Computational Photonics
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0. Introduction and Motivation ................................................................. 3
  0.1 Why computational photonics? .......................................................... 3
  0.2 Maxwell’s equations ......................................................................... 4
    0.2.1 Maxwell’s equations in time domain . .......................................... 4
    0.2.2 Maxwell’s equations in frequency domain ...................................... 5
  0.3 Basic numerical operations ............................................................. 5
    0.3.1 Differentiation ............................................................................. 5
    0.3.2 Integration ................................................................................ 6
    0.3.3 Root Finding & Minimization/ Maximization ................................. 7
    0.3.4 Linear systems of equations ......................................................... 10
    0.3.5 Eigenvalue problems .................................................................. 11
    0.3.6 Discrete (Fast) Fourier transform - FFT ....................................... 11
    0.3.7 Ordinary differential equations (ODEs) ........................................ 12

1. Matrix method for stratified media ....................................................... 15
   1.1 Optical layer systems .................................................................... 15
   1.2 Derivation of the transfer matrix ................................................... 16
   1.3 Guided modes in layer systems ...................................................... 19

2. Finite-difference method for waveguide modes .................................... 23
   2.1 Stationary solutions of the scalar Helmholtz equation ....................... 23
   2.2 Matrix notation of the eigenvalue equation ...................................... 24
   2.3 Boundary conditions ..................................................................... 26

3. Beam Propagation Method (BPM) ....................................................... 27
   3.1 Categorization of Partial Differential Equation (PDE) problems ........ 27
   3.2 Slowly Varying Envelope Approximation (SVEA) ............................ 29
   3.3 Differential equations of BPM ....................................................... 30
   3.4 Semi-vector BPM ......................................................................... 31
   3.5 Scalar BPM .................................................................................. 32
   3.6 Crank-Nicholson method ............................................................... 32
   3.7 Alternating Direction Implicit (ADI) ............................................... 33
   3.8 Boundary condition ...................................................................... 33
   3.8.1 Absorbing Boundary Conditions (ABC) ....................................... 33
   3.8.2 Transparent Boundary Condition (TBC) ...................................... 35
   3.8.3 Perfectly matched layer boundaries (PML) .................................. 36
   3.9 Conformal mapping regions ........................................................... 37
   3.10 Wide-angle BPM based on Padé operators .................................... 39
     3.10.1 Fresnel approximation – Padé 0th order .................................. 40
     3.10.2 Wide angle (WA) approximation – Padé (1,1) .......................... 41

4. Finite Difference Time Domain Method (FDTD) .................................. 42
   4.1 Maxwell’s equations ...................................................................... 42
   4.2 1D problems ................................................................................ 43
     4.2.1 Solution with finite difference method in the time domain for $E_z$ .... 43
     4.2.2 Yee grid in 1D and Leapfrog time steps .................................... 46
   4.3 3D problems ............................................................................... 47
     4.3.1 Yee grid in 3D ....................................................................... 48
     4.3.2 Physical interpretation ............................................................. 49
     4.3.3 Divergence-free nature of the Yee discretization ......................... 50
     4.3.4 Computational procedure ....................................................... 51
<table>
<thead>
<tr>
<th>Section</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4</td>
<td>Simplification to 2D problems</td>
<td>52</td>
</tr>
<tr>
<td>4.5</td>
<td>Implementing light sources</td>
<td>52</td>
</tr>
<tr>
<td>4.6</td>
<td>Relation between frequency and time domain</td>
<td>53</td>
</tr>
<tr>
<td>4.7</td>
<td>Dispersive and nonlinear materials</td>
<td>55</td>
</tr>
<tr>
<td>4.8</td>
<td>Boundary conditions</td>
<td>57</td>
</tr>
<tr>
<td>5.1.1</td>
<td>The general eigenvalue problem for scalar fields</td>
<td>58</td>
</tr>
<tr>
<td>5.1.2</td>
<td>Properties of guided modes</td>
<td>58</td>
</tr>
<tr>
<td>5.1.3</td>
<td>Cylinder symmetric waveguides</td>
<td>60</td>
</tr>
<tr>
<td>5.1.4</td>
<td>Bessel’s differential equation</td>
<td>61</td>
</tr>
<tr>
<td>5.1.5</td>
<td>Analytical solutions of Bessel’s differential equation</td>
<td>62</td>
</tr>
<tr>
<td>5.1.6</td>
<td>Specifying the numerical problem</td>
<td>63</td>
</tr>
<tr>
<td>5.1.7</td>
<td>Solving the second order singularity</td>
<td>64</td>
</tr>
<tr>
<td>5.1.8</td>
<td>Numerical integration methods</td>
<td>64</td>
</tr>
<tr>
<td>5.1.9</td>
<td>Eigenvalue search</td>
<td>67</td>
</tr>
<tr>
<td>5.1.10</td>
<td>Calculation examples</td>
<td>67</td>
</tr>
<tr>
<td>5.1.11</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5.1.12</td>
<td></td>
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<td>5.1.13</td>
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<tr>
<td>5.99</td>
<td></td>
<td></td>
</tr>
<tr>
<td>6.1</td>
<td>Formulation of the problem in 2D for TE</td>
<td>71</td>
</tr>
<tr>
<td>6.2</td>
<td>Scalar theory for thin elements</td>
<td>72</td>
</tr>
<tr>
<td>6.3</td>
<td>Rigorous grating solver</td>
<td>74</td>
</tr>
<tr>
<td>6.3.1</td>
<td>Calculation of eigenmodes in Fourier space</td>
<td>75</td>
</tr>
<tr>
<td>6.3.2</td>
<td>Explicit derivation for 2D problems</td>
<td>79</td>
</tr>
</tbody>
</table>
0. Introduction and Motivation

0.1 Why computational photonics?
- it’s a numerical experiment
- provides insides to inaccessible domain
- permits to interpret and understand experimental results
- simplifies the design of functional elements
- explores prospective applications presently not realizable
- with available large scale computational resources it became an inevitable tool in the world of micro- and nanooptics

What is light?
- „Light is like an odor an emanation of our body“
  Epikur (Greek philosopher, 341-271 BC)
- Straight „Light-Ray“ as an abstract imagination
  Euklid in „Elements“ (365 - ca. 300 BC)
- Light is an electromagnetic wave
  J. C. Maxwell 1873 (Propagation and interaction of light with matter)
- Light consists of particles (Photons)
  A. Einstein 1905 (Creation and absorption)
- Light is particle and wave
  De Broglie 1923 (quantum mechanics)

Formulation of the problem:
For a specific geometry and a particular set of boundary conditions Maxwell's equations have to be solved (with or without approximations)
⇒ Description of the interaction of electromagnetic waves with matter
- Initially published 1873 by James Clark Maxwell
- Experimental proof by Heinrich Rudolf Hertz 1884 (speed of radio waves corresponds to the speed of light)
0.2 Maxwell’s equations

0.2.1 Maxwell’s equations in time domain

\[
\begin{align*}
\text{rot } \mathbf{E}(r,t) &= -\frac{\partial \mathbf{B}(r,t)}{\partial t}, \\
\text{rot } \mathbf{H}(r,t) &= \mathbf{j}_{\text{makr}}(r,t) + \frac{\partial \mathbf{D}(r,t)}{\partial t}, \\
\text{div } \mathbf{D}(r,t) &= \mathbf{\rho}_{\text{ext}}(r,t), \\
\text{div } \mathbf{B}(r,t) &= 0,
\end{align*}
\]

(1)

\( - \mathbf{E}(r,t) \) electric field \([\text{V m}^{-1}]\)

\( - \mathbf{H}(r,t) \) magnetic field \([\text{A m}^{-1}]\)

\( - \mathbf{D}(r,t) \) dielectric flux density \([\text{As m}^{-2}]\)

\( - \mathbf{B}(r,t) \) magnetic flux density \([\text{Vs m}^{-2}]\)

\( - \mathbf{\rho}_{\text{ext}}(r,t) \) external charge density \([\text{As m}^{-3}]\)

\( - \mathbf{j}_{\text{makr}}(r,t) \) macroscopic current density \([\text{A m}^{-2}]\)

(Usually there are no external charges or currents in optics.)

\textbf{Matter equations in time domain}

\[
\begin{align*}
\mathbf{D}(r,t) &= \varepsilon_0 \mathbf{E}(r,t) + \mathbf{P}(r,t), \\
\mathbf{B}(r,t) &= \mu_0 \mathbf{H}(r,t) + \mathbf{M}(r,t)
\end{align*}
\]

(2)

\( - \mathbf{P}(r,t) \) dielectric polarization \([\text{As m}^{-2}]\)

\( - \mathbf{M}(r,t) \) magnetic polarization (magnetization) \([\text{Vs m}^{-2}]\)

\( - \varepsilon_0 \) permittivity of vacuum \(\varepsilon_0 = (\mu_0 c_0^2)^{-1} = 8.85 \times 10^{-12} \text{ As/Vm}\)

\( - \mu_0 \) permeability of vacuum \(\mu_0 = 4\pi \times 10^{-12} \text{ Vs/Am}\)

in linear, local, isotropic Media in optics

\[
\begin{align*}
\mathbf{P}(r,t) &= \varepsilon_0 \int_0^\infty \mathbf{R}(r,t')\mathbf{E}(r,t-t')\,dt', \\
\mathbf{M}(r,t) &= 0
\end{align*}
\]

(3)

with \( \mathbf{R}(r,t') \) being the response function
0.2.2 Maxwell’s equations in frequency domain
Using Fourier transformation to transform into frequency space
\[ \mathbf{V}(\mathbf{r}, t) = \int_{-\infty}^{\infty} \mathbf{\tilde{V}}(\mathbf{r}, \omega) \exp(-i\omega t) d\omega, \quad \mathbf{\tilde{V}}(\mathbf{r}, \omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathbf{V}(\mathbf{r}, t) \exp(i\omega t) dt. \] (4)

Maxwell’s equations in frequency domain by \( \frac{\partial}{\partial t} \mathbf{\tilde{F}}(\mathbf{r}, \omega) = -i\omega \mathbf{\tilde{F}}(\mathbf{r}, \omega) \)
\[ \text{rot} \mathbf{\tilde{E}}(\mathbf{r}, \omega) = i\omega \mathbf{\tilde{B}}(\mathbf{r}, \omega), \quad \text{rot} \mathbf{\tilde{H}}(\mathbf{r}, \omega) = -i\omega \mathbf{\tilde{D}}(\mathbf{r}, \omega), \]
\[ \text{div} \mathbf{\tilde{D}}(\mathbf{r}, \omega) = \rho(\mathbf{r}, \omega), \quad \text{div} \mathbf{\tilde{B}}(\mathbf{r}, \omega) = 0. \] (5)

\[ \text{Matter equations in frequency domain} \]
\[ \chi(\mathbf{r}, \omega) = \int_{-\infty}^{\infty} R(\mathbf{r}, t) \exp(i\omega t) \partial t \] (6)
with \( \chi(\mathbf{r}, \omega) \) being the material’s susceptibility, which is connected to the dielectric constant \( \varepsilon(\mathbf{r}, \omega) \) by
\[ \varepsilon(\mathbf{r}, \omega) = 1 + \chi(\mathbf{r}, \omega) \]
\[ \mathbf{\tilde{P}}(\mathbf{r}, \omega) = \varepsilon_0 \chi(\mathbf{r}, \omega) \mathbf{\tilde{E}}(\mathbf{r}, \omega) \quad \mathbf{\tilde{D}}(\mathbf{r}, \omega) = \varepsilon_0 \chi(\mathbf{r}, \omega) \mathbf{\tilde{E}}(\mathbf{r}, \omega) \]
\[ \mathbf{\tilde{M}}(\mathbf{r}, \omega) = 0 \quad \mathbf{\tilde{B}}(\mathbf{r}, \omega) = \mu_0 \mathbf{\tilde{H}}(\mathbf{r}, \omega) \] (7)

0.3 Basic numerical operations

0.3.1 Differentiation
Derived from the definition of differentiation, e.g. right-sided/forward difference equation
\[ \frac{\partial f(x)}{\partial x} = f'(x) = \lim_{h \to 0} \frac{f(x + h) - f(x)}{h} \]
for finite \( h \)
\[ f''(x) \approx D_h[f(x)] = \frac{f(x + h) - f(x)}{h} \]
or left-sided/backward
\[ D_h[f(x)] = \frac{f(x) - f(x - h)}{h} \]
or central operator
\[ D_h[f(x)] = \frac{f(x + h) - f(x - h)}{2h} \]
higher order differentiation
\[ f''(x) \approx D_h^2[f(x)] = \frac{f(x-h) - 2f(x) + f(x+h)}{h^2} \]

### 0.3.2 Integration

\[ A = \int_a^b dx \, f(x) = \sum_{i=0}^{N-1} \int_{x_i}^{x_{i+1}} dx \, f(x) \]

with \( I_i = [x_i, x_{i+1}] \) where \( x_{i+1} = x_i + h \) and \( h = (b-a) / N \) with \( x_0 = a \), \( x_N = b \)

\[ \text{Decomposition of the full integration interval } [a, b] \text{ into } N \text{ equivalent partial intervals } I_i = [x_i, x_{i+1}] \].

Implementation example: rectangle rule

in each interval the mean value of the function is approximated by

\[ \bar{f}(x_i) \approx f_i \frac{1}{2} = f\left(x_i + \frac{h}{2}\right) \]

resulting in an integral approximation

\[ A \approx \sum_{i=0}^{N-1} \int \frac{1}{2} dx f_i \frac{1}{2} = \sum_{i=0}^{N-1} h f_i \frac{1}{2} = \frac{b-a}{N} \sum_{i=0}^{N-1} f_i \frac{1}{2} \]

\[ \text{Rectangle rule for approximation of integrals.} \]
0.3.3 Root Finding & Minimization/Maximization

Root finding of a single isolated root in one dimension.

**Secant method for 1D**

Iterative solution by

\[ x_{i+1} = x_i - f(x_i) \frac{x_i - x_{i-1}}{f(x_i) - f(x_{i-1})} \]

until

\[ |f(x_i) - f(x_{i-1})| \leq 10 \varepsilon |f(x_i)| \]

with \( \varepsilon \) determined by the desired accuracy.

Illustration of the secant method (The individual points are numbered in the order of the iterations.)
function [x,i,status] = secant_method(x0,x1,tol1,tol2,no)

% Secant method
% x0, x1: start value
% tol1, tol2: tolerance
% no: maximum number iterations

% graphic output
ab = -0.4; x_old=1000; fx_old=1000;
axis on;
plot([-5 5],[0 0]); % plotting x-axis
hold on;
set(findobj(gca,'Type','line','Color', [0 0 1]),'Color','black','LineWidth',1)
p=(-5):0.1:(5);
for i=1:1:(101)
    f(i) = f1(p(i));
end
plot(p,f,'LineWidth',1);

i = 0; fa = f1(x0); fb = f1(x1);
if abs(fa) > abs(fb)
a = x0; b = x1;
else
    a = x1; b = x0; tmp = fb; fb = fa; fa = tmp;
end

% iteration of the secant
while i < no
    s=fb/fa; r=1-s;
t=s*(a-b); % ascent between two points of the secant
    x=b-t/r; % step towards root
    fx=f1(x); % converging towards root
    % output of points of the secant
    if abs(x_old-x)<0.3 && abs(fx_old-fx)<0.3
        ab=ab-0.2;
    end
    x_old=x; fx_old=fx;
    plot(x,fx,'ro','LineWidth',1);
text(x+ab, fx,num2str(i+1),'HorizontalAlignment','left')
end
if t == 0
    status = 'Method did not converge.'; return
end
if abs(fx) < tol1
    status = 'Method converged and calculated solution.'; return
end
if abs(x-b) < tol2*(1+abs(x))
    status = 'Method converged and calculated solution.'; return
end
45        end
46        i = i+1;
47        if abs(fx) > abs(fb)
48            a = x; fa = fx;
49        else
50            a = b; fa = fb; b = x; fb = fx;
51        end
52    end
53    status = 'Number iterations exceeded.';

**Minima of higher-dimensional functions by minimization along alternating directions**

Approach: solution of multiple one-dimensional minimizations in alternating directions.

Starting from point $\mathbf{P}_1$ into direction $\mathbf{u}_1$

$$\{\mathbf{P}_1, \mathbf{u}_1\}$$

and iteratively minimizing

$$\min \left(f\left(\mathbf{P}_1 + \lambda_i \mathbf{u}_1\right)\right) \quad \mathbf{P}_2 = \mathbf{P}_1 + \lambda_i \mathbf{u}_1$$

$$\min \left(f\left(\mathbf{P}_2 + \lambda_i \mathbf{u}_2\right)\right) \quad \mathbf{P}_3 = \mathbf{P}_2 + \lambda_i \mathbf{u}_2$$

$$\vdots$$

$$\min \left(f\left(\mathbf{P}_n + \lambda_i \mathbf{u}_i\right)\right) \quad \mathbf{P}_i = \mathbf{P}_{i-1} + \lambda_i \mathbf{u}_i$$

until no further improvement can be obtained along any direction.

