Resonances of thin photonic membranes

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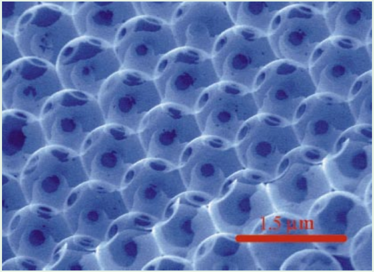
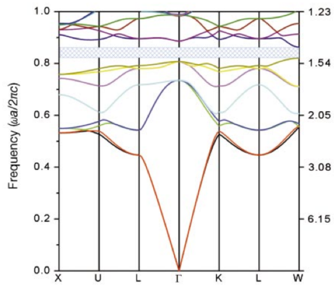
Photonic crystals

Periodic structures with strong dielectric contrast can exhibit bandgaps.

Example (experimental)





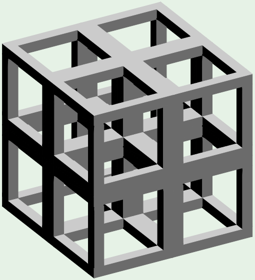
SEM image of a fabricated 3D PBG structure [Blanco et al, *Nature*, 2000]

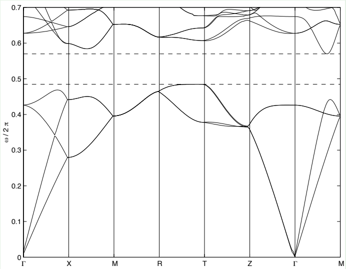
Localization of light having frequencies in the bandgap can be achieved by introducing "defects" in the periodic pattern.

Photonic crystals

Periodic structures with strong dielectric contrast can exhibit bandgaps.

Example (computational)



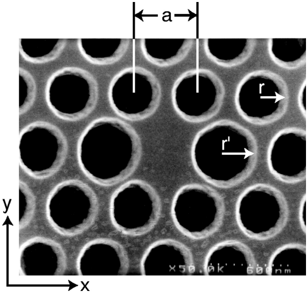


Infinite 3D scaffold structure analyzed in [Dobson, G, & Pasciak, *JCP*, 2000]

Localization of light having frequencies in the bandgap can be achieved by introducing "defects" in the periodic pattern.

Photonic membranes

- Practical photonic structures are finite and have truncated periodic pattern. (They are hence open and lossy.)
- It is practically easier to fabricate (etch) 2-dimensional "membranes" on which periodically spaced air holes can be created.
- Even if they have no bandgaps, they can have useful resonant modes.



An SEM image of a free-standing PBG membrane with a "defect".
[Painter et al, *Science*, 1999]

The mathematical problem

- Compute resonant frequencies k and corresponding resonant modes of thin photonic membranes.
- Identify resonance modes that have high localization within fabricated "defect" regions.

Resonance k is a complex number for which there is a non-trivial function u satisfying

$$\begin{aligned} \Delta u + k^2 \varepsilon(x) u = 0 & \qquad \text{in all } \mathbb{R}^n, \\ u \text{ is "outgoing"} & \qquad \text{at infinity.} \end{aligned}$$

Here ε = refractive index, and "outgoing" has many definitions...

Outgoing wave

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- For *real* k, the standard definition of the "outgoing" condition is the Sommerfeld's radiation condition
$$\lim_{r\to\infty} r^{1/2}\Big|\frac{\partial u}{\partial r} - iku\Big| = 0.$$
However this is not correct for general complex k.

- For *complex* k, expressions that are analytic continuations of expressions in the real k case are used to define "outgoing" waves:
  - Series representation (2d): u is outgoing if
$$u(r,\theta) = \sum_{n=-\infty}^{\infty} c_n e^{in\theta} H_n^1(kr).$$
  - Volume integral representation:
$$u(x) = \int_D G_k(x;y)\, f(y)\, dy$$
where G_k is the free-space Green's function.

