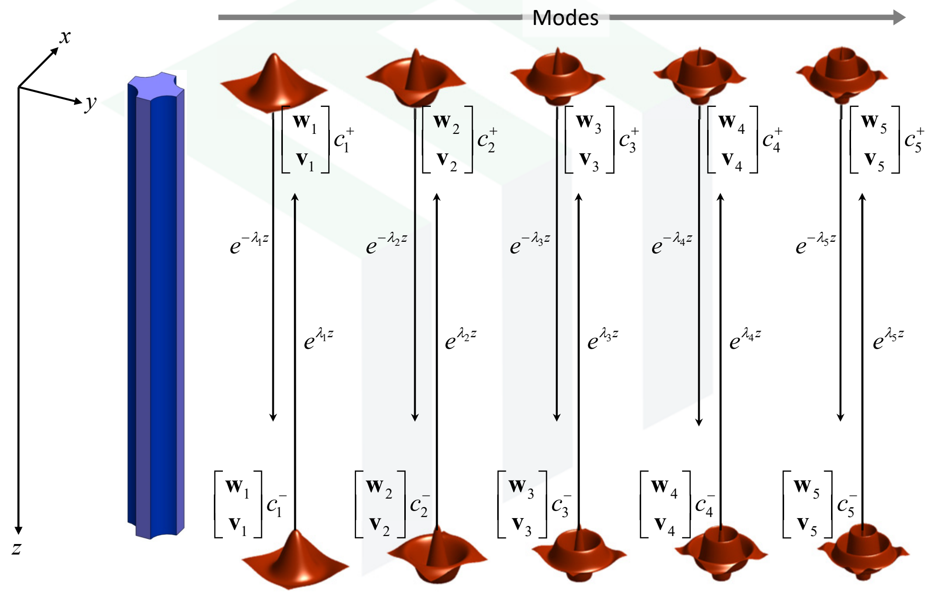
Visualization of this Solution



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Solution in Homogeneous Layers

Recall that in homogeneous layers **P** and **Q** are

$$\mathbf{P} = \varepsilon_r^{-1}\begin{bmatrix}\tilde{\mathbf{K}}_x\tilde{\mathbf{K}}_y & \mu_r\varepsilon_r\mathbf{I}-\tilde{\mathbf{K}}_x^2\\ \tilde{\mathbf{K}}_y^2-\mu_r\varepsilon_r\mathbf{I} & -\tilde{\mathbf{K}}_y\tilde{\mathbf{K}}_x\end{bmatrix} \qquad \mathbf{Q} = \frac{\varepsilon_r}{\mu_r}\mathbf{P}$$

The solution to the eigen-value problem is

$$\mathbf{\Omega}^2 = \mathbf{PQ} \qquad \text{Eigen-Vectors:}\ \ \mathbf{W} = \begin{bmatrix}\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{I}\end{bmatrix}$$

$$\text{Eigen-Values:}\ \ \boldsymbol{\lambda}^2 = \begin{bmatrix}-\tilde{\mathbf{K}}_z^2 & \mathbf{0}\\ \mathbf{0} & -\tilde{\mathbf{K}}_z^2\end{bmatrix} \qquad \boldsymbol{\lambda} = \begin{bmatrix}j\tilde{\mathbf{K}}_z & \mathbf{0}\\ \mathbf{0} & j\tilde{\mathbf{K}}_z\end{bmatrix}$$

$$\tilde{\mathbf{K}}_z = \left(\sqrt{\mu_r^*\varepsilon_r^*\mathbf{I}-\tilde{\mathbf{K}}_x^2-\tilde{\mathbf{K}}_y^2}\right)^*$$

The eigen-modes for the magnetic fields are simply

$$\mathbf{V} = \mathbf{Q}\boldsymbol{\lambda}^{-1}$$

Thus, no need to actually solve the eigen-value problem in homogeneous layers.

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Multilayer Framework: Scattering Matrices

R. C. Rumpf, "Improved formulation of scattering matrices for semi-analytical methods that is consistent with convention," PIERS B, Vol. 35, 241-261, 2011.

