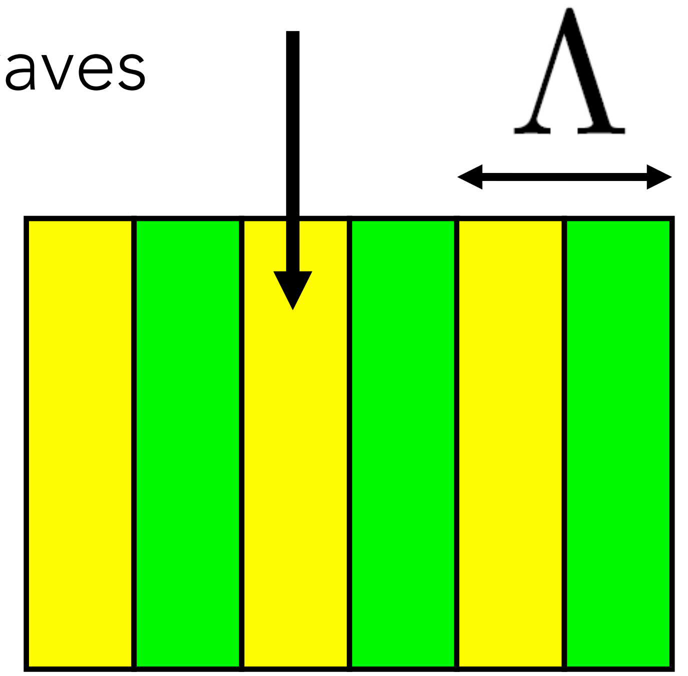
Computational Photonics

Basics of grating theories - eigenmodes for a 1D and 2D grating

Strategy for the grating algorithm

- expanding the fields in the different domains in terms of modes (mode=solution of a wave equation)
  - for incident and transmitted region modes are plane waves
  - in grating region modes are waveguide modes that fulfil periodic boundary conditions



⇨ mode profile is determined numerically *(analytical solutions can be used in special cases)*

- deriving the proper boundary conditions and solving for the unknown amplitudes of each mode

⇨ comparable to the plane interface problem

⇨ tangential electric and magnetic field are continuous + transversal wave vector component

Outline of the algorithm

- ⟹ calculate all wave vector components of interest
- ⟹ Fourier transforming the permittivity distribution
- ⟹ calculating the eigenvalues and the eigenvectors of the eigenmodes as supported by the structure in Fourier space
- ⟹ solving the system of linear equations that provide the amplitude of all relevant field components
- ⟹ calculating derived quantities of interest, such as diffraction efficiency and/or field distributions in the plane of interest
- ⟹ note that the algorithm thus far requires invariance of the structure in the propagation direction

Guided modes in a plane wave basis

- start with Maxwell's equations for a time harmonic field
- magnetic field scaled by impedance

$$\nabla \times \mathbf{E}(\mathbf{r}) = ik_0\mathbf{H}(\mathbf{r})$$
$$\nabla \times \mathbf{H}(\mathbf{r}) = -ik_0\epsilon(\mathbf{r})\mathbf{E}(\mathbf{r})$$

- combining equations to eliminate the z-component of the field
  (unambiguously determined by the divergence equations)
- e.g.: $$\frac{\partial}{\partial z}E_y = \frac{\partial}{\partial y}E_z - ik_0H_x$$
- and $$\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x = -ik_0\epsilon(\mathbf{r})E_z$$

$$\frac{\partial}{\partial z}E_y = \frac{1}{-ik_0}\frac{\partial}{\partial y}\left[\frac{1}{\epsilon}\left(\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x\right)\right] - ik_0H_x$$

Guided modes in a plane wave basis

$$\frac{\partial}{\partial z}E_x = \frac{1}{-ik_0}\frac{\partial}{\partial x}\left[\frac{1}{\epsilon}\left(\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x\right)\right] + ik_0 H_y$$

$$\frac{\partial}{\partial z}E_y = \frac{1}{-ik_0}\frac{\partial}{\partial y}\left[\frac{1}{\epsilon}\left(\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x\right)\right] - ik_0 H_x$$

$$\frac{\partial}{\partial z}H_x = \frac{1}{ik_0}\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x\right) - ik_0\epsilon E_y$$

