Computational Photonics

– Matrix Method for Stratified Media –

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Recap of the last lecture
Recap: Basic Structure

- numerical 1D problem
- **here:** only homogeneous, isotropic materials

possible tasks:
- transmission & reflection as a function of angle of incidence, wavelength, polarization
- EM fields in & outside the structure
- dispersion relation & EM fields of guided waves (finite stack)
- dispersion relation & EM fields of Bloch modes (infinite structure)

in the last lecture, we learned to solve this task analytically using a transfer matrix for the field components. Computers just aid us with the many algebraic operations!
Application examples for Multilayer Structures
Applications

• **Anti-reflection coatings**
  
  – single quarter wave layer on substrate can cancel reflection entirely if
    \[ n = \sqrt{n_{in}n_{out}} \]
  
  – more layers lift material limitation or broaden spectral bandwidth

Reflectance of a single quarter wave layer with varying refractive index on a substrate with \( n_{out} = 2.25 \) and incidence from air.

Applications

• Bragg mirror
  – reflection: phase shift of $\pi$
  – idea: constructively interfere waves which have that shift!
  – this means, the optical thickness of two alternate layers should match $\lambda_0/2$!
  – this is easily achieved, if each layer has an optical thickness of $\lambda_0/4$ ("quarter wave stack")

20 layers, $n_1 = 1.5$, $n_2 = 2.0$, $\lambda_0 = 600$ nm
Applications

- Bragg mirror
  - efficiency increases with layer number
Applications

• Spectral filters
  – introducing a “defect” in a periodic stack will couple light evanescently through the structure and produce a very sharp spectral dip / peak!
Calculating the electromagnetic fields of the scattering problem*

*this is a supplementary topic, for details, see seminar
Calculating EM fields

• Problem with transfer matrix:
  – we got rid of the C coefficients for up- & downward propagating amplitudes → can’t directly derive fields in the stack

• Strategy:
  – normalize transmitted field, then calculate piecewise backward

\[
\begin{bmatrix}
F(x) \\
G(x)
\end{bmatrix} = \begin{bmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{bmatrix}^{-1} \begin{bmatrix}
1 \\
iq_{\text{out}} k_{x}^{\text{out}}
\end{bmatrix}
= \begin{bmatrix}
M_{11} & M_{12} \\
M_{21} & M_{22}
\end{bmatrix} \begin{bmatrix}
1 \\
-iq_{\text{out}} k_{x}^{\text{out}}
\end{bmatrix}
\]
Calculating guided modes of the stack*

* This is a supplementary topic
Guided modes of the stack

• Seeing the basic structure in a different way:

• Guided waves are evanescent in cladding & substrate (no “in” & “out”, total internal reflection at substrate & cladding interface)
Guided modes of the stack

• Dispersion relation still unchanged:

\[
\left[ k_x^{(i)} \right]^2 + k_z^2 = |\mathbf{k}|^2 = \frac{\omega^2}{c^2} \epsilon_i(\omega)
\]

• for \( k_x \) to be imaginary on both sides, \( k_z \) has to be larger than \( |\mathbf{k}| \) on both sides!! (“outside the light line/cone”)
Guided modes of the stack

• Algebraically, this leads to “imaginary angles of incidence”

• We can use the very same matrix algorithm and observe singularities of the scattering problem:
Guided modes of the stack

- Recalling formulas for reflection/transmission:

\[
\begin{align*}
    r &= \frac{F_r}{F_{\text{in}}} = \frac{q_{\text{in}} k_{x}^{\text{in}} M_{22} - q_{\text{out}} k_{x}^{\text{out}} M_{11} - i(M_{21} + q_{\text{in}} k_{x}^{\text{in}} q_{\text{out}} k_{x}^{\text{out}} M_{12})}{q_{\text{in}} k_{x}^{\text{in}} M_{22} + q_{\text{out}} k_{x}^{\text{out}} M_{11} + i(M_{21} - q_{\text{in}} k_{x}^{\text{in}} q_{\text{out}} k_{x}^{\text{out}} M_{12})} \\
    t &= \frac{F_t}{F_{\text{in}}} = \frac{2 q_{\text{in}} k_{x}^{\text{in}}}{q_{\text{in}} k_{x}^{\text{in}} M_{22} + q_{\text{out}} k_{x}^{\text{out}} M_{11} + i(M_{21} - q_{\text{in}} k_{x}^{\text{in}} q_{\text{out}} k_{x}^{\text{out}} M_{12})}
\end{align*}
\]

- Singularities occur for a vanishing denominator

- The roots of the denominator are the guided modes of the stack!

