A Dirichlet-to-Neumann approach for the exact computation of guided modes in photonic crystal waveguides

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Talk Abstract
This works deals with one dimensional infinite perturbation - namely line defects - in periodic media. In optics, such defects are created to construct an (open) waveguide that concentrates light. The existence and the computation of the eigenmodes is a crucial issue. This is related to a selfadjoint eigenvalue problem associated to a PDE in an unbounded domain (in the directions orthogonal to the line defect), which makes both the analysis and the computations more complex. Using a Dirichlet-to-Neumann (DtN) approach, we show that this problem is equivalent to one set on a small neighborhood of the defect. Conversely to existing methods, this one is exact but there is a price to be paid : the reduction of the problem leads to a nonlinear eigenvalue problem of a fixed point nature.

Introduction
The propagation model we consider is a simple 2D space-($\mathbf{x} = (x, y)$) time domain scalar problem and we look for w satisfying the wave equation

$$\rho(\mathbf{x})\frac{\partial^2 w}{\partial t^2} - \triangle w = 0, \quad \mathbf{x} \in \Omega,\ t \geq 0 \qquad (\mathcal{P})$$

The domain of propagation Ω is infinite in the two directions, its geometry is periodic in the $y-$direction with the period L_y in the whole domain and periodic in the $x-$direction with the period L_x outside a straight band

$$\Omega_0 =]-a, a[\times \mathbb{R}$$

The function ρ is periodic as well in $\Omega_+ \cup \Omega_- = \Omega \setminus \Omega_0$ ($\Omega_\pm = (\Omega \setminus \Omega_0) \cap (\mathbb{R}^\pm \times \mathbb{R})$), with the same periodicity than the geometry (see figure 1)

$$\rho(x,y) = \left| \begin{array}{lll} \rho_p(x,y) & \text{in} & \Omega_+ \cup \Omega_- \\ \rho_0(x,y) & \text{in} & \Omega_0 \end{array} \right.$$

$$\text{with} \quad \begin{array}{rll} \rho_p(x \pm L_x, y \pm L_y) = & \rho_p(x,y) & \forall\,(x,y) \in \Omega \\ \rho_0(x, y \pm L_y) = & \rho_0(x,y) & \forall\,(x,y) \in \Omega_0 \end{array}$$

A mode of this problem is by definition a solution w to ($\mathcal{P}$) which can be written in the form

$$w(x,y) = v(x,y)\, e^{\imath(\beta y - \omega t)}$$

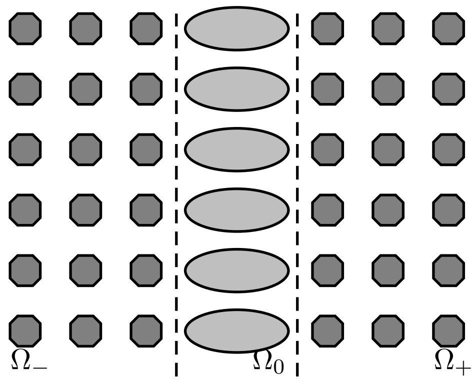


Figure 1: Domain of propagation : typically $\rho = 1$ in the white region, $\rho = 2$ in the dark grey regions and $\rho = 3$ in the light grey regions.

where, in full generality, the quasi period β is in $]-\pi/L_y, \pi/L_y[+\imath\mathbb{R}$, the frequency $\omega \in \mathbb{R}^+$ and v is periodic in the $y-$direction with period L_y. Let us denote B one period of the domain in the y-direction (see figure 2):

$$B = \mathbb{R}\times]-\frac{L_y}{2}, \frac{L_y}{2}[.$$

We focus here exclusively on the "guided" modes which

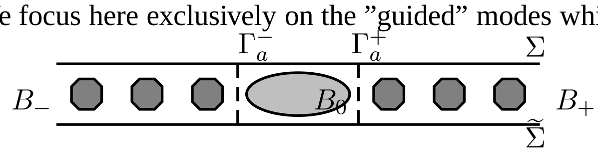


Figure 2: The band B.

correspond to a solution w for which $\beta \in]-\pi/L_y, \pi/L_y[$ and $v \in L^2(B)$. This corresponds to finding couples (ω^2, β) such that there exists $u \in H^1(B)$, $u \neq 0$ solution of

$$\left| \begin{array}{l} -\dfrac{1}{\rho}\triangle u = \omega^2 u, \quad \text{in } B \\ u\big|_\Sigma = e^{\imath\beta}\, u\big|_{\widetilde{\Sigma}}, \quad \partial_y u\big|_\Sigma = e^{\imath\beta}\, \partial_y u\big|_{\widetilde{\Sigma}} \end{array} \right.$$

where (see figure 2) $\Sigma = \mathbb{R}\times\left\{\frac{L_y}{2}\right\}$ and $\widetilde{\Sigma} = \mathbb{R}\times\left\{-\frac{L_y}{2}\right\}$.