Choosing directions along steepest descent (opposite to gradient)

$$\mathbf{P}_{i+1} = \mathbf{P}_i - \lambda_i \nabla f(\mathbf{P}_i) \text{ mit } \lambda_i = \min_{t \in \mathbb{R}} \left(f\left(\mathbf{P}_i - t \nabla f(\mathbf{P}_i)\right)\right)$$

Examples of easy and difficult converging surfaces.
0.3.4 Linear systems of equations

System of algebraic equations

\[
\begin{align*}
    a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1n}x_n &= b_1 \\
    a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2n}x_n &= b_2 \\
    a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \ldots + a_{3n}x_n &= b_3 \\
    \vdots \\
    a_{m1}x_1 + a_{m2}x_2 + a_{m3}x_3 + \ldots + a_{mn}x_n &= b_m
\end{align*}
\]

in matrix representation

\[
\hat{A}\vec{x} = \vec{b}
\]

with \(\hat{A}\) being a coefficient matrix and \(\vec{b}\) a column vector

\[
\hat{A} = \begin{pmatrix}
    a_{11} & a_{12} & \ldots & a_{1n} \\
    a_{21} & a_{22} & \ldots & a_{2n} \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{m1} & a_{m2} & a_{m3} & a_{m4}
\end{pmatrix}, \quad \vec{b} = \begin{pmatrix}
    b_1 \\
    b_2 \\
    \vdots \\
    b_m
\end{pmatrix}
\]

alternative formulation of the problem \(f(\vec{x}) = 0\) with

\[
f_i(\vec{x}) = \sum_{j=1}^{n} a_{ij}x_j - b_i \quad \text{and} \quad j = 1, \ldots, n; \quad i = 1, \ldots, m
\]

Types of problems:

- \(\hat{A}\vec{x} = \vec{b}\)
- calculating the inverse matrix \(\hat{A}^{-1}\) with \(\hat{A}\hat{A}^{-1} = \hat{E} \Rightarrow\) equivalent to
  \(\hat{A}\vec{x}_j = \vec{b}_j\) with \(j = 1, \ldots, N\) and \(b_j = 1\), and all other 0, then \(\hat{A}^{-1} = (\vec{x}_1, \ldots, \vec{x}_N)\)

Important matrix properties:

1. \(n = m \Rightarrow\) same number of equations and unknowns
2. hermite matrix \(\Rightarrow\) \(\hat{A}^\dagger = \hat{A}\) (komplex conjugate and transposed)
3. positiv definite \(\Rightarrow\) \(\vec{v}^\dagger \hat{A} \vec{v} > 0 \quad \forall \vec{v}\)
4. band matrix

5. sparse matrix \(\Rightarrow\) most matrix coefficients are zero
   \(\Rightarrow\) always use adapted solution schemes
0.3.5 Eigenvalue problems

\[ \hat{M} \cdot \vec{x} = \lambda \vec{x} \quad \text{with} \quad \lambda = \frac{\Omega^2}{\omega^2} \rightarrow (\hat{M} - \lambda \hat{E}) \vec{x} = 0 \]

\[ \Rightarrow \] characteristic polynomial \[ \det[\hat{M} - \lambda \hat{E}] = P(\lambda) = 0 \] to have solutions of \[ (\hat{M} - \lambda \hat{E}) \vec{x} = 0 \] which are not identical zero

0.3.6 Discrete (Fast) Fourier transform - FFT

Starting from periodic function \[ f(x \pm L) = f(x) \]

Periodic original space with set of discrete points with period \( L \) and step size \( a \)

\[ \{x\} = \{0, a, 2a, \ldots, L - a\} \]

Periodic frequency space with set of discrete frequencies

\[ \{k\} = \{0, 1 \cdot \frac{2\pi}{L}, 2 \cdot \frac{2\pi}{L}, \ldots, [\frac{L}{a} - 1] \cdot \frac{2\pi}{L}\} \quad \text{with} \quad \frac{L}{a} = N \]

Definition of discrete Fourier transform (FT)

\[ \tilde{f}(k) = a \sum_{x} e^{-ikx} f(x) \]

with \( N = \frac{L}{a}, \quad k = n \cdot \frac{2\pi}{L} \quad (0 \leq n < N), \quad x = n \cdot a \)

and inverse discrete Fourier transform (FT⁻¹)

\[ f(x) = \frac{1}{L} \sum_{k} e^{ikx} \tilde{f}(k) \]

General property: \( f(x) \rightarrow \text{FT} \rightarrow \tilde{f}(k) \rightarrow \text{FT}^{-1} \rightarrow f(x) \)
Illustration of decomposition of periodic function into harmonic functions.

**Generalization for higher dimensions**

with \((x \rightarrow x'; k \rightarrow k')\), e.g. for 3 dimensions

\[

tilde{f}(\tilde{k}) = a^3 \sum_x e^{-i\tilde{k}\tilde{x}} f(\tilde{x})
\]

\[
f(\tilde{x}) = \frac{1}{L^3} \sum_k e^{i\tilde{k}\tilde{x}} \tilde{f}(\tilde{k})
\]

**0.3.7 Ordinary differential equations (ODEs)**

General form of ordinary differential equation

\[
\frac{d^n f(t)}{dt^n} = G(f, f', \ldots, f^{(n-1)}, t)
\]

distinction of initial value problems and boundary value problems

**Initial value problems (AWA)**

initial values

\[
f(t = 0), f'(t = 0), \ldots, f^{(n-1)}(t = 0)
\]
equivalent to system of coupled first order differential equations

\[
\begin{align*}
\frac{df_1(t)}{dt} &= G_1(f_1, f_2, \ldots, f_n, t) \\
\frac{df_2(t)}{dt} &= G_2(f_1, f_2, \ldots, f_n, t) \\
\frac{df_3(t)}{dt} &= G_3(f_1, f_2, \ldots, f_n, t) \\
&\vdots \\
\frac{df_n(t)}{dt} &= G_n(f_1, f_2, \ldots, f_n, t)
\end{align*}
\]

Simple solution method

**Forward Euler scheme**

problem:

\[ f'(t) = G(f(t), t) \]

transformed into difference equation:

\[ f'(t) = D_{\Delta t} \left[ f(t) \right] = \frac{f(t + \Delta t) - f(t)}{\Delta t} = G(f(t), t) \]

with discretization \( \Delta t \): \( f_n := f(n \cdot \Delta t) \)

results in difference equation

\[ \frac{f_{n+1} - f_n}{\Delta t} = G(f_n, t) \]

and recursion formula for the solution of the ODE

\[ f_{n+1} = f_n + \Delta t \cdot G(f_n, t) \]
**Limitation: global error**

![Graph showing error vs. discretization and round off error](image)

**Limitation: instability**

![Graph showing instability scheme of harmonic oscillator equation](image)

*Instability scheme of harmonic oscillator equation.*
1. Matrix method for stratified media

1.1 Optical layer systems

Previously: transmission problems

– Bragg mirrors
– chirped mirrors for dispersion compensation
– interferometers

Today: guided modes

– multi layer waveguides
– Bragg waveguides

Fields in the layer system

Prerequisites:
– stationary
– layers in y-z-plane
– incident fields in x-z-plane

Ansatz:
\[ E_r(x, z, t) = \text{Re} \left[ E(x) \exp(ik_z z - i\omega t) \right] \]
\[ H_r(x, z, t) = \text{Re} \left[ H(x) \exp(ik_z z - i\omega t) \right] \]

Decomposition in TE and TM fields:
1.2 Derivation of the transfer matrix

Transition conditions
Fields: \( E_t \) and \( H_t \) continuous \( \Rightarrow \) TE: \( E_y \) and \( H_z \) \( \Rightarrow \) Calculation of tangential components (normal components can be derived from them)

wave vector component \( k_z \) \( \Rightarrow \) conserved throughout the layer system (determined by incidence angle)

wave vector component \( k_x \) \( \Rightarrow \) constant in a single homogeneous layer but varies from layer to layer

\[
k_{x_i}^2 = \frac{\omega^2}{c^2} \varepsilon_i(\omega) - k_z^2
\]

Field calculation of continuous components (TE)

\[
\begin{bmatrix}
\frac{\partial^2}{\partial x^2} + \frac{\omega^2}{c^2} \varepsilon_i(\omega) - k_{x_i}^2
\end{bmatrix} E_y(x) = 0 \quad \text{and} \quad H_x(x) = -\frac{i}{\omega \mu_0} \frac{\partial}{\partial x} E_y(x)
\]

Solution:

\[
E_y(x) = C_1 \cos(k_{x_i} x) + C_2 \sin(k_{x_i} x)
\]

\[
i \omega \mu_0 H_z(x) = \frac{\partial}{\partial x} E_y(x) = k_{x_i} \left[ -C_1 \sin(k_{x_i} x) + C_2 \cos(k_{x_i} x) \right]
\]

Determination of \( C_1, C_2 \) by \( E_y(0) = C_1 \) and \( \left. \frac{\partial}{\partial x} E_y \right|_0 = k_{x_i} C_2 \)

TE:

\[
E_y(x) = \cos(k_{x_i} x) E_y(0) + \frac{1}{k_{x_i}} \sin(k_{x_i} x) \left. \frac{\partial}{\partial x} E_y \right|_0
\]

\[
\frac{\partial}{\partial x} E_y = -k_{x_i} \sin(k_{x_i} x) E_y(0) + \cos(k_{x_i} x) \left. \frac{\partial}{\partial x} E_y \right|_0
\]
TM:

\[
H_y(x) = \cos\left(k_{\perp} x\right)H_y(0) + \frac{\varepsilon_i}{k_{\perp}} \sin\left(k_{\perp} x\right) \frac{1}{\varepsilon_i} \frac{\partial}{\partial x} H_y(0)
\]

\[
\frac{1}{\varepsilon_i} \frac{\partial}{\partial x} H_y = -\frac{k_{\perp}}{\varepsilon_i} \sin\left(k_{\perp} x\right) H_y(0) + \cos\left(k_{\perp} x\right) \frac{1}{\varepsilon_i} \frac{\partial}{\partial x} H_y(0)
\]

Combined TE/TM:

\[
F(x) = \cos\left(k_{\perp} x\right)F(0) + \frac{1}{\alpha_i k_{\perp}} \sin\left(k_{\perp} x\right)G(0)
\]

\[
G(x) = -\alpha_i k_{\perp} \sin\left(k_{\perp} x\right)F(0) + \cos\left(k_{\perp} x\right)G(0)
\]

TE: \( F = E_y \), \( G = i\omega\mu_0 H_z = \frac{\partial}{\partial x} E_y \), \( \alpha_i = 1 \)

TM: \( F = H_y \), \( G = -i\omega\varepsilon_0 E_z = \alpha_i \frac{\partial}{\partial x} H_y \), \( \alpha_i = 1/\varepsilon_i \)

Summary matrix method:

given: \( F(0), G(0), k_z, \varepsilon_i, d_i \)

\[
k_{\perp}(k_z, \omega) = \left(\frac{2\pi}{\lambda_0}\right)^2 \varepsilon_i(\omega) - k_z^2
\]

to be calculated fields: \( F(D), G(D) \)

\[
\begin{pmatrix}
F \\
G
\end{pmatrix}_D = \prod_{i=1}^{N} \hat{m}_i(d_i) \begin{pmatrix}
F \\
G
\end{pmatrix}_0 = \hat{M} \begin{pmatrix}
F \\
G
\end{pmatrix}_0
\]

with \( \hat{m}_i(x) = \begin{bmatrix}
\cos(k_{\perp}d_i) & \frac{1}{k_{\perp}} \sin(k_{\perp}d_i) \\
-k_{\perp} \alpha_i & \cos(k_{\perp}d_i)
\end{bmatrix} \)

TE: \( F = E_y \), \( G = \frac{\partial}{\partial x} E_y \), \( \alpha_i = 1 \)

TM: \( F = H_y \), \( G = \alpha_i \frac{\partial}{\partial x} H_y \), \( \alpha_i = 1/\varepsilon_i \)
Reflection and transmission coefficients for fields

Transmission coefficient (T) and reflection coefficient (R)

$$T = \frac{F_T}{F_{in}}$$

$$R = \frac{F_R}{F_{in}}$$

$$R = \frac{\alpha_s k_{sx} M_{22} - \alpha_c k_{cx} M_{11} - \mathfrak{i}(M_{21} + \alpha_s k_{sx} \alpha_c k_{cx} M_{12})}{N}$$

$$T = \frac{2\alpha_s k_{sx}}{N}$$

$$N = \alpha_s k_{sx} M_{22} + \alpha_c k_{cx} M_{11} + \mathfrak{i}(M_{21} - \alpha_s k_{sx} \alpha_c k_{cx} M_{12})$$

$$k_{s/c x}^2 = \left(\frac{2\pi}{\lambda_0}\right)^2 \frac{\varepsilon_{s/c}}{(\lambda_0)} - k_z^2$$

Energy flux

defined by the normal component of the Poynting vectors sx

$$\tau = \frac{S_{xT}}{S_{sx in}}$$

$$\rho = \frac{S_{xR}}{S_{sx in}}$$

$$\rho = |R|^2$$

$$\tau = \frac{\alpha_c \text{Re}(k_{cx})}{\alpha_s \text{Re}(k_{sx})} |T|^2$$
Field distribution

Aim: Calculation of \( F(x) \) in the entire structure

Starting point: known shape of transmitted vector

\[
\begin{pmatrix} F \\ G \end{pmatrix}_D = \begin{pmatrix} F \\ \alpha_c \frac{\partial F}{\partial x} \end{pmatrix}_D = F_T \begin{pmatrix} 1 \\ i \alpha_c k_{xx} \end{pmatrix}
\]

now: \( F_T \equiv 1 \)

1. invert structure (vector transforms into \( \{1, -i\alpha_c k_{xx}\} \))
2. calculate field vector up to the next layer boundary
3. calculate towards the current \( x \)-value, starting from the layer boundary
4. save the first component of the vector
5. turn back the derived field and structure

Calculating the real fields

\[
\begin{align*}
E_r(x,z,t) &= \text{Re} \left[ E(x) \exp \left( i k_z z - i \omega t \right) \right] \\
H_r(x,z,t) &= \text{Re} \left[ H(x) \exp \left( i k_z z - i \omega t \right) \right]
\end{align*}
\]

with

\[
\begin{align*}
\text{TE:} & \quad E(x) = F(x) e_y \\
\text{TM:} & \quad H(x) = F(x) e_y
\end{align*}
\]

1.3 Guided modes in layer systems

\( \Rightarrow \) no \( y \) dependence, phase rotation in \( z \) direction
waves propagating without diffraction
- miniaturization of optics
- optical signal communication

How can waves be bound by the layer system?

\[ \text{principle mechanism is total internal reflection} \]

Field distribution:

- plane wave in propagation direction: \( \exp(ik_z z) \)
- evanescent wave in substrate and cladding \( k_z^2 > \frac{\omega^2}{c^2} \max\{\varepsilon_{s,c}(\omega)\} \)
- oscillating solution in core \( (A \sin(k_{\phi}x) + B \cos(k_{\phi}x)) \Rightarrow k_z^2 < \frac{\omega^2}{c^2} \max\{\varepsilon_i(\omega)\} \)
- general condition for guided waves \( \frac{\omega}{c} \max\{\varepsilon_{s,c}(\omega)\} < k_z^2 < \frac{\omega^2}{c^2} \max\{\varepsilon_i(\omega)\} \)

**Modes are resonances of the system**

Dispersion relation of guided waves \( \Rightarrow \) singularities of \( R \) and \( T \)

\[
R = \frac{F_R}{F_I} = \left( \alpha_s k_{s} M_{22} - \alpha_c k_{c} M_{11} \right) - \frac{i}{\mu} \left( M_{21} + \alpha_s k_{s} \alpha_c k_{c} M_{12} \right)
\]

\[
F_I = \left( \alpha_s k_{s} M_{22} + \alpha_c k_{c} M_{11} \right) + \frac{i}{\mu} \left( M_{21} - \alpha_s k_{s} \alpha_c k_{c} M_{12} \right)
\]

\( \Rightarrow \) singularity: \( \left( \alpha_s k_{s} M_{22} + \alpha_c k_{c} M_{11} \right) + \frac{i}{\mu} \left( M_{21} - \alpha_s k_{s} \alpha_c k_{c} M_{12} \right) = 0 \)

The problem of finding a guided mode is reduced to finding a root.

with: \( k_{s} = i\mu_s, \quad k_{c} = i\mu_c, \quad \mu_{s,c} = \sqrt{k_z^2 - \frac{\omega^2}{c^2} \varepsilon_{s,c}(\omega)} > 0 \)

\( \Rightarrow \alpha_s \mu_s M_{22}^{TE,TM} + \alpha_c \mu_c M_{11}^{TE,TM} + M_{21}^{TE,TM} + \alpha_c \mu_c \alpha_s \mu_s M_{12}^{TE,TM} = 0 \)
Roots of the denominator correspond to modes guided along the layer system.

A physical explanation of the correspondence of roots and modes can be seen in the singularities of the reflection and transmission coefficients. Hence there is a field in the layer without an input field.

