Modal expansion methods for modeling of photonic devices

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1 Introduction

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 \( \vec{E} \), \( c\vec{B} \)

Maxwell equations

Convention: To keep formulation as simple as possible we use \( c\vec{B} \) instead of \( \vec{H} \) and dimensionless coordinates

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

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

\[
\vec{\nabla} \times c\vec{B} = i\varepsilon\vec{E} \tag{1}
\]

\[
\vec{\nabla} \times \vec{E} = -i\varepsilon\vec{B} \tag{2}
\]
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

\[
\begin{align*}
\epsilon(x, y, z) &= \epsilon(x, y) \quad (2D \text{ task}) \\
\epsilon(x, y, z) &= \epsilon(y) \quad (1D \text{ task}) \\
\{ \vec{E}(x, y, z) \}_{c \vec{B}(x, y, z)} &= \left\{ \vec{E}_\nu(x, y) \right\}_{c \vec{B}_\nu(x, y)} \exp(-i\beta_\nu z) \\
\text{mode profile? propagation constant?}
\end{align*}
\]

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.

2 Eigenmode expansion

Eigenmode expansion

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:

\[
\begin{align*}
\{ \vec{E}(x, y, z) \}_{c \vec{B}(x, y, z)} &= \sum_{\nu \in \mathbb{N}} \left[ f_\nu \left\{ \vec{E}_\nu(x, y) \right\}_{c \vec{B}_\nu(x, y)} \exp(-i\beta_\nu z) + b_\nu \left\{ \vec{E}_{-\nu}(x, y) \right\}_{c \vec{B}_{-\nu}(x, y)} \exp(i\beta_\nu z) \right]. \\
\end{align*}
\]
3 Analysis of 1D structure – $\varepsilon(y)$

One-dimensional structure

$$\varepsilon = \varepsilon(y)$$

If we suppose

$$\frac{\partial}{\partial x} \left\{ \hat{E} \hat{B} \right\} = 0$$

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

3.1 TE and TM modes

TE modes

$$\left\{ \begin{array}{c} E_x \\ E_y \\ E_z \\ cB_x \\ cB_y \\ cB_z \end{array} \right\} = \left\{ \begin{array}{c} \varphi_{hk}(y) \\ 0 \\ 0 \\ \beta_{hk}\varphi_{hk}(y) \\ -i\varphi_{hk}'(y) \\ \varphi_{hk}'(y) \end{array} \right\} \exp(-i\beta_{hk}z)$$

(9)

$$\varphi_{hk}'(y) + \varepsilon(y)\varphi_{hk}(y) = \beta_{hk}^2\varphi_{hk}(y)$$

(10)

TM modes

$$\left\{ \begin{array}{c} E_x \\ E_y \\ E_z \\ cB_x \\ cB_y \\ cB_z \end{array} \right\} = \left\{ \begin{array}{c} 0 \\ -\beta_{ek}\varphi_{ek}(y)/\varepsilon(y) \\ i\varphi_{ek}'(y)/\varepsilon(y) \\ \varphi_{ek}(y) \\ 0 \\ 0 \end{array} \right\} \exp(-i\beta_{ek}z)$$

(11)

$$\left[ \frac{1}{\varepsilon(y)}\varphi_{ek}'(y) \right]' + \varphi_{ek}(y) = \frac{\beta_{ek}^2}{\varepsilon(y)}\varphi_{ek}(y)$$

(12)

Eigenvalue problem

Eqs. (10) and (12) can be written in unique form

$$\hat{L}_p(y)\varphi_{pk}(y) = \beta_{pk}^2\eta_p(y)\varphi_{pk}(y)$$

(13)

$$\hat{L}_p(y)\varphi_{pk}(y) \equiv \left[ \eta_p(y)\varphi_{pk}'(y) \right]' + \eta_p(y)\varepsilon(y)\varphi_{pk}(y)$$

(14)

$$\eta_p(y) \equiv \left\{ \begin{array}{ll} 1 & p = h \\ 1/\varepsilon(y) & p = e \end{array} \right.$$  \hspace{1cm} (15)

Note:
- $\beta_{pk}^2$ and $\varphi_{pk}(y)$ are eigenvalues and eigenfunctions of $\hat{L}_p(y)$
- for each $\beta_{pk}^2$ 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>$c\vec{B}<em>z = 0$ i.e. $\varphi</em>{hk}' = 0$, $\varphi_{ek} = 0$</td>
</tr>
</tbody>
</table>

