Photonic crystals, PHYS-605

Ecole doctorale photonique

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Summer semester 2017

II Theory

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   ...
Background

- Hamiltonian operator
- Floquet-Bloch theorem
- Crystal lattice
- Reciprocal space and Brillouin zone
- Dispersion diagram and band structure

Complements:
- basic lecture on quantum mechanics
- basic lecture on solid state physics and crystallography

Maxwell equations

\[ \nabla \cdot \mathbf{D} = \rho \] \[ \mathbf{E}: \text{electric field (champ électrique)} \]

\[ \nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J} \] \[ \mathbf{D}: \text{electric displacement (induction électrique)} \]

\[ \nabla \cdot \mathbf{B} = 0 \] \[ \mathbf{B}: \text{magnetic field/induction (induction magnétique)} \]

\[ \nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0 \] \[ \mathbf{H}: \text{magnetic/magnetizing field (champ magnétique)} \]

\[ \mathbf{J}: \text{current density (densité de courant)} \]

\[ \rho: \text{charge density (densité de charges libres)} \]

Continuity relations

(included in Maxwell equations if taken as distributions)

Continuity of the parallel component of \( \mathbf{E} \): \[ n_{12} \wedge (E_2 - E_1) = 0 \]

Discontinuity of the parallel component of \( \mathbf{H} \): \[ n_{12} \wedge (H_2 - H_1) = J_z \]

Discontinuity of the normal component of \( \mathbf{D} \): \[ n_{12} (D_2 - D_1) = \rho \]

Continuity of the normal component of \( \mathbf{B} \): \[ n_{12} (B_2 - B_1) = 0 \]

\( n_{12} \): normal unit vector at the interface between medium 1 and 2
\( \rho, J_z \): surface charge and current densities at interface 1,2
Constitutive relations of the medium

\[ D = \varepsilon_0 E + P = \varepsilon_0 \varepsilon_r E = \varepsilon E \quad \text{P: polarisation} \]
\[ B = \mu_0 H + M = \mu_0 \mu_r H \quad \text{M: magnetisation (aimantation)} \]

\( \varepsilon_0 \): dielectric constant / vacuum permittivity  
permitivité du vide / constante diélectrique

\( \varepsilon_r \): relative permittivity (permittivité relative)

\( \mu_0 \): magnetic permeability (perméabilité du vide)

\( \mu_r \): relative permeability (perméabilité relative)

Dielectric photonic crystals

\(*\) Linear regime:  \( \varepsilon \) independant of \( E \)

\(*\) No free currents and charges:  \( \rho, J = 0 \)

\(*\) Isotropic dielectric materials:  \( \varepsilon \) scalar  
\( \mu_r = 1 \)

\(*\) Loss-less dielectrics:  \( \varepsilon \) real
Dielectric photonic crystals

Dielectric constant is periodic (lattice + motif) in one, two or three directions of space

\[
\varepsilon(\vec{r} + \vec{T}) = \varepsilon(\vec{r})
\]

\[
\vec{T} = \sum_{i=1,2,3} n_i \vec{a}_i, \quad n_i \in \mathbb{Z}
\]

Propagation equations

\[
\nabla \cdot \mathbf{E} = 0
\]

\[
\nabla \times \mathbf{H} - \varepsilon_0 \varepsilon(\mathbf{r}) \frac{\partial \mathbf{E}}{\partial t} = 0
\]

\[
\nabla \cdot \mathbf{H} = 0
\]

\[
\nabla \times \mathbf{E} + \frac{\partial \mathbf{H}}{\partial t} = 0
\]

for harmonic fields:

\[
\mathbf{H}(\mathbf{r}, t) = \mathbf{H}(\mathbf{r}) e^{j \omega t}
\]

\[
\nabla \times \mathbf{H}(\mathbf{r}) - j \omega \varepsilon_0 \varepsilon(\mathbf{r}) \mathbf{E}(\mathbf{r}) = 0
\]

\[
\mathbf{E}(\mathbf{r}, t) = \mathbf{E}(\mathbf{r}) e^{j \omega t}
\]

\[
\nabla \times \mathbf{E}(\mathbf{r}) + j \omega \mu_0 \mathbf{H}(\mathbf{r}) = 0
\]
E-field equation

after elimination of H

\[ \hat{\Delta} \mathbf{E}_\omega (\mathbf{r}) = \left( \frac{\omega}{c} \right)^2 \mathbf{E}_\omega (\mathbf{r}) \quad \text{avec} \quad \hat{\Delta} = \frac{1}{\varepsilon(\mathbf{r})} \nabla \times \nabla \times \]

H-field equation

or after elimination of E

\[ \hat{\Theta} \mathbf{H}_\omega (\mathbf{r}) = \left( \frac{\omega}{c} \right)^2 \mathbf{H}_\omega (\mathbf{r}) \quad \text{avec} \quad \hat{\Theta} = \nabla \times \left[ \frac{1}{\varepsilon(\mathbf{r})} \nabla \times \right] \]

Field equation as an eigenvalues equation

\[ \hat{\Delta} \mathbf{E}_\omega (\mathbf{r}) = \left( \frac{\omega}{c} \right)^2 \mathbf{E}_\omega (\mathbf{r}) \quad \text{eigenvalue} \ (\omega/c)^2 \]

\[ \hat{\Theta} \mathbf{H}_\omega (\mathbf{r}) = \left( \frac{\omega}{c} \right)^2 \mathbf{H}_\omega (\mathbf{r}) \]

Especially interesting if the operator is self-adjoint (hermitian)
Hermiticity of the field operator

There is a confusing literature on the Hermiticity of the field operator

Most common misconception:

This is true for the H-operator:

$$\hat{\Theta} = \nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times \right]$$

but not for the E-operator:

$$\hat{\Xi} = \frac{1}{\varepsilon(r)} \nabla \times \nabla \times$$

Hermiticity of the field operator

Proof for H-operator is a bit tedious. Integrate twice by parts:

$$\langle F | \Theta G \rangle = \int_{\Omega} d^3r \cdot F^* \nabla \wedge \left( \frac{1}{\varepsilon(r)} \nabla \wedge G \right)$$

$$= \int_{\Omega} d^3r (\nabla \wedge F)^* \frac{1}{\varepsilon(r)} \nabla \wedge G$$

$$= \int_{\Omega} d^3r \left( \nabla \wedge \left( \frac{1}{\varepsilon(r)} \nabla \wedge F \right) \right)^* G$$

$$= \langle \Theta F | G \rangle$$

using:

$$\nabla (a \wedge b) = b \cdot \nabla \wedge a - a \cdot \nabla \wedge b$$

and notice that the integrals of a gradient can be transformed in integrals of a flux of a periodic function, that are equal to zero.
Hermiticity of the field operator

Yes, but:

Eigenvalues of an operator do not depend of the inner product $<F|G>$ that is used

Some inner product are better than other

like e.g. , an inner that corresponds to a quantity with a physical meaning, or which is conserved

For example in quantum mechanics:

$$\langle \Psi | \Psi' \rangle = \int \Psi^* (r) \Psi (r) d^3 r = 1$$

Hermiticity of the field operator

For an electromagnetic wave, the inner product related to the total energy is a good choice:

$$\langle (E,H) | (E',H') \rangle = \int (E(r) \varepsilon(r) E'(r) + H(r) \mu(r) H'(r)) d^3 r$$

Using this inner product, both operators

$$\hat{\Theta} = \nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times \right]$$

are Hermitian

$$\hat{\Xi} = \frac{1}{\varepsilon(r)} \nabla \times \nabla \times$$

(same kind of tedious proof)

Nevertheless, common practice is to solve the equation on $H$ instead of $E$.

