Modal expansion methods for modeling of photonic devices

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How does light propagate in photonic device?

Answer: Maxwell equations.
Strategy:

- we suppose time-harmonic field $\sim \exp(i\omega t)$ with given $\omega$ or $\lambda$, i.e. we solve in frequency domain
- the device is described with refractive index $n(x, y, z)$ or relative permittivity $\varepsilon(x, y, z)$ – these functions are complex and depend on $\omega$
- then we solve Maxwell equations to find $\vec{E}$, $c\vec{B}$
Convention: To keep formulation as simple as possible we use $c\vec{B}$ instead of $\vec{H}$ and dimensionless coordinates

$$(x, y, z) = \frac{2\pi}{\lambda}(X, Y, Z) = \frac{\omega}{c}(X, Y, Z)$$

$$\beta = n_{\text{eff}}, \quad k_{\text{vacuum}} = 1$$

$$\vec{\nabla} \times c\vec{B} = i\varepsilon \vec{E} \quad (1)$$

$$\vec{\nabla} \times \vec{E} = -ic\vec{B} \quad (2)$$
Rigorous methods

- Finite-difference
- Finite-element
- Modal expansion methods ("Mode-matching")
- Method of lines
- Spectral index
- ...

...
Tasks to be solved

1. Searching for waveguide modes and propagation constants - “Mode solvers”
   – stationary state, eigenvalue problem

2. Modeling of light propagation (i.e. evolution of the em field) in photonic devices (e.g. “BPM” = Beam propagation method)
   – evolving state
Mode solvers

\[
\varepsilon(x, y, z) = \varepsilon(x, y) \quad (2D \text{ task})
\]

\[
\varepsilon(x, y, z) = \varepsilon(y) \quad (1D \text{ task})
\]

\[
\begin{aligned}
\left\{ \begin{array}{l}
\vec{E}(x, y, z) \\
c\vec{B}(x, y, z)
\end{array} \right\} &= \left\{ \begin{array}{l}
\vec{E}_\nu(x, y) \\
c\vec{B}_\nu(x, y)
\end{array} \right\} \exp(-i\beta_\nu z)
\end{aligned}
\]

mode profile? propagation constant?
Example: Mode profiles of step-index optical fiber

\[ n_1 = 1, 5, \quad n_2 = 1, 495, \quad a/\lambda = 10 \]
Light propagation

- device can change along \( z \)
- we know incident field i.e. \( \vec{E}, c\vec{B} \) at \( z = 0 \)
- we search for \( \vec{E}, c\vec{B} \) for any \( z \)

Two kinds of methods:
(i) **one-way methods** use paraxial approximation, reflections are neglected
(ii) **bi-directional methods** can deal with reflected field, can calculate reflected and transmitted power and loss.
BPM example
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See e.g. [1].

Suppose that the waveguide structure is uniform for $z \in (z_1, z_2)$. General solution of the Maxwell equations in $(z_1, z_2)$ is a sum of forward and backward-traveling modes:

$$
\begin{align*}
\vec{E}(x, y, z) \\
c \vec{B}(x, y, z)
\end{align*}
= \sum_{\nu \in \mathbb{N}} \left[ f_{\nu} \left\{ \vec{E}_\nu(x, y) \right\} \exp(-i\beta_{\nu}z) + b_{\nu} \left\{ \vec{E}_{-\nu}(x, y) \right\} \exp(i\beta_{\nu}z) \right].
\tag{6}
$$
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One-dimensional structure

\[ \varepsilon = \varepsilon(y) \] (7)

If we suppose

\[ \frac{\partial}{\partial x} \left\{ \begin{array}{c} \vec{E} \\ c\vec{B} \end{array} \right\} = 0 \] (8)

we obtain TE and TM solutions (modes) of the Maxwell equations.
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TE modes

\begin{align*}
\begin{pmatrix}
E_x \\
E_y \\
E_z \\
cB_x \\
cB_y \\
cB_z
\end{pmatrix} &= 
\begin{pmatrix}
\varphi_{hk}(y) \\
0 \\
0 \\
0 \\
\beta_{hk}\varphi_{hk}(y) \\
-i\varphi'_{hk}(y)
\end{pmatrix} 
\exp(-i\beta_{hk}z) 
\tag{9}
\end{align*}

\varphi''_{hk}(y) + \varepsilon(y)\varphi_{hk}(y) = \beta_{hk}^2\varphi_{hk}(y) 
\tag{10}
TM modes

\[
\begin{pmatrix}
E_x \\
E_y \\
E_z \\
cB_x \\
cB_y \\
cB_z \\
\end{pmatrix}
= 
\begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
-\beta_{ek} \varphi_{ek}(y)/\varepsilon(y) & i\varphi_{ek}^{'}(y)/\varepsilon(y) & \varphi_{ek}(y) & 0 & 0 & 0 \\
\end{pmatrix}
\text{exp}(-i\beta_{ek}z) \tag{11}
\]

\[
\left[ \frac{1}{\varepsilon(y)} \varphi_{ek}^{'}(y) \right]^{'} + \varphi_{ek}(y) = \beta_{ek}^2 \frac{1}{\varepsilon(y)} \varphi_{ek}(y) \tag{12}
\]
Eqs. (10) and (12) can be written in unique form

$$\hat{L}_p(y) \varphi_{pk}(y) = \beta^2_{pk} \eta_p(y) \varphi_{pk}(y)$$  \hspace{1cm} (13)

$$\hat{L}_p(y) \varphi_{pk}(y) \equiv \left[ \eta_p(y) \varphi'_{pk}(y) \right]' + \eta_p(y) \varepsilon(y) \varphi_{pk}(y)$$ \hspace{1cm} (14)

$$\eta_p(y) \equiv \begin{cases} 1 & p = h \\ 1/\varepsilon(y) & p = e \end{cases}$$ \hspace{1cm} (15)