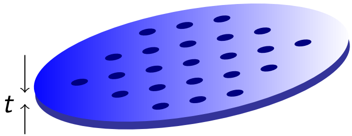
Two approaches

We will report results obtained by approaching the problem using two very different computational techniques:

1. Discretize an asymptotic limit of a Lippman-Schwinger-type integral formulation for the resonance problem.
   - Results in a *small* *dense* *nonlinear* *eigenproblem*.
2. Discretize using finite elements combined with the perfectly matched layer (PML).
   - Results in a *large* *sparse* *generalized* *eigenproblem*.

Thin, high-contrast membranes

- Geometry:



Dielectric membrane occupies the volume

$$D = \Omega \times (-\frac{t}{2}, \frac{t}{2}).$$

- Assume that the membrane thickness t is small:

$$t \ll \mathrm{diam}(\Omega).$$

- Assume high contrast dielectric:

$$\varepsilon(x_1, x_2, x_3) = \begin{cases} \dfrac{\varepsilon_0(x_1, x_2)}{t}, & \text{if } |x_3| < t/2 \text{ and } (x_1, x_2) \in \Omega, \\ 1, & \text{otherwise.} \end{cases}$$

Resonance via Lippman-Schwinger

- The source problem was analyzed in [Moskow, Santosa & Zhang, 2005] by asymptotics on the Lippman-Schwinger equation.
- Follow along the same lines for the resonance problem:

$$\begin{aligned} & \Delta u + k^2 \varepsilon\, u = 0 \\ \Longrightarrow \quad & \Delta u + \quad k^2 u = (1-\varepsilon) k^2 u. \end{aligned}$$

Using the outgoing fundamental solution $G_k(x; y)$, we thus formally obtain a Lippman-Schwinger type volume integral equation for the resonance:

$$\Longrightarrow \qquad u(x) = k^2 \int_D G_k(x;y) \big(1 - \varepsilon(y)\big)\, u(y)\, dy.$$

For our thin membrane, this implies

$$u(x) = k^2 \int_\Omega \int_{-t/2}^{t/2} G_k(x;y) \left(1 - \frac{\varepsilon_0(y_1, y_2)}{t}\right) u(y)\, dy.$$

Scaled operators

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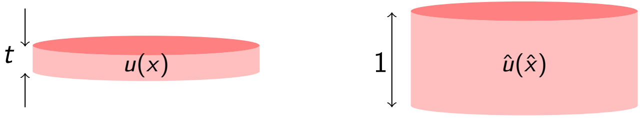
From previous slide	$$u(x) = k^2 \int_\Omega \int_{-t/2}^{t/2} G_k(x;y) \left(1 - \frac{\varepsilon_0(y_1,y_2)}{t}\right) u(y)\, dy.$$

We map to a fixed scaled domain $\hat{D}$,



$D = \Omega \times (-t/2, t/2)$ $\qquad$ $\hat{D} = \Omega \times (-1/2, 1/2)$

and recast the problem: $\hat{u} = k^2 T_t(k)\, \hat{u},$ $\qquad T_t(k) : L^2(\hat{D}) \mapsto L^2(\hat{D}),$

$$T_t(k)\hat{u}\,(\hat{x}) = \int_\Omega \int_{-1/2}^{1/2} G_k(\hat{x}_1, \hat{x}_2, t\hat{x}_3; \hat{y}_1, \hat{y}_2, t\hat{y}_3)\big(t - \varepsilon_0(\hat{y}_1, \hat{y}_2)\big)\, \hat{u}(\hat{y})\, d\hat{y}.$$

The formal asymptotic limit (as $t \to 0$) is now clear.

1st approach: Asymptotic limit

Limiting operator $T_0(k)$:

$$T_0(k)\hat{v}\,(\hat{x}) = -\int_\Omega \int_{-1/2}^{1/2} G_k(\hat{x}_1, \hat{x}_2, 0; \hat{y}_1, \hat{y}_2, 0)\, \varepsilon_0(\hat{y}_1, \hat{y}_2)\, \hat{v}(\hat{y})\; d\hat{y}.$$

Limiting resonance problem: Find $\{k_0, u_0\}$ satisfying

$$u_0 = k_0^2\, T_0(k_0)\, u_0.$$

(nonlinear eigenproblem)

Discretization: Collocation scheme using piecewise linear continuous approximants with respect to a uniform grid.

