High order FEM computation of resonances in nanostructures

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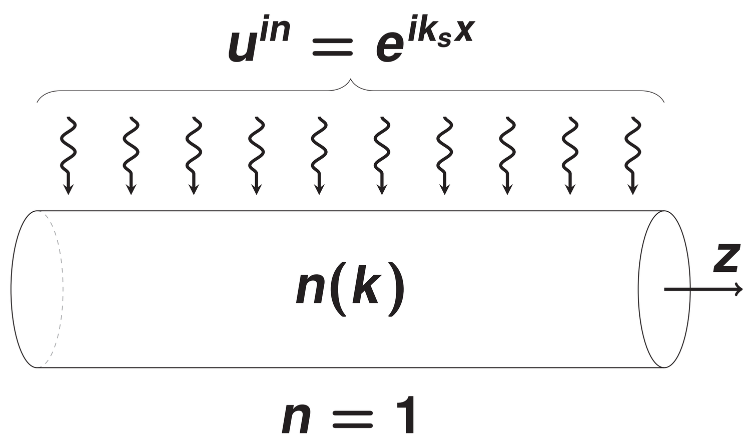
1) Scattering in dielectric resonators (TM)

Objective: Accurate computation of resonances in nano structures. Specifically, we study light confinement in prism-scatterers with arbitrarily shaped faces. Applications: design optimization of sensors, optical filters.

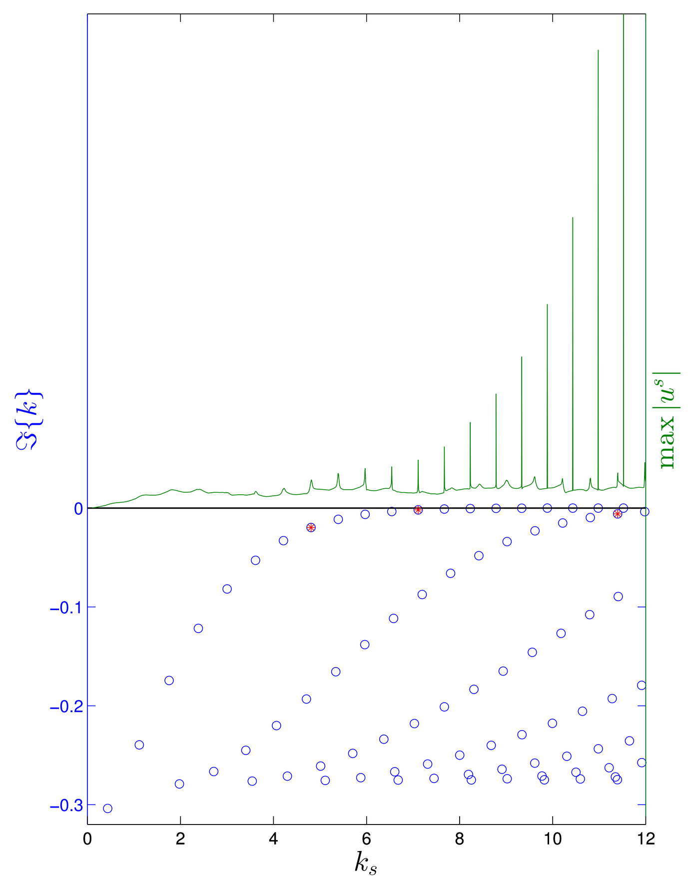
Model:
- Maxwell equations in Fourier space $\partial_t \to -i\omega$ with $k^2 = \varepsilon_0\mu_0\omega^2$
- Infinitely long dielectric ($\partial_z \to 0$) in exterior domain
- TM-polarization $\mathbf{E} = [0, 0, u(x, y)]$, $H_z = 0$. We reduce to 2D, where u satisfies: $\mathcal{L}(k)\, u := \Delta u + k^2 n^2(\mathrm{r}, k) u = 0$
- $n(\mathrm{r}, k)$: refractive index, where $n \neq 1$, for $\mathrm{r} \in \Omega_s$ (dielectric)
- Scattering problem: $k_s \in \mathbb{R}$ and u^i are given, then we solve for **outgoing** solutions u^{out} of $\mathcal{L}(k_s)\, u = 0$



