Numerical Methods for Scattering Poles

Jiguang Sun

Michigan Technological University

Joint with Gong, Lin, Ma, Xi and Xiao

Numerical methods for spectral problems: theory and applications
August 5 - 9, 2024 Guiyang, China.

Research funded in part by NSF and SIMONS Foundation

Scattering Resonances/Poles

- Scattering poles/resonances play a significant role in scattering theory and carry important physical information - acoustics, electromagnetics, quantum mechanic, etc.
- They are the poles of the meromorphic continuation of the scattering operator.
- There exist many computational papers from the engineering community and limited studies from the numerical analysis community.
- The problems are nonlinear and defined on unbounded domains. The spectrum can be way more complicated than spectrum of compact self-adjoint operators (e.g., Laplace eigenvalue problem and Maxwell's eigenvalue problem).
- Existing results can be misleading and wrong.

[Lax and Phillips 1989], [Taylor,1996], [Dyatlov and Zworski 2019]

Scattering Poles for a Sound Soft Obstacle

Let $D \subset \mathbb{R}^2$ be a bounded simply connected smooth domain. The scattering problem is to find $u \in H^1_{loc}(\mathbb{R}^2 \setminus \overline{D})$ such that

$$\begin{aligned} &\Delta u + k^2 u = 0 && \text{in } \mathbb{R}^2 \setminus \overline{D}, \\ &u = g && \text{on } \partial D, \\ &\lim_{r\to\infty} \sqrt{r}\left(\frac{\partial u}{\partial r} - iku\right) = 0, && \end{aligned} \tag{1}$$

where $k \in \mathbb{C}$ is the wave number, $g \in L^2(\partial D)$, and $r = |x|$.

For k, $\mathrm{Im}(k) \geq 0$, there exists a unique solution u to (7). The scattering operator $\mathcal{B}(k)$ is defined as $u = \mathcal{B}(k)g$.

The operator $\mathcal{B}(k)$ is holomorphic on the upper half-plane of $\mathbb{C}$ and can be meromorphically continued to the lower half complex plane.

The poles of $\mathcal{B}(k)$ is the discrete set $\{k \in \mathbb{C} : \mathrm{Im}(k) < 0\}$, which are called the scattering poles.

Holomorphic Operator Functions

Definition

Let $\Lambda \subset \mathbb{C}$ be open and connected. Let X and Y be Banach spaces. A function $\Lambda \ni \eta \mapsto F(\eta) \in \mathcal{L}(X, Y)$ is holomorphic if

$$\lim_{h \to 0} \frac{F(\eta + h) - F(\eta)}{h}$$

exists for all $\eta \in \Lambda$.

Assume that $F(\eta)$ is Fredholm. A complex $\lambda \in \Lambda$ is an eigenvalue of F if there exists a nontrivial $x \in X$ such that

$$F(\lambda)x = 0.$$

The resolvent set of F is $\rho(F) := \{\eta \in \Lambda : F(\eta)^{-1} \in \mathcal{L}(Y, X)\}$. The spectrum $\sigma(F) := \Lambda \setminus \rho(F)$.

Goal: To compute eigenvalues of $F(\cdot)$.

Abstract Approximation Theory

Abstract approximation theory for eigenvalue problems of holomorphic Fredholm operator functions was studied in [Grigorieff 1975, Vainikko 1976, Karma 1996].

Let $X_n, \; Y_n, \; n \in \mathbb{N}$, be Banach spaces. Consider a sequence of operator functions $F_n(\cdot)$. Denote by $\mathcal{P}$ and $\mathcal{Q}$ two sequences of operators $\mathcal{P} = \{p_n\}_{n\in\mathbb{N}}$, $\mathcal{Q} = \{q_n\}_{n\in\mathbb{N}}$ with $p_n \in \mathcal{L}(X, X_n)$ and $q_n \in \mathcal{L}(Y, Y_n)$.

A sequence $\{y_n\}_{n\in\mathbb{N}}$ with $y_n \in Y_n$ is discrete-compact if, for each subsequence $\{y_n\}_{n\in\mathbb{N}'}$, $\mathbb{N}' \subset \mathbb{N}$, there exists $\mathbb{N}'' \subset \mathbb{N}'$ and $y \in Y$ s.t. $\|y_n - q_n y\|_{Y_n} \to 0$, $n \to \infty$, $n \in \mathbb{N}''$.

