Rigorous Coupled-Wave Analysis

A numerical Fourier-space modal method for layered periodic structures

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Special syllabus, June 18, 2018

Outline

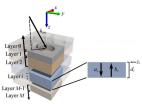
- Background
 - Introduction
 - Preparing Maxwell's equations for CEM
- Formulation of RCWA
 - Semi-analytical form of Maxwell's equations in Fourier space
 - Matrix form of Maxwell's equations
 - Matrix wave equation
 - Solution to the matrix wave equation
- Multilayer framework: Scattering matrices
 - Intro to multilayer framework for RCWA
 - S-matrices for semi-analytical methods
 - Multilayer device
- Calculating reflected and transmitted power
 - Reflected and transmitted fields
 - Reflectance and transmittance

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Layered photonic media Computational electromagnetism (CEM)

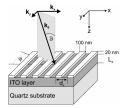
- There are several general-purpose tools available for computational electromagnetism (CEM) that can be adapted to simulate 3D structures with 2D periodicity.
- Rigorous Coupled-Wave Analysis is a CEM method that is specifically designed to model layered structures with in-plane periodicity.



Layered structure which is periodic in the xy-plane, and piecewise constant in the z-direction.

Rigorous Coupled-Wave Analysis (RCWA)

- Developed in early 1980's by Moharam and Gaylord¹
- Alternate names:
 - Fourier modal method
 - · Rigorous coupled-wave analysis
 - Transfer matrix method with a plane wave basis
 - Scattering matrix method
- What can it compute?
 - Transmission/reflection/absorption-spectra of structures composed of periodic, patterned, planar layers.
 - Electromagnetic fields throughout the structure may also be obtained.
 - Energy density within a layer, stress tensor...



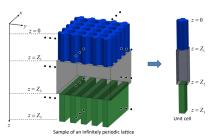
Published example of a metal grating transmission spectrum using RCWA

Christ, A., Zentgraf, T. and Kuhl, J., "Optical properties of planar metallic photonic crystal structures:Experiment and theory", Phys. Rev. B, 70, 125113 (2004).

¹M. G. Moharam and T. K. Gaylord, "Rigorous coupled-wave analysis of planar-grating diffraction," J. Opt. Soc. Am. 71. 811-818 (1981).

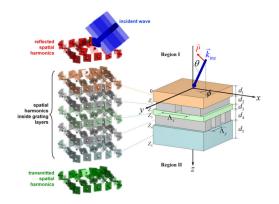
RCWA basic idea (1/2)

- RCWA is particularly suitable for structures composed of layers invariant in the direction normal to the periodicity, due to its Fourier basis representation.
- In order to solve EM-fields throughout a 3D structure, a typical RCWA-code applies the method to compute modal expansions within layers, then joins together the layers by combining it with a scattering matrix (S-matrix) algorithm.²



 $^{^2}$ For example, the S^4 code uses S-matrix formalism https://web.stanford.edu/group/fam/S4/+ Ξ + - Ξ \sim \circ

RCWA basic idea (2/2)



- RCWA is a semi-analytical method.
- Field in each layer is represented as a set of plane waves at different angles (Fourier space).
- Plane waves describe propagation through each layer.
- Fields are computed in the transverse plane for each layer and propagated analytically in the z-direction.
- Layers are connected by boundary conditions (using S-matrices).
- Transmission through entire stack of layers is then known and transmitted/reflected fields can be computed.

Benefits and drawbacks

BENEFITS

- Excellent for modeling diffraction from periodic dielectric structures.
- Very fast and efficient for all-dielectric structures with low-moderate index contrast
- Layer thickness does not affect numerical cost, because you only look at the xy-plane cross-section of each layer
- Easily incorporates polarization and angle of incidence.
- Accurate and robust

DRAWBACKS

- Very slow convergence of the Fourier series representation due to Gibbs phenomenon for discontinuous functions. In particular problematic for metals (high contrast dielectric function).
- Scales poorly in transverse dimensions.
- Layers must have the same periodic length (there exists workarounds)

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Simplifying Maxwell's equations

 $\textbf{ 4 Ssume no charges or current sources: } \rho = 0, \vec{J} = 0 \text{: } ^3$

$$\begin{split} \nabla \cdot \vec{B} &= 0 & \nabla \times \vec{H} = \partial \vec{D} / \partial t & \vec{D}(t) = [\varepsilon(t)] * \vec{E}(t) \\ \nabla \cdot \vec{D} &= 0 & \nabla \times \vec{E} = -\partial \vec{B} / \partial t & \vec{B}(t) = [\mu(t)] * \vec{H}(t) \end{split}$$

Transform Maxwell's equations to frequency domain:

Substitute constitutive relations into Maxwell's equations:

$$\nabla \cdot ([\mu] \vec{H}) = 0 \qquad \nabla \times \vec{H} = j\omega[\varepsilon] \vec{E}$$

$$\nabla \cdot ([\varepsilon] \vec{E}) = 0 \qquad \nabla \times \vec{E} = -j\omega[\mu] \vec{H}$$



^{3*} means convolution. [] means tensor.

Isotropic materials

Will assume isotropic materials, so that the permittivity and permeability tensors reduce to a single quantity:

$$[\varepsilon] = \begin{pmatrix} \varepsilon & 0 & 0 \\ 0 & \varepsilon & 0 \\ 0 & 0 & \varepsilon \end{pmatrix} = \varepsilon \qquad \qquad [\mu] = \begin{pmatrix} \mu & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \mu \end{pmatrix} = \mu$$

Maxwell's equations can then be written as

$$\nabla \cdot (\mu_r \vec{H}) = 0 \qquad \nabla \times \vec{H} = j\omega \varepsilon_0 \varepsilon_r \vec{E}$$

$$\nabla \cdot (\varepsilon_r \vec{E}) = 0 \qquad \nabla \times \vec{E} = -j\omega \mu_0 \mu_r \vec{H}$$

Normalize the magnetic field

• Standard form of Maxwell's curl equations:

$$\nabla \times \vec{E} = -j\omega \mu_0 \mu_r \vec{H}$$

$$\nabla \times \vec{H} = j\omega \varepsilon_0 \varepsilon_r \vec{E}$$

Normalized magnetic field:

$$\frac{\vec{E}}{\vec{H}} \approx \frac{377}{n}$$

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

Note:
$$k_0 = \omega \sqrt{\mu_0 \varepsilon_0}$$

Normalized Maxwell's equations:

$$\nabla \times \vec{E} = k_0 \mu_r \vec{\tilde{H}}$$

$$\nabla \times \vec{\tilde{H}} = k_0 \varepsilon_r \vec{E}$$

Starting point for most CEM methods

We arrive at the following set of equations

$$\begin{split} \frac{\partial E_z}{\partial y} &- \frac{\partial E_y}{\partial z} = k_0 \mu_r \tilde{H}_x \\ \frac{\partial E_x}{\partial z} &- \frac{\partial E_z}{\partial x} = k_0 \mu_r \tilde{H}_y \\ \frac{\partial E_y}{\partial x} &- \frac{\partial E_x}{\partial y} = k_0 \mu_r \tilde{H}_z \end{split}$$

$$\begin{split} \frac{\partial \tilde{H}_z}{\partial y} &- \frac{\partial \tilde{H}_y}{\partial z} = k_0 \varepsilon_r E_x \\ \frac{\partial \tilde{H}_x}{\partial z} &- \frac{\partial \tilde{H}_z}{\partial x} = k_0 \varepsilon_r E_y \\ \frac{\partial \tilde{H}_y}{\partial x} &- \frac{\partial \tilde{H}_x}{\partial y} = k_0 \varepsilon_r E_z \end{split}$$

Magnetic field normalized according to

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

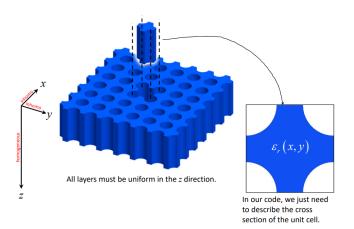
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Matrix wave equation

Solution to the matrix wave equation

The 2D unit cell



Fourier expansion of Maxwell's equations

Start with Maxwell's equations in the form

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

$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0 \varepsilon_r E_x$$

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0 \mu_r \tilde{H}_y$$

$$\frac{\partial \tilde{H}_x}{\partial z} - \frac{\partial \tilde{H}_z}{\partial x} = k_0 \varepsilon_r E_y$$

$$\frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} = k_0 \mu_r \tilde{H}_z$$

$$\frac{\partial \tilde{H}_y}{\partial x} - \frac{\partial \tilde{H}_z}{\partial y} = k_0 \varepsilon_r E_z$$