- Dense nonlinear eigenproblem
- Small eigenproblem (due to the dimension reduction)
- Can solve using Residual Inverse Iteration [Neumaier, 1985].

To obtain rate of convergence using [Osborn, 1975], we assume:

- k_t is a resonance of T_t. $\qquad u_t = k_t^2\, T_t(k_t)\, u_t.$
- k_t converges to some k_0 in $\mathbb{C}$.
- k_0 is a simple resonance of T_0. $\qquad u_0 = k_0^2\, T_0(k_0)\, u_0.$
- Normalize $\langle u_0, u_0 \rangle = 1$ and assume $k_0^2 \langle D(k_0) u_0, u_0 \rangle \neq -1$, where $D(k)v = \frac{\partial}{\partial k}(k T_0(k) v)$.

Theorem (Rate of convergence)

There exists C independent of t such that

$$|k_t - k_0| \leq C\, t,$$

and furthermore

$$k_t = k_0 + k_0^2 \frac{\langle (T_0(k_0) - T_t(k_0)) u_0, u_0 \rangle}{1 + k_0^2 \langle D(k_0) u_0, u_0 \rangle} + O(t^2).$$

2nd approach: Apply PML

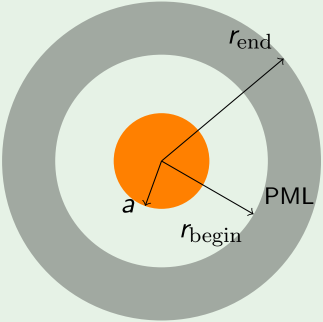
- PML [Berenger 1994] extensively used for source problems.
- Does it work for resonance computations?
  - Airplane noise (slat resonance) [Hein, Hohage, Koch, Schöberl, 2007]
  - Often used in engineering. Spurious modes reported.
- To validate PML, consider a problem with calculable exact resonances.

Example: Resonances of a disk

A circular homogeneous dielectric disk ($\varepsilon = 4$) of radius $a = 1$ is placed in infinite vacuum.

Compute using finite elements with PML set in region $r_{\text{begin}} < r < r_{\text{end}}$.

At PML truncation $r = r_{\text{end}}$, set zero b.c.

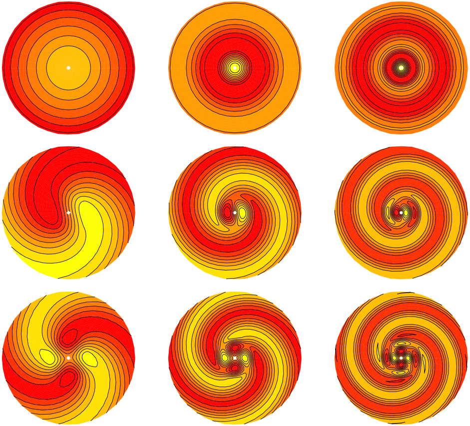


Example: Exact solution

$n = 0$
(simple modes)

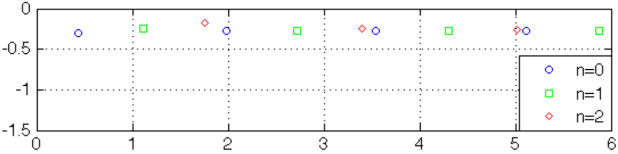
$n = 1$
(multiplicity 2)

$n = 2$
(multiplicity 2)



Figures show region $r < 3$.

Corresponding k-values in the complex plane



Things to learn from the example

1. Approximations can seem to converge, but to the wrong solution!

Apparent order of convergence	Difference in resonances with successive mesh refinements			
	$\lvert k^{(h)} - k^{(h/2)}\rvert$	$\lvert k^{(h/2)} - k^{(h/4)}\rvert$	$\lvert k^{(h/4)} - k^{(h/8)}\rvert$	$\lvert k^{(h/8)} - k^{(h/16)}\rvert$
1.90	0.0100	0.0029	0.0007	0.0002

Actual order of convergence	Actual errors in computed resonances			
	$\lvert k^{(h)} - k\rvert$	$\lvert k^{(h/2)} - k\rvert$	$\lvert k^{(h/4)} - k\rvert$	$\lvert k^{(h/8)} - k\rvert$
0.01	0.0971	0.0957	0.0954	0.0953

