Photonic crystals, PHYS-605

Ecole doctorale photonique

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II Theory

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  - Thermal photovoltaic
  - …

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

$$\nabla \cdot \mathbf{D} = \rho$$
$$\nabla \times \mathbf{H} - \frac{\partial \mathbf{D}}{\partial t} = \mathbf{J}$$
$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \times \mathbf{E} + \frac{\partial \mathbf{B}}{\partial t} = 0$$

E: electric field (champ électrique)
D: electric displacement (induction électrique)
B: magnetic field/induction (induction magnétique)
H: magnetic/magnetizing field (champ magnétique)
J: current density (densité de courant)
ρ: charge density (densité de charges libres)

Continuity relations

(included in Maxwell equations if taken as distributions)

Continuity of the parallel component of E : $n_{12} \wedge (E_2 - E_1) = 0$
Discontinuity of the parallel component of H : $n_{12} \wedge (H_2 - H_1) = J_s$
Discontinuity of the normal component of D : $n_{12} . (D_2 - D_1) = \rho_s$
Continuity of the normal component of B : $n_{12} . (B_2 - B_1) = 0$

$\mathbf{n_{12}}$: normal unit vector at the interface between medium 1 and 2

ρ_s, J_s : surface charge and current densities at interface 1,2

Constitutive relations of the medium

$$D = \varepsilon_0 E + P = \varepsilon_0 \varepsilon_r E = \varepsilon E$$ P: polarisation

$$B = \mu_0 H + M = \mu_0 \mu_r H$$ M: magnetisation (aimantation)

ε_0 : dielectric constant / vacuum permittivity
permittivité du vide / constante diélectrique

ε_r : relative permittivity (permittivité relative)

μ_0 : magnetic permeability (perméabilité du vide)

μ_r : relative permeability (perméabilité relative)

Dielectric photonic crystals

✳Linear regime: ε independant of E

✳No free currents and charges: ρ, J = 0

✳Isotropic dielectric materials: ε scalar
$\mu_r = 1$

✳Loss-less dielectrics: ε real

Dielectric photonic crystals

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

$$\varepsilon\left(\vec{r}+\vec{T}\right)=\varepsilon\left(\vec{r}\right)$$

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

Propagation equations

$$\begin{aligned}\nabla \cdot \mathbf{E} &= 0\\ \nabla \times \mathbf{H} - \varepsilon_0 \varepsilon(\mathbf{r}) \frac{\partial \mathbf{E}}{\partial t} &= 0\\ \nabla \cdot \mathbf{H} &= 0\\ \nabla \times \mathbf{E} + \frac{\partial \mathbf{H}}{\partial t} &= 0\end{aligned}$$

for harmonic fields :

$$\mathbf{H}(\mathbf{r},t) = \mathbf{H}(\mathbf{r}) e^{j\omega t}$$
$$\mathbf{E}(\mathbf{r},t) = \mathbf{E}(\mathbf{r}) e^{j\omega t}$$

$$\nabla \times \mathbf{H}(\mathbf{r}) - j\omega\varepsilon_0\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) = 0$$
$$\nabla \times \mathbf{E}(\mathbf{r}) + j\omega\mu_0\mathbf{H}(\mathbf{r}) = 0$$

E-field equation

after elimination of H

$$\hat{\Xi}\,\mathbf{E}_\omega(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{E}_\omega(\mathbf{r}) \quad \textbf{avec} \quad \hat{\Xi} = \frac{1}{\varepsilon(\mathbf{r})}\nabla\times\nabla\times$$

H-field equation

or after elimination of E

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

Field equation as an eigenvalues equation

$$\hat{\Xi}\,\mathbf{E}_\omega(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{E}_\omega(\mathbf{r})$$

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

eigenvalue $(\omega/c)^2$

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

but *not* for the E-operator : $\hat{\Xi} = \frac{1}{\varepsilon(\mathbf{r})}\nabla \times \nabla\times$

Hermiticity of the field operator

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

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

using : $\nabla(a\wedge b) = b.\nabla\wedge a - a.\nabla\wedge b$

and notice that the integrals of a gradient car 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 :

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

Using *this* inner product, both operators

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

are Hermitian

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

(same kind of tedious proof)

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

For a more detailed discussion, see lecture notes from S. G. Johnson: http://ocw.mit.edu/courses/mathematics/18-369-mathematical-methods-in-nanophotonics-spring-2008/readings/wave_equations.pdf

Scaling laws

In contrast to electrons in solids, there is no fundamental length scale in Maxwell equations

If the dielectric map ε is expanded or contracted by a factor s : $\varepsilon'(\mathbf{r}) = \varepsilon(\mathbf{r}/s) = \varepsilon(\mathbf{r}')$

Solutions of : $$\nabla \times \frac{1}{\varepsilon(\mathbf{r})} \nabla \times \mathbf{H}_\omega(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}_\omega(\mathbf{r})$$

become : $$\nabla' \times \frac{1}{\varepsilon(\frac{\mathbf{r}}{s})} \nabla' \times \mathbf{H}_\omega\left(\frac{\mathbf{r}}{s}\right) = \left(\frac{\omega}{c \cdot s}\right)^2 \mathbf{H}_\omega\left(\frac{\mathbf{r}}{s}\right)$$

$$\mathbf{H}(\mathbf{r})' = \mathbf{H}(\mathbf{r}/s) \qquad \omega' = \omega / s$$

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

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

and further wavevector : (in a couple of slides) $\tilde{k} = \dfrac{ka}{2\pi}$

a : paramètre de maille

Scaling laws

2^{nd} scaling law on the dielectric constant :

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

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

Field map and wavevector are unchanged

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

Scaling laws

Spatial homothety	Homothety on ε
$r \to r' = r.s$ $\varepsilon(r) \to \varepsilon(r')$ $k \to k' = k/s$ $\omega \to \omega' = \dfrac{\omega}{s}$ $H(r) \to H(r') \quad idem \quad E(r), B(r), D(r)$	$r \to r$ $\varepsilon(r) \to \varepsilon(r)\, s^2$ $k \to k$ $\omega \to \omega' = \dfrac{\omega}{s}$ $H(r) \to H(r) \quad idem \quad E(r), B(r), D(r)$

Floquet-Bloch theorem

Exactly like in solid state physics

Periodicity of ε allows to look for solutions on the form :

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

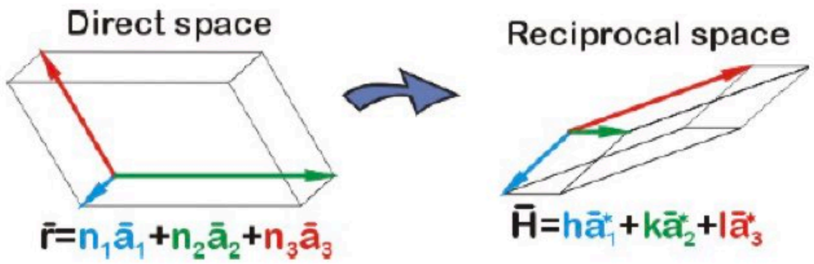
with $u_k(r)$ function with the same periodicity and symmetries as ε

$$\varepsilon\left(\vec{r} + \vec{T}\right) = \varepsilon(\vec{r}) \quad \text{then} \quad u_k\left(\vec{r} + \vec{T}\right) = u_k(\vec{r})$$

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

with k, wavevector, vector of the reciprocal space

Reminder, reciprocal space and Brillouin zones



$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

$$\vec{a}_i \bullet \vec{a}_j{}^* = 2\pi\delta_{ij}$$

Real (direct) space — Reciprocal space

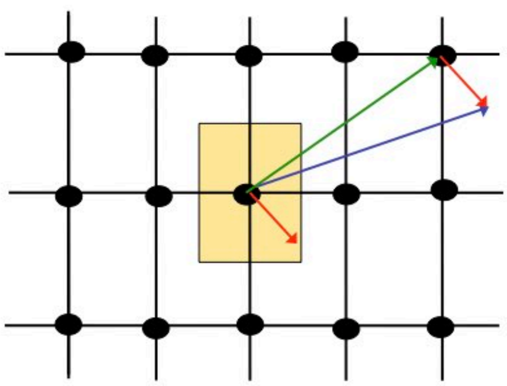
dimension of r is a length
dimension of h is a wavevector (inverse of a length)

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

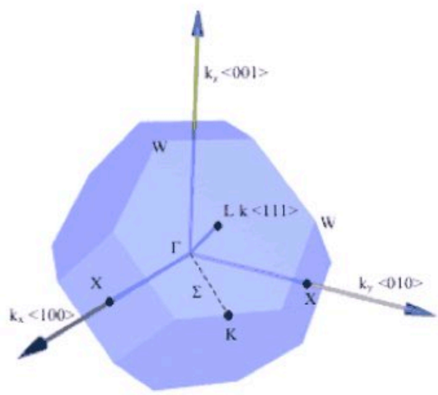
Reminder, reciprocal space and Brillouin zones

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



Case of the zinc-blende structure

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

Eigenvalues equation with u_k

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

with : $H_k(r) = u_k(r)\, e^{ikr}$ et $\hat{\Theta} = \nabla \times \left[\frac{1}{\varepsilon(\mathbf{r})}\nabla\times\right.$

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, ω'= ω/s et k'=k/s

reduced units $\tilde{k} = \frac{ka}{2\pi}$

Band structure
Dispersion diagram

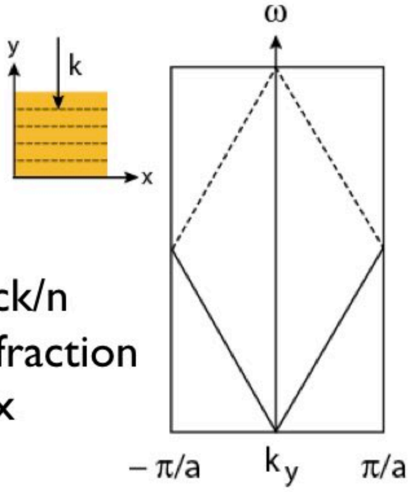
r: real space lattice
k: wavevector, reciprocal space
n: integer, 1, 2, 3 ...

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

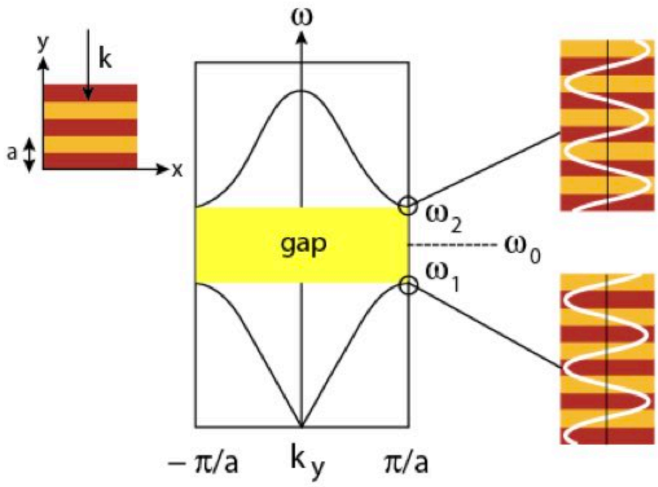
Free space



$\omega = ck/n$

n: refraction index

Coupled modes



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

Air band and dielectric band

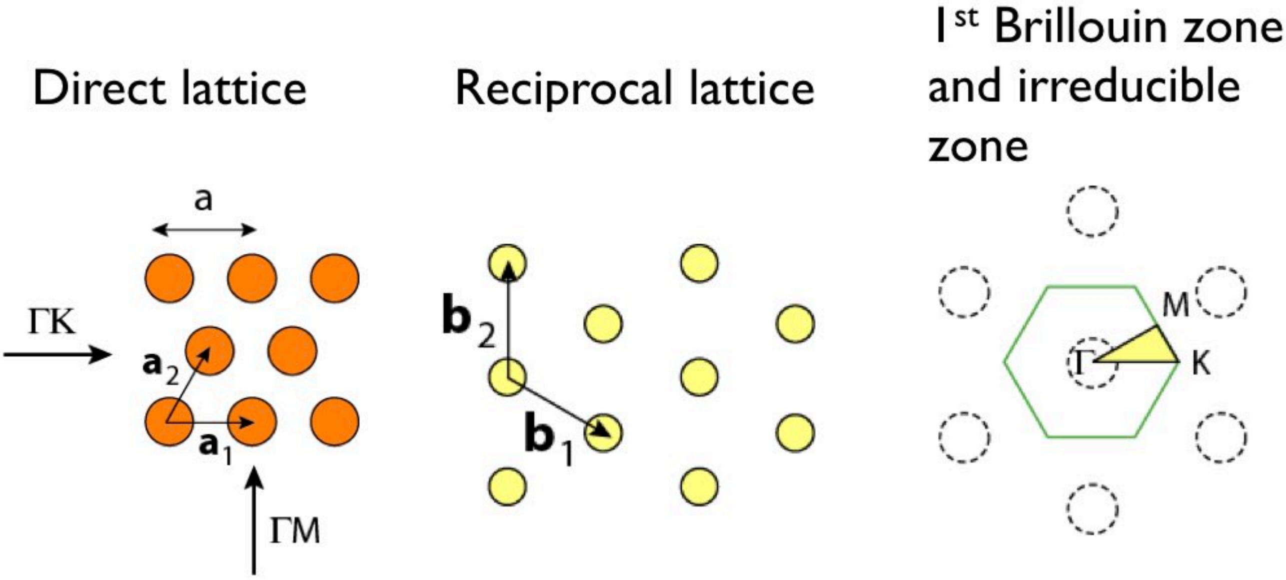
As a general rule, it can be shown that the electric displacement field D of high symmetry states is concentrated either in *high* or *low* index regions

Dielectric band — Air band

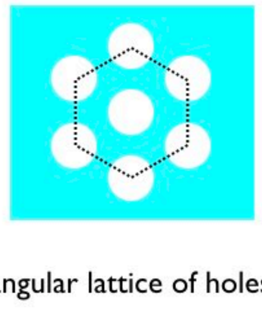
The fundamental state maximise the field overlap with the high index dielectric, the next state, in order to ensure orthogonality minimise the overlap

Note: for a demonstration, refer for example to : Photonic crystals : molding the flow of light / John D. Joannopoulos, Robert D. Meade, Joshua N. Winn, Princeton, New Jersey : Princeton University Press, pages 16-17

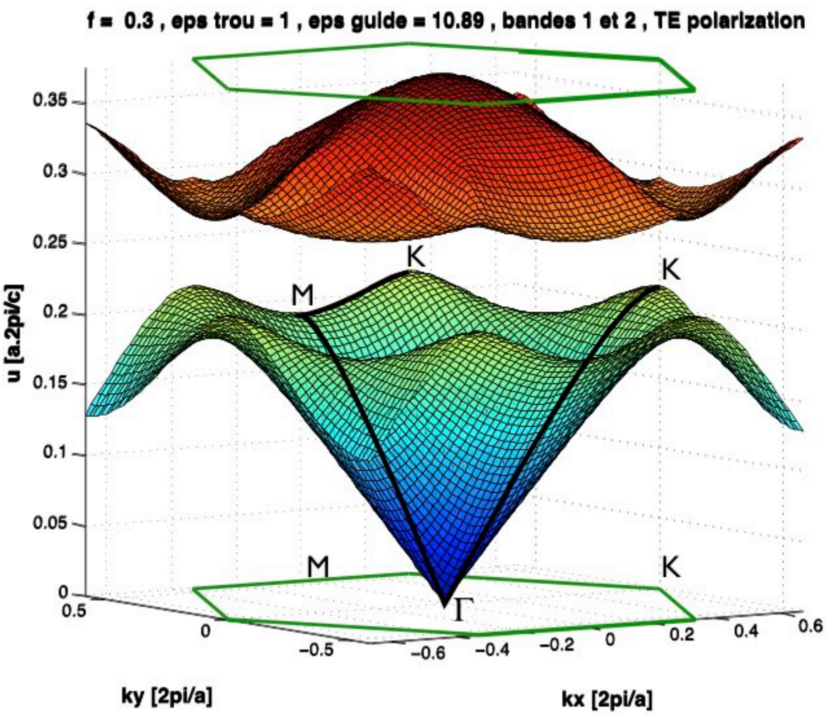
Band structure
Dispersion diagram
Examples : Two dimensions 2D