Magnetic field normalized according to

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

Fourier expansion of the materials

Assuming the device is infinitely periodic in the (x,y)-plane, the permittivity and permeability functions can be expanded into Fourier series

$$\varepsilon_r(x,y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} a_{m,n} e^{j \left(\frac{2\pi mx}{\Lambda_x} + \frac{2\pi my}{\Lambda_y} \right)}$$

$$a_{m,n} = \frac{1}{\Lambda_x \Lambda_y} \int_{-\Lambda_x/2}^{\Lambda_x/2} \int_{-\Lambda_y/2}^{\Lambda_y/2} \varepsilon_r(x,y) e^{-j\left(\frac{2\pi mx}{\Lambda_x} + \frac{2\pi my}{\Lambda_y}\right)} dxdy$$

$$\mu_r(x,y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,n} e^{j\left(\frac{2\pi mx}{\Lambda x} + \frac{2\pi my}{\Lambda y}\right)}$$

$$b_{m,n} = \frac{1}{\Lambda_x \Lambda_y} \int_{-\Lambda_x/2}^{\Lambda_x/2} \int_{-\Lambda_y/2}^{\Lambda_y/2} \mu_r(x,y) e^{-j\left(\frac{2\pi mx}{\Lambda_x} + \frac{2\pi my}{\Lambda_y}\right)} dxdy$$

Fourier expansion of the fields

Field expansions are slightly different because a wave could travel in any direction $\vec{\beta} = < k_{x,\mathrm{inc}}, k_{y,\mathrm{inc}}, 0 >$ along the (x,y)-plane. The expansions must satisfy Floquet periodic boundary conditions.

$$\begin{split} E_x(x,y,z) &= e^{-j\vec{\beta}\cdot\vec{r}} \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_x(m,n;z) e^{j\left(\frac{2\pi mx}{\Lambda_x} + \frac{2\pi ny}{\Lambda_y}\right)} \\ &= \sum_m \sum_n S_x(m,n;z) e^{-j\left(\vec{\beta} - \frac{2\pi mx}{\Lambda_x} - \frac{2\pi ny}{\Lambda_y}\right)\cdot\vec{r}} \\ &= \sum_m \sum_n S_x(m,n;z) e^{-j\vec{k}(m,n)\cdot\vec{r}} \\ &= \sum_m \sum_n S_x(m,n;z) e^{-j\left[k_x(m)x + k_y(n)y\right]} \end{split}$$

with transverse wave vector components

$$k_x(m) = k_{x, {
m inc}} - rac{2\pi m}{\Lambda_x}$$
 $k_y(n) = k_{y, {
m inc}} - rac{2\pi n}{\Lambda}$



Fourier expansions of the fields

Doing the same for the remaining fields we get

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

$$E_{y}(x, y, z) = \sum_{m = -\infty}^{\infty} \sum_{m = -\infty}^{\infty} S_{y}(m, n; z) e^{-j[k_{x}(m)x + k_{y}(n)y]}$$

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

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

$$\tilde{H}_{y}(x, y, z) = \sum_{m=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} U_{y}(m, n; z) e^{-j[k_{x}(m)x + k_{y}(n)y]}$$

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

Substitute expansions into Maxwell's equations

$$E_{z}(x,y,z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_{z}(m,n;z) \cdot e^{-\int \left[k_{z}(m)x+k_{y}(n)y\right]} \qquad \mu_{r}(x,y) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,n} e^{\left(\frac{2\pi mx_{z}}{A_{z}}, \frac{2\pi ny}{A_{y}}\right)}$$

$$E_{y}(x,y,z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_{y}(m,n;z) \cdot e^{-\int \left[k_{z}(m)x+k_{y}(n)y\right]}$$

$$\tilde{H}_{x}(x,y,z) = \sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_{x}(m,n;z) \cdot e^{-\int \left[k_{z}(m)x+k_{y}(n)y\right]}$$

$$\frac{\partial E_{z}}{\partial y} - \frac{\partial E_{y}}{\partial z} = k_{0} \mu_{r} \tilde{H}_{x}$$

$$\frac{\partial}{\partial y} \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_z\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] - \frac{\partial}{\partial z} \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_y\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] = k_0 \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,v} e^{\left(\frac{j\pi m}{\lambda_z},\frac{j\pi m}{\lambda_y}\right)} \right] \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_x\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] - \frac{\partial}{\partial z} \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_y\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] = k_0 \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,v} e^{\left(\frac{j\pi m}{\lambda_z},\frac{j\pi m}{\lambda_y}\right)} \right] \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_x\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] - \frac{\partial}{\partial z} \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} S_y\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] = k_0 \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} b_{m,v} e^{\left(\frac{j\pi m}{\lambda_z},\frac{j\pi m}{\lambda_y}\right)} \right] \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} U_x\left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] - \frac{\partial}{\partial z} \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \left(m,n;z\right) \cdot e^{-j\left[k_z(n)z+k_z(n)z\right]} \right] \left[\sum_{m=-\infty}^{\infty} \sum_{n=-\infty}^{\infty} \sum_{n=-\infty}^{$$

$$\sum_{m=-\infty}^{\infty}\sum_{k=-m}^{\infty}-jk_{\gamma}\left(m\right)S_{z}\left(m,n;z\right)\cdot e^{-j\left[k_{z}\left(m\right)+k_{z}\left(z\right)\right]}-\left[\sum_{m=-\infty}^{\infty}\sum_{k=-m}^{\infty}\frac{\partial S_{\gamma}\left(m,n;z\right)}{\partial z}\cdot e^{-j\left[k_{z}\left(m\right)+k_{z}\left(z\right)\right]}\right]\\ =k_{0}\sum_{m=-\infty}^{\infty}\sum_{m=-m}^{\infty}\int_{-\infty}^{\infty}\sum_{r=-m}^{\infty}b_{m-q,n-r}e^{-j\left[k_{z}\left(m-z\right)+\frac{2z(n-r)p}{\lambda_{z}}\right]}U_{z}\left(q,r;z\right)e^{-j\left[k_{z}\left(m\right)+k_{z}\left(z\right)\right]}$$

$$\sum_{m=-\infty}^{\infty}\sum_{m=-\infty}^{\infty}\left\{-jk_{y}\left(m\right)S_{z}\left(m,n;z\right)\cdot e^{-j\left[k_{z}\left(m\right)z+k_{z}\left(n\right)r\right]}-\frac{\partial S_{y}\left(m,n;z\right)}{\partial z}e^{-j\left[k_{z}\left(m\right)z+k_{z}\left(n\right)r\right]}\right]=k_{0}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,x-r}e^{-j\left[\frac{2\pi\left(m-q\right)z}{\Lambda_{z}}+\frac{2\pi\left(m-r\right)r}{\Lambda_{y}}\right]}U_{x}\left(q,r;z\right)e^{-j\left[k_{z}\left(q\right)z+k_{z}\left(r\right)r\right]}$$

$$-jk_{_{y}}(m)S_{z}(m,n;z) - \frac{dS_{_{y}}(m,n;z)}{dz} = k_{_{0}}\sum_{g=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{g=-g,r-r}U_{x}(q,r;z)$$
The derivative is ordinary because z is the only in the constant possible left.

independent variable left.



