Theory of Photonic Crystal Slabs by the Guided-Mode Expansion Method

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Where is Pavia???

Pavia is 25 Km far from Milano.

A nice small town with an ancient (~XIII century) university tradition.
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2D photonic crystals embedded in planar waveguides (photonic crystal slabs)

GaAs membrane (air bridge)

GaAs/AlGaAs PhC slab with internal source

W1 waveguide in Si membrane
Novel effects with 3D control of light

Guiding light through a $90^\circ$ bent waveguide: Loncar et al., APL (2000)

3D confinement of light $\rightarrow$ ultra-high Q nanocavities ($Q \sim 10^6$ recently measured)

Song et al., Nature Mat. (2005)
Novel effects with 3D control of light


Outline

The Guided Mode Expansion (GME) method
Theory, convergence tests, comparisons with other methods

Overview of applications
Disorder-induced losses in PhC slab waveguides
PhC slab cavities Q-factors
Triangular holes in PhC slabs
Quantum theory of radiation-matter interaction
Reminder: eigenmodes in planar dielectric slabs

1D Helmholtz equation:
\[ \frac{\partial^2 \Psi(z)}{\partial z^2} + \left( \epsilon(z) \frac{\omega^2}{c^2} - k_x^2 \right) \Psi(z) = 0 \]

\[ \beta_j^2 = \epsilon_j \frac{\omega^2}{c^2} - k_x^2, \quad j = 1, 2, 3 \]

Exact solution!
Photonic crystal slabs: dispersion, losses, and the light-line issue

Periodically textured planar waveguide

Modified light dispersion

- Dispersion
- Losses
- Light-line issue
Basic ideas of guided-mode expansion (GME)

- **Motivation**: fast and accurate frequency-domain solver

- Photonic crystal slabs combine the features of

  2D photonic crystals: control of light propagation in the \( xy \) plane by Bragg diffraction

  Slab waveguides: control of light propagation in the vertical (\( z \)) direction by total internal reflection

\[ \Rightarrow \] Electromagnetic field is a combination of 2D plane waves in \( xy \) and guided modes along \( z \)
Guided-Mode Expansion method

- Equation for the magnetic field: \[ \nabla \times \left( \frac{1}{\varepsilon(r)} \nabla \times H(r) \right) = \frac{\omega^2}{c^2} H(r), \quad \nabla \cdot H(r) = 0 \]

- Expand magnetic field in a finite basis set, \[ H(r) = \sum_\mu c_\mu H_\mu(r) \]
  \[ \rightarrow \] linear eigenvalue problem
  \[ \sum_\nu H_{\mu\nu} c_\nu = \frac{\omega^2}{c^2} c_\mu \]

  “Hamiltonian” \[ H_{\mu\nu} = \int \varepsilon^{-1}(r)(\nabla \times H^*_\mu(r)) \cdot (\nabla \times H_\nu(r)) dr \]

- Basis states \( H_\mu(r) \): **guided modes** of effective waveguide, where each layer is taken to have an average dielectric constant \( \rightarrow \) **approximation**

- Off-diagonal components \( \left( \frac{1}{\varepsilon} \right)_{G,G'} \) \( \rightarrow \) folding and splitting of PhC bands

- Modes above the light line are coupled to radiative waveguide modes: Fermi’s golden rule \( \rightarrow \) **radiative losses**
Consider a PhC slab with semi-infinite claddings. For the basis states $H_{\mu}(r)$, we choose the guided modes of an effective homogeneous waveguide with an average dielectric constant $\bar{\varepsilon}_j$ in each layer $j=1,2,3$. 

We usually take $\bar{\varepsilon}_j$ to be the spatial average of $\varepsilon_j(xy)=\varepsilon_j(\rho)$ in each layer: 

$$\bar{\varepsilon}_j = \frac{1}{A} \int_{\text{cell}} \varepsilon_j(\rho) d\rho,$$

where $A=$unit cell area.