Band structure
Dispersion diagram

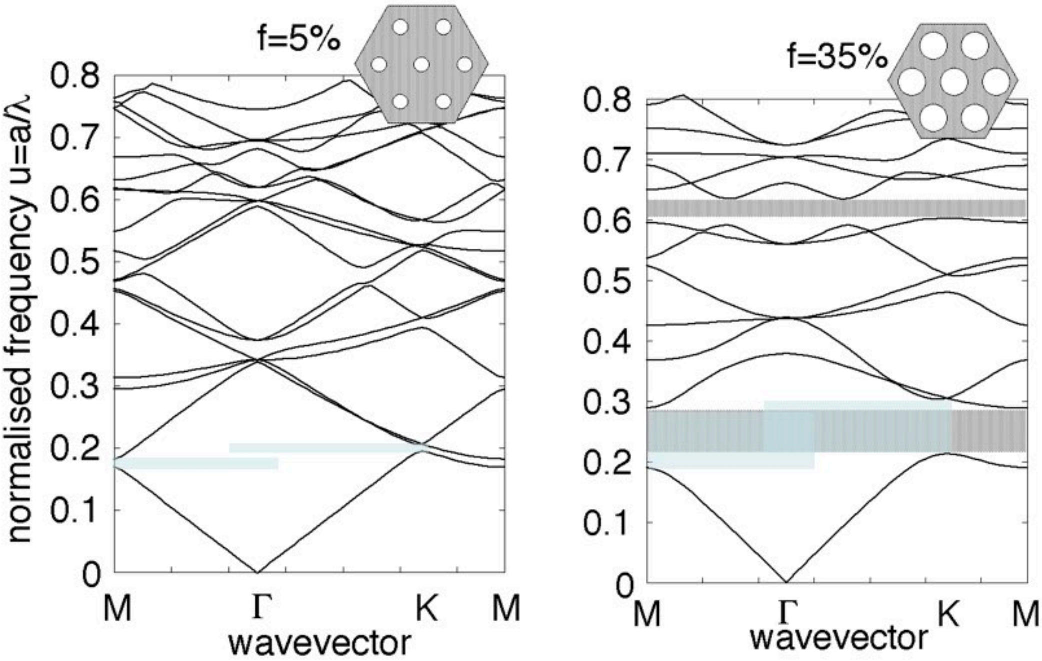


Triangular lattice of holes



Band structure
Dispersion diagram
Examples : Two dimensions 2D

TE



Band structure
Dispersion diagram

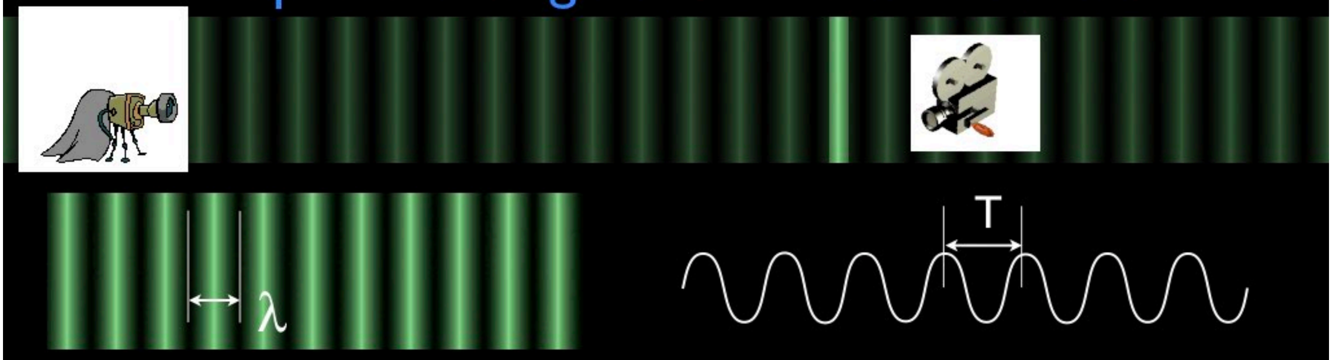
Two important conclusions :

✳The forbidden bands in different directions do not necessarily overlap

✳The forbidden bands for both polarisations do not necessarily overlap

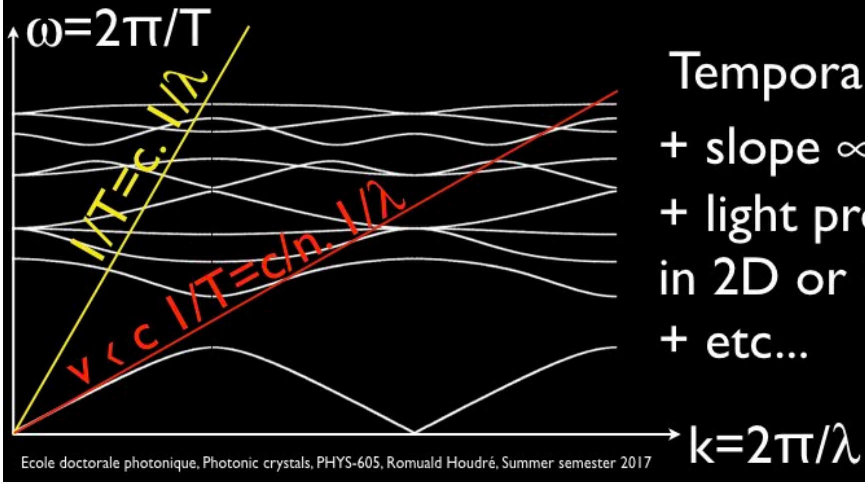
As a consequence : Full forbidden bands will exist only for specific structures and sufficient index contrast

Dispersion diagram : what is it about ?



spatial periodicity → spatial frequency

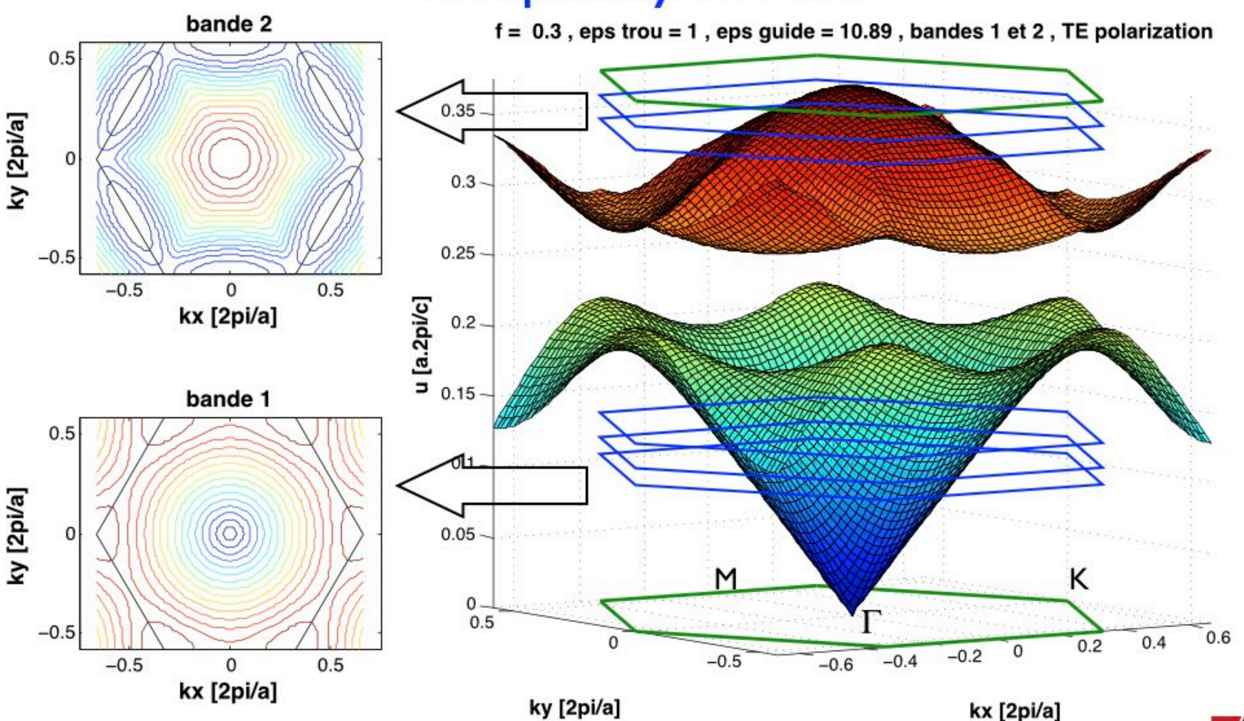
temporal frequency



Temporal *vs.* spatial aspects

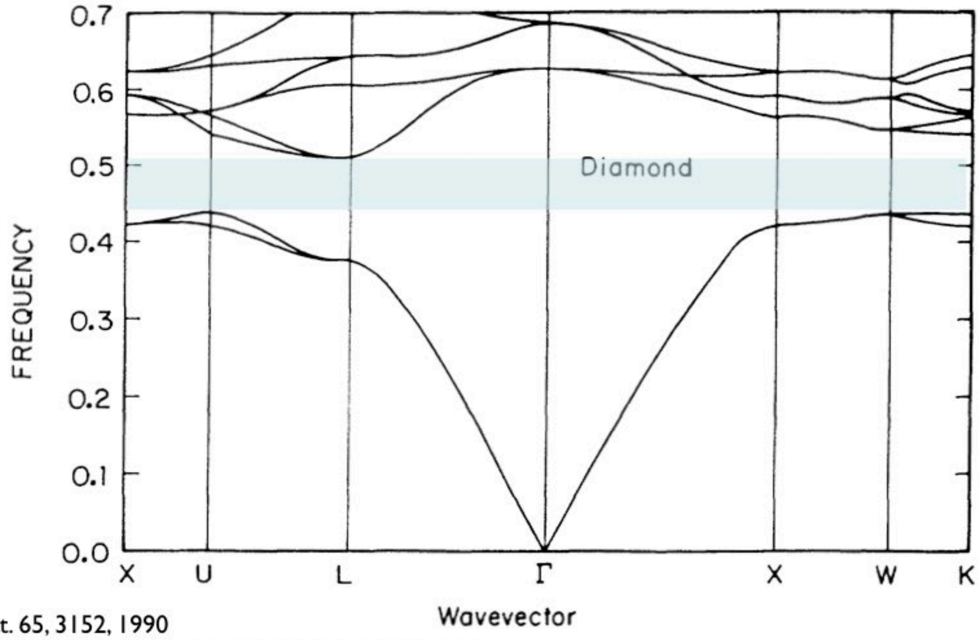
+ slope ∝ group velocity
+ light propagation direction in 2D or 3D representation
+ etc...

Band structure Dispersion diagram and equi-frequency curves



Band structure
Dispersion diagram
Examples : Three dimensions 3D

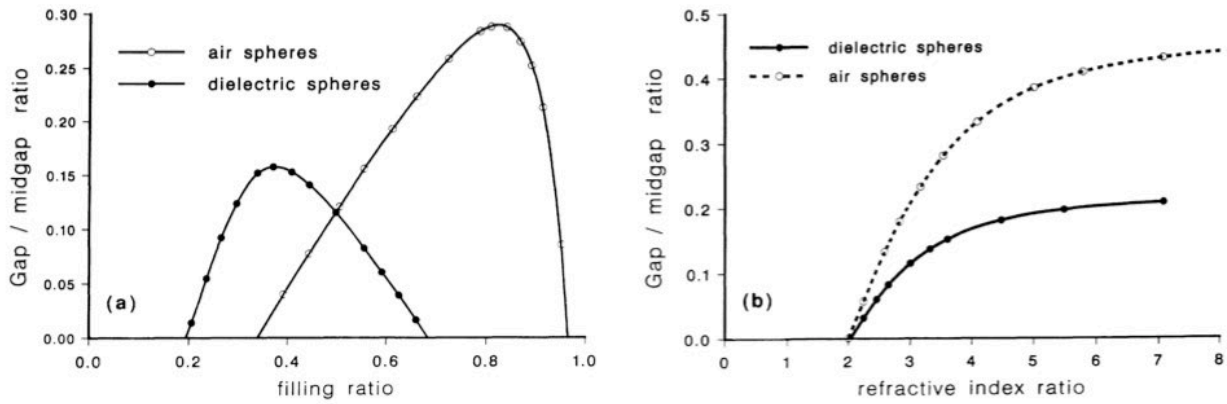
Stacking of dielectric spheres with a diamond structure



Phys. Rev. Lett. 65, 3152, 1990

Band structure
Dispersion diagram
Examples : Three dimensions 3D

Stacking of dielectric spheres with a diamond structure



Threshold on filling factor

Threshold on index contrast

Phys. Rev. Lett. 65, 3152, 1990

Band structure computation
Plane wave expansion method

Eigenvalue equations on u_k :

$$\hat{\Theta}\mathbf{H}_\omega(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}_\omega(\mathbf{r}) \qquad \hat{\Theta} = \nabla \times \left[\frac{1}{\varepsilon(\mathbf{r})}\nabla\times\right.$$

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), ε(r) or 1/ε(r)

$E(r) = \sum_{G \in \text{réseau réciproque}} E_G \; e^{i(k+G)r}$	$H(r) = \sum_{G \in \text{réseau réciproque}} H_G \; e^{i(k+G)r}$
$\varepsilon(r) = \sum_{G \in \text{réseau réciproque}} \varepsilon_G \; e^{iGr}$	$\varepsilon(r)^{-1} = \sum_{G \in \text{réseau réciproque}} \varepsilon_G^{-1} \; e^{iGr}$

Note : Réseau réciproque = reciprocal lattice in French

Note : variables ω and k are omitted in $E_\omega(r)$ and E^k_G

in order to write $\hat{\Theta}\mathbf{H}_\omega(\mathbf{r}) = \left(\frac{\omega}{c}\right)^2 \mathbf{H}_\omega(\mathbf{r})$

as a matrix eigenvalue equation :

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

$$\left[M^k_{G_n,G_m}\right]\left[H^k_m\right] = \left(\frac{\omega_k}{c}\right)^2\left[H^k_m\right]$$

Plane wave expansion method

More technically : $\nabla H = 0$ implies transversality of H

H(r) can be written : $H(r) = \sum_{G' \in \text{réseau réciproque}} \left(h_{1,G'} \vec{u}_{1,G'} + h_{2,G'} \vec{u}_{2,G'} \right) e^{i(k+G')r}$

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

$$\nabla \wedge H = \sum_{G' \in R.R.} i \left| k + G' \right| \left(h_{1,G'} \vec{u}_{2,G'} - h_{2,G'} \vec{u}_{1,G'} \right) e^{i(k+G')r}$$

$$\varepsilon(r)^{-1} = \sum_{G'' \in R.R.} \varepsilon_{G''}^{-1} e^{iG''r}$$

$$\varepsilon(r)^{-1} \nabla \wedge H = i \sum_{G',G'' \in R.R.} \varepsilon_{G''}^{-1} \left| k + G' \right| \left(h_{1,G'} \vec{u}_{2,G'} - h_{2,G'} \vec{u}_{1,G'} \right) e^{i(k+G'+G'')r}$$

which is more convenient to write with G=G'+G"

$$\varepsilon(r)^{-1} \nabla \wedge H = i \sum_{G,G' \in R.R.} \varepsilon_{G-G'}^{-1} \left| k + G' \right| \left(h_{1,G'} \vec{u}_{2,G'} - h_{2,G'} \vec{u}_{1,G'} \right) e^{i(k+G)r}$$

Plane wave expansion method

after the second curl :

$$\nabla \wedge \varepsilon(r)^{-1} \nabla \wedge H = \sum_{G,G' \in R.R.} \varepsilon_{G-G'}^{-1} \left| k + G' \right| \left| k + G \right| \begin{bmatrix} \vec{u}_{2,G} . \vec{u}_{2,G'} & -\vec{u}_{2,G} . \vec{u}_{1,G'} \\ -\vec{u}_{1,G} . \vec{u}_{2,G'} & \vec{u}_{1,G} . \vec{u}_{1,G'} \end{bmatrix} \begin{bmatrix} h_{1,G'} \\ h_{2,G'} \end{bmatrix} e^{i(k+G)r}$$

$$\nabla \wedge \varepsilon(r)^{-1} \nabla \wedge H = \left(\frac{\omega_k}{c} \right)^2 H = \left(\frac{\omega_k}{c} \right)^2 \sum_{G \in R.R.} H_G e^{i(k+G)r}$$

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

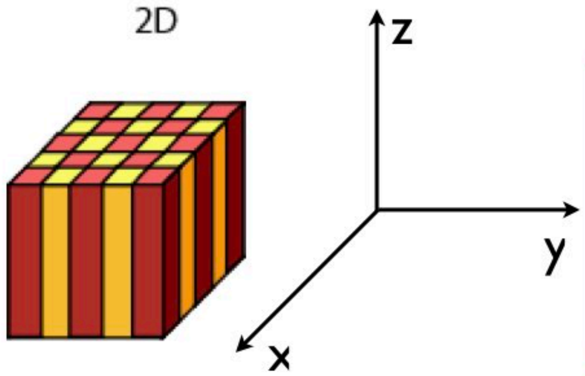
$$\left\{ \sum_{G' \in R.R.} \varepsilon_{G-G'}^{-1} \left| k + G' \right| \left| k + G \right| \begin{bmatrix} \vec{u}_{2,G} . \vec{u}_{2,G'} & -\vec{u}_{2,G} . \vec{u}_{1,G'} \\ -\vec{u}_{1,G} . \vec{u}_{2,G'} & \vec{u}_{1,G} . \vec{u}_{1,G'} \end{bmatrix} \begin{bmatrix} h_{1,G'} \\ h_{2,G'} \end{bmatrix}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

which, we will limit to m vectors of the reciprocal lattice. The equation reduces to a diagonalisation problem of a 2mX2m 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

$$\nabla \times \mathbf{H}(\mathbf{r}) - j\omega\varepsilon_0\varepsilon(\mathbf{r})\mathbf{E}(\mathbf{r}) = 0$$
$$\nabla \times \mathbf{E}(\mathbf{r}) + j\omega\mu_0\mathbf{H}(\mathbf{r}) = 0$$

link H_z with E_x,E_Y and E_z with H_x,H_Y (z-derivatives vanish)

Field equations on H_z and E_z are decoupled :