Scaling laws

In contrast to electrons in solids, there is no fundamental length scale in Maxwell equations. If the dielectric map $\varepsilon$ is expanded or contracted by a factor $s$:

$$\varepsilon'(r) = \varepsilon(r/s) = \varepsilon(r')$$

Solutions of:

$$\nabla \times \frac{1}{\varepsilon(r)} \nabla \times H_\omega(r) = \left(\frac{\omega}{c}\right)^2 H_\omega(r)$$

become:

$$\nabla' \times \frac{1}{\varepsilon'(s)} \nabla' \times H_\omega\left(\frac{r}{s}\right) = \left(\frac{\omega}{c \cdot s}\right)^2 H_\omega\left(\frac{r}{s}\right)$$

$$H(r')' = H(r/s) \quad \omega' = \omega / s$$

As a consequence, energies and later on wavevector are often expressed in reduced units:

**energy:**  $u = \frac{a}{\lambda} = \frac{\omega a}{2\pi c}$

and further

**wavevector:**  $\tilde{k} = \frac{ka}{2\pi}$

(a : paramètre de maille)

Scaling laws

2\textsuperscript{nd} scaling law on the dielectric constant:

$$\varepsilon(r) = \frac{\varepsilon'(r)}{s^2}$$

$$\nabla \times \frac{1}{\varepsilon'(r)} \nabla \times H_\omega(r) = \left(\frac{\omega}{c \cdot s}\right)^2 H_\omega(r)$$

Field map and wavevector are unchanged.

Physics is solely determined by the ratio of the dielectric constants $\varepsilon_1/\varepsilon_2$
Scaling laws

<table>
<thead>
<tr>
<th>Spatial homothety</th>
<th>Homothety on $\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r \rightarrow r' = rs$</td>
<td>$r \rightarrow r$</td>
</tr>
<tr>
<td>$\varepsilon(r) \rightarrow \varepsilon(r')$</td>
<td>$\varepsilon(r) \rightarrow \varepsilon(r)s^2$</td>
</tr>
<tr>
<td>$k \rightarrow k' = k/s$</td>
<td>$k \rightarrow k$</td>
</tr>
<tr>
<td>$\omega \rightarrow \omega' = \frac{\omega}{s}$</td>
<td>$\omega \rightarrow \omega' = \frac{\omega}{s}$</td>
</tr>
<tr>
<td>$H(r) \rightarrow H(r')$ idem $E(r), B(r), D(r)$</td>
<td>$H(r) \rightarrow H(r)$ idem $E(r), B(r), D(r)$</td>
</tr>
</tbody>
</table>

Floquet-Bloch theorem

Exactly like in solid state physics

Periodicity of $\varepsilon$ allows to look for solutions on the form:

$$H_k(r) = u_k(r) e^{ikr}$$

with $u_k(r)$ function with the same periodicity and symmetries as $\varepsilon$

$\varepsilon(\vec{r} + \vec{T}) = \varepsilon(\vec{r})$ then $u_k(\vec{r} + \vec{T}) = u_k(\vec{r})$

$\varepsilon(S(\vec{r})) = \varepsilon(\vec{r})$ then $u_k(S(\vec{r})) = u_k(\vec{r})$

with $k$, wavevector, vector of the reciprocal space
Reminder, reciprocal space and Brillouin zones

\[
\begin{align*}
\vec{a}_i \cdot \vec{a}_j^* &= 2\pi \delta_{ij} \\
\begin{aligned}
b_1 &= 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\
b_2 &= 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \\
b_3 &= 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}
\end{aligned}
\end{align*}
\]

Dimension of \( r \) is a length
Dimension of \( h \) is a wavevector (inverse of a length)

Technically, the reciprocal lattice is the Fourier transform of the real space lattice

Reminder, reciprocal space and Brillouin zones

Elementary cell of the reciprocal lattice

As in real space, knowledge in an elementary unit cell is sufficient to describe the lattice in the entire reciprocal space, these zones are called Brillouin zones

Exemple in two dimensions

Exercice: draw the three first Brillouin zones of a square lattice

Case of the zinc-blende structure
**Eigenvalues equation with** $u_k$

\[
\hat{\Theta} H_\omega(r) = \left(\frac{\omega}{c}\right)^2 H_\omega(r) \\
\text{with: } H_k(r) = u_k(r) e^{ikr} \quad \text{et} \quad \hat{\Theta} = \nabla \times \left[ \frac{1}{\varepsilon(r)} \nabla \times \right] \\
\text{becomes: } \nabla \wedge \left( \frac{1}{\varepsilon(r)} \nabla \wedge u_k(r) e^{ikr} \right) = \left( \frac{\omega(k)}{c} \right)^2 u_k(r) e^{ikr} \\
(ik + \nabla) \wedge \left( \frac{1}{\varepsilon(r)} (ik + \nabla) \wedge u_k(r) \right) = \left( \frac{\omega(k)}{c} \right)^2 u_k(r) \\
\Theta_k u_k(r) = \left( \frac{\omega(k)}{c} \right)^2 u_k(r) \\
\]

**with the new operator:** \[\Theta_k = (ik + \nabla) \wedge \left( \frac{1}{\varepsilon(r)} (ik + \nabla) \wedge \right] \]

Note: idem scaling law, \[r' = r/s, \quad \omega' = \omega/s \quad \text{et} \quad k' = k/s\]

**reduced units** \[\tilde{k} = \frac{ka}{2\pi}\]

---

**Band structure**

**Dispersion diagram**

\[r: \text{real space lattice} \]
\[k: \text{wavevector, reciprocal space} \]
\[n: \text{integer, } 1, 2, 3 \ldots\]

**The set of the curves** $\omega_n(k)$ **are the dispersion curves of the Bloch modes in the crystal: it is also called the band structure**

---

The same way it is sufficient to know $\varepsilon(r)$ or $u_k(r)$ within a unit cell of the crystal, curves $\omega_n(k)$ have the same symmetries than the reciprocal lattice and it is sufficient to know $\omega_n(k)$ in one Brillouin zone.
Band structure
Dispersion diagram
Examples: One dimension 1D

Free space

Coupled modes

**\( \omega = ck/n \)**

\( n: \) refraction index

Presence of a forbidden band around normal incidence as soon as \( \varepsilon_1 \neq \varepsilon_2 \)

Air band and dielectric band

As a general rule, it can be shown that the electric displacement field \( D \) of high symmetry states is concentrated either in *high* or *low* index regions

The fundamental state maximise the field overlap with the high index dielectric, the next state, in order to ensure orthogonality minimise the overlap

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Band structure
Dispersion diagram
Examples: Two dimensions 2D

Direct lattice

Reciprocal lattice

1st Brillouin zone and irreducible zone

Triangular lattice of holes

Band structure
Dispersion diagram
Band structure
Dispersion diagram
Examples: Two dimensions 2D

TE

Two important conclusions:

✱ The forbidden bands in different directions do not necessarily overlap

✱ The forbidden bands for both polarisations do not necessarily overlap

As a consequence: Full forbidden bands will exist only for specific structures and sufficient index contrast
Dispersion diagram: what is it about?