...
3.2 Transfer matrix method

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 \( n, n = 0..N - 1 \).

\[
\begin{array}{c|c|c}
\varepsilon_{N-1}, d_{N-1} & y_N \\
\varepsilon_{N-2}, d_{N-2} & y_{N-1} \\
\vdots & \vdots \\
\varepsilon_2, d_2 & y_3 \\
\varepsilon_1, d_1 & y_2 \\
\varepsilon_0, d_0 & y_1 \\
\end{array}
\]

Solution in layer \( n \)

Choose \( y_n = 0 \)

\[
\varphi_n(y) = f_n \exp(-i\alpha_n y) + b_n \exp(i\alpha_n y)
\]
\[
= f_n \exp[i\alpha_n (d_n - y)] + b_n \exp[-i\alpha_n (d_n - y)]
\]
\[
= A_n \cos(\alpha_n y) + \frac{B_n}{\alpha_n} \sin(\alpha_n y)
\]
\[
= A_n \cos[\alpha_n (d_n - y)] - \frac{B_n}{\alpha_n} \sin[\alpha_n (d_n - y)]
\]
\[
= \ldots
\]
\[
\alpha_n = \sqrt{\varepsilon_n - \beta^2}.
\]

Transfer matrix and “matching” conditions

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

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

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.

\[
\Delta_n(\beta^2) = A_n^+ B_n^- - A_n^- B_n^+ = (B_n^+ - A_n^-) \begin{pmatrix}
A_n^+ \\
B_n^+
\end{pmatrix} = 0
\]

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].
3.3 Orthogonality relations

**Orthogonality relations**

For simplicity we suppose closed boundary conditions.

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

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

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.)

3.4 E- and H-type modes

**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

\[
\vec{E}_{pk} = (k_{xpk}, 0, k_{zpk}) \tag{26}
\]

Instead of (5) we have

\[
\begin{bmatrix}
E_x(x, y, z) \\
E_y(x, y, z) \\
E_z(x, y, z) \\
cB_x(x, y, z) \\
cB_y(x, y, z) \\
cB_z(x, y, z)
\end{bmatrix}
= \beta_{hk}
\begin{bmatrix}
k_{zhk} \varphi_{hk}(y) \\
0 \\
-k_{zhk} \varphi_{hk}(y) \\
-k_i k_{zhk} \varphi'_{hk}(y) \\
\beta^2_{hk} \varphi_{hk}(y) \\
-i k_i k_{zhk} \varphi'_{hk}(y)
\end{bmatrix}
\exp \left( -i k_{zhk} x - i k_{zhk} z \right) \tag{27}
\]

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

\[
\beta^2_{pk} = k^2_{xpk} + k^2_{zpk} \tag{28}
\]

**Rotation of TE mode**

\[
\begin{aligned}
&u \\
&k_x \vec{e}_x \\
&k_z \vec{e}_z
\end{aligned}
\]

**H-modes**

Transformation of (9)

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

Transformation of (11)

\[
\begin{pmatrix}
E_x \\
E_y \\
E_z \\
cB_x \\
cB_y \\
cB_z
\end{pmatrix} = \frac{1}{\beta_{\epsilon k}} \begin{pmatrix}
\beta_{z k} \eta_c(y) \varphi_{z k}'(y) \\
-\beta_{k y} \eta_c(y) \varphi_{x k}'(y) \\
\beta_{x k} \eta_c(y) \varphi_{y k}'(y) \\
0 \\
0 \\
0
\end{pmatrix} \exp(-ik_{z k}x - ik_{z k}z)
\] (30)

4 Propagation in 2D structure \( \varepsilon(y, z) \)

Propagation in 2D structure \( \varepsilon(y, z) \)

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

![Model of 2D structure](image)

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.