The classical approach for solving this eigenvalue problem set in an unbounded domain is the Supercell Method [5] which is based on the exponentially decreasing property of the mode in the $x-$ direction and consists in truncating the band B far enough. The main drawback of this strategy relies on the increase of the computational cost when a mode is not well confined.

Here we propose a novel method based on a DtN approach, which is originally developed for scattering problems and offer a rigorously justified alternative to existing methods such as the super-cell method. Compared to this latter method, the DtN method allows us to reduce the numerical computation to a small neighborhood of the defect independently from the confinement of the computed guided modes. Moreover, as the method is exact, we improve the accuracy for non well-confined guided modes. Obviously, there is a price to be paid: the reduction of the problem leads to a nonlinear eigenvalue problem, of a fixed point nature.

1 Spectral theory

We have reduced the problem of finding the guided modes to the following problem :

$$\begin{aligned} &\text{Find } \beta \in]-\frac{\pi}{L_y}, \frac{\pi}{L_y}[,\ \omega^2 \in \mathbb{R}^+, \\ &\text{s.t. } \exists u \in H^1(B),\ u \neq 0, \\ &A(\beta)u = \omega^2 u \end{aligned} \qquad (\mathcal{E})$$

where

$$\left| \begin{array}{l} A(\beta) = -\frac{1}{\rho}\triangle \\ D(A(\beta)) = \{u \in H^1(\triangle, B), \left| \begin{array}{l} u|_\Sigma = e^{\imath\beta} u|_{\widetilde{\Sigma}} \\ \partial_y u|_\Sigma = e^{\imath\beta}\partial_y u|_{\widetilde{\Sigma}} \end{array} \right. \}. \end{array} \right.$$

with $H^1(\triangle, B) = \{u \in H^1(B),\ \triangle u \in L^2(B)\}$.

To solve ($\mathcal{E}$), there are two different approaches: the $\omega-$formulation (which consists in fixing β and looking for ω) and the $\beta-$formulation (which consists in fixing ω and looking for β). To simplify the presentation, we choose here the first one but the method extends to the other formulation - which could be more adapted for dispersive media for example, $\rho(\omega)$.

Using [3] and proving that $A(\beta)$ is the compact perturbation of an operator with perfectly periodic coefficient, we can show that

Proposition 1 (Properties of $A(\beta)$)
The operator $A(\beta)$ is selfadjoint in $L^2(B, \rho dxdy)$, positive and its essential spectrum satisfies

$$\sigma_{ess}(\beta) = \mathbb{R} \setminus \bigcup_{n\in[\![1,N(\beta)]\!]}]a_n(\beta), b_n(\beta)[$$

where $0 \leq a_n(\beta) < b_n(\beta)$ and $N(\beta) \leq +\infty$. The intervals $]a_n(\beta), b_n(\beta)[$ are called the gaps of the essential spectrum.

Remark *The classical characterization of the essential spectrum involves the eigenvalues of a cell problem with quasi periodic conditions. In Section 2.3, we will give another characterization of the essential spectrum with a by-product of the method.*

Let us suppose now that at least one gap exists (see [1] for a comprehensive study on the existence of gaps). We are interested in characterizing and then computing the eigenvalues $(\lambda_m(\beta))_m$ which are in the gaps of the essential spectrum (see [6] -optical waveguides- and [4] -photonic crystal waveguides- for existence of eigenvalues inside gaps).

Proposition 2 (Properties of each $\lambda_m(\beta)$)
The dispersion curves $\beta \mapsto \lambda_m(\beta)$ are continuous, $2\pi/L_y$-periodic and even.

So, we suppose in the following that $\beta \in [0, \pi/L_y]$.

2 The non linear eigenvalue problem

We focus, from this point, on the eigenvalues $\omega^2 \notin \sigma_{ess}(\beta)$.