Spatial periodicity → spatial frequency

Temperal frequency

\[ \omega = \frac{2\pi}{T} \]

Temporal vs. spatial aspects
+ slope \( \propto \) group velocity
+ light propagation direction in 2D or 3D representation
+ etc...

\[ k = \frac{2\pi}{\lambda} \]

Band structure
Dispersion diagram and equi-frequency curves
Band structure
Dispersion diagram
Examples: Three dimensions 3D
Stacking of dielectric spheres with a diamond structure

Ecole doctorale photonique, Photonic crystals, PHYS-605, Romuald Houdré, Summer semester 2017
Band structure computation
Plane wave expansion method

Eigenvalue equations on $u_k$:

$$\hat{\Theta} H_\omega(r) = \left( \frac{\omega}{c} \right)^2 H_\omega(r)$$

with:

$$H_k(r) = u_k(r) e^{ikr}$$

becomes:

$$\Theta_k u_k(r) = \left( \frac{\omega(k)}{c} \right)^2 u_k(r)$$

with the new operator:

$$\Theta_k = (ik + \nabla) \wedge \left( \frac{1}{\varepsilon(r)} (ik + \nabla) \wedge \right)$$

Plane wave expansion method

Method consists in exploiting the periodicity of fields and of the dielectric map and in proceeding to a Fourier transform of $E(r)$, $H(r)$, $\varepsilon(r)$ or $1/\varepsilon(r)$

\[
\begin{array}{c|c}
E(r) &= \sum_{G \in \text{réseau réciproque}} E_G e^{i(k+G)r} \\
H(r) &= \sum_{G \in \text{réseau réciproque}} H_G e^{i(k+G)r} \\
\varepsilon(r) &= \sum_{G \in \text{réseau réciproque}} \varepsilon_G e^{iGr} \\
(\varepsilon(r))^{-1} &= \sum_{G \in \text{réseau réciproque}} \varepsilon_G^{-1} e^{iGr}
\end{array}
\]

Note: Réseau réciproque = reciprocal lattice in French
Note: variables $\omega$ and $k$ are omitted in $E_\omega(r)$ and $E_G$

in order to write

$$\hat{\Theta} H_\omega(r) = \left( \frac{\omega}{c} \right)^2 H_\omega(r)$$

as a matrix eigenvalue equation:

after truncation to a finite number $N$ of plane waves, $m=1...N$

$$\begin{bmatrix} M_G^k \end{bmatrix} \begin{bmatrix} H_m^k \end{bmatrix} = \left( \frac{\omega_k}{c} \right)^2 \begin{bmatrix} H_m^k \end{bmatrix}$$
Plane wave expansion method

More technically: \( \nabla H = 0 \) implies transversality of \( H \)

\( H(r) \) can be written:

\[
H(r) = \sum_{G \in \text{réseau réciproque}} \left( h_{1,G} \bar{u}_{1,G} + h_{2,G} \bar{u}_{2,G} \right) e^{i(k+G) \cdot r}
\]

with \( \{u_{1,G}, u_{2,G}, k+G\} \) direct dihedral. Note: \( k+G = |k+G| \cdot u_{1,G} \wedge u_{2,G} \)

\[
\nabla \times \nabla = \sum_{G \in R.R.} \varepsilon^{-1}_{G} |k+G| \begin{bmatrix}
  h_{1,G} \bar{u}_{1,G} & -h_{2,G} \bar{u}_{1,G} \\
  -h_{2,G} \bar{u}_{2,G} & h_{1,G} \bar{u}_{2,G}
\end{bmatrix} e^{i(k+G) \cdot r}
\]

\[
\varepsilon(r)^{-1} \nabla \times H = i \sum_{G \wedge G' \in R.R.} \varepsilon_{G-G'}^{-1} |k+G| \begin{bmatrix}
  h_{1,G} \bar{u}_{1,G} & -h_{2,G} \bar{u}_{1,G} \\
  -h_{2,G} \bar{u}_{2,G} & h_{1,G} \bar{u}_{2,G}
\end{bmatrix} e^{i(k+G') \cdot r}
\]

which is more convenient to write with \( G = G' + G'' \)

\[
\varepsilon(r)^{-1} \nabla \times H = i \sum_{G \wedge G' \in R.R.} \varepsilon_{G-G'}^{-1} |k+G| \begin{bmatrix}
  h_{1,G} \bar{u}_{1,G} & -h_{2,G} \bar{u}_{1,G} \\
  -h_{2,G} \bar{u}_{2,G} & h_{1,G} \bar{u}_{2,G}
\end{bmatrix} e^{i(k+G') \cdot r}
\]

Plane wave expansion method

after the second curl:

\[
\nabla \times \varepsilon(r)^{-1} \nabla \times H = \sum_{G \wedge G' \in R.R.} \varepsilon_{G-G'}^{-1} |k+G| \begin{bmatrix}
  \bar{u}_{2,G} & \bar{u}_{2,G} \\
  -\bar{u}_{1,G} & \bar{u}_{1,G}
\end{bmatrix} \begin{bmatrix}
  h_{1,G} \\
  h_{2,G}
\end{bmatrix} e^{i(k+G) \cdot r}
\]

\[
\nabla \times \varepsilon(r)^{-1} \nabla \times H = \left( \frac{\omega}{c} \right)^2 H = \left( \frac{\omega}{c} \right)^2 \sum_{G \in R.R.} H_{G} e^{i(k+G) \cdot r}
\]

this leads to a set equations on the \( \{G\} \) plane waves:

\[
\left\{ \sum_{G \in R.R.} \varepsilon_{G-G'}^{-1} |k+G| \begin{bmatrix}
  \bar{u}_{2,G} & \bar{u}_{2,G} \\
  -\bar{u}_{1,G} & \bar{u}_{1,G}
\end{bmatrix} \begin{bmatrix}
  h_{1,G} \\
  h_{2,G}
\end{bmatrix} \right\}_{G \in R.R.}
\]

which, we will limit to \( m \) vectors of the reciprocal lattice. The equation reduces to a diagonalisation problem of a \( 2m \times 2m \) hermitian matrix with eigenvalues \( (\omega/c)^2 \) and eigenvectors \( \{H_G\} \)
Plane wave expansion method
2D systems

The method requires very quickly a large amount of CPU time, several thousands of plane waves are required to compute the band structure of a diamond lattice stack of spheres.

