0. Introduction

1. Reminder:
   E-Dynamics in homogenous media and at interfaces

2. Photonic Crystals
   2.1 Introduction
   2.2 1D Photonic Crystals
   2.3 2D and 3D Photonic Crystals
   2.4 Numerical Methods
      2.4.1 FDTD
      2.4.2 Plane-Wave Expansion
      2.4.3 T-Matrix, Scalar-Wave-Approximation, S-Matrix
   2.5 Fabrication
   2.6 Chiral Photonic Crystals
   2.7 Photonic Crystal Fibers – „Holey“ Fibers
   2.8 Quantumoptics
   2.9 Quasicrystals

3. Metamaterials
Multiple interfaces

- Finite 1D Photonic Crystal with N-1 layers and N interfaces

\[
\begin{pmatrix}
E_0 \\
r
\end{pmatrix}
= \mathbf{M}^{x_0 + a(N-1)} \cdots \mathbf{M}^{x_0}
\begin{pmatrix}
t \\
E_1
\end{pmatrix}
\]
Multiple interfaces

- Finite 1D Photonic Crystal with N-1 layers and N interfaces

\[(\text{Fields on left side}) = T\text{-Matrix} \ast (\text{Fields on right side})\]
Same problem – different approach

• Finite 1D Photonic Crystal with N-1 layers and N interfaces

\[ E_0 \text{ r} \] (Outgoing fields) = S-Matrix * \( (\text{Incident Fields}) \)

T-Matrix works fine? Why do we need another method?

The **T-Matrix** formalism is inherently unstable since it deals with exponentially decaying and **exponentially growing fields**.

Therefore, the **T-Matrix** formalism is not suited for more complicated problems (e.g. 2D or 3D metallic structures).

In contrast to this, **exponentially growing fields** do not appear in the **S-Matrix** formalism.
S-Matrix formalism for finite 3D Photonic Crystals

Finite extent in $z$-direction

Periodic in $xy$-direction

Note:
The electromagnetic field is a superposition of partial waves (diffraction!) with wavevectors

\[
\vec{k}_G = \begin{pmatrix}
  k_x + G_x \\
  k_y + G_y \\
  \sqrt{\frac{\omega^2 \varepsilon}{c^2} - (k_x + G_x)^2 - (k_y + G_y)^2}
\end{pmatrix}
\]

(Outgoing fields) = S-Matrix * (Incident Fields)
How to calculate the S-Matrix?

1.) Decompose the structure into layers which are homogenous in \( \textit{z}\)-direction and periodic in \( \textit{xy}\)-direction.

2.) Calculate the \textit{eigenmodes} of each layer (2D Photonic Crystal problem!).

3.) Calculate \textit{transfer matrix} for each layer and \textit{interface matrices} for adjacent layers.

4.) \textbf{Construct the S-Matrix} of the whole 3D Photonic Crystal by an iterative procedure from the transfer- and interface matrices.

How to calculate the S-Matrix?

1.) Decompose the structure into layers which are **homogenous** in \( z \)-direction and **periodic** in \( xy \)-direction.

2.) Calculate the eigenmodes of each layer (2D Photonic Crystal problem!).

3.) Calculate transfer matrix for each layer and interface matrices for adjacent layers.

4.) Construct the S-Matrix of the whole 3D Photonic Crystal by an iterative procedure from the transfer- and interface matrices.
Decompose the structure into layers which are homogenous in $z$-direction and periodic in $xy$-direction.

Example:

For each layer:

$$\eta (\vec{G}) = \frac{1}{S} \int d\vec{r} \frac{1}{\varepsilon (\vec{r})} e^{i\vec{G} \cdot \vec{r}}$$

Area of unit cell

Define matrix $\eta^{\rightarrow}$ with elements:

$$\eta_{\vec{G}, \vec{G}'} = \eta (\vec{G} - \vec{G}')$$
How to calculate the S-Matrix?

1.) Decompose the structure into layers which are homogenous in $z$-direction and periodic in $xy$-direction.

2.) Calculate the **eigenmodes** of each layer (2D Photonic Crystal problem!).

3.) Calculate transfer matrix for each layer and interface matrices for adjacent layers.