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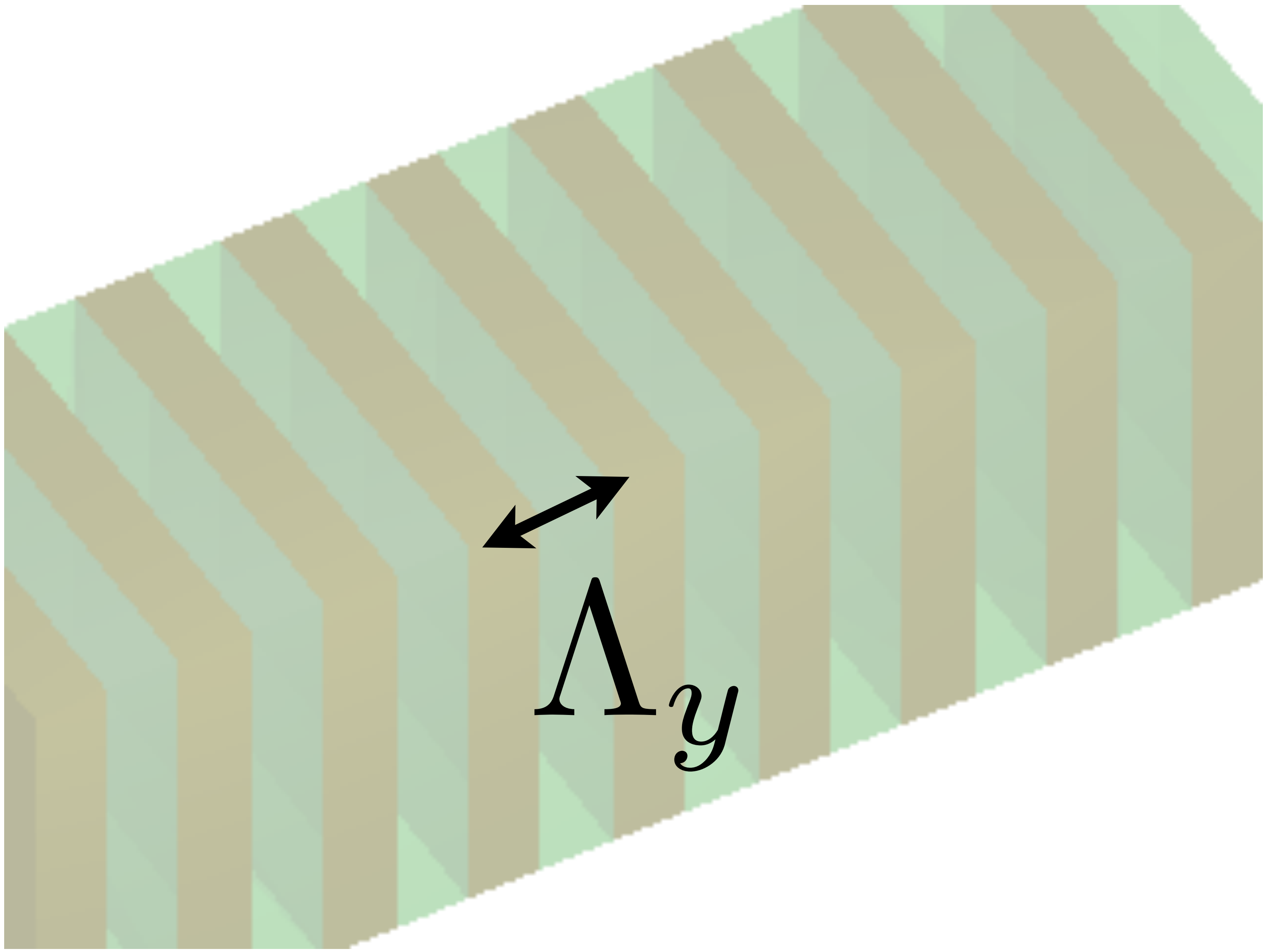
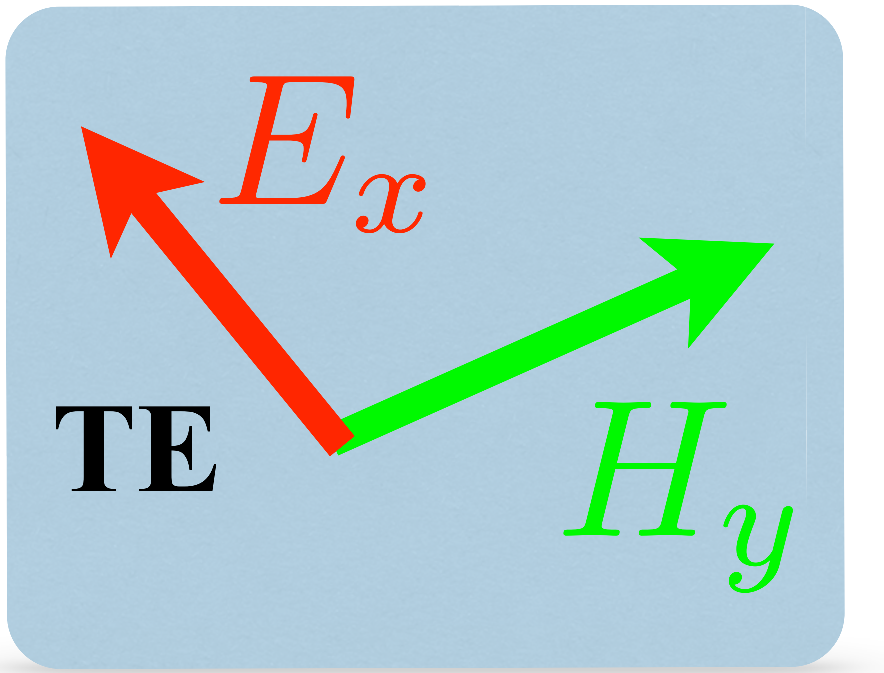
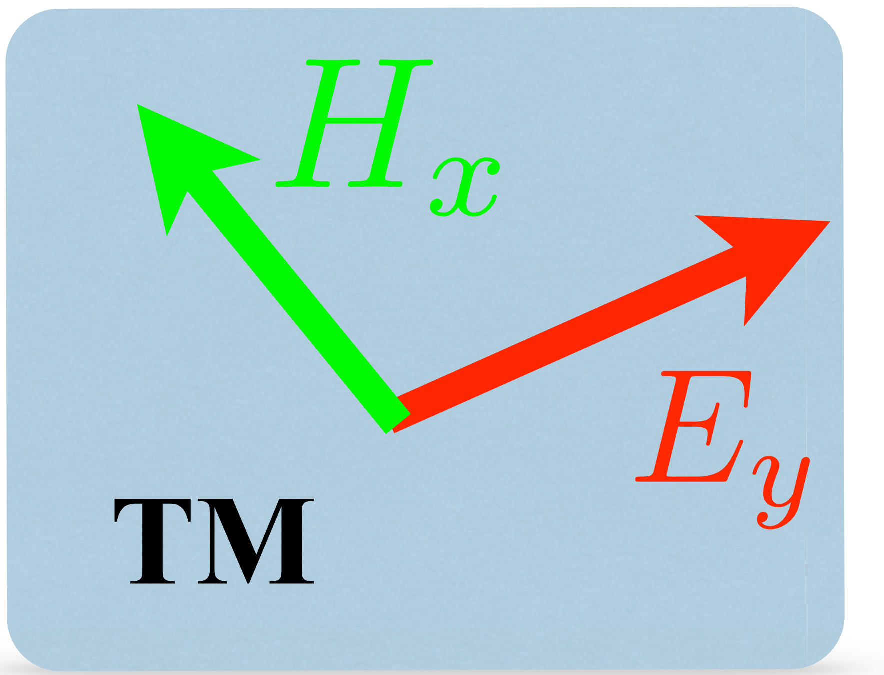
(Li et al., Phys. Rev. E, Vol. 67, 046607 2003)

Simplification to a 2D problem

⇨ decomposition into two orthogonal states of polarisation (TE/TM)







E.g. for TE polarisation

$$\frac{\partial}{\partial z}H_y = \frac{1}{ik_0}\frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x\right) + ik_0\epsilon E_x$$

$$\frac{\partial}{\partial x} = 0 \quad \Longrightarrow \quad \frac{\partial}{\partial z}H_y = -\frac{1}{ik_0}\frac{\partial^2}{\partial y^2}E_x + ik_0\epsilon E_x$$

$$\frac{\partial}{\partial z}E_x = \frac{1}{-ik_0}\frac{\partial}{\partial x}\left[\frac{1}{\epsilon}\left(\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x\right)\right] + ik_0 H_y$$

$$\frac{\partial}{\partial x} = 0 \quad \Longrightarrow \quad \frac{\partial}{\partial z}E_x = ik_0 H_y$$

Fourier expansion of all fields

$$\frac{\partial}{\partial z}E_x = ik_0 H_y$$

$$\frac{\partial}{\partial z}E_x = \frac{\partial}{\partial z}\sum_m E_{m,x}e^{ik_{m,y}y}$$

$$ik_0 H_y = ik_0 \sum_m H_{m,y}e^{ik_{m,y}y}$$

$$\frac{\partial}{\partial z}\sum_m E_{m,x}e^{ik_{m,y}y} = ik_0 \sum_m H_{m,y}e^{ik_{m,y}y}$$

multiplying both sides with reciprocal grating vector

$$\frac{\partial}{\partial z}\sum_m E_{m,x}e^{ik_{m,y}y}e^{-ik_{j,y}y} = ik_0 \sum_m H_{m,y}e^{ik_{m,y}y}e^{-ik_{j,y}y}$$