It is mainly used with 2D systems restricted to propagation in the x,y plane z-derivatives vanish

Plane wave expansion method
2D systems
TE and TM polarization

\[ \nabla \times \mathbf{H}(r) - j \omega \varepsilon_0 \varepsilon(r) \mathbf{E}(r) = 0 \]
link \( H_z \) with \( E_x, E_y \) and \( E_z \) with \( H_x, H_y \)

\[ \nabla \times \mathbf{E}(r) + j \omega \mu_0 \mathbf{H}(r) = 0 \]
(z-derivatives vanish)

Field equations on \( H_z \) and \( E_z \) are decoupled:

\[ \frac{1}{\varepsilon(x,y)} \nabla^2 E_z = -\left( \frac{\omega}{c} \right)^2 E_z \]

\[ \nabla \left( \frac{1}{\varepsilon(x,y)} \nabla H_z \right) = -\left( \frac{\omega}{c} \right)^2 H_z \]
Plane wave expansion method  
2D systems  
TE and TM polarisations

Two independent polarization:

- $H_z = 0, \ E_z \neq 0$  \hspace{1cm} TM ou $s$
  - Transverse mode for $E$
  - $H$ in the perpendicular plane

- $H_z \neq 0, \ E_z = 0$  \hspace{1cm} TE ou $p$
  - Transverse mode for $H$
  - $E$ in the perpendicular plane

Note: TE and TM polarization

In the case of a planar waveguide with a mirror symmetry, it is still possible to define even and odd modes and the field structure *in the mirror plane only* has a TE-like or TM-like structure. They are commonly, but improperly, still named TE and TM

- $H_z(z=0) = 0, \ E_z(z=0) \neq 0$  \hspace{1cm} "TM" ou $s$
  - Transverse mode for $E$
  - $H$ in the mirror plane

- $H_z(z=0) \neq 0, \ E_z(z=0) = 0$  \hspace{1cm} "TE" ou $p$
  - Transverse mode for $H$
  - $E$ in the mirror plane

If there is no mirror symmetry, TE and TM polarization can not be separated
Note: TE and TM polarization

**Polarization**

Odd and even modes, abusively referred as TE and TM

Transverse (to the mirror plane) H mode
E in the plane normal to H

Transverse (to the mirror plane) E mode
H in the plane normal to E

---

**Plane wave expansion method**

after the second curl:

\[
\nabla \times \epsilon(r)^{-1} \nabla \times H = \sum_{G,G' \in \mathbb{R},R} \epsilon_{G-G'}^{-1} |k + G'| |k + G| \begin{bmatrix} u_{2,G} u_{2,G'} & -u_{2,G} u_{1,G'} \\ -u_{1,G} u_{2,G'} & u_{1,G} u_{1,G'} \end{bmatrix} \begin{bmatrix} h_{1,G} \\ h_{2,G} \end{bmatrix} e^{i(k+G)r} 
\]

\[
\nabla \times \epsilon(r)^{-1} \nabla \times H = \left(\omega_k / c\right)^2 H = \left(\omega_k / c\right)^2 \sum_{G \in \mathbb{R},R} H_G e^{i(k+G)r} 
\]

this leads to a set equations on the \{G\} plane waves:

\[
\sum_{G' \in \mathbb{R},R} \epsilon_{G-G'}^{-1} |k + G'| |k + G| \begin{bmatrix} u_{2,G} u_{2,G'} & -u_{2,G} u_{1,G'} \\ -u_{1,G} u_{2,G'} & u_{1,G} u_{1,G'} \end{bmatrix} \begin{bmatrix} h_{1,G'} \\ h_{2,G'} \end{bmatrix} = \left(\omega / c\right)^2 \begin{bmatrix} h_{1,G} \\ h_{2,G} \end{bmatrix} \forall G \in \mathbb{R},R
\]

which, we will limit to m vectors of the reciprocal lattice. The equation reduces to a diagonalisation problem of a 2m\times2m hermitian matrix with eigenvalues \((\omega/c)^2\) and eigenvectors \{H_G\}
Plane wave expansion method
2D systems

$k+G$ lies in the $x,y$ plane
$u_{1,G}$ can be chosen along $Oz$ and $u_{2,G}$ in order to
define the direct basis $\{u_{1,G}, u_{2,G}, k+G\}$

$$\sum_{G' \in R.R.} \epsilon^{-1}_{G-G'} |k + G'| k + G \begin{bmatrix} \vec{u}_{2,G} & \vec{u}_{1,G} \\ -\vec{u}_{1,G} & \vec{u}_{2,G} \end{bmatrix} \begin{bmatrix} h_{1,G} \\ h_{2,G} \end{bmatrix} = \left( \frac{\omega}{c} \right)^2 \begin{bmatrix} h_{1,G} \\ h_{2,G} \end{bmatrix} \forall G \in R.R.$$  

writes:

**TM** : $h_{1G} = 0$ for any $G$, $u_{1,G} = u_{1,G'}$ and $u_{2,G} = u_{1,G}$

$$\text{TM} \quad \sum_{G' \in R.R.} \epsilon^{-1}_{G-G'} |k + G'| k + G h_{2,G'} = \left( \frac{\omega}{c} \right)^2 h_{2,G} \forall G \in R.R.$$  

Plane wave expansion method
2D systems

for m plane waves in the reciprocal lattice, the equation is reduced
to the diagonalisation problem of a $m \times m$ hermitian matrix with
eigenvalues $(\omega/c)^2$ and eigenvectors $\{H_G\}$

**TM**

$$\begin{bmatrix} |k + G_1| & |k + G_1| & \cdots & |k + G_1| & |k + G_m| & \cdots & |k + G_1| & |k + G_m| \\ |k + G_1| & |k + G_1| & \cdots & |k + G_1| & |k + G_m| & \cdots & |k + G_1| & |k + G_m| \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\ |k + G_1| & |k + G_1| & \cdots & |k + G_1| & |k + G_m| & \cdots & |k + G_1| & |k + G_m| \\ |k + G_1| & |k + G_1| & \cdots & |k + G_1| & |k + G_m| & \cdots & |k + G_1| & |k + G_m| \\ \end{bmatrix} \begin{bmatrix} \delta(G_1 - G_1) & \cdots & \delta(G_1 - G_m) \\ \delta(G_m - G_1) & \cdots & \delta(G_m - G_m) \\ \delta(G_m - G_1) & \cdots & \delta(G_m - G_m) \\ \end{bmatrix} \begin{bmatrix} C_1 \\ C_m \end{bmatrix} = \left( \frac{\omega}{c} \right)^2 \begin{bmatrix} C_1 \\ C_m \end{bmatrix}$$

$$\vec{\kappa}(x,y) = \frac{1}{\epsilon(x,y)}$$
Plane wave expansion method
2D systems