4.) Construct the S-Matrix of the whole 3D Photonic Crystal by an iterative procedure from the transfer- and interface matrices.
Ansatz for the eigenmodes (magnetic field) in each layer:

\[ \vec{H}_n(\vec{r}_\parallel, z, t) = \sum_G \left[ \Phi_{x,n}(\vec{G}) \ast \left( \vec{e}_x - \frac{1}{q_n} (k_x + G_x) \vec{e}_z \right) \right. \]
\[ \left. + \Phi_{y,n}(\vec{G}) \ast \left( \vec{e}_y - \frac{1}{q_n} (k_y + G_y) \vec{e}_z \right) \right] e^{i(\vec{k}_\parallel + \vec{G}) \cdot \vec{r}_\parallel} e^{i q_n z} e^{-i \omega \, t} \]

Out-of-plane propagation!

Numerical simulations:

• truncate summation after \( N_g \) reciprocal lattice vectors!
• check for convergence !!!

\( \Phi_{x,n}(\vec{G}) \) and \( \Phi_{y,n}(\vec{G}) \) refers to the eigenmodes in the \( x \) and \( y \) directions, respectively, with wave vectors \( \vec{k}_\parallel \) and \( \vec{G} \) in the parallel and reciprocal space, respectively.
Inserting the ansatz into Maxwell’s equations yields the following matrix eigenproblem:

\[
\begin{pmatrix}
\eta^- & 0 \\
0 & \eta^-
\end{pmatrix}^{-1}
\begin{pmatrix}
\varepsilon_0 \mu_0 \omega^2 & 1 \\
1 & \tilde{Z} - \tilde{K}
\end{pmatrix}
\begin{pmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{pmatrix} = q_n^2
\begin{pmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{pmatrix}
\]

Good exercise: derive this equation!
Inserting the ansatz into Maxwell’s equations yields the following matrix eigenproblem:

\[
\begin{bmatrix}
\hat{\eta} & 0 \\
0 & \hat{\eta}
\end{bmatrix}^{-1} \begin{bmatrix}
\varepsilon & 0 \\
0 & \mu
\end{bmatrix} \omega^2 \mathbf{I} - \mathbf{Z} - \mathbf{K} \begin{bmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{bmatrix} = q_n^2 \begin{bmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{bmatrix}
\]

Unit matrix

\[
\begin{bmatrix}
\hat{K}_y \\
\hat{K}_x
\end{bmatrix}_{\tilde{G}, \tilde{G}'} = \left( k_y + G_y \right) \delta_{\tilde{G}, \tilde{G}'}
\]

\[
\begin{bmatrix}
\hat{K}_y \\
\hat{K}_x
\end{bmatrix}_{\tilde{G}, \tilde{G}'} = \left( k_x + G_x \right) \delta_{\tilde{G}, \tilde{G}'}
\]

\[
\mathbf{Z} = \begin{bmatrix}
\hat{K}_y \hat{\eta} \hat{K}_y & - \hat{K}_y \hat{\eta} \hat{K}_x \\
- \hat{K}_x \hat{\eta} \hat{K}_y & \hat{K}_x \hat{\eta} \hat{K}_x
\end{bmatrix}
\]

Inserting the ansatz into Maxwell’s equations yields the following matrix eigenproblem:

\[ \mathbf{K} = \begin{pmatrix} \mathbf{K}_x \mathbf{K}_x & \mathbf{K}_x \mathbf{K}_y \\ \mathbf{K}_y \mathbf{K}_x & \mathbf{K}_y \mathbf{K}_y \end{pmatrix} \]

\[
\begin{pmatrix} \eta & 0 \\ 0 & \eta \end{pmatrix}^{-1} \left( \varepsilon \mu \omega^2 \mathbf{1} - \mathbf{Z} \right) \mathbf{K} \begin{pmatrix} \Phi_{x,n} \\ \Phi_{y,n} \end{pmatrix} = q_n^2 \begin{pmatrix} \Phi_{x,n} \\ \Phi_{y,n} \end{pmatrix}
\]

\[
\left( \mathbf{K}_y \right)_{\tilde{G},\tilde{G}'} = \left( k_y + G_y \right) \delta_{\tilde{G},\tilde{G}'}
\]

\[
\left( \mathbf{K}_x \right)_{\tilde{G},\tilde{G}'} = \left( k_x + G_x \right) \delta_{\tilde{G},\tilde{G}'}
\]