Note:
- $\beta^2_{pk}$ and $\varphi_{pk}(y)$ are eigenvalues and eigenfunctions of $\hat{L}_p(y)$
- for each $\beta^2_{pk}$ there are two modes $\pm \beta_{pk}$ propagating in $\pm z$
- to solve the problem in $\langle y_{\text{min}}, y_{\text{max}} \rangle$ we need to know boundary conditions at $y_{\text{min}}$ and $y_{\text{max}}$
## Boundary conditions

<table>
<thead>
<tr>
<th>Name</th>
<th>Condition at $y_{\text{min}}$ or $y_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Open B.C.</td>
<td>$\varphi_{pk}, \varphi'_{pk}$ are finite</td>
</tr>
<tr>
<td>Closed B.C. – Electric wall</td>
<td>$\vec{E}<em>t = 0$ i.e. $\varphi</em>{hk} = 0, \varphi'_{ek} = 0$</td>
</tr>
<tr>
<td>Closed B.C. – Magnetic wall</td>
<td>$c\vec{B}<em>t = 0$ i.e. $\varphi'</em>{hk} = 0, \varphi_{ek} = 0$</td>
</tr>
<tr>
<td>...</td>
<td></td>
</tr>
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Transfer matrix method

is technique for solving Eq.(13) in multilayer waveguide [4, 5, 6, 7]. The waveguide consists of $N$ layers. $d_n$ and $\varepsilon_n$ are thickness and relative permittivity of layer $n$, $n = 0..N - 1$. 

\[
\begin{array}{c}
\varepsilon_{N-1}, d_{N-1} \\
\varepsilon_{N-2}, d_{N-2} \\
\vdots \\
\varepsilon_1, d_1 \\
\varepsilon_0, d_0 \\
y_0 \\
y_1 \\
y_2 \\
y_{N-1} \\
y_N
\end{array}
\]
Choose $y_n = 0$

\[
\varphi_n(y) = f_n \exp(-i\alpha_n y) + b_n \exp(i\alpha_n y) \quad (16)
\]

\[
= \bar{f}_n \exp[i\alpha_n (d_n - y)] + \bar{b}_n \exp[-i\alpha_n (d_n - y)] \quad (17)
\]

\[
= A_n \cos(\alpha_n y) + \frac{B_n}{\alpha_n} \sin(\alpha_n y) \quad (18)
\]

\[
= \bar{A}_n \cos[\alpha_n (d_n - y)] - \frac{\bar{B}_n}{\alpha_n} \sin[\alpha_n (d_n - y)] \quad (19)
\]

\[
= \ldots \quad (20)
\]

\[
\alpha_n = \sqrt{\varepsilon_n - \beta^2}. \quad (21)
\]
Realizing that $A_n$ and $B_n$ are values of function $\varphi(y)$ and its derivative at $y = y_n$ and using continuity conditions for normal and tangential components of electric and magnetic field we obtain

\[
\begin{pmatrix}
A_{n+1} \\
B_{n+1}\eta_{n+1}
\end{pmatrix}
= \begin{pmatrix}
\cos(\alpha_n d_n) & \sin(\alpha_n d_n) / (\alpha_n \eta_n) \\
-\alpha_n \eta_n \sin(\alpha_n d_n) & \cos(\alpha_n d_n)
\end{pmatrix}
\begin{pmatrix}
A_n \\
B_n \eta_n
\end{pmatrix}
\]

(22)

for any $n = 0..N-1$. 
Dispersion equation

As a consequence if we know $\beta$ and $A_n, B_n$ for some $n$ we can calculate the all $A_n, B_n$. This can be used to find radiation modes and reflection and transmission coefficients. On the other hand if we know $A_0, B_0$ and $A_N, B_N$ we can obtain implicit dispersion equation for unknown $\beta^2$. We choose layer $n$ and compare $A_n^+, B_n^+$ with $A_n^-, B_n^-$. $A_n^+, B_n^+$ are calculated from known $A_0, B_0$ and $A_n^-, B_n^-$ are calculated from known $A_N, B_N$. Values of $A_0, B_0, A_N$ and $B_N$ depend on type of boundary conditions used.

$$\Delta_n(\beta^2) = A_n^+ B_n^- - A_n^- B_n^+ = (B_n^-, -A_n^-) \left( \begin{array}{c} A_n^+ \\ B_n^+ \end{array} \right) = 0$$  \hspace{1cm} (23)
Root searching

Roots on real axis $\beta^2$ (bound modes of a waveguide with real index profile) are searched using standard numerical routines [8]. Complex roots (leaky modes, active or passive waveguide) are searched using “root-tracking” technique [9] or rigorous technique that uses analyticity of the dispersion function [10, 11, 12, 13], see also [14, 15, 16, 17].
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For simplicity we suppose closed boundary conditions.