3) Motivation: Energy peaks

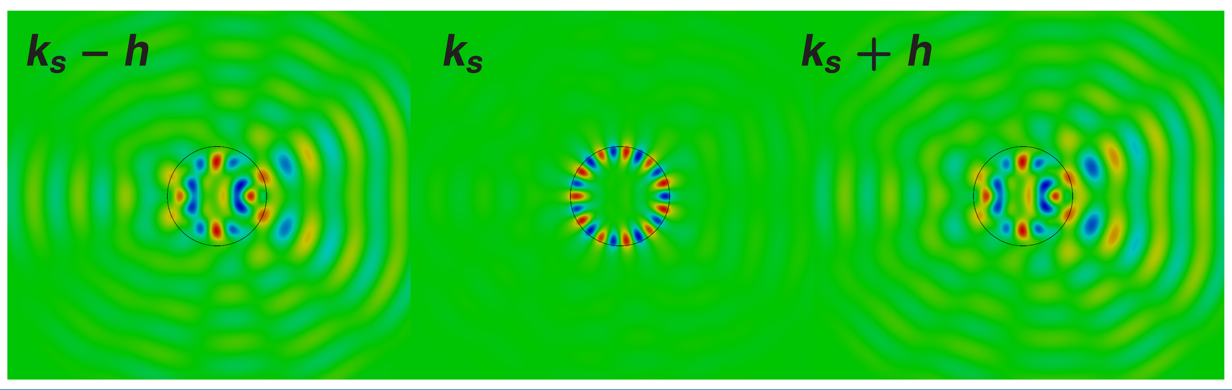
- Incident plane waves with wave number $k_s \in \mathbb{R}$ excite amplitude peaks.
- Finding k_s by frequency sweeps is generally computationally expensive.
- Resonator's quality factor: $$Q_m = \frac{\Re\{k_m\}}{2|\Im\{k_m\}|}$$
- Peaks and resonances k_m are related by the scattering problem through Q_m:

Take $k_s = \Re\{k_m\}$ provided Q_m is large.



Scattering example

$k_m = 7.109 – 0.0018i$
$h = 0.005$
$k_s = 7.109$



5) Modeling exterior domains: Dirichlet-to-Neumann map

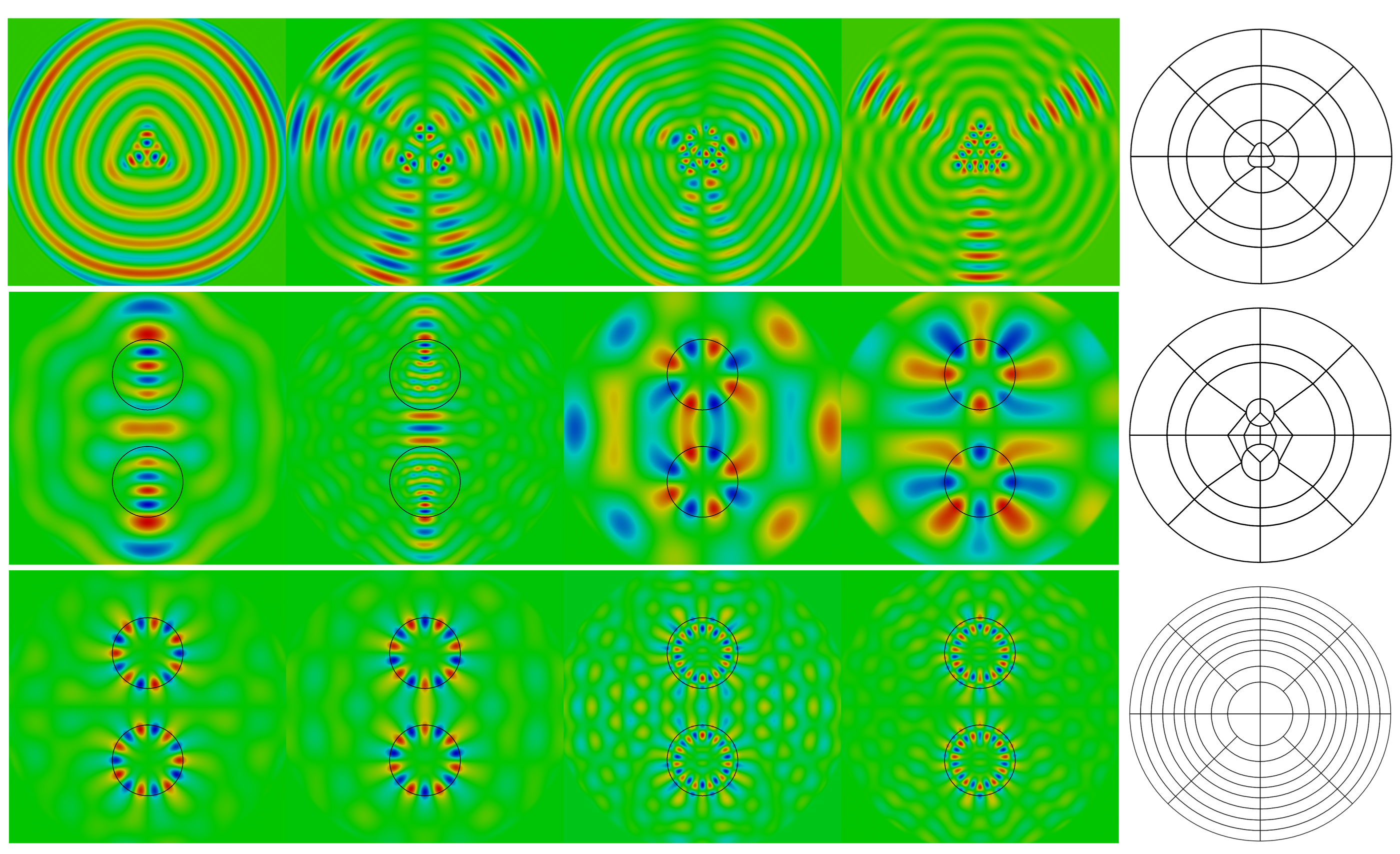
- Introduce an outer circle Γ_a with radius $r = a$ containing the scatterer Ω_s and use the exact series for outgoing waves in $\mathrm{r} \in \Omega^+ \equiv \mathbb{R}^2 \setminus \Omega_a$