For comparison this is the reflectivity and transmissivity of the same layer system in the $k_z$-domain corresponding to the reflection/transmission problem addressed in the previous section.
Field distributions of guided modes inside a single high-index layer embedded into low-index substrate and cladding.
2. Finite-difference method for waveguide modes

Starting from the wave equation

\[ \text{rot} \ \text{rot} \ E(r, \omega) = \frac{\omega^2}{c^2} \varepsilon(r, \omega) E(r, \omega) \]

Neglecting the divergence of the electric field

\[ \text{div} \ D(r, \omega) = 0 \Rightarrow \varepsilon_0 \varepsilon(\omega) \text{div} E(r, \omega) \approx 0 \]

We obtain the Helmholtz equation

\[ \Delta E(r, \omega) + \frac{\omega^2}{c^2} \varepsilon(r, \omega) E(r, \omega) = 0 \]

Neglecting the vectorial properties of the electric field \( \Rightarrow \) scalar Helmholtz equation

\[ \Delta v(r) + k^2(r, \omega) v(r) = 0 \quad \text{with} \quad k^2(r, \omega) = \frac{\omega^2}{c^2} \varepsilon(r, \omega) \]

2.1 Stationary solutions of the scalar Helmholtz equation

Now we search for the stationary states (modes) of the problem with \( \varepsilon(r, \omega) = \varepsilon(x, y, \omega) \)

\[ v(r) = u(x, y) \exp(\text{i} \beta z) \]

which results in an eigenvalue equation for the propagation constant \( \beta \)

\[ \Delta^{(2)} u(x, y) + \left[ k^2(x, y, \omega) - \beta^2(\omega) \right] u(x, y) = 0 \]

This eigenvalue problem is to be solved by a finite difference scheme

\[ \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right] u(x, y) + \left[ k^2(x, y, \omega) - \beta^2(\omega) \right] u(x, y) = 0 \]

with the discrete Laplace operator for two dimensions

\[ \frac{\partial^2 u(x, y)}{\partial x^2} + \frac{\partial^2 u(x, y)}{\partial y^2} \]
linear equation for each variable \( U_{j,k} \)

\[
\begin{align*}
\Delta_{(x,y)} U & \rightarrow \quad (\Delta U)_{j,k} \\
\text{• quadratic area of size } a \times a \\
\text{• equidistant discretization of the area with } N \times N \text{ points}
\end{align*}
\]

\[
\begin{align*}
\frac{d^2U}{dx^2} \bigg|_{x_j,y_k} & \approx \frac{U(x_{j+1},y_k) - 2U(x_j,y_k) + U(x_{j-1},y_k)}{h^2} \\
\frac{d^2U}{dy^2} \bigg|_{x_j,y_k} & \approx \frac{U(x_j,y_{k+1}) - 2U(x_j,y_k) + U(x_j,y_{k-1})}{h^2}
\end{align*}
\]

\[
\frac{d^2U}{dx^2} + \frac{d^2U}{dy^2} \bigg|_{x_j,y_k} \approx (\Delta U)_{j,k} = \frac{-4U_{j,k} + U_{j+1,k} + U_{j-1,k} + U_{j,k+1} + U_{j,k-1}}{h^2}
\]

\[
+ \left[ k^2(x,y,\omega) - \beta^2(\omega) \right] u(x,y) = 0
\]

\[
\begin{align*}
\Delta (x,y) U & \rightarrow \quad (\Delta U)_{j,k} \\
\text{• quadratic area of size } a \times a \\
\text{• equidistant discretization of the area with } N \times N \text{ points}
\end{align*}
\]

\[
(\Delta U)_{2,3} = \frac{-4U_{2,3} + U_{3,3} + U_{1,3} + U_{2,4} + U_{2,2}}{h^2}
\]

2.2 Matrix notation of the eigenvalue equation

\( U_{j,k} \): originally 2D variable depending on x-direction (j) and y-direction (k)

\( \rightarrow \) unfolding of \( U_{j,k} \) into a 1D vector

\( \rightarrow \) for each vector component \( U_{j,k} \) results an individual linear equation

matrix dimension: number variables in x times number variables in y
Matrix equation: schematic picture

\[
\begin{bmatrix}
-4 & 1 & 0 & 0 & \cdots & 0 & 1 & 0 & 0 & 0 & \cdots \\
1 & -4 & 1 & 0 & \cdots & 0 & 0 & 1 & 0 & 0 & \cdots \\
0 & 1 & -4 & 1 & \cdots & 0 & 0 & 0 & 1 & 0 & \cdots \\
0 & 0 & 1 & -4 & \cdots & 0 & 0 & 0 & 0 & 1 & \cdots \\
0 & 0 & 0 & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
\end{bmatrix}
\begin{bmatrix}
U_{1,1} \\
U_{1,2} \\
\vdots \\
U_{N-1,2} \\
U_{2,3} \\
U_{3,3} \\
\vdots \\
U_{N-2,3} \\
U_{N-2,4} \\
U_{N-1,4} \\
\vdots \\
\end{bmatrix}
= 0
\]

\[x \text { iterates first}\]

- accounts for the 1D – problem (tridiagonal matrix)
- occurs for 2D problems

matrix: small number of non-zero values – ’sparse matrix’
2.3 Boundary conditions

- boundaries of the grid?
  example:
  \[ (\Delta U)_{1,3} = \frac{-4U_{1,3} + U_{2,3} + U_{0,3} + U_{1,4} + U_{1,2}}{h^2} \]

outside the grid

\[ \Rightarrow \text{boundary conditions} \]

(compare with theory of partial differential equation)

Example: Metal boundaries (Metal tube with boundaries \(\partial \Omega_i\))

\[ U|_{\partial \Omega} = U_i = \text{const} \]

grid with metal boundaries (\(U|_{\partial \Omega} = 0\))

\[ (\Delta U)_{j,k} = \frac{-4U_{j,k} + U_{j+1,k} + U_{j-1,k} + U_{j,k+1} + U_{j,k-1}}{h^2} = 0 \]

\[ \Rightarrow (N-2) \times (N-2) - \text{equations} \]

\[ \Rightarrow (N-2) \times (N-2) - \text{unknown} \]
3. Beam Propagation Method (BPM)

• up to this point we only dealt with eigenmodes
  – required invariance of the structure in the third dimension
  – What happens if light propagation occurs in a medium where the index distribution weakly changes?
• accurately model a very wide range of devices
  – linear and nonlinear light propagation in axially varying waveguide systems, as e.g.
    o curvilinear directional couplers,
    o branching and combining waveguides,
    o S-shaped bent waveguides,
    o tapered waveguides
  – ultra short light pulse propagation in optical fibers
• implementation
  – finite difference BPM solves Maxwell's equations by using finite differences in place of partial derivatives
  – computational intensive
  – entirely in the frequency domain ⇒ only weak nonlinearities can be modeled
  – use of a slowly varying envelope approximation in the paraxial direction ⇒ the device it is assumed to have an optical axis, and that most of the light travels approximately in this direction, (paraxial approximation) ⇒ allows to rely on first order differential equations

3.1 Categorization of Partial Differential Equation (PDE) problems

general second-order Partial Differential Equation
\[
p \frac{\partial^2 f}{\partial x^2} + q \frac{\partial^2 f}{\partial x \partial y} + r \frac{\partial^2 f}{\partial y^2} + s \frac{\partial f}{\partial x} + t \frac{\partial f}{\partial y} + u \cdot f + v = 0 \tag{8}
\]

The following different types of partial differential equations are distinguished

1. \( q^2 < 4pr \) : elliptic PDE
2. \( q^2 = 4pr \) : parabolic PDE
3. \( q^2 > 4pr \) : hyperbolic PDE

Elliptic PDE
\[
\frac{\partial^2 u(x,y)}{\partial x^2} + \frac{\partial^2 u(x,y)}{\partial y^2} = \rho(x,y) \quad \text{Poisson equation}
\]

⇒ Boundary Value Problem (BVP) ⇒ limited mainly by computing memory
Hyperbolic PDE

\[ \frac{\partial^2 u(x, y)}{\partial t^2} = v^2 \frac{\partial^2 u(x, y)}{\partial y^2} \]

1D wave equation

Parabolic PDE

\[ \frac{\partial u(x, t)}{\partial t} = \frac{\partial}{\partial x} \left( D \frac{\partial u(x, t)}{\partial x} \right) \]

diffusion equation (IVP)

⇒ both are Initial Value Problem (IVP) ⇒ limited mainly by computing time
3.2 Slowly Varying Envelope Approximation (SVEA)

Assumptions

- a component of the optical electromagnetic field is primarily a periodic (harmonic) function of position
- it changes most rapidly along the optical axis \( z \) (with a period on the order of the optical wavelength \( \lambda \))

**Slowly Varying Envelope Approximation (SVEA)**

- replace the quickly varying component, \( \Phi \), with a slowly varying one, \( \phi \), as
  \[
  \Phi(x, y, z) = \phi(x, y, z) \exp(-iknz) \quad \text{with} \quad k = \frac{2\pi}{\lambda}
  \]
- introduction of a reference index \( n_0 \) → light is travelling mostly parallel to the \( z \) axis (paraxial approximation), and is monochromatic with wavelength \( \lambda \)
  → requirements on the mesh to represent derivatives by finite differences are relaxed → choose fewer mesh points → higher speed of the calculation without compromising accuracy
  → BPM: accurate calculations using step sizes \( \Delta z > \lambda \)

**SVEA Problems**

- if part of the light strongly deviates from the direction of the axis \( z \)
  solution: wide angle BPM
- if structure has large index contrast → no accurate global choice of \( n_0 \) → finer mesh needed
  solution: if variation is in \( z \) direction → \( n_0(z) \)

quality of choice of \( n_0 \) can be checked by evaluating the speed of phase evolution of \( \phi \) in the numerics
3.3 Differential equations of BPM

starting from Maxwell’s equations in the frequency domain with an inhomogeneous distribution of the dielectric properties $\varepsilon(x, y, z)$

$$\nabla \times \mathbf{E} = -i\omega \mu_0 \mathbf{H}$$
$$\nabla \times \mathbf{H} = i\omega \varepsilon_0 \varepsilon(x, y, z) \mathbf{E}$$

+ no charges $\Rightarrow$ $\nabla \cdot (n^2 \mathbf{E}) = 0$
$$\nabla \cdot \mathbf{H} = 0$$

magnetic field can be eliminated by taking curl of curl $\mathbf{E}$-equation

$$\nabla \times \nabla \times \mathbf{E} = k^2 \varepsilon(x, y, z) \mathbf{E} \quad \text{with} \quad k = \omega \sqrt{\varepsilon_0 \mu_0}$$

using the vector identity $\nabla \times \nabla \times = \nabla (\nabla \cdot) - \nabla^2$ one gets the wave equation

$$\nabla^2 \mathbf{E} + k^2 \varepsilon(x, y, z) \mathbf{E} = \nabla (\nabla \cdot \mathbf{E})$$

since BPM is biased for the $z$-axis, it is natural to treat $z$-components of $\mathbf{E}$ and $\nabla$ separately from the transverse components $x$ and $y$

$$\mathbf{E} = \mathbf{E}_t + \hat{z} E_z \quad \text{and} \quad \nabla = \nabla_t + \hat{z} \frac{\partial}{\partial z}$$

the transverse component of the wave equation becomes

$$\nabla_t^2 \mathbf{E}_t + \frac{\partial^2 \mathbf{E}_t}{\partial z^2} + k^2 \varepsilon(x, y, z) \mathbf{E}_t = \nabla_t \left( \nabla_t \cdot \mathbf{E}_t + \frac{\partial E_z}{\partial z} \right) \quad (9)$$

which is inconsistent since it contains transverse and longitudinal components.

Splitting also the divergence equation in the transverse and longitudinal components

$$\nabla_t \cdot \left( \varepsilon(x, y, z) \mathbf{E}_t \right) + \frac{\partial \varepsilon(x, y, z)}{\partial z} E_z + \varepsilon(x, y, z) \frac{\partial E_z}{\partial z} = 0$$

and neglecting the second term ($\varepsilon$ is assumed to change slowly in $z$)

$$\nabla_t \cdot \left( \varepsilon(x, y, z) \mathbf{E}_t \right) + \varepsilon(x, y, z) \frac{\partial E_z}{\partial z} \approx 0$$

one can eliminate the longitudinal term in the right hand side of the wave equation (9)

$$\nabla_t^2 \mathbf{E}_t + \frac{\partial^2 \mathbf{E}_t}{\partial z^2} + k^2 \varepsilon(x, y, z) \mathbf{E}_t = \nabla_t \left[ \nabla_t \cdot \mathbf{E}_t - \frac{1}{\varepsilon(x, y, z)} \nabla_t \cdot \left( \varepsilon(x, y, z) \mathbf{E}_t \right) \right]$$

applying the chain rule on the second divergence term on the right hand side, the first divergence term is canceled out

$$\nabla_t^2 \mathbf{E}_t + \frac{\partial^2 \mathbf{E}_t}{\partial z^2} + k^2 \varepsilon(x, y, z) \mathbf{E}_t = -\nabla_t \left[ \frac{1}{\varepsilon(x, y, z)} (\nabla_t \varepsilon(x, y, z)) \cdot \mathbf{E}_t \right] \quad (10)$$

up to now: $\mathbf{E}_t$ is varying slowly in $x$ and $y$, but rapidly in $z$

now SVEA is introduced
\[ \mathbf{E}_i(x, y, z) = \mathbf{e}_i(x, y, z) \exp(-in_0kz) \]

\( \Rightarrow \) the new field \( \mathbf{e}_i(x, y, z) \) is slowly varying in all coordinates (compared to \( \lambda \))

substituting SVEA ansatz into wave equation (10)

\[ \frac{\partial^2 \mathbf{e}_i}{\partial z^2} - 2jkn_0 \frac{\partial \mathbf{e}_i}{\partial z} + k^2(\varepsilon(x, y, z) - n_0^2)\mathbf{e}_i + \nabla_i^2 \mathbf{e}_i + \nabla_i \left[ \frac{1}{\varepsilon(x, y, z)} \nabla \varepsilon(x, y, z) \cdot \mathbf{e}_i \right] = 0 \]

if reference index \( n_0 \) was chosen correctly, the first term will be much smaller than the second and hence can be neglected

\( \Rightarrow \) results in a first order equation in \( z \)

\( \Rightarrow \) collect the transverse 2. order operators on the right hand side

\[ 2jkn_0 \frac{\partial}{\partial z} \begin{bmatrix} e_x \\ e_y \end{bmatrix} = \begin{bmatrix} P_{xx} & P_{xy} \\ P_{yx} & P_{yy} \end{bmatrix} \begin{bmatrix} e_x \\ e_y \end{bmatrix} \]

with the components of the operator being

\[ P_{xx} = \frac{\partial}{\partial x} \left[ \frac{1}{\varepsilon(x, y, z)} \frac{\partial}{\partial x} \varepsilon(x, y, z) \cdot \right] + \frac{\partial^2}{\partial y^2} + k^2(\varepsilon(x, y, z) - n_0^2) \]

\[ P_{xy} = \frac{\partial}{\partial x} \left[ \frac{1}{\varepsilon(x, y, z)} \frac{\partial}{\partial y} \varepsilon(x, y, z) \cdot \right] + \frac{\partial^2}{\partial x \partial y} \]

\[ P_{yx} = \frac{\partial}{\partial y} \left[ \frac{1}{\varepsilon(x, y, z)} \frac{\partial}{\partial x} \varepsilon(x, y, z) \cdot \right] + \frac{\partial^2}{\partial y \partial x} \]

\[ P_{yy} = \frac{\partial}{\partial y} \left[ \frac{1}{\varepsilon(x, y, z)} \frac{\partial}{\partial y} \varepsilon(x, y, z) \cdot \right] + \frac{\partial^2}{\partial x^2} + k^2(\varepsilon(x, y, z) - n_0^2) \]

**Summary of the results**

- paraxial vector wave equation for the optical electric field
- initial value problem: knowledge of the electric field in some transverse plane \((z = \text{const.})\) is enough
- reflections of light are neglected
- in a finite differencing scheme the operator \( \mathbf{P} \) is a large sparse matrix

### 3.4 Semi-vector BPM

before: full vector character of the electromagnetic field is included

now: if the modeled device operates mainly on a single field component, the other component’s contribution can often be neglected

\( \Rightarrow \) semi vector TE equation for E-field being mainly transversely polarized

\[ 2jkn_0 \frac{\partial e_x}{\partial z} = P_{xx} e_x \]

\( \Rightarrow \) of semi vector TM equation for H-field being mainly transversely polarized
\[ 2jkn_0 \frac{\partial e_y}{\partial z} = P_{yy} e_y \]

**Properties**
- correctly models differences of TE and TM wave propagation
- neglects coupling to other field component

### 3.5 Scalar BPM

if structure has very low index contrast, the \( \frac{\partial \varepsilon}{\partial x} \) and \( \frac{\partial \varepsilon}{\partial y} \) term can be neglected → operators commute → \( P_{xx} \) and \( P_{yy} \) reduce to scalar operator

\[ P = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + k^2(\varepsilon(x, y, z) - n_0^2) \]

### 3.6 Crank-Nicholson method

formal solution of BPM equation can be written as

\[
e_t(z_i) = \exp \left[ \frac{\Delta z}{2jn_0k} P \right] e_t(z_0) \quad \text{with} \quad \Delta z = z_i - z_0
\]

however, a rational function is needed to approximate the exponent of the operator

a simple approximation would be

\[
\exp[x] = \frac{1 + (1 - \alpha)x}{1 - \alpha x}
\]

**The case \( \alpha = 0.5 \)**
- called Padé(1,1) approximation
- accurate for small \( x \) → small step size \( \Delta z \) (higher order Padé approximations can be used, see below)
- generates the first three terms of the MacLaurin series expansion for \( \exp[x] \)

→ leads to Crank-Nicholson scheme

\[
\left[ I - \frac{\Delta z}{4jn_0k} P \right] e_t(z_i) = \left[ I + \frac{\Delta z}{4jn_0k} P \right] e_t(z_0)
\]

since the operator \( P \) is applied to the unknown \( e_t(z_i) \) it is an implicit method
→ requires solution of set of linear equations

Variable \( \alpha \) is called scheme parameter, for \( \alpha = 0.5 \) the method is stable and energy conserving
3.7 Alternating Direction Implicit (ADI)
- Solving the implicit problem in 2D leads to a huge set of linear equations.
  \( \rightarrow \) time consuming numerical solution
- However, 1D problems result only in a simple tridiagonal matrix which can be solved very fast.