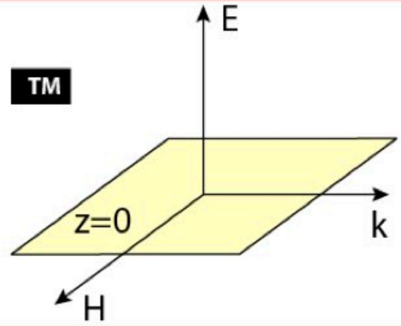
$$\frac{1}{\varepsilon(x,y)}\nabla^2 E_z = -\left(\frac{\omega}{c}\right)^2 E_z \quad \nabla\left(\frac{1}{\varepsilon(x,y)}\nabla H_z\right) = -\left(\frac{\omega}{c}\right)^2 H_z$$

Plane wave expansion method
2D systems
TE and TM polarisations

Two independent polarization :

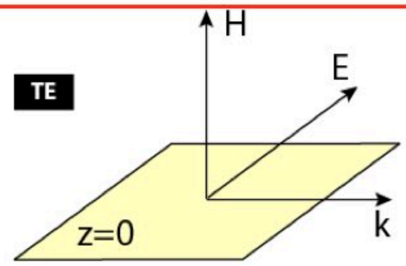
$H_z=0, E_z \neq 0$ TM ou s

Transverse mode for E
H in the perpendicular plane



$H_z \neq 0, E_z=0$ TE ou p

Transverse mode for H
E in the perpendicular plane



Note: TE and TM polarization

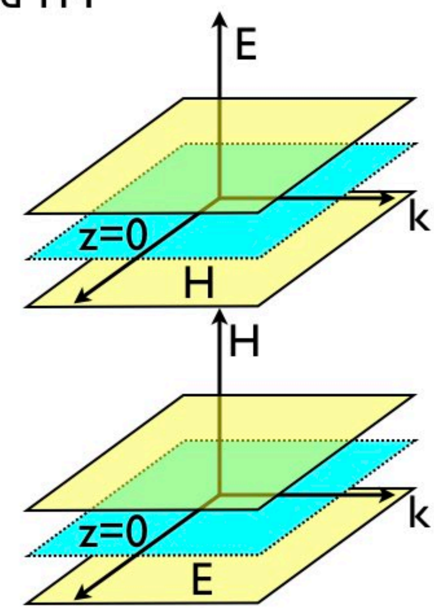
In the case of a planar waveguide with a mirror symmetry, it is still possible to define even and odd modes and the field structure *in the mirror plane only* has a TE-like or TM-like structure. They are commonly, but improperly, still named TE and TM

$H_z(z=0)=0, E_z(z=0) \neq 0$ "TM" ou s

Transverse mode for E
H in the mirror plane

$H_z\ (z=0) \neq 0, E_z(z=0)=0$ "TE" ou p

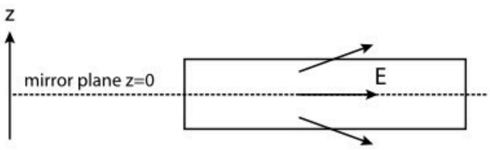
Transverse mode for H
E in the mirror plane

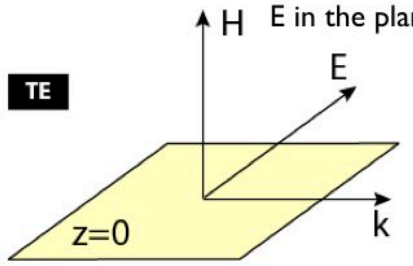


If there is no mirror symmetry,
TE and TM polarization can not be separated

Note: TE and TM polarization

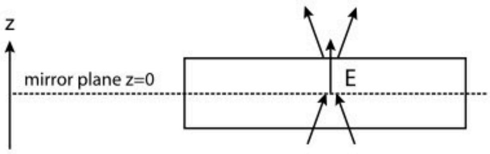
Polarization

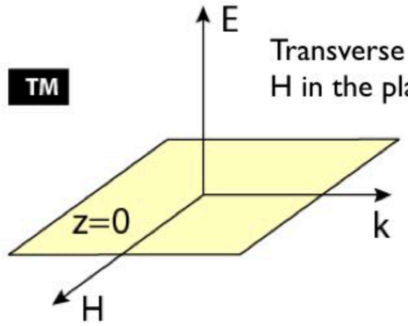




Transverse (to the mirror plane) H mode
E in the plane normal to H

Odd and even modes, abusively referred as TE and TM





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

Plane wave expansion method

after the second curl :

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

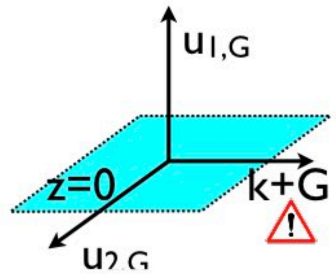
$$\nabla \wedge \varepsilon(r)^{-1} \nabla \wedge H = \left(\frac{\omega_k}{c}\right)^2 H = \left(\frac{\omega_k}{c}\right)^2 \sum_{G \in R.R.} H_G e^{i(k+G)r}$$

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

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

which, we will limit to m vectors of the reciprocal lattice. The equation reduces to a diagonalisation problem of a 2mX2m 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 $\{u_{1,G}, u_{2,G}, k+G\}$

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

writes :

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

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

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 x m hermitian matrix with eigenvalues $(\omega/c)^2$ and eigenvectors $\{H_G\}$

TM

$$\left[\begin{pmatrix} |\mathbf{k}+\mathbf{G}_1|\cdot|\mathbf{k}+\mathbf{G}_1| & \cdots & |\mathbf{k}+\mathbf{G}_1|\cdot|\mathbf{k}+\mathbf{G}_m| & \cdots & |\mathbf{k}+\mathbf{G}_1|\cdot|\mathbf{k}+\mathbf{G}_N| \\ \vdots & \ddots & \vdots & & \vdots \\ |\mathbf{k}+\mathbf{G}_n|\cdot|\mathbf{k}+\mathbf{G}_1| & \cdots & |\mathbf{k}+\mathbf{G}_n|\cdot|\mathbf{k}+\mathbf{G}_m| & \cdots & |\mathbf{k}+\mathbf{G}_n|\cdot|\mathbf{k}+\mathbf{G}_N| \\ \vdots & & \vdots & \ddots & \vdots \\ |\mathbf{k}+\mathbf{G}_N|\cdot|\mathbf{k}+\mathbf{G}_1| & \cdots & |\mathbf{k}+\mathbf{G}_N|\cdot|\mathbf{k}+\mathbf{G}_m| & \cdots & |\mathbf{k}+\mathbf{G}_N|\cdot|\mathbf{k}+\mathbf{G}_N| \end{pmatrix} \begin{pmatrix} \hat{\kappa}(\mathbf{G}_1-\mathbf{G}_1) & \cdots & \hat{\kappa}(\mathbf{G}_1-\mathbf{G}_m) & \cdots & \hat{\kappa}(\mathbf{G}_1-\mathbf{G}_N) \\ \vdots & \ddots & \vdots & & \vdots \\ \hat{\kappa}(\mathbf{G}_n-\mathbf{G}_1) & \cdots & \hat{\kappa}(\mathbf{G}_n-\mathbf{G}_m) & \cdots & \hat{\kappa}(\mathbf{G}_n-\mathbf{G}_N) \\ \vdots & & \vdots & \ddots & \vdots \\ \hat{\kappa}(\mathbf{G}_N-\mathbf{G}_1) & \cdots & \hat{\kappa}(\mathbf{G}_N-\mathbf{G}_m) & \cdots & \hat{\kappa}(\mathbf{G}_N-\mathbf{G}_N) \end{pmatrix}\right] \cdot \begin{pmatrix} C_1 \\ \vdots \\ C_n \\ \vdots \\ C_N \end{pmatrix} = \frac{\omega^2}{c^2} \begin{pmatrix} C_1 \\ \vdots \\ C_n \\ \vdots \\ C_N \end{pmatrix}$$

$$\hat{\kappa}(x,y) = \frac{1}{\varepsilon(x,y)}$$

Plane wave expansion method
2D systems

TE : $h_{2G}=0$ for any G and $u_{1,G}.\,u_{2,G'}=0$

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')

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

writes :

TE

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

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 x m hermitian matrix with eigenvalues $(\omega/c)^2$ and eigenvectors $\{H_G\}$

TE

$$\left[\begin{pmatrix}(\mathbf{k}+\mathbf{G}_1)\cdot(\mathbf{k}+\mathbf{G}_1) & \cdots & (\mathbf{k}+\mathbf{G}_1)\cdot(\mathbf{k}+\mathbf{G}_m) & \cdots & (\mathbf{k}+\mathbf{G}_1)\cdot(\mathbf{k}+\mathbf{G}_N)\\ \vdots & \ddots & \vdots & & \vdots\\ (\mathbf{k}+\mathbf{G}_n)\cdot(\mathbf{k}+\mathbf{G}_1) & \cdots & (\mathbf{k}+\mathbf{G}_n)\cdot(\mathbf{k}+\mathbf{G}_m) & \cdots & (\mathbf{k}+\mathbf{G}_n)\cdot(\mathbf{k}+\mathbf{G}_N)\\ \vdots & & \vdots & \ddots & \vdots\\ (\mathbf{k}+\mathbf{G}_N)\cdot(\mathbf{k}+\mathbf{G}_1) & \cdots & (\mathbf{k}+\mathbf{G}_N)\cdot(\mathbf{k}+\mathbf{G}_m) & \cdots & (\mathbf{k}+\mathbf{G}_N)\cdot(\mathbf{k}+\mathbf{G}_N)\end{pmatrix}\begin{pmatrix}\hat{\kappa}(\mathbf{G}_1-\mathbf{G}_1) & \cdots & \hat{\kappa}(\mathbf{G}_1-\mathbf{G}_m) & \cdots & \hat{\kappa}(\mathbf{G}_1-\mathbf{G}_N)\\ \vdots & \ddots & \vdots & & \vdots\\ \hat{\kappa}(\mathbf{G}_n-\mathbf{G}_1) & \cdots & \hat{\kappa}(\mathbf{G}_n-\mathbf{G}_m) & \cdots & \hat{\kappa}(\mathbf{G}_n-\mathbf{G}_N)\\ \vdots & & \vdots & \ddots & \vdots\\ \hat{\kappa}(\mathbf{G}_N-\mathbf{G}_1) & \cdots & \hat{\kappa}(\mathbf{G}_N-\mathbf{G}_m) & \cdots & \hat{\kappa}(\mathbf{G}_N-\mathbf{G}_N)\end{pmatrix}\right]\cdot\begin{pmatrix}A_1\\ \vdots\\ A_n\\ \vdots\\ A_N\end{pmatrix}=\frac{\omega^2}{c^2}\begin{pmatrix}A_1\\ \vdots\\ A_n\\ \vdots\\ A_N\end{pmatrix}$$

$$\hat{\kappa}(x,y)=\frac{1}{\varepsilon(x,y)}$$

Plane wave expansion method
2D systems

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

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

which leads to :

$$\text{"TE"} \quad \sum_n H_n (k+G_m).(k+G_m)\varepsilon^{-1}_{G_m-G_n} = \left(\frac{\omega}{c}\right)^2 H_n \quad \forall G_m \in R.R.$$

$$\text{"TM"} \quad \sum_n E_n (k+G_n).(k+G_m)\varepsilon^{-1}_{G_m-G_n} = \left(\frac{\omega}{c}\right)^2 E_n \quad \forall G_m \in R.R.$$

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

$$C_m = |k+G_m| E_m$$

$$\text{"TM"} \quad \sum_n C_n |k+G_m||k+G_n| \varepsilon^{-1}_{G_m-G_n} = \left(\frac{\omega}{c}\right)^2 C_n \quad \forall G_m \in R.R.$$

Plane wave expansion method
2D systems

A last technical effort before a pause

---

remains the computation of the Fourier transform of 1/ε(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 examples for circular pillars or holes :

$$\varepsilon(G) = \varepsilon_a \delta_{G,0} + (\varepsilon_a - \varepsilon_b) \frac{2\pi R^2}{S_{cellule}} \frac{J_1(|G|R)}{|G|R}$$

where J_1 is a 1st order Bessel function
+ summation over the entire lattice

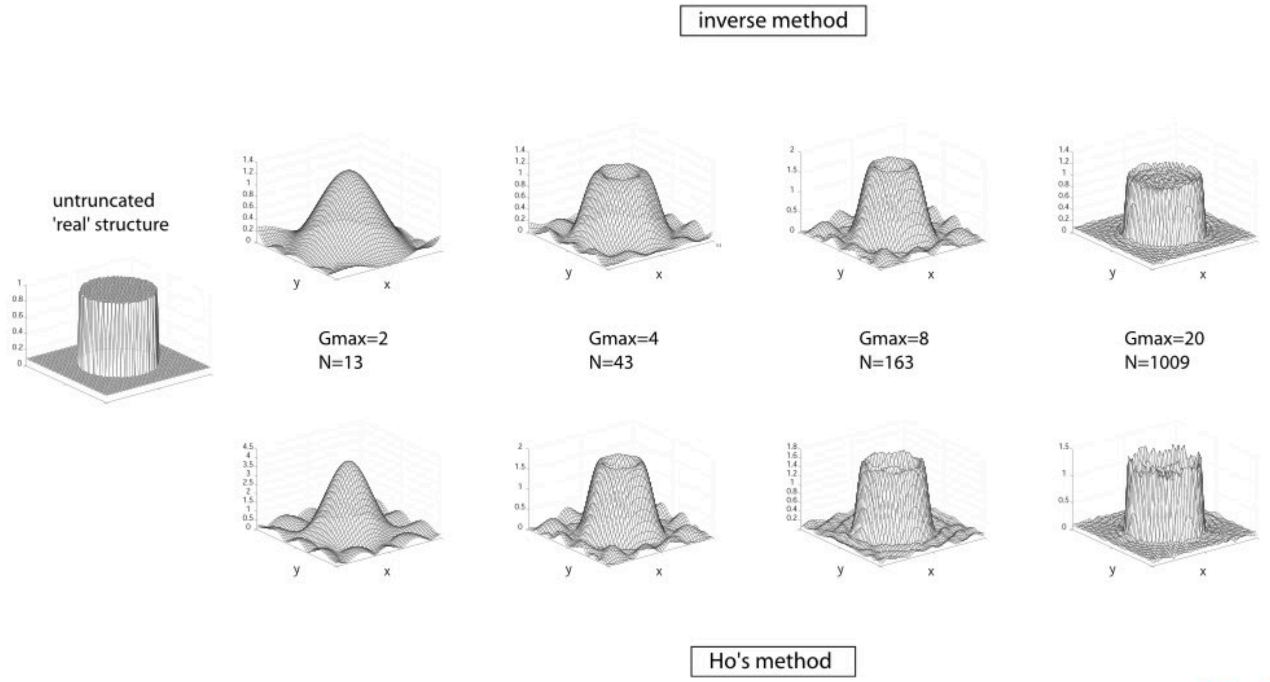
Plane wave expansion method
2D systems
Inverse method and Ho's method

As it was developed here, the formalism requires the Fourier transform of $1/\varepsilon$, it is also possible to use the Fourier transform of ε 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.

Step	Inverse method	Ho's method
✳1 Computation of the Fourier transform	$\varepsilon^{-1}(G)=TF(1/\varepsilon)$	$\varepsilon(G)=TF(\varepsilon)$
✳Truncation	$[\varepsilon^{-1}(G)]_N$	$[\varepsilon(G)]_N$
✳3 Inversion	-	$[\varepsilon^{-1}(G)]_{N, Ho}=[\varepsilon(G)]_N^{-1}$

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
2D systems
Inverse method and Ho's method



Plane wave expansion method limitations

✳2D & 3D

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

	2D	3D
Nb of plane waves per dimension	α	α
Nb of plane waves	α^2	α^3
Memory	$(\alpha^2)^2 = \alpha^4$	$(2\alpha^3)^2 = 4\alpha^6$
Computation time	$2(\alpha^2)^3 = 2\alpha^6$	$(2\alpha^3)^3 = 8\alpha^9$

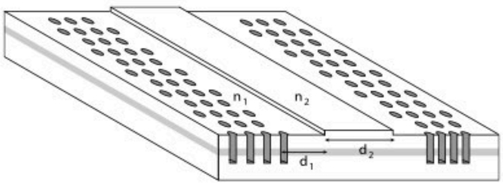
(2: polarisation cannot be decoupled)

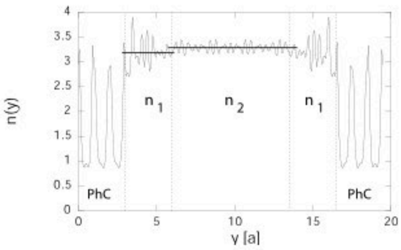
✳Losses, complex refractive index and dispersive medium or non-linear medium

lifetime (E+iγ), penetration depth (k+iρ), absorption (n+ik), $\varepsilon(\lambda)$ ...