TE : $h_{2G} = 0$ for any $G$ and $u_{1,G} \cdot u_{2,G} = 0$
the angle $u_{2,G}, u_{2,G'}$ is identical to the angle $(k+G), (k+G')$
and $|k+G||k+G'|u_{2,G}u_{2,G'} = (k+G).(k+G')$

$$\sum_{G' \in R,R.} \varepsilon_{G-G'}^{-1} (k + G') (k + G) \begin{bmatrix} \tilde{u}_{2,G} \tilde{u}_{2,G'} & -\tilde{u}_{2,G} \tilde{u}_{1,G'} \\ -\tilde{u}_{1,G} \tilde{u}_{2,G'} & \tilde{u}_{1,G} \tilde{u}_{1,G'} \end{bmatrix} \begin{bmatrix} h_{1,G'} \\ h_{2,G'} \end{bmatrix} = \left(\frac{\omega}{c}\right)^2 \begin{bmatrix} h_{1,G} \\ h_{2,G} \end{bmatrix} \quad \forall G \in R,R.$$

writes:

$$\left\{ \begin{array}{l} \sum_{G' \in R,R.} \varepsilon_{G-G'}^{-1} (k + G') (k + G) h_{1,G'} = \left(\frac{\omega}{c}\right)^2 h_{1,G} \\ \forall G \in R,R. \end{array} \right.$$ 

for $m$ plane waves in the reciprocal lattice, the equation is reduced to the diagonalisation problem of a $m \times m$ hermitian matrix with eigenvalues $(\omega/c)^2$ and eigenvectors $\{H_G\}$

$$\begin{pmatrix} (k + G_1) & (k + G_2) & \cdots & (k + G_m) \\ (k + G_2) & (k + G_3) & \cdots & (k + G_m) \\ \vdots & \vdots & \ddots & \vdots \\ (k + G_m) & (k + G_2) & \cdots & (k + G_1) \end{pmatrix} \begin{pmatrix} \delta(G_1 - G_1) & \delta(G_1 - G_2) & \cdots & \delta(G_1 - G_m) \\ \delta(G_2 - G_1) & \delta(G_2 - G_2) & \cdots & \delta(G_2 - G_m) \\ \vdots & \vdots & \ddots & \vdots \\ \delta(G_m - G_1) & \delta(G_m - G_2) & \cdots & \delta(G_m - G_m) \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_m \end{pmatrix} = \frac{\omega}{c}^2 \begin{pmatrix} A_1 \\ A_2 \\ \vdots \\ A_m \end{pmatrix}$$

$$\tilde{\hat{\kappa}}(x,y) = \frac{1}{\varepsilon(x,y)}$$
Plane wave expansion method
2D systems

Note: it is also possible to derive the same equations with the development on a plane wave basis from the equations:

\[ \nabla \times \frac{1}{\varepsilon(r)} \nabla \times H_\omega(r) = \left( \frac{\omega}{c} \right)^2 H_\omega(r) \quad \text{and} \quad \frac{1}{\varepsilon(r)} \nabla \times \nabla \times E_\omega(r) = \left( \frac{\omega}{c} \right)^2 E_\omega(r) \]

which leads to:

"TE" \[ \sum_n H_n (k + G_m) \cdot (k + G_n) \varepsilon_n^{-1} = \left( \frac{\omega}{c} \right)^2 H_n \quad \forall G_m \in \mathbb{R} \mathbb{R}. \]

"TM" \[ \sum_n E_n (k + G_m) \cdot (k + G_n) \varepsilon_n^{-1} = \left( \frac{\omega}{c} \right)^2 E_n \quad \forall G_m \in \mathbb{R} \mathbb{R}. \]

this E-field equation is not Hermitian. It is possible to convert it in an Hermitian problem with the variable change:

\[ C_m = |k + G_m| E_m. \]

"TM" \[ \sum_n C_n |k + G_m| |k + G_n| \varepsilon_n^{-1} = \left( \frac{\omega}{c} \right)^2 C_n \quad \forall G_m \in \mathbb{R} \mathbb{R}. \]

Plane wave expansion method
2D systems

A last technical effort before a pause remains the computation of the Fourier transform of \(1/\varepsilon(x,y)\)

In the general case, this has to be done numerically, exploiting as much as possible the crystal symmetries and performing the computations in the irreducible Brillouin zone. Usually with FFT algorithms.

In specific cases, there exist analytical solutions, for example for circular pillars or holes:

\[ \varepsilon(G) = \varepsilon_n \delta_{G,0} + (\varepsilon_n - \varepsilon_p) \frac{2\pi R^2}{S_{\text{cellule}}} J_1 \left( |G| R \right) \]

where \(J_1\) is a 1st order Bessel function + summation over the entire lattice
Plane wave expansion method  
2D systems  
Inverse method and Ho's method

As it was developed here, the formalism requires the Fourier transform of $1/\varepsilon$, it is also possible to use the Fourier transform of $\varepsilon$ and inverse further the operator.  
For a finite number of plane waves, both approaches differ. As a general rule, the direct method of Ho converges faster.

<table>
<thead>
<tr>
<th>Step</th>
<th>Inverse method</th>
<th>Ho’s method</th>
</tr>
</thead>
<tbody>
<tr>
<td>*1</td>
<td>$\varepsilon^{-1}(G) = TF(1/\varepsilon)$</td>
<td>$\varepsilon(G) = TF(\varepsilon)$</td>
</tr>
<tr>
<td>*Truncation</td>
<td>$[\varepsilon^{-1}(G)]_N$</td>
<td>$[\varepsilon(G)]_N$</td>
</tr>
<tr>
<td>*3 Inversion</td>
<td>-</td>
<td>$[\varepsilon^{-1}(G)]<em>{N, Ho} = [\varepsilon(G)]</em>{N^{-1}}$</td>
</tr>
</tbody>
</table>

ref: Phys. Rev. Lett. 65, 3152, 1990 and JOSA B, 13, 1870, 1996, for a more detailed discussion, see e.g. V. Zabelin, PhD thesis EPFL, n° 4315.
**Plane wave expansion method limitations**

*2D & 3D*

PWE method is mainly used for 2D systems, as it converges slowly.

<table>
<thead>
<tr>
<th></th>
<th>2D</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nb of plane waves per dimension</td>
<td>$\alpha$</td>
<td>$\alpha$</td>
</tr>
<tr>
<td>Nb of plane waves</td>
<td>$\alpha^2$</td>
<td>$\alpha^3$</td>
</tr>
<tr>
<td>Memory</td>
<td>$(\alpha^2)^2 = \alpha^4$</td>
<td>$(2\alpha^3)^2 = 4\alpha^6$</td>
</tr>
<tr>
<td>Computation time</td>
<td>$2(\alpha^2)^3 = 2\alpha^6$</td>
<td>$(2\alpha^3)^3 = 8\alpha^9$</td>
</tr>
</tbody>
</table>

*Losses, complex refractive index and dispersive medium or non-linear medium*

lifetime (E+i\gamma), penetration depth (k+ip), absorption (n+ik), \varepsilon(\lambda) ... possible but delicate

*Small and large index steps simultaneously*

![Diagram](image)