Definitions of Convergence

- $F_n \in \mathcal{L}(X_n, Y_n)$ converges to $F \in \mathcal{L}(X, Y)$ if

$$\|F_n p_n x - q_n F x\|_{Y_n} \to 0, \quad n \to \infty, \quad \forall x \in X.$$

- $F_n \in \mathcal{L}(X_n, Y_n)$ converges uniformly to $F \in \mathcal{L}(X, Y)$ if

$$\|F_n p_n - q_n F\| \to 0, \quad n \to \infty.$$

- $F_n \in \mathcal{L}(X_n, Y_n)$ converges compactly to $F \in \mathcal{L}(X, Y)$ if F_n converges to F, meanwhile $\|x_n\|_{X_n} \leqslant C, \forall n \in \mathbb{N}$ implies $\{F_n x_n\}$ is $\mathcal{Q}$-compact.
- $F_n \in \mathcal{L}(X_n, Y_n)$ converges stably to $F \in \mathcal{L}(X, Y)$ if F_n converges to F, meanwhile there exists n_0 s.t. F_n is invertible with $\|F_n^{-1}\| \leqslant C, \forall n \geqslant n_0$.
- $F_n \in \mathcal{L}(X_n, Y_n)$ converges regularly to $F \in \mathcal{L}(X, Y)$ if F_n converges to F, meanwhile $\{F_n x_n\}$ is $\mathcal{Q}$-compact implies $\{x_n\}$ is $\mathcal{P}$-compact.

Abstract Convergence Theorem

Let Λ_0 be a compact subset of Λ such that $\partial\Lambda_0 \subset \rho(F)$ and $\sigma(F) \cap \Lambda_0 = \{\lambda\}$. If the following three properties hold,

1. The operators p_n and q_n satisfy

$$\lim_{n\to\infty} \|p_n u\|_{X_n} = \|u\|_X,\ \forall u \in X, \quad \lim_{n\to\infty} \|q_n v\|_{Y_n} = \|v\|_Y,\ \forall v \in Y;$$

2. $\{F_n(\cdot)\}_{n\in\mathbb{N}}$ is equibounded on any compact $\Lambda_0 \subset \Lambda$, i.e.,

$$\|F_n(\lambda)\| \leq C, \quad \forall\lambda \in \Lambda_0,\ n \in \mathbb{N},$$

3. $\{F_n(\lambda)\}_{n\in\mathbb{N}}$ converges regularly to $F(\lambda)$ for every $\lambda \in \Lambda$,

then, for sufficiently large n, there exist $\lambda_n \in \sigma(F_n) \cap \Lambda_0$ such that

$$|\lambda_n - \lambda| \leqslant C\epsilon_n^{1/r},$$

where

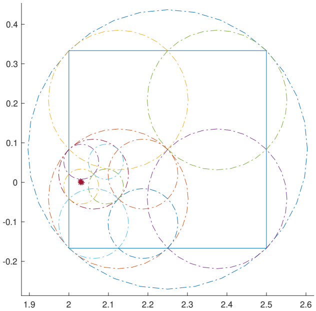
$$\epsilon_n = \sup_{\substack{\eta\in\partial\Lambda_0 \\ u\in G(\lambda),\|u\|_1=1}} \|F_n(\eta)p_n u - q_n F(\eta)u\|_{Y_n},$$

and r is the maximum length of Jordan chain of λ.

Parallel Multistep Spectral Indicator Method

Consider a sequence of approximations $F_n : \Lambda \to \mathcal{L}(X_n, Y_n), n \in \mathbb{N}$.

Define $P : Y_n \to X_n$ such that $P = \dfrac{1}{2\pi i} \int_\Gamma F_n(\eta)^{-1} d\eta$.



- Xi and S., *Parallel Multi-step Spectral Indicator Method for Nonlinear Eigenvalue Problems.* arXiv:2312.13117
- Huang, S., and Yang, *Recursive integral method with Cayley transformation.* Numer. Linear Algebra Appl. 25 (2018), no. 6, e2199.

Scattering Poles for a Sound Soft Obstacle

Let $D \subset \mathbb{R}^2$ be a bounded simply connected smooth domain. The scattering problem is to find $u \in H^1_{loc}(\mathbb{R}^2 \setminus \overline{D})$ such that

$$\begin{aligned} &\Delta u + k^2 u = 0 && \text{in } \mathbb{R}^2 \setminus \overline{D}, \\ &u = g && \text{on } \partial D, \\ &\lim_{r\to\infty} \sqrt{r} \left(\frac{\partial u}{\partial r} - iku \right) = 0, && \end{aligned} \tag{2}$$

where $k \in \mathbb{C}$ is the wave number, $g \in L^2(\partial D)$, and $r = |x|$.