The definition of the DtN operators involves the half-band problems: for given φ in $H^{1/2}(\Gamma_a^\pm)$

$$\begin{array}{l} \text{Find } u^\pm \in H^1(B^\pm) \\ \left| \begin{array}{l} -\triangle u^\pm - \rho_p\omega^2 u^\pm = 0 \quad \text{in } B^\pm \\ u|_{\Gamma_a^\pm} = \varphi \\ u|_{\Sigma^\pm} = e^{\imath\beta}u|_{\widetilde{\Sigma}^\pm}, \quad \partial_y u|_{\Sigma^\pm} = e^{\imath\beta}\partial_y u|_{\widetilde{\Sigma}^\pm}. \end{array} \right. \end{array} \qquad (\mathcal{P}^\pm)$$

where $B^\pm = B \cap \Omega^\pm$, $\Sigma^\pm = \Sigma \cap \Omega^\pm$ and $\widetilde{\Sigma}^\pm = \widetilde{\Sigma} \cap \Omega^\pm$.

Theorem 1 (Well-posedness of the problems ($\mathcal{P}^\pm$))
If $\omega^2 \notin \sigma_{ess}(\beta)$, the problem ($\mathcal{P}^\pm$) is well-posed in H^1 except for a countable set of frequencies.
If the periodicity cell is symmetric with respect to the axis $x = 0$ and if $\omega^2 \notin \sigma_{ess}(\beta)$, the problem ($\mathcal{P}^\pm$) is always well-posed in H^1.

Suppose that the problems are well posed. Then, the DtN operators $\Lambda^\pm(\beta,\omega) \in \mathcal{L}(H^{1/2}(\Gamma_a^\pm), H^{-1/2}(\Gamma_a^\pm))$ are given by

$$\forall\varphi \in H^{1/2}(\Gamma_a^\pm), \quad \Lambda^\pm(\beta,\omega)\varphi = \mp\partial_x u^\pm(\beta,\omega;\varphi),$$

where $\Gamma_a^\pm = \{\pm a\}\times] - L_y/2, L_y/2[$ (see figure 2) and $u^\pm(\beta,\omega;\varphi)$ is the unique H^1 solution to ($\mathcal{P}^\pm$).
The next theorem is therefore straightforward.

Theorem 2 (Problem with DtN conditions)
The problem ($\mathcal{E}$) *is equivalent to the problem posed on* $B_0 = B \cap \Omega_0$

$$\textit{Find } \omega^2 \notin \sigma_{ess}(\beta), \textit{ s.t. } \exists u_0 \in H^1(B_0),\ u_0 \neq 0$$

$$-\frac{1}{\rho}\triangle u_0 = \omega^2 u_0, \quad \textit{in } B_0 \qquad (\mathcal{E}_0)$$

u_0 *satisfying the boundary conditions*

$$(BC_0)\left|\begin{array}{l} +\partial_x\, u_0 + \Lambda^+(\beta,\omega)\, u_0 = 0, \quad \textit{on } \Gamma_a^+ \\ -\partial_x\, u_0 + \Lambda^-(\beta,\omega)\, u_0 = 0, \quad \textit{on } \Gamma_a^-, \\ u_0|_{\Sigma_0} = e^{\imath\beta} u_0|_{\widetilde{\Sigma}_0},\ \partial_y u_0|_{\Sigma_0} = e^{\imath\beta}\partial_y u_0|_{\widetilde{\Sigma}_0}. \end{array}\right.$$

where $\Sigma_0 = \Sigma \cap \Omega_0$ *and* $\widetilde{\Sigma}_0 = \widetilde{\Sigma} \cap \Omega_0$.

These problems are equivalent in the sense that if (ω, u) is solution of ($\mathcal{E}$) then $(\omega, u|_{B_0})$ is solution of ($\mathcal{E}_0$). Conversely, if (u_0, ω) is solution of ($\mathcal{E}_0$) then u defined by

$$\left|\begin{array}{l} u|_{B_0} = u_0 \\ u|_{B^\pm} = u^\pm(\beta,\omega,\varphi), \quad \text{where } \varphi = u_0|_{\Gamma_a^\pm} \end{array}\right.$$

associated to the same value ω is solution of ($\mathcal{E}$). Moreover, the multiplicity of ω is the same for the two problems.