**ADI approximation**
- splitting the n-dimensional operator into n subsequent 1-dimensional operators
  \( \rightarrow \) each operation only on a single dimension
  \( \rightarrow \) fast algorithm: periodic application of 1D operators in \( x \) and \( y \) direction

3.8 Boundary condition

**Easiest boundary condition: reflecting boundaries (electric walls)**
- assuming that the field is zero at the boundary \( \rightarrow \) perfect reflection

**Advanced boundary conditions: fields can radiate out of simulation area**
- fields radiating out, e.g. from waveguide, should not disturb the evolution by being reflected back from the boundaries \( \rightarrow \) let the radiation fields out
- do not create any additional effects (e.g. instability, dissipation etc.)

**Typical advanced boundary condition**
- absorbing boundary conditions (ABC)
- transparent boundary conditions (TBC)
- perfectly matched layer boundaries (PML)

3.8.1 Absorbing Boundary Conditions (ABC)

**problem:**
- field at the boundary of the computational window is not wanted

**solution:**
- remove field at boundaries by multiplication with factor \(<1\)
  \( \rightarrow \) can be introduced by \( \Im(n) > 0 \) at the boundary

**however:**
- all inhomogeneities of the optical properties induce reflections themselves, this can be shown by computing Fresnel reflection at interface where just the imaginary part of the dielectric function changes

**improvement:**
- soft onset of the absorbing layer

**technical realization:**
- multiplication of the field in each iteration step with a filter function, e.g. in 1D:

\[ e_{p}^{\text{abs}} = e_{p} \left[ 1 - A_{\text{abs}} \exp\left( -\frac{p}{N_{\text{abs}}} \right) - A_{\text{abs}} \exp\left( \frac{p - P}{N_{\text{abs}}} \right) \right] \quad \text{with} \quad N_{\text{abs}} = 3...5 \]

drawback:
- absorption strength $A_{\text{abs}}$ and absorption width $N_{\text{abs}}$ are difficult to adjust for the smallest reflection
- individual optimal parameters for each problem
3.8.2 Transparent Boundary Condition (TBC)

**Goal:**
- simulates a nonexistent boundary
- radiation is allowed to freely escape from the simulated area without reflection
- radiation flux back into the problem region is prevented

**Method:**
- assuming that the field in the vicinity of the virtual boundary consists of an outgoing plane wave and does not include the reflected wave from the virtual boundary

\[ \text{wave function for the left-traveling wave with the } x \text{-directed wave number } k_x \text{ is expressed as} \]

\[ \phi(x, z) = A(z) \exp(j k_x x) \]

**Derivation**

projecting the field onto the following lattice

\[ \phi(x_p) = \phi_p \]

Nodes \( p = -1 \) and \( p = m \) are outside the computational window

hence the relation of the field at neighboring mesh points can be expressed as

\[ \exp(j k_x \Delta x) = \frac{\phi_1}{\phi_0} \quad \text{with} \quad \Delta x = x_i - x_0 \]

from which we can calculate the \( x \)-directed wave number \( k_x \)

\[ k_x = \frac{1}{j \Delta x} \ln \left( \frac{\phi_1}{\phi_0} \right) \]

if \( \Re(k_x) > 0 \) \( \Rightarrow \) plane wave is traveling outwards

if \( \Re(k_x) < 0 \) \( \Rightarrow \) plane wave is traveling inwards
since inward waves should not exist
\[ \Re(k_x) \text{ must be positive} \Rightarrow \Re(k_x) \geq 0 \]

**Implementation**

- \( k_x \) is calculated at the boundary
- another mesh point at \( p = -1 \) is artificially added to the mesh
- the field at \( p = -1 \) is assumed to be determined by the same plane wave function
  \[ \exp(jk_x\Delta x) = \frac{\phi_0}{\phi_{-1}} \quad \text{with} \quad \Delta x = x_i - x_0 = x_0 - x_{-1} \]
- assuming that the \( k_x \)-vector is preserved by the wave
  \[ \frac{\phi_1}{\phi_0} = \exp(jk_x\Delta x) = \frac{\phi_0}{\phi_{-1}} \rightarrow 0 = \phi_{-1}\phi_1 - \phi_0\phi_0 \]
- trick: calculate \( k_x^{n-1} \) one step \( \Delta z \) before applying it to the boundary
  \[ 0 = \phi_{-1}^{n-1}\phi_1^n - \phi_0^{n-1}\phi_0^n \]

### 3.8.3 Perfectly matched layer boundaries (PML)

**Definition**

perfectly matched layer = artificial absorbing layer for wave equations used to truncate computational regions in numerical methods to simulate problems with open boundaries

**Property**

waves incident upon the PML from a non-PML medium do not reflect at the interface \( \Rightarrow \) strongly absorb outgoing waves from the interior of a computational region without reflecting them back into the interior (impedance matching required)

**Different formulations**

nice one: stretched-coordinate PML (Chew and Weedon)
coordinate transformation in which one (or more) coordinates are mapped to complex numbers \( \Rightarrow \) analytic continuation of the wave equation into complex coordinates, replacing propagating (oscillating) waves by exponentially decaying waves

**Technical description**

to absorb waves propagating in the x direction, the following transformation is applied to the wave equation:
al x derivative \( \partial/\partial x \) are replaced by
\[
\frac{\partial}{\partial x} \rightarrow \frac{1 + i\sigma(x)}{\omega} \frac{\partial}{\partial x}
\]

with \(\omega\) being the angular frequency and \(\sigma\) some positive function of \(x\). Hence, propagating waves in +x direction \((k>0)\) become attenuated

\[
\exp[i(kx - \omega t)] \rightarrow \exp[i(kx - \omega t) - \frac{k}{\omega} \int^x \sigma(x') \partial x']
\]

which corresponds to the coordinate transformation (analytic continuation to complex coordinates)

\[
x \rightarrow x + \frac{i}{\omega} \int^x \sigma(x') \partial x' \quad \text{or equivalently} \quad \partial x \rightarrow \partial x(1 + i\sigma/\omega)
\]

**Properties**

- for real valued \(\sigma\) the PML attenuate only propagating waves
- purely evanescent waves oscillate in the PML but do not decay more quickly
  - attenuation of evanescent waves can be accelerated by including a real coordinate stretching in the PML
  - corresponds to complex valued \(\sigma\)
- PML is reflectionless only for the exact wave equation
  - discretized simulation shows small numerical reflections
  - can be minimized by gradually turn on (e.g. with quadratic spatial profile) the absorption coefficient \(\sigma\) from zero over a short distance on the scale of the wavelength of the wave

**3.9 Conformal mapping regions**

- used to simulate curved optical waveguides
- solving bends by BPM directly leads to large errors due to the paraxial approximation
- can be used to treat losses in curved waveguides
- radii of curvature need not to be restricted to large values, when first order approximation of the conformal mapping is used (corresponding to linear index gradient)

**Method**

- conformal mapping in the complex plane to transform a curved waveguide in coordinates \((x,y)\) into a straight waveguide with a modified refractive index in new coordinates \((u,v)\)
conformal mapping is an angle-preserving transformation in a complex plane

- typical example for local angle preserving transformation: word maps

\[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 n^2(x, y) = 0 \]

Demonstration for 2D scalar wave equation

\[ \left[ \frac{\partial}{\partial x^2} + \frac{\partial}{\partial z^2} + k^2 n^2(x, y) \right] \phi = 0 \]

general transformation

\[ W = u + iv = f(x + iz) = f(Z) \]

for \( f \) being an analytical function in the complex plane

to straighten a bend radius of \( R \) in the \((u,v)\) plane, \( f \) should be taken as

\[ W = R \ln(Z / R) \]

applying the transformation to the wave equation gives

\[ \left[ \frac{\partial}{\partial u^2} + \frac{\partial}{\partial v^2} + k^2 \left( \frac{dZ}{dW} \right)^2 n^2(x(u,v), y(u,v)) \right] \phi = 0 \]

with the Jacobian of the transformation being

\[ \left| \frac{dZ}{dW} \right| = \exp(u / R) \]
a bended waveguide is transformed into straight waveguide with modified refractive index

\[ \frac{dZ}{dW} n(x, y) \]

- limitations imposed by the paraxial approximation are avoided
- in first order approximation a linear index gradient is added to account for the bending

### 3.10 Wide-angle BPM based on Padé operators

**Principle**

expansion via Padé is more accurate than Taylor expansion for the same order of terms \( \Rightarrow \) larger angles / higher index contrast / more complex mode interference can be analyzed as the Padé order increases

**Derivation**

starting from scalar wave equation without neglecting second order \( z \) derivative, the equation can be formally rewritten as

\[ \frac{\partial \phi}{\partial z} = -j \frac{P/2k_0n_0}{1 + (j/2k_0n_0)(\partial / \partial z)} \phi \tag{*} \]

which can be reduced to

\[ \frac{\partial \phi}{\partial z} = -j \frac{N}{D} \phi \]

with \( N \) and \( D \) being polynomials determined by the operator \( P \)

applying a finite difference scheme we get to iteration equation

\[ \phi^{l+1} = \frac{D - j\Delta z(1-\alpha)N}{D + j\Delta z\alpha N} \phi^l \]

with \( \alpha \) being a control parameter of the finite difference scheme ranging between 0 and 1 (\( \alpha = 0 \) fully implicit scheme; \( \alpha = 1 \) fully explicit scheme; \( \alpha = 0.5 \) Crank-Nicolson scheme)

the numerator \( D - j\Delta z(1-\alpha)N \) can be factorized as

\[ (A_{\text{Nom}} P^N + B_{\text{Nom}} P^{N-1} + C_{\text{Nom}} P^{N-2} + ...) = (1+c_N P) ... (1+c_2 P)(1+c_1 P) \]

with coefficients \( c_1, c_2, ..., c_N \) which can be obtained from the solution of the algebraic equation

\[ (D - j\Delta z(1-\alpha)N) = (A_{\text{Nom}} P^N + B_{\text{Nom}} P^{N-1} + C_{\text{Nom}} P^{N-2} + ...) = 0 \]

similarly the denominator \( D + j\Delta z\alpha N \) can be factorized as

\[ (A_{\text{Den}} P^N + B_{\text{Den}} P^{N-1} + C_{\text{Den}} P^{N-2} + ...) = (1+d_N P) ... (1+d_2 P)(1+d_1 P) \]

with coefficients \( d_1, d_2, ..., d_N \) which can be obtained from the solution of the algebraic equation
\[ (D + j \Delta z \alpha N) = \sum_{i=0}^{N} d_i P^i = 0 \]

with \( c_0 = d_0 = P^0 = 1 \)

Thus, the unknown field \( \phi^{i+1} \) at \( z + \Delta z \) is related to the known field \( \phi^i \) at \( z \) as

\[
\phi^{i+1} = \frac{A_N P^N + B_N P^{N-1} + C_N P^{N-2} + \ldots + \phi^i}{A_D P^N + B_D P^{N-1} + C_D P^{N-2} + \ldots}
\]

or

\[
\phi^{i+1} = \frac{(1 + c_N P)(1 + c_2 P)(1 + c_1 P) \phi^i}{(1 + d_N P)(1 + d_2 P)(1 + d_1 P)}
\]

3.10.1 Fresnel approximation – Padé 0th order

starting again from wave equation (*) we account for the z-derivative by the recursion equation

\[
\frac{\partial}{\partial z}_{|n} = -j \frac{P/2 k_0 \eta_0}{1 + (j/2 k_0 \eta_0) \frac{\partial}{\partial z}_{|n-1}} (**)
\]

which is used to replace the z-derivative in the denominator of (**)

in paraxial approximation \( \frac{\partial}{\partial z}_{|0} = -j \frac{P/a}{1 + (j/a) \frac{\partial}{\partial z}_{|-1}} = -j \frac{P}{a} \)

with \( a = 2 k_0 \eta_0 \) and \( \frac{\partial}{\partial z}_{|-1} \approx 0 \)

comparison to the expansion equations gives

\[ D = 1 \quad \text{and} \quad N = P/a \]

and therefore the nominator becomes

\[ D - j \Delta z (1 - \alpha) N = 1 - j \Delta z (1 - \alpha) \frac{P}{a} = 1 + A_N P \]

and the denominator analogously

\[ D + j \Delta z \alpha N = 1 + j \Delta z \alpha \frac{P}{a} = 1 + A_D P \]

with

\[ A_N = -j \frac{\Delta z (1 - \alpha)}{a} \]

\[ A_D = j \frac{\Delta z \alpha}{a} \]

thus the unknown field \( \phi^{i+1} \) at \( z + \Delta z \) is related to the known field \( \phi^i \) at \( z \) as
The unknown field \( \phi^{l+1} \) at \( z + \Delta z \) is related to the known field \( \phi^l \) at \( z \) again as

\[
(A_{\text{Den}} P + 1) \phi^{l+1} = (A_{\text{Nom}} P + 1) \phi^l
\]

which includes now higher order corrections.
4. Finite Difference Time Domain Method (FDTD)

- ab initio, direct solution of Maxwell’s equations
- probably the most often used numerical technique, as an implementation is straight forward (but cumbersome implementation of proper boundary conditions)
- requires excessive computational resources for reasonable problems in 3D (implementation for clusters)
- implementation is absolutely general but often doesn’t take explicit advantage of symmetries
- principally all kinds of materials are treatable (dispersive or nonlinear materials)

4.1 Maxwell’s equations

\[
\begin{align*}
\text{rot } \mathbf{E}(\mathbf{r}, t) &= -\frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t}, \\
\text{rot } \mathbf{H}(\mathbf{r}, t) &= \frac{\partial \mathbf{D}(\mathbf{r}, t)}{\partial t} + j_{\text{makr}}(\mathbf{r}, t), \\
\text{div } \mathbf{D}(\mathbf{r}, t) &= \rho_{\text{ext}}(\mathbf{r}, t), \\
\text{div } \mathbf{B}(\mathbf{r}, t) &= 0,
\end{align*}
\]

MWEQ in linear isotropic and dispersionless dielectric Media

\[
\begin{align*}
\mathbf{D}(\mathbf{r}, t) &= \varepsilon_0 \varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}, t), \\
\mathbf{B}(\mathbf{r}, t) &= \mu_0 \mathbf{H}(\mathbf{r}, t), \\
\text{rot } \mathbf{E}(\mathbf{r}, t) &= -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t}, \\
\text{rot } \mathbf{H}(\mathbf{r}, t) &= \varepsilon_0 \varepsilon(\mathbf{r}) \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} + j_{\text{makr}}, \\
\text{div } \varepsilon_0 \varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) &= 0, \\
\text{div } \mathbf{H}(\mathbf{r}, t) &= 0,
\end{align*}
\]

rot-equations for individual components

\[
(a) \quad \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t} = -\frac{1}{\mu_0} \text{rot } \mathbf{E}(\mathbf{r}, t)
\]
\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu_0} \left[ \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - j_x \right], \\
\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \left[ \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - j_y \right], \\
\frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \left[ \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - j_z \right]
\]

(b) \[ \frac{\partial E(r,t)}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \text{rot} \mathbf{H}(r,t) \]

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \left[ \frac{\partial H_y}{\partial z} - \frac{\partial H_z}{\partial y} \right], \\
\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \left[ \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right], \\
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \left[ \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} \right]
\]

4.2 1D problems

Assuming that there is no dependence on y and z → all dynamics in x

(a) \[ \frac{\partial H_x}{\partial t} = 0, \quad \frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_z}{\partial x}, \quad \frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_y}{\partial x} \]

(b) \[ \frac{\partial E_x}{\partial t} = 0, \quad \frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \frac{\partial H_z}{\partial x}, \quad \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \frac{\partial H_y}{\partial x} \]

grouping together all non-mixing transverse electromagnetic components (TEM)

z-polarized E-field \[ \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \frac{\partial H_y}{\partial x}, \quad \frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_z}{\partial x} \]

y-polarized E-field \[ \frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \frac{\partial H_z}{\partial x}, \quad \frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_y}{\partial x} \]

Without loss of generality we concentrate on the first case \((E_z)\)

4.2.1 Solution with finite difference method in the time domain for \(E_z\)

**Discretization of derivative operators**

symmetric discretization is second order accurate
\[ \frac{\partial f_n}{\partial x} \bigg|_N \approx \frac{f_{N+1} - f_{N-1}}{x_{N+1} - x_{N-1}} + O\left[ \frac{(x_{N+1} - x_{N-1})^2}{x_{N+1} - x_{N-1}} \right] \]

while the unsymmetric discretization is just first order accurate

\[ \frac{\partial f_n}{\partial x} \bigg|_N \approx \frac{f_{N} - f_{N-1}}{x_{N} - x_{N-1}} + O\left[ \frac{(x_{N} - x_{N-1})}{x_{N} - x_{N-1}} \right] \]

\( \Rightarrow \) always use symmetric discrete operators

\( (i, n) = (i\Delta x, n\Delta t) \):

\[ E_z(i\Delta x, n\Delta t) = E_i^n \Rightarrow \frac{\partial E_i^n}{\partial x} = \frac{E_{i+1}^n - E_{i-1}^n}{2\Delta x} + O\left[ (\Delta x)^2 \right] \]

\[ \frac{\partial E_i^n}{\partial t} = \frac{E_{i+1}^{n+1} - E_{i-1}^{n+1}}{2\Delta t} + O\left[ (\Delta t)^2 \right] \]

\[ H_y(i\Delta x, n\Delta t) = H_i^n \Rightarrow \frac{\partial H_i^n}{\partial x} = \frac{H_{i+1}^n - H_{i-1}^n}{2\Delta x} + O\left[ (\Delta x)^2 \right] \]

\[ \frac{\partial H_i^n}{\partial t} = \frac{H_{i+1}^{n+1} - H_{i-1}^{n+1}}{2\Delta t} + O\left[ (\Delta t)^2 \right] \]

\[ \varepsilon(i\Delta x) = \varepsilon_i \]

**Maxwell’s equations**

\[ \frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon_r(r)} \frac{\partial H_y}{\partial x} \Rightarrow \frac{\partial E_i^n}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon_i} \frac{\partial H_i^n}{\partial x} \]

\[ \frac{E_{i+1}^n - E_{i-1}^{n+1}}{2\Delta t} \approx \frac{1}{\varepsilon_0 \varepsilon_i} \frac{H_{i+1}^n - H_{i-1}^n}{2\Delta x} \]

\[ \Rightarrow E_i^n \approx E_i^{n+1} + \frac{1}{\varepsilon_0 \varepsilon_i} \frac{\Delta t}{\Delta x} \left[ H_{i+1}^n - H_{i-1}^n \right] \]

\[ \frac{\partial H_y}{\partial t} = \frac{\partial E_z}{\partial \mu_0} \Rightarrow \frac{\partial H_i^n}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_i^n}{\partial x} \]

\[ \frac{H_{i+1}^n - H_{i-1}^{n+1}}{2\Delta t} \approx \frac{1}{\mu_0} \frac{E_{i+1}^n - E_{i-1}^n}{2\Delta x} \]

\[ \Rightarrow H_i^{n+1} \approx H_i^{n+1} + \frac{1}{\mu_0} \frac{\Delta t}{\Delta x} \left[ E_{i+1}^n - E_{i-1}^n \right] \]
**FDTD Discretization for the H field:**

![Diagram of FDTD discretization for the H field]

**FDTD Discretization for the E field:**

![Diagram of FDTD discretization for the E field]
4.2.2 Yee grid in 1D and Leapfrog time steps

Equations for a single space-time step

\[
E_i^{n+1} \approx E_i^n + \frac{1}{\varepsilon_0 c_s} \frac{\Delta t}{\Delta x} \left[ H_{i+0.5}^{n+0.5} - H_{i-0.5}^{n+0.5} \right]
\]
\[
H_{i+0.5}^{n+0.5} \approx H_{i+0.5}^{n-0.5} + \frac{1}{\mu_0} \frac{\Delta t}{\Delta x} \left[ E_{i+1}^n - E_i^n \right]
\]

Properties

Divergence?