Fourier expansion of all fields

$$\frac{\partial}{\partial z}\sum_m E_{m,x}e^{ik_{m,y}y}e^{-ik_{j,y}y} = ik_0\sum_m H_{m,y}e^{ik_{m,y}y}e^{-ik_{j,y}y}$$

integration across the unit cell

$$\frac{\partial}{\partial z}\sum_m E_{m,x}\int dye^{ik_{m,y}y}e^{-ik_{j,y}y} = ik_0\sum_m H_{m,y}\int dye^{ik_{m,y}y}e^{-ik_{j,y}y}$$

employing orthogonality in plane wave expansion

$$\frac{\partial}{\partial z}\sum_m E_{m,x}\delta_{m,j} = ik_0\sum_m H_{m,y}\delta_{m,j}$$

short notation

$$\frac{\partial}{\partial z}E_{j,x} = ik_0 H_{j,y}$$

Final matrix expression

$$\frac{\partial}{\partial z}E_{0,x} = ik_0 H_{0,y}$$

$$\frac{\partial}{\partial z}E_{1,x} = ik_0 H_{1,y}$$

$$\vdots$$

$$\frac{\partial}{\partial z}E_{n,x} = ik_0 H_{n,y}$$

$$\Rightarrow \frac{\partial}{\partial z}\begin{bmatrix} E_{0,x} \\ E_{1,x} \\ \cdot \\ \cdot \\ \cdot \\ E_{n,x} \end{bmatrix} = \begin{bmatrix} ik_0 & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & ik_0 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & \cdot & ik_0 \end{bmatrix} \begin{bmatrix} H_{0,y} \\ H_{1,y} \\ \cdot \\ \cdot \\ \cdot \\ H_{n,y} \end{bmatrix}$$

$$\frac{\partial}{\partial z}E_x = T_1 H_y$$

$$T_1^{j;n} = ik_0 \delta_{jn}$$

E.g. for TE polarisation

$$\frac{\partial}{\partial z}H_y = -\frac{1}{ik_0}\frac{\partial^2}{\partial y^2}E_x + ik_0\epsilon E_x$$

$$\frac{\partial}{\partial z}H_y = \frac{\partial}{\partial z}\sum_m H_{m,y}e^{i(k_{m,y}y)}$$

$$\Rightarrow \quad \frac{\partial}{\partial z}H_{i,y}$$

$$\frac{i}{k_0}\frac{\partial^2}{\partial y^2}E_x = \frac{i}{k_0}\frac{\partial^2}{\partial y^2}\sum_m E_{m,x}e^{i(k_{m,y}y)}$$

$$= -\frac{i}{k_0}\sum_m k_{m,y}^2 E_{m,x}e^{i(k_{m,y}y)}$$

$$\Rightarrow \quad -\frac{i}{k_0}k_{i,y}^2 E_{i,x}$$

E.g. for TE polarisation

$$ik_0 \epsilon E_x = ik_0 \sum_m \epsilon_m e^{i\mathbf{G}_m y} \sum_n E_{n,x} e^{ik_{n,y} y}$$

$$= ik_0 \sum_m \sum_n \epsilon_m E_{n,x} e^{i(\mathbf{G}_m y + k_{n,y} y)}$$

$$\Rightarrow \quad ik_0 \sum_m \sum_n \epsilon_m E_{n,x} e^{i(\mathbf{G}_m y + k_{n,y} y - k_{i,y} y)}$$

$$= ik_0 \sum_m \sum_n \epsilon_m E_{n,x} e^{i(m\frac{2\pi}{\Lambda_y} y + n\frac{2\pi}{\Lambda_y} y + k_y^0 y - i\frac{2\pi}{\Lambda_y} y - k_y^0 y)}$$

$$= ik_0 \sum_m \sum_n \epsilon_m E_{n,x} e^{i(m\frac{2\pi}{\Lambda_y} y + n\frac{2\pi}{\Lambda_y} y - i\frac{2\pi}{\Lambda_y} y)}$$

E.g. for TE polarisation

$$\Longrightarrow \quad ik_0 \sum_m \sum_n \epsilon_m E_{n,x} \int dy e^{i(m\frac{2\pi}{\Lambda_y}y + n\frac{2\pi}{\Lambda_y}y - i\frac{2\pi}{\Lambda_y}y)}$$

$$\int dy e^{i(m\frac{2\pi}{\Lambda_y}y + n\frac{2\pi}{\Lambda_y}y - i\frac{2\pi}{\Lambda_y}y)} = \delta_{m=i-n}$$

$$\Longrightarrow \quad ik_0 \sum_n \epsilon_{i-n} E_{n,x}$$

permittivity appears here as a Toeplitz matrix

E.g. for TE polarisation

$$\frac{\partial}{\partial z} H_y = -\frac{1}{ik_0}\frac{\partial^2}{\partial y^2} E_x + ik_0 \epsilon E_x$$

$$\frac{\partial}{\partial z} H_{i,y} = -\frac{i}{k_0} k_{i,y}^2 E_{i,x} + ik_0 \sum_n \epsilon_{i-n} E_{n,x}$$

$$\frac{\partial}{\partial z}\begin{bmatrix} H_{0,y} \\ H_{1,y} \\ \cdot \\ \cdot \\ \cdot \\ H_{n,x} \end{bmatrix} = \frac{i}{k_0}\begin{bmatrix} -k_{0,y}^2 + k_0^2\epsilon_0 & k_0^2\,\epsilon_{-1} & k_0^2\,\epsilon_{-2} & \cdot & \cdot & k_0^2\,\epsilon_{-n} \\ k_0^2\,\epsilon_1 & -k_{1,y}^2 + k_0^2\epsilon_0 & k_0^2\epsilon_{-1} & \cdot & \cdot & k_0^2\,\epsilon_{1-n} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & \cdot & \cdot & k_0^2\epsilon_1 & -k_{n,y}^2 + k_0^2\epsilon_0 \end{bmatrix}\begin{bmatrix} E_{0,x} \\ E_{1,x} \\ \cdot \\ \cdot \\ \cdot \\ E_{n,x} \end{bmatrix}$$

$$\frac{\partial}{\partial z} H_y = T_2 E_x$$

Eigenvalue problem in 2D

➡ **TE:**

$$\frac{\partial^2}{\partial z^2} E_x = (T_1 T_2)\, E_x$$

$$T_1^{j;n} = i k_0 \delta_{jn} \qquad T_2^{j;n} = \frac{i}{k_0}\left(-k_{j,y}^2 \delta_{jn} + k_0^2 \epsilon_{j-n}\right)$$