Whereas the problem ($\mathcal{E}$) was linear with respect to the eigenvalue ω^2 but defined on an unbounded domain, the problem ($\mathcal{E}_0$) is set on a bounded domain but non linear. Note that the problem ($\mathcal{E}_0$) is also non linear with respect to β (whereas the problem ($\mathcal{E}$) can be rewritten as a quadratic eigenvalue problem). In other words, this difficulty would be present if we decided to fix ω and look for β.

We now introduce the solution algorithm of the non linear eigenvalue problem and explain how to compute the DtN operators in the case where $\omega^2 \notin \sigma_{ess}(\beta)$.

2.1 Solution algorithm

For $\omega^2 \notin \sigma_{ess}(\beta)$, we denote by $A_0(\beta,\omega)$ the operator

$$\left|\begin{array}{l} A_0(\beta,\omega) = -\dfrac{1}{\rho_0}\triangle \\ D(A_0(\beta,\omega)) = \left\{u \in H^1(\triangle, B_0),\ u \text{ satisfying } (BC0)\right\}. \end{array}\right.$$

The operator $A_0(\beta,\omega)$ is selfadjoint and with compact resolvant so its spectrum is a pure point one and consists of a sequence of eigenvalues $(\mu_n(\omega))_n$ of finite multiplicity tending to $+\infty$. The explicit expression of these eigenvalues using the Min-Max principle yields some regularity properties of each eigenvalue with respect of ω.

Consequently, the solutions of the non-linear problem ($\mathcal{E}_0$) are the roots of the equations :

$$\omega^2 \notin \sigma_{ess}(\beta) \quad \text{and } \mu_m(\omega) = \omega^2, \text{ for } m \geq 1.$$

We then infer the iterative algorithm for the computation of the guided modes and associated eigenvalues with two nested loops:

- the outer loop consists in a fixed point algorithm to solve the non linear equation:

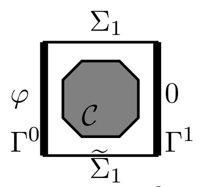
$$\mu_m(\omega) = \omega^2, \quad \omega^2 \notin \sigma_{ess}(\beta);$$

- each iteration of this fixed point algorithm requires the computation of the $m-$th eigenvalue $\mu_m(\alpha)$ of the operator $A_0(\beta,\alpha)$ (and possibly the derivative of $\mu_m(\alpha)$ with respect to α if a Newton method is used to solve the fixed point problem).

This algorithm is quite classical for the computation of guided modes in open waveguides (see [6]). Here the novelty comes from the fact that the eigenvalues ω^2 could belong to any gap of the spectrum and moreover that the operators $\Lambda^\pm(\beta,\omega)$ have no analytical expression, however they can be computed numerically.

2.2 Characterization of $\Lambda^\pm(\beta,\omega)$

As explained in [2], the construction of the operators $\Lambda^\pm(\beta,\omega)$ is based only on the resolution of a family of cell problems and the resolution of a stationary Ricatti equation. For the sake of clarity, we shall recall the method for the construction of Λ^+. Let $e_0(\beta,\varphi)$ and $e_1(\beta,\varphi)$ be the unique solutions in $H^1(\mathcal{C})$ to the following elementary cell problems



The periodicity cell $\mathcal{C}$

$$-\triangle e_\ell - \rho_p\, \omega^2 e_\ell = 0 \quad \text{in } \mathcal{C}, \qquad \ell \in \{0,1\}$$

satisfying β-quasi periodic boundary conditions on $\Sigma_1 = \Sigma \cap \mathcal{C}$ and $\widetilde{\Sigma}_1 = \widetilde{\Sigma} \cap \mathcal{C}$

$$e_\ell|_{\Sigma_1} = e^{\imath\beta}\, e_\ell|_{\widetilde{\Sigma}_1} \qquad \partial_y e_\ell|_{\Sigma_1} = e^{\imath\beta}\partial_y\, e_\ell|_{\widetilde{\Sigma}_1}.$$

and Dirichlet boundary conditions on Γ^0 and Γ^1

$$\left|\begin{array}{l} e_0|_{\Gamma^0} = \varphi \\ e_0|_{\Gamma^1} = 0 \end{array}\right. \quad \text{and} \quad \left|\begin{array}{l} e_1|_{\Gamma^0} = 0 \\ e_1|_{\Gamma^1} = \varphi \end{array}\right.$$