Semi-analytical form of Maxwell's equations in Fourier space

Doing this for all of Maxwell's equations, we get

Real space

$$\frac{\partial \tilde{H}_{z}}{\partial y} - \frac{\partial \tilde{H}_{y}}{\partial z} = k_{0} \varepsilon_{r} E_{x}$$

$$\frac{\partial \tilde{H}_{x}}{\partial z} - \frac{\partial \tilde{H}_{z}}{\partial x} = k_{0} \varepsilon_{r} E_{y}$$

$$\frac{\partial \tilde{H}_{y}}{\partial x} - \frac{\partial \tilde{H}_{x}}{\partial y} = k_{0} \varepsilon_{r} E_{z}$$

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

$$\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} = k_0 \mu_r \tilde{H}_y$$

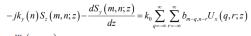
$$\frac{\partial E_{y}}{\partial x} - \frac{\partial E_{x}}{\partial y} = k_{0} \mu_{r} \tilde{H}_{z}$$

Fourier space

$$-jk_{y}(n)U_{z}(m,n;z) - \frac{dU_{y}(m,n;z)}{dz} = k_{0} \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} a_{m-q,n-r}S_{x}(q,r;z)$$

$$\frac{dU_{x}\left(m,n;z\right)}{dz}+jk_{x}\left(m\right)U_{z}\left(m,n;z\right)=k_{0}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a_{m-q,n-r}S_{y}\left(q,r;z\right)$$

$$-jk_{x}\left(m\right)U_{y}\left(m,n;z\right)+jk_{y}\left(n\right)U_{x}\left(m,n;z\right)=k_{0}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}a_{m-q,n-r}S_{z}\left(q,r;z\right)$$



$$\frac{dS_x(m,n;z)}{dz} + jk_x(m)S_z(m,n;z) = k_0 \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} b_{m-q,n-r}U_y(q,r;z)$$

$$-jk_{x}(m)S_{y}(m,n;z) + jk_{y}(n)S_{x}(m,n;z) = k_{0}\sum_{q=-\infty}^{\infty}\sum_{r=-\infty}^{\infty}b_{m-q,n-r}U_{z}(q,r;z)$$

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

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Normalize the Fourier-space equations

Define normalized wave vectors and z-coordinate:

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

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

$$j\tilde{k}_x(m)U_z(m,n;\bar{z}) + \frac{dU_x(m,n;\bar{z})}{d\bar{z}} = \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} a_{m-q,n-r}S_y(q,r;\bar{z})$$

$$-j\tilde{k}_x(m)U_y(m,n;\bar{z}) + j\tilde{k}_y(n)U_x(m,n;\bar{z}) = \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} a_{m-q,n-r}S_z(q,r;\bar{z})$$

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

Matrix form of Maxwell's equations (1/2)

Starting with the first equation...

$$-j\tilde{k}_{y}(n)U_{z}(m,n;\tilde{z}) - \frac{dU_{y}(m,n;\tilde{z})}{d\tilde{z}} = \sum_{q=-M/2}^{M/2} \sum_{r=-N/2}^{N/2} a_{m-q,n-r}S_{x}(q,r;\tilde{z})$$

This equation is written once for each spatial harmonic. (total spatial harmonics $= M \cdot N$)

This large set of equations are in matrix form as

$$-j\tilde{\mathbf{K}}_y\mathbf{u}_z - \frac{d}{d\tilde{z}}\mathbf{u}_y = \llbracket \varepsilon_r \rrbracket \, \mathbf{s}_x$$

where

$$\mathbf{u}_z = \begin{pmatrix} U_z(1,1) \\ U_z(1,2) \\ \vdots \\ U_z(M,N) \end{pmatrix} \mathbf{u}_y = \begin{pmatrix} U_y(1,1) \\ U_y(1,2) \\ \vdots \\ U_y(M,N) \end{pmatrix} \mathbf{s}_z = \begin{pmatrix} S_x(1,1) \\ S_x(1,2) \\ \vdots \\ S_x(M,N) \end{pmatrix} \mathbf{K}_y = \begin{pmatrix} \tilde{k}_y(1,1) & \mathbf{0} \\ & \tilde{k}_y(1,2) \\ & & \ddots \\ \mathbf{0} & & \tilde{k}_y(M,N) \end{pmatrix}$$

$$\llbracket arepsilon_r
rbracket = \left(egin{array}{c} \operatorname{Convolution matrix}
ight. \end{array}
ight)$$

Matrix form of Maxwell's equations (2/2)

Analytical equations

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

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

Numerical equations

$$-j\tilde{\mathbf{K}}_{y}\mathbf{u}_{z} - \frac{d}{d\tilde{z}}\mathbf{u}_{y} = [\![\varepsilon_{r}]\!]\mathbf{s}_{x}$$
$$j\tilde{\mathbf{K}}_{x}\mathbf{u}_{z} + \frac{d}{d\tilde{z}}\mathbf{u}_{x} = [\![\varepsilon_{r}]\!]\mathbf{s}_{y}$$
$$\tilde{\mathbf{K}}_{x}\mathbf{u}_{y} - \tilde{\mathbf{K}}_{y}\mathbf{u}_{x} = j[\![\varepsilon_{r}]\!]\mathbf{s}_{z}$$

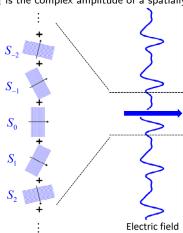
$$-j\tilde{\mathbf{K}}_{y}\mathbf{s}_{z} - \frac{d}{d\tilde{z}}\mathbf{s}_{y} = \llbracket \mu_{r} \rrbracket \mathbf{u}_{x}$$
$$j\tilde{\mathbf{K}}_{x}\mathbf{s}_{z} + \frac{d}{d\tilde{z}}\mathbf{s}_{x} = \llbracket \mu_{r} \rrbracket \mathbf{u}_{y}$$
$$\tilde{\mathbf{K}}_{x}\mathbf{s}_{y} - \tilde{\mathbf{K}}_{y}\mathbf{s}_{x} = j \llbracket \mu_{r} \rrbracket \mathbf{u}_{z}$$

Extra: Interpreting the column vectors

Each element of the column vector \mathbf{s}_i is the complex amplitude of a spatially harmonic

$$\mathbf{s}_{i} = \begin{bmatrix} \vdots \\ S_{-2} \\ S_{-1} \\ S_{0} \\ S_{1} \\ S_{2} \\ \vdots \end{bmatrix}$$

Column vector



Spatial harmonics

Extra: Constructing the convolution matrices

Alternate derivation of ME in Fourier space

Start with
$$\frac{\partial \tilde{H}_z}{\partial y} - \frac{\partial \tilde{H}_y}{\partial z} = k_0 \varepsilon_r E_x$$
.

Fourier transform this equation in x and y, resulting in

$$-jk_y(n)U_z(m,n;z) - \frac{dU_y(m,n;z)}{dz} = k_0a * S_x$$

I.e. we realize that the double summation in the r.h.s. of the analytical Maxwell's equations in Fourier space is actually a 2D convolution in Fourier space,

$$a * S_x \to \sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} a_{m-q,n-r} S_x(q,r;z)$$

$$a = \mathsf{FT}\{\varepsilon_r\} \qquad S_x = \mathsf{FT}\{E_x\}$$

Extra: Constructing the convolution matrices

The convolution matrix

There are two matrices that must be constructed that perform a 2D convolution in Fourier space: $\llbracket \varepsilon_r \rrbracket$ and $\llbracket \mu_r \rrbracket$.

These are constructed by placing the Fourier coefficients in the proper order in each row in the matrix.

$$a_{m,n} = \frac{1}{\Lambda_x \Lambda_y} \int\limits_{-\Lambda_x/2}^{\Lambda_x/2} \int\limits_{-\Lambda_y/2}^{\Lambda_y/2} \varepsilon_r(x,y) e^{-j\left(\frac{2\pi mx}{\Lambda_x} + \frac{2\pi my}{\Lambda_y}\right)} dx dy$$

This can be calculated using a 2D Fast Fourier Transform.

$$\llbracket arepsilon_r
rbracket = \left(egin{array}{c} {}_{
m row\,m,n} & {}_{
m column\,q,r} \end{array}
ight)$$

$$\sum_{q=-\infty}^{\infty} \sum_{r=-\infty}^{\infty} a_{m-q,n-r} S_x(q,r;\tilde{z})$$

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Solve for longitudinal field components

Goal: eliminate longitudinal field components thus reducing number of equations from six to four; re-write the resulting matrix equations in block matrix form; finally derive a wave equation.