\[
\int_{y_{\text{min}}}^{y_{\text{max}}} \eta_p(y) \varphi_{p_k}(y) \varphi_{p_l}(y) dy = \delta_{kl}
\] (24)

\[
\frac{1}{\beta_{el}^2} \int_{y_{\text{min}}}^{y_{\text{max}}} \eta_e(y) \varphi_{h_k}(y) \varphi'_{el}(y) dy + \frac{1}{\beta_{hk}^2} \int_{y_{\text{min}}}^{y_{\text{max}}} \eta_e(y) \varphi'_{h_k}(y) \varphi_{el}(y) dy = 0
\] (25)

The both relations can be derived from (13) [3, 2]. Note that these relations are valid for \( \varepsilon \) complex. (For \( \varepsilon \) real we can also use relations with complex conjugate fields.)
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E- and H-type modes

See e.g. [2]

We do not suppose (8). As \( \varepsilon \) does not depend on \( x \) and \( z \) the solution of the Maxwell equations can be expressed using

\[
\vec{k}_{pk} = (k_{xpk}, 0, k_{zpk})
\]  \hspace{1cm} (26)

Instead of (5) we have

\[
\begin{cases}
\vec{E}(x, y, z) \\
c\vec{B}(x, y, z)
\end{cases}
= \begin{cases}
\vec{E}_{pk}(y) \\
c\vec{B}_{pk}(y)
\end{cases}
\exp(-ik_{xpk}x - ik_{zpk}z)
\]  \hspace{1cm} (27)

Choose system \((u, y, v)\) in such a way that \(\vec{k}_{pk} = (0, 0, \beta_{pk})\)

\[
\beta_{pk}^2 = k_{xpk}^2 + k_{zpk}^2
\]  \hspace{1cm} (28)
Rotation of TE mode
H-modes

Transformation of (9)

\[
\begin{pmatrix}
E_x \\
E_y \\
E_z \\
cB_x \\
cB_y \\
cB_z
\end{pmatrix} = \frac{1}{\beta_{hk}} \begin{pmatrix}
k_{zhk}\varphi_{hk}(y) \\
0 \\
-k_{xhk}\varphi_{hk}(y) \\
-ik_{xhk}\varphi'_{hk}(y) \\
\beta^2_{hk}\varphi_{hk}(y) \\
-ik_{zhk}\varphi'_{hk}(y)
\end{pmatrix} \exp\left(-ik_{xhk}x - ik_{zhk}z\right) 
\] (29)
E-modes

Transformation of (11)

\[
\begin{bmatrix}
E_x \\
E_y \\
E_z \\
cB_x \\
cB_y \\
cB_z \\
\end{bmatrix}
= \frac{1}{\beta_{ek}} \begin{bmatrix}
ik_{xek}\eta_e(y)\varphi'_{ek}(y) \\
-\beta_{ek}^2\eta_e(y)\varphi_{ek}(y) \\
iki_{zek}\eta_e(y)\varphi'_{ek}(y) \\
1k_{zek}\varphi_{ek}(y) \\
0 \\
-k_{xek}\varphi_{ek}(y) \\
\end{bmatrix} \exp\left(-ik_{xek}x - ik_{zek}z\right)
\]
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The technique is often called “Bi-directional eigenmode expansion and propagation method” – BEP, [18, 19]

- The 2D waveguide is divided into a sequence of \( M \) uniform sections which are separated by vertical lines. The refractive index in each section is function of \( y \) coordinate only. The total field in each section is expanded into set of TE or TM modes of that section (= local eigenmodes). The mode spectrum is discretised by closing computational domain in \( y \) direction by electric or magnetic conductors.

- (“Mode Matching”) At the interfaces between all neighbouring sections the conditions for continuity of electric and magnetic field are used.
Model of 2D structure

\[ \varepsilon^{(m-1)}(y) \quad \varepsilon^{(m)}(y) \quad \varepsilon^{(m+1)}(y) \]

\[ d^{(m-1)} \quad d^{(m)} \quad d^{(m+1)} \]

\[ y_{\text{min}} \quad \ldots \quad y_{\text{max}} \]

\[ x \rightarrow z \]

Electric or magnetic walls
Approximations

1. The continuous part of local eigenmodes spectra has to be discretised and this is achieved by closing computational domain in transverse direction by suitable artificial boundaries.

2. Spatial resolution of the method depends on the number of local eigenmodes used [20].

3. Staircase approximation is used to model curvature interfaces.
Note that 1 does not apply for devices which are closed or periodic in transverse direction as the local eigenmodes are naturally discrete. However, for open devices this approximation causes serious problem which can be solved using various techniques, for example the Perfectly Matched Layers (PML). Approximations 2 and 3 do not cause complications in most cases as fast convergence of results with increasing number of local eigenmodes or stairs is usually observed.
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Field expansion in section \( m \)

**TE solution**

\[
E_x(y, z) = \sum_k u_k(z) \varphi_k(y) \tag{31}
\]

\[
cB_y(y, z) = i \sum_k u'_k(z) \varphi_k(y) \tag{32}
\]

\[
cB_z(y, z) = -i \sum_k u_k(z) \varphi'_k(y) \tag{33}
\]