4.1 Field expansion

Field expansion in section \( m \)

TE solution

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

\[
cB_y(y, z) = i \sum_k u_k'(z) \varphi_k(y)
\] (32)

\[
cB_z(y, z) = -i \sum_k u_k(z) \varphi_k'(y)
\] (33)
TM solution

\[ cB_x(y, z) = \sum_k u_k(z)\varphi_k(y) \]  \hspace{1cm} (34)

\[ E_y(y, z) = -i\eta(y) \sum_k u'_k(z)\varphi_k(y) \]  \hspace{1cm} (35)

\[ E_z(y, z) = i\eta(y) \sum_k u_k(z)\varphi'_k(y) \]  \hspace{1cm} (36)

choose \( z^{(m)} = 0 \)

\[ u_k(z) = f_k \exp(-i\beta_k z) + b_k \exp(i\beta_k z) \]  \hspace{1cm} (37)

\[ A_k \cos(\beta_k z) + B_k \beta_k \sin(\beta_k z) \]  \hspace{1cm} (39)

\[ u'_k(z) = \cdots \]  \hspace{1cm} (41)

4.2 Mode matching

Mode matching

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

\[ \sum_k u_k^{(m)}(z^{(m+1)})\varphi_k^{(m)}(y) = \sum_k u_k^{(m+1)}(z^{(m+1)})\varphi_k^{(m+1)}(y) \]  \hspace{1cm} (32)

\[ \sum_k A_k^{(m)}\varphi_k^{(m)} = \sum_k A_k^{(m+1)}\varphi_k^{(m+1)} \]  \hspace{1cm} (42)

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

\[ \int_{y_{\text{min}}}^{y_{\text{max}}} \bar{A}_l^{(m)}(\varphi_l^{(m)}\eta^{(m)}\varphi_l^{(m)}) dy = \sum_k \int_{y_{\text{min}}}^{y_{\text{max}}} A_k^{(m+1)}(\varphi_k^{(m+1)}\eta^{(m)}\varphi_l^{(m)}) dy \]  \hspace{1cm} (43)

use (24)

\[ \bar{A}_l^{(m)} = \sum_{k=0}^{m} Q_{lk}^{(m,m+1)} A_k^{(m+1)} \]  \hspace{1cm} (44)

\[ Q_{lk}^{(m,n)} \equiv \int_{y_{\text{min}}}^{y_{\text{max}}} \eta^{(m)}\varphi_l^{(m)}\varphi_k^{(n)} dy \]  \hspace{1cm} (45)

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

\[ A_k^{(m+1)} = \sum_k Q_{lk}^{(m+1,m)} A_k^{(m)} \]  \hspace{1cm} (46)

Continuity of \( cB_y \) or \( E_y \)

\[ \bar{B}_l^{(m)} = \sum_{k=0}^{m} O_{lk}^{(m,m+1)} B_k^{(m+1)} \]  \hspace{1cm} (47)

\[ B_l^{(m+1)} = \sum_{k=0}^{m} O_{lk}^{(m+1,m)} B_k^{(m)} \]  \hspace{1cm} (48)

\[ O_{lk}^{(m,n)} \equiv \int_{y_{\text{min}}}^{y_{\text{max}}} \eta^{(m)}\varphi_l^{(m)}\varphi_k^{(n)} dy. \]
Relations among overlap integrals

It follows from (43) – (46)

\[
\begin{align*}
\left[O_{lk}^{(n,m)}\right]^{-1} &= O_{lk}^{(m,n)} \equiv Q_{kl}^{(n,m)}, \\
\left[Q_{lk}^{(n,m)}\right]^{-1} &= Q_{lk}^{(m,n)} \equiv O_{kl}^{(m,n)}.
\end{align*}
\]

(49)  (50)

For TE only:

\[
\begin{align*}
Q_{lk}^{(m,n)} &= O_{lk}^{(m,n)}, \\
O_{lk}^{(m,n)} &= Q_{kl}^{(n,m)}.
\end{align*}
\]

(51)  (52)

4.3 \textbf{S-matrix method}

\textbf{S-matrix method}

Motivation: solution using transfer matrix is \textit{unstable} because we add \( \exp(i\beta_\varepsilon z) \) and \( \exp(-i\beta_\varepsilon z) \) and these can be big and small numbers. The source of instability:

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

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

\textbf{What is \textit{S}-matrix?}

It provides relation between amplitudes of output and input modes

\[
\begin{pmatrix}
  f^{(2)} \\
  b^{(1)}
\end{pmatrix} =
\begin{pmatrix}
  t & \bar{r} \\
  r & \bar{t}
\end{pmatrix}
\begin{pmatrix}
  f^{(1)} \\
  b^{(2)}
\end{pmatrix} \equiv S
\begin{pmatrix}
  f^{(1)} \\
  b^{(2)}
\end{pmatrix}
\]