  → use numerical root finding algorithm to solve
Alternative formulation: transmission matrix*

* This is a supplementary topic following Pochi Yeh, “Optical Waves in Layered Media”, Wiley 1988
Alternative formulation: T-Matrix

- Treating the single interface:
  - incoming & outgoing waves
  - Maxwell boundary conditions:

\[
\begin{align*}
E_1 + E_1' &= E_2 + E_2' \\
\sqrt{\epsilon_1}(E_1 - E_1') \cos \theta_1 &= \sqrt{\epsilon_2}(E_2 - E_2') \cos \theta_2 \\
(E_1 + E_1') \cos \theta_1 &= (E_2 + E_2') \cos \theta_2 \\
\sqrt{\epsilon_1}(E_1 - E_1') &= \sqrt{\epsilon_2}(E_2 - E_2')
\end{align*}
\]  

(TE)  
(TM)

- boundary conditions as a matrix notation:

\[
\hat{D}_1 \begin{bmatrix} E_1 \\ E_1' \end{bmatrix} = \hat{D}_2 \begin{bmatrix} E_2 \\ E_2' \end{bmatrix}
\]
Alternative formulation: T-Matrix

- many layers:
  - formulation for for- & backward amplitudes A and B:

\[
\begin{bmatrix}
A_1 \\
B_1
\end{bmatrix} = \hat{D}_1^{-1} \hat{D}_2 \begin{bmatrix}
A'_2 \\
B'_2
\end{bmatrix}
\]

\[
\begin{bmatrix}
A'_2 \\
B'_2
\end{bmatrix} = \hat{P}_2 = \begin{bmatrix}
\exp(ik_x^{(2)}d) & 0 \\
0 & \exp(-ik_x^{(2)}d)
\end{bmatrix} \begin{bmatrix}
A_2 \\
B_2
\end{bmatrix}
\]

\[
\begin{bmatrix}
A_2 \\
B_2
\end{bmatrix} = \hat{D}_2^{-1} \hat{D}_3 \begin{bmatrix}
A'_3 \\
B'_3
\end{bmatrix}
\]

\[
\begin{bmatrix}
A_{in} \\
B_{in}
\end{bmatrix} = \begin{bmatrix}
T_{11} & T_{12} \\
T_{21} & T_{22}
\end{bmatrix} \begin{bmatrix}
A'_{out} \\
B'_{out}
\end{bmatrix}
\]

\[
\hat{T} = \hat{D}_{in}^{-1} \prod_{l=1}^{N} \hat{D}_l \hat{P}_l \hat{D}_l^{-1} \hat{D}_{out}
\]

\[
r = \frac{T_{21}}{T_{11}}
\]

\[
t = \frac{1}{T_{11}}
\]
Alternative formulation: T-matrix

- allows to derive symmetry properties for lossless structures:
  \[ T_{21} = T_{12}^*, \quad T_{22} = T_{11}^* \]
  \[ \det(\hat{T}) = \frac{n_{out} \cos \theta_{out}}{n_{in} \cos \theta_{in}} \]

- reciprocity:
  \[ r = \frac{T_{21}}{T_{11}}, \quad t = \frac{1}{T_{11}} \]
  \[ r' = -\frac{T_{12}}{T_{11}}, \quad t' = \frac{\det(\hat{T})}{T_{11}} \]

- **advantage**: scattering parameters, fields & symmetries straight-forward to calculate
- **problem**: numerical stability not guaranteed due to exponential factors of different signs!
Another alternative formulation: S-Matrix*

* This is a supplementary topic following Lifeng Li, “Formulation and comparison of two recursive matrix algorithms for modeling layered diffraction gratings”, JOSAA 13(5), p. 1024, (1996)
Layers as ports: the S-matrix

- A layer describes a 'gate' with 'ports' for the E-field
- Simple optical scattering problem: described by scattering matrix

\[
\begin{bmatrix}
E^f \\
E^b_i
\end{bmatrix}
= \begin{pmatrix}
T_f & R_b \\
R_f & T_b
\end{pmatrix}
\begin{bmatrix}
E^f_i \\
E^b
\end{bmatrix}
\]

Compare to electronics: in and out going currents at a junction
Constructing layers

- For homogeneous media there are two kinds of layers:

  - Propagators
  - Interfaces

  A general layer is defined by a propagator and two interfaces.