**TM solution**

\[
cB_x(y, z) = \sum_k u_k(z) \varphi_k(y) \tag{34}
\]

\[
E_y(y, z) = -i \eta(y) \sum_k u'_k(z) \varphi_k(y) \tag{35}
\]

\[
E_z(y, z) = i \eta(y) \sum_k u_k(z) \varphi'_k(y) \tag{36}
\]
choose \( z^{(m)} = 0 \)

\[
\begin{align*}
  u_k(z) &= f_k \exp(-i\beta_k z) + b_k \exp(i\beta_k z) \\
  &= \bar{f}_k \exp[i\beta_k (d - z)] + \bar{b}_k \exp[-i\beta_k (d - z)] \\
  &= A_k \cos(\beta_k z) + \frac{B_k}{\beta_k} \sin(\beta_k z) \\
  &= \bar{A}_k \cos[\beta_k (d - z)] - \frac{\bar{B}_k}{\beta_k} \sin[\beta_k (d - z)] \\
  u'_k(z) &= \cdots
\end{align*}
\]
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Mode matching

Compare field at \( z^{(m+1)} \):
Continuity of \( E_x \) or \( cB_x \), see (31) or (34)

\[
\sum_k u_k^{(m)}(z^{(m+1)}) \varphi_k^{(m)}(y) = \sum_k u_k^{(m+1)}(z^{(m+1)}) \varphi_k^{(m+1)}(y)
\]

\[
\sum_k \bar{A}_k^{(m)} \varphi_k^{(m)} = \sum_k A_k^{(m+1)} \varphi_k^{(m+1)} \tag{42}
\]

multiply \( \eta^{(m)} \varphi_i^{(m)} \) and integrate

\[
\sum_k \int_{y_{\text{min}}}^{y_{\text{max}}} \bar{A}_k^{(m)} \varphi_k^{(m)} \eta^{(m)} \varphi_i^{(m)} \, dy = \sum_k \int_{y_{\text{min}}}^{y_{\text{max}}} A_k^{(m+1)} \varphi_k^{(m+1)} \eta^{(m)} \varphi_i^{(m)} \, dy
\]

use (24)
\[ \bar{A}_l^{(m)} = \sum_k Q_{lk}^{(m,m+1)} A_k^{(m+1)} \]  
(43)

\[ Q_{lk}^{(m,n)} \equiv \int_{y_{\min}}^{y_{\max}} \eta^{(m)}(m) \varphi_l^{(m)}(m) \varphi_k^{(n)} dy \]  
(44)

Alternatively Eq. (42) can be solved with respect to \( A_k^{(m+1)} \)

\[ A_l^{(m+1)} = \sum_k Q_{lk}^{(m+1,m)} \bar{A}_l^{(m)} \]  
(45)
Continuity of $cB_y$ or $E_y$

\[
\tilde{B}_l^{(m)} = \sum_k O_{lk}^{(m,m+1)} B_k^{(m+1)},
\]  
(46)

\[
B_l^{(m+1)} = \sum_k O_{lk}^{(m+1,m)} \bar{B}_k^{(m)},
\]  
(47)

\[
O_{lk}^{(m,n)} \equiv \int_{y_{\min}}^{y_{\max}} \eta^{(n)}(\varphi_l^{(m)} \varphi_k^{(n)}) dy.
\]  
(48)
It follows from (43) – (46)

$$\left[ O_{lk}^{(n,m)} \right]^{-1} = O_{lk}^{(m,n)} \equiv Q_{kl}^{(n,m)},$$  \hspace{1cm} (49)

$$\left[ Q_{lk}^{(n,m)} \right]^{-1} = Q_{lk}^{(m,n)} \equiv O_{kl}^{(n,m)}. $$  \hspace{1cm} (50)

For TE only:

$$Q_{lk}^{(m,n)} = O_{lk}^{(m,n)}, \hspace{1cm} (51)$$

$$O_{lk}^{(m,n)} = Q_{kl}^{(n,m)}. \hspace{1cm} (52)$$
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Motivation: solution using transfer matrix is unstable because we add \( \exp(i\beta_k z) \) and \( \exp(-i\beta_k z) \) and these can be big and small numbers. The source of instability:

\[
(Big + Small) - Big = 0 \quad \text{not} \quad Small!
\]

Solution: \( S \)- or \( R \)-matrix technique [22]. \( S \)-matrix is used in e.g. [19, 21].
What is $S$-matrix?

It provides relation between amplitudes of output and input modes

$$
\begin{pmatrix}
  f^{(2)} \\
  b^{(1)}
\end{pmatrix} = \begin{pmatrix}
  t & \tilde{r} \\
  r & \tilde{t}
\end{pmatrix} \begin{pmatrix}
  f^{(1)} \\
  b^{(2)}
\end{pmatrix} \equiv S \begin{pmatrix}
  f^{(1)} \\
  b^{(2)}
\end{pmatrix}
$$