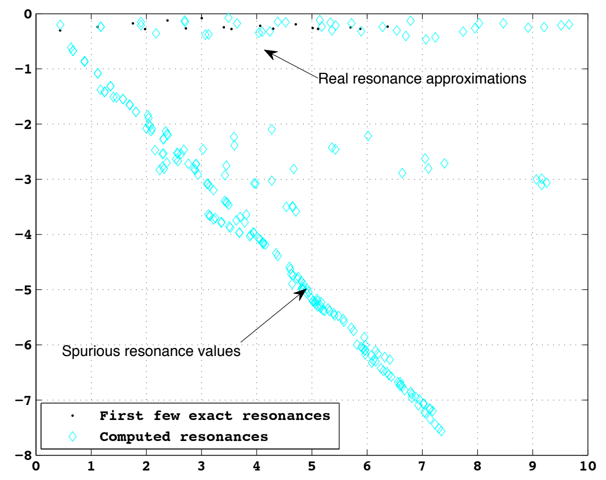
(Here h = initial meshsize, $k^{(h)}$ = computed resonance, k = exact resonance.)

Explanation: PML truncation alters the exact spectrum. Discrete spectrum tries to converge to the altered spectrum.

Moral: Truncation distance r_{end} should be carefully chosen.

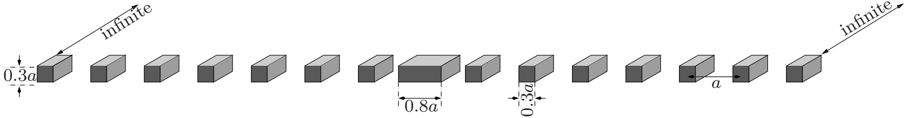
Things to learn from the example

1. Approximations can seem to converge, but to the wrong solution!
2. Spurious modes can arise!

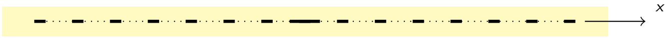


A simple 2D photonic membrane

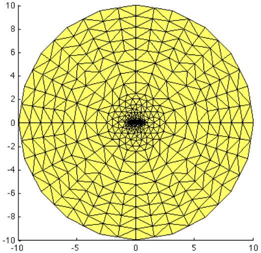
We apply both approaches to an example from [Fan et al, 1995]:



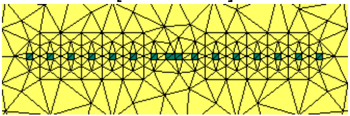
1. Asymptotic approach uses a uniform 1D mesh. (size: 2,289)



2. PML approach uses 2D mesh. (size: 221,201)



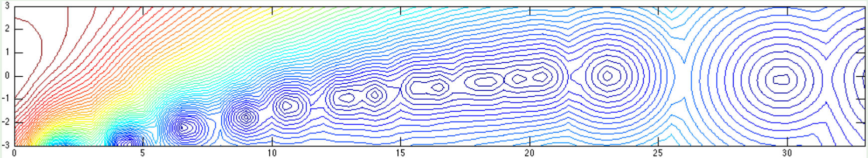
[zoomed in]



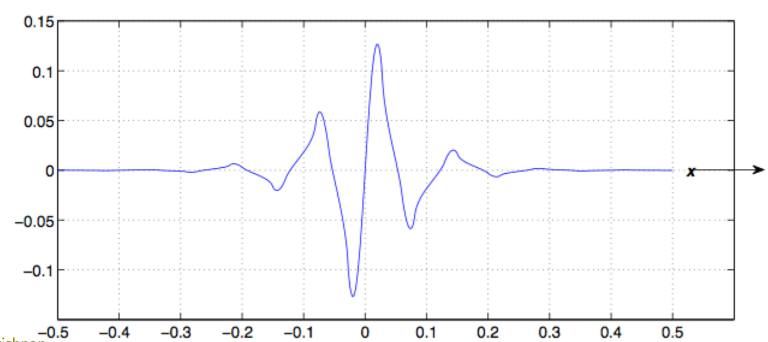
This mesh is further refined 4 times.