Start by solving for the longitudinal field components \mathbf{s}_z and \mathbf{u}_z from the 3rd and 6th equation...

$$-j\tilde{\mathbf{K}}_{y}\mathbf{u}_{z} - \frac{d}{d\tilde{z}}\mathbf{u}_{y} = \llbracket \varepsilon_{r} \rrbracket \mathbf{s}_{x}$$

$$j\tilde{\mathbf{K}}_{x}\mathbf{u}_{z} + \frac{d}{d\tilde{z}}\mathbf{u}_{x} = \llbracket \varepsilon_{r} \rrbracket \mathbf{s}_{y}$$

$$\tilde{\mathbf{K}}_{x}\mathbf{u}_{y} - \tilde{\mathbf{K}}_{y}\mathbf{u}_{x} = j \llbracket \varepsilon_{r} \rrbracket \mathbf{s}_{z}$$

$$-j\tilde{\mathbf{K}}_{y}\mathbf{s}_{z} - \frac{d}{d\tilde{z}}\mathbf{s}_{y} = \llbracket \mu_{r} \rrbracket \mathbf{u}_{x}$$

$$j\tilde{\mathbf{K}}_{x}\mathbf{s}_{z} + \frac{d}{d\tilde{z}}\mathbf{s}_{x} = \llbracket \mu_{r} \rrbracket \mathbf{u}_{y}$$

$$\tilde{\mathbf{K}}_{x}\mathbf{s}_{y} - \tilde{\mathbf{K}}_{y}\mathbf{s}_{x} = j \llbracket \mu_{r} \rrbracket \mathbf{u}_{x}$$

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

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

Then substitute \mathbf{s}_z and \mathbf{u}_z back into the remaining four equations



Eliminate the longitudinal field components

Substituting \mathbf{s}_z and \mathbf{u}_z back into the remaining equations we get

$$-\tilde{\mathbf{K}}_{y} \llbracket \mu_{r} \rrbracket^{-1} (\tilde{\mathbf{K}}_{x} \mathbf{s}_{y} - \tilde{\mathbf{K}}_{y} \mathbf{s}_{x}) - \frac{d}{d\tilde{z}} \mathbf{u}_{y} = \llbracket \varepsilon_{r} \rrbracket \mathbf{s}_{x}$$

$$\tilde{\mathbf{K}}_{x} \left[\!\left[\mu_{r}\right]\!\right]^{-1} \left(\tilde{\mathbf{K}}_{x} \mathbf{s}_{y} - \tilde{\mathbf{K}}_{y} \mathbf{s}_{x}\right) + \frac{d}{d\tilde{z}} \mathbf{u}_{x} = \left[\!\left[\varepsilon_{r}\right]\!\right] \mathbf{s}_{y}$$

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

$$\tilde{\mathbf{K}}_{x} \left[\varepsilon_{r} \right]^{-1} \left(\tilde{\mathbf{K}}_{x} \mathbf{u}_{y} - \tilde{\mathbf{K}}_{y} \mathbf{u}_{x} \right) + \frac{d}{d\tilde{z}} \mathbf{s}_{x} = \left[\mu_{r} \right] \mathbf{u}_{y}$$

Re-arrange the terms

Now expand the equations and re-arrange

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

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

$$\begin{split} &\frac{d}{d\tilde{z}}\mathbf{u}_{y} = (\tilde{\mathbf{K}}_{y} \, \llbracket \mu_{r} \rrbracket^{-1} \, \tilde{\mathbf{K}}_{y} - \llbracket \varepsilon_{r} \rrbracket) \mathbf{s}_{x} - \tilde{\mathbf{K}}_{y} \, \llbracket \mu_{r} \rrbracket^{-1} \, \tilde{\mathbf{K}}_{x} \mathbf{s}_{y} \\ &\frac{d}{d\tilde{z}} \mathbf{u}_{x} = \tilde{\mathbf{K}}_{x} \, \llbracket \mu_{r} \rrbracket^{-1} \, \tilde{\mathbf{K}}_{y} \mathbf{s}_{x} + (\llbracket \varepsilon_{r} \rrbracket - \tilde{\mathbf{K}}_{x} \, \llbracket \mu_{r} \rrbracket^{-1} \, \tilde{\mathbf{K}}_{x}) \mathbf{s}_{y} \end{split}$$

$$\begin{split} &\frac{d}{d\tilde{z}}\mathbf{s}_{y} = (\tilde{\mathbf{K}}_{y} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{y} - \left[\!\left[\boldsymbol{\mu}_{r}\right]\!\right] \mathbf{u}_{x} - \tilde{\mathbf{K}}_{y} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{x} \mathbf{u}_{y} \\ &\frac{d}{d\tilde{z}}\mathbf{s}_{x} = \tilde{\mathbf{K}}_{x} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{y} \mathbf{u}_{x} + (\left[\!\left[\boldsymbol{\mu}_{r}\right]\!\right] - \tilde{\mathbf{K}}_{x} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{x}) \mathbf{u}_{y} \end{split}$$

Block matrix form

These matrix equations can be written in block matrix form as

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

$$\begin{split} &\frac{d}{d\tilde{z}}\mathbf{s}_{x} = \tilde{\mathbf{K}}_{x} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{y} \mathbf{u}_{x} + (\left[\!\left[\boldsymbol{\mu}_{r}\right]\!\right] - \tilde{\mathbf{K}}_{x} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{x}) \mathbf{u}_{y} \xrightarrow{} \\ &\frac{d}{d\tilde{z}}\mathbf{s}_{y} = (\tilde{\mathbf{K}}_{y} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{y} - \left[\!\left[\boldsymbol{\mu}_{r}\right]\!\right]) \mathbf{u}_{x} - \tilde{\mathbf{K}}_{y} \left[\!\left[\boldsymbol{\varepsilon}_{r}\right]\!\right]^{-1} \tilde{\mathbf{K}}_{x} \mathbf{u}_{y} \end{split}$$

$$\frac{d}{d\bar{z}} \begin{pmatrix} \mathbf{u}_x \\ \mathbf{u}_y \end{pmatrix} = \mathbf{Q} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix}$$

$$\mathbf{Q} = \begin{pmatrix} \tilde{\mathbf{K}}_x \llbracket \mu_r \rrbracket^{-1} \tilde{\mathbf{K}}_y & \llbracket \varepsilon_r \rrbracket - \tilde{\mathbf{K}}_x \llbracket \mu_r \rrbracket^{-1} \tilde{\mathbf{K}}_x \end{pmatrix}$$

$$\mathbf{Q} = \begin{pmatrix} \tilde{\mathbf{K}}_x \left[\!\left[\boldsymbol{\mu}_r\right]\!\right]^{-1} \tilde{\mathbf{K}}_y & \left[\!\left[\boldsymbol{\varepsilon}_r\right]\!\right] - \tilde{\mathbf{K}}_x \left[\!\left[\boldsymbol{\mu}_r\right]\!\right]^{-1} \tilde{\mathbf{K}}_x \\ -\tilde{\mathbf{K}}_y \left[\!\left[\boldsymbol{\mu}_r\right]\!\right]^{-1} \tilde{\mathbf{K}}_x - \left[\!\left[\boldsymbol{\varepsilon}_r\right]\!\right] & -\tilde{\mathbf{K}}_y \left[\!\left[\boldsymbol{\mu}_r\right]\!\right]^{-1} \tilde{\mathbf{K}}_x \end{pmatrix}$$

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

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

Matrix wave equation

$$\frac{d}{d\tilde{z}}\begin{pmatrix} \mathbf{u}_x \\ \mathbf{u}_y \end{pmatrix} = \mathbf{Q}\begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} \tag{1a}$$

First differentiate eq (1b) w.r.t. z:

$$\frac{d^2}{d\tilde{z}^2} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} = \mathbf{P} \frac{d}{d\tilde{z}} \begin{pmatrix} \mathbf{u}_x \\ \mathbf{u}_y \end{pmatrix}$$
 (2)

Then substitute eq (1a) into eq (2) to eliminate the magnetic fields:

$$\frac{d^2}{d\tilde{z}^2} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} = \mathbf{PQ} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} \tag{3}$$

Finally, the matrix wave equation is

$$rac{d^2}{d ilde{z}^2}inom{\mathbf{s}_x}{\mathbf{s}_y}-\mathbf{\Omega}^2inom{\mathbf{s}_x}{\mathbf{s}_y}=\mathbf{0} \qquad \qquad \mathbf{\Omega}^2=\mathbf{PQ}$$

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Analytical solution in the z-direction

Matrix wave equation:

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

This is actually a very large set of ordinary differential equations where each can be solved analytically. The system of equations can be solved as a single matrix equation as:

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

- $s^+(0)$ and $s^-(0)$ are initial values for this differential equation.
- The superscripts ± shows whether they are forward propagating waves (+) or backward propagating waves (-).