Inserting the ansatz into Maxwell’s equations yields the following matrix eigenproblem:

\[
\begin{pmatrix}
\Phi_{x,n}(\vec{G}_1) \\
\vdots \\
\Phi_{x,n}(\vec{G}_{2N_g})
\end{pmatrix}
\begin{pmatrix}
(\eta^\top \ 0) \ \ \ \ (\frac{1}{\eta^\top} \ \ 0) \\
(0 \ \ \ 0)
\end{pmatrix}^{-1}
\begin{pmatrix}
(\varepsilon_0 \mu_0 \omega^2 \mathbf{1} - \hat{Z}) \ \ \hat{K}
\end{pmatrix}
\begin{pmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{pmatrix}
= q_n^2
\begin{pmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{pmatrix}
\begin{pmatrix}
\Phi_{y,n}(\vec{G}_1) \\
\vdots \\
\Phi_{y,n}(\vec{G}_{2N_g})
\end{pmatrix}
\]
Inserting the ansatz into Maxwell’s equations yields the following matrix eigenproblem:

\[
\begin{pmatrix}
\hat{\eta} & 0 \\
0 & \hat{\eta}
\end{pmatrix}^{-1}
\begin{pmatrix}
\varepsilon \mu_0 \omega^2 \hat{1} - \hat{Z}
\end{pmatrix}
\begin{pmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{pmatrix}
= q_n^2
\begin{pmatrix}
\Phi_{x,n} \\
\Phi_{y,n}
\end{pmatrix}
\]

Note: In contrast to “normal” band structure calculations, we solve for \( q_n \) (z-component of the wave vector) and not the frequency \( \omega \)!

How to calculate the S-Matrix?

1.) Decompose the structure into layers which are homogenous in $z$-direction and periodic in $xy$-direction.

2.) Calculate the eigenmodes of each layer (2D Photonic Crystal problem!).

3.) Calculate transfer matrix for each layer and interface matrices for adjacent layers.

4.) Construct the S-Matrix of the whole 3D Photonic Crystal by an iterative procedure from the transfer- and interface matrices.
Define for each eigenmode $n$ a $2N_g$ dimensional vector:

$$\vec{\Phi}_{||,n} = \begin{pmatrix} \Phi_{x,n}(\vec{G}_1) \\ \vdots \\ \Phi_{x,n}(\vec{G}_{N_g}) \\ \Phi_{y,n}(\vec{G}_1) \\ \vdots \\ \Phi_{y,n}(\vec{G}_{N_g}) \end{pmatrix}$$

Important: $\vec{\Phi}_{||,n}$ does not depend on $z$!
Define two $2N_g \times 2N_g$ dimensional matrices:

$$\tilde{H}_\parallel = \left( \Phi_{\parallel,1}, \ldots, \Phi_{\parallel,2N_g} \right)$$

The eigenvectors $\tilde{\Phi}_{\parallel,n}$ form the columns of this matrix.

and

$$\tilde{\kappa} = \begin{pmatrix} q_1 & 0 & 0 & \ldots & 0 \\ 0 & q_2 & 0 & \ldots & 0 \\ 0 & 0 & \ddots & \ddots & \ddots \\ \vdots & \vdots & \ddots & \ddots \ddots & \ddots \\ 0 & 0 & \ldots & \ldots & q_{2N_g} \end{pmatrix}$$

The eigenvalues $q_n$ are the diagonal elements of this matrix.
The total magnetic field in each plane $z$ can be written as a superposition of the eigenmodes, propagating along and opposite to the $z$-axis, i.e. $\propto \exp (iq_n z - i\omega t)$ and $\propto \exp (-iq_n z - i\omega t)$, respectively.

Define $4N_g$ dimensional vector of amplitudes:

$$\vec{A}(z) = \begin{pmatrix} \vec{A}^+(z) \\ \vec{A}^-(z) \end{pmatrix}$$

- Amplitude of $2N_g$ modes propagating in $z$ direction.
- Amplitude of $2N_g$ modes propagating in $-z$ direction.

Note: the vector of amplitudes depends only on $z$, while the eigenmodes only depend on $x$ and $y$!
Alternatively, the total magnetic field can also be Fourier-decomposed into a sum of partial waves (plane wave expansion).