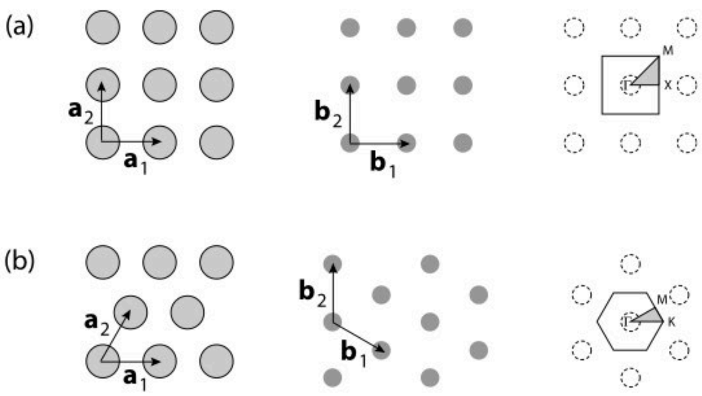
possible but delicate

✳Small and large index steps simultaneously





Bestiary of common 2D systems



$$|\Gamma X| = \frac{\pi}{a} \quad |\Gamma X|_{réduit} = \pm\frac{1}{2}$$

$$|\Gamma M| = \sqrt{2}\,\frac{\pi}{a} \quad |\Gamma M|_{réduit} = \pm\frac{\sqrt{2}}{2}$$

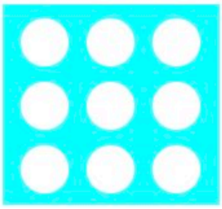
$$|\Gamma M| = 2\frac{\sqrt{3}}{3}\frac{\pi}{a} \quad |\Gamma M|_{réduit} = \pm\frac{\sqrt{3}}{3}$$

$$|\Gamma K| = \frac{4}{3}\frac{\pi}{a} \quad |\Gamma K|_{réduit} = \pm\frac{2}{3}$$

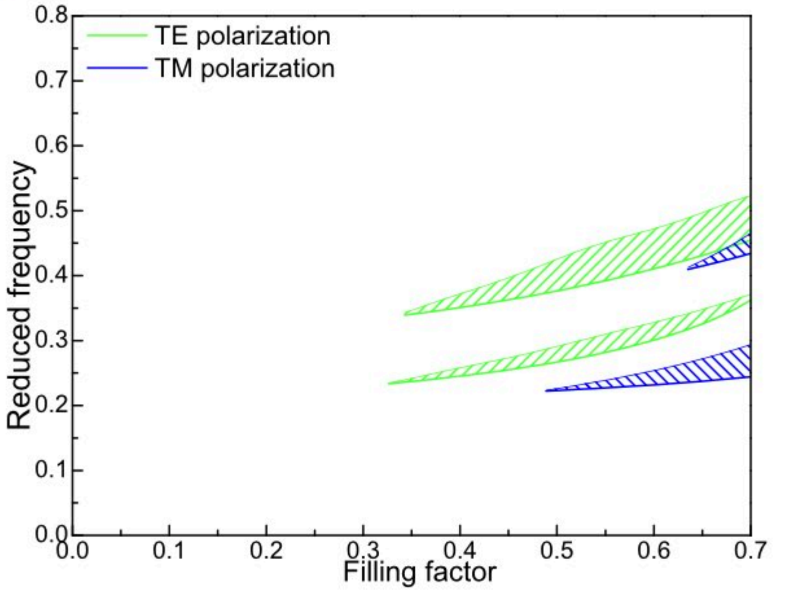
Attention : in contrast to intuition the modulus of ΓK is *not* π/a

	geometry	
	square lattice	triangular lattice
direct vectors	$\mathbf{a}_1 = (1,0);\ \mathbf{a}_2 = (0,1)$	$\mathbf{a}_1 = (1,0);\ \mathbf{a}_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$
reciprocal vectors	$\mathbf{b}_1 = \frac{2\pi}{a}(1,0);\ \mathbf{b}_2 = \frac{2\pi}{a}(0,1)$	$\mathbf{b}_1 = \frac{2\pi}{a}(1, -\frac{1}{3}\sqrt{3});\ \mathbf{b}_2 = \frac{2\pi}{a}(0, \frac{2}{3}\sqrt{3})$
f	$\frac{R^2\pi}{a^2}$	$\frac{2\pi}{\sqrt{3}}\frac{R^2}{a^2}$
unit cell surface	a^2	$\frac{\sqrt{3}}{2}a^2$

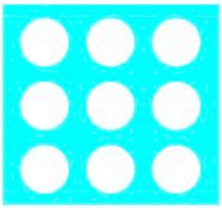
Bestiary of common 2D systems
Square lattice, holes



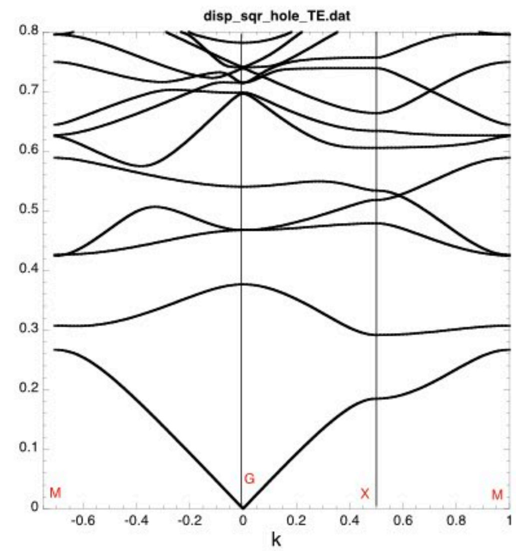
filling factor = f_{air}
n=3.36

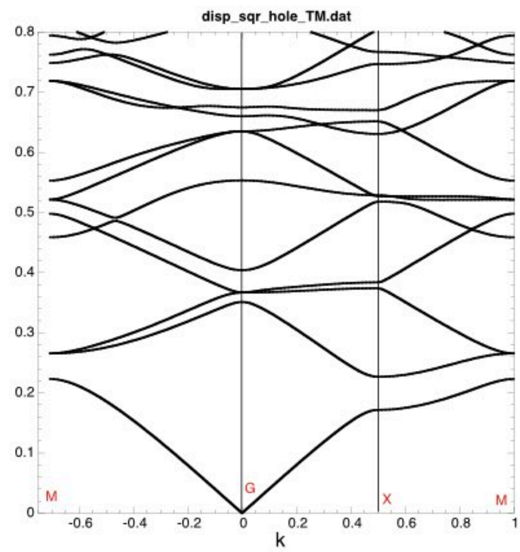


Bestiary of common 2D systems
Square lattice, holes



filling factor = f_{air} = 50 %
n=3.36



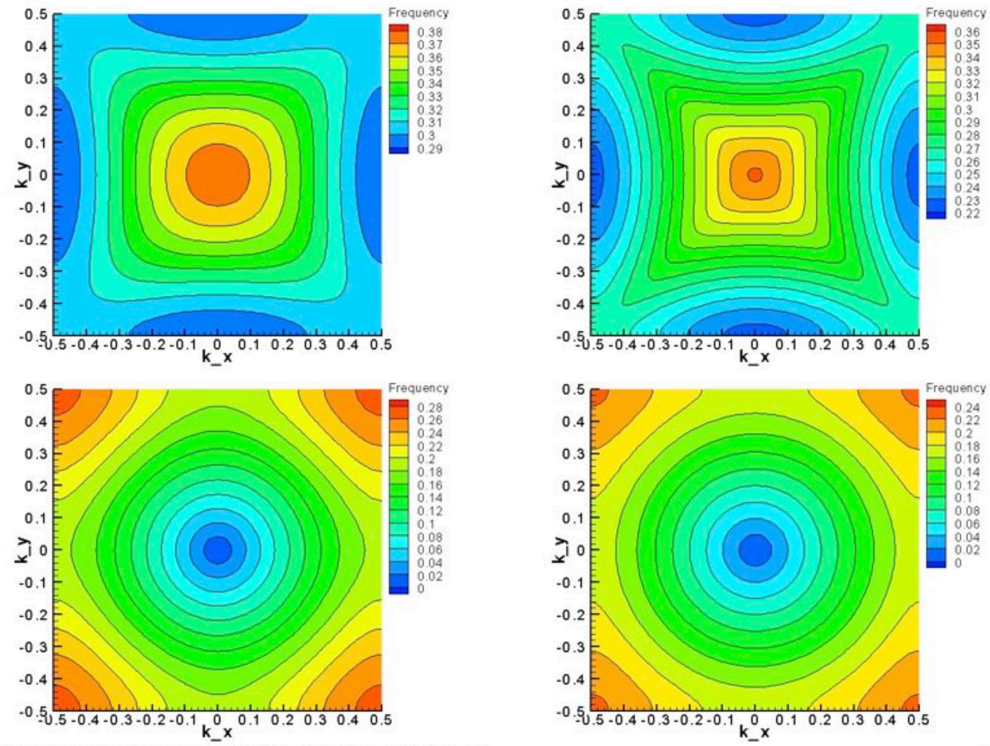


Bestiary of common 2D systems
Square lattice, holes

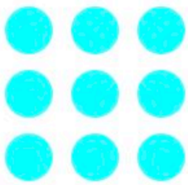
TE TM

2

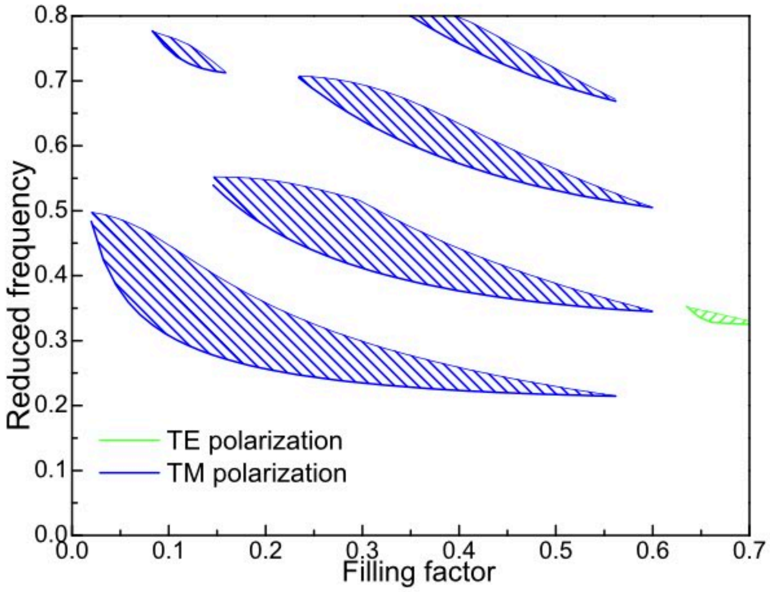
1



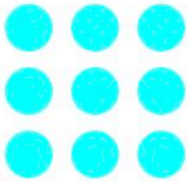
Bestiary of common 2D systems
Square lattice, pillars



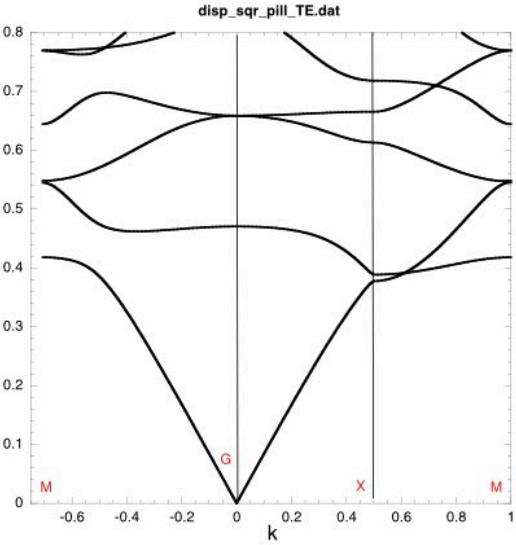
filling factor = f_{diel}
n=3.36

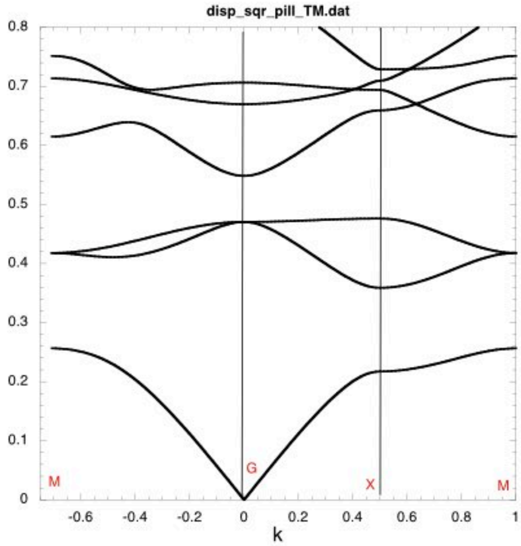


Bestiary of common 2D systems
Square lattice, pillars

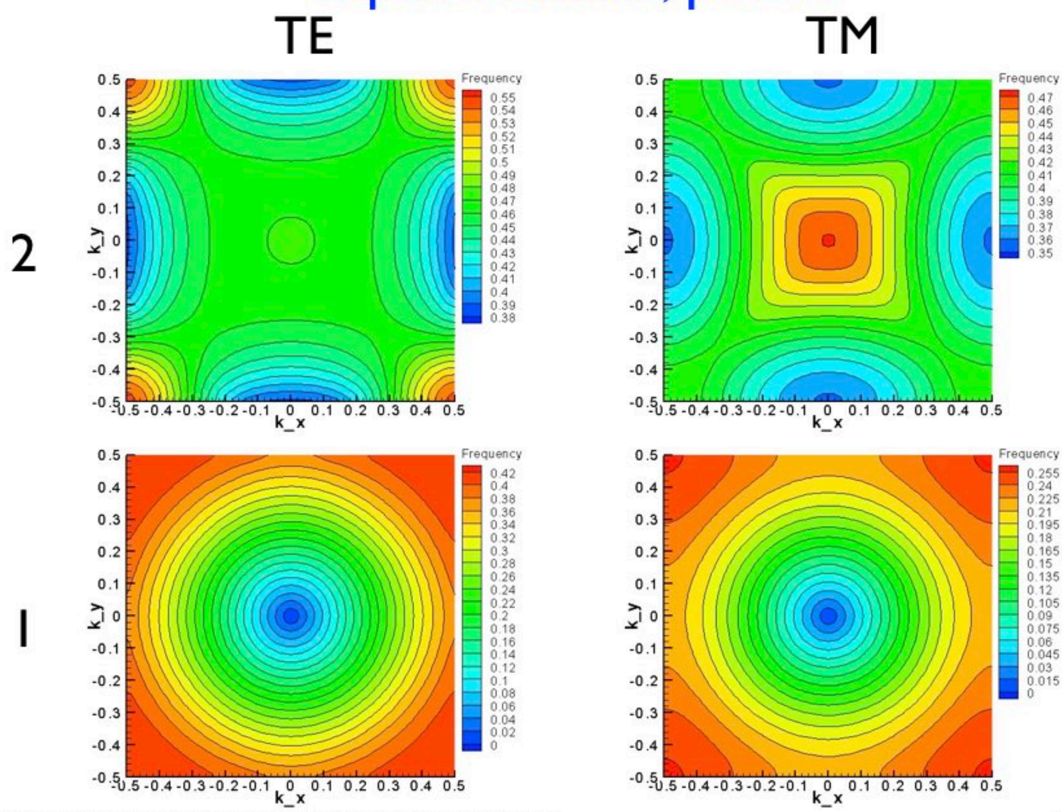


filling factor = f_{diel} = 20 %
n=3.36

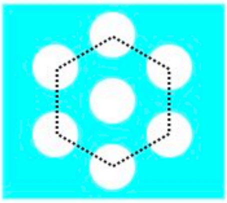




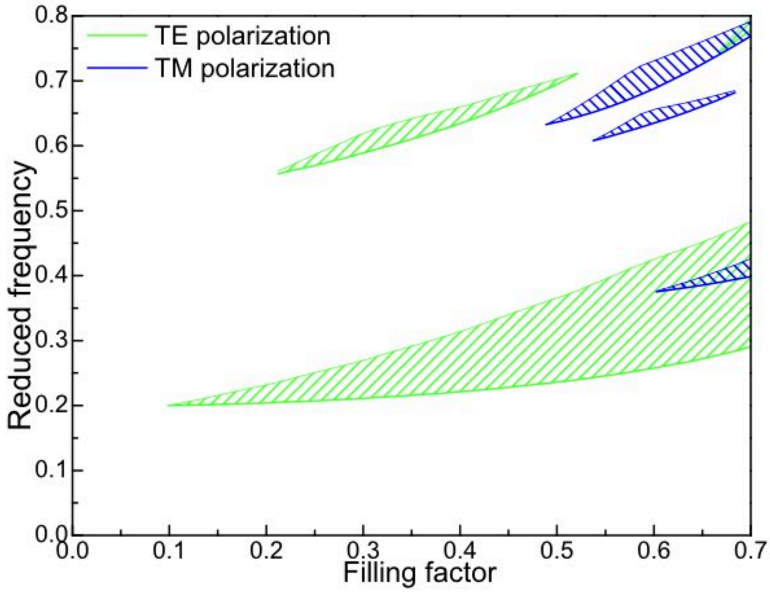
Bestiary of common 2D systems
Square lattice, pillars



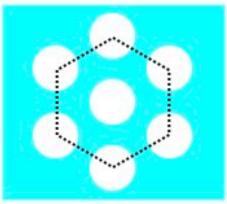
Bestiary of common 2D systems
Triangular lattice, holes