Results from 1st approach (asymptotic)

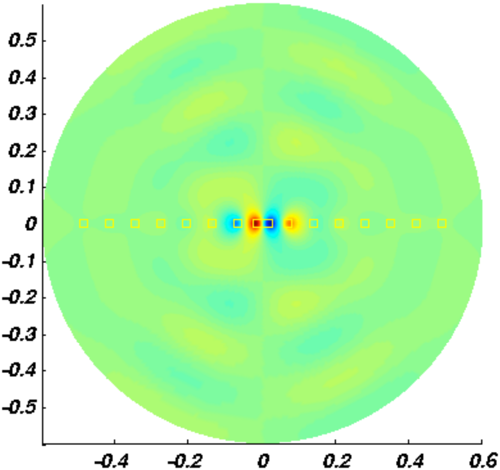
A coarse pseudospectra-type plot: $\sigma_{\min}(I - k^2 T_0^{\mathrm{aprx}}(k))$ on $\mathbb{C}$



A localized eigenfunction: $k = 28.0236 - 0.0005i$

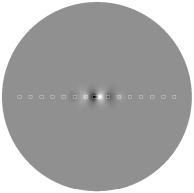


Results from 2nd approach (PML)



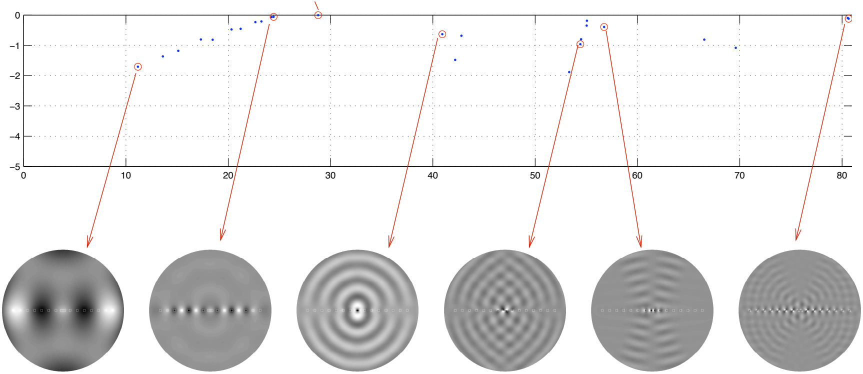
A highly localized resonance mode found at $k = 28.7878 - 0.0017i$

Results from 2nd approach (PML)



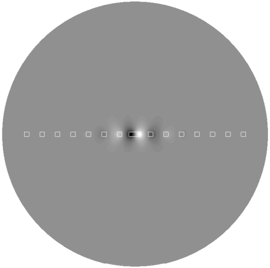
← The localized resonance mode.

↓ First few resonances
(after removing spurious ones and adjusting truncation distance "by hand").

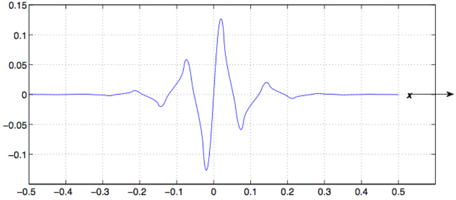


Comparison

Our result from the PML approach

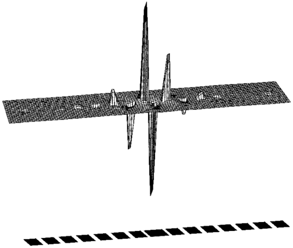


Our result from the asymptotic approach



As we see, the interesting mode is captured by all the three experiments.

FDTD result: Figure from [Fan et al, 1995]



Conclusions

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- For thin high-contrast membranes, we formulated and analyzed a dimension reduced asymptotic limit.
- The asymptotic approach is very effective for calculating resonances of thin photonic membranes.
  - Need better nonlinear eigensolvers.
- The PML approach is also effective, once we remove spurious modes and choose truncation distance correctly.
  - Need to automate spurious mode removal and truncation choices.
- Our two approaches when applied to a simple 2D photonic membrane, yielded results close to those obtained in literature by FDTD simulations.

Reference: [G., Moskow & Santosa, SIAP, 2008] Asymptotic and numerical techniques for resonances of thin photonic structures, ☞doi: 10.1137/070701388.