$$\Delta u + k^2 n^2(k, \mathrm{r}) u = 0, \qquad \mathrm{r} \in \Omega_a$$
$$\nabla u \cdot \mathrm{n} = \mathcal{G}u, \qquad \mathrm{r} \in \Gamma_a \quad \text{(DtN map)}$$

$$\mathcal{G}u \equiv -\frac{\partial u^+}{\partial r}\bigg|_{r=a} = -\frac{1}{2\pi}\sum_{m=-\infty}^{\infty} k\frac{H_m'(ka)}{H_m(ka)} e^{im\theta}\int_0^{2\pi} u(a, \theta')\, e^{-im\theta'}\, d\theta'$$

- Truncate the series until $|m| = l$, with $l > a\Re\{k\}$
- Weak form: Find eigenpairs (u, k) such that: (nonlinear in k)
$$(\nabla u, \nabla \bar{v})_{\Omega_a} - k^2(n^2(k, \mathrm{r})u, \bar{v})_{\Omega_a} + (\mathcal{G}^l(k)u, \bar{v})_{\Gamma_a} = 0, \quad u, v \in H^1(\Omega_a)$$
- Nonlinear eigenvalue problem, solver: NEPCISS in SLEPc-3.6.0.

7) Resonances of arbitrarily shaped scatterers



- We use curved elements (*Manifolds* in Deal.II library) and polynomial order $p = 20$

2) Problem description and challenges

- A **resonance** state is a long-lived state of an open system and can be determined by applying a DtN-map formulation or by a perfectly matched layer (PML) to $\mathcal{L}(k)\, u = 0$; resonances $k_m \in \mathbb{C}$.
- Solutions $u_m \notin L^2(\mathbb{R}^2)$ grow as $e^{|\Im\{k_m\}|d}$, with d the distance from Ω_s. This makes the u_m difficult to compute by any discretization method.
- Sectors in the k-plane may have large resolvent norms, which results in spurious solutions for poor discretizations (spectral pollution). Example: allowing large *air* regions in the computational domain.
- Identifying spurious solutions is an unsolved problem.
- We discretize by using FEM with high polynomial degree. We use *Gauss-Lobatto* shape functions and curvilinear elements in **deal.II**.