For k, $\mathrm{Im}(k) \geq 0$, there exists a unique solution u to (7). The scattering operator $\mathcal{B}(k)$ is defined as $u = \mathcal{B}(k)g$.

The operator $\mathcal{B}(k)$ is holomorphic on the upper half-plane of $\mathbb{C}$ and can be meromorphically continued to the lower half complex plane.

The poles of $\mathcal{B}(k)$ is the discrete set $\{k \in \mathbb{C} : \mathrm{Im}(k) < 0\}$, which are called the scattering poles.

A Model Problem

Let D be the unit disc. Using polar coordinates, one seeks

$$u(r,\theta) = \frac{1}{2}\alpha_0 H_0^{(1)}(kr) + \sum_{\nu=1}^{\infty} \alpha_\nu H_\nu^{(1)}(kr)\cos\nu\theta + \sum_{\nu=1}^{\infty} \beta_\nu H_\nu^{(1)}(kr)\sin\nu\theta, \; r > 1,$$

where $H_\nu^{(1)}$ is the Hankel function. On ∂D,

$$u(\theta) = \frac{1}{2}\alpha_0 H_0^{(1)}(k) + \sum_{\nu=1}^{\infty} \alpha_\nu H_\nu^{(1)}(k)\cos\nu\theta + \sum_{\nu=1}^{\infty} \beta_\nu H_\nu^{(1)}(k)\sin\nu\theta.$$

Assume that $g(\theta) = \frac{1}{2}a_0 + \sum_{\nu=1}^{\infty} a_\nu \cos(\nu\theta) + \sum_{\nu=1}^{\infty} b_\nu \sin(\nu\theta)$. Matching u and g on ∂D, we obtain

$$\alpha_0 = \frac{a_0}{H_0^{(1)}(k)}, \quad \alpha_\nu = \frac{a_\nu}{H_\nu^{(1)}(k)}, \quad \beta_\nu = \frac{b_\nu}{H_\nu^{(1)}(k)}, \quad \nu = 1, 2, \ldots$$

The scattering poles for the unit disc are the zeros of $H_\nu^{(1)}(k)$.

Exact Zeros of Hankel Functions

Zeros of Hankel functions were studied by many researchers. Table III of [Doring 1966].

Table: Some small zeros of Hankel functions in the fourth quadrant of $\mathbb{C}$.

ν	zeros of $H_\nu^{(1)}(k)$
2	$0.4294849652 - 1.2813737977i$
3	$1.3080120323 - 1.6817888047i$
4	$2.2043719815 - 1.9781618635i$
	$0.4326966486 - 2.6286711680i$
5	$3.1130829450 - 2.2186262746i$
	$1.3038823977 - 3.1351328447i$

Exact Zeros of Hankel Functions

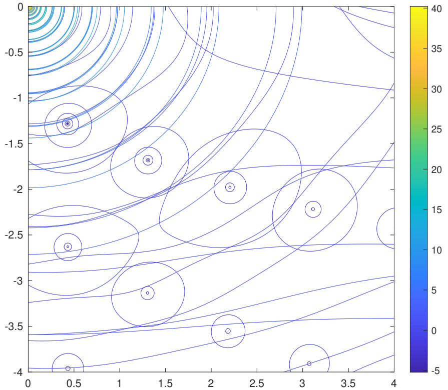


Figure: Absolute value of $H_{\nu}^{(1)}(k)$, $\nu = 2, \ldots, 7$, in log scale.

Integral Formulations

For $\phi \in L^2(\partial D)$, define the single and double layer operators as

$$(S(k)\phi)(x) := 2\int_{\partial D} \Phi(x,y,k)\phi(y)ds(y), \quad x \in \partial D, \tag{3}$$

and

$$(K(k)\phi)(x) := 2\int_{\partial D} \frac{\partial \Phi(x,y,k)}{\partial n(y)}\phi(y)ds(y), \quad x \in \partial D, \tag{4}$$

$S(k)$ and $K(k)$ are compact operators on $L^2(\partial D)$ for each $k \in \mathbb{C}$ with holomorphic dependence on k [Taylor 1996].

We seek u in the form of

$$u(x) = \int_{\partial D} \frac{\partial \Phi(x,y,k)}{\partial n(y)}\phi(y)ds(y), \quad x \in \mathbb{R}^2 \setminus \partial D$$

with the unknown density ϕ.