➡ **TM:**

$$\frac{\partial^2}{\partial z^2} E_y = (T_1 T_2)\, E_y$$

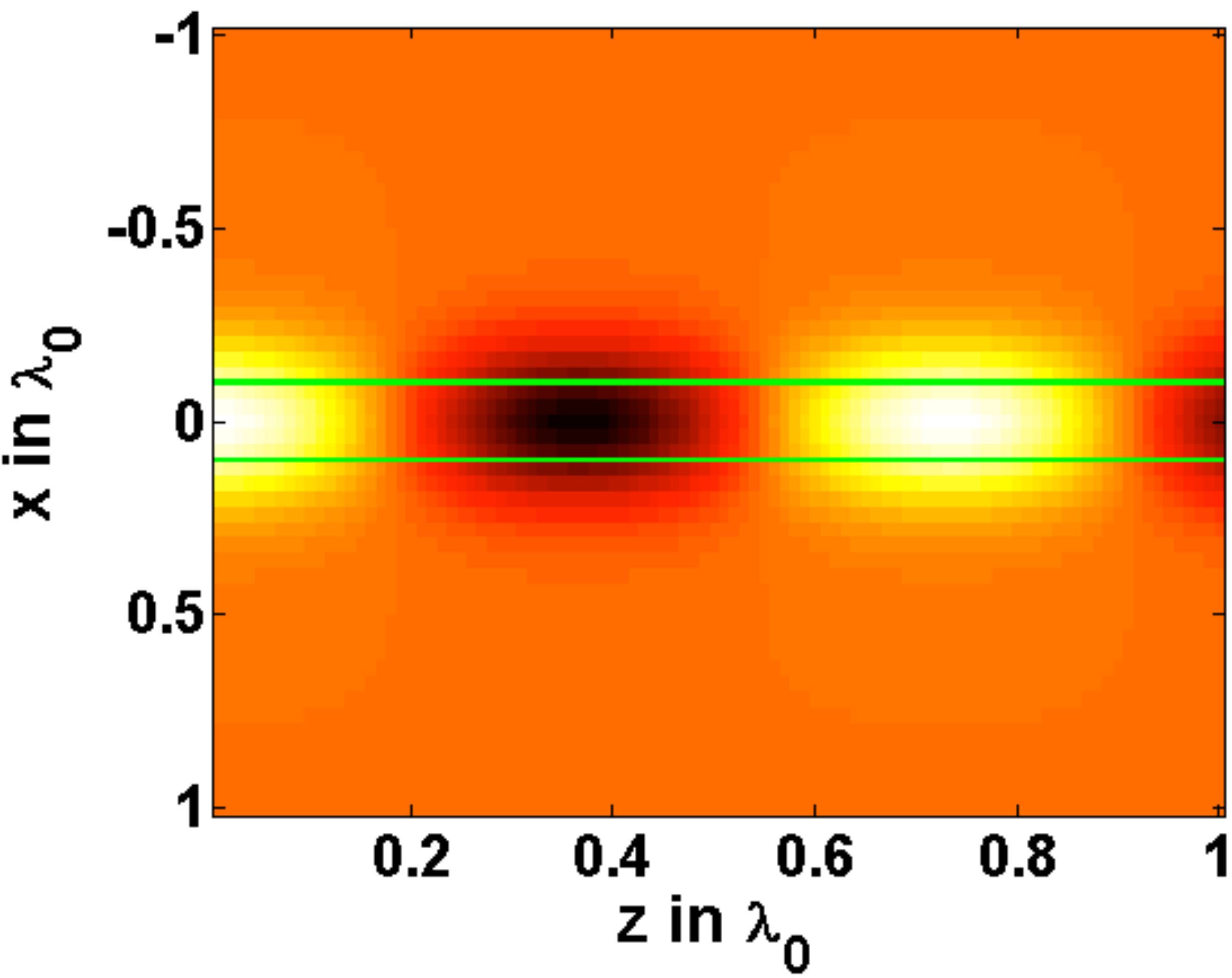
$$T_1^{j;n} = \frac{i}{k_0}\left(k_{j,y} \epsilon_{j-n}^{-1} k_{n,y} - k_0^2 \delta_{jn}\right) \qquad T_2^{j;n} = -i k_0 \left[1/\epsilon\right]_{j-n}^{-1}$$

➡ eigenvalues are propagation constants

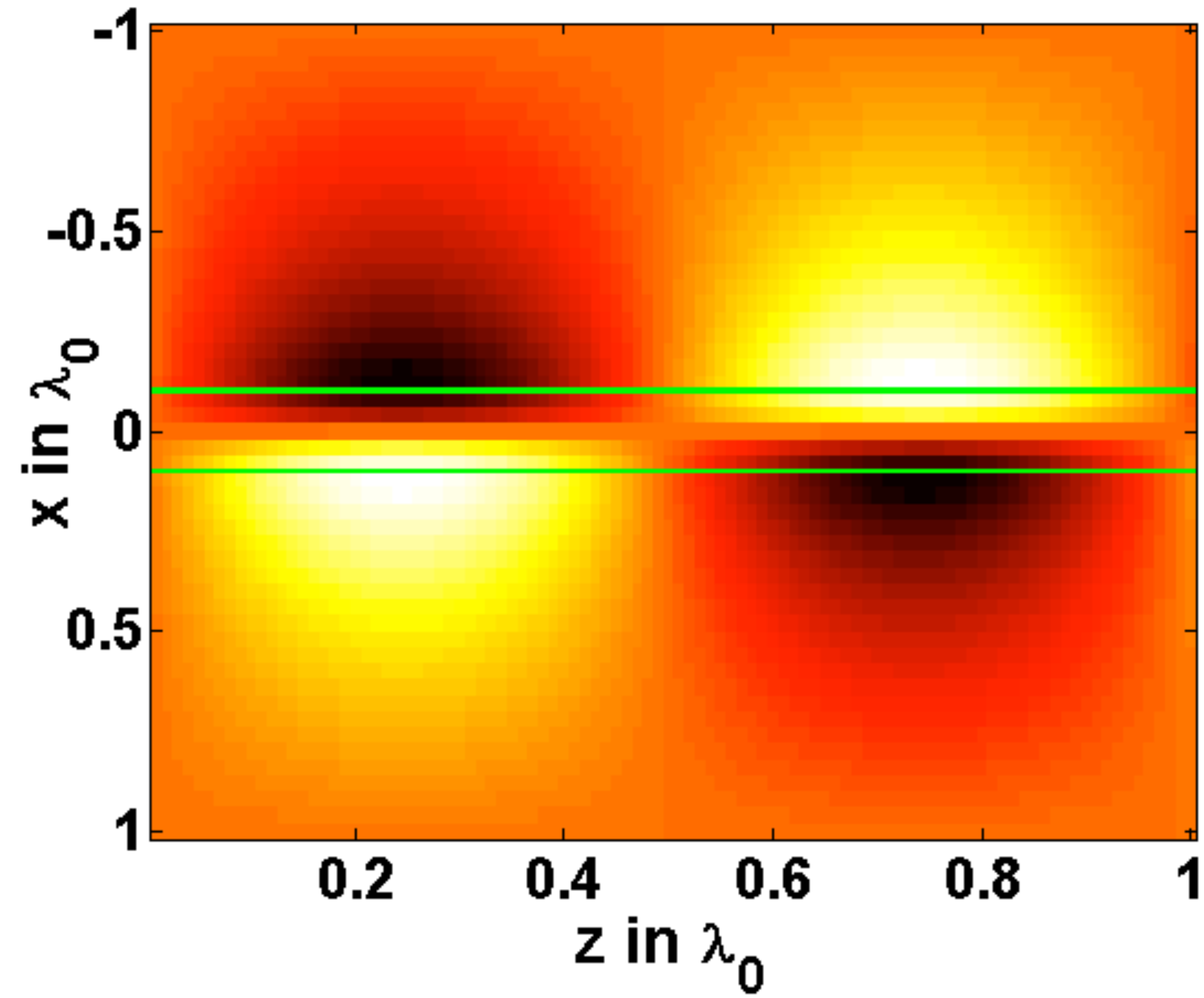
➡ eigenvectors are plane wave amplitudes of the respective mode