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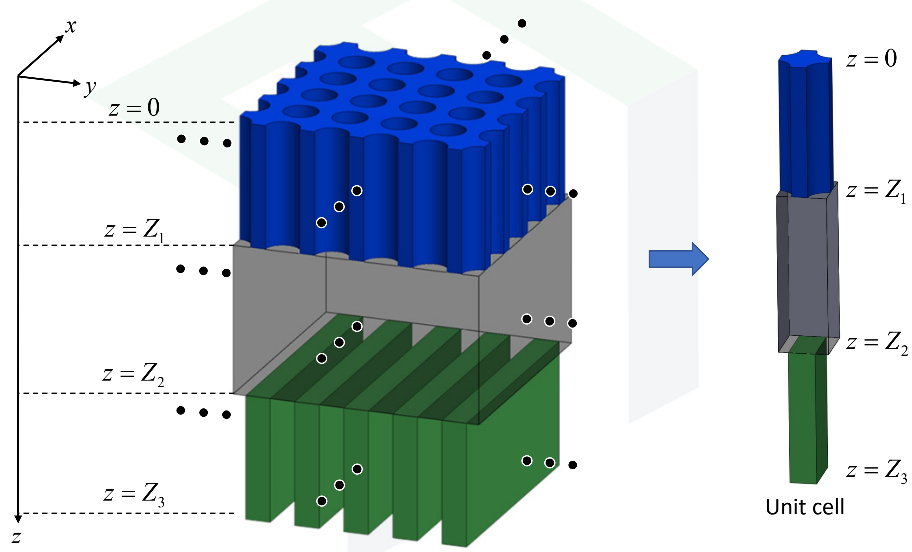
Geometry of a Multilayer Device



Sample of an infinitely periodic lattice

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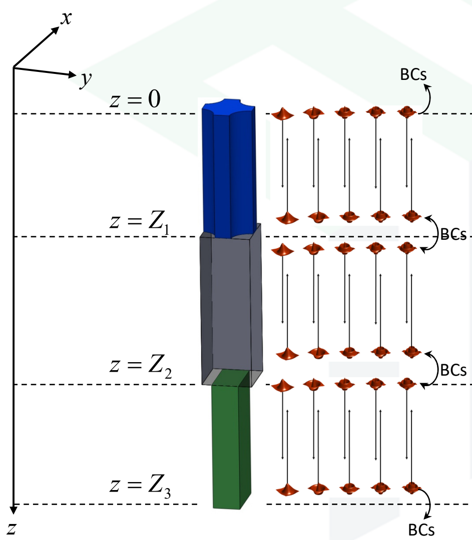
Eigen System in Each Layer

Boundary conditions require that all layers have the same $\mathbf{K}_x$ and $\mathbf{K}_y$ matrices.



$$\mathbf{P}_1=\begin{bmatrix} \tilde{\mathbf{K}}_x [\![\varepsilon_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_y & \boldsymbol{\mu}_{r,1} - \tilde{\mathbf{K}}_x [\![\varepsilon_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\varepsilon_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_y - \boldsymbol{\mu}_{r,1} & -\tilde{\mathbf{K}}_y [\![\varepsilon_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\mathbf{Q}_1=\begin{bmatrix} \tilde{\mathbf{K}}_x [\![\mu_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\varepsilon_{r,1}]\!] - \tilde{\mathbf{K}}_x [\![\mu_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\mu_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\varepsilon_{r,1}]\!] & -\tilde{\mathbf{K}}_y [\![\mu_{r,1}]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\boldsymbol{\Omega}_1^2 = \mathbf{P}_1\mathbf{Q}_1 \;\rightarrow\; \mathbf{W}_1, \boldsymbol{\lambda}_1 \;\rightarrow\; \mathbf{V}_1 \qquad \mathbf{c}_1^+, \mathbf{c}_1^-$$