Then ϕ satifies

$$\frac{1}{2}\left(I + K(k)\right)\phi = g \quad \text{on } \partial D. \tag{5}$$

Scattering Operator

If $I + K(k)$ is invertible, which is true for k such that $\mathrm{Im}(k) > 0$, one can write the scattering operator as

$$\mathcal{B}(k) := 2\,(I + K(k))^{-1}\,. \tag{6}$$

The poles of $\mathcal{B}(k)$ are the zeros of $I + K(k)$. Furthermore, according to the analysis in [Taylor 1996] (Section 7, Chp. 9), the scattering poles coincides with the zeros of the single layer operator $S(k)$. Consequently, for scattering poles for the sound soft obstacle, one can compute the zeros of either $S(k)$ or $I + K(k)$.

We employ Nyström method (see, e.g., Section 3.6 of [Colton&Kress 2019]) to obtain the discrete operators $S_m(k)$ and $K_m(k)$, respectively. Here m is the number of the discretization points on ∂D. To compute the zeros of $S_m(k)$ or $I + K_m(k)$, we use the contour integral method.

Numerical Examples - Unit Disc

∂D is parametrized by $\partial D := \{(\cos\theta, \sin\theta) | 0 \leq \theta \leq 2\pi\}$.

Table: Two small scattering poles computed as the zeros of $I + K_m(k)$.

m	$0.4294849652 - 1.2813737977i$ (reference)	$1.3080120323 - 1.6817888047i$ (reference)
8	$0.429484965220538 - 1.281373797654556i$	$1.308012211586915 - 1.681788586461922i$
16	$0.429484965208720 - 1.281373797656096i$	$1.308012032273949 - 1.681788804745846i$
32	$0.429484965208720 - 1.281373797656096i$	$1.308012032273949 - 1.681788804745844i$
64	$0.429484965208720 - 1.281373797656097i$	$1.308012032273949 - 1.681788804745846i$
128	$0.429484965208719 - 1.281373797656096i$	$1.308012032273950 - 1.681788804745847i$

Table: Two small scattering poles computed as the zeros of $S_m(k)$.

m	$0.4294849652 - 1.2813737977i$ (reference)	$1.3080120323 - 1.6817888047i$ (reference)
8	$0.429484965209784 - 1.281373797647466i$	$1.308012112162007 - 1.681788678655068i$
16	$0.429484965207398 - 1.281373797652153i$	$1.308012032269924 - 1.681788804740671i$
32	$0.429484965208059 - 1.281373797654125i$	$1.308012032271937 - 1.681788804743257i$
64	$0.429484965208390 - 1.281373797655110i$	$1.308012032272943 - 1.681788804744552i$
128	$0.429484965208554 - 1.281373797655603i$	$1.308012032273445 - 1.681788804745198i$

Numerical Examples - Kite

$$\partial D := \{(\cos\theta + 0.65\cos(2\theta) - 0.65, 1.5\sin\theta) | 0 \leq \theta \leq 2\pi\}.$$

Table: Two small scattering poles computed as the zeros of $I + K_m(k)$.

$m = 8$	$0.308427187555871 - 0.926456704613979i$	$0.344630757029365 - 1.041445850336002i$
$m = 16$	$0.308141675774348 - 0.925041061981904i$	$0.344645070326207 - 1.041658853585890i$
$m = 32$	$0.308142570520245 - 0.925045454944318i$	$0.344645288036283 - 1.041658669884707i$
$m = 64$	$0.308142570519161 - 0.925045454943916i$	$0.344645288043423 - 1.041658669891838i$
$m = 128$	$0.308142570519161 - 0.925045454943915i$	$0.344645288043423 - 1.041658669891838i$

Table: Two small scattering poles computed as the zeros of $S_m(k)$.

$m = 8$	$0.308116677919850 - 0.924972176995767i$	$0.344669978664697 - 1.041739017739591i$
$m = 16$	$0.308142605717916 - 0.925045560824190i$	$0.344645284088626 - 1.041658613095357i$
$m = 32$	$0.308142570518591 - 0.925045454942228i$	$0.344645288042992 - 1.041658669889854i$
$m = 64$	$0.308142570518898 - 0.925045454943098i$	$0.344645288043049 - 1.041658669890614i$
$m = 128$	$0.308142570519027 - 0.925045454943508i$	$0.344645288043234 - 1.041658669891226i$

Scattering Poles for a Sound Hard Obstacle

Let $D \subset \mathbb{R}^2$ be a bounded simply connected smooth domain. The scattering problem is to find $u \in H^1_{loc}(\mathbb{R}^2 \setminus \overline{D})$ such that

$$\begin{aligned} &\Delta u + k^2 u = 0 && \text{in } \mathbb{R}^2 \setminus \overline{D}, \\ &\partial u / \partial \nu = g && \text{on } \partial D, \\ &\lim_{r\to\infty} \sqrt{r} \left(\frac{\partial u}{\partial r} - iku \right) = 0, && \end{aligned} \tag{7}$$

where $k \in \mathbb{C}$ is the wave number, $g \in L^2(\partial D)$, and $r = |x|$.