(Li et al., Phys. Rev. E, Vol. 67, 046607 2003)

Eigenvalue problem in 2D



fundamental mode

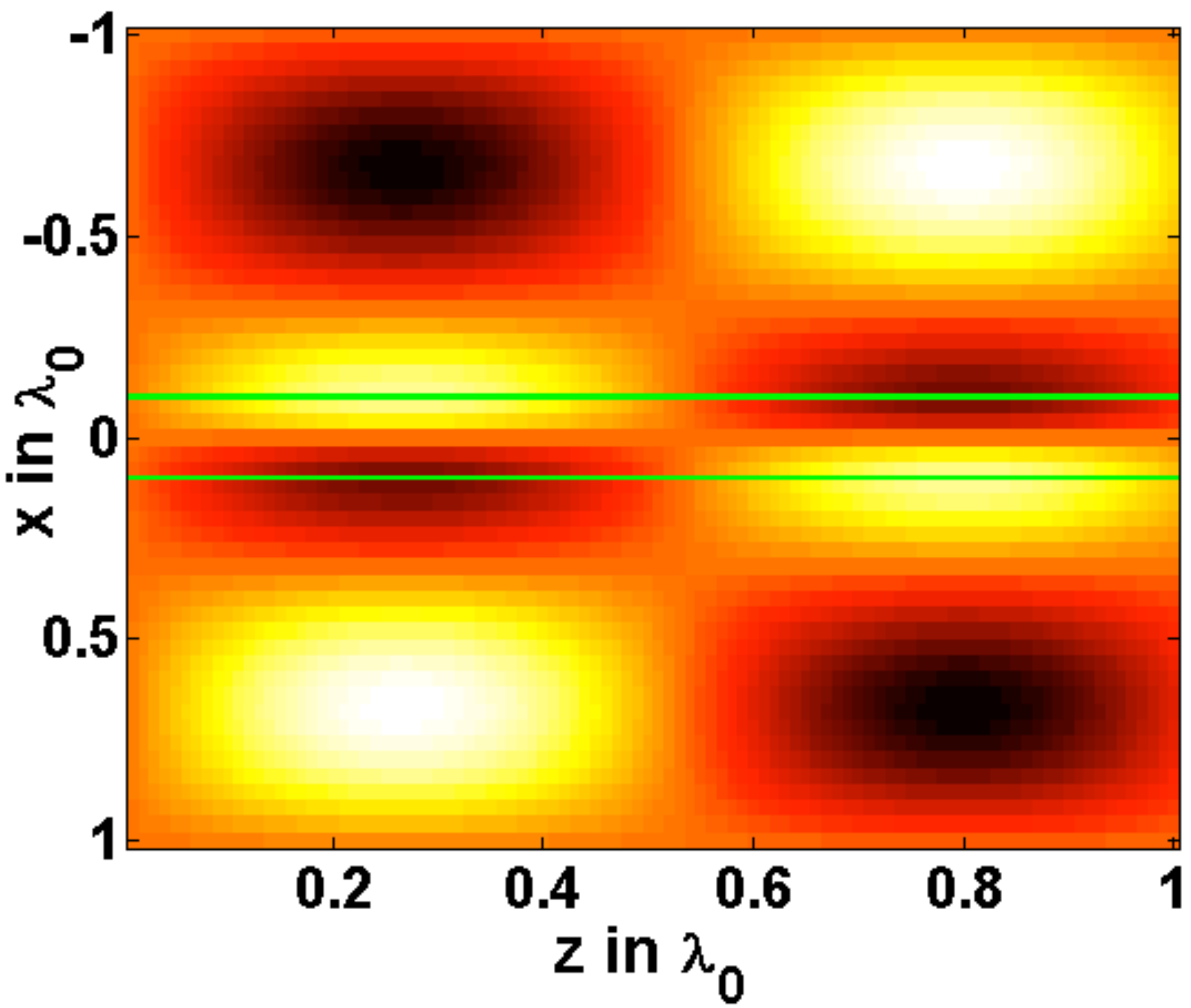


higher order guided mode

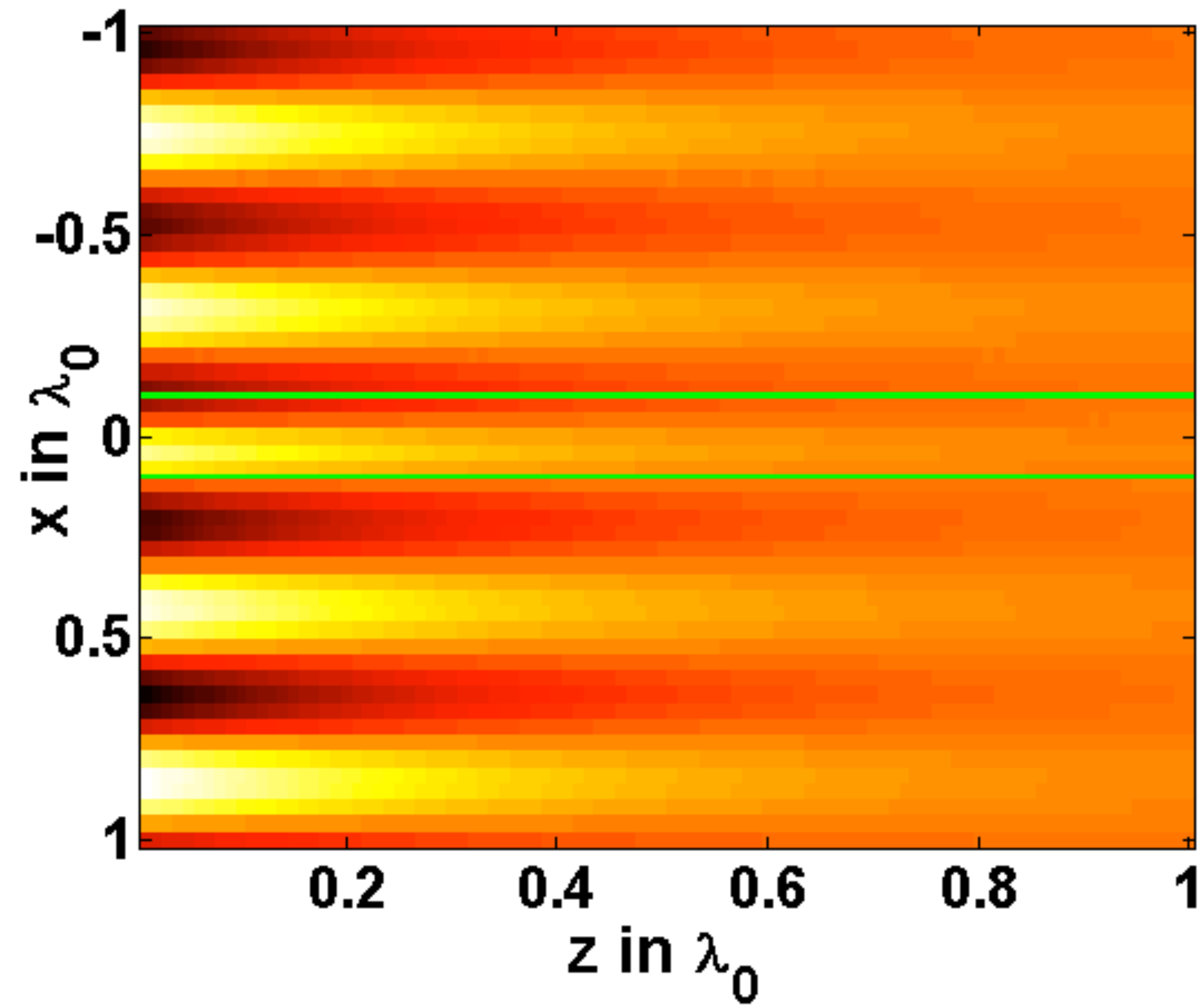
1D periodic waveguide array

(shown is the electric field upon propagating through a waveguide in z-direction)

Eigenvalue problem in 2D



guided mode with field localisation between the waveguides



evanescent mode

all possible eigenmodes are calculated using the method

Returning to the full 3D problem

$$\frac{\partial}{\partial z}E_x = \frac{1}{-ik_0}\frac{\partial}{\partial x}\left[\frac{1}{\epsilon}\left(\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x\right)\right] + ik_0 H_y$$

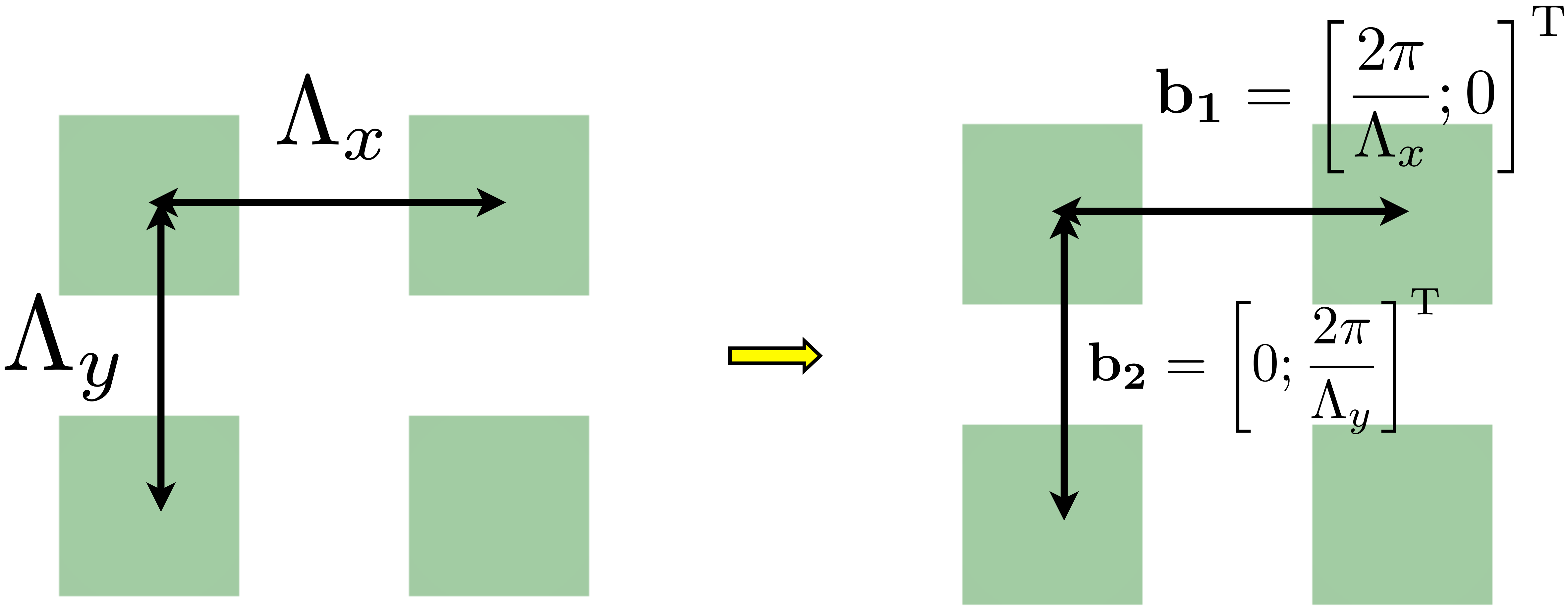
$$\frac{\partial}{\partial z}E_y = \frac{1}{-ik_0}\frac{\partial}{\partial y}\left[\frac{1}{\epsilon}\left(\frac{\partial}{\partial x}H_y - \frac{\partial}{\partial y}H_x\right)\right] - ik_0 H_x$$

$$\frac{\partial}{\partial z}H_x = \frac{1}{ik_0}\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x\right) - ik_0\epsilon E_y$$

$$\frac{\partial}{\partial z}H_y = \frac{1}{ik_0}\frac{\partial}{\partial y}\left(\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x\right) + ik_0\epsilon E_x$$

(Li et al., Phys. Rev. E, Vol. 67, 046607 2003)

Fourier expansion of all quantities



Real space **Reciprocal space**

- Fourier transformation in the x- and y-direction
- all quantities: $\mathbf{E}(\mathbf{r})$, $\mathbf{H}(\mathbf{r})$, $\epsilon(\mathbf{r})$, and $\epsilon^{-1}(\mathbf{r})$