The average dielectric constants must fulfill $\bar{\varepsilon}_2 > \bar{\varepsilon}_1, \bar{\varepsilon}_3$. 
Diffraction losses by perturbation theory

Modes above the light line are coupled to radiative PhC slab modes, yielding an imaginary part of mode frequencies:

\[- \Im \left( \frac{\omega_k^2}{c^2} \right) = \pi \sum_{G',\lambda,j} \left| H_{k,\text{rad}} \right|^2 \rho_j \left( k + G'; \frac{\omega^2}{c^2} \right).\]

The matrix element between a quasi-guided and a radiative mode is

\[H_{k,\text{rad}} = \int \frac{1}{\varepsilon(r)} (\nabla \times H_k^*(r)) \cdot (\nabla \times H_{k+G',\lambda,j}(r)) dr\]

The sum is over
- \(G'\) \(\rightarrow\) reciprocal lattice vectors (out-of-plane diffraction channels)
- \(\lambda=\text{TE, TM}\) \(\rightarrow\) polarization of radiative PhC slab modes
- \(j=1,3\) \(\rightarrow\) radiative modes that are outgoing in medium 1,3

Approximation: radiative PhC slab modes are replaced with those of the effective waveguide.
Quality factor and propagation losses

The quality factor of a photonic mode is defined as

\[ Q = \frac{\omega}{2 \text{Im}(\omega)}. \]

Spatial attenuation is described by an imaginary part of the wavevector:

\[ \text{Im}(k) = \frac{\text{Im}(\omega)}{v_g}, \]

where

\[ v_g = \frac{d\omega}{dk} \]

is the mode group velocity. Propagation losses in dB are obtained as

\[ \alpha_{\text{loss}} = 4.34 \cdot 2 \text{Im}(k). \]

To treat line and point defects (linear waveguides and nanocavities):

→ use an in-plane supercell
Discussion of GME method

Approximations (besides numerical ones):
- For dispersion: the basis set of guided modes of the effective waveguide is not complete, since leaky modes are not included.
- For losses: radiative PhC slab modes are replaced with those of the effective homogeneous waveguide.

Advantages:
- Guided and quasi-guided photonic modes are obtained, without any artificial layers (PML…) in the vertical direction.
- For thin slabs a few guided modes are sufficient → numerical effort is comparable to that of a 2D plane-wave calculation.
- Diffraction losses by perturbation theory → very efficient procedure, little additional numerical effort beyond dispersion.
- Calculated values for losses are more accurate when they are small → good for line defects and for high-Q nanocavities.
2D periodicity: the triangular lattice

Symmetry plane: horizontal mid-plane \((x,y)\)

Even modes w.r.t. reflection through \((x,y)\) have a band gap

Defect modes with parity \(\sigma_{xy} = +1\) can be engineered!
Convergence tests

Triangular lattice on membrane, $\varepsilon = 12.11$, $d/a = 0.5$, $r/a = 0.3$

Few guided modes are sufficient for convergence

Use of average $\varepsilon$ is justified
Comparison with MIT PBG code

Triangular lattice on membrane, \( \varepsilon=12, \ d/a=0.6, \ r/a=0.45 \)

S.G. Johnson et al., PRB 60, 5751 (1999)

Guided-mode expansion
Comparison with FDTD*

Triangular lattice on membrane, $\varepsilon=11.56$, $d/a=0.65$, $r/a=0.25$

*T. Ochiai and K. Sakoda, PRB 63, 125107 (2001)
Losses in W1 waveguide: comparisons

Membrane, $\varepsilon=11.56$, $h=0.6a$, $r=0.3016a$

Energy (eV) vs Wavevector $ka/\pi$

Loss (dB/mm) vs Wavelength (nm)

FDTD & Fourier: M. Cryan et al., IEEE-PTL 17, 58 (2005)