$$\mathbf{P}_2=\begin{bmatrix} \tilde{\mathbf{K}}_x [\![\varepsilon_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_y & \boldsymbol{\mu}_{r,2} - \tilde{\mathbf{K}}_x [\![\varepsilon_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\varepsilon_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_y - \boldsymbol{\mu}_{r,2} & -\tilde{\mathbf{K}}_y [\![\varepsilon_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\mathbf{Q}_2=\begin{bmatrix} \tilde{\mathbf{K}}_x [\![\mu_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\varepsilon_{r,2}]\!] - \tilde{\mathbf{K}}_x [\![\mu_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\mu_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\varepsilon_{r,2}]\!] & -\tilde{\mathbf{K}}_y [\![\mu_{r,2}]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\boldsymbol{\Omega}_2^2 = \mathbf{P}_2\mathbf{Q}_2 \;\rightarrow\; \mathbf{W}_2, \boldsymbol{\lambda}_2 \;\rightarrow\; \mathbf{V}_2 \qquad \mathbf{c}_2^+, \mathbf{c}_2^-$$

$$\mathbf{P}_3=\begin{bmatrix} \tilde{\mathbf{K}}_x [\![\varepsilon_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\mu_{r,3}]\!] - \tilde{\mathbf{K}}_x [\![\varepsilon_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\varepsilon_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\mu_{r,3}]\!] & -\tilde{\mathbf{K}}_y [\![\varepsilon_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\mathbf{Q}_3=\begin{bmatrix} \tilde{\mathbf{K}}_x [\![\mu_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_y & [\![\varepsilon_{r,3}]\!] - \tilde{\mathbf{K}}_x [\![\mu_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_x \\ \tilde{\mathbf{K}}_y [\![\mu_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_y - [\![\varepsilon_{r,3}]\!] & -\tilde{\mathbf{K}}_y [\![\mu_{r,3}]\!]^{-1} \tilde{\mathbf{K}}_x \end{bmatrix}$$

$$\boldsymbol{\Omega}_3^2 = \mathbf{P}_3\mathbf{Q}_3 \;\rightarrow\; \mathbf{W}_3, \boldsymbol{\lambda}_3 \;\rightarrow\; \mathbf{V}_3 \qquad \mathbf{c}_3^+, \mathbf{c}_3^-$$

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Field Relations & Boundary Conditions

Field inside the i^{th} layer:

$$\boldsymbol{\psi}_i(\tilde{z}) = \begin{bmatrix} \mathbf{s}_{x,i}(\tilde{z}) \\ \mathbf{s}_{y,i}(\tilde{z}) \\ \mathbf{u}_{x,i}(\tilde{z}) \\ \mathbf{u}_{y,i}(\tilde{z}) \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\boldsymbol{\lambda}_i \tilde{z}} & \mathbf{0} \\ \mathbf{0} & e^{\boldsymbol{\lambda}_i \tilde{z}} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Boundary conditions at the first interface:

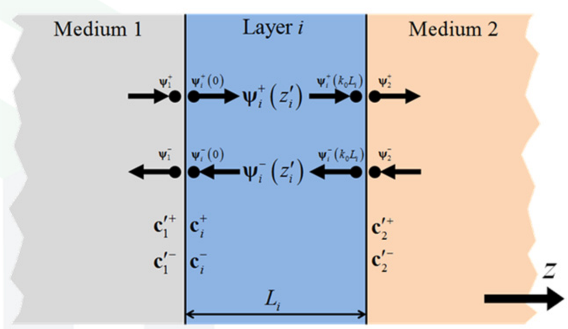
$$\boldsymbol{\psi}_1 = \boldsymbol{\psi}_i(0)$$

$$\begin{bmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ -\mathbf{V}_1 & \mathbf{V}_1 \end{bmatrix} \begin{bmatrix} \mathbf{c}_1'^+ \\ \mathbf{c}_1'^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix}$$

Boundary conditions at the second interface:

$$\boldsymbol{\psi}_i(k_0 L_i) = \boldsymbol{\psi}_2$$

$$\begin{bmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{bmatrix} \begin{bmatrix} e^{-\boldsymbol{\lambda}_i k_0 L_i} & \mathbf{0} \\ \mathbf{0} & e^{\boldsymbol{\lambda}_i k_0 L_i} \end{bmatrix} \begin{bmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{bmatrix} = \begin{bmatrix} \mathbf{W}_2 & \mathbf{W}_2 \\ -\mathbf{V}_2 & \mathbf{V}_2 \end{bmatrix} \begin{bmatrix} \mathbf{c}_2'^+ \\ \mathbf{c}_2'^- \end{bmatrix}$$



Note: k_0 has been incorporated to normalize L_i.