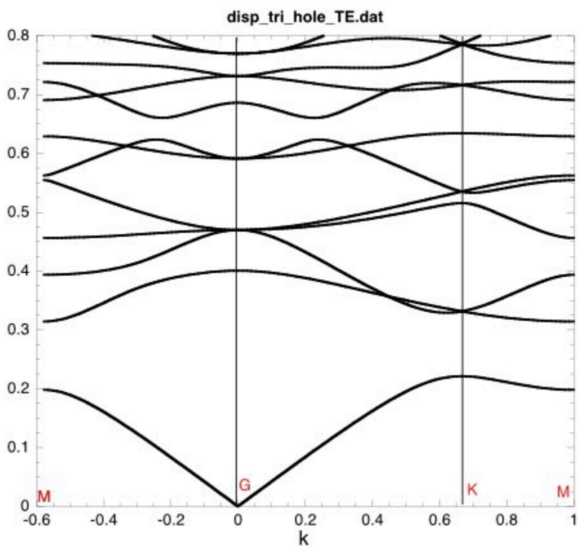
filling factor = f_{air}
n=3.36

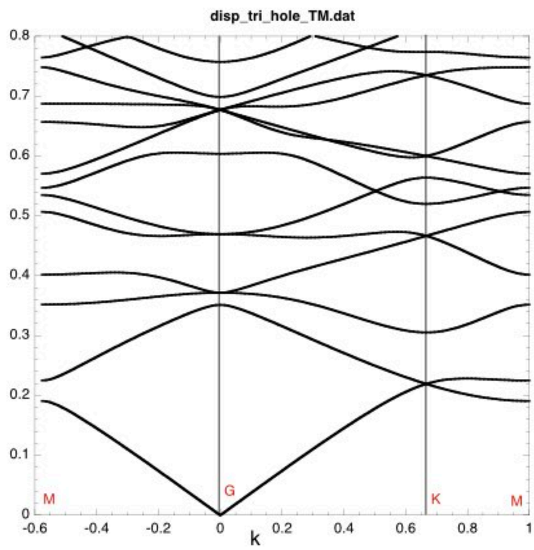


Bestiary of common 2D systems
Triangular lattice, holes



filling factor = f_{air} = 40 %
n=3.36



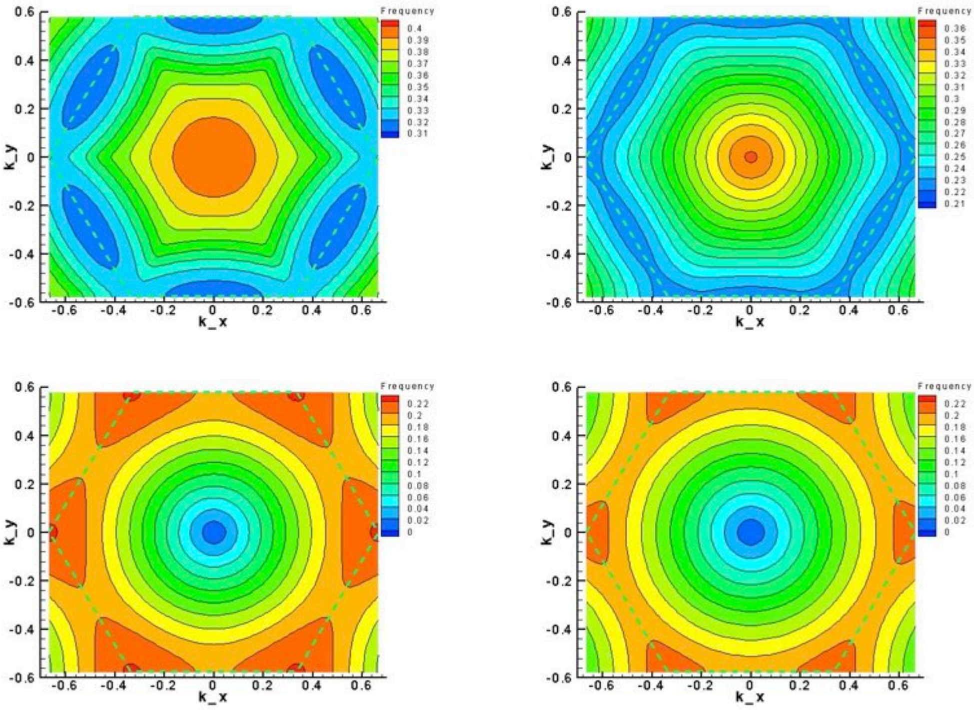


Bestiary of common 2D systems
Triangular lattice, holes

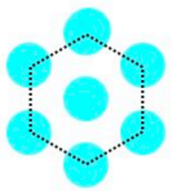
TE | TM

2

1

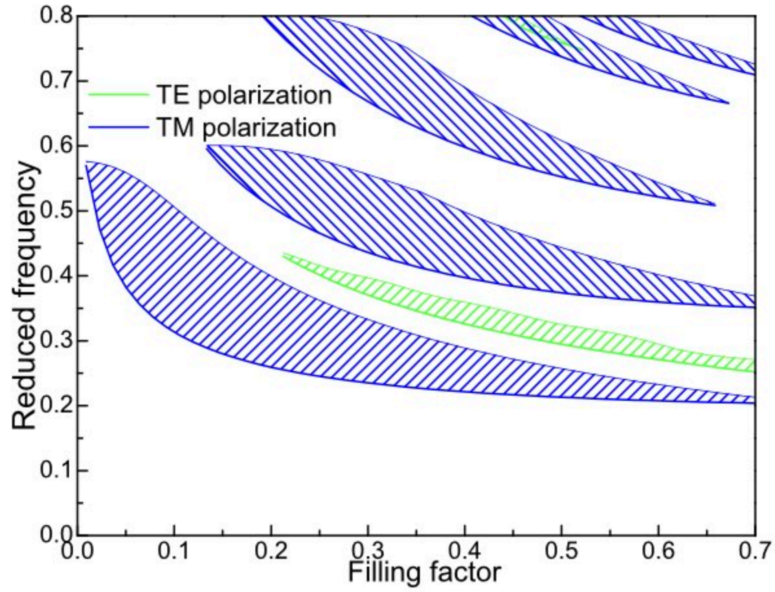


Bestiary of common 2D systems
Triangular lattice, pillars

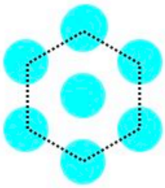


filling factor = f_{diel}

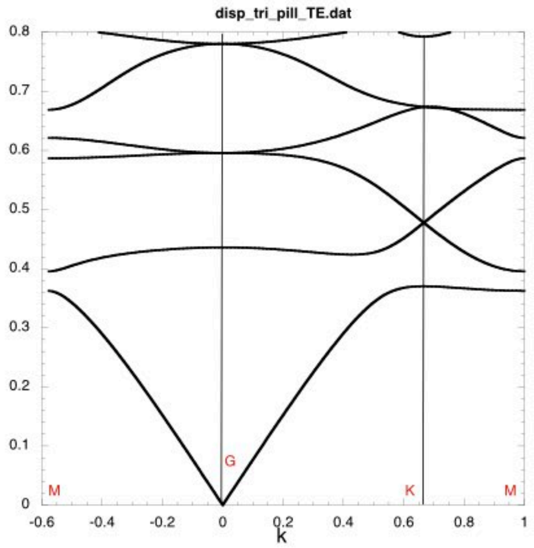
n=3.36

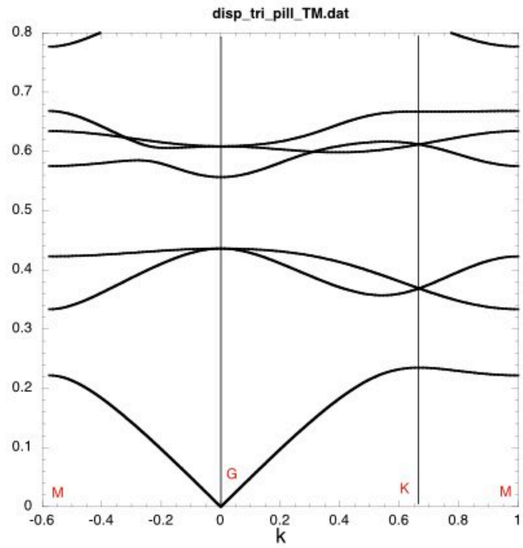


Bestiary of common 2D systems
Triangular lattice, pillars



filling factor = f_{diel} = 30 %
n=3.36

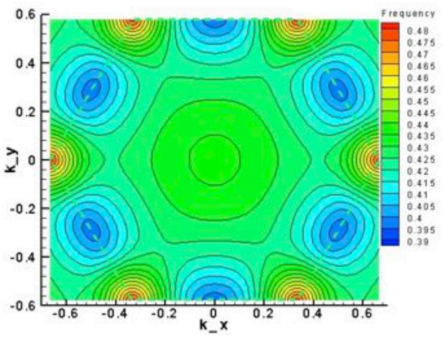


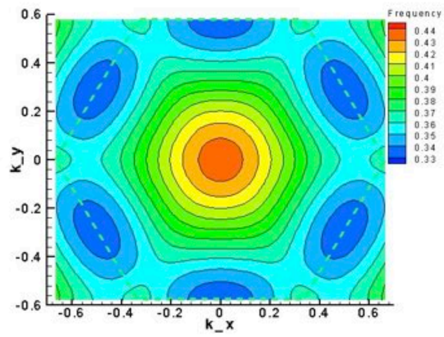


Bestiary of common 2D systems
Triangular lattice, pillars

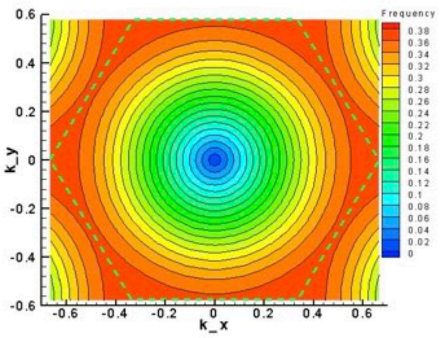
TE TM

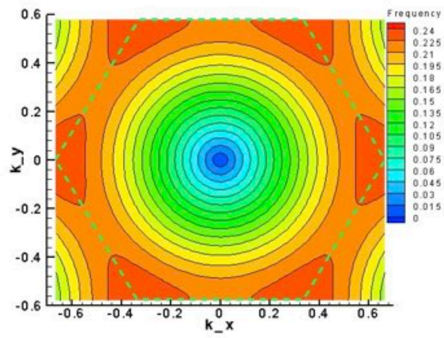
2



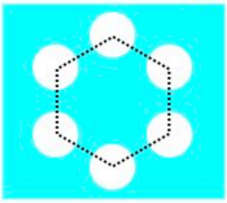


1

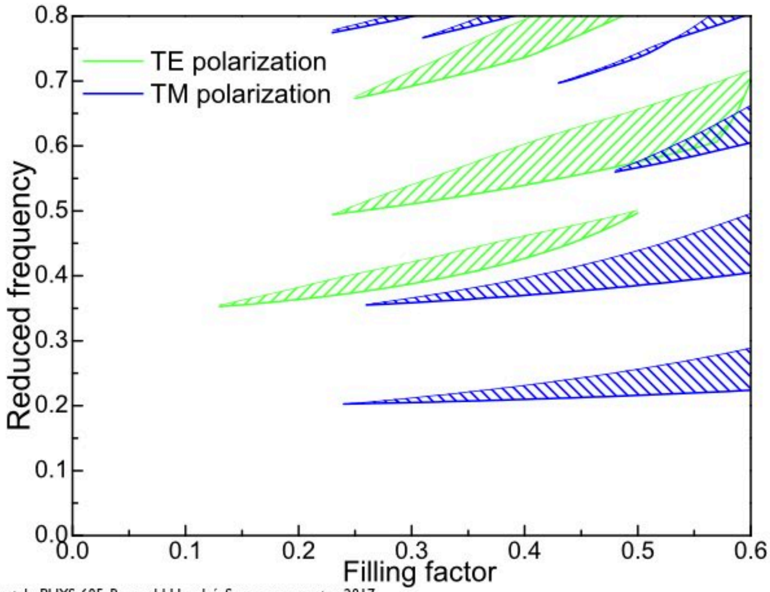




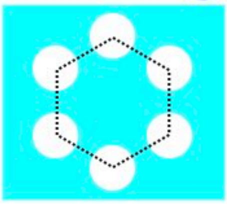
Bestiary of common 2D systems Graphite/Honeycomb lattice, holes