Fourier expansion of all quantities

$$\mathbf{E}(\mathbf{r}) = \sum_{ij} \mathbf{E}_{ij}(z) e^{i(k_{ij,x}x + k_{ij,y}y)}$$

$$\mathbf{H}(\mathbf{r}) = \sum_{ij} \mathbf{H}_{ij}(z) e^{i(k_{ij,x}x + k_{ij,y}y)}$$

$$\mathbf{k_{ij}} = (k_{ij,x}, k_{ij,y}) = (k_{0x}, k_{0y}) + i\mathbf{b_1} + j\mathbf{b_2}$$

i and j run from $-\infty$ till ∞ have to be numerically truncated

Fourier expansion of all quantities

$$\epsilon(\mathbf{r}) = \sum_{ij} \epsilon_{ij} e^{i\mathbf{G}_{ij}\cdot\mathbf{r}}$$

$$\epsilon(\mathbf{r})^{-1} = \sum_{ij} \epsilon_{ij}^{-1} e^{i\mathbf{G}_{ij}\cdot\mathbf{r}}$$

$$\mathbf{G}_{ij} = i\mathbf{b_1} + j\mathbf{b_2}$$

i and j run from $-\infty$ till ∞ have to be numerically truncated

Fourier expansion of all quantities

⇨ plugging those Fourier expansions, e.g. into the third equation

e.g. $$\frac{\partial}{\partial z}H_x = \frac{1}{ik_0}\frac{\partial}{\partial x}\left(\frac{\partial}{\partial x}E_y - \frac{\partial}{\partial y}E_x\right) - ik_0\epsilon E_y$$

$$\frac{\partial}{\partial z}H_x = \frac{\partial}{\partial z}\sum_{mn} H_{mn,x}e^{i(k_{mn,x}x+k_{mn,y}y)}$$

$$\begin{aligned}\frac{\partial}{\partial x}E_y &= \frac{\partial}{\partial x}\sum_{mn} E_{mn,y}e^{i(k_{mn,x}x+k_{mn,y}y)} \\ &= \sum_{mn} ik_{mn,x}E_{mn,y}e^{i(k_{mn,x}x+k_{mn,y}y)}\end{aligned}$$

$$\epsilon E_y = \sum_{mn}\epsilon_{mn}e^{i(G_{mn,x}x+G_{mn,y}y)}\sum_{mn} E_{mn,y}e^{i(k_{mn,x}x+k_{mn,y}y)}$$