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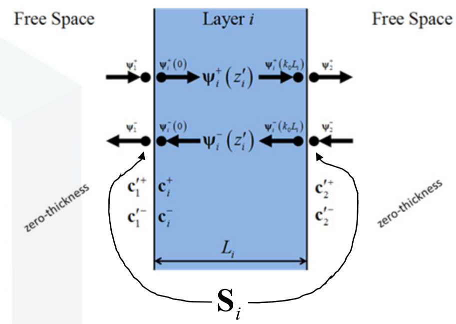
Adopt the Symmetric S-Matrix Approach

The scattering matrix $\mathbf{S}_i$ of the i^{th} layer is still defined as:

$$\begin{bmatrix} \mathbf{c}_1'^- \\ \mathbf{c}_2'^+ \end{bmatrix} = \mathbf{S}^{(i)} \begin{bmatrix} \mathbf{c}_1'^+ \\ \mathbf{c}_2'^- \end{bmatrix} \qquad \mathbf{S}^{(i)} = \begin{bmatrix} \mathbf{S}_{11}^{(i)} & \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{21}^{(i)} & \mathbf{S}_{22}^{(i)} \end{bmatrix}$$



But the elements are calculated as

$$\mathbf{S}_{11}^{(i)} = \left(\mathbf{A}_i - \mathbf{X}_i\mathbf{B}_i\mathbf{A}_i^{-1}\mathbf{X}_i\mathbf{B}_i\right)^{-1}\left(\mathbf{X}_i\mathbf{B}_i\mathbf{A}_i^{-1}\mathbf{X}_i\mathbf{A}_i - \mathbf{B}_i\right)$$

$$\mathbf{S}_{12}^{(i)} = \left(\mathbf{A}_i - \mathbf{X}_i\mathbf{B}_i\mathbf{A}_i^{-1}\mathbf{X}_i\mathbf{B}_i\right)^{-1}\mathbf{X}_i\left(\mathbf{A}_i - \mathbf{B}_i\mathbf{A}_i^{-1}\mathbf{B}_i\right)$$

$$\mathbf{S}_{21}^{(i)} = \mathbf{S}_{12}^{(i)}$$

$$\mathbf{S}_{22}^{(i)} = \mathbf{S}_{11}^{(i)}$$

- Layers are symmetric so the scattering matrix elements have redundancy.
- Scattering matrix equations are simplified.
- Fewer calculations.
- Less memory storage.

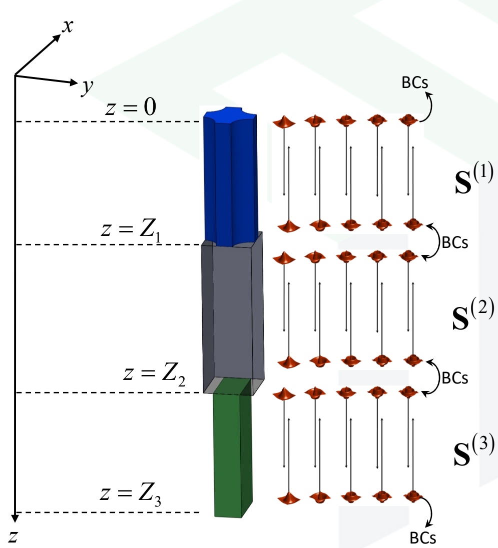
$$\mathbf{A}_i = \mathbf{W}_i^{-1}\mathbf{W}_0 + \mathbf{V}_i^{-1}\mathbf{V}_0$$

$$\mathbf{B}_i = \mathbf{W}_i^{-1}\mathbf{W}_0 - \mathbf{V}_i^{-1}\mathbf{V}_0$$

$$\mathbf{X}_i = e^{-\boldsymbol{\lambda}_i k_0 L_i}$$

```
X = expm(-LAM*k0*L(nlay));
```