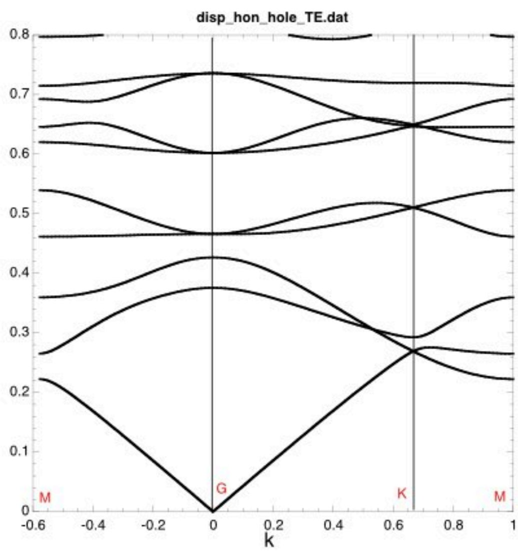
filling factor = f_{air}
n=3.36

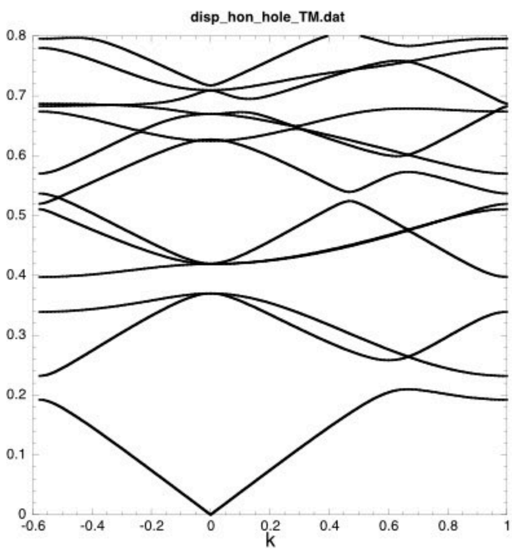


Bestiary of common 2D systems Graphite/Honeycomb lattice, holes



filling factor = f_{air} = 40 %
n=3.36



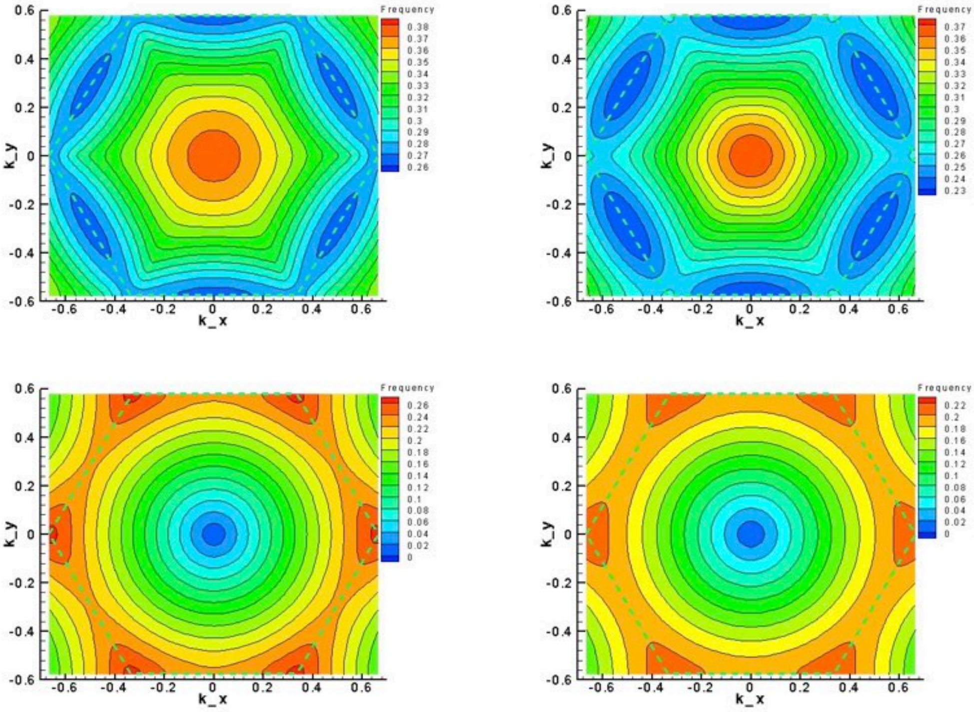


Bestiary of common 2D systems
Graphite/Honeycomb lattice, holes

TE TM

2

1

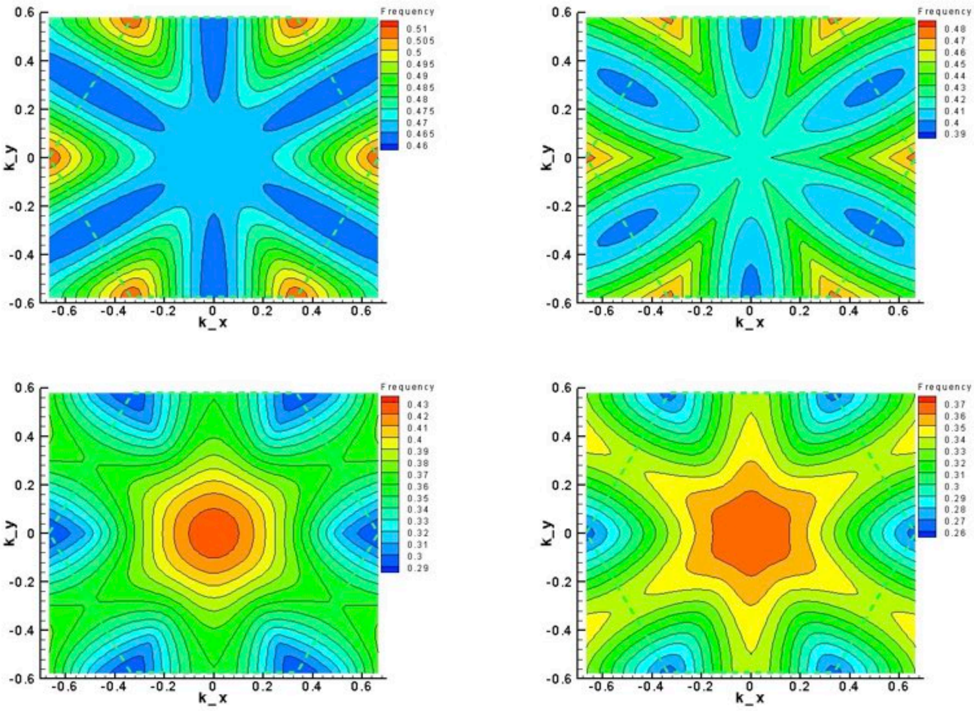


Bestiary of common 2D systems
Graphite/Honeycomb lattice, holes

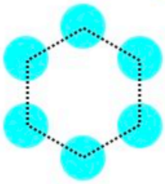
TE TM

4

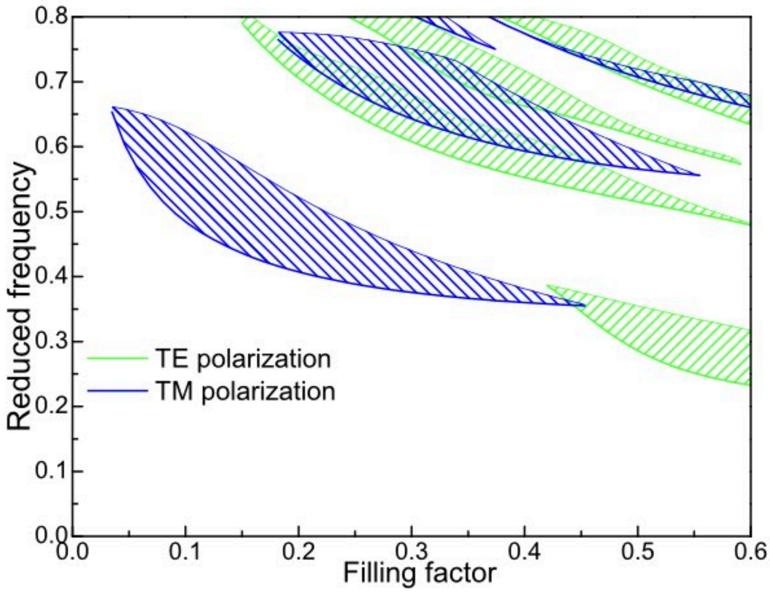
3



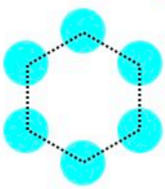
Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars



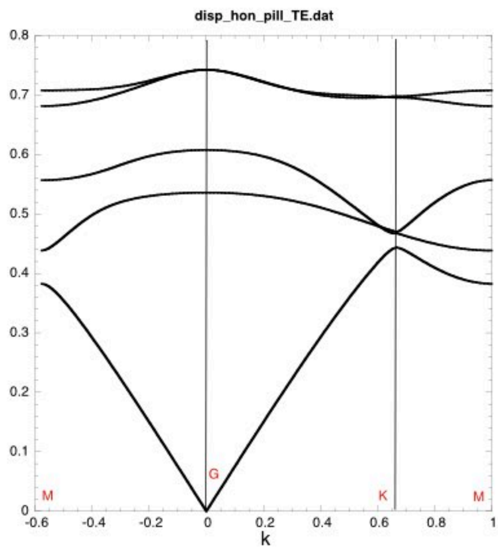
filling factor = f_{diel}
n=3.36

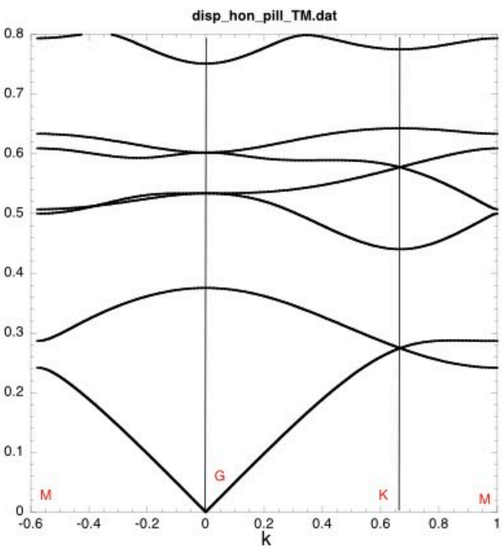


Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars



filling factor = f_{diel} = 30 %
n=3.36



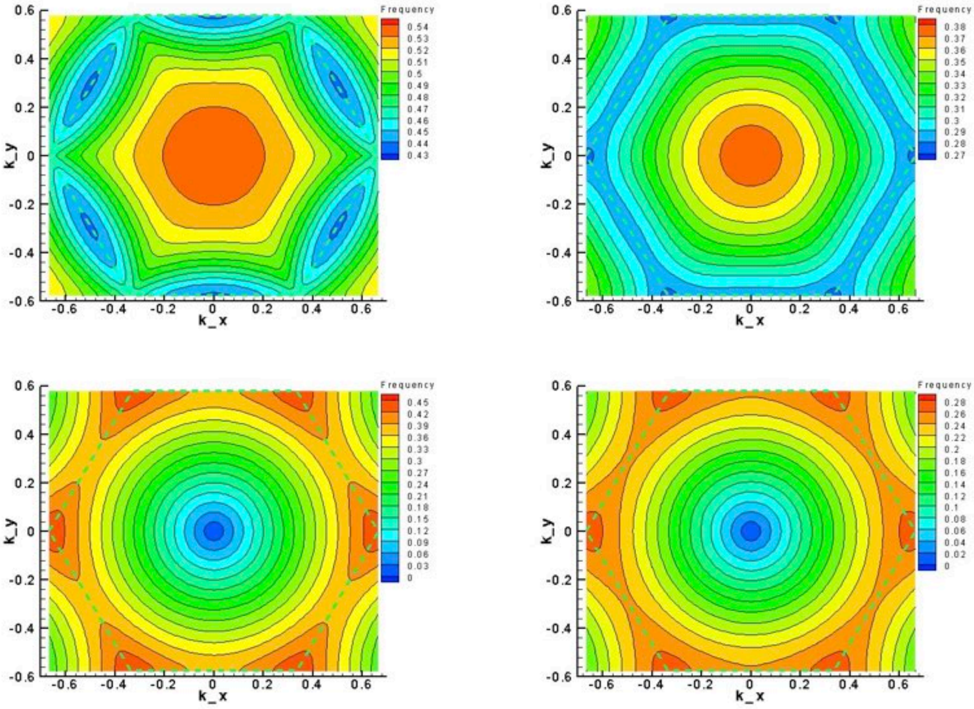


Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars

TE TM

2

1

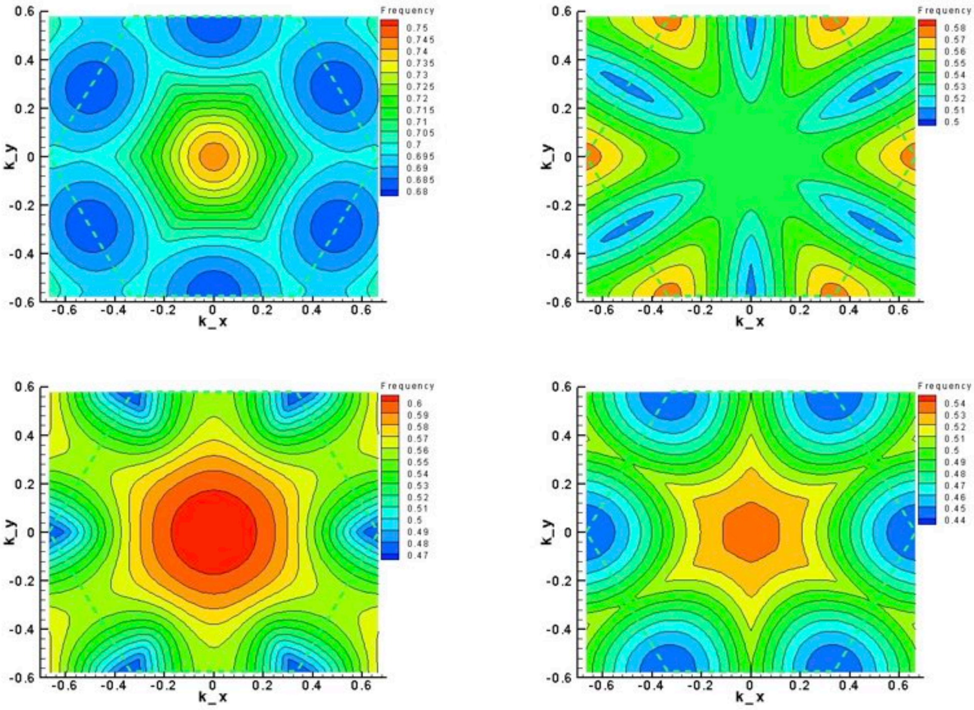


Bestiary of common 2D systems
Graphite/Honeycomb lattice, pillars

TE TM

4

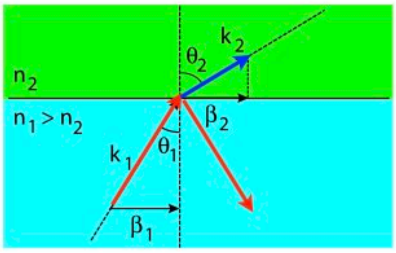
3



Out of plane propagation in 2D systems
Light cone

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

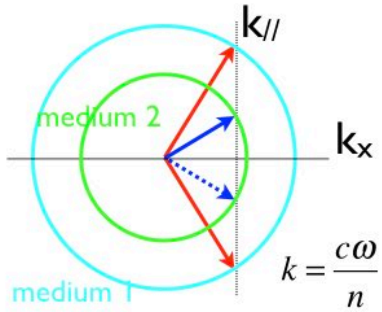
Ibn Sahl (*c.* 984) (also known as Snell-Descartes law, *c.*1631) :

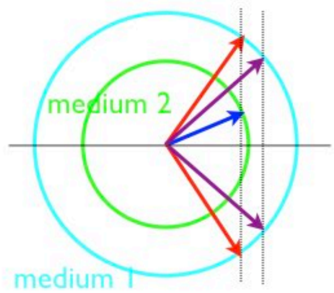


$$\frac{\sin\theta_1}{\sin\theta_2} = \frac{n_2}{n_1}$$

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

$$k_0 n_1 \sin\theta_1 = k_0 n_2 \sin\theta_2 \qquad \beta_1 = \beta_2$$



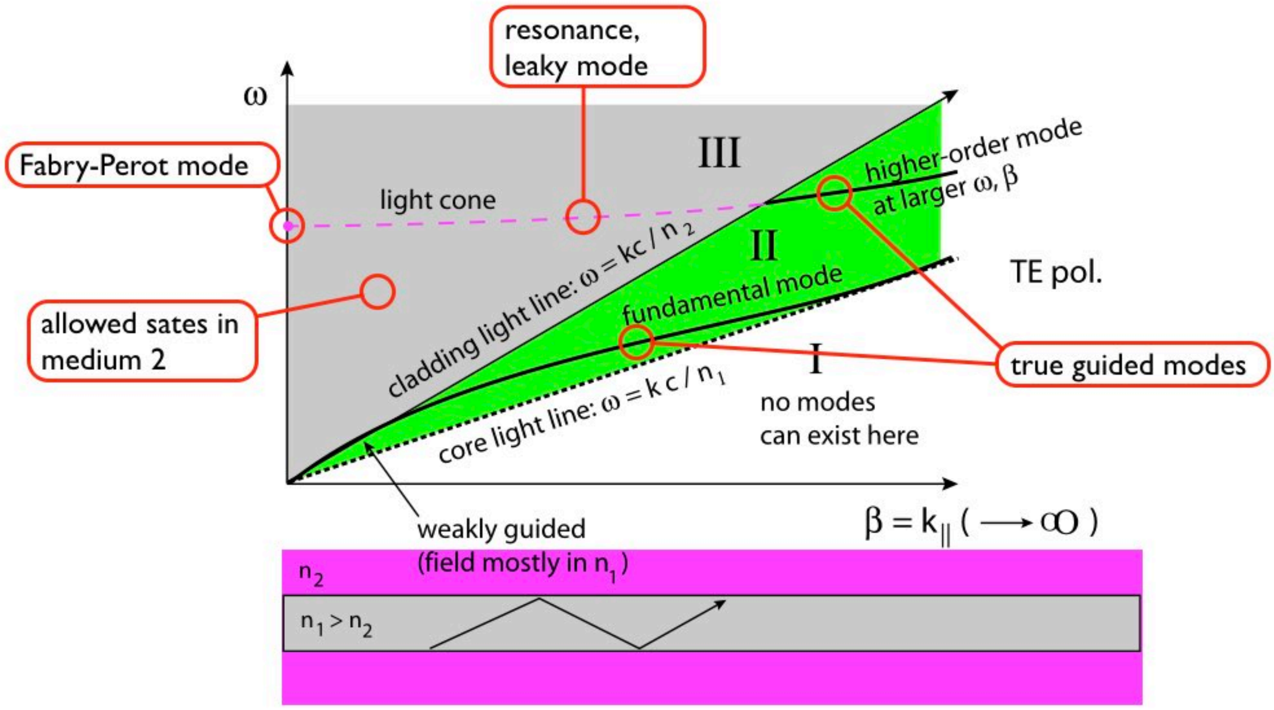


Total internal reflection :

✳ $k < n_2\omega/c$: couplage 1 to 2 allowed

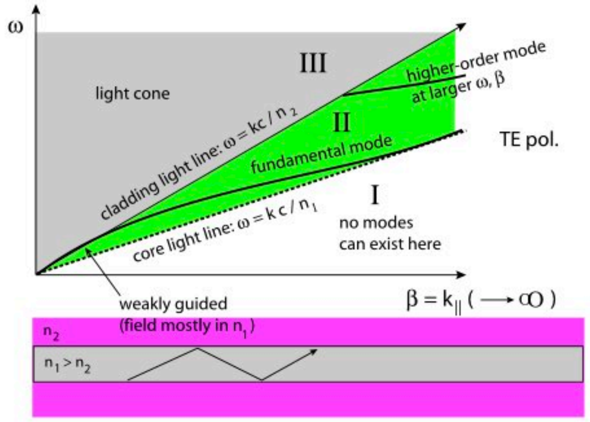
✳ $k > n_2\omega/c$: couplage 1 to 2 forbidden

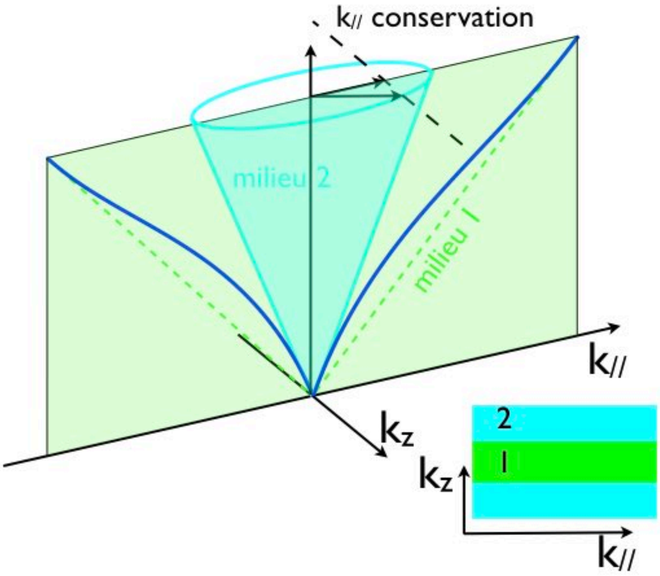
Out of plane propagation in 2D systems
Light cone