**Bestiary of common 2D systems**

(a) ![Diagram](image)

\[ |\Gamma X| = \frac{\pi}{a}, \quad |\Gamma X|_{\text{reduct}} = \pm \frac{1}{2} \]

\[ |\Gamma M| = \sqrt{2} \frac{\pi}{a}, \quad |\Gamma M|_{\text{reduct}} = \pm \frac{\sqrt{2}}{2} \]

(b) ![Diagram](image)

\[ |\Gamma M| = 2 \frac{\sqrt{3} \pi}{3} \frac{\pi}{a}, \quad |\Gamma M|_{\text{reduct}} = \pm \frac{\sqrt{3}}{3} \]

\[ |\Gamma K| = \frac{4 \pi}{3} \frac{\pi}{a}, \quad |\Gamma K|_{\text{reduct}} = \pm \frac{2}{3} \]

Attention: in contrast to intuition the modulus of $\Gamma K$ is not $\pi/a$

<table>
<thead>
<tr>
<th>geometry</th>
<th>square lattice</th>
<th>triangular lattice</th>
</tr>
</thead>
<tbody>
<tr>
<td>direct vectors</td>
<td>$a_1 = (1, 0)$; $a_2 = (0, 1)$</td>
<td>$a_1 = (1, 0)$; $a_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$</td>
</tr>
<tr>
<td>reciprocal vectors</td>
<td>$b_1 = \frac{2\pi}{a}(1, 0)$; $b_2 = \frac{2\pi}{a}(0, 1)$</td>
<td>$b_1 = \frac{2\pi}{a}(1, -\frac{1}{3} \sqrt{3})$; $b_2 = \frac{2\pi}{a}(0, \frac{2}{3} \sqrt{3})$</td>
</tr>
<tr>
<td>$f$</td>
<td>$\frac{R^2 \pi}{a^2}$</td>
<td>$\frac{2\sqrt{3}}{3} \frac{R^2}{a^2}$</td>
</tr>
<tr>
<td>unit cell surface</td>
<td>$a^2$</td>
<td>$\frac{\sqrt{3}}{2} a^2$</td>
</tr>
</tbody>
</table>
Bestiary of common 2D systems
Square lattice, holes

filling factor $= f_{\text{air}}$
$n = 3.36$

Bestiary of common 2D systems
Square lattice, holes

filling factor $= f_{\text{air}} = 50\%$
$n = 3.36$
Bestiary of common 2D systems
Square lattice, holes

Bestiary of common 2D systems
Square lattice, pillars

filling factor = $f_{\text{dil}}$
$n=3.36$
Bestiary of common 2D systems
Square lattice, pillars

filling factor = $f_{\text{die}} = 20\%$
$n=3.36$

Ecole doctorale photonique, Photonic crystals, PHYS-605, Ramuald Hébard, Summer semester 2017
Bestiary of common 2D systems
Triangular lattice, holes

filling factor = \( f_{\text{air}} \)
\[ n = 3.36 \]
Bestiary of common 2D systems
Triangular lattice, holes

![Graphs showing TE and TM modes for triangular lattice with holes.]

Ecole doctorale photonique, Photonic crystals, PHYS-605, Ramuald Houdré, Summer semester 2017

Bestiary of common 2D systems
Triangular lattice, pillars

filling factor = \( f_{\text{diele}} \)
n=3.36

![Graph showing reduced frequency vs filling factor for TE and TM polarizations.]
Bestiary of common 2D systems
Triangular lattice, pillars

filling factor = $f_{\text{die}} = 30\%$

$n=3.36$
Bestiary of common 2D systems
Graphite/Honeycomb lattice, holes

filling factor = $f_{air}$
n=3.36

Bestiary of common 2D systems
Graphite/Honeycomb lattice, holes

filling factor = $f_{air} = 40\%$
n=3.36
Bestiary of common 2D systems
Graphite/Honeycomb lattice, holes

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Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars

filling factor = $f_{\text{die}}$

$n=3.36$

Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars

filling factor = $f_{\text{die}} = 30\%$

$n=3.36$
Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars

TE

TM

2

1

Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars

TE

TM

4

3

Ecole doctorale photonique, Photonic crystals, PHYS-605, Ramualdi Heudrü, Summer semester 2017
Out of plane propagation in 2D systems
Light cone

Reminder: refraction and reflection can be understood as scattering processes between two dispersion curves.

Ibn Sahl (c. 984) (also known as Snell-Descartes law, c. 1631):

\[
\frac{\sin \theta_1}{\sin \theta_2} = \frac{n_2}{n_1}
\]

is nothing but the \( k_{\|} \) conservation at the interface (due to in-plane translational invariance):

\[
k_0 n_1 \sin \theta_1 = k_0 n_2 \sin \theta_2 \\
\beta_1 = \beta_2
\]

Total internal reflection:
- \( k < n_2 \omega/c \):
  - coupling 1 to 2 allowed
- \( k > n_2 \omega/c \):
  - coupling 1 to 2 forbidden

Out of plane propagation in 2D systems
Light cone

- Fabry-Perot mode
- allowed states in medium 2
- resonance, leaky mode
- TE pol.
- higher-order mode at larger \( \omega, \beta \)
- weakly guided
- thin slab waveguide
Out of plane propagation in 2D systems
Light cone

Note: the continuum of states inside the light cone originates from the projection on k// of the dispersion diagram of the semi-infinite cladding medium

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Out of plane propagation in 2D systems
Light cone

Ecole doctorales photoniques, Photonic crystals, PHY5-405, Ramuald Houdré. Summer semester 2017
Out of plane propagation in 2D systems
Light cone

Note: the continuum of states inside the light cone originates from the projection on \( k// \) of the dispersion diagram of the semi-infinite cladding medium and folded back on the first Brillouin zone.

Intersection of the light cone \( \omega=kc/n_2 \)
with the planes \( \Gamma M, MK \) and \( K\Gamma \)
= dispersion curve of zero index contrast photonic crystal
\( n_{\text{hole}}=n_{\text{dielectric}}=n_{\text{air}} \)

2D systems and defect modes
super-cell

Goal: computation of defect modes

New larger unit cell \( \alpha \) time larger in direction \( a_1 \) and \( \beta \) time larger in \( a_2 \) compared to the original unit cell.

Linear defect (waveguide)

For the same accuracy, \( \alpha \beta \) more plane waves are needed

\[
N = \frac{G_{\text{max}}^2 \pi}{(2\pi/\alpha a) (2\pi/\beta a)} = \alpha \beta N_0
\]
2D systems and defect modes
super-cell and projected band structure

1D defect (wave guide)

Only $k_x$ remains a good quantum number

square lattice

Once again, we must project on $k_x$ the dispersion diagram of the cladding medium (now the photonic crystal in-plane)

2D systems and defect modes
super-cell and projected band structure

Square lattice

Projection on $\Gamma M$

Projection on $\Gamma X$
2D systems and defect modes
super-cell and projected band structure

The triangular lattice case is a bit more subtle: the ΓK length is not the same in a 1D lattice and a triangular lattice with identical period a.

One finds such obscure schemes in the literature. This is no mystery...