Global Scattering Matrix



Scattering matrix for all layers.

$$\mathbf{S}^{(\text{device})} = \mathbf{S}^{(1)} \otimes \mathbf{S}^{(2)} \otimes \mathbf{S}^{(3)}$$

Connection to outside regions

$$\mathbf{S}^{(\text{global})} = \mathbf{S}^{(\text{ref})} \otimes \mathbf{S}^{(\text{device})} \otimes \mathbf{S}^{(\text{trn})}$$

Recall this procedure from Lecture 5.

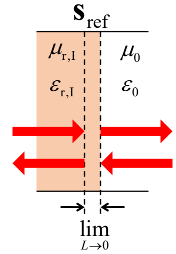
Reflection/Transmission Side Scattering Matrices

The reflection-side scattering matrix is

$$\mathbf{S}_{11}^{(\text{ref})} = -\mathbf{A}_{\text{ref}}^{-1}\mathbf{B}_{\text{ref}}$$
$$\mathbf{S}_{12}^{(\text{ref})} = 2\mathbf{A}_{\text{ref}}^{-1}$$
$$\mathbf{S}_{21}^{(\text{ref})} = 0.5\left(\mathbf{A}_{\text{ref}} - \mathbf{B}_{\text{ref}}\mathbf{A}_{\text{ref}}^{-1}\mathbf{B}_{\text{ref}}\right)$$
$$\mathbf{S}_{22}^{(\text{ref})} = \mathbf{B}_{\text{ref}}\mathbf{A}_{\text{ref}}^{-1}$$

$$\mathbf{A}_{\text{ref}} = \mathbf{W}_0^{-1}\mathbf{W}_{\text{ref}} + \mathbf{V}_0^{-1}\mathbf{V}_{\text{ref}}$$
$$\mathbf{B}_{\text{ref}} = \mathbf{W}_0^{-1}\mathbf{W}_{\text{ref}} - \mathbf{V}_0^{-1}\mathbf{V}_{\text{ref}}$$

```
A = W0\Wref + V0\Vref;
B = W0\Wref - V0\Vref;
SR.S11 = -A\B;
SR.S12 = 2*inv(A);
SR.S21 = 0.5*(A - B/A*B);
SR.S22 = B/A;
```

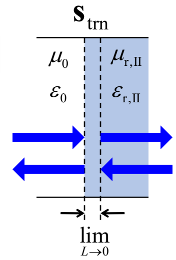


The transmission-side scattering matrix is

$$\mathbf{S}_{11}^{(\text{trn})} = \mathbf{B}_{\text{trn}}\mathbf{A}_{\text{trn}}^{-1}$$
$$\mathbf{S}_{12}^{(\text{trn})} = 0.5\left(\mathbf{A}_{\text{trn}} - \mathbf{B}_{\text{trn}}\mathbf{A}_{\text{trn}}^{-1}\mathbf{B}_{\text{trn}}\right)$$
$$\mathbf{S}_{21}^{(\text{trn})} = 2\mathbf{A}_{\text{trn}}^{-1}$$
$$\mathbf{S}_{22}^{(\text{trn})} = -\mathbf{A}_{\text{trn}}^{-1}\mathbf{B}_{\text{trn}}$$

$$\mathbf{A}_{\text{trn}} = \mathbf{W}_0^{-1}\mathbf{W}_{\text{trn}} + \mathbf{V}_0^{-1}\mathbf{V}_{\text{trn}}$$
$$\mathbf{B}_{\text{trn}} = \mathbf{W}_0^{-1}\mathbf{W}_{\text{trn}} - \mathbf{V}_0^{-1}\mathbf{V}_{\text{trn}}$$

```
A = W0\Wtrn + V0\Vtrn;
B = W0\Wtrn - V0\Vtrn;
ST.S11 = B/A;
ST.S12 = 0.5*(A - B/A*B);
ST.S21 = 2*inv(A);
ST.S22 = -A\B;
```



EMPossible External regions are homogeneous so we do not need to construct convolution matrices.