Let us now introduce the four corresponding local DtN operators :

$$\forall (i,j) \in \{0,1\}, \quad T_{ij}(\beta)\varphi = (-1)^{j+1} \partial_x e_i(\beta, \varphi)\Big|_{\Gamma^j}$$

We can show, by linearity of the problem, that the DtN operator can be expressed as

$$\Lambda^+(\beta, \omega) = T_{00}(\beta) + T_{10}(\beta)\, P(\beta)$$

where $P(\beta)$ is called the propagation operator.
Finally, to determine $P(\beta)$, we use the property that for any β, if $\omega^2 \notin \sigma_{ess}(\beta)$, $P(\beta)$ is the unique compact operator of spectral radius strictly less than 1, $\rho(P(\beta)) < 1$, solution to the stationary Ricatti equation ($\mathcal{E}_R$):

$$T_{10}(\beta)P(\beta)^2 + (T_{00}(\beta) + T_{11}(\beta))\, P(\beta) + T_{01}(\beta) = 0.$$

2.3 *Characterization of the essential spectrum*

The determination of the essential spectrum and then of the gaps is a by-product of the determination of the DtN operators. Indeed, in [2], we have shown that when ω^2 lies in the essential spectrum $\sigma_{ess}(\beta)$, not only the spectral radius of the propagation operator is equal to 1 but in addition this operator is no more the unique solution of the Ricatti equation ($\mathcal{E}_R$). Consequently, we can give this characterization of the essential spectrum of A

Theorem 3 *The Ricatti equation ($\mathcal{E}_R$) has a unique solution whose spectral radius is strictly less than one if and only if $\omega^2 \notin \sigma_{ess}(\beta)$.*

3 Numerical results

We plot on Figure 3 the isovalue lines of the function $\mu_1(\omega) - \omega^2$ for $\beta \in [0, \pi/L_y]$ and $\omega^2 \in [0, 20] \setminus \sigma_{ess}(\beta)$. For a fixed β, the white regions corresponds to the essential spectrum $\sigma_{ess}(\beta)$. Note that the function $\mu_1(\omega) - \omega^2$ vanishes several times in this interval but once per gap. The dispersion curves are given by the green lines corresponding to the null isovalue. We then represent in Figure 4 the guided modes for two values of β in eight periods from each side of the line defect. Figure 4(a) corresponds to the eigenvalue in the first gap of $A(0.5)$ with a well confined mode whereas in Figure 4(b) the eigenvalue belongs to the fourth gap of $A(1.9)$) and the associated guided mode is not well confined.

4 Towards the computation of the leaky modes

We have shown that this method is well adapted to the computation of guided modes which are not well confined. This DtN strategy can be applied to a β-formulation which is more adapted for dispersive media.

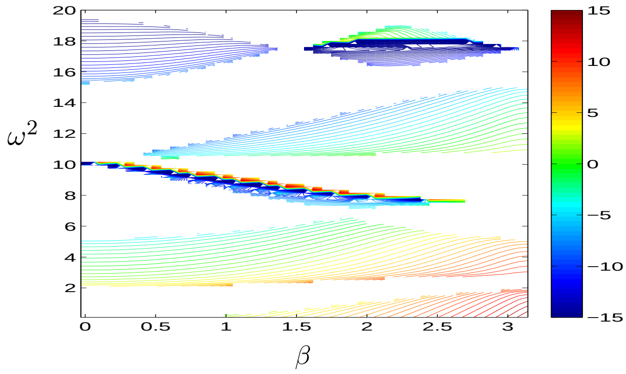
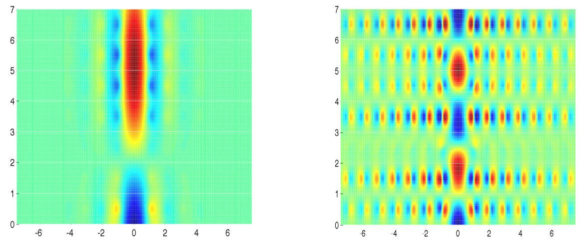


Figure 3: Contours of $\mu_1(\omega) - \omega^2$; $\beta \in [0, \pi/L]$, $\omega^2 \in [0, 20]$



(a) $\beta = 0.5$, $\omega^2 = 3.465$ (b) $\beta = 1.9$, $\omega^2 = 10.565$

Figure 4: Modes: well confined (left); not well confined (right).

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