(53)

Composition law

\[
\begin{align*}
1 & \quad \text{\( b^{(1)} \)} & \quad 2 & \quad \text{\( f^{(1)} \)} & \quad 3 & \quad \text{\( z \)} \\
\text{\( S^{(1)} \)} & \quad \text{\( S^{(2)} \)} & \quad \text{\( z \)}
\end{align*}
\]

\[
\begin{align*}
1 & \quad \text{\( b^{(1)} \)} & \quad 2 & \quad \text{\( f^{(1)} \)} & \quad 3 & \quad \text{\( z \)} \\
\text{\( S = S^{(1)} \otimes S^{(2)} \)} & \quad \text{\( z \)}
\end{align*}
\]
\[
\begin{pmatrix}
  f^{(2)}_1 \\
  \bar{b}^{(1)}_1
\end{pmatrix}
= S^{(1)} \begin{pmatrix}
  f^{(1)}_1 \\
  \bar{b}^{(2)}_1
\end{pmatrix},
\begin{pmatrix}
  f^{(3)}_1 \\
  \bar{b}^{(2)}_1
\end{pmatrix}
= S^{(2)} \begin{pmatrix}
  f^{(2)}_1 \\
  \bar{b}^{(3)}_1
\end{pmatrix}
\]

\[
S \equiv S^{(1)} \otimes S^{(2)} = \begin{pmatrix}
  t^{(2)} \bar{J}^{-1} t^{(1)} & t^{(2)} \bar{P}^{-1} t^{(2)} + \bar{f}^{(2)} \\
  \bar{q}^{(1)} t^{-1} r^{(1)} + r^{(1)} & \bar{q}^{(1)} t^{-1} \bar{q}^{(2)}
\end{pmatrix}
\]

\[
J \equiv 1 - \bar{P}^{-1} t^{(2)} r^{(1)}, \quad K \equiv 1 - r^{(2)} \bar{P}^{-1}
\]

Definitions

\[
\begin{align*}
  u^{(m)}(z) &= \{ u_k^{(m)}(z) \} \\
  f^{(m)} &= \{ f_k^{(m)} \} \\
  \bar{f}^{(m)} &= \{ \bar{f}_k^{(m)} \} \\
  g^{(m)} &= \{ g_k^{(m)} \} \\
  \bar{g}^{(m)} &= \{ \bar{g}_k^{(m)} \} \\
  K^{(m)} &= \{ K_{kk}^{(m)} \} \\
  P^{(m)}(d) &= \exp(-K^{(m)} d)
\end{align*}
\]

Expression for the field

\[
\begin{align*}
  u^{(m)}(z) &= P^{(m)} \left( z - z^{(m)} \right) f^{(m)} + P^{(m)} \left( z^{(m+1)} - z \right) \bar{g}^{(m)} \\
  \left[ u^{(m)}(z) \right]^T &= -K^{(m)} \left[ P^{(m)} \left( z - z^{(m)} \right) f^{(m)} - P^{(m)} \left( z^{(m+1)} - z \right) \bar{g}^{(m)} \right]
\end{align*}
\]

S-matrix of uniform section

\[
\begin{pmatrix}
  \bar{f}^{(m)} \\
  \bar{g}^{(m)}
\end{pmatrix}
= \begin{pmatrix}
  P^{(m)} (d^{(m)}) & 0 \\
  0 & P^{(m)} (d^{(m)})
\end{pmatrix}
\begin{pmatrix}
  f^{(m)} \\
  \bar{g}^{(m)}
\end{pmatrix}
\equiv S^{(m)} \begin{pmatrix}
  f^{(m)} \\
  \bar{g}^{(m)}
\end{pmatrix}
\]

S-matrix at boundary

It follows from (45) and (47)

\[
\begin{align*}
  f^{(m+1)} + \bar{g}^{(m+1)} &= O^{(m+1,m)} \left( \bar{f}^{(m)} + \bar{g}^{(m)} \right), \\
  K^{(m+1)} \left( f^{(m+1)} - \bar{g}^{(m+1)} \right) &= O^{(m+1,m)} K^{(m)} \left( \bar{f}^{(m)} - \bar{g}^{(m)} \right).
\end{align*}
\]