Thin slab waveguide

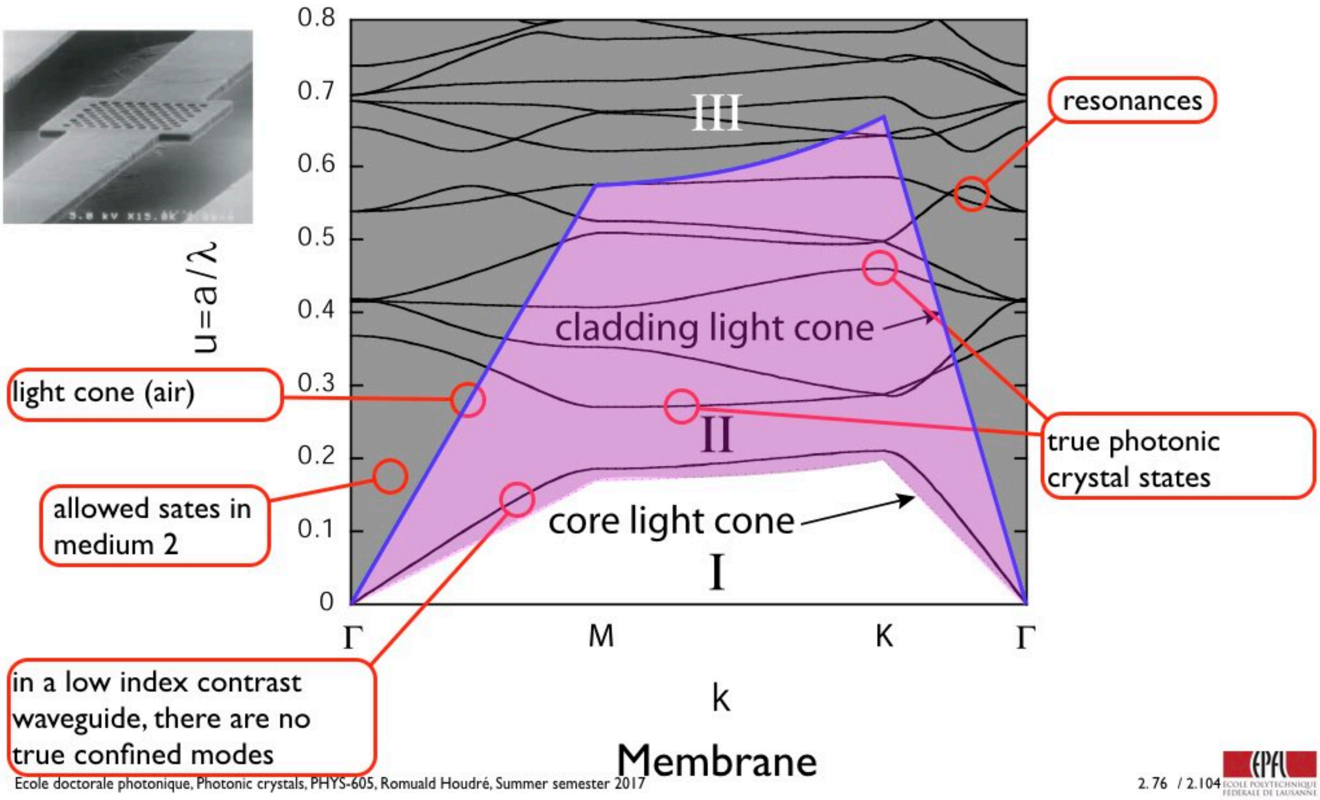
Out of plane propagation in 2D systems
Light cone





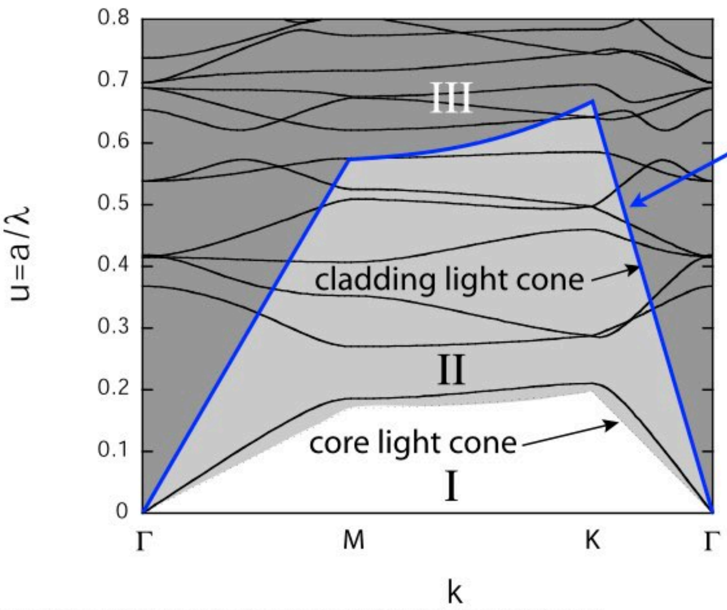
Note: the continuum of states inside the light cone originates from the projection on $k_{//}$ of the dispersion diagram of the semi-infinite cladding medium

Out of plane propagation in 2D systems
Light cone



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

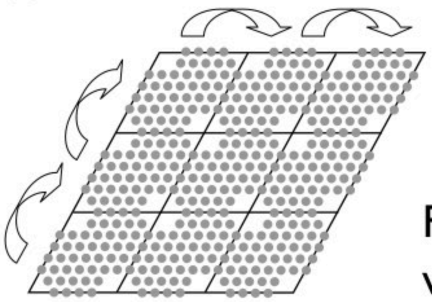


Intersection of the light cone $\omega=kc/n_2$ with the planes ΓM, MK and KΓ = dispersion curve of zero index contrast photonic crystal $n_{hole}=n_{dielectric}=n_{air}$

2D systems and defect modes
super-cell

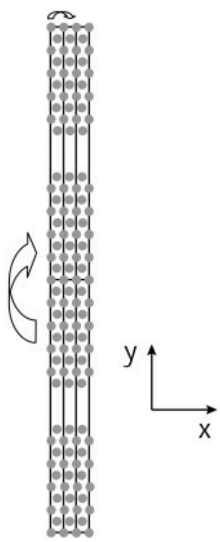
Goal: computation of defect modes

New larger unit cell α time larger in direction a_1 and β time larger in a_2 compared to the original unit cell



Point defect

Linear defect (waveguide)

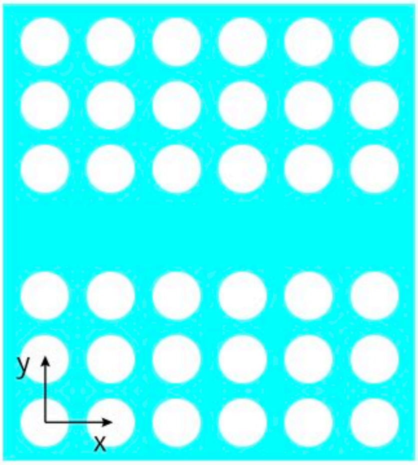


For the same accuracy, αβ more plane waves are needed

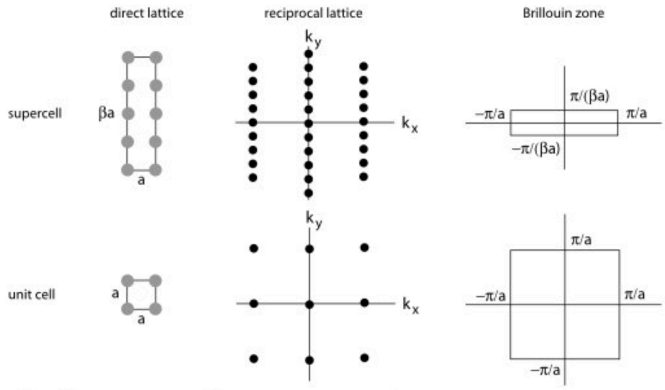
$$N = \frac{G_{\max}^2 \pi}{\left(\frac{2\pi}{\alpha a}\right)\left(\frac{2\pi}{\beta a}\right)} = \alpha\beta N_0$$

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

1D defect (wave guide)



square lattice

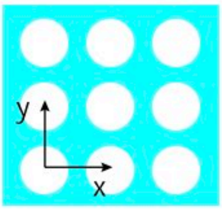


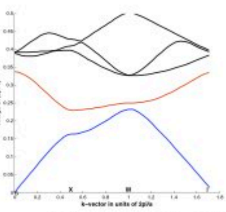
Only k_x remains a good quantum number

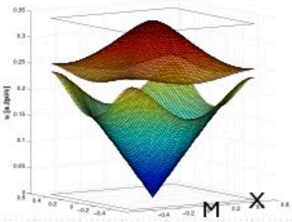
Once again, we must project on k_x the dispersion diagram of the cladding medium (now the photonic crystal in-plane)

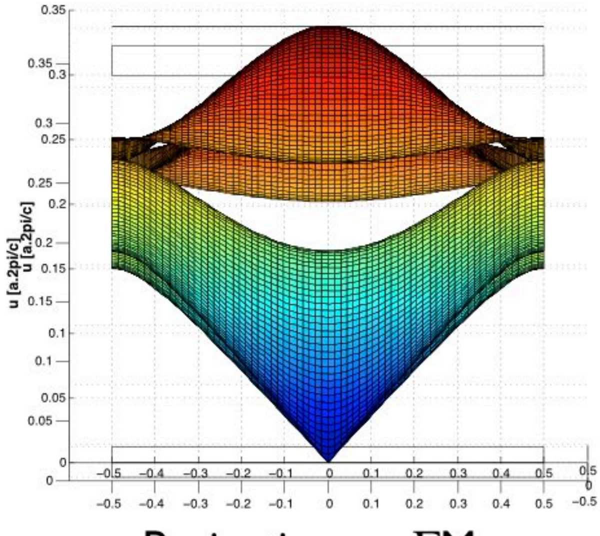
2D systems and defect modes
super-cell and projected band structure

Square lattice

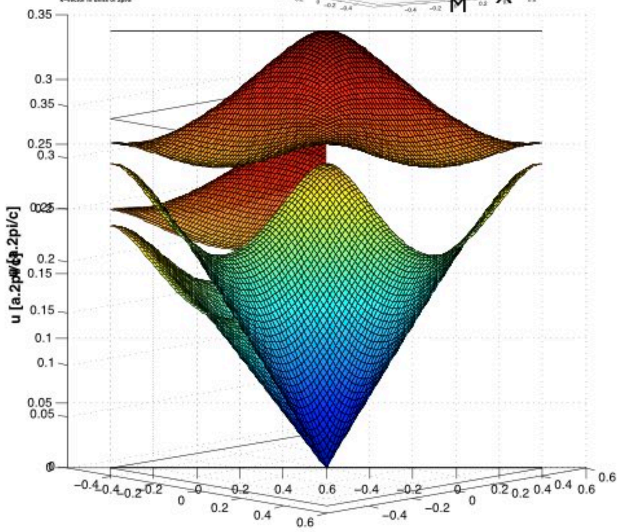








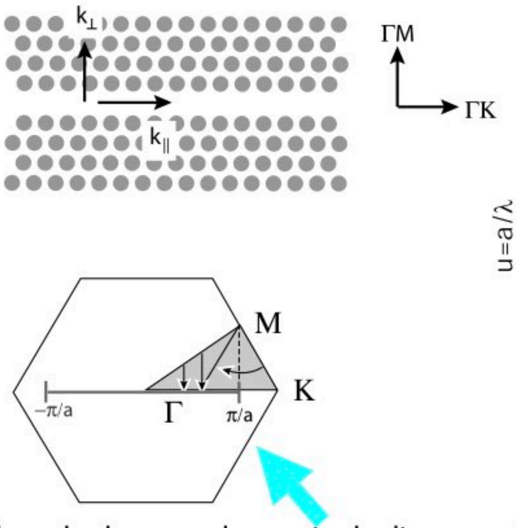
Projection on ΓM

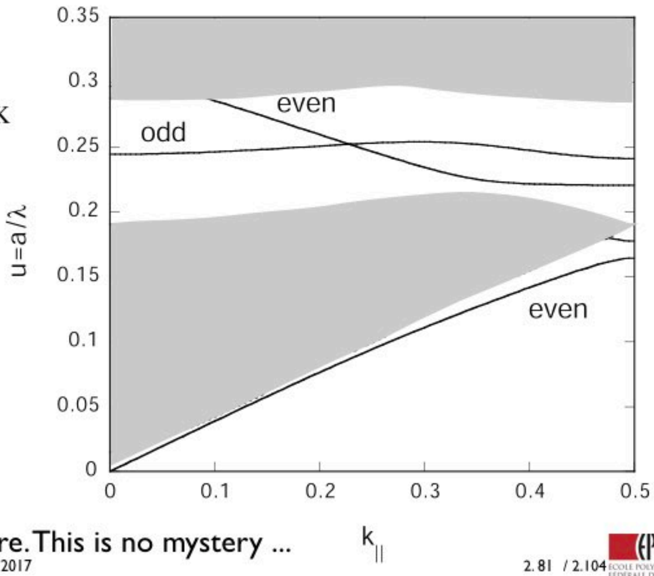


Projection on ΓX

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



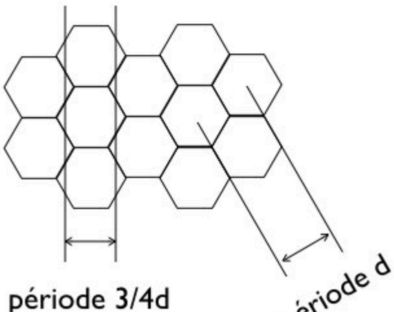


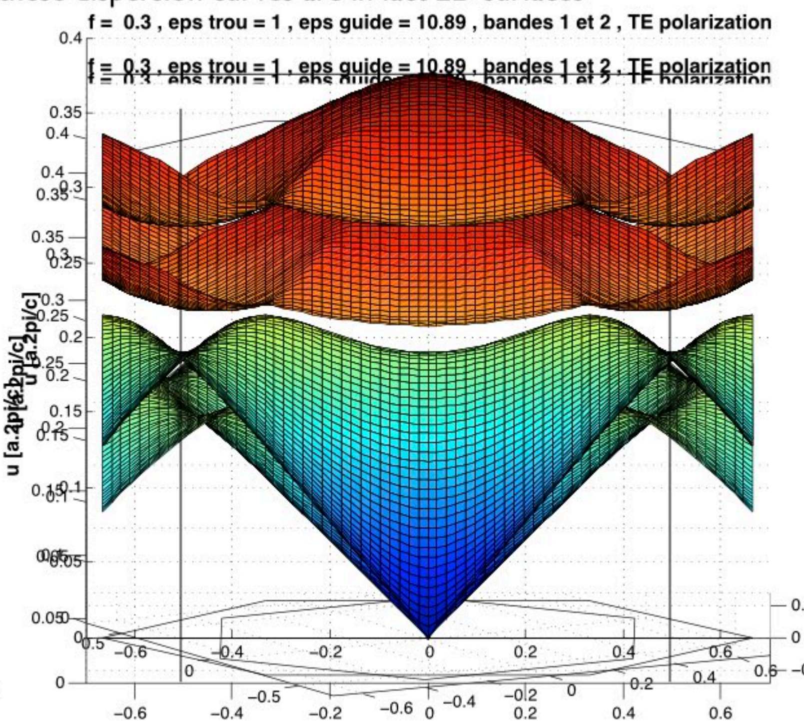
One finds such obscure schemes in the literature. This is no mystery ...