(53)
Composition law

\[
\begin{array}{ccc}
1 & S^{(1)} & 2 & S^{(2)} & 3 \\
\leftarrow b^{(1)} & \rightarrow f^{(1)} & \leftarrow b^{(2)} & \rightarrow f^{(2)} & \leftarrow b^{(3)} & \rightarrow f^{(3)} \\
\end{array}
\]

\[
\begin{array}{cc}
1 & 3 \\
\leftarrow b^{(1)} & \leftarrow b^{(3)} \\
\rightarrow f^{(1)} & \rightarrow f^{(3)} \\
\end{array}
\]

\[
S = S^{(1)} \otimes S^{(2)} \rightarrow z
\]
\[
\begin{align*}
\begin{pmatrix}
  f^{(2)} \\
  b^{(1)}
\end{pmatrix}
&= S^{(1)} \begin{pmatrix}
  f^{(1)} \\
  b^{(2)}
\end{pmatrix},
\begin{pmatrix}
  f^{(3)} \\
  b^{(2)}
\end{pmatrix}
= S^{(2)} \begin{pmatrix}
  f^{(2)} \\
  b^{(3)}
\end{pmatrix} \\
\begin{pmatrix}
  f^{(3)} \\
  b^{(1)}
\end{pmatrix}
&= S \begin{pmatrix}
  f^{(1)} \\
  b^{(3)}
\end{pmatrix}
\end{align*}
\]

\[
S \equiv S^{(1)} \otimes S^{(2)} = \begin{pmatrix}
  t^{(2)} J^{-1} t^{(1)} & t^{(2)} \tilde{r}^{(1)} K^{-1} \tilde{t}^{(2)} + \tilde{r}^{(2)} \\
  \tilde{t}^{(1)} r^{(2)} J^{-1} t^{(1)} + r^{(1)} & \tilde{t}^{(1)} K^{-1} \tilde{t}^{(2)}
\end{pmatrix}
\]

\[
J \equiv 1 - \tilde{r}^{(1)} r^{(2)}, \quad K \equiv 1 - r^{(2)} \tilde{r}^{(1)}
\]
Definitions

\[ u^{(m)}(z) = \{u^{(m)}_k(z)\} \]
\[ f^{(m)} = \{f^{(m)}_k\} \quad b^{(m)} = \{b^{(m)}_k\} \]
\[ \bar{f}^{(m)} = \{\bar{f}^{(m)}_k\} \quad \bar{b}^{(m)} = \{\bar{b}^{(m)}_k\} \]

\[ K^{(m)} = \{K^{(m)}_{kk}\} = \{i\beta^{(m)}_k\}, \]
\[ P^{(m)}(d) = \exp\left(-K^{(m)}d\right) \]
Expression for the field

\[ u^{(m)}(z) = P^{(m)} \left( z - z^{(m)} \right) f^{(m)} + P^{(m)} \left( z^{(m+1)} - z \right) \bar{b}^{(m)} \]

\[ \left[ u^{(m)}(z) \right]' = -K^{(m)} \left[ P^{(m)} \left( z - z^{(m)} \right) f^{(m)} - P^{(m)} \left( z^{(m+1)} - z \right) \bar{b}^{(m)} \right] \]
$S$-matrix of uniform section

\[
\begin{pmatrix}
\bar{f}^{(m)} \\
b^{(m)}
\end{pmatrix} = \begin{pmatrix}
P^{(m)} & (d^{(m)}) \\
0 & P^{(m)} & (d^{(m)})
\end{pmatrix} \begin{pmatrix}
f^{(m)} \\
\bar{b}^{(m)}
\end{pmatrix}
\equiv S^{(m)} \begin{pmatrix}
f^{(m)} \\
\bar{b}^{(m)}
\end{pmatrix}
\]
It follows from (45) and (47)

\[ f^{(m+1)} + b^{(m+1)} = Q^{(m+1,m)} \left( \bar{f}^{(m)} + \bar{b}^{(m)} \right), \]

\[ K^{(m+1)} \left( f^{(m+1)} - b^{(m+1)} \right) = O^{(m+1,m)} K^{(m)} \left( \bar{f}^{(m)} - \bar{b}^{(m)} \right). \]

This can be rewritten into form

\[
\begin{pmatrix}
  f^{(m+1)} \\
  \bar{b}^{(m)}
\end{pmatrix}
= S^{(m,m+1)} \begin{pmatrix}
  \bar{f}^{(m)} \\
  b^{(m+1)}
\end{pmatrix}
\]

\[ S^{(m,m+1)} \equiv \begin{pmatrix}
  2 \left( K^{(m)} D^{(+)1} \right)^T - \left( D^{(-)} D^{(+)1} \right)^T \\
  D^{(+)1} D^{(-)} \\
  2D^{(+)1} K^{(m+1)}
\end{pmatrix} \]

\[ D^{(\pm)} \equiv O^{(m+1,m)} K^{(m)} \pm K^{(m+1)} Q^{(m+1,m)} \]
$S$-matrix of the whole structure

$$S = S^{(0)} \otimes S^{(0,1)} \otimes S^{(1)} \otimes S^{(1,2)} \otimes \ldots \otimes S^{(M-2,M-1)} \otimes S^{(M-1)}$$

$$\begin{pmatrix} f^{(M)} \\ b^{(0)} \end{pmatrix} = S \begin{pmatrix} f^{(0)} \\ \bar{b}^{(M)} \end{pmatrix}$$
Example: Waveguide with Bragg grating