4) Modeling exterior domains: Radial PML

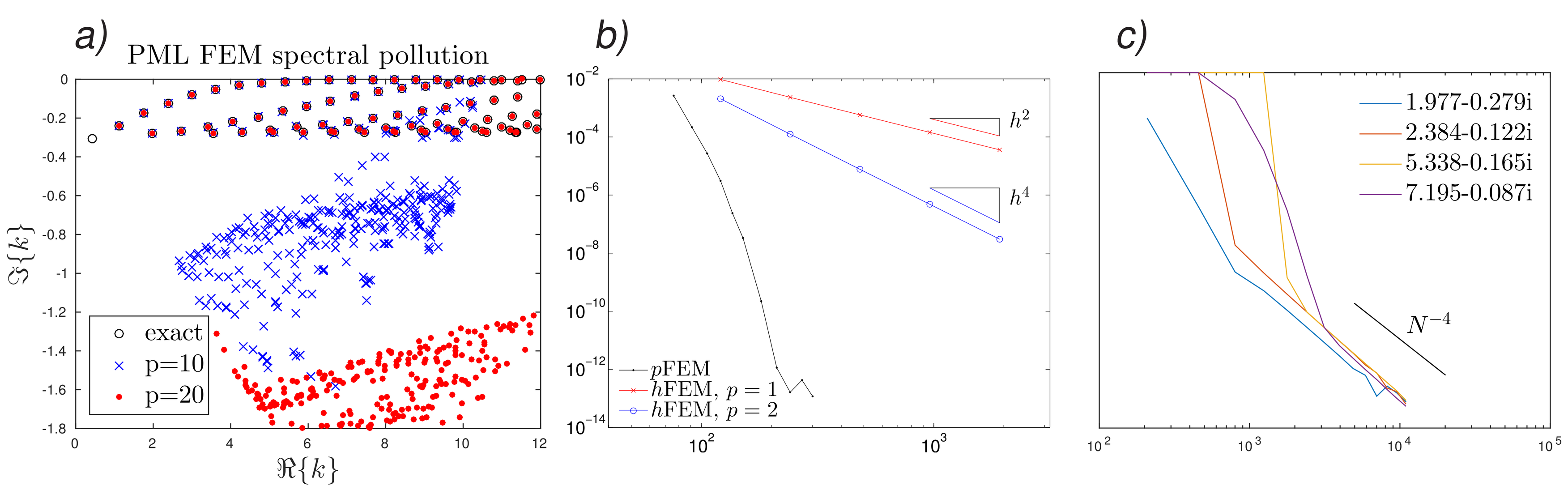
- Coordinate stretching $\nabla \cdot (\mathcal{A}\nabla u) + k^2 n^2 \mathcal{B}\, u = 0, \;\; \mathrm{r} \in \Omega_d$; $\;u = 0, \;\; \mathrm{r} \in \Gamma_d$

with definitions $\alpha := 1 + i\sigma(r)$,

$$\mathcal{A}(\mathrm{r}) = \begin{pmatrix} \frac{\tilde\alpha}{\alpha}\cos^2\theta + \frac{\alpha}{\tilde\alpha}\sin^2\theta & \left(\frac{\tilde\alpha}{\alpha} - \frac{\alpha}{\tilde\alpha}\right)\sin\theta\cos\theta \\ \left(\frac{\tilde\alpha}{\alpha} - \frac{\alpha}{\tilde\alpha}\right)\sin\theta\cos\theta & \frac{\tilde\alpha}{\alpha}\sin^2\theta + \frac{\alpha}{\tilde\alpha}\cos^2\theta \end{pmatrix}, \quad \mathcal{B}(\mathrm{r}) = \alpha\tilde\alpha$$

- Weak form: Find eigenpairs (u, k^2) s.t:
$$(\mathcal{A}\nabla u, \nabla \bar{v})_{\Omega_d} - k^2(n^2(k, \mathrm{r})\mathcal{B}u, \bar{v})_{\Omega_d} = 0; \quad u, v \in H_0^1(\Omega_d)$$
- $\mathcal{A}$ is the identity in air/scatterer, and has diagonal form for $r > r_2$
- Parameters: domain's truncation d and strenght σ_0
- Generalized linear eigenvalue problem for $n(k, \mathrm{r}) \equiv n(\mathrm{r})$ and $\lambda \equiv k^2$
- Solver: *EPSKRYLOVSCHUR* in SLEPc.

6) Convergence and comparison



- In *a)* we show examples of spectral pollution from PML computations. It is evident that improving the mesh quality (increasing the polynomial degree p) moves spurious eigenvalues away from the area of interest.
- In *b)* we show relative errors for the 3^{rd} eigenvalue in the PML 1D case. The simplicity of the problem allow us to study convergence for *i) hFEM*: where we keep p fixed and decrease the mesh size h, and *ii) pFEM*: where h is fixed and we increase p. In *i)* we obtain h^{2p} convergence, where in *ii)* we obtain exponential convergence.
- In *c)* we show relative errors for the 2D disk computed with the DtN method and $l = 30$ (truncation index) for selected eigenvalues. We used the nonlinear eigenvalue solver NEPCISS in SLEPc.

8) PML vs DtN for linear materials: $n(\mathrm{r}, k) \equiv n(\mathrm{r})$

PML:
+ Linear eigenvalue problem.
+ Easy to implement.
– Nonphysical eigenvalues satisfy the PML PDE.
– Resonances with small $|\Re\{k\}|$ require large σ_0, more dofs!
– Parameters σ_0 and d are not straight forward to control.
– Requires extra cells/dofs for the PML layer.
– Spurious eigenvalues appear for poor discretizations.

DtN:
+ Exact boundary condition, only resonances are eigenvalues.
+ The only parameter is l (truncation of the series).
+ Only physical cells are required (fewer dofs).
– Resonance problem: nonlinear eigenvalue problem (quadratic in 1D).
– Implementation requires keeping $2l + 1$ DtN dense boundary matrices.
– Spurious eigenvalues appear for poor discretizations.

- Spectral pollution can be diminished by using finer discretizations.
- Eigenvalue computation of non-self adjoint operators is a challenging task.