– That there is no divergence of the fields is always fulfilled in 1D, since fields are always transversally polarized to the direction of field change

Resolution of discretization $\Delta x$ and $\Delta t$? (from physical arguments)

– spatial grid resolution $\Delta x$ must be fine enough to display the finest structures of the $e$ distribution and the fields $\Rightarrow$ rule of thumb
\[ \Delta x \leq \frac{\lambda}{(20n_{\text{max}})}, \text{ with } n_{\text{max}} \text{ being the highest refractive index in the simulation domain} \]

- temporal stepsize \( \Delta t \) is limited by the speed of light, i.e. the interaction in space can reach only up to the next neighbor \( \mapsto \) sets upper limit to the phase velocity \( \mapsto \Delta t \leq \Delta x / c \) in higher dimensions

\[ \Delta t \leq \frac{1}{c} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right)^{1/2} \]

**Boundaries?**

- finite grid size, e.g. with metallic borders \( (E = 0 \text{ at the boundary}) \)

**Sources?**

- either initial field distribution or sources in the simulation domain
- initial field is difficult in higher dimensions since field must have zero divergence
- sources as e.g. currents:

\[ E_i^{n+1} \approx E_i^n + \frac{1}{\varepsilon_n \varepsilon_i} \frac{\Delta t}{\Delta x} \left[ H_{i+0.5}^{n+0.5} - H_{i-0.5}^{n+0.5} \right] + \frac{\Delta t}{\varepsilon_n \varepsilon_i} f_{i+0.5}^{n+0.5} \]

### 4.3 3D problems

**space grid**

\[ (i, j, k, n) = (i \Delta x, j \Delta y, k \Delta z, n \Delta t) \]

\[ \Rightarrow E_x(i \Delta x, j \Delta y, k \Delta z, n \Delta t) = E_x_{ijk}^n \]

\[ \varepsilon(i \Delta x, j \Delta y, k \Delta z) = \varepsilon_{ijk} \]

**Finite differencing in space and time**

\[ \frac{\partial E_x_{ijk}^n}{\partial y} = \frac{E_x_{i+j+1k}^n - E_x_{ijk}^n}{2 \Delta y} + O[(\Delta y)^2] \]

\[ \frac{\partial E_x_{ijk}^n}{\partial t} = \frac{E_x_{ij+k}^{n+1} - E_x_{ijk}^{n-1}}{2 \Delta t} + O[(\Delta t)^2] \]
4.3.1 Yee grid in 3D

**Properties**
- no divergence
- Leapfrog time steps
- central differencing \(\rightarrow\) second order explicit method

Discretizing MWEQ
\[
\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon(r)} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - j_x \right]
\]

\[
E_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = E_x|_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\varepsilon_0 \varepsilon_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \left( \frac{H_z|_{i+1,j+\frac{1}{2},k+\frac{1}{2}} - H_z|_{i,j+\frac{1}{2},k+\frac{1}{2}}}{\Delta y} - \frac{H_y|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - H_y|_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{\Delta z} - j_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \right)
\]

Other equations:
\[
E_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = E_y|_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\varepsilon_0 \varepsilon_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \left( \frac{H_y|_{i+1,j+\frac{1}{2},k+\frac{1}{2}} - H_y|_{i,j+\frac{1}{2},k+\frac{1}{2}}}{\Delta z} - \frac{H_z|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - H_z|_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{\Delta x} - j_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \right)
\]
\[
E_z|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = E_z|_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\varepsilon_0 \varepsilon_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}} \left( \frac{H_z|_{i+1,j+\frac{1}{2},k+\frac{1}{2}} - H_z|_{i,j+\frac{1}{2},k+\frac{1}{2}}}{\Delta x} - \frac{H_x|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - H_x|_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{\Delta z} - j_z|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} \right)
\]
\[
H_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = H_x|_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\mu_0} \left( \frac{E_x|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - E_x|_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{\Delta y} - \frac{E_x|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - E_x|_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta x} \right)
\]
\[
H_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = H_y|_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\mu_0} \left( \frac{E_y|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - E_y|_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{\Delta z} - \frac{E_y|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - E_y|_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta y} \right)
\]
\[
H_z|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} = H_z|_{i,j+\frac{1}{2},k+\frac{1}{2}} + \frac{\Delta t}{\mu_0} \left( \frac{E_z|_{i+\frac{1}{2},j+1,k+\frac{1}{2}} - E_z|_{i+\frac{1}{2},j+\frac{1}{2},k+1}}{\Delta x} - \frac{E_z|_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - E_z|_{i-\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}}{\Delta z} \right)
\]
\[
H_y^{n+1}_{i,j+1/2,k} = H_y^n_{i,j+1/2,k} + \frac{\Delta t}{\mu_0} \left( \frac{E_z^{n+1/2}_{i+1/2,j,k+1} - E_z^{n+1/2}_{i-1/2,j,k+1}}{\Delta x} - \frac{E_y^{n+1/2}_{i,j+1/2,k+1} - E_y^{n+1/2}_{i,j-1/2,k+1}}{\Delta z} \right)
\]

\[
H_z^{n+1}_{i,j,k+1} = H_z^n_{i,j,k+1} + \frac{\Delta t}{\mu_0} \left( \frac{E_x^{n+1/2}_{i+1/2,j,k} - E_x^{n+1/2}_{i-1/2,j,k}}{\Delta y} - \frac{E_y^{n+1/2}_{i,j+1/2,k} - E_y^{n+1/2}_{i,j-1/2,k}}{\Delta z} \right)
\]

**Grid size**

\[
E_x^{n+1/2}(N_x, N_y + 1, N_z + 1) \quad H_x^n(N_x + 1, N_y, N_z)
\]

\[
E_y^{n+1/2}(N_x + 1, N_y, N_z + 1) \quad H_y^n(N_x, N_y + 1, N_z)
\]

\[
E_z^{n+1/2}(N_x + 1, N_y + 1, N) \quad H_z^n(N_x, N_y, N_z + 1)
\]

**Simple boundary conditions: Perfect Electric Conductor (PEC)**

\[
E_x(:,:,1) = 0, \quad E_x(:,:,;1) = 0
\]

\[
E_x(:,:,N_y + 1) = 0, \quad E_x(:,:,;N_z + 1) = 0
\]

\[
E_x(1,:,;) = 0, \quad E_x(;;;,1) = 0
\]

\[
E_y(N_x + 1,:,;) = 0, \quad E_y(;;;,N_z + 1) = 0
\]

\[
E_z(1,:,;) = 0, \quad E_z(:,:,1) = 0
\]

\[
E_z(N_x + 1,:,;) = 0, \quad E_z(:,:,N_y + 1;) = 0
\]

**4.3.2 Physical interpretation**

**3D Yee grid & Amper’s law**

\[
\frac{\partial}{\partial t} \int_{\mathcal{F}} \epsilon_0 \mathbf{e}(\mathbf{r}) \mathbf{E}(\mathbf{r}, t) \partial \mathbf{f} = \int_{(F)} \mathbf{H}(\mathbf{r}, t) \partial \mathbf{s}
\]
\[ H_x(i-1/2,j+1,k) \]
\[ H_x(i-1/2,j+1,k-1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ H_y(i-1,j+1/2,k) \]
\[ H_y(i-1,j+1/2,k) \]
\[ E_z(i-1/2,j+1/2,k) \]
\[ E_z(i-1/2,j+1/2,k) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ H_x(i-1/2,j+1,k) \]
\[ H_x(i-1/2,j+1,k) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ H_x(i-1/2,j+1,k) \]
\[ H_x(i-1/2,j+1,k) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ H_x(i-1/2,j+1,k) \]
\[ H_x(i-1/2,j+1,k) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ H_x(i-1/2,j+1,k) \]
\[ H_x(i-1/2,j+1,k) \]
\[ E_y(i-1/2,j+1,k+1/2) \]
\[ E_y(i-1/2,j+1,k+1/2) \]

\[ \varepsilon_0 \varepsilon_{i,j+\frac{1}{2},k+\frac{1}{2}} \left( \frac{E_z^{i-\frac{1}{2},j+\frac{1}{2},k} - E_z^{i-\frac{1}{2},j-\frac{1}{2},k}}{\Delta t} \right) \Delta x \Delta y \]

\[ = H_x^{i-\frac{1}{2},j+\frac{1}{2},k} \Delta x + H_y^{i+\frac{1}{2},j+\frac{1}{2},k} \Delta y - H_x^{i-\frac{1}{2},j+\frac{3}{2},k} \Delta x - H_y^{i-1,j+\frac{1}{2},k} \Delta y \]

solving for the unknown component:

\[ E_z^{i-\frac{1}{2},j+\frac{1}{2},k} = E_z^{i-\frac{1}{2},j+\frac{1}{2},k} + \frac{\Delta t}{\varepsilon_0 \varepsilon_{i,j+\frac{1}{2},k+\frac{1}{2}}} \left( \frac{H_x^{i-\frac{1}{2},j+\frac{1}{2},k} - H_x^{i-\frac{1}{2},j-\frac{1}{2},k}}{\Delta x} + \frac{H_y^{i+\frac{1}{2},j+\frac{1}{2},k} - H_y^{i-\frac{1}{2},j+\frac{3}{2},k}}{\Delta y} \right) \]

3D Yee grid & Faraday’s law

\[ \frac{\partial}{\partial t} \int_{\mathcal{F}} \mu_0 \mathbf{H}(\mathbf{r},t) \partial \mathbf{F} = - \int_{\mathcal{F}} \mathbf{E}(\mathbf{r},t) \partial \mathbf{F} \]

4.3.3 Divergence-free nature of the Yee discretization

\[ \nabla \times \mathbf{E}(\mathbf{r},t) = -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r},t)}{\partial t}, \quad \nabla \times \mathbf{H}(\mathbf{r},t) = \varepsilon_0 \varepsilon(\mathbf{r}) \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} + \mathbf{j}_{\text{magn}}, \]

\[ \nabla \cdot [\varepsilon_0 \varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r},t)] = 0, \quad \nabla \cdot \mathbf{H}(\mathbf{r},t) = 0, \]
\[
\frac{\partial}{\partial t} \text{div} (\varepsilon_0 \mathbf{E}) = \nabla \cdot (\varepsilon_0 \mathbf{E}) = \varepsilon_0 \frac{\partial}{\partial t} \left( \int \int \int_{\text{Yee cell}} \text{div} (\varepsilon_0 \mathbf{E}) \, dV \right) = \frac{\partial}{\partial t} \int \int \int_{\text{Yee cell}} \varepsilon_0 \mathbf{E} \cdot d\mathbf{f}
\]

\[
\frac{\partial}{\partial t} \int \int \int_{\text{Yee cell}} \varepsilon_0 \mathbf{E} \cdot d\mathbf{f} = \varepsilon_0 \frac{\partial}{\partial t} \left( \left[ E_x |_{l_i, j + \frac{1}{2}, k + \frac{1}{2}} - E_x |_{l_i, j - \frac{1}{2}, k + \frac{1}{2}} \right] \Delta y \Delta z \right)
\]

\[
+ \varepsilon_0 \frac{\partial}{\partial t} \left( \left[ E_y |_{l_i, j + \frac{1}{2}, k + \frac{1}{2}} - E_y |_{l_i, j - \frac{1}{2}, k + \frac{1}{2}} \right] \Delta x \Delta z \right)
\]

\[
+ \varepsilon_0 \frac{\partial}{\partial t} \left( \left[ E_z |_{l_i, j + \frac{1}{2}, k + \frac{1}{2}} - E_z |_{l_i, j - \frac{1}{2}, k + \frac{1}{2}} \right] \Delta x \Delta y \right)
\]

substitute Term 1 with rot equation \( \frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon_0 (\mathbf{r})} \left[ \frac{\partial \mathbf{H}}{\partial y} - \frac{\partial \mathbf{H}}{\partial z} \right] \)

Term 1 = \[
\frac{H_z |_{l_i, j + 1, k + \frac{1}{2}} - H_z |_{l_i, j - \frac{1}{2}, k + \frac{1}{2}}}{\Delta y} - \frac{H_y |_{l_i, j + 1, k + \frac{1}{2}} - H_y |_{l_i, j + \frac{1}{2}, k + \frac{1}{2}}}{\Delta z}
\] - \[
\frac{H_z |_{l_i, j - 1, k + \frac{1}{2}} - H_z |_{l_i, j + \frac{1}{2}, k + \frac{1}{2}}}{\Delta y} - \frac{H_y |_{l_i, j - 1, k + \frac{1}{2}} - H_y |_{l_i, j + \frac{1}{2}, k + \frac{1}{2}}}{\Delta z}
\]

collecting the contributions from Term 1, Term 2 and Term 3 results in vanishing of all contributions:

\[
\frac{\partial}{\partial t} \int \int \int_{\text{Yee cell}} \varepsilon_0 \mathbf{E} \cdot d\mathbf{f} = (\text{Term 1}) \Delta y \Delta z + (\text{Term 2}) \Delta x \Delta z + (\text{Term 3}) \Delta x \Delta y = 0
\]

\[\Rightarrow\] hence, if the field was divergence-free at some time it will conserve this property

\[
\int \int \int_{\text{Yee cell}} \text{div} [\varepsilon_0 \mathbf{E}(t = 0)] \, dV = 0 \quad \& \quad \frac{\partial}{\partial t} \int \int \int_{\text{Yee cell}} \text{div} (\varepsilon_0 \mathbf{E}) \, dV = 0 \quad \Rightarrow \quad \text{div} [\varepsilon_0 \mathbf{E}] = 0
\]

\[\Rightarrow\] it is important that sources do not introduce artificial divergence

### 4.3.4 Computational procedure

- Using the spatial differences of the \( \mathbf{E} \) Field that are known for the time step \( n \Delta t \) to calculate the \( \mathbf{H} \) field at the time step \((n+1/2) \Delta t\)
- Using the spatial differences of the \( \mathbf{H} \) Field that are known for the time step \((n+1/2) \Delta t\) to calculate the \( \mathbf{E} \) field at the time step \((n+1) \Delta t\)
- Using the spatial differences of the \( \mathbf{E} \) Field that are known for the time step \((n+1) \Delta t\) to calculate the \( \mathbf{H} \) field at the time step \((n+3/2) \Delta t\)
- …
Properties of the algorithm

- Leap-Frog algorithm \(\rightarrow\) discretization applies to all components
- Close to the physical world as the spatial and temporal propagation is exactly simulated

4.4 Simplification to 2D problems

- Problems are often invariant in one spatial direction, taking \(z\) (e.g. grating, cylindrical objects)
- Derivations of the field along this directions are zero

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu_0} \left[ \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - j_x \right]
\]
\[
\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon_0(\mathbf{r})} \left[ \frac{\partial H_z}{\partial y} - \frac{\partial H_x}{\partial z} \right]
\]
\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \left[ \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - j_y \right]
\]
\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon_0(\mathbf{r})} \left[ \frac{\partial H_x}{\partial x} - \frac{\partial H_y}{\partial z} \right]
\]
\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \left[ \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - j_z \right]
\]
\[
\frac{\partial H_x}{\partial t} = \frac{1}{\varepsilon_0(\mathbf{r})} \left[ \frac{\partial E_y}{\partial x} - \frac{\partial E_x}{\partial y} \right]
\]
\[
\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon_0(\mathbf{r})} \left[ \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial y} \right]
\]

\(\Rightarrow\) Maxwell can be decoupled into 2 sets of each 3 differential equations

TE polarization  TM polarization

4.5 Implementing light sources

- arbitrary light sources can be modeled simply by adding the source field to the field in the computational domain
- a physical model for sources is a makroskopic current density

\[
\text{rot} \mathbf{E}(\mathbf{r},t) = -\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t}, \quad \text{rot} \mathbf{H}(\mathbf{r},t) = \frac{\partial \mathbf{D}(\mathbf{r},t)}{\partial t} + \mathbf{j}_{\text{makr}}(\mathbf{r},t)
\]

- Simplyfied implementation by adding a source term to the electric field, which corresponds to an externaly driven dipole polarization

Examples for temporal variation

x-polarized cw-source \(E_{x_{i,j,k}} = E_{x_{i,j,k}} + \sin(n\Delta t\omega)\)

x-polarized impulse \(E_{x_{i,j,k}} = E_{x_{i,j,k}} + \delta_{n,n'}\)

Examples for spatial variation of the light source
x-polarized Gaussian wave \( E_{x_{i,j,k}}^{m} = E_{x_{i,j,k}}^{m} + e^{-\left(\frac{\Delta x}{\sigma_x}\right)^2} e^{-\left(\frac{\Delta y}{\sigma_y}\right)^2} \sin(n \Delta t \omega) \)

**Example calculations (2D-configuration, TM, Hy)**

plane wave  
homogeneous medium  
Cylinder with \( n=2 \) and \( D=2 \times \lambda \)

point source  
homogeneous medium  
Cylinder with \( n=2 \) and \( D=2 \times \lambda \)

### 4.6 Relation between frequency and time domain

If one would like to determine the response of an optical system for different wavelength of excitation one can perform many calculations for different cw excitations, where one has to wait for a long computing time until the stationary state of the calculation is reached.