For k, $\mathrm{Im}(k) \geq 0$, there exists a unique solution u to (7). The scattering operator $\mathcal{B}(k)$ is defined as $u = \mathcal{B}(k)g$.

The operator $\mathcal{B}(k)$ is holomorphic on the upper half-plane of $\mathbb{C}$ and can be meromorphically continued to the lower half complex plane.

The poles of $\mathcal{B}(k)$ is the discrete set $\{k \in \mathbb{C} : \mathrm{Im}(k) < 0\}$, which are called the scattering poles.

DtN Map

For $\mathrm{Im}(k) \geq 0$, the radiating condition of $u(x)$ is equivalent to the series expansion of u in the form

$$u(x) = \sum_{m=0}^{\infty} a_m H_m^{(1)}(kr) e^{im\theta}, \quad |x| > r_0, \tag{8}$$

where $H_m^{(1)}$ is the first kind Hankel function of order m.

Let Γ_R be a circle centered at the origin with radius R with D inside. Let the set of zeros of Hankel function $H_n^1(kR)$ be Z_n and $Z = \bigcup_{n=0}^{\infty} Z_n$. Define $\Lambda = \mathbb{C} \setminus (\mathbb{R}^- \cup Z)$. For $k \in \Lambda$, the DtN operator $T(k) : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$ is defined as

$$T(k)\varphi = {\sum_{n=0}^{+\infty}}' \frac{k}{\pi} \frac{H_n^{(1)'}(kR)}{H_n^{(1)}(kR)} \int_0^{2\pi} \varphi(\phi) \cos(n(\theta - \phi)) \mathrm{d}\phi, \tag{9}$$

where the summation with a prime $'$ means that the zero-th term is factored by $1/2$ [Hsiao et al. 2011].

Equivalent Problem on the Bounded Domain

Given $g \in H^{1/2}(\Gamma_R)$, find $u \in H^1(\Omega)$ such that

$$\left\{ \begin{array}{rcll} \Delta u + k^2 u &=& 0, & \text{in } \Omega, \\ \frac{\partial u}{\partial \nu} &=& g, & \text{on } \Gamma, \\ \frac{\partial u}{\partial \nu} &=& T(k)u, & \text{on } \Gamma_{\mathrm{R}}. \end{array} \right. \tag{10}$$

The variational formulation for (10) is to find $u \in H^1(\Omega)$ such that

$$(\nabla u, \nabla v) - k^2(u, v) - \langle T(k)u, v\rangle_{\Gamma_R} = \langle g, v\rangle, \quad \forall v \in H^1(\Omega). \tag{11}$$

Define $B(k)$ such htat

$$(B(k)u, v)_1 = (\nabla u, \nabla v) - k^2(u, v) - \langle T(k)u, v\rangle_{\Gamma_R}, \quad \forall v \in H^1(\Omega).$$

The eigenvalue problem is to find $(k, u) \in \mathbb{C} \times H^1(\Omega)$ such that

$$B(k)u = 0 \quad \text{in } H^1(\Omega). \tag{12}$$

Truncated DtN Operator

Lemma

The operator function $B(k)$ is holomorphic Fredholm on Λ.

Define $T^N(k) : H^{1/2}(\Gamma_R) \to H^{-1/2}(\Gamma_R)$

$$T^N(k)\varphi = {\sum_{n=0}^{N}}' \frac{k}{\pi} \frac{H_n^{(1)'}(kR)}{H_n^{(1)}(kR)} \int_0^{2\pi} \varphi(\phi)\cos(n(\theta-\phi))\mathrm{d}\phi,$$

The approximation $B^N(k)$ of $B(k)$ is then given by

$$(B^N(k)u, v)_1 = (\nabla u, \nabla v) - k^2(u, v) - \langle T^N(k)u, v\rangle_{\Gamma_R} \quad \forall v \in H^1(\Omega).$$