Fourier expansion of all quantities

⟹ multiply all terms with $e^{-i(k_{ij,x}x+k_{ij,y}y)}$

⟹ integrate over x and y

$$\iint e^{-i(k_{ij,x}x+k_{ij,y}y)}e^{i(k_{mn,x}x+k_{mn,y}y)}dxdy = \delta_{ij,mn}$$

$$\begin{aligned}\frac{\partial}{\partial z}\sum_{mn}\iint H_{mn,x}e^{i(k_{mn,x}x+k_{mn,y}y)}e^{-i(k_{ij,x}x+k_{ij,y}y)}dxdy &= \frac{\partial}{\partial z}\sum_{mn}H_{mn,x}\delta_{ij,mn}\\ &= \frac{\partial}{\partial z}H_{ij,x}\end{aligned}$$

⟹ doing the same with all the other terms

Introduction of the Fourier expansion

$$\frac{\partial}{\partial z}E_{ij,x} = \frac{-ik_{ij,x}}{k_0}\sum_{mn}\epsilon^{-1}_{ij;mn}(k_{mn,x}H_{mn,y} - k_{mn,y}H_{mn,x}) + ik_0 H_{ij,y}$$

$$\frac{\partial}{\partial z}E_{ij,y} = \frac{-ik_{ij,y}}{k_0}\sum_{mn}\epsilon^{-1}_{ij;mn}(k_{mn,x}H_{mn,y} - k_{mn,y}H_{mn,x}) - ik_0 H_{ij,x}$$

$$\frac{\partial}{\partial z}H_{ij,x} = \frac{ik_{ij,x}}{k_0}\sum_{mn}\delta_{ij;mn}(k_{mn,x}E_{mn,y} - k_{mn,y}E_{mn,x}) - ik_0\sum_{mn}\epsilon_{ij;mn}E_{mn,y}$$

$$\frac{\partial}{\partial z}H_{ij,y} = \frac{ik_{ij,x}}{k_0}\sum_{mn}\delta_{ij;mn}(k_{mn,x}E_{mn,y} - k_{mn,y}E_{mn,x}) + ik_0\sum_{mn}\epsilon_{ij;mn}E_{mn,x}$$

$$\epsilon_{ij,mn} = \epsilon_{i-m,j-n}$$

⇨ writing this system of equations in a matrix form simplifies life

Matrix form

$$\frac{\partial}{\partial z}E = T_1 H$$

$$\frac{\partial}{\partial z}H = T_2 E$$

$$E = (\cdots, E_{ij,x}, E_{ij,y}, \cdots)^T \quad H = (\cdots, H_{ij,x}, H_{ij,y}, \cdots)^T$$

$$T_1^{ij;mn} = \frac{i}{k_0}\begin{pmatrix} k_{ij,x}\epsilon^{-1}_{ij;mn}k_{mn,y} & -k_{ij,x}\epsilon^{-1}_{ij;mn}k_{mn,x} + k_0^2\delta_{ij;mn} \\ k_{ij,y}\epsilon^{-1}_{ij;mn}k_{mn,y} - k_0^2\delta_{ij;mn} & -k_{ij,y}\epsilon^{-1}_{ij;mn}k_{mn,x} \end{pmatrix}$$

$$T_2^{ij;mn} = \frac{i}{k_0}\begin{pmatrix} -k_{ij,x}\delta_{ij;mn}k_{mn,y} & k_{ij,x}\delta_{ij;mn}k_{mn,x} - k_0^2\epsilon_{ij;mn} \\ -k_{ij,y}\delta_{ij;mn}k_{mn,y} + k_0^2\epsilon_{ij;mn} & k_{ij,y}\delta_{ij;mn}k_{mn,x} \end{pmatrix}$$

2nd order DGL system

$$\frac{\partial^2}{\partial z^2} E = (T_1 T_2)\, E$$

- ⟹ Eigenvalue equation can be solved with standard routines
- ⟹ the infinite Fourier expansion is truncated up to

$$N_0 = (-N, ..., 0, ..., N)$$

- ⟹ $2N_0$ eigenvalues β_i^2 with $\Im(\beta_i) \geq 0$
  - ⟹ correspond to forward or backward propagating solution
  - ⟹ eigenvectors are associated with the eigenvalues
- ⟹ provide the Fourier components of the guided eigenmodes

Eigenmodes

- Eigenvectors are given in a matrix S_a with size $(2N_0) \times (2N_0)$
- fields are forward and backward propagating eigenmode

$$E = S_a \left(E_a^+ + E_a^- \right)$$

$$E_a^+ = \left[\ldots, E_{a,l}^+(z), \ldots \right]^T \qquad E_a^- = \left[\ldots, E_{a,l}^-(z), \ldots \right]^T$$