Alternatively one can perform this calculation in the frequency domain:

- The frequency spectrum used for the illumination is given by the Fourier-transformation of the time dependent incident field
• With a single calculation we can calculate the entire frequency response by detecting the temporal evolution of the field behind a structure and taking the Fourier transform of the time series of the field.

• For a high resolution in the wavelength domain, we have to record the temporal evolution of the field for a long time ($N_t =$ total number of time steps) \(\Rightarrow\) long computing time.

**Example of a grating waveguide coupler**

*Periodically structured slab waveguide \(\Rightarrow\) corresponds to one-dimensional Photonic Crystal waveguide ($n_1=1.58$, $n_2=1.87$, $d_1=d_2=165$ nm, TE)*

*Transmission spectrum - The dips are waveguide resonances that are excited if the transverse $k$-vector (i.e. the momentum) provided by the grating matches the propagation constant of a waveguide mode.*
Field distributions obtained for calculations with cw-excitation at frequencies of dips in spectrum, corresponding to guided modes in the grating waveguide.

4.7 Dispersive and nonlinear materials

- FDTD is not directly applicable for materials with \( \varepsilon < 0 \) as e.g. (metals)
- Material properties depend strongly on the wavelength (dispersion)
- Inclusion of nonlinear response (instantaneous or non-instantaneous) of the material
- There exists a great diversity of approaches, but usually all of them require the simulation of the dynamics of an additional quantity
- So far we have taken into account \( \vec{E} \) and \( \vec{H} \)
- Now we include: \( \vec{J} \) current density, \( \vec{P} \) polarization, and \( \vec{D} \) displacement

Metals
Maxwell’s equations

\[
\text{rot } \mathbf{E}(\mathbf{r}, t) = -\mu_0 \frac{\partial \mathbf{H}(\mathbf{r}, t)}{\partial t}, \quad \text{rot } \mathbf{H}(\mathbf{r}, t) = \varepsilon_0 \frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} + \mathbf{j}(\mathbf{r}, t)
\]

in addition we need an equation relating current and electric field (Drude model, mean drift velocity of electrons in a field)

\[
\frac{\partial \mathbf{j}}{\partial t} + \gamma \mathbf{j} = \varepsilon_0 \omega_p^2 \mathbf{E}
\]

with \( \omega_p \) the plasma frequency and \( 1 / \gamma \) the relaxation time \( \tau \)

This is usually solved in the frequency domain as

\[
\varepsilon(\nu) = 1 + \frac{i \frac{\pi \omega_p^2}{2 \pi \nu(1 - i2\pi\nu)}}{2\pi(1 - i2\pi\nu)}
\]
Epsilon function of a metal described by the Drude model

**Dielectrics**

Assuming a 2D geometry (y-z plane) with TM polarization

$$E = E_x \hat{x}$$

The dielectric material response results in an induced polarization

$$P = P_x \hat{x}$$

which can be approximated by an Lorentz model (frequency domain similar to Drude model but with non-zero resonance frequency)

Lorentz dispersion in frequency domain:

$$P_{x,\omega} = \frac{\varepsilon_0 \omega_0^2 \chi_L}{\omega_0^2 - \omega^2 + j\omega \Gamma} E_{x,\omega}$$

Transforming into time domain by Fourier transform

Lorentz dispersion in time domain:

$$\frac{\partial^2 P_x}{\partial t^2} + \Gamma \frac{\partial P_x}{\partial t} + \omega_0^2 P_x = \varepsilon_0 \omega_0^2 \chi_L E_x$$

(see also R.W. Ziolkowski et al., JOSA A, Vol. 16, No. 4, 980)

**Nonlinear materials**

Maxwell’s equations

$$\text{rot } E(r,t) = -\frac{\partial B(r,t)}{\partial t}, \quad \text{rot } H(r,t) = \frac{\partial D(r,t)}{\partial t} + j \text{makr} (r,t),$$

$$\text{div } D(r,t) = \rho_{\text{ext}} (r,t), \quad \text{div } B(r,t) = 0,$$

Linear material response: $$D = \varepsilon E$$

Nonlinear material response: $$D = \varepsilon_0 E + P$$

with $$P = \varepsilon_0 (\chi^{(1)} E + \chi^{(2)} E^2 + \chi^{(3)} E^3 + ...)$$

Example: instantaneous Kerr $$\chi^{(3)}$$ nonlinearity

$$D = \varepsilon_0 \varepsilon E$$ with intensity dependent refractive index
\[ \varepsilon = n^2 = \left( n_0 + n_2 |E|^2 \right)^2 \approx n_0^2 + 2n_0n_2 |E|^2 \]

Refractive index depends on the square of the E-Field (for \( n_2 \ll n_0 \))

Problem: implicit equation and solution by Newton iterative procedure necessary

4.8 **Boundary conditions**

⇒ see separate presentation
5. Fiber waveguides

5.1.1 The general eigenvalue problem for scalar fields

Restrictions:
- weakly guiding structure \((\Delta n \ll 1 \Rightarrow \nabla \ln \varepsilon(x, y; \omega) \approx 0)\)
- linearly polarized field

Scalar wave equation for a scalar mode field \(u\)

\[
\Delta u(x, y) + \left[k^2 \varepsilon(x, y, \omega) - \beta^2(\omega)\right] u(x, y) = 0
\]

The mode solution \(u(x, y)\) can be assumed to correspond to the power density \(u = \sqrt{E \cdot H}\) and it has two important properties:
- \(u\) and \(u'\) must be continuous and bound, since the second derivative of \(u\) must be finite due to the finite refractive index discontinuities.
- \(u\) and \(u'\) converge to zero as \(x, y \to \infty\), since physically relevant fields should have finite energy.

These properties determine the eigenvalue problem for the propagation constant \(\beta\) of guided modes.

The discrete solutions are called guided modes.

5.1.2 Properties of guided modes

Orthogonality and normalization

Two solutions \(u_a\) and \(u_b\) of the scalar wave equation with the respective propagation constants \(\beta_a\) and \(\beta_b\) read as

\[
\Delta u(x, y) + \left[k^2 \varepsilon(x, y, \omega) - \beta_a^2(\omega)\right] u_a(x, y) = 0
\]

\[
\Delta u(x, y) + \left[k^2 \varepsilon(x, y, \omega) - \beta_b^2(\omega)\right] u_b(x, y) = 0
\]

By multiplying the first equation with \(u_b\) and the second with \(u_a\) and subtracting the results one obtains

\[
(\beta_a^2 - \beta_b^2) u_a u_b = u_b \Delta_i u_a - u_a \Delta_i u_b
\]

Integration over the infinite cross section of the waveguide \(A\infty\)

\[
(\beta_a^2 - \beta_b^2) \int_{A\infty} u_a u_b \, dA = \int_{A\infty} u_b \Delta_i u_a - u_a \Delta_i u_b \, dA
\]

Using Green’s law to transform the surface integral on the right side into a line integral, one can show that the right side is equivalent to zero, since the mode field is assumed to tend to zero at infinity

\[
(\beta_a^2 - \beta_b^2) \int_{A\infty} u_a u_b \, dA = 0
\]

To fulfill the equation for different \(\beta\) the integral must be zero

\[
\int_{A\infty} u_a u_b \, dA = \delta_{a,b}
\]
This requires the normalization of the fields according to
\[ \int_{A_{\infty}} u^2 \, dA = 1 \]
For cylinder symmetric problems we will later see that this reads as
\[ \int_{r_{\infty}} Y_a(r)Y_b(r) \, r \, dr = \delta_{a,b} \]

**Phase velocity**
The propagation velocity of the phase fronts is called phase velocity
\[ v_p = \frac{\omega}{\beta} = \frac{2\pi c}{\lambda \beta} \]
with \( \lambda \) as the vacuum wavelength and \( c \) as the speed of light in vacuum

**Group velocity**
The propagation velocity of the energy is called group velocity
\[ v_g = \frac{\partial \omega}{\partial \beta} = \frac{2\pi c}{\lambda^2} \frac{\partial \lambda}{\partial \beta} \]
which can be calculated very accurately by the following approach:
Take two solutions at two different wavelength \( \lambda \) and \( \lambda' \)
\[ \left[ \Delta_i + k^2(\lambda)\varepsilon(\lambda) - \beta^2(\lambda) \right] u(\lambda) = 0 \]
\[ \left[ \Delta_i + k^2(\lambda')\varepsilon(\lambda') - \beta^2(\lambda') \right] u(\lambda') = 0 \]
Do the same as done for deriving the orthogonality relation: multiply the first equation with \( u(\lambda) \) and the second with \( u(\lambda') \) and subtracting the results one obtains
\[ \left( (\beta^2(\lambda) - \beta^2(\lambda')) - (k^2(\lambda)\varepsilon(\lambda) - k^2(\lambda')\varepsilon(\lambda')) \right) u(\lambda)u(\lambda') = u(\lambda')\Delta_i u(\lambda) - u(\lambda)\Delta_i u(\lambda') \]
as before integrate over the infinite waveguide cross section \( A_{\infty} \), transform into a line integral using Green’s law, and show that the right side is equivalent to zero
\[ \int_{A_{\infty}} \frac{\beta^2(\lambda) - \beta^2(\lambda')}{\lambda - \lambda'} u(\lambda)u(\lambda') \, \partial A = \frac{4\pi}{\lambda - \lambda'} \int_{A_{\infty}} \left( \frac{\varepsilon(\lambda)}{\lambda^2} - \frac{\varepsilon(\lambda')}{\lambda'^2} \right) u(\lambda)u(\lambda') \, \partial A \]
with \( \lambda \to \lambda' \) one obtains
\[ \frac{1}{\beta(\lambda)} \frac{\partial \beta(\lambda)}{\partial \lambda} \int_{A_{\infty}} u^2(\lambda) \, \partial A = 4\pi \int_{A_{\infty}} u^2(\lambda) \frac{\partial}{\partial \lambda} \left( \frac{\varepsilon(\lambda)}{\lambda^2} \right) \, \partial A \]
using this expression to substitute \( \partial \lambda / \partial \beta \) in our definition for the group velocity we obtain
\[ v_g = \frac{-4\pi c \beta(\lambda)}{\lambda^2} \frac{\int_{A_{\infty}} u^2(\lambda) \, \partial A}{\int_{A_{\infty}} u^2(\lambda) \frac{\partial}{\partial \lambda} \left( \frac{\varepsilon(\lambda)}{\lambda^2} \right) \, \partial A} \]
**Group velocity dispersion**

The dependence of the group velocity on the wavelength is expressed by the Group velocity dispersion coefficient

\[ D = \frac{\partial \frac{1}{v}}{\partial \lambda} \]

5.1.3 Cylinder symmetric waveguides

In particular for fibers, the refractive index profile of the waveguide is very often cylinder symmetric

\[ \varepsilon(x, y) = \varepsilon(r) = n^2(r) \]

For fibers, the index profile is often characterized by special parameters

**Fiber parameter**

\[ V = \frac{2\pi a}{\lambda} \left( n_{co}^2 - n_{cl}^2 \right)^{1/2} \]

with

- \( a \) - core radius
- \( n_{co} \) - maximal refractive index in the core
- \( n_{cl} \) - constant refractive index in the cladding surrounding the core

**Index difference**

\[ \Delta = \frac{1}{2} \left( \frac{n_{co}^2 - n_{cl}^2}{n_{co}^2} \right) \]

**Index profile**

\[ n^2 = n_{co}^2 \left( 1 - 2\Delta f(r) \right) \]

with

\[ f(r) = \begin{cases} 
1 & r \leq a \\
\leq 1 & r > a 
\end{cases} \]

**Index dispersion**

To describe the wavelength dependence of \( \text{SiO}_2 \), which is the standard fiber material, often the Sellmaier equation is used

\[ n^2(\lambda) = 1 + \sum_{i} \frac{a_i \lambda^2}{\lambda_i^2 - C} \]

which takes into account electronic transitions in the UV and molecular vibrations in the IR by
$C = 1.53714322 \text{m}^2$

$a_1 = 1.968198 \times 10^{14}$

$a_2 = 1.4108754 \times 10^{10}$

$b_1 = 1.790244 \times 10^{14}$

$b_2 = 1.572513 \times 10^{10}$

### 5.1.4 Bessel’s differential equation

Using the Laplace operator in cylindrical coordinates

$$\Delta u(r, \varphi) = \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \varphi^2}$$

the scalar Helmholtz equation reads as

$$\frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \varphi^2} + \left[ k^2 \varepsilon(r) - \beta^2 \right] u = 0$$

Applying the product Ansatz

$$u(r, \varphi) = u_r(r) u_\varphi(\varphi)$$

the scalar cylindrical Helmholtz equation reads as

$$\frac{\partial^2 u_r}{\partial r^2} u_\varphi + \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial u_r}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u_\varphi}{\partial \varphi^2} + \left[ k^2 \varepsilon(r) - \beta^2 \right] u_r u_\varphi = 0$$

Multiplying with $r^2/(u_r u_\varphi)$ the equation can be separate in terms depending only on $r$ and terms depending only on $\varphi$

$$\frac{r^2 \frac{\partial^2 u_r}{\partial r^2}}{u_r} + \frac{r \frac{\partial u_r}{\partial r}}{u_r} + r^2 \left[ k^2 \varepsilon(r) - \beta^2 \right] = \frac{1}{u_\varphi} \frac{\partial^2 u_\varphi}{\partial \varphi^2}$$

Since both sides of the equations are independent, the equation can be solved non-trivially only when both sides are equivalent to a constant $m^2$

$$\frac{\partial^2 u_r}{\partial r^2} + \frac{1}{r} \frac{\partial u_r}{\partial r} + \left[ k^2 \varepsilon(r) - \beta^2 - \frac{m^2}{r^2} \right] u_r = 0$$

$$\frac{\partial^2 u_\varphi}{\partial \varphi^2} + m^2 u_\varphi = 0$$

The $r$-equation is the Bessel’s differential equation.

The $\varphi$-equation can be solved analytically as

$$u_\varphi = A \cos m\varphi + B \sin m\varphi = C \cos(m\varphi + \varphi_0).$$

To obtain a continuous field the so-called azimuthal mode constant must obey

$$m \in \mathbb{N}$$

Bessel’s differential equation can be simplified further by introducing the dimensionless modal parameters
\[ U = a\left(k^2 n_{co}^2 - \beta^2 \right)^{1/2} \text{ in the core} \]
\[ W = a\left(\beta^2 - k^2 n_{ci}^2 \right)^{1/2} \text{ in the cladding} \]

which are connected by
\[ V^2 = U^2 + W^2 \]

With \( n^2 = n_{co}^2 \left(1 - 2\Delta f(r)\right) \) we can express \( k^2 n^2 - \beta^2 \) as
\[ k^2 n^2 - \beta^2 = k^2 n_{co}^2 - \beta^2 - 2\Delta k n_{co}^2 f(r) \text{ and hence } k^2 n^2 - \beta^2 = \frac{U^2 - V^2 f(r)}{a^2} \]

Now we can rewrite Bessel’s differential equation for \( Y_m(\rho) = u_r(r) \) with the normalized radius \( \rho = r/a \) in the final form
\[
\frac{\partial^2 Y_m(\rho)}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial Y_m(\rho)}{\partial \rho} + \left[ U^2 - V^2 f(\rho) - \frac{m^2}{\rho^2} \right] Y_m(\rho) = 0
\]

### 5.1.5 Analytical solutions of Bessel’s differential equation

Bessel’s differential equation can be solved analytically for some specific profiles \( f(\rho) \) or in segments where \( f(\rho) \) is constant. Even though we are interested in the numeric solution of the general problem, we need particular analytic solutions to derive some general properties of the numeric solution, as e.g. the boundary conditions.

Introducing
\[ G(\rho) = U^2 - V^2 f(\rho) \]

the analytic solution in an interval with constant refractive index \((f(\rho) = \text{const.})\) reads as
\[ Y_m(\rho) = AJ_m(\rho G(0)) \]

with \( A \) being an arbitrary scaling constant and \( J_m(\rho) \) being the Bessel function of the first kind and \( m^{th} \) order. The other solutions of Bessel’s differential equation can be ruled out by physical reasoning due to their infinite value at the origin or their unboundedness for growing arguments.