Note: Here we assume a sign convention of $e^{-j\beta z}$ for forward propagation in the +z-direction.



Functions of matrices Computation of $e^{\pm\Omega\tilde{z}}$

It is sometimes necessary to evaluate the function of a matrix A,

$$f(\mathbf{A}) = ?$$

To do this, first calculate the eigenvectors and eigenvalues of the matrix A

$$A \to \left\{ \begin{array}{ll} W & \text{eigenvector matrix of } A \\ \lambda & \text{eigenvalue matrix of } A. \end{array} \right.$$

$$oldsymbol{\lambda} = egin{pmatrix} \lambda_1 & & & \mathbf{0} \\ & \lambda_2 & & \\ & & \ddots & \\ \mathbf{0} & & & \lambda_N \end{pmatrix}$$

The function of the matrix is then evaluated as

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

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

In our case, we have the following matrix differential equation and general solution

$$\frac{d^2}{d\tilde{z}^2} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} - \mathbf{\Omega}^2 \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} = \mathbf{0} \quad \rightarrow \quad \begin{pmatrix} \mathbf{s}_x(\tilde{z}) \\ \mathbf{s}_y(\tilde{z}) \end{pmatrix} = e^{-\mathbf{\Omega}\tilde{z}} \mathbf{s}^+(0) + e^{\mathbf{\Omega}\tilde{z}} \mathbf{s}^-(0)$$

We can evaluate the matrix exponential using the eigenvalues and eigenvectors of the matrix Ω with the relation $f(\mathbf{A}) = \mathbf{W} \cdot f(\lambda) \cdot \mathbf{W}^{-1}$

$$e^{-\Omega \tilde{z}} = \mathbf{W} e^{-\lambda \tilde{z}} \mathbf{W}^{-1}$$

$$e^{\mathbf{\Omega}\tilde{z}} = \mathbf{W}e^{\mathbf{\lambda}\tilde{z}}\mathbf{W}^{-1}$$

 ${f W}\equiv$ Eigenvector matrix calculated from ${f \Omega}^2$

$$oldsymbol{\lambda}^2 \equiv \mathsf{Diagonal}$$
 eigenvalue matrix of $oldsymbol{\Omega}^2$

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

Solution to the matrix wave equation

$$\begin{pmatrix} \mathbf{s}_{x}(\tilde{z}) \\ \mathbf{s}_{y}(\tilde{z}) \end{pmatrix} = e^{-\Omega \tilde{z}} \mathbf{s}^{+}(0) + e^{\Omega \tilde{z}} \mathbf{s}^{-}(0) \quad (4)$$

$$e^{-\Omega \tilde{z}} = \mathbf{W} e^{-\lambda \tilde{z}} \mathbf{W}^{-1}$$

$$e^{\Omega \tilde{z}} = \mathbf{W} e^{\lambda \tilde{z}} \mathbf{W}^{-1}$$

$$(5)$$

Substitute eq (5) into eq (4) gives us

$$\begin{pmatrix} \mathbf{s}_{x}(\tilde{z}) \\ \mathbf{s}_{y}(\tilde{z}) \end{pmatrix} = \mathbf{W}e^{-\lambda\tilde{z}}\mathbf{W}^{-1}\mathbf{s}^{+}(0) + \mathbf{W}e^{\lambda\tilde{z}}\mathbf{W}^{-1}\mathbf{s}^{-}(0)$$

$$= \mathbf{W}e^{-\lambda\tilde{z}}\mathbf{c}^{+} + \mathbf{W}e^{\lambda\tilde{z}}\mathbf{c}^{-}$$

where we have defined the mode coefficients c^+ and c^- .

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

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

$$\mathbf{c}^+ = \mathbf{W}^{-1} \mathbf{s}^{+(0)}$$
$$\mathbf{c}^- = \mathbf{W}^{-1} \mathbf{s}^{-(0)}$$

Solution for the magnetic fields (1/2)

Similarly, for the magnetic field

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

Must calculate V from the eigenvalue solution of Ω^2 .

To put this equation in terms of the electric field, we differentiate with respect to z

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

We can now use this together with eq (1a) and our electric field solution to find the magnetic field.

$$\frac{d}{d\tilde{z}} \begin{pmatrix} \mathbf{u}_x \\ \mathbf{u}_y \end{pmatrix} = \mathbf{Q} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} \tag{1a}$$



Solution for the magnetic fields (2/2)

Recall

$$\frac{d}{d\bar{z}}\begin{pmatrix} \mathbf{u}_x \\ \mathbf{u}_y \end{pmatrix} = \mathbf{Q}\begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} \qquad \text{and} \qquad \begin{pmatrix} \mathbf{s}_x(\bar{z}) \\ \mathbf{s}_y(\bar{z}) \end{pmatrix} = \mathbf{W}e^{-\lambda\bar{z}}\mathbf{c}^+ + \mathbf{W}e^{\lambda\bar{z}}\mathbf{c}^-$$

Inserting these into the differentiated solution of the magnetic field from the previous slide we get

$$\begin{aligned} \frac{d}{d\tilde{z}} \begin{pmatrix} \mathbf{u}_x(\tilde{z}) \\ \mathbf{u}_y(\tilde{z}) \end{pmatrix} &= \mathbf{V} \lambda e^{-\lambda \tilde{z}} \mathbf{c}^+ + \mathbf{V} \lambda e^{\lambda \tilde{z}} \mathbf{c}^- \\ &= \mathbf{Q} \begin{pmatrix} \mathbf{s}_x \\ \mathbf{s}_y \end{pmatrix} \\ &= \mathbf{Q} \mathbf{W} e^{-\lambda \tilde{z}} \mathbf{c}^+ + \mathbf{Q} \mathbf{W} e^{\lambda \tilde{z}} \mathbf{c}^- \end{aligned}$$

Comparing these equations we see that

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



Overall field solution

The field solutions to the electric field and magnetic field are

$$\begin{pmatrix} \mathbf{s}_{x}(\tilde{z}) \\ \mathbf{s}_{y}(\tilde{z}) \end{pmatrix} = \mathbf{W}e^{-\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{+} + \mathbf{W}e^{\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{-}$$

$$\begin{pmatrix} \mathbf{u}_{x}(\tilde{z}) \\ \mathbf{u}_{y}(\tilde{z}) \end{pmatrix} = -\mathbf{V}e^{-\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{+} + \mathbf{V}e^{\boldsymbol{\lambda}\tilde{z}}\mathbf{c}^{-}$$

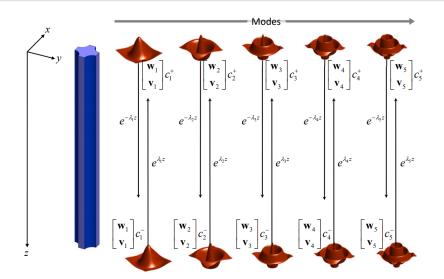
$$\mathbf{V} = \mathbf{Q}\mathbf{W}\boldsymbol{\lambda}^{-1}$$

Combining these into a single matrix equation yields

$$egin{aligned} \Psi(ilde{z}) = egin{pmatrix} \mathbf{s}_x(ilde{z}) \\ \mathbf{s}_y(ilde{z}) \\ \mathbf{u}_x(ilde{z}) \\ \mathbf{u}_y(ilde{z}) \end{pmatrix} = egin{pmatrix} \mathbf{W} & \mathbf{W} \\ -\mathbf{V} & \mathbf{V} \end{pmatrix} egin{pmatrix} e^{-oldsymbol{\lambda} ilde{z}} & \mathbf{0} \\ \mathbf{0} & e^{oldsymbol{\lambda} ilde{z}} \end{pmatrix} egin{pmatrix} \mathbf{c}^+ \\ \mathbf{c}^- \end{pmatrix} \end{aligned}$$

Semi-analytical form of Maxwell's equations in Fourier spac Matrix form of Maxwell's equations Matrix wave equation Solution to the matrix wave equation