GME
Applications of GME method

- Photonic band dispersion and gap maps: 1D and 2D lattices
- Linear waveguides: propagation losses
- Nanocavities: Q-factors optimization
- Geometry optimization, design, comparison with expts…
- Extrinsic losses: effects of disorder
- Radiation-matter interaction: exciton-polaritons, weak/strong coupling

Main reference on the method (see also refs. therein):

The code is freely available on the web at
http://fisicavolta.unipv.it/dipartimento/ricerca/fotonici/
Disorder-induced losses in W1 waveguides

The losses show a quadratic behavior as a function of the disorder parameter…typical of Rayleigh scattering


$\Delta r \rightarrow$ r.m.s. deviation from average hole radius $\Delta r/a << 1$
Comparison with experimental results*

membrane W1 waveguide, d/a=0.494, r/a=0.37, a=445 nm, Δr=5 nm

Point defects in PC slabs behave as 0D cavities with full photonic confinement in very small volumes. The Q-factor can be increased by shifting the position of nearby holes.

Q-factor of photonic crystal cavities

Supercell in two directions + Golden Rule
→ \text{Im}(\omega) \text{ and } Q = \frac{\omega}{2\text{Im}(\omega)}


Andreani, Gerace, Agio, Photonics and Nanostructures 2, 103 (2004)
Effect of size disorder on cavity Q-factors

Triangular lattice with triangular holes

\[ \sigma_{xy} = +1 \]
\[ \sigma_{xy} = -1 \]

\[ d/a = 0.68, L/a = 0.85: \text{no complete photonic gap (closed by 2}^{\text{nd}}\text{-order mode)} \]

\[ d/a = 0.5, L/a = 0.8: \text{even gap at } \omega, \text{odd gap at } 2\omega \]

Takayama et al., APL 87, 061107 (2006); Andreani&Gerace, PRB 73, 235114 (2006)
PhC slab with embedded quantum wells

Quantum-well exciton resonance in interaction with photonic modes
→ possibility of strong-coupling regime or photonic crystal polaritons
(analogous to polaritons in bulk crystals or in planar microcavities)
Weak and strong coupling regimes: radiative PhC slab polaritons

Strong coupling regime with vacuum Rabi splitting occurs when photonic mode linewidth is smaller than exciton-photon coupling ~ a few meV

Gerace & Andreani, PRB 75, 235325 (2007)
Experimental configuration and parametric processes: polariton stimulation?

Gerace & Andreani, PRB 75, 235325 (2007)
More on GME method...
Photonic crystal slabs: structures

(a) Air bridge
(b) GaAs/AlGaAs
(c) Silicon-on-Insulator (SOI)

(d) Air bridge
(e) GaAs/AlGaAs
(f) Silicon-on-Insulator (SOI)
Expansion in the basis of guided modes

\[ H_k(r) = \sum_{G,\alpha} c(k + G, \alpha) H_{k+G,\alpha}^{\text{guided}}(r) \]

**\( k \)** = Bloch vector, chosen to be in the first Brillouin zone

**\( G \)** = reciprocal lattice vectors of the 2D Bravais lattice

**\( \alpha \)** = index of guided mode

**\( H_{k+G,\alpha}^{\text{guided}}(r) \)** = guided modes of effective waveguide at \( k + G \)

Dimension of linear eigenvalue problem is \((N_{PW} N_\alpha) \times (N_{PW} N_\alpha)\).

Since the guided modes are simple trigonometric functions, the matrix elements can be calculated analytically.

Both TE and TM guided modes appear in the expansion of a PhC slab mode. The index \( \alpha \) includes mode order and polarization.
Matrix elements: the dielectric tensor

The matrix elements between guided modes depend on the inverse dielectric matrices in the three layers,

\[ \eta_j(G, G') = \frac{1}{A} \int \varepsilon_j^{-1}(\rho) e^{i(G'-G) \cdot \rho} d\rho \]

Like in 2D plane-wave expansion, they are evaluated from numerical inversion of the direct dielectric matrices:

\[ \eta_j(G, G') = [\varepsilon_j(G, G')]^{-1} \]

\[ \varepsilon_j(G, G') = \frac{1}{A} \int \varepsilon_j(\rho) e^{i(G'-G) \cdot \rho} d\rho \]

Convergence properties, possible optimization beyond the Ho-Chan-Soukoulis procedure are similar to 2D plane-wave expansion.