2D systems and defect modes
super-cell and projected band structure

...provided one keeps in mind that these dispersion curves are in fact 2D surfaces.

Triangular lattice
Other methods

Guided mode expansion method GME

* Same method as plane wave expansion method but with the basis set of the planar waveguide guided modes or Bloch modes
  1. Expand onto electromagnetic modes of a homogeneous slab
  2. Include radiation modes to lowest order (Fermi’s golden rule)

- More complex to implement but more accurate and fast
- In 2016, one PhC cavity : $\approx 1$ minute on one CPU core
- One optimisation : $\approx 10,000$ simulations $\approx 2$ days on a small cluster

- V. Zabelin, PhD thesis EPFL, n° 4315
- M. Minkov, PhD thesis EPFL, n° 6857
- M. Minkov and V. Savona, Scientific Reports 4, 5124 (2014)

---

GME

2D guided modes in the slab

Elementary super-cell

$$H_{G\alpha}(r) = \sum_{G,\alpha} c_{\alpha}(k + G,\alpha) H_{G,\alpha}(r)$$
Other methods

Guided mode expansion method GME

- Very efficient for 2D structures
- In 1D, not very well suited, FDTD is faster and easier to implement
- In 3D GME = PWE!

Note: more in the high Q cavities chapter

Bloch mode expansion method

- Same method as GME but with the basis set of the PhC Bloch modes
- More complex to implement but more accurate and fast
- Used to compute defects states, cavity modes etc...

Other methods

Tight binding method

- Basis of localized functions
- Periodic structure and overlap integrals
- There are no convenient localized enough basis functions
- Matrices elements are computed ab initio or deduced from plane wave computations
- Suitable to the description of localized states

Korringa-Kohn-Rostocker method (KKR)

- Diffraction matrix of the unit cell + Green function of the periodic structure
- More complex to implement but more stable
- Compute directly the density of states and the local density of states
Modelling
Finite Difference in the Time Domain

Solve numerically the Maxwell's equations as a function of time using finite difference techniques on grid

Finite Difference in the Time Domain

✱ Direct computation of the time evolution of the electromagnetic field in the dielectric structure and the optical response (transmission, reflectivity, ...)

✱ but only indirect access to more fundamental physical quantities (eigenstates, dispersion curves, ...)

✱ it is difficult, but possible to some extend, to include dispersive or non-linear materials

⚠️ numerical methods: "an avalanche of numbers in a desert of ideas"
Finite Difference in the Time Domain

More technically:

replace derivations operator by finite differences

\[
\frac{df}{dx}(x) = \lim_{h \to 0} \frac{f(x + h) - f(x)}{h} = \frac{f(x + h) - f(x)}{h}
\]

preferably written in a centered form:

\[
\frac{df}{dx}(x) \approx \frac{f(x + h) - f(x - h)}{2h}
\]

The aim of the FDTD method is to find the appropriate grid and compute only the necessary field components in order to minimize memory requirement and computation time.


Finite Difference in the Time Domain

Maxwell's equations:

\[
\nabla \times \vec{E} = -\mu \frac{\partial \vec{H}}{\partial t}
\]

\[
\nabla \times \vec{H} = \sigma \vec{E} + \varepsilon \frac{\partial \vec{E}}{\partial t}
\]

6 scalar equations:

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right)
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right)
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right)
\]

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_y}{\partial z} - \frac{\partial H_z}{\partial y} - \sigma E_x \right)
\]

\[
\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} - \sigma E_y \right)
\]

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left( \frac{\partial H_x}{\partial y} - \frac{\partial H_y}{\partial x} - \sigma E_z \right)
\]
Finite Difference in the Time Domain

Grid: step size $\Delta x, \Delta y, \Delta z$

$$(i, j, k) = (i\Delta x, j\Delta y, k\Delta z)$$

$$F^n(i, j, k) = F(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$$

derivatives / finite differences:

$$\frac{\partial F^n(i, j, k)}{\partial x} = \frac{F^n(i + 1/2, j, k) - F^n(i - 1/2, j, k)}{\Delta x}$$

$$\frac{\partial F^n(i, j, k)}{\partial t} = \frac{F^{n+1/2}(i, j, k) - F^{n-1/2}(i, j, k)}{\Delta t}$$

the 6 scalar equations become:

<table>
<thead>
<tr>
<th>Equation 1</th>
<th>Equation 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_x^{n+1}(i+1/2,j,k)=A_{i,j,k}E_x^n(i+1/2,j,k)$</td>
<td>$H_y^{n+1/2}(i+1/2,j,k+1/2)=H_y^{n+1/2}(i+1/2,j,k+1/2)$</td>
</tr>
<tr>
<td>$+B_{i,j,k}[H_y^{n+1/2}(i+1/2,j,k+1/2)-H_y^{n+1/2}(i+1/2,j,k-1/2)]$</td>
<td>$+\frac{\Delta t}{\mu}\left[E_y^n(i,j+1/2,k+1) - E_y^n(i,j+1/2,k)\right]$</td>
</tr>
<tr>
<td>$+H_y^{n+1/2}(i+1/2,j,k-1/2)-H_y^{n+1/2}(i+1/2,j,k+1/2)]$</td>
<td>$+E_y^n(i,j,k+1/2)-E_y^n(i,j,k+1/2)]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Equation 3</th>
<th>Equation 4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_y^{n+1}(i,j+1/2,k)=A_{i,j,k}E_y^n(i,j+1/2,k)$</td>
<td>$H_x^{n+1/2}(i+1/2,j,k+1/2)=H_x^{n+1/2}(i+1/2,j,k+1/2)$</td>
</tr>
<tr>
<td>$+B_{i,j,k}[H_x^{n+1/2}(i+1/2,j,k+1/2)-H_x^{n+1/2}(i+1/2,j,k-1/2)]$</td>
<td>$+\frac{\Delta t}{\mu}\left[E_x^n(i+1,j,k+1) - E_x^n(i+1,j,k)\right]$</td>
</tr>
<tr>
<td>$+H_x^{n+1/2}(i+1/2,j,k-1/2)-H_x^{n+1/2}(i+1/2,j,k+1/2)]$</td>
<td>$+E_x^n(i+1/2,k)+E_x^n(i+1/2,k+1)]$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Equation 5</th>
<th>Equation 6</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_z^{n+1}(i,j,k+1/2)=A_{i,j,k}E_z^n(i,j,k+1/2)$</td>
<td>$H_x^{n+1/2}(i+1/2,j,k+1/2)=H_x^{n+1/2}(i+1/2,j,k+1/2)$</td>
</tr>
<tr>
<td>$+B_{i,j,k}[H_y^{n+1/2}(i+1/2,j,k+1/2)-H_y^{n+1/2}(i+1/2,j,k-1/2)]$</td>
<td>$+\frac{\Delta t}{\mu}\left[E_z^n(i,j+1/2,k+1) - E_z^n(i,j+1/2,k)\right]$</td>
</tr>
<tr>
<td>$+H_y^{n+1/2}(i+1/2,j,k-1/2)-H_y^{n+1/2}(i+1/2,j,k+1/2)]$</td>
<td>$+E_z^n(i,j,k+1/2)-E_z^n(i,j,k+1/2)]$</td>
</tr>
</tbody>
</table>

with:

$$A_{i,j,k} = \frac{1 - \sigma(i,j,k)}{\varepsilon(i,j,k)}$$

$$B_{i,j,k} = \frac{\Delta t}{\varepsilon(i,j,k)\delta}$$
Finite Difference in the Time Domain

these equations are such that:

<table>
<thead>
<tr>
<th>((n-1/2)\Delta t)</th>
<th>(n\Delta t)</th>
<th>((n+1/2)\Delta t)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(H_{(n-1/2)\Delta t})</td>
<td>(E_{(n-1)\Delta t}) → (E_{n\Delta t})</td>
<td>(E_{n\Delta t}) → (H_{(n+1/2)\Delta t})</td>
</tr>
</tbody>
</table>

It is sufficient to compute \(E\) and \(H\) on two interlaced grids at alternate odd and even time steps \(E(n\Delta t)\) et \(H(m\Delta t)\)

Finite Difference in the Time Domain

Stability requirement / step size:

\(v_{\text{max}}\) : maximum propagation speed of the electromagnetic wave  
\(\Delta t\) : temporal step  
\(\delta\) : grid lattice  
\(N\) : dimensionality

\[
\frac{v_{\text{max}} \Delta t}{\delta} = \frac{1}{\sqrt{N}}
\]

with different \(\Delta x, \Delta y, \Delta z\) along \(x, y\) and \(z\)

\[
v_{\text{max}} \Delta t = \left(\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right)^{-1/2}
\]

in practice:

\[
\delta = \lambda/10
\]
Finite Difference in the Time Domain

Sources:

Spatial shape:
- plane wave
- point source, Gaussian, ...

Time structure:
- harmonic excitation (eigenstates ?)
- pulse excitation (spectral response)

Exemples:

\[ E^\text{time}(x, y, z) = E_0(x, y, z) \sin(\omega t) \]

Gaussian source

\[ E_i(t+1/2, j, k_0) = E_0(i+1/2, j, k_0) \sin(2\pi f_n \delta t) \]

plane wave

Technically this is more complex than it looks like. There are two types of approaches:

- total field / scattered field
- champ total / champ diffracté


Finite Difference in the Time Domain

Boundary conditions.

Finite size of the computation domain. The field at the boundary is not properly computed as some components are missing.

**Strategy 1** : ignore the missing components (= 0). Very bad. Generates non physical parasitic reflections.
Finite Difference in the Time Domain

Ideal boundary conditions: perfectly absorbing layer, \( T=0 \) and \( R=0 \)

By order of merit but also difficulty of implementation:

**Strategy 2**: Murs conditions. Simulates the propagation of an outward going wave at the boundary

**Strategy 3**: Liao conditions. Interpolation of the field at the boundary, in space and time

**Strategy 4**: Perfectly matched layer (PML). Simulate, over a few period, a perfectly absorbing medium. Gives excellent results with only a few periods
Journal of Computational Physics, 114, 185, 1994

Finite Difference in the Time Domain
Examples
Continuous wave (harmonic)

**Polariser filter**

**Add/Drop filter**

![Image of polariser filter](image)

![Image of add/drop filter](image)
Finite Difference in the Time Domain
Examples

Pulsed regime, spectral response

Example: transmission across 8 rows, triangular lattice of holes, direction ΓK,
TE:

Transfer matrices method

Transfer matrices techniques for stack of thin layers:

\[
\begin{pmatrix}
S_+ \\
S_-
\end{pmatrix} =
\begin{pmatrix}
a & b \\
c & d
\end{pmatrix}
\begin{pmatrix}
E_+ \\
E_-
\end{pmatrix}
\]

Transfer matrix

\[
\begin{pmatrix}
E_+ \\
E_-
\end{pmatrix} =
\begin{pmatrix}
\alpha & \beta \\
\gamma & \delta
\end{pmatrix}
\begin{pmatrix}
E_+ \\
E_-
\end{pmatrix}
\]

Diffusion matrix

Entire structure:

\[
\begin{pmatrix}
S_+ \\
S_-
\end{pmatrix} = \prod_{i=1}^{n} T_i
\begin{pmatrix}
E_+ \\
E_-
\end{pmatrix}
\]

With \( T_i \) transfer matrix of an interface or propagatoin matrix

Ref: any good book on optics
Transfer matrices method

Transmission and reflection coefficients are computed setting to 0 the incoming wave in the final layer

\[
\begin{pmatrix}
0 \\
S_-
\end{pmatrix} = \prod_{i=1..n} T_i \begin{pmatrix}
E_+ \\
E_-
\end{pmatrix}
\]

\[
R = \frac{|E_-|^2}{|E_+|^2} \quad T = \frac{|S_+|^2}{|E_+|^2}
\]

⚠️ beware of initial and final refractive indices

Ref: any good book on optics
Ecole Doctorale Photonique, Photonic Crystals, PHYS-405, Ramuald Houédrey, Summer semester 2017

Sakoda and other transfer matrices method

Generalisation of transfer matrices methods including diffracted modes

\[
\begin{pmatrix}
S_+^i \\
S_-^i
\end{pmatrix} = \begin{pmatrix}
a \\
b
\end{pmatrix} \begin{pmatrix}
E_+
\end{pmatrix}
\]

Main difficulty lies in the computation of the diffusion coefficients

- Pure Appl. Opt., 3, 975, 1994
- Implementation of such techniques in 2D photonic crystals by S. Sakoda

These techniques often have serious numerical instability issues
Other techniques

Other techniques less frequently used:

- Finite element (FEM), becoming more commonly used nowadays
- BPM beam propagation method
- multipolar
- integral equations / Green functions
- differential method / coupled waves
- homogenisation
- envelope function / "effective mass"
- ...

For a review of these techniques refer for example to:

Photonic crystals : towards nanoscale photonic devices / J.-M. Lourtioz, Berlin : Springer

Codes

FDTD : http://www.thefullwiki.org/Finite-difference_time-domain_method
FEM : http://www.thefullwiki.org/Finite_element_method

Open sources

- Meep http://ab-initio.mit.edu/wiki/index.php/Meep
- CAMFR http://camfr.sourceforge.net
- Geo-Radar http://carsten-welcomes-you.com/radarfdtd
- GFDTD http://ostatic.com/gfdtd
- BigBoy http://sourceforge.net/projects/bigboy
- EM Explorer http://www.emexplorer.net/news.htm
- GprMax http://www.gprmax.org/

Commercial

- Photon Design (CrystalWave, OmniSim, FIMMPROP) http://www.photond.com/
- COMSOL (FEM) http://www.comsol.com/
- Lumerical http://www.lumerical.com/  ⋄ cluster option
- RFsoft http://www.rfsoftinc.com/
- EM Photonics http://www.empophotonics.com/
- Optiwave http://www.optiwave.com/
- Apollo Photonics http://www.apollophoton.com/apollo/