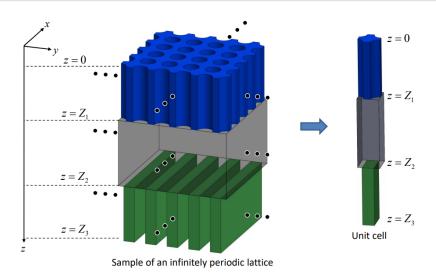
Visualization of this solution



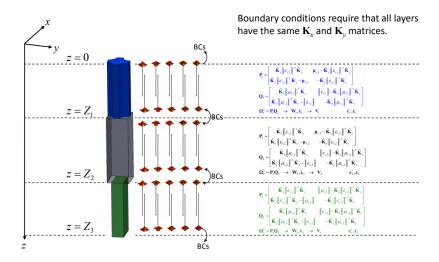
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Geometry of a multilayer device

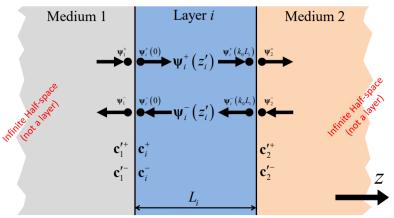


Eigen-system in each layer



Geometry of a single layer

• Indicates a point that lies on an interface, but associated with a particular side.



$$\psi_i^{\pm}(z) \equiv \text{ field within } i^{\text{th}} \text{ layer}$$

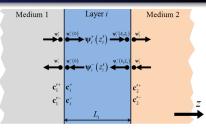
 $\mathbf{c}_{i}^{\pm} \equiv \text{mode coefficients inside } i^{\text{th}} \text{ layer}$ $\mathbf{c}_{i}^{\prime \pm} \equiv \text{mode coefficients outside } i^{\text{th}} \text{ layer}$

◆□ → ◆圖 → ◆差 → ◆差 → ● り へ ⊙

Field relations and boundary conditions

Field inside ith layer:

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



Boundary conditions at the first interface

$$\begin{split} & \boldsymbol{\Psi}_1 = \boldsymbol{\Psi}_i(0) \\ \begin{pmatrix} \mathbf{W}_1 & \mathbf{W}_1 \\ -\mathbf{V}_1 & \mathbf{V}_1 \end{pmatrix} \begin{pmatrix} \mathbf{c}_1^+ \\ \mathbf{c}_1^- \end{pmatrix} = \begin{pmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{pmatrix} \begin{pmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{pmatrix}$$

Boundary conditions at the second interface

$$\begin{split} & \Psi_i(k_0L_i) = \Psi_2 \\ \begin{pmatrix} \mathbf{W}_i & \mathbf{W}_i \\ -\mathbf{V}_i & \mathbf{V}_i \end{pmatrix} \begin{pmatrix} e^{-\boldsymbol{\lambda}_i k_0 L_i} & \mathbf{0} \\ \mathbf{0} & e^{\boldsymbol{\lambda}_i k_0 L_i} \end{pmatrix} \begin{pmatrix} \mathbf{c}_i^+ \\ \mathbf{c}_i^- \end{pmatrix} = \begin{pmatrix} \mathbf{W}_2 & \mathbf{W}_2 \\ -\mathbf{V}_2 & \mathbf{V}_2 \end{pmatrix} \begin{pmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{pmatrix} \end{split}$$

Outline

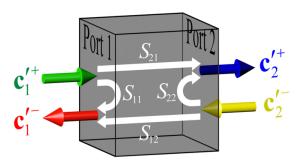
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Definition of a S-matrix

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

$$\mathbf{S}_{11} \equiv \text{reflection}$$

 $\mathbf{S}_{21} \equiv \text{transmission}$



Derivation of the S-matrix (1/2)

Solve the two boundary conditions from before with respect to the intermediate coefficients \mathbf{c}_i^+ and \mathbf{c}_i^- :

$$\begin{pmatrix} \mathbf{c}_{i}^{+} \\ \mathbf{c}_{i}^{-} \end{pmatrix} = \begin{pmatrix} \mathbf{W}_{i} & \mathbf{W}_{i} \\ -\mathbf{V}_{i} & \mathbf{V}_{i} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{W}_{1} & \mathbf{W}_{1} \\ -\mathbf{V}_{1} & \mathbf{V}_{1} \end{pmatrix} \begin{pmatrix} \mathbf{c}_{1}^{+} \\ \mathbf{c}_{1}^{-} \end{pmatrix}$$
(6)

$$\begin{pmatrix} \mathbf{c}_{i}^{+} \\ \mathbf{c}_{i}^{-} \end{pmatrix} = \begin{pmatrix} e^{-\lambda_{i}k_{0}L_{i}} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_{i}k_{0}L_{i}} \end{pmatrix} \begin{pmatrix} \mathbf{W}_{i} & \mathbf{W}_{i} \\ -\mathbf{V}_{i} & \mathbf{V}_{i} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{W}_{2} & \mathbf{W}_{2} \\ -\mathbf{V}_{2} & \mathbf{V}_{2} \end{pmatrix} \begin{pmatrix} \mathbf{c}_{2}^{+} \\ \mathbf{c}_{2}^{-} \end{pmatrix}$$
 (7)

Both equations have a common term

$$\begin{pmatrix} \mathbf{W}_{i} & \mathbf{W}_{i} \\ -\mathbf{V}_{i} & \mathbf{V}_{i} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{W}_{j} & \mathbf{W}_{j} \\ -\mathbf{V}_{j} & \mathbf{V}_{j} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \mathbf{A}_{ij} & \mathbf{B}_{ij} \\ -\mathbf{B}_{ij} & \mathbf{A}_{ij} \end{pmatrix}$$
(8)
$$\mathbf{A}_{ij} \equiv \mathbf{W}_{i}^{-1} \mathbf{W}_{j} + \mathbf{V}_{i}^{-1} \mathbf{V}_{j}$$
$$\mathbf{B}_{ij} \equiv \mathbf{W}_{i}^{-1} \mathbf{W}_{j} - \mathbf{V}_{i}^{-1} \mathbf{V}_{j}$$

Substitute eq (8) into both eqs (6) and (7), then set them equal eachother (6) = (7)

$$\begin{pmatrix} \mathbf{A}_{i1} & \mathbf{B}_{i1} \\ -\mathbf{B}_{i1} & \mathbf{A}_{i1} \end{pmatrix} \begin{pmatrix} \mathbf{c}_1^+ \\ \mathbf{c}_1^- \end{pmatrix} = \begin{pmatrix} e^{-\lambda_i k_0 L_i} & \mathbf{0} \\ \mathbf{0} & e^{\lambda_i k_0 L_i} \end{pmatrix} \begin{pmatrix} \mathbf{A}_{i2} & \mathbf{B}_{i2} \\ -\mathbf{B}_{i2} & \mathbf{A}_{i2} \end{pmatrix} \begin{pmatrix} \mathbf{c}_2^+ \\ \mathbf{c}_2^- \end{pmatrix}$$

Now separate this block-matrix equation into two matrix equations and reorganize the terms so that they have the form of a scattering matrix equation

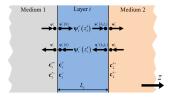
$$\begin{pmatrix} \mathbf{c}_1^- \\ \mathbf{c}_2^+ \end{pmatrix} = \begin{pmatrix} ? & ? \\ ? & ? \end{pmatrix} \begin{pmatrix} \mathbf{c}_1^+ \\ \mathbf{c}_2^- \end{pmatrix}$$



Derivation of the S-matrix (2/2)

The S-matrix $\mathbf{S}^{(i)}$ of the i^{th} layer is defined as

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



Doing the algebra, we get the components of the scattering matrix to be as follows

$$\begin{split} \mathbf{S}_{11}^{(i)} &= \left(\mathbf{A}_{i1} - \mathbf{X}_{i} \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{X}_{i} \mathbf{B}_{i1}\right)^{-1} \left(\mathbf{X}_{i} \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{X}_{i} \mathbf{A}_{i1} - \mathbf{B}_{i1}\right) & \mathbf{A}_{ij} &= \mathbf{w}_{i}^{-1} \mathbf{w}_{j} + \mathbf{v}_{i}^{-1} \mathbf{v}_{j} \\ \mathbf{S}_{12}^{(i)} &= \left(\mathbf{A}_{i1} - \mathbf{X}_{i} \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{X}_{i} \mathbf{B}_{i1}\right)^{-1} \mathbf{X}_{i} \left(\mathbf{A}_{i2} - \mathbf{B}_{i2} \mathbf{A}_{i2}^{-1} \mathbf{B}_{i2}\right) \\ \mathbf{S}_{21}^{(i)} &= \left(\mathbf{A}_{i2} - \mathbf{X}_{i} \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{X}_{i} \mathbf{B}_{i2}\right)^{-1} \mathbf{X}_{i} \left(\mathbf{A}_{i1} - \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{B}_{i1}\right) \\ \mathbf{S}_{22}^{(i)} &= \left(\mathbf{A}_{i2} - \mathbf{X}_{i} \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{X}_{i} \mathbf{B}_{i2}\right)^{-1} \left(\mathbf{X}_{i} \mathbf{B}_{i1} \mathbf{A}_{i1}^{-1} \mathbf{X}_{i} \mathbf{A}_{i2} - \mathbf{B}_{i2}\right) & \mathbf{X}_{i} &= e^{\mathbf{\lambda}_{i} k_{0} L_{i}} \end{split}$$

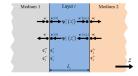
i is the layer number.

j=1,2 is the external medium being referenced.