Calculating Transmission and Reflection

Calculating the Transmitted and Reflected Fields

The electric field source is calculated assuming unit amplitude polarization vector $\vec{P}$.

$$\mathbf{s}_{\mathrm{T}}^{\mathrm{inc}} = \begin{bmatrix} p_x \boldsymbol{\delta}_{0,pq} \\ p_y \boldsymbol{\delta}_{0,pq} \end{bmatrix} \qquad \mathbf{c}_{\mathrm{inc}} = \mathbf{W}_{\mathrm{ref}}^{-1} \mathbf{s}_{\mathrm{T}}^{\mathrm{inc}} \qquad \vec{P} = \begin{bmatrix} p_x \\ p_y \\ p_z \end{bmatrix} \qquad |\vec{P}| = 1$$

Given the global scattering matrix, the coefficients for the reflected and transmitted fields are

$$\text{delta function} \equiv \boldsymbol{\delta}_{0,pq} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \leftarrow p,q \text{ position}$$

$$\mathbf{c}_{\mathrm{ref}} = \mathbf{S}_{11} \mathbf{c}_{\mathrm{inc}} \qquad \mathbf{c}_{\mathrm{trn}} = \mathbf{S}_{21} \mathbf{c}_{\mathrm{inc}}$$

The transverse components of the reflected and transmitted fields are then

$$\mathbf{r}_{\mathrm{T}} = \mathbf{s}_{\mathrm{T}}^{\mathrm{ref}} = \mathbf{W}_{\mathrm{ref}} \mathbf{c}_{\mathrm{ref}} = \mathbf{W}_{\mathrm{ref}} \mathbf{S}_{11} \mathbf{c}_{\mathrm{inc}}$$

$$\mathbf{t}_{\mathrm{T}} = \mathbf{s}_{\mathrm{T}}^{\mathrm{trn}} = \mathbf{W}_{\mathrm{trn}} \mathbf{c}_{\mathrm{trn}} = \mathbf{W}_{\mathrm{trn}} \mathbf{S}_{21} \mathbf{c}_{\mathrm{inc}}$$

$$\mathbf{r}_{\mathrm{T}} = \begin{bmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{bmatrix} \qquad \mathbf{t}_{\mathrm{T}} = \begin{bmatrix} \mathbf{t}_x \\ \mathbf{t}_y \end{bmatrix}$$

These are amplitude coefficients of the transverse components of the spatial harmonics, not reflectance or transmittance.

Calculating the Longitudinal Components

The longitudinal field components are calculated from the transverse components using the divergence equation (see TMM).

$$\mathbf{r}_z = -\tilde{\mathbf{K}}_{z,\mathrm{ref}}^{-1} \left(\tilde{\mathbf{K}}_x \mathbf{r}_x + \tilde{\mathbf{K}}_y \mathbf{r}_y \right)$$

$$\mathbf{t}_z = -\tilde{\mathbf{K}}_{z,\mathrm{trn}}^{-1} \left(\tilde{\mathbf{K}}_x \mathbf{t}_x + \tilde{\mathbf{K}}_y \mathbf{t}_y \right)$$

$$\tilde{\mathbf{K}}_{z,\mathrm{ref}} = -\left(\sqrt{\mu_{\mathrm{r,ref}}^* \varepsilon_{\mathrm{r,ref}}^* \mathbf{I} - \tilde{\mathbf{K}}_x^2 - \tilde{\mathbf{K}}_y^2} \right)^*$$

$$\tilde{\mathbf{K}}_{z,\mathrm{trn}} = \left(\sqrt{\mu_{\mathrm{r,trn}}^* \varepsilon_{\mathrm{r,trn}}^* \mathbf{I} - \tilde{\mathbf{K}}_x^2 - \tilde{\mathbf{K}}_y^2} \right)^*$$