  - \( N \) layers of a stratified medium is defined by \( N \) propagators and \( 2N+1 \) interfaces.

  Fresnel equations

\[
S_P = \begin{pmatrix} \exp(ink_0d) & 0 \\ 0 & \exp(ink_0d) \end{pmatrix}, \quad
S_{n_1,n_2} = \begin{pmatrix} \frac{2n_1}{n_1+n_2} & \frac{n_2-n_1}{n_1+n_2} \\ \frac{n_1-n_2}{n_1+n_2} & \frac{2n_2}{n_1+n_2} \end{pmatrix}
\]

Phase sign preserved in forward coordinate system.
Combining layers

• S-matrices are combined using the ‘star product’

\[
S = S_1 \ast S_2 = \begin{pmatrix} \hat{T}_1^f & \hat{R}_1^b \\ \hat{R}_1^f & \hat{T}_1^b \end{pmatrix} \ast \begin{pmatrix} \hat{T}_2^f & \hat{R}_2^b \\ \hat{R}_2^f & \hat{T}_2^b \end{pmatrix} = \begin{pmatrix} \hat{T}_1^f \left( \mathbb{I} - \hat{R}_1^b \hat{R}_2^f \right)^{-1} \hat{T}_1^f & \hat{R}_2^b + \hat{T}_2^f \hat{R}_1^b \left( \mathbb{I} - \hat{R}_2^f \hat{R}_1^b \right)^{-1} \hat{T}_2^b \\ \hat{R}_1^f + \hat{T}_1^b \hat{R}_2^f \left( \mathbb{I} - \hat{R}_1^b \hat{R}_2^f \right)^{-1} \hat{T}_1^b & \hat{T}_1^b \left( \mathbb{I} - \hat{R}_2^f \hat{R}_1^b \right)^{-1} \hat{T}_2^b \end{pmatrix}
\]

– entries are scalar or matrices

• single layer in air

\[
\begin{array}{c}
\text{n}_{\text{air}} \\
n_1 \\
\text{n}_{\text{air}}
\end{array}
\]

\[
S_1 = S_{n_{1,\text{air}}} \ast S_{P_1} \ast S_{n_{\text{air}},n_1}
\]

• 3 layers (equal height) in air

\[
\begin{array}{c}
\text{n}_{\text{air}} \\
n_1 \\
n_2 \\
n_3 \\
\text{n}_{\text{air}}
\end{array}
\]

\[
S_3 = S_{n_{1,\text{air}}} \ast S_{P_1} \ast S_{n_{2,n_1}} \ast S_{P_2} \ast S_{n_{3,n_2}} \ast S_{P_3} \ast S_{n_{\text{air}},n_3}
\]

– example: transmission coefficient:

\[
T_1^f = \frac{4n_1 e^{i d k_0 n_1}}{(n_1 + 1)^2 - (n_1 - 1)^2 e^{2i d k_0 n_1}}
\]

includes interference from reflection between interfaces!
Research: nano-structured layers

- layers with nano-structures have complex S-matrices
- combined with star product: full response of layered system

nano-structured layered system
Summary: Matrix Method for Stratified Media
• **We derived the transfer matrix method**
  – completely analytically
  – separates in TE/TM due to symmetry of the problem
  – transfer matrix connects EM fields at different $x$ positions
  – continuity of tangential EM fields allows treatment by simple matrix multiplication
  – we can solve analytically for $r$, $t$, $R$, and $T$
  – guided modes are poles of the scattering problem ($r$, $t$ diverge there!)
  – EM fields need to be calculated separately by a trick
1. Recall Maxwells equations, Helmholtz equation, dispersion relation of plane waves and boundary conditions for the fields

2. Understand the basic concepts of the transfer matrix method derivation

3. Being able to implement the given formulas as a computer program

4. Being able to write a program to calculate scattering parameters (R,T) for a structure for a given wavelength range or angle of incidence
1. Being able to calculate the EM fields

2. Being able to find guided modes from the poles of the scattering problem

3. Writing a program that calculates the dispersion relation of guided modes of an arbitrary stack

4. Knowing different variants of matrix methods implementations and their specific advantages