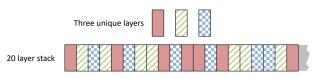
Limitation of a conventional S-matrix approach

Note that the elements of a S-matrix are a function of the materials outside the layer.



⇒ Interchanging S-matrices arbitrarily becomes very difficult.

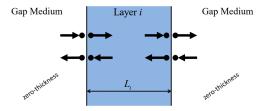
Take this example of a 20 layer structure consisting of three unique layers. Even though there are only three unique layers, 20 different S-matrices have to be computed.



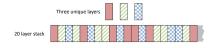
Solution Limitation of a conventional S-matrix approach

This problem can be solved by surrounding each layer with external regions of zero thickness.

- This lets us connect S-matrices in any order because all of them calculate fields in layers that have the same external mediums.
- This has no effect electromagnetically as long as the external regions have zero thickness between layers.

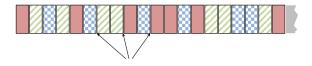


Visualization of the technique



Calculate the scattering matrices only for the three unique layers.

Then manipulate these same three scattering matrices to build the global scattering matrix



Gaps between layers have zero thickness

- Faster
- Simpler
- Less memory needed



Calculating the revised Scattering matrices

The S-matrix $\mathbf{S}^{(i)}$ of the i^{th} layer is still defined as

$$\begin{pmatrix} \mathbf{c}_1^- \\ \mathbf{c}_2^+ \end{pmatrix} = \mathbf{S}^{(i)} \begin{pmatrix} \mathbf{c}_1^+ \\ \mathbf{c}_2^- \end{pmatrix},$$

$$\mathbf{S}^{(i)} = \begin{pmatrix} \mathbf{S}_{11}^{(i)} & \mathbf{S}_{12}^{(i)} \\ \mathbf{S}_{21}^{(i)} & \mathbf{S}_{22}^{(i)} \end{pmatrix}$$

But the elements are now calculated as

$$\begin{aligned} \mathbf{S}_{11}^{(i)} &= \left(\mathbf{A}_{i} - \mathbf{X}_{i} \mathbf{B}_{i} \mathbf{A}_{i}^{-1} \mathbf{X}_{i} \mathbf{B}_{i}\right)^{-1} \left(\mathbf{X}_{i} \mathbf{B}_{i} \mathbf{A}_{i}^{-1} \mathbf{X}_{i} \mathbf{A}_{i} - \mathbf{B}_{i}\right) & \mathbf{A}_{i} &= \mathbf{W}_{i}^{-1} \mathbf{W}_{0} + \mathbf{V}_{i}^{-1} \mathbf{V}_{0} \\ \mathbf{S}_{12}^{(i)} &= \left(\mathbf{A}_{i} - \mathbf{X}_{i} \mathbf{B}_{i} \mathbf{A}_{i}^{-1} \mathbf{X}_{i} \mathbf{B}_{i}\right)^{-1} \mathbf{X}_{i} \left(\mathbf{A}_{i} - \mathbf{B}_{i} \mathbf{A}_{i}^{-1} \mathbf{B}_{i}\right) & \mathbf{B}_{i} &= \mathbf{W}_{i}^{-1} \mathbf{W}_{0} + \mathbf{V}_{i}^{-1} \mathbf{V}_{0} \\ \mathbf{S}_{21}^{(i)} &= \mathbf{S}_{12}^{(i)} & \mathbf{X}_{i} &= e^{\mathbf{\lambda}_{i} k_{0} L_{i}} \end{aligned}$$

- Layers are symmetric so the scattering matrix have redundancy
- Fewer calculations
- Less memory storage

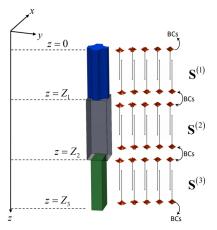


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Global scattering matrix

The scattering matrix method consists of working through the device one layer at a time and calculating an overall scattering matrix.



 \otimes is the Redheffer star product

Scattering matrix for all layers

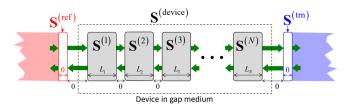
$$\mathbf{S}^{(\text{device})} = \mathbf{S}^{(1)} \otimes \mathbf{S}^{(2)} \otimes \mathbf{S}^{(3)}$$

Connection to outside regions (ambient/substrate)

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

Putting it all together

Connect the device scattering matrix to the external regions to get the global scattering matrix.



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

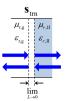
Reflection/transmission region scattering matrices

The reflection-side scattering matrix is

$$\begin{split} \mathbf{S}_{11}^{(ref)} &= -\mathbf{A}_{ref}^{-1} \mathbf{B}_{ref} \\ \mathbf{S}_{12}^{(ref)} &= 2\mathbf{A}_{ref}^{-1} \\ \mathbf{S}_{21}^{(ref)} &= 0.5 \Big(\mathbf{A}_{ref} - \mathbf{B}_{ref} \mathbf{A}_{ref}^{-1} \mathbf{B}_{ref} \Big) \end{split} \qquad \mathbf{A}_{ref} &= \mathbf{W}_g^{-1} \mathbf{W}_{ref} + \mathbf{V}_g^{-1} \mathbf{V}_{ref} \\ \mathbf{B}_{ref} &= \mathbf{W}_g^{-1} \mathbf{W}_{ref} - \mathbf{V}_g^{-1} \mathbf{V}_{ref} \\ \mathbf{S}_{22}^{(ref)} &= \mathbf{B}_{ref} \mathbf{A}_{ref}^{-1} \end{split}$$

The transmission-side scattering matrix is

$$\begin{split} \mathbf{S}_{11}^{(tm)} &= \mathbf{B}_{tm} \mathbf{A}_{tm}^{-1} \\ \mathbf{S}_{12}^{(tm)} &= 0.5 \Big(\mathbf{A}_{tm} - \mathbf{B}_{tm} \mathbf{A}_{tm}^{-1} \mathbf{B}_{tm} \Big) \\ \mathbf{S}_{12}^{(tm)} &= 2 \mathbf{A}_{tm}^{-1} \\ \mathbf{S}_{21}^{(tm)} &= 2 \mathbf{A}_{tm}^{-1} \\ \mathbf{S}_{22}^{(tm)} &= - \mathbf{A}_{tm}^{-1} \mathbf{B}_{tm} \end{split}$$



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Solution using Scattering matrices Transversal components

ullet The electric field source is, when assuming unit amplitude polarization vector \vec{P} , as follows

$$\mathbf{s}_T^{\mathsf{inc}} = \begin{pmatrix} p_x oldsymbol{\delta}_{0,pq} \\ p_y oldsymbol{\delta}_{0,pq} \end{pmatrix} \qquad \qquad ec{P} = \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix}, \qquad |ec{P}| = 1 \qquad \qquad \delta_{0,pq} = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow p,q \quad \mathsf{position}$$

The external fields (incident wave, reflected wave, transmitted wave) are related through the global scattering matrix

$$egin{pmatrix} egin{pmatrix} \mathbf{c}_{\mathsf{ref}} \\ \mathbf{c}_{\mathsf{trn}} \end{pmatrix} = \mathbf{S}^{(\mathsf{global})} egin{pmatrix} \mathbf{c}_{\mathsf{inc}} \\ \mathbf{0} \end{pmatrix} \qquad \qquad \mathbf{c}_{\mathsf{inc}} = \mathbf{W}_{\mathsf{ref}}^{-1} \mathbf{s}_{T}^{\mathsf{inc}}$$