This can be rewritten into form

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

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

\[
D^{(\pm)} \equiv O^{(m+1,m)} K^{(m)} \pm K^{(m+1)} Q^{(m+1,m)}
\]
\[ S = S(0) \otimes S^{(0,1)} \otimes S^{(1)} \otimes \ldots \otimes S^{(M-2,M-1)} \otimes S^{(M-1)} \]

\[
\begin{pmatrix}
\tilde{f}^{(M)} \\
\tilde{b}^{(0)}
\end{pmatrix} = S \begin{pmatrix}
f^{(0)} \\
b^{(0)}
\end{pmatrix}
\]

4.4 Perfectly matched layer (PML)

**How to represent radiation modes?**

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 \((d_0 \text{ or } d_{N-1})\) is complex. \((\beta^2 \text{ gets complex, we need to use root-tracking technique in which we change } \text{Im}(d))\).

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.

\[ \text{Im}(y) = \frac{\text{Re}(y)}{\text{Re}(d)} \text{Im}(d) \]

4.5 Bloch modes

**Bloch modes**

Solution of the Maxwell equations in periodic media [36]. If we know \(S\)-matrix of the period with length \(a\) then

\[
\begin{pmatrix}
\tilde{f}^{(M)} \\
\tilde{b}^{(M)}
\end{pmatrix} = \gamma \begin{pmatrix}
f^{(0)} \\
b^{(0)}
\end{pmatrix} \equiv \exp(-ik_{FB}a) \begin{pmatrix}
f^{(0)} \\
b^{(0)}
\end{pmatrix}
\]

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

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

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

Bloch modes can be used to improve BEP performance see e.g. [37].
5 Modes of 3D waveguide – $\varepsilon(x, y)$

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].

5.1 Full vector expansion in uniform section

Full vector expansion in section $m$

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

\[
\begin{pmatrix}
\vec{E}(x, y, z) \\
c\vec{B}(x, y, z)
\end{pmatrix}
= \sum_{p_k}^{} \left[ f_{p_k} \begin{pmatrix}
\vec{E}_{p_k}(y, z) \\
c\vec{B}_{p_k}(y, z)
\end{pmatrix}\exp(-ik_{x_{p_k}}x) +
+b_{p_k} \begin{pmatrix}
\vec{E}_{-p_k}(y, z) \\
c\vec{B}_{-p_k}(y, z)
\end{pmatrix}\exp(ik_{x_{p_k}}x) \right]
\]

Full vector expansion in section $m$

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

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

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

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

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

\[
cB_z(x, y) = -ik_z \sum_k u_{hk}(x)\varphi'_{hk}(y) - i \sum_k u'_{ek}(x)\varphi_{ek}(y)
\]

Full vector expansion in section $m$

\[
k_{x_{p_k}} = (\beta^2_{p_k} - k_z^2)^{1/2}
\]
\[ u_{pk}(x) = \frac{A_{pk}}{\beta_{pk}} \cos(k_{xpk}x) + \frac{B_{pk}}{k_{xpk}} \sin(k_{xpk}x) \]  
\[ u_{pk}'(x) = \ldots \]  
\[ \tilde{A}_{pk} = \frac{A_{pk}}{\beta_{pk}^2} \cos(k_{xpk}d) + \frac{B_{pk}}{k_{xpk}} \sin(k_{xpk}d) \]  
\[ \tilde{B}_{pk} = -k_{xpk} \frac{A_{pk}}{\beta_{pk}^2} \sin(k_{xpk}d) + B_{pk} \cos(k_{xpk}d) \]  

Matrix formulation

diagonal matrices \( T_p^{(m)} \) and \( S_p^{(m)} \) in section \( m \)

\[ T_p^{(m)} = \frac{k_{xpk}^{(m)}}{\beta_{pk}^{(m)/2} \tan[k_{xpk}^{(m)}d_x^{(m)}]} \]  
\[ S_p^{(m)} = \frac{k_{xpk}^{(m)}}{\beta_{pk}^{(m)/2} \sin[k_{xpk}^{(m)}d_x^{(m)}]} \]