The following equation allows us to switch between the description of the total magnetic field in terms of amplitudes of the eigenmodes and the in-plane coefficients of the partial waves:

\[
\begin{pmatrix}
H_x(z) \\
H_y(z)
\end{pmatrix} = \vec{H}_\parallel(z) = (\vec{H}_\parallel, \vec{H}_\parallel) \vec{A}(z)
\]

where

\[
H_x(z) = \begin{pmatrix}
H_x(\vec{G}_1, z) \\
\vdots \\
H_x(\vec{G}_{2N_g}, z)
\end{pmatrix}
\]

and

\[
H_y(z) = \begin{pmatrix}
H_y(\vec{G}_1, z) \\
\vdots \\
H_y(\vec{G}_{2N_g}, z)
\end{pmatrix}
\]
Analog, we can calculate the coefficients of the in-plane electric field components of the plane waves from the amplitudes of the eigenmodes by

\[
\begin{pmatrix}
- E_y(z) \\
E_x(z)
\end{pmatrix} = \vec{E}_\parallel(z) = \\
= \left( \frac{1}{\omega \varepsilon_0} \left( \varepsilon_0 \mu_0 \omega^2 \mathbf{1} - \mathbf{Z} \right) \mathbf{H}_\parallel \mathbf{\kappa}^{-1}, - \frac{1}{\omega \varepsilon_0} \left( \varepsilon_0 \mu_0 \omega^2 \mathbf{1} - \mathbf{Z} \right) \mathbf{H}_\parallel \mathbf{\kappa}^{-1} \right) \vec{A}(z)
\]

where \( E_x(z) = \begin{pmatrix} E_x(\mathbf{G}_1, z) \\ \vdots \\ E_x(\mathbf{G}_{2N_g}, z) \end{pmatrix} \) and \( E_y(z) = \begin{pmatrix} E_y(\mathbf{G}_1, z) \\ \vdots \\ E_y(\mathbf{G}_{2N_g}, z) \end{pmatrix} \).
Next, we define the transfer matrix $\mathbf{\tilde{T}}_L$ which connects the amplitudes at different planes $z$ and $z+L$ within one layer:

$$\tilde{A}(z + L) = \mathbf{\tilde{T}}_L \tilde{A}(z)$$

It can be written as a diagonal matrix:

$$\mathbf{\tilde{T}}_L = \begin{pmatrix} \exp(i \tilde{\kappa}^\perp L) & 0 \\ 0 & \exp(-i \tilde{\kappa}^\perp L) \end{pmatrix}$$

Diagonal matrices with $\exp(\pm i q_j L), j = 1, 2, \ldots, 2 N_g$ on the main diagonal.
The in-plane components of the electric and magnetic field must be continuous across the interface between two layers $a$ and $b$ at $z = z_{a,b}$:

\[
\begin{pmatrix}
\vec{E}_\parallel (z) \\
\vec{H}_\parallel (z)
\end{pmatrix}
_{z_{a,b}^- 0} =
\begin{pmatrix}
\vec{E}_\parallel (z) \\
\vec{H}_\parallel (z)
\end{pmatrix}
_{z_{a,b}^+ 0}
\]

In order to connect the amplitudes at the interfaces between adjacent layers, we define the interface matrix $\tilde{T}_{b,a}$:

\[
\tilde{A}(z_{a,b}^+ 0) = \tilde{T}_{b,a} \tilde{A}(z_{a,b}^- 0)
\]
In order to calculate $T_{b,a}$, we define the material matrix $\mathbf{F}$ of the layer by:

$$
\begin{pmatrix}
\vec{E}_\parallel(z) \\
\vec{H}_\parallel(z)
\end{pmatrix} = \mathbf{F} \vec{A}(z)
$$

where

$$
\mathbf{F} = \left( \begin{array}{cc}
\frac{1}{\omega} \left( \varepsilon_0 \mu_0 \omega^2 \mathbf{1} - \mathbf{Z} \right) \mathbf{H}_\parallel \kappa^{-1} & - \frac{1}{\omega} \left( \varepsilon_0 \mu_0 \omega^2 \mathbf{1} - \mathbf{Z} \right) \mathbf{H}_\parallel \kappa^{-1} \\
\mathbf{H}_\parallel & \mathbf{H}_\parallel
\end{array} \right)
$$

Thus, the interface matrix is given by:

$$
\mathbf{T}_{b,a} = \mathbf{F}_b^{-1} \mathbf{F}_a
$$
How to calculate the S-Matrix?

1.) Decompose the structure into layers which are homogenous in $z$-direction and periodic in $xy$-direction.

2.) Calculate the eigenmodes of each layer (2D Photonic Crystal problem!).