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





Projection on ΓK

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

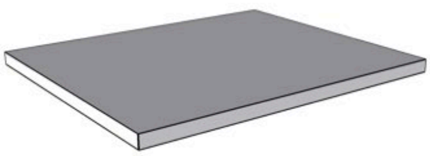
1. Expand onto electromagnetic modes of a homogeneous slab
2. Include radiation modes to lowest order (Fermi's golden rule)

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

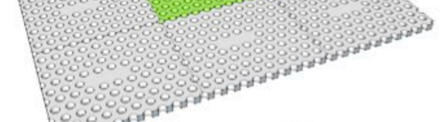
- L.C. Andreani and D. Gerace Phys. Rev. B 73, 235114 (2006)
- V. Zabelin, PhD thesis EPFL, n°4315
- M. Minkov, PhD thesis EPFL, n°6857
- M. Minkov and V. Savona, Scientific Reports **4**, 5124 (2014)

GME

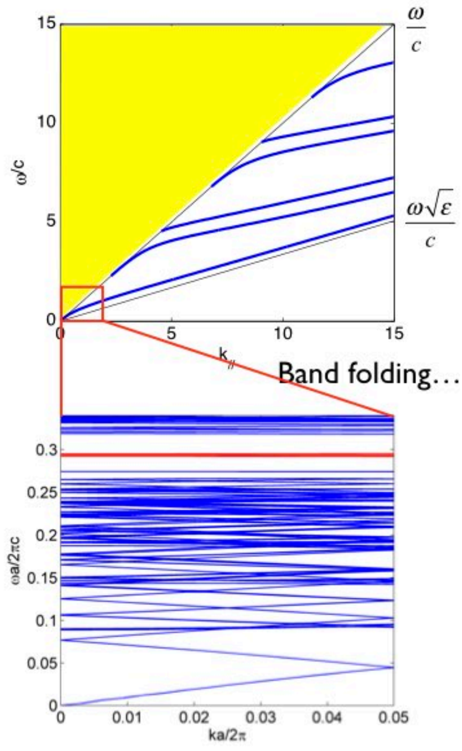
2D guided modes in the slab



Elementary super-cell



$$\mathbf{H}_{\mathbf{k}n}(\mathbf{r}) = \sum_{\mathbf{G},\alpha} c_n(\mathbf{k}+\mathbf{G},\alpha)\mathbf{H}^{(g)}_{\mathbf{k}+\mathbf{G},\alpha}(\mathbf{r})$$



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 highQ 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 localised states

-Phys. Rev. Lett., 81, 1405, 1998 (Mie resonance)
-Phys. Rev. B, 61, 4381, 2000

Korringa-Kohn-Rostocker method (KKR)

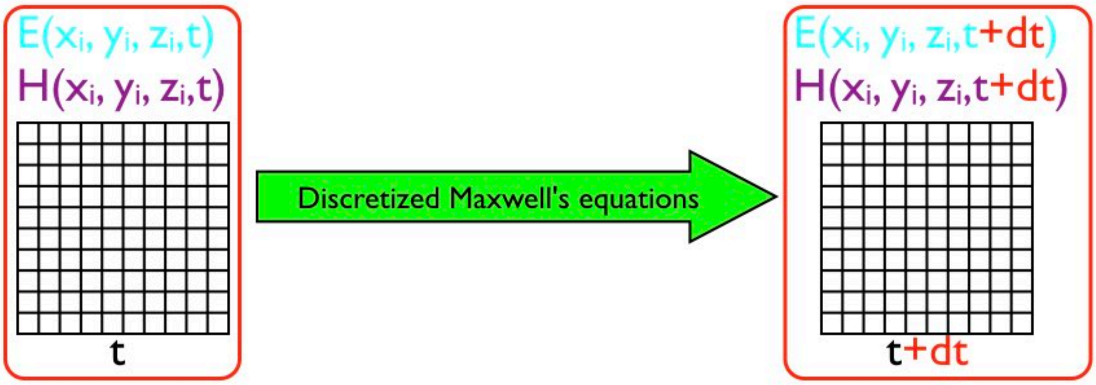
✳ Diffraction matrix of the unit cell + Green function of the periodic structure

- More complex to implement but more stable
- Compute directly the density of states and the local density of states

-J. Phys. Cond. Matt. 6, 171, 1994
-Phys. Rev. B, 51, 2068, 1995

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

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

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

Original article : IEEE Transactions on Antennas and Propagation, vol. AP-14, 302-307, 1966

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 :

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

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

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

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

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

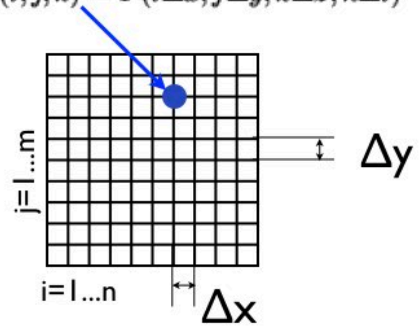
$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - \sigma E_z\right)$$

Finite Difference in the Time Domain

Grid : step size Δx, Δy, Δz

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

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



derivatives / finite differences :

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

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

Finite Difference in the Time Domain

the 6 scalar equations become :

$E_x^{n+1}(i+1/2,j,k)=A_{i+1/2,j,k}E_x^n(i+1/2,j,k)$ $+B_{i+1/2,j,k}[H_z^{n+1/2}(i+1/2,j+1/2,k)-H_z^{n+1/2}(i+1/2,j-1/2,k)$ $+H_y^{n+1/2}(i+1/2,j,k-1/2)-H_y^{n+1/2}(i+1/2,j,k+1/2)]$	$H_x^{n+1/2}(i,j+1/2,k+1/2)=H_x^{n-1/2}(i,j+1/2,k+1/2)$ $+\frac{\Delta t}{\mu\delta}[E_y^n(i,j+1/2,k+1)-E_y^n(i,j+1/2,k)$ $+E_z^n(i,j,k+1/2)-E_z^n(i,j+1,k+1/2)]$
$E_y^{n+1}(i,j+1/2,k)=A_{i,j+1/2,k}E_y^n(i,j+1/2,k)$ $+B_{i,j+1/2,k}[H_x^{n+1/2}(i,j+1/2,k+1/2)-H_x^{n+1/2}(i,j+1/2,k-1/2)$ $+H_z^{n+1/2}(i-1/2,j+1/2,k)-H_z^{n+1/2}(i+1/2,j+1/2,k)]$	$H_y^{n+1/2}(i+1/2,j,k+1/2)=H_y^{n-1/2}(i+1/2,j,k+1/2)$ $+\frac{\Delta t}{\mu\delta}[E_z^n(i+1,j,k+1/2)-E_z^n(i,j,k+1/2)$ $+E_x^n(i+1/2,j,k)-E_x^n(i+1/2,j,k+1)]$
$E_z^{n+1}(i,j,k+1/2)=A_{i,j,k+1/2}E_z^n(i,j,k+1/2)$ $+B_{i,j,k+1/2}[H_y^{n+1/2}(i+1/2,j,k+1/2)-H_y^{n+1/2}(i-1/2,j,k+1/2)$ $+H_x^{n+1/2}(i,j-1/2,k+1/2)-H_x^{n+1/2}(i,j+1/2,k+1/2)]$	$H_z^{n+1/2}(i+1/2,j+1/2,k)=H_z^{n-1/2}(i+1/2,j+1/2,k)$ $+\frac{\Delta t}{\mu\delta}[E_x n(i+1/2,j+1,k)-E_x^n(i+1/2,j,k)$ $+E_y^n(i,j+1/2,k)-E_y^n(i+1,j+1/2,k)]$

with :

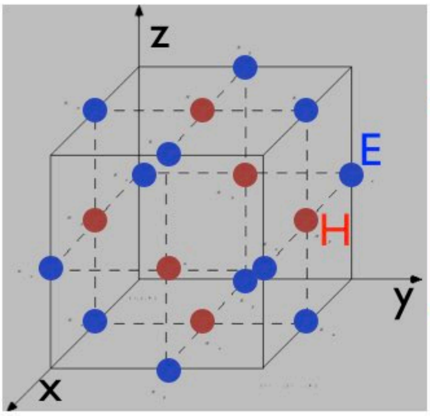
$$A_{i,j,k} = 1 - \frac{\sigma(i,j,k)}{\varepsilon(i,j,k)}$$

$$B_{i,j,k} = \frac{\Delta t}{\varepsilon(i,j,k)\delta}$$

Finite Difference in the Time Domain

these equations are such that :

(n-1/2)Δt	nΔt	(n+1/2)Δt
$H_{(n-1/2)\Delta t}$	$E_{(n-1)\Delta t}$, $H_{(n-1/2)\Delta t}$ → $E_{n\Delta t}$	$E_{n\Delta t}$, $H_{(n-1/2)\Delta t}$ → $H_{(n+1/2)\Delta t}$



It is sufficient to compute E and H on two interlaced grids at alternate odd and even time steps E(nΔt) et H(mΔt)

Finite Difference in the Time Domain

Stability requirement / step size :

v_{max} : maximum propagation speed of the electromagnetic wave
Δt : temporal step
δ : grid lattice
N : dimensionality

$$\frac{v_{\max}\Delta t}{\delta} = \frac{1}{\sqrt{N}}$$

with different Δx, Δy, Δz along x,y and z

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

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 :

$E^{inc}=E_o e^{-(x-x_o)^2/w^2}$

Gaussian source

$E^{inc}(x,y,z) = E_o(x,y,z)\sin(\omega t)$

$E_x^{inc}(i+1/2,j,k_s) = E_o(i+1/2,j,k_s)\sin(2\pi f n\delta t)$

plane wave

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

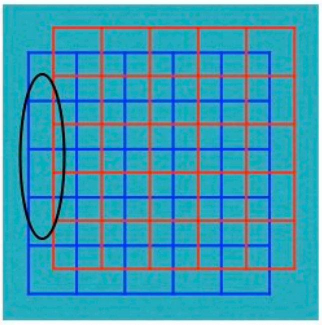
total field / scattered field — IEEE Trans. Electromagnetic Compatibility, vol. 24, 397, 1982.
champ total / champ diffracté

pure scattered field — The Finite Difference Time Domain Method for Electromagnetics. CRC Press, 1993.
champ diffracté pur

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 : Mur conditions. Simulates the propagation of an outward going wave at the boundary
IEEE Tansactions on Electromagnetic Compatibility, vol. EMC-23, 377, 1981

Strategy 3 : Liao conditions. Interpolation of the field at the boundary, in space and time
Sci. Sin., Ser. A, 27,1063, 1984

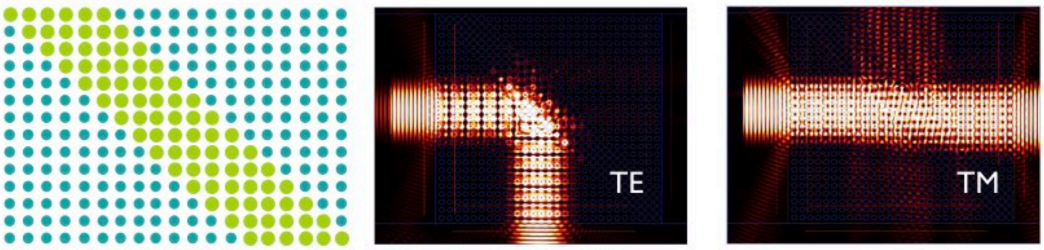
Strategy 4 : Perfectly matched layer (PML). Simulate, over a few period, a perfectly absorbing medium. Gives excellent results with only a few periods

Journal of Computational Physics, 114,185, 1994

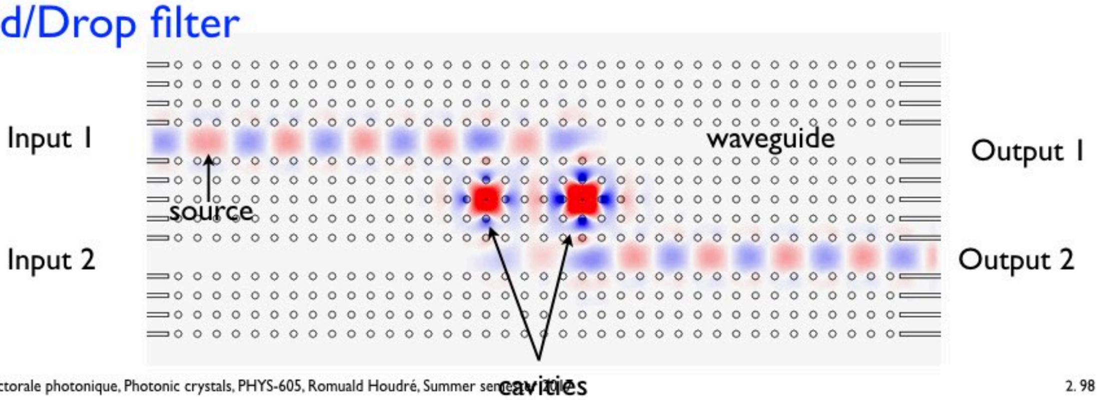
Finite Difference in the Time Domain Examples

Continuous wave (harmonic)

Polariser filter

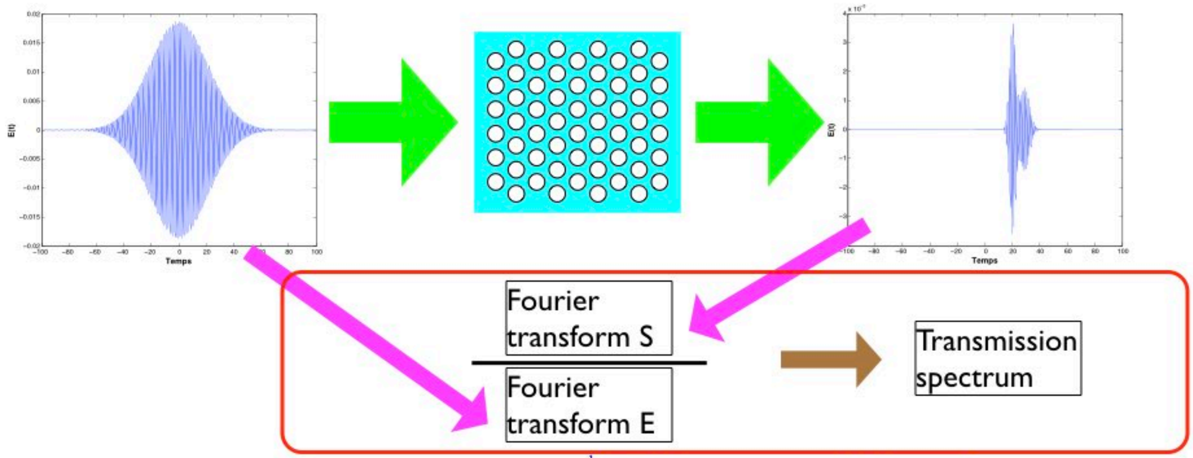


Add/Drop filter

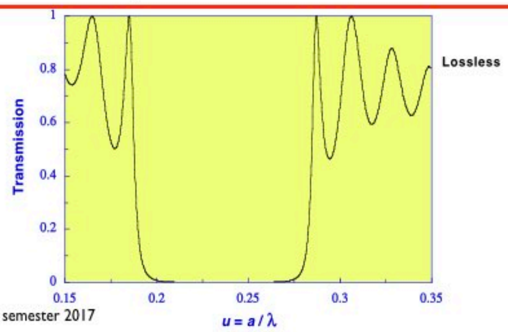


Finite Difference in the Time Domain Examples

Pulsed regime, spectral response

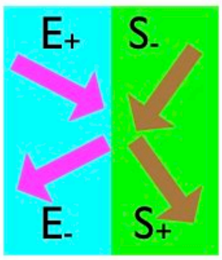


Example: transmission across 8 rows, triangular lattice of holes, direction ΓK, TE :



Transfer matrices method

Transfer matrices techniques for stack of thin layers :



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

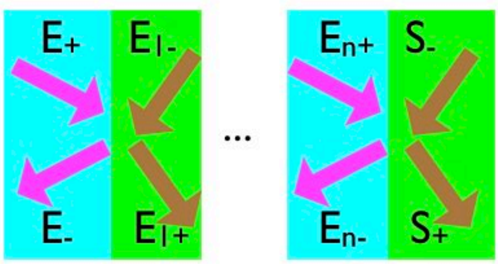
transfer matrix

$$\begin{pmatrix} E_- \\ S_- \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \begin{pmatrix} E_+ \\ S_{+-} \end{pmatrix}$$

diffusion matrix

a, b ... computed according to Fresnel law

Entire structure :



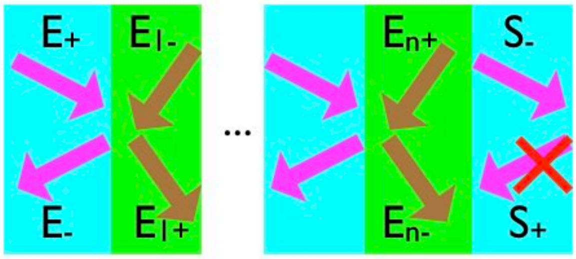
$$\begin{pmatrix} S_+ \\ S_- \end{pmatrix} = \prod_{i=1..n} T_i \begin{pmatrix} E_+ \\ E_- \end{pmatrix}$$

with T_i transfer matrix of an interface or propagatrion 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



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

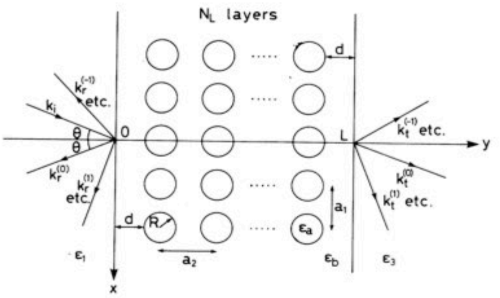
$$R = \frac{\left|E_-\right|^2}{\left|E_+\right|^2} \qquad T = \frac{\left|S_+\right|^2}{\left|E_+\right|^2}$$

⚠ beware of initial and final refractive indices

Ref : any good book on optics

Sakoda and other transfer matrices method

Generalisation of transfer matrices methods including diffracted modes



$$\begin{pmatrix} \left[S_+^i\right] \\ \left[S_-^i\right] \end{pmatrix} = \begin{pmatrix} [a] & [b] \\ [c] & [d] \end{pmatrix} \begin{pmatrix} E_+^i \\ E_-^i \end{pmatrix}$$

infinite size matrices truncated to the size nXn

Main difficulty lies in the computation of the diffusion coefficients

- "Diffraction gratings", SPIE Milestone series, vol. MS83, 1993
- Pure Appl. Opt., 3, 975, 1994

Implementation of such techniques in 2D photonic crystals by S. Sakoda

- Phys. Rev. B, 52, 8992, 1995

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
Les cristaux photoniques ou la lumière en cage / J.-M. Lourtioz, Paris : Hermes-Sciences

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
- MIT Photonic Band http://ab-initio.mit.edu/wiki/index.php/MIT_Photonic_Bands
- CAMFR http://camfr.sourceforge.net
- Geo-Radar http://carsten.welcomes-you.com/radarfdtd
- GFDTD http://ostatic.com/gfdtd
- BigBoy http://sourceforge.net/projects/bigboy
- EMP3 http://www.fieldp.com/emp3.html
- 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/ $\exists$ cluster option
- RSoft http://www.rsoftinc.com/
- ISE / Synopsishttp://www.synopsys.com/Tools/OpticalDesign/
- EM photonics http://www.emphotonics.com/
- Optiwave http://www.optiwave.com/
- Apollo Photonics http://www.apollophoton.com/apollo/
- SEMCAD http://www.iis.ee.ethz.ch/research/bioemc/em_simulation_platform.en.html