Similarly the solution in the cladding (where \( f(\rho) = 1 \)) is based on the modified Hankel function
\[ Y_m(\rho) = BK_m(\rho W^2) \text{ where } \rho > 1 \]

with \( B \) being an arbitrary constant.

Using the requirement that the general solution and its derivative need to be continuous we can derive the following conditions at the core-cladding interface, which can be written as a set of linear equations using the arbitrary variables \( A \) and \( B \)
\[
AY_m(\rho = 1) - BK_m(W^2(\rho = 1)) = 0
AY_m'(\rho = 1) - BWK'_m(W^2(\rho = 1)) = 0
\]
the determinant of which must vanish to obtain unambiguous solutions
\[ W Y_m(\rho = 1)K'_m(W^2(\rho = 1)) - Y'_m(\rho = 1)K_m(W^2(\rho = 1)) = F(U^2) = 0 \]
This characteristic equation \( F(U^2) \) is only solved for discrete values of the parameters \( W \) or \( U \) which selects a finite number of modes. Usually it is solved as a function of \( U^2 \) which can vary in the interval \( 0 < U^2 < V^2 \).

The modes are often categorized in their linearly polarized form as \( \text{LP}_{mp} \) -modes, where the index \( m \) corresponds to the azimuthal mode number and \( p \) selects the modes according to the above equation. \( p \) is therefore often called the radial mode number.

\( \text{LP}_{mp} \)-modes: \( m \) - azimuthal mode number \( m \geq 0, m \in \mathbb{N} \)
\( p \) - radial mode number \( p \geq 1, p \in \mathbb{N} \)

5.1.6 Specifying the numerical problem
Repeating the governing equation
\[ \frac{\partial^2 Y_m(\rho)}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial Y_m(\rho)}{\partial \rho} + \left[ U^2 - V^2f(\rho) - \frac{m^2}{\rho^2} \right] Y_m(\rho) = 0 \]

The numerical problem consists in finding discrete modal solutions for a given azimuthal mode index \( m \) with an unknown eigenvalue \( U \).

First we need to define the boundary condition. Starting from the core center at \( \rho = 0 \) we assume that solution \( Y(\rho) \) for \( \rho \to 0 \) behaves like the Bessel function \( Y_m(\rho) = AJ_m(\rho G(0)) \) of the analytic solution. Since the Bessel function can be expressed as a series like
\[ J_m(\rho) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!(n + m + 1)} \left( \frac{\rho}{2} \right)^{2n+m} \]
we can use an ansatz function like
\[ Y_m(\rho) = \rho^m X(\rho) \]
where \( X(\rho) \) is an analytic finite valued function for finite arguments. From this ansatz we can also take the derivative of the solution as
\[ Y'_m(\rho) = m\rho^{(m-1)}X(\rho) + \rho^m X'(\rho) \]

Hence the boundary condition in the center read as
\[ m = 0: \ Y(0) = X(0) \]
\[ Y'(0) = X'(0) \]
\[ m = 1: \ Y(0) = 0 \]
\[ Y'(0) = X(0) \]
\[ m > 1: \ Y(0) = 0 \]
\[ Y'(0) = 0 \]
As was demonstrated in the “Analytic solution” section the boundary conditions at infinity ($\rho \to \infty$) can be transformed to the position of the core cladding interface as

$$F(U^2) = W Y_m'(\rho = 1) K'_m(W^2(\rho = 1)) - Y_m(\rho = 1) K_m(W^2(\rho = 1)) = 0$$

### 5.1.7 Solving the second order singularity

The governing Bessel’s differential equation possesses a second order singularity at $\rho = 0$ which makes it very hard to integrate numerically. Using again the ansatz function

$$Y_m(\rho) = \rho^m X_m(\rho)$$

we obtain a new differential equation for $X(\rho)$ as

$$\frac{\partial^2 X_m(\rho)}{\partial \rho^2} + \frac{2m + 1}{\rho} \frac{\partial X_m(\rho)}{\partial \rho} + \left[U^2 - V^2 f(\rho)\right] X_m(\rho) = 0$$

which possesses only an ordinary singularity at $\rho = 0$. At the same time the boundary conditions must be transformed. Since $X(\rho)$ is an analytic function it can be expressed as a power series following the series representation of the Bessel function as

$$X_m(\rho) = \sum_{n=0}^{\infty} c_n \rho^n$$

Hence the new boundary conditions at $\rho = 0$ are independent of $m$

$$X(0) = c_0 \quad \text{and} \quad X'(0) = 0$$

Similarly the boundary condition at $\rho = 1$ becomes

$$F(U^2) = \left[ W \frac{K'_m(W)}{K_m(W)} - m \right] X_m(\rho = 1) - X'_m(\rho = 1) = 0$$

with $F(U^2)$ being a characteristic function. We have to keep in mind that, once found, the new solution $X_m(\rho)$ has to be transformed back to $Y_m(\rho)$ to derive some physical meaning.

### 5.1.8 Numerical integration methods

Up to now the problem is a boundary value problem which would require e.g. a relaxation method for its numerical solution and to find the desired parameter $U^2$. Using the shooting method the problem can be transformed into an initial value problem starting at $\rho = 0$ which depends on the parameter $U^2$. Different $U^2$ result in different solutions at $\rho = 1$ and hence also different $F(U^2)$. The aim must be to find a parameter $U = U^*$ with

$$F(U^{*2}) = 0$$
Then the solutions of the initial value problem would also solve the boundary value problem.

For the numerical integration of the differential equation for $X_m(\rho)$ we have to take into account the following properties:

- at $\rho = 0$ the function $X_m(\rho)$ has a first-order singularity, which depending on $m$ can lead to instabilities of the numeric solution
- the profile function $f(\rho)$ can possess discontinuities in the integration interval, which can reduce the order of the integration methods
- the coefficients of the series representation of $X_m(\rho)$ can go through zero in the integration interval, which can change the continuity properties of the solution

Hence one should refer to implicit integration methods.

In the beginning we transform the second order differential equation into a set of coupled first order differential equations with

$$
\begin{align*}
Z_m(\rho) = \begin{pmatrix} Z_m^1(\rho) \\ Z_m^2(\rho) \end{pmatrix} = \begin{pmatrix} X_m(\rho) \\ X'_m(\rho) \end{pmatrix}
\end{align*}
$$

as

$$
\frac{\partial Z_m^1(\rho)}{\partial \rho} = Z_m^2(\rho)
$$

$$
\frac{\partial Z_m^2(\rho)}{\partial \rho} = \left( V^2 f(\rho) - U^2 \right) Z_m^1(\rho) - \frac{2m+1}{\rho} Z_m^2(\rho)
$$

Now we have to discretize the integration interval $\Omega = [0,1] \subset \mathbb{R}$, e.g. with very simple equidistant spacing $h$ as:

$$
\Omega_h = \left\{ \rho_j \mid \rho_j = jh, \ j = 0(1)N, \ h = \frac{1}{N} \right\}
$$

then the discrete approximation of the solution can be written as

$$
Z_j \approx Z(\rho_j), \ \rho_j \notin \Omega_h
$$

**Implicit Runge-Kutta-Midpoint-Method of 2\textsuperscript{nd} order**

In matrix representation the differential equation reads as

$$
\frac{\partial Z_m(\rho)}{\partial \rho} = \begin{pmatrix} 0 & 1 \\ V^2 f(\rho) - U^2 & -\frac{2m+1}{\rho} \end{pmatrix} Z_m(\rho) = K(Z_{m(j)}, \rho_j)
$$

The midpoint-method has the following Runge-Kutta parameter table (Butcher scheme)

$$
\begin{array}{r|c}
0.5 & 0.5 \\
1 & 1
\end{array}
$$

This is a single step implicit method which results in an iteration step like
\[ Z_{j+1} = Z_j + h \Phi(\rho_j, Z_j, h), \quad (j = 0, 1, ..., N) \]

\[ \Phi(\rho_j, Z_j, h) = K \left( Z_j + \frac{1}{2} \Phi(\rho_j, Z_j, h), \rho_j + \frac{h}{2} \right) \]

applying this method to our particular problem gives

\[ \Phi(\rho_j, Z_j, h) = \left( \begin{array}{c} \varphi_1 \\ \varphi_2 \end{array} \right) = \left( \begin{array}{c} 0 \\ \frac{1}{2} \end{array} \right) \begin{bmatrix} V^2 f \left( \rho_j + \frac{h}{2} \right) - U^2 & - \frac{2m+1}{\rho_j + \frac{h}{2}} \\ \frac{Z_{1(j)} + \frac{h}{2} \varphi_1}{Z_{2(j)} + \frac{h}{2} \varphi_2} \end{bmatrix} \]

since we are dealing with a linear problem we can avoid the otherwise necessary iterative numerical solution of the above problem and solve it explicitly

\[ Z_{1(j+1)} = Z_{1(j)} + h \frac{h}{2} \left( V^2 f \left( \rho_j + \frac{h}{2} \right) - U^2 \right) \frac{Z_{1(j)} + Z_{2(j)}}{1 + \frac{h}{2} \frac{2m+1}{\rho_j + \frac{h}{2}} - \frac{h}{4} \left( V^2 f \left( \rho_j + \frac{h}{2} \right) - U^2 \right)} \]

\[ Z_{2(j+1)} = Z_{2(j)} + h \frac{h}{2} \left( V^2 f \left( \rho_j + \frac{h}{2} \right) - U^2 \right) \frac{Z_{1(j)} + \frac{h}{2} \left( V^2 f \left( \rho_j + \frac{h}{2} \right) - U^2 \right) - \frac{2m+1}{\rho_j + \frac{h}{2}}}{1 + \frac{h}{2} \frac{2m+1}{\rho_j + \frac{h}{2}} - \frac{h}{4} \left( V^2 f \left( \rho_j + \frac{h}{2} \right) - U^2 \right)} \]

The solution accuracy of the method is second order in \( h \). The discretization grid \( \Omega_h \) should be chosen such that the discontinuity points \( \rho_D \) of the profile function \( f(\rho) \) coincide with grid points of \( \Omega_h \)

\[ \rho_D \in \Omega_h \]

This ensures that the differential equation is only evaluated in continuous intervals at \( x_D + 0.5h \). Consequently the second order solution accuracy is preserved also for discontinuous profiles \( f(\rho) \).

**Implicit Runge-Kutta-Method of 4th order**

To improve the accuracy one could also use the following Gaussian type forth order method with the Butcher scheme

\[
\begin{array}{ccc}
\frac{1}{2} + \frac{\sqrt{3}}{6} = \gamma_1 & \frac{1}{2} = \beta_{11} & \frac{1}{2} + \frac{\sqrt{3}}{6} = \beta_{12} \\
\frac{1}{2} - \frac{\sqrt{3}}{6} = \gamma_2 & \frac{1}{2} - \frac{\sqrt{3}}{6} = \beta_{21} & \frac{1}{4} = \beta_{11} \\
1 & \frac{1}{2} = \beta_1 & \frac{1}{2} = \beta_2
\end{array}
\]
5.1.9 Eigenvalue search

Since we have transformed the original boundary value problem into an initial value problem using a shooting method, the search for the eigenvalues $U^2$ is a simple search for the roots of $F(U^2)$ for parameter $m$. However for each calculation of $F(U^2)$ we have to compute the full differential equation problem in the interval $\Omega = [0,1]$.

The eigenvalue interval for guided modes is restricted to $0 < U^2 < V^2$ containing a finite number of roots. To find all roots the interval can be scanned for sign changes with a fixed step size $\Delta U^2$. The resulting subintervals can be refined using e.g. a converging secant method.

5.1.10 Calculation examples

Example of $F(U^2)$ in the interval $U \in (0,V)$ for a step index profile with $m = 0$
Examples of calculated mode field for a ring index fiber.
Examples of calculated mode field for a ring index fiber.

(a) $\lambda = 1064 \, \text{nm}, \, m = 2, \, p = 1$

(b) $\lambda = 804 \, \text{nm}, \, m = 3, \, p = 4$
6. Fourier Modal Method for periodic systems

**Aim**
- rigorous solution of the diffraction of light at periodic structures (gratings)

**Methods**
- A) thin element approximation
- B) formulating the eigenvalue problem in the Fourier space and deriving boundary conditions imposed onto the modes in order to be matched properly to the homogenous space

**Examples of diffraction gratings**

![1D grating](image1)

![2D grating (biperiodic)](image2)

Gratings are characterized by a periodic variation of the dielectric constant in $x$ and $y$ direction with periods $\Lambda_x$ and $\Lambda_y$.

**Illustration of the problem by understanding a grating as a periodic waveguide array embedded between two homogenous media**

![Illustration](image3)

Dielectric waveguide with rectangular cross section ➔ Periodically arranged dielectric waveguide with rectangular cross section
6.1 Formulation of the problem in 2D for TE

Rigorously calculated field distribution around a binary grating for plane wave TE excitation and sketch of the diffraction problem

Incident field
\[ E_{\text{inc},y} = \exp\left[i k_{0} n_{\text{i}} (\sin \theta x + \cos \theta z)\right] \text{ with } \theta \text{ being the angle of incidence} \]

Diffraction field in different diffraction orders \( i \)
\[ E_{\text{I},y} = E_{\text{inc},y} + \sum R_{i} \exp\left[i (k_{x,i} x - k_{z,i} z)\right] \text{ for } z < 0 \]
\[ E_{\text{II},y} = \sum T_{i} \exp\left[i (k_{x,i} x + k_{z,i} (z - d))\right] \text{ for } z > d \]

Remaining question: What is the direction and strength of the reflected and transmitted amplitudes??

The wave number of each wave is given by
\[ k = \frac{2 \pi}{\lambda} n = \sqrt{k_{x}^2 + k_{z}^2} \]

The incident wave is characterized by
\[ k_{z,i} = \frac{2 \pi}{\lambda_{0}} n_{\text{i}} \cos(\theta), \quad k_{x,i} = \frac{2 \pi}{\lambda_{0}} n_{\text{i}} \sin(\theta) \]

The grating provides a momentum for each diffraction order of
\[ k_{x,i} = i \frac{2 \pi}{\Lambda} \text{ with } i \in \mathbb{Z} \text{ being the index of the diffraction order} \]

Hence the diffracted waves are characterized by
\[ k_{x,i} = i \frac{2 \pi}{\Lambda} + k_{0} n_{\text{i}} \sin(\theta), \quad k_{z,\text{I/II},zi} = \sqrt{k_{0}^2 n_{\text{I/II}}^2 - k_{x,i}^2} \]

- The propagation directions of the diffraction orders are only determined by the grating period \( \Lambda \), the angle of incidence \( \theta \) and the refractive indices \( n_{\text{I/II}} \) of the surrounding media.
- The character of the diffraction orders is determined by
  \[ k_{x,i}^2 \leq k_{0}^2 n_{\text{I/II}}^2 \Rightarrow \text{propagating wave} \]
  \[ k_{x,i}^2 > k_{0}^2 n_{\text{I/II}}^2 \Rightarrow \text{evanescent field} \]
6.2 Scalar theory for thin elements

The field after the structure is given by the incident field multiplied by the transfer function

\[ U_T(x, y) = T(x, y)U_0(x, y) \quad \text{with} \quad U = E_0 \hat{y} \]

\[ T(x, y) = |T(x, y)|\exp(i\phi(x, y)) \]

For a pure phase grating the amplitude transmission function equals unity and the phase is given by

\[ \phi(x) = k_0 \left(n_{II} - n_I\right)f(x) \]

Hence for perpendicular plane wave illumination the field after the structure is given by

\[ \exp(i\phi(x)) \]

The amplitudes of the planewaves in the direction of the diffraction orders are given by the Fourier transform of the transmission function

\[ T_n = FT\left(\exp(i\phi(x))\right) = \frac{1}{\Lambda} \int_0^\Lambda \exp\left(ik_0 \left(n_{II} - n_I\right)f(x)\right)\exp(-ik_{sn}x)\,dx \]

Physical interpretation of diffraction efficiency

- The diffraction efficiency corresponds to the energy transferred into a diffraction order normalized to the incident energy (given by the Poynting vector) \( S = E \times H \)
- Introducing the plane waves into the equation leads to
\[ \eta_{\text{TE}} = \left| \frac{k_{II}}{k_0} \right|^2 \text{Re} \left( \frac{k_{II}}{k_0} \right) R_0^2 \text{ with } p_{II} = 1 \text{ for TE and } p_{III} = \epsilon_{III} \text{ for TM} \]

\[ \eta_{\text{TM}} = \left| \frac{k_{III}}{k_0} \right|^2 \text{Re} \left( \frac{k_{III}}{k_0} \right) R_0^2 \]

- Energy must be conserved for loss-less materials!

**Examples for the validity of the thin element approximation**

Sinusoidal long period grating \((\Lambda = 10\lambda)\) illuminated with a plane wave

\(\Lambda\) is much larger than \(\lambda\) \(\Rightarrow\) The thin element approach is justified.

Sinusoidal short period grating \((\Lambda = 2.1\lambda)\) illuminated with a plane wave

\(\Lambda\) is comparable to \(\lambda\) \(\Rightarrow\) Diffractive effects can already be observed inside the grating volume \(\Rightarrow\) The thin element approach would fail.
**Limitations of the scalar method**

**Phase of the field directly after a sinusoidal grating with different grating periods**

*grating profile with depth $h = \lambda$, $n_1 = 1$, $n_2 = 2$, TE illumination.*

- Scalar theory fails if the period gets comparable to the wavelength and the thickness of the grating is significant.
- Proper description of the field inside the grating ($0 < z < d$) is impossible.
  $\Rightarrow$ Maxwell's equations must be solved also inside the grating!