<u>Derivation</u>

$$\nabla \bullet \vec{E} = 0$$

$$\frac{\partial E_x}{\partial x} + \frac{\partial E_y}{\partial y} + \frac{\partial E_z}{\partial z} = 0$$

$$-jk_x(m,n) S_x(m,n) - jk_y(m,n) S_y(m,n) - jk_z(m,n) S_z(m,n) = 0$$

$$k_x(m,n) S_x(m,n) + k_y(m,n) S_y(m,n) + k_z(m,n) S_z(m,n) = 0$$

$$\tilde{\mathbf{K}}_x \mathbf{s}_x + \tilde{\mathbf{K}}_y \mathbf{s}_y + \tilde{\mathbf{K}}_z \mathbf{s}_z = \mathbf{0}$$

$$\tilde{\mathbf{K}}_z \mathbf{s}_z = -\tilde{\mathbf{K}}_x \mathbf{s}_x - \tilde{\mathbf{K}}_y \mathbf{s}_y$$

$$\mathbf{s}_z = -\tilde{\mathbf{K}}_z^{-1} \left(\tilde{\mathbf{K}}_x \mathbf{s}_x + \tilde{\mathbf{K}}_y \mathbf{s}_y \right)$$

Calculating the Diffraction Efficiencies

The diffraction efficiencies $\mathbf{R}$ and $\mathbf{T}$ are calculated as

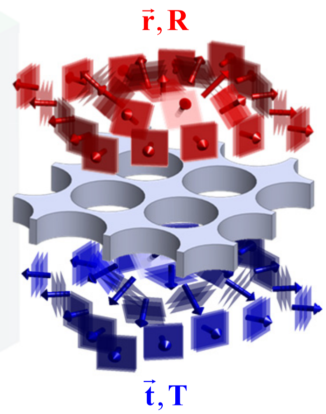
$$\left|\vec{\mathbf{r}}\right|^2 = \left|\mathbf{r}_x\right|^2 + \left|\mathbf{r}_y\right|^2 + \left|\mathbf{r}_z\right|^2$$

$$\left|\vec{\mathbf{t}}\right|^2 = \left|\mathbf{t}_x\right|^2 + \left|\mathbf{t}_y\right|^2 + \left|\mathbf{t}_z\right|^2$$

$$\mathbf{R} = \frac{\mathrm{Re}\left[-\tilde{\mathbf{K}}_{z,\mathrm{ref}} / \mu_{\mathrm{r,ref}}\right]}{\mathrm{Re}\left[k_z^{\mathrm{inc}} / \mu_{\mathrm{r,ref}}\right]}\left|\vec{\mathbf{r}}\right|^2$$

$$\mathbf{T} = \frac{\mathrm{Re}\left[\tilde{\mathbf{K}}_{z,\mathrm{trn}} / \mu_{\mathrm{r,trn}}\right]}{\mathrm{Re}\left[k_z^{\mathrm{inc}} / \mu_{\mathrm{r,inc}}\right]}\left|\vec{\mathbf{t}}\right|^2$$

Remember that these equations assume a unit amplitude source.



Don't forget to reshape $\mathbf{R}$ and $\mathbf{T}$ back to 2D arrays!

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Calculating Overall Reflectance and Transmittance

The overall reflectance R and transmittance T are calculated by summing all of the diffraction efficiencies.

$$R = \sum \mathbf{R}$$

$$T = \sum \mathbf{T}$$

Reflectance and Transmittance on a Decibel Scale

$$R_{\mathrm{dB}} = 10\log_{10} R \qquad T_{\mathrm{dB}} = 10\log_{10} T$$

Be careful NOT to use 20log10!

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Power Conservation

It is always good practice to check for conservation of power.

$$A + R + T = 1$$

When no loss or gain is incorporated into the simulation (i.e. $A = 0$), conservation reduces to

$$R + T = 1 \qquad \text{no loss or gain}$$