The off-diagonal components of \( \eta_j(G, G') \) are responsible for the folding of photonic bands in the first BZ, gap formation, splittings etc.
Discussion of GME method (dispersion)

Main drawback: the basis set of guided modes of the effective waveguide is not complete, since leaky modes are not included.

⇒ the GME method is an APPROXIMATE one

Main advantage: folded photonic modes in the first Brillouin zone may fall above the light line ⇒ guided and quasi-guided photonic modes are obtained, without the need of introducing any artificial layers (PML…) in the vertical direction.

When a few guided modes are sufficient, as it often happens, the numerical effort is comparable to that of a 2D plane-wave calculation. Very suited for parameter optimization, design…

The dispersion of photonic bands in a PhC slab can be compared with that of the ideal 2D system and with the dispersion of free waveguide modes. Multimode slabs are naturally treated.
Symmetry properties, TE/TM mixing

When the PhC slab is symmetric under reflection in the xy plane: separation of even ($\sigma_{xy}=+1$) and odd ($\sigma_{xy}=+1$) modes

\[
\begin{align*}
q \sin \frac{qd}{2} - \chi_1 \cos \frac{qd}{2} &= 0 \quad \text{TE, } \sigma_{xy} = +1 \\
q \cos \frac{qd}{2} + \chi_1 \sin \frac{qd}{2} &= 0 \quad \text{TE, } \sigma_{xy} = -1 \\
\frac{q}{\epsilon_2} \cos \frac{qd}{2} + \frac{\chi_1}{\epsilon_1} \sin \frac{qd}{2} &= 0 \quad \text{TM, } \sigma_{xy} = +1 \\
\frac{q}{\epsilon_2} \sin \frac{qd}{2} - \frac{\chi_1}{\epsilon_1} \cos \frac{qd}{2} &= 0 \quad \text{TM, } \sigma_{xy} = -1
\end{align*}
\]

Low-lying photonic modes are dominated by lowest-order modes of the effective waveguide:

- $\sigma_{xy}=+1$ modes are dominated by TE waveguide modes $\rightarrow$ quasi-TE
- $\sigma_{xy}=-1$ modes are dominated by TM waveguide modes $\rightarrow$ quasi-TM

However, in general, any PhC mode contains both TE and TM waveguide modes $\rightarrow$ only the symmetry labels $\sigma_{xy}=\pm 1$ have a rigorous meaning.
Coupling matrix element

Using the guided-mode expansion for the magnetic field of a PhC slab mode, the matrix element with a radiative mode is

\[ H_{k,\text{rad}} = \sum_{G,\alpha} c(k + G, \alpha)^* H_{\text{guided, rad}} \]

where

\[ H_{k,\text{rad}} = \int \frac{1}{\varepsilon(r)} (\nabla \times H_k^*(r)) \cdot (\nabla \times H_{k+G',\lambda,j}^\text{rad}(r)) dr \]

are matrix elements between guided and radiation modes of the effective waveguide, which are calculated analytically.

Both guided and radiation modes are normalized according to

\[ \int H_\mu^*(r) \cdot H_\nu(r) dr = \delta_{\mu\nu} \]

(within a large box for radiation modes).
Each hole is subdivided into N sections of length $L_c = \frac{2\pi r}{N}$, where $L_c$ is a correlation length of size fluctuations.

Micro-roughness is characterized by two parameters: $\sigma$ and $L_c$, in analogy to the Marcuse-Payne-Lacey model for strip waveguides.