3.) Calculate transfer matrix for each layer and interface matrices for adjacent layers.

4.) **Construct the S-Matrix** of the whole 3D Photonic Crystal by an iterative procedure from the transfer- and interface matrices.
We could now calculate the total transfer matrix through the whole 3D Photonic Crystal:

\[
\mathbf{T}_{\text{total}} = \mathbf{T}_{s,a_N} \mathbf{T}_{L_N} \mathbf{T}_{a_N,a_{N-1}} \cdots \mathbf{T}_{L_1} \mathbf{T}_{a_1,v}
\]

However, the transfer-matrix calculations are numerically unstable (exponentially growing fields for evanescent modes)!
The total scattering matrix $\tilde{S}_{v,s}$ connects the incident field with the outgoing field:

$$\begin{pmatrix} \vec{A}_s^+ \\ \vec{A}_v^- \end{pmatrix} = \tilde{S}_{v,s} \begin{pmatrix} \vec{A}_v^+ \\ \vec{A}_s^- \end{pmatrix}$$
The total scattering matrix $\vec{S}_{M+1}$ of a system containing $M+1$ layers can be constructed from the total scattering matrix $\vec{S}_M$ of the system with $M$ layers

$$\vec{S}_M = \begin{pmatrix} \vec{S}_{11} & \vec{S}_{12} \\ \vec{S}_{21} & \vec{S}_{22} \end{pmatrix}$$

and the inverse transfer matrix $\vec{T}$ through the additional (M+1)th layer

$$\vec{T} = \begin{pmatrix} \vec{T}_{11} & \vec{T}_{12} \\ \vec{T}_{21} & \vec{T}_{22} \end{pmatrix}$$

For example, if we add an interface with interface matrix $\vec{T}_{b,a}$, then $\vec{T} = \vec{T}_{a,b} = \vec{T}_{b,a}$. 
The **scattering matrix** connects the amplitudes for the existing \( M \) layers:

\[
\begin{pmatrix}
\vec{A}_M^+ \\
\vec{A}_M^-
\end{pmatrix} = \begin{pmatrix}
\vec{S}_{11} & \vec{S}_{12} \\
\vec{S}_{21} & \vec{S}_{22}
\end{pmatrix}\begin{pmatrix}
\vec{A}_v^+ \\
\vec{A}_M^-
\end{pmatrix}
\]

The **inverse transfer matrix** connects the amplitudes between layers \( M \) and \( M+1 \):

\[
\begin{pmatrix}
\vec{A}_M^+ \\
\vec{A}_M^-
\end{pmatrix} = \begin{pmatrix}
\vec{T}_{11} & \vec{T}_{12} \\
\vec{T}_{21} & \vec{T}_{22}
\end{pmatrix}\begin{pmatrix}
\vec{A}_{M+1}^+ \\
\vec{A}_{M+1}^-
\end{pmatrix}
\]

This yields a system of equations for the amplitudes in layer \( M+1 \). Solving for the amplitudes in layer \( M+1 \) yields...
... (after a lengthy calculation) the construction rule:

\[ \vec{S}_{M+1} = \left( \begin{array}{ccc} \vec{Q}\vec{S}_{11} & \vec{Q}\vec{P} \\ \vec{S}_{21} + \vec{S}_{22}\vec{T}_{21}\vec{Q}\vec{S}_{11} & \vec{S}_{22}\vec{T}_{21}\vec{Q}\vec{P} + \vec{S}_{22}\vec{T}_{22} \end{array} \right) \]

where \[ \vec{P} = \left( \vec{S}_{12}\vec{T}_{22} - \vec{T}_{12} \right) \quad \text{and} \quad \vec{Q} = \left( \vec{T}_{11} - \vec{S}_{12}\vec{T}_{21} \right)^{-1}. \]

Exercise: derive this formula for the 1D case!
The total scattering matrix of the system can be calculated iteratively:

• We start from the obvious condition \( \hat{S}_{v,v} = \hat{1} \).

• Next, we add the interface of the first layer and calculate the corresponding scattering matrix by the procedure described above.

• Then, we account for the first layer itself and calculate the new scattering matrix.

• ...

• Finally, we add the interface between the last layer and the substrate and obtain the total scattering matrix.
And again: comparison to experiments

- Experimental spectra at different angles
And again: comparison to experiments

- Bandstructure expectations