$$E_{a,l}^+(z) = A_l e^{i\beta_l z} \qquad E_{a,l}^-(z) = B_l e^{-i\beta_l z}$$

amplitudes have to be found from boundary problem

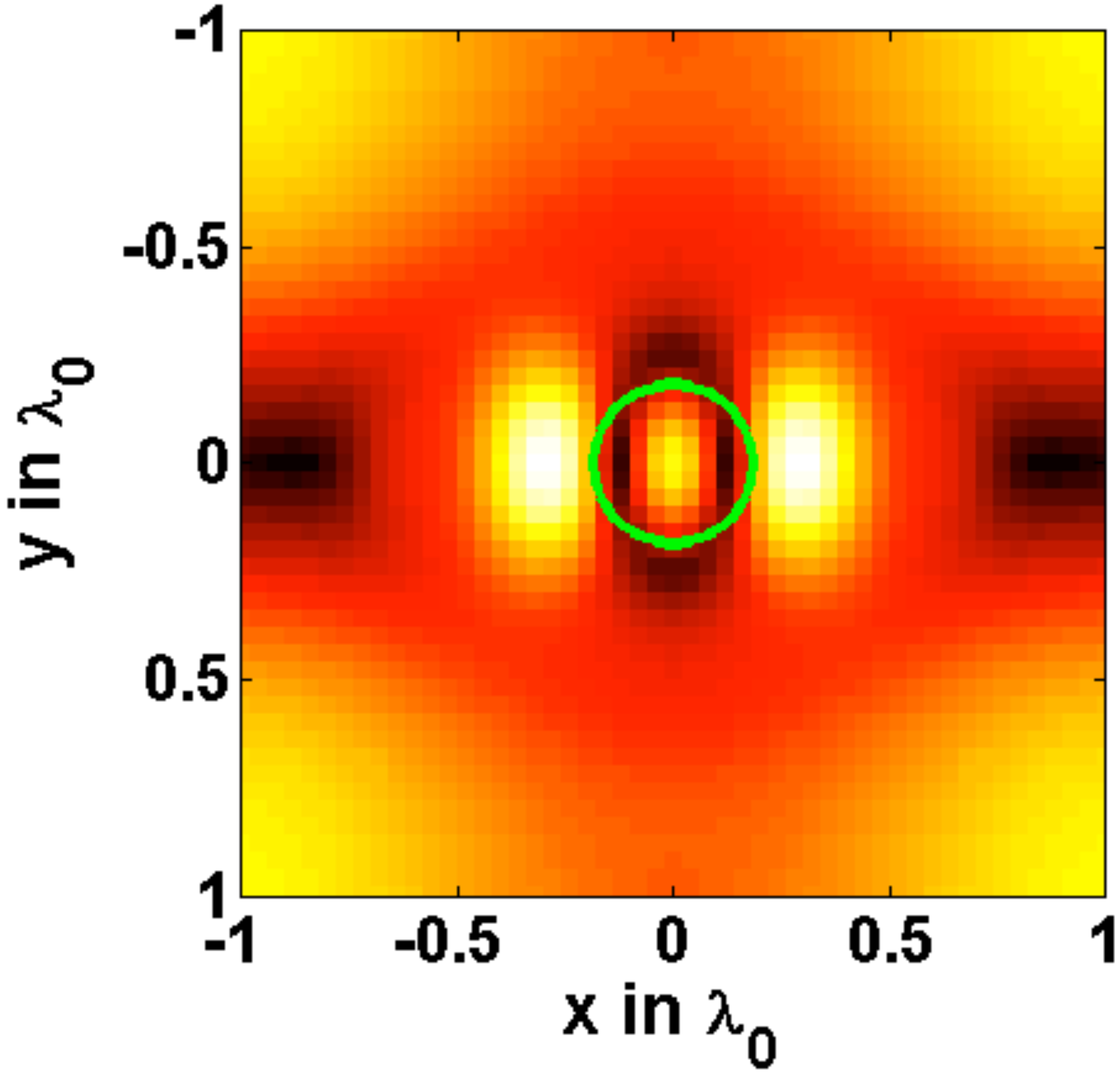
Magnetic field of eigenmodes

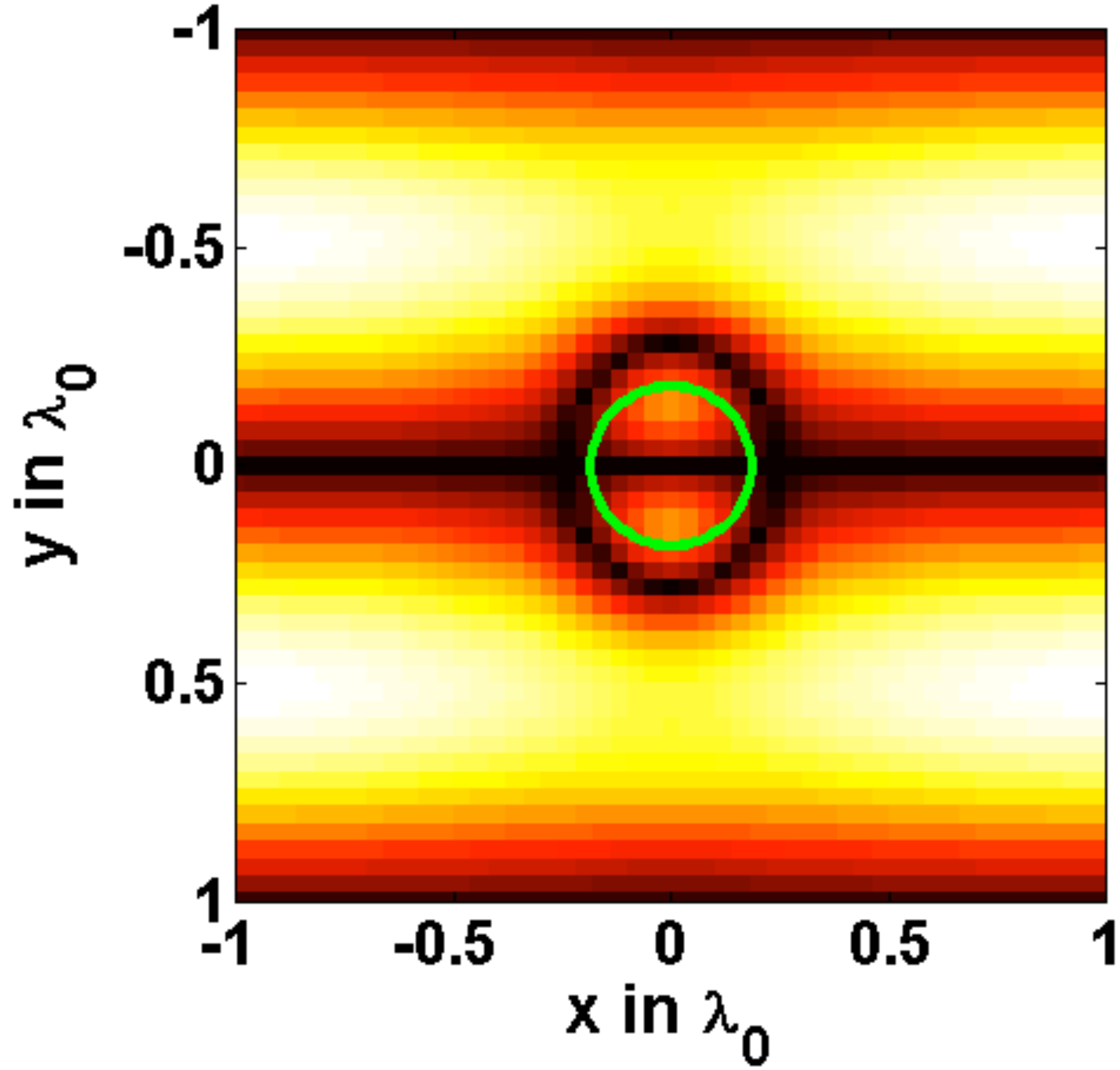
⇨ take the DGL 1st order from before

$$
\begin{aligned}
H &= T_1^{-1} \frac{\partial}{\partial z} E \\
&= T_1^{-1} S_a \frac{\partial}{\partial z} \left(E_a^+ + E_a^-\right) \\
&= T_1^{-1} S_a i\beta \left(E_a^+ + E_a^-\right) \\
&= T_a \left(E_a^+ + E_a^-\right)
\end{aligned}
$$

with: $$T_a = T_1^{-1} S_a i\beta$$

Examples of Eigenmodes





eigenmodes propagate in the waveguide normal to this plane

(periodic boundaries)

Computational Photonics

Basics of grating theories
- eigenmodes for a 1D grating