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

\[ B_p^{(m)} = -T_p^{(m)} A_p^{(m)} + S_p^{(m)} \tilde{A}_p^{(m)} \]  
\[ \tilde{B}_p^{(m)} = -S_p^{(m)} A_p^{(m)} + T_p^{(m)} \tilde{A}_p^{(m)} \]

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

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

\[ B_p^{(M-1)} = -T_p^{(M-1)} A_p^{(M-1)}, \]  
\[ \tilde{B}_p^{(0)} = T_p^{(0)} \tilde{A}_p^{(0)}. \]  

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

\[ T_p^{(b)} = \frac{k_{xpk}^{(b)}}{\beta_{pk}^{(b)/2} \tan[k_{xpk}^{(b)}d_x^{(m)}]}, \quad b = 0, M - 1. \]

For open boundary

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

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

\[ T_p^{(b)} = \frac{k_{xpk}^{(b)}}{\beta_{pk}^{(b)/2}} \]

5.2 Mode matching and numerical technique

Mode matching

\[ \tilde{A}_h^{(m)} = O_h^{(m,m+1)} A_h^{(m+1)} \]  
\[ \tilde{B}_h^{(m)} = O_h^{(m,m+1)} B_h^{(m+1)} - k_z O_h^{(m,m+1)} A_c^{(m+1)} \]  
\[ A_c^{(m)} = O_c^{(m,m+1)} A_c^{(m+1)} \]  
\[ B_c^{(m)} = O_c^{(m+1,m)} B_c^{(m+1)} + k_z O_h^{(m+1,m)} A_h^{(m+1)} \]
Overlap integrals

\[ O_{pplk}^{(m,n)} \equiv \int_{y_{\min}}^{y_{\max}} \int_{y_{\min}}^{y_{\max}} \eta_{p}^{(n)} \varphi_{pl}^{(m)} \varphi_{pk} dy \]  

\[ Q_{pplk}^{(m,n)} \equiv \int_{y_{\min}}^{y_{\max}} \int_{y_{\min}}^{y_{\max}} \eta_{p}^{(m)} \varphi_{pl}^{(n)} \varphi_{pk} dy \]  

\[ X_{helk}^{(m,n)} \equiv \frac{1}{\rho_{ek}^{(n)^2}} \int_{y_{\min}}^{y_{\max}} \eta_{e}^{(m)} \varphi_{el}^{(n)} \varphi_{ek}^{(n)} dy \]  

\[ Y_{helk}^{(m,n)} \equiv \frac{1}{\rho_{hk}^{(n)^2}} \int_{y_{\min}}^{y_{\max}} \eta_{e}^{(m)} \varphi_{el}^{(n)} \varphi_{hk}^{(n)} dy \]  

\[ O_{helk}^{(m,n)} \equiv Y_{he}^{(n,m)^T} + X_{he}^{(m,n)} \]  

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]

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

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.

\[ \mathcal{M} = \begin{pmatrix} 
A_b^{(1)} & A_e^{(1)} & A_{hc}^{(2)} & A_e^{(2)} & \cdots \\
A_b^{(M-1)} & A_e^{(M-1)} 
\end{pmatrix} \]

\[ U = \begin{pmatrix} 
A_b^{(1)} \\
A_e^{(1)} \\
A_b^{(2)} \\
A_e^{(2)} \\
\vdots \\
A_b^{(M-1)} \\
A_e^{(M-1)} 
\end{pmatrix} \]

Dimension of \(\mathcal{M}\) is \(2(M - 1)L\)
\[ P^{(m)}_p \equiv O^{(m-1,m)}_{pp} T_{pp}^{(m-1)} O^{(m-1,m)}_{pp} + T^{(m)}_p, \]
\[ W^{(m)}_p \equiv -O^{(m-1,m)}_{pp} T_{pp}^{(m-1)} S_p, \]
\[ R^{(m)}_p \equiv -O^{(m,m+1)}_{pp} S_p^{(m)}, \]
\[ Z^{(m)}_h \equiv k_z O^{(m-1,m)}_{hh} T O^{(m-1,m)}_{he}, \]
\[ Z^{(m)}_e \equiv -k_z O^{(m-1,m)}_{ee} T O^{(m,m-1)}_{he} \]

6 Conclusions

Conclusions

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
References