 $\mathbf{c}_{\text{inc}}^{\text{right}}$ is usually null, so our input mode-coefficients are only $\mathbf{c}_{\text{inc}}^{\text{left}}=\mathbf{c}_{\text{inc}}.$

$$\Longrightarrow \mathbf{c}_{\mathsf{ref}} = \mathbf{S}_{11}\mathbf{c}_{\mathsf{inc}}$$
 $\mathbf{c}_{\mathsf{trn}} = \mathbf{S}_{21}\mathbf{c}_{\mathsf{inc}}$

The transverse components of the reflected and transmitted fields are then

$$\mathbf{r}_T \equiv \mathbf{s}_T^{\mathsf{ref}} = \mathbf{W}_{\mathsf{ref}} \mathbf{c}_{\mathsf{ref}} = \mathbf{W}_{\mathsf{ref}} \mathbf{S}_{11} \mathbf{c}_{\mathsf{inc}} \ \mathbf{t}_T \equiv \mathbf{s}_T^{\mathsf{trn}} = \mathbf{W}_{\mathsf{trn}} \mathbf{c}_{\mathsf{trn}} = \mathbf{W}_{\mathsf{trn}} \mathbf{S}_{21} \mathbf{c}_{\mathsf{inc}}$$

Transversal components of reflected/transmitted fields

$$\begin{split} \mathbf{r}_T &= \begin{pmatrix} \mathbf{r}_x \\ \mathbf{r}_y \end{pmatrix} = \mathbf{W}_{\mathsf{ref}} \mathbf{S}_{11} \mathbf{W}_{\mathsf{ref}}^{-1} \mathbf{s}_T^{\mathsf{inc}} \\ \mathbf{t}_T &= \begin{pmatrix} \mathbf{t}_x \\ \mathbf{t}_y \end{pmatrix} = \mathbf{W}_{\mathsf{trn}} \mathbf{S}_{21} \mathbf{W}_{\mathsf{ref}}^{-1} \mathbf{s}_T^{\mathsf{inc}} \end{split}$$

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

Calculating the longitudinal components

Still missing the longitudinal field components on either side of the layer stack.

These are calculated from the transverse components using the divergence equation.

$$\begin{split} \mathbf{r}_z &= -\tilde{\mathbf{K}}_{z,\mathrm{ref}}^{-1} \left(\tilde{\mathbf{K}}_x \mathbf{r}_x + \tilde{\mathbf{K}}_y \mathbf{r}_y \right) & \qquad \qquad \tilde{\mathbf{K}}_{z,\mathrm{ref}}^{-1} = - \left(\sqrt{\mu_{r,\mathrm{ref}}^* \varepsilon_{r,\mathrm{ref}}^* \mathbf{I} - \tilde{\mathbf{K}}_x^2 - \tilde{\mathbf{K}}_y^2} \right) \\ \mathbf{t}_z &= -\tilde{\mathbf{K}}_{z,\mathrm{trn}}^{-1} \left(\tilde{\mathbf{K}}_x \mathbf{t}_x + \tilde{\mathbf{K}}_y \mathbf{t}_y \right) & \qquad \tilde{\mathbf{K}}_{z,\mathrm{trn}}^{-1} = \left(\sqrt{\mu_{r,\mathrm{trn}}^* \varepsilon_{r,\mathrm{trn}}^* \mathbf{I} - \tilde{\mathbf{K}}_x^2 - \tilde{\mathbf{K}}_y^2} \right) \end{split}$$

DERIVATION

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

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

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

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

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

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

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

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Calculating the diffraction efficiencies (1/2)

Power flow described by Poynting vector

$$\vec{\wp} = \tfrac{1}{2} \mathsf{Re}[\vec{E} \times \vec{H}] = \tfrac{1}{2} \mathsf{Re} \left[\tfrac{\vec{k}}{|\vec{k}|} |\vec{E}| |\vec{H}| \right] = \tfrac{1}{2} \mathsf{Re} \left[\tfrac{\vec{k}}{|\vec{k}|} \tfrac{|\vec{E}|^2}{\eta} \right]$$

· Only interested in power leaving the device

$$\wp_z = \frac{1}{2} \text{Re} \left[\frac{k_z}{|\vec{k}|} \frac{|\vec{E}|^2}{\eta} \right]$$

• Our field scattered from the periodic device is decomposed into a Fourier series, where $\vec{S}(m,n)$ is the amplitude and polarization of the $(m,n)^{\text{th}}$ harmonic. Power flow away from the device due to the $(m,n)^{\text{th}}$ diffracted order is therefore

$$\wp_z(m,n) = \frac{1}{2} \text{Re} \left[\frac{\tilde{k}_z(m,n)}{|\vec{\tilde{k}}(m,n)|} \frac{|\vec{S}(m,n)|^2}{\eta} \right]$$

• Diffraction efficiency (DE) is defined as the power in a specified order divided by the applied incident power: $\mathsf{DE}(m,n) = \wp_z(m,n)/\wp_z^{\mathrm{inc}}$

$$\begin{split} \Rightarrow & \quad \mathsf{DE}^{\mathsf{ref}}(m,n) = \mathsf{Re}\left[\frac{\hat{k}_{z,\mathsf{ref}}(m,n)}{\hat{k}_z^{\mathsf{inc}}}\right] \cdot \frac{|\vec{S}^{\mathsf{ref}}(m,n)|^2}{|\vec{S}_{\mathsf{inc}}|^2} \\ \Rightarrow & \quad \mathsf{DE}^{\mathsf{trn}}(m,n) = \mathsf{Re}\left[\frac{\hat{k}_{z,\mathsf{trn}}(m,n)}{\hat{k}_z^{\mathsf{inc}}} \frac{\mu_r^{\mathsf{inc}}}{\mu_r^{\mathsf{trn}}}\right] \cdot \frac{|\vec{S}^{\mathsf{trn}}(m,n)|^2}{|\vec{S}_{\mathsf{inc}}|^2} \end{split}$$

Calculating the diffraction efficiencies (2/2)

The diffraction efficiencies for all modes ${f R}$ and ${f T}$ are calculated as

$$\begin{split} \mathbf{R} &= \mathrm{Re}\left[\frac{\tilde{\mathbf{K}}_{z,\mathrm{ref}}}{k_{z,\mathrm{inc}}}\right] \cdot |\vec{\mathbf{r}}|^2 \\ \mathbf{T} &= \mathrm{Re}\left[\frac{\mu_{r,\mathrm{inc}}}{\mu_{r,\mathrm{trn}}}\frac{\tilde{\mathbf{K}}_{z,\mathrm{trn}}}{k_{z,\mathrm{inc}}}\right] \cdot |\vec{\mathbf{t}}|^2 \end{split}$$

where

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

ř, R

Remember notation for reflected/transmitted fields: $\mathbf{r}_x = \mathbf{s}_x^{\mathsf{ref}}$, $\mathbf{t}_x = \mathbf{s}_x^{\mathsf{trn}}$ etc.

Overall reflectance and transmittance

The overall reflectance ${\cal R}$ and transmittance ${\cal T}$ are calculated by summing the diffraction efficiencies of all the modes

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

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

Always good practice to check for for conservation of power

$$A + R + T = 1$$

When no loss or gain is in the simulation

$$R + T = 1$$

End

Literature

- R. C. Rumpf, "Improved formulation of scattering matrices for semi-analytical methods that is consistent with convention," PIERS B, Vol. 35, 241-261, 2011. http://ww.ipier.org/PIERB/pierb35/13.11083107.pdf
- EE 5337 Computational Electromagnetics, University of Texas at El Paso http://emlab.utep.edu/ee5390cem.htm
- Lifeng Li. Fourier Modal Method. E. Popov, ed. Gratings: Theory and Numeric Applications, Second Revisited Edition, 2014. https://hal.archives-ouvertes.fr/hal-00985928/document
- S⁴: A free electromagnetic solver for layered periodic structures, Victor Liu, Shanhui Fan, Computer Physics Communications 183 (2012) 2233-2244
 https://web.stanford.edu/group/fan/publication/Liu_ComputerPhysicsCommunications_ 183_2233_2012.pdf

Images taken from

- https://web.stanford.edu/group/fan/publication/Liu_ComputerPhysicsCommunications_ 183_2233_2012.pdf
- http://emlab.utep.edu/ee5390cem.htm