Calculate modal power reflectance $R$, transmittance $T$ and loss $L = 1 - R - T$. For details see: www.ure.cas.cz/dpt130/cost268 and [23].
Convergence with increasing number of local modes
Poynting vector
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Continuous spectrum of radiation modes can be discretised using:
- closed boundary conditions – electric or magnetic walls
- leaky modes [24, 25]
- direct sampling [26]
- adaptive sampling [27, 28]
- transparent boundary condition [29] (TBC), originally used in BPM [30]
Perfectly matched layer (PML)

Problem: We should avoid parasitic reflections. PML is an artificial material that can absorb radiation without any parasitic reflection at its interface, regardless of wavelength, incidence angle or polarisation [31, 32, 33, 34]. According to [29], the most efficient way is to use closed boundary conditions + PML.
Complex coordinate stretching

is one form of PML [33, 35] particularly suitable for our method [19, 29]. Thickness of PML (\(d_0\) or \(d_{N-1}\)) is complex. \((\beta^2\) gets complex, we need to use root-tracking technique in which we change \(\text{Im}(d)\)). If \(\varepsilon_0 = \varepsilon_1\) there are no reflections at \(y_1\). The wave inside of PML

\[
\exp(-i\alpha y)
\]

is absorbed because \(y\) is complex, e.g.

\[
\text{Im}(y) = \frac{\text{Re}(y)}{\text{Re}(d)}\text{Im}(d)
\]
Movement of roots during searching of PML modes
Example: calculation with and without PML
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Solution of the Maxwell equations in periodic media [36]. If we know the $S$-matrix of the period with length $a$ then

\[
\begin{align*}
\begin{pmatrix} f^{(M)} \\ b^{(M)} \end{pmatrix} & = \gamma \begin{pmatrix} f^{(0)} \\ b^{(0)} \end{pmatrix} \\
\Rightarrow & \exp (-i k_{FB} a) \begin{pmatrix} f^{(0)} \\ b^{(0)} \end{pmatrix}
\end{align*}
\]

\[
\begin{pmatrix} \gamma f^{(0)} \\ \gamma^{-1} b^{(M)} \end{pmatrix} = S \begin{pmatrix} f^{(0)} \\ b^{(M)} \end{pmatrix} \equiv \begin{pmatrix} t & \tilde{r} \\ r & \tilde{t} \end{pmatrix} \begin{pmatrix} f^{(0)} \\ b^{(M)} \end{pmatrix}
\]

This can be rewritten into (linear) form of the generalized eigenvalue problem

\[
\begin{pmatrix} t & \tilde{r} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} f^{(0)} \\ b^{(M)} \end{pmatrix} = \gamma \begin{pmatrix} 1 & 0 \\ r & \tilde{t} \end{pmatrix} \begin{pmatrix} f^{(0)} \\ b^{(M)} \end{pmatrix}.
\] (54)

Bloch modes can be used to improve BEP performance see e.g. [37].
Example: Modeling of 2D photonic crystals

- One of the most exciting developments in physics is discovery of photonic crystals [36].
- Plane wave method, PWM
- Hexagonal lattice, \( \Gamma-K \), empty pillars in InP with \( \varepsilon=10.5 \), crystal length is \( 10a \), area of holes/area of crystal is 0.4
Dependence $R, T$ on $a/\lambda$ for TE wave

![Graph showing the dependence of $R$ and $T$ on $a/\lambda$ for TE wave.](image-url)
Electric field profiles

In band-gap $a/\lambda = 0.280$.

![Electric field profile in band-gap (a/λ = 0.280).](image)

high $T$: $a/\lambda = 0.351$

![Electric field profile at high temperature (a/λ = 0.351).](image)
Band structure

\[ \omega a/2\pi \]

- **symmetric modes**
- **antisymmetric modes**

\[ \frac{k a}{2\pi} \]
Example: Line defect

\[ t/T = 0.25 \]
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The technique is often called “Mode matching method” – MMM, [2, 38, 7, 1, 20].
The waveguide cross-section is divided into a sequence of $M$ uniform sections which are separated by vertical lines. Each section can be viewed as a part of a 2D waveguide (the refractive index in each section is function of $y$ coordinate only) and TE and TM modes (= local modes) of such a 2D waveguide can be found and normalized. The mode spectrum is discretised by closing computational domain in $y$ direction by electric or magnetic walls. The computational domain is not limited in $x$ direction, except possible walls resulting from waveguide symmetry. MMM is based on the expansion of the unknown modal field into local modes in each section. Consequently tangential components of the modal field are matched at the section interfaces and this results in a nonlinear eigenvalue problem. The spatial resolution of the method depends on the number of local mode pairs used [20].
Model of the waveguide cross-section

\[\varepsilon^{(m-1)}(y) \quad d^{(m-1)} \quad \varepsilon^{(m)}(y) \quad d^{(m)} \quad \varepsilon^{(m+1)}(y) \quad d^{(m+1)}\]