### 6.3 Rigorous grating solver

**Ansatz**

- expanding the fields in the different domains in terms of modes
  (mode = eigen solution of a wave equation)
  - Modes are just plane waves in the incidence and transmitted region.
  - In grating region the modes are waveguide modes propagating along $z$, that fulfill the periodic boundary conditions in the transverse direction.
  - The mode profil must be 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 wavevector 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 amplitudes 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.)

6.3.1 Calculation of eigenmodes in Fourier space
• starting from Maxwell’s equations for a time harmonic field with magnetic field scaled by impedance
\[
\nabla \times \mathbf{E}(r) = i k_0 \mathbf{H}(r) \quad \nabla \times \mathbf{H}(r) = -i k_0 \varepsilon(r) \mathbf{E}(r)
\]
• plugging equations together and eliminating the z-component of the field (unambiguously determined by the divergence equations)
\[
\frac{\partial}{\partial z} E_y = \frac{\partial}{\partial y} E_z - i k_0 H_x \quad \frac{\partial}{\partial z} H_y - \frac{\partial}{\partial y} H_x = -i k_0 \varepsilon(r) E_z
\]
results in the following dynamic equations
\[
\frac{\partial}{\partial z} E_y = \frac{1}{-i k_0} \frac{\partial}{\partial y} \left[ \frac{1}{\varepsilon} \left( \frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x \right) \right] - i k_0 H_x
\]
\[
\frac{\partial}{\partial z} E_x = \frac{1}{-i k_0} \frac{\partial}{\partial x} \left[ \frac{1}{\varepsilon} \left( \frac{\partial}{\partial y} H_y - \frac{\partial}{\partial y} H_x \right) \right] + i k_0 H_y
\]
\[
\frac{\partial}{\partial z} H_y = \frac{1}{i k_0} \frac{\partial}{\partial y} \left[ \frac{\partial}{\partial x} E_y - \frac{\partial}{\partial y} E_x \right] + i k_0 \varepsilon H_y
\]
\[
\frac{\partial}{\partial z} H_x = \frac{1}{i k_0} \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial y} E_y - \frac{\partial}{\partial y} E_x \right] - i k_0 \varepsilon H_y
\]
(For details see Li et al., Phys. Rev. E 67, 046607 (2003).)

**Fourier expansion of all quantities**
To solve the eigenvalue problem derived from the above equations all quantities are transformed into Fourier space: \( \mathbf{E}(r) \rightarrow \mathbf{E}(k) \), \( \mathbf{H}(r) \rightarrow \mathbf{H}(k) \), \( \varepsilon(r) \rightarrow \varepsilon(k) \), and also \( \varepsilon^{-1}(r) \rightarrow \varepsilon^{-1}(k) \).
\[ E(r) = \sum_{ij} E_{ij}(z) \exp\left[ i \left( k_{ij,x} x + k_{ij,y} y \right) \right] \]
\[ H(r) = \sum_{ij} H_{ij}(z) \exp\left[ i \left( k_{ij,x} x + k_{ij,y} y \right) \right] \]
\[ \varepsilon(r) = \sum_{ij} \varepsilon_{ij} \exp\left[ i G_{ij} r \right] \]
\[ \varepsilon(r)^{-1} = \sum_{ij} \varepsilon_{ij}^{-1} \exp\left[ i G_{ij} r \right] \]

with \( k_{ij} = (k_{ij,x}, k_{ij,y}) = (k_{0,x}, k_{0,y}) + i b_1 + j b_2 \) and \( G_{ij} = i b_1 + j b_2 \)

The integers \( i, j \) run from \(-\infty\) to \(\infty\), which has to be truncated for numerical calculations.

Now these Fourier expansions are inserted into the dynamic field equations, here for the following example

\[ \frac{\partial}{\partial z} H_x = \frac{1}{ik_0} \frac{\partial}{\partial x} \left[ \frac{\partial}{\partial y} E_y - \frac{\partial}{\partial y} E_x \right] - ik_0 \varepsilon H_y \]
the individual terms are substituted

\[ \frac{\partial}{\partial z} H_x = \frac{\partial}{\partial z} \sum_{mn} H_{mn,x} \exp\left[ i \left( k_{mn,x} x + k_{mn,y} y \right) \right] \]

\[ \frac{\partial}{\partial x} E_y = \frac{\partial}{\partial x} \sum_{mn} E_{mn,y} \exp\left[ i \left( k_{mn,x} x + k_{mn,y} y \right) \right] = \sum_{mn} ik_{mn,x} E_{mn,y} \exp\left[ i \left( k_{mn,x} x + k_{mn,y} y \right) \right] \]

\[ \varepsilon E_y = \sum_{mn} \varepsilon_{mn} \exp\left[ i \left( k_{mn,x} x + k_{mn,y} y \right) \right] \sum_{mn} E_{mn,y} \exp\left[ i \left( k_{mn,x} x + k_{mn,y} y \right) \right] \]

now all terms are multiplied with \( \exp\left[ -i \left( k_{ij,x} x + k_{ij,y} y \right) \right] \) and integrated over \( x \) and \( y \) as

\[ \iint \exp\left[ -i \left( k_{ij,x} x + k_{ij,y} y \right) \right] \exp\left[ i \left( k_{mn,x} x + k_{mn,y} y \right) \right] \partial x \partial y = \delta_{ij,mn} \]

This results in the following example
\[
\frac{\partial}{\partial z} \sum_{mn} \iint H_{mn,x} \exp\left[-i(k_{ij,x}x + k_{ij,y}y)\right] \exp\left[i(k_{mn,x}x + k_{mn,y}y)\right] \partial x \partial y = \frac{\partial}{\partial z} \sum_{mn} H_{mn,x} \delta_{ij,mn}
\]

which has to be done with all equations

This results in the following set of equations

\[
\frac{\partial}{\partial z} E_{ij,x} = -\frac{ik_{ij,x}}{k_0} \sum_{mn} \varepsilon_{ij,mn}^{-1} (k_{mn,x} H_{mn,y} - k_{mn,y} H_{mn,x}) + ik_0 H_{ij,y}
\]
\[
\frac{\partial}{\partial z} E_{ij,y} = -\frac{ik_{ij,y}}{k_0} \sum_{mn} \varepsilon_{ij,mn}^{-1} (k_{mn,x} H_{mn,y} - k_{mn,y} H_{mn,x}) - ik_0 H_{ij,x}
\]
\[
\frac{\partial}{\partial z} H_{ij,x} = \frac{ik_{ij,x}}{k_0} \sum_{mn} \delta_{ij,mn} (k_{mn,x} E_{mn,y} - k_{mn,y} E_{mn,x}) - ik_0 \sum_{mn} \varepsilon_{ij,mn} E_{mn,y}
\]
\[
\frac{\partial}{\partial z} H_{ij,y} = \frac{ik_{ij,y}}{k_0} \sum_{mn} \delta_{ij,mn} (k_{mn,x} E_{mn,y} - k_{mn,y} E_{mn,x}) + ik_0 \sum_{mn} \varepsilon_{ij,mn} E_{mn,x}
\]

with \( \varepsilon_{ij,mn} = \varepsilon_{i-m,j-n} \)

These equations can be conveniently written in matrix form as

\[
\frac{\partial}{\partial z} E = T_1 H \quad \frac{\partial}{\partial z} H = T_2 E
\]

where

\[
E = \begin{pmatrix}
E_{ij,x} \\
E_{ij,y} \\
\vdots
\end{pmatrix} \quad H = \begin{pmatrix}
H_{ij,x} \\
H_{ij,y} \\
\vdots
\end{pmatrix}
\]

and

\[
T_1^{ij,mn} = \frac{i}{k_0} \begin{pmatrix}
\delta_{ij,mn} k_{mn,y} & -k_{ij,x} \varepsilon_{ij,mn}^{-1} k_{mn,x} + k_0^2 \delta_{ij,mn} \\
k_{ij,x} \varepsilon_{ij,mn}^{-1} k_{mn,y} & \delta_{ij,mn} k_{mn,x} & -k_{ij,y} \varepsilon_{ij,mn}^{-1} k_{mn,y} + k_0^2 \delta_{ij,mn}
\end{pmatrix}
\]
\[
T_2^{ij,mn} = \frac{i}{k_0} \begin{pmatrix}
-k_{ij,x} \delta_{ij,mn} k_{mn,y} + k_0^2 \varepsilon_{ij,mn}^{-1} & k_{ij,x} \delta_{ij,mn} k_{mn,x} + k_0^2 \varepsilon_{ij,mn}^{-1} \\
-k_{ij,y} \delta_{ij,mn} k_{mn,x} & \delta_{ij,mn} k_{mn,y} + k_0^2 \varepsilon_{ij,mn}^{-1}
\end{pmatrix}
\]

This set of two coupled 1\(^{st}\) order differential equations for \( E \) and \( H \) can be combined into a single 2\(^{nd}\) order equation for \( E \)

\[
\frac{\partial^2}{\partial z^2} E = (T_1 T_2) E
\]

**Eigenvalues**

- This eigenvalue equation can be solved for its eigenvalues with standard routines.
The infinite Fourier expansions are truncated up to $N_0 = (-N,\ldots,0,\ldots,N)$ for numerical solution. This results in $2N_0$ eigenvalues $\beta_i^2$ with $\Im(\beta_i) \geq 0$ which correspond to forward or backward propagating solutions.

**Eigenvectors**

- Eigenvectors are associated with the eigenvalues and are given in a matrix $S_a$ with size $(2N_0) \times (2N_0)$.
- They provide the Fourier components of the guided eigenmodes.
- Eigenfields are given by the forward and backward propagating eigenmode

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

with

$$E_a^+ = \begin{pmatrix} \vdots \\ E_{a,i}^+(z) \\ \vdots \end{pmatrix} \quad E_a^- = \begin{pmatrix} \vdots \\ E_{a,i}^-(z) \\ \vdots \end{pmatrix}$$

where

$$E_{a,i}^+(z) = E_i^+ \exp(i\beta_i z) \quad E_{a,i}^-(z) = E_i^- \exp(-i\beta_i z)$$

Here $E_i^+$ and $E_i^-$ are unknown (free) amplitudes.

(For details see Li et al., Phys. Rev. E 67, 046607 (2003).)

The magnetic fields can be determined from the 1st order differential equations as

$$H = T_1^{-1} \frac{\partial}{\partial z} E$$

$$= T_1^{-1} S_a \frac{\partial}{\partial z} \left( E_a^+ + E_a^- \right)$$

$$= T_1^{-1} S_a i\beta \left( E_a^+ + E_a^- \right)$$

$$= T_a \left( E_a^+ + E_a^- \right)$$

with $T_a = T_1^{-1} S_a i\beta$
Examples of eigenfields

Eigenmodes propagate in the waveguide normal to this plane (periodic boundaries)

6.3.2 Explicit derivation for 2D problems

E.g. for TE polarization

\[
\begin{align*}
\frac{\partial}{\partial z} H_y &= \frac{1}{ik_0} \frac{\partial}{\partial y} \left( \frac{\partial}{\partial x} E_y - \frac{\partial}{\partial y} E_x \right) + ik_0 \varepsilon E_x \\
\frac{\partial}{\partial x} &= 0 \quad \Rightarrow \quad \frac{\partial}{\partial z} H_y = \frac{1}{ik_0} \frac{\partial^2}{\partial y^2} E_x + ik_0 \varepsilon E_x \\
\text{and} \\
\frac{\partial}{\partial z} E_x &= \frac{1}{-ik_0} \frac{\partial}{\partial x} \left[ \frac{1}{\varepsilon} \left( \frac{\partial}{\partial x} H_y - \frac{\partial}{\partial y} H_x \right) \right] + ik_0 H_y
\end{align*}
\]

\( E_x \), \( H_y \), \( H_x \), \( E_y \)

\( \Lambda_y \)
We substitute the fields by their Fourier series representations. We start from
\[
\frac{\partial}{\partial x} E_x = i k_0 H_x
\]
and insert
\[
\frac{\partial}{\partial z} E_x = \frac{\partial}{\partial z} \sum_m E_{m,x} \exp(ik_{m,y} y) \quad \text{and} \quad ik_0 H_y = ik_0 \sum_m H_{m,y} \exp(ik_{m,y} y)
\]
We get
\[
\frac{\partial}{\partial z} \sum_m E_{m,x} \exp(ik_{m,y} y) = ik_0 \sum_m H_{m,y} \exp(ik_{m,y} y)
\]
Multiplying with the periodic function \( \exp(-ik_{j,y} y) \) results in
\[
\frac{\partial}{\partial z} \sum_m E_{m,x} \exp(ik_{m,y} y) \exp(-ik_{j,y} y) = ik_0 \sum_m H_{m,y} \exp(ik_{m,y} y) \exp(-ik_{j,y} y)
\]
Integrated over \( y \) as
\[
\frac{\partial}{\partial z} \sum_m E_{m,x} \int \exp(ik_{m,y} y) \exp(-ik_{j,y} y) = ik_0 \sum_m H_{m,y} \int \exp(ik_{m,y} y) \exp(-ik_{j,y} y)
\]
gives
\[
\frac{\partial}{\partial z} \sum_m E_{m,x} \delta_{m,j} = ik_0 \sum_m H_{m,y} \delta_{m,j} \Rightarrow \frac{\partial}{\partial z} E_{j,x} = ik_0 H_{j,y}
\]
which are individual equations for to different Fourier components of the fields, as
\[
\begin{align*}
\frac{\partial}{\partial z} E_{0,x} &= ik_0 H_{0,y} \\
\frac{\partial}{\partial z} E_{1,x} &= ik_0 H_{1,y} \\
\vdots \quad \Rightarrow \quad \frac{\partial}{\partial z} E_{n,x} &= ik_0 H_{n,y}
\end{align*}
\]
which in matrix notation reads as
\[
\frac{\partial}{\partial z} E_x = T_1 H_y \quad \text{with} \quad T_1^{j,n} = ik_0 \delta_{j,n}
\]
The other equation we treat equivalently
\[
\frac{\partial}{\partial z} H_y = \frac{1}{ik_0} \frac{\partial^2}{\partial y^2} E_x + ik_0 \varepsilon E_x
\]
By substituting
\[ \frac{\partial}{\partial z} H_y = \frac{\partial}{\partial z} \sum_m H_{m,y} \exp(ik_{m,y}y) \]

and, as above, multiplying with the periodic function and integrating over \( y \) we get directly

\[ \Rightarrow \frac{\partial}{\partial z} H_{i,y} \]

We apply the same procedure to the second term by substituting

\[ \frac{i}{k_0} \frac{\partial^2}{\partial y^2} E_x = \frac{i}{k_0} \frac{\partial^2}{\partial y^2} \sum_m E_{m,x} \exp(ik_{m,y}y) = -\frac{i}{k_0} \sum_m k^2_{m,y} E_{m,x} \exp(ik_{m,y}y) \]

results in

\[ \Rightarrow -\frac{i}{k_0} k^2_{i,y} E_{i,x} \]

For the third term

\[ ik_0 \varepsilon E_x = ik_0 \varepsilon \sum_m E_{m,y} \exp(ik_{m,y}) \sum_n E_{n,x} \exp(ik_{n,x}) = ik_0 \sum_m \sum_n \varepsilon_m E_{n,x} \exp(iG_{m,y} + k_{n,y} - k_{i,y}y) \]

\[ \Rightarrow ik_0 \sum_m \sum_n \varepsilon_m E_{n,x} \exp(i(m \frac{2\pi}{\Lambda_y} y + n \frac{2\pi}{\Lambda_y} y - \frac{2\pi}{\Lambda_y} y + k_{i,y}y)) \]

\[ = ik_0 \sum_m \sum_n \varepsilon_m E_{n,x} \exp(i(m \frac{2\pi}{\Lambda_y} y + n \frac{2\pi}{\Lambda_y} y - \frac{2\pi}{\Lambda_y} y)) \]

\[ \Rightarrow ik_0 \sum_m \sum_n \varepsilon_m E_{n,x} \int dy e^{i(m \frac{2\pi}{\Lambda_y} y + n \frac{2\pi}{\Lambda_y} y - \frac{2\pi}{\Lambda_y} y)} \]

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

\[ \Rightarrow ik_0 \sum_n \varepsilon_{i-n} E_{n,x} \]
\[
\frac{\partial}{\partial z} H_y = -\frac{1}{i k_0} \frac{\partial^2}{\partial y^2} E_x + i k_0 \epsilon E_x
\]

\[
\frac{\partial}{\partial z} H_{i,y} = -\frac{i}{k_0} k_{i,y}^2 E_{i,x} + i k_0 \sum_n \epsilon_i - n E_{n,x}
\]

\[
\frac{\partial}{\partial z} H_y = T_2 E_x
\]

**Eigenvalue problem in 2D**

\[
\begin{bmatrix}
H_{0,y} \\
H_{1,y} \\
\vdots \\
H_{n,x}
\end{bmatrix}
= i \frac{k_0}{k_0} \begin{bmatrix}
-k_0^2 \epsilon_0 + k_0^2 \epsilon_0 \\
k_0^2 \epsilon_1 - k_0^2 \epsilon_0 \\
-k_0^2 \epsilon_2 + k_0^2 \epsilon_1 \\
\vdots \\
k_0^2 \epsilon_{1-n} - k_0^2 \epsilon_{1-n}
\end{bmatrix}
\begin{bmatrix}
E_{0,x} \\
E_{1,x} \\
\vdots \\
E_{n,x}
\end{bmatrix}
\]

**Example**

- 1D periodic waveguide array
- All possible eigenmodes are calculated using the method
- shown is the electric field upon propagating through a waveguide in z-direction

Fundamental mode

Higher order guided mode

Guided mode with field localization between the waveguides

Evanescent mode