Electric or magnetic walls
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As (8) is not valid we have to use E- and H-modes (29) and (30). These modes can be viewed as “propagating” in \( \pm x \) directions so that (6) takes the form

\[
\begin{align*}
\left\{ \begin{array}{l}
\vec{E}(x, y, z) \\
\vec{cB}(x, y, z)
\end{array} \right\} &= \sum_{pk} \left[ f_{pk} \left\{ \begin{array}{l}
\vec{E}_{pk}(y, z) \\
\vec{cB}_{pk}(y, z)
\end{array} \right\} \exp(-i k_{xpk} x) + \\
+ b_{pk} \left\{ \begin{array}{l}
\vec{E}_{-pk}(y, z) \\
\vec{cB}_{-pk}(y, z)
\end{array} \right\} \exp(i k_{xpk} x) \right]
\end{align*}
\]
Full vector expansion in section $m$

\[
E_x(x, y) = k_z \sum_k u_{hk}(x) \varphi_{hk}(y) - \frac{1}{\varepsilon(y)} \sum_k u'_{ek}(x) \varphi'_{ek}(y) \tag{55}
\]

\[
E_y(x, y) = -\frac{1}{\varepsilon(y)} \sum_k u_{ek}(x) \beta^2_{ek} \varphi_{ek}(y) \tag{56}
\]

\[
E_z(x, y) = -i \sum_k u'_{hk}(x) \varphi_{hk}(y) + \frac{ik_z}{\varepsilon(y)} \sum_k u_{ek}(x) \varphi'_{ek}(y) \tag{57}
\]

\[
cB_x(x, y) = \sum_k u'_{hk}(x) \varphi'_{hk}(y) + k_z \sum_k u_{ek}(x) \varphi_{ek}(y) \tag{58}
\]

\[
cB_y(x, y) = \sum_k u_{hk}(x) \beta^2_{hk} \varphi_{hk}(y) \tag{59}
\]

\[
cB_z(x, y) = -ik_z \sum_k u_{hk}(x) \varphi'_{hk}(y) - i \sum_k u'_{ek}(x) \varphi_{ek}(y) \tag{60}
\]
Full vector expansion in section $m$

\[ k_{xpk} = (\beta^2_{pk} - k_z^2)^{1/2} \quad (61) \]

\[ u_{pk}(x) = \frac{A_{pk}}{\beta^2_{pk}} \cos(k_{xpk}x) + \frac{B_{pk}}{k_{xpk}} \sin(k_{xpk}x) \quad (62) \]

\[ = \frac{\bar{A}_{pk}}{\beta^2_{pk}} \cos[k_{xpk}(d - x)] - \frac{\bar{B}_{pk}}{k_{xpk}} \sin[k_{xpk}(d - x)] \quad (63) \]

\[ u'_{pk}(x) = \cdots \quad (64) \]

\[ \frac{\bar{A}_{pk}}{\beta^2_{pk}} = \frac{A_{pk}}{\beta^2_{pk}} \cos(k_{xpk}d) + \frac{B_{pk}}{k_{xpk}} \sin(k_{xpk}d) \quad (65) \]

\[ \bar{B}_{pk} = -k_{xpk} \frac{A_{pk}}{\beta^2_{pk}} \sin(k_{xpk}d) + B_{pk} \cos(k_{xpk}d) \quad (66) \]
diagonal matrices $T^{(m)}_p$ and $S^{(m)}_p$ in section $m$

\begin{align}
T^{(m)}_{pkk} & \equiv \frac{k^{(m)}_{xpk}}{\beta^{(m)}_p \tan \left[ k^{(m)}_{xpk} d^{(m)}_x \right]} \\
S^{(m)}_{pkk} & \equiv \frac{k^{(m)}_{xpk}}{\beta^{(m)}_p \sin \left[ k^{(m)}_{xpk} d^{(m)}_x \right]} 
\end{align}

(67) (68)

rewrite (65) a (66) into stable form used in $R$-matrix technique [22, 7]

\begin{align}
B^{(m)}_p & = -T^{(m)}_p A^{(m)}_p + S^{(m)}_p \bar{A}^{(m)}_p \\
\bar{B}^{(m)}_p & = -S^{(m)}_p A^{(m)}_p + T^{(m)}_p \bar{A}^{(m)}_p
\end{align}

(69) (70)
Boundary conditions at \( z^{(0)} \) or \( z^{(M)} \)

If \( A_p^{(0)} = 0 \) or \( \bar{A}_p^{(M-1)} = 0 \), Eqs. (69), (70) turn into form

\[
B_p^{(M-1)} = -T_p^{(M-1)} A_p^{(M-1)},
\]

\[
\bar{B}_p^{(0)} = T_p^{(0)} \bar{A}_p^{(0)}.
\]

If \( B_p^{(0)} = 0 \) or \( \bar{B}_p^{(M-1)} = 0 \), we use again (71), (72), with

\[
T_{pkk}^{(b)} \equiv -\frac{k_{xpk}^{(b)}}{\beta_{pk}^{(b)2}} \tan \left[ k_{xpk}^{(b)} d_x^{(m)} \right], \quad b = 0, M - 1.
\]

For open boundary

\[
u_{pk}^{(b)'} = \pm ik_{xpk}^{(b)} \nu_{pk}^{(b)}, \quad b = 0, M - 1
\]

we use again (71), (72), with

\[
T_{pkk}^{(b)} \equiv \pm \frac{k_{xpk}^{(b)}}{\beta_{pk}^{(b)2}}
\]
Mode matching

\[ \bar{A}_h^{(m)} = O_{hh}^{(m,m+1)} A_h^{(m+1)} \]  \hspace{1cm} (73)
\[ \bar{B}_h^{(m)} = O_{hh}^{(m,m+1)} B_h^{(m+1)} - k_z O_{he}^{(m,m+1)} A_e^{(m+1)} \]  \hspace{1cm} (74)
\[ \bar{A}_e^{(m)} = O_{ee}^{(m,m+1)} A_e^{(m+1)} \]  \hspace{1cm} (75)
\[ \bar{B}_e^{(m)} = O_{ee}^{(m+1,m)} T B_e^{(m+1)} + k_z O_{he}^{(m+1,m)} T A_h^{(m+1)} \]  \hspace{1cm} (76)
Overlap integrals

\[ O_{pplk}^{(m,n)} \equiv \int_{y_{\text{min}}}^{y_{\text{max}}} \eta^{(n)}_{p} \varphi^{(m)}_{pl} \varphi^{(n)}_{pk} \, dy \]  \hspace{1cm} (77)

\[ Q_{pplk}^{(m,n)} \equiv \int_{y_{\text{min}}}^{y_{\text{max}}} \eta^{(m)}_{p} \varphi^{(m)}_{pl} \varphi^{(n)}_{pk} \, dy \]  \hspace{1cm} (78)

\[ X_{helk}^{(m,n)} \equiv \frac{1}{\beta^{(n)}_{ek}} \int_{y_{\text{min}}}^{y_{\text{max}}} \eta^{(n)}_{e} \varphi^{(m)}_{hl} \varphi^{(n)'}_{ek} \, dy \]  \hspace{1cm} (79)

\[ Y_{helk}^{(m,n)} \equiv \frac{1}{\beta^{(n)}_{hk}} \int_{y_{\text{min}}}^{y_{\text{max}}} \eta^{(m)}_{e} \varphi^{(m)}_{el} \varphi^{(n)'}_{hk} \, dy \]  \hspace{1cm} (80)

\[ O_{helk}^{(m,n)} \equiv Y^{(n,m)T}_{he} + X^{(m,n)}_{he} \]  \hspace{1cm} (81)
Dispersion equation

Using (69), (70) \((0 < m < M - 1)\), (71), (72) and (73), (75) we remove \(B, \bar{B}\) and \(\bar{A}\) from Eqs. (74) and (76). The result is set of nonlinear equations for eigenvector \(A_p^{(m)}\) and eigenvalue \(k_z\) [7]

\[
\mathcal{M}(k_z) \mathcal{U} = 0 \tag{82}
\]

This problem can be solved by searching for roots of determinant of \(\mathcal{M}\) with the inverse iteration technique. The “root tracking” technique was used to find eigenvalues in the complex plane.
\[ \mathcal{U} \equiv \begin{pmatrix} A_h^{(1)} \\ A_e^{(1)} \\ A_h^{(2)} \\ A_e^{(2)} \\ \vdots \\ \vdots \\ A_h^{(M-1)} \\ A_e^{(M-1)} \end{pmatrix} \]
\[
\mathcal{M} \equiv \\
\begin{pmatrix}
P_h^{(1)} & Z_h^{(1)} & R_h^{(1)} \\
Z_e^{(1)} & P_e^{(1)} & 0 & R_e^{(1)} \\
W_h^{(2)} & 0 & P_h^{(2)} & Z_h^{(2)} & R_h^{(2)} \\
W_e^{(2)} & Z_e^{(2)} & P_e^{(2)} & 0 & R_e^{(2)} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
W_h^{(M-1)} & 0 & P_h^{(M-1)} & Z_h^{(M-1)} \\
W_e^{(M-1)} & Z_e^{(M-1)} & P_e^{(M-1)}
\end{pmatrix}
\]

Dimension of \( \mathcal{M} \) is \( 2(M-1)L \)
\[ P_p^{(m)} \equiv O_{pp}^{(m-1,m)} T_p^{(m-1)} O_{pp}^{(m-1,m)} + T_p^{(m)}, \]
\[ W_p^{(m)} \equiv -O_{pp}^{(m-1,m)} T_p S_p^{(m-1)}, \]
\[ R_p^{(m)} \equiv -O_{pp}^{(m,m+1)} S_p^{(m)}, \]
\[ Z_h^{(m)} \equiv k_z O_{hh}^{(m-1,m)} T O_{he}^{(m-1,m)}, \]
\[ Z_e^{(m)} \equiv -k_z O_{ee}^{(m-1,m)} T O_{he}^{(m,m-1)} T \]
Example: Dominant modes of rib waveguide
Example: Surface plasmon mode

Au, $\varepsilon_{Au} = -11.46 + i1.39$

"Superstrate"

$n_3 = 1.30 \div 1.45$

$\lambda = 800 \text{ nm}$

$\text{guide } n_g = 1.456$

$\text{SiO}_2, n_{\text{sub}} = 1.453$

$5 \mu m$

$6 \mu m$

$50 \text{ nm}$

Graph showing the relationship between the index of the superstrate ($n_a$) and the real part of the propagation constant ($\text{Re}(\beta)$) with two peaks at different values of $n_a$.
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Advantages

- straightforward, no hidden parameters
- no need to generate mesh
- accurate, no approximations
- can be used for quick estimation
- relatively fast

Disadvantages

- complicated formulation
- nonlinear eigenvalue problem


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