The eigenvalue problems using the truncated DtN map is to find $(k, u) \in \mathbb{C} \times H^1(\Omega)$ satisfying

$$B^N(k)u = 0 \quad \text{in } H^1(\Omega),$$

Convergence Theorem

Let $\mathcal{T}_n := \mathcal{T}_{h_n}$ be a regular triangular mesh for Ω with mesh size h_n. Let $V_n \subseteq H^1(\Omega)$ be the linear Lagrange finite element spaces on $\mathcal{T}_n$. For $k \in \Lambda$, define $B_n^N(k) : V_n \to V_n$ for all $v_n \in V_n$ such that

$$(B_n^N(k)u_n, v_n)_1 = (\nabla u_n, \nabla v_n) - k^2(u_n, v_n) - \langle T^N(k)u_n, v_n\rangle_{\Gamma_R}.$$

Theorem

Let Λ_0 be a compact subset of Λ such that $\partial\Lambda_0 \subset \rho(B)$ and $\sigma(B) \cap \Lambda_0 = \{k\}$. Then for sufficiently large N and n, there exist $k^N \in \sigma(B^N) \cap \Lambda_0$ and $k_n^N \in \sigma(B_n^N) \cap \Lambda_0$, having the same multiplicity as k, such that

$$|k^N - k| \leqslant C \left(\sup_{\substack{u \in G(k) \\ \|u\|_1 = 1}} \gamma(N, u) + \frac{1}{\sqrt{N}} \right)^{1/r},$$

$$|k_n^N - k^N| \leqslant C \sup_{\substack{u \in G(k^N) \\ \|u\|_1 = 1}} \|u - p_n u\|_{1/2+\epsilon}^{1/r_N}.$$

Numerical Examples - Unit Disk

The solution to the scattering problem can be written in the form

$$u(r,\theta) := \Sigma_{m=0}^{\infty} \alpha_m H_m^{(1)}(kr) e^{im\theta}. \tag{13}$$

Assume that the incident wave u^{inc} is given by

$$u^{\mathrm{inc}}(r,\theta) = \Sigma_{m=0}^{\infty} \beta_m J_m(kr) e^{im\theta}. \tag{14}$$

Then $g(r,\theta) = \partial u^{\mathrm{inc}}/\partial \nu$. Using (13) to match $u(r,\theta)$ and $g(r,\theta)$ on ∂D $(r = 1)$, one has that

$$\alpha_m = -\frac{\beta_m J_m'(k)}{H_m^{(1)'}(k)}. \tag{15}$$

Hence the scattering poles for the sound hard unit disk are the zeros of $H_m^{(1)'}(k)$.

Exact and Computed Poles

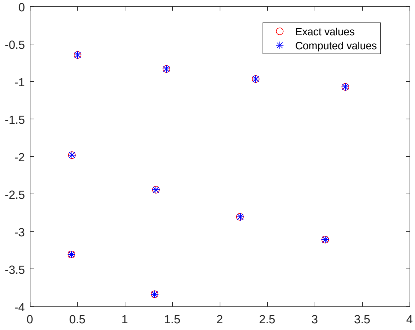


Figure: The computed scattering poles and exact poles in $[0, 4] \times [-4, 0]$ for the unit disk.

Convergence Orders

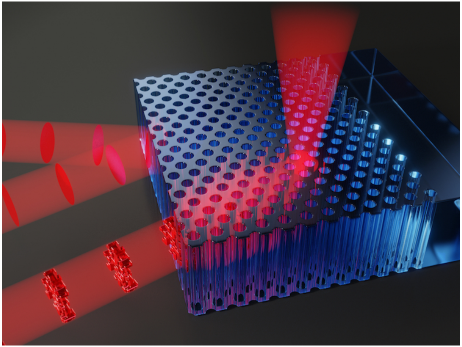
Table: The smallest three scattering poles and their convergence orders for the unit disk.

	k_1	Order	k_2	Order	k_3	Order
h_1	0.5013-0.6441i		1.4357-0.8364i		0.4434-1.9897i	
h_2	0.5012-0.6437i		1.4348-0.8350i		0.4415-1.9837i	
h_3	0.5012-0.6436i	1.9896	1.4345-0.8347i	2.0013	0.4410-1.9821i	1.9915
h_4	0.5012-0.6436i	1.9956	1.4344-0.8346i	2.0009	0.4408-1.9817i	1.9924
h_5	0.5012-0.6435i	1.9985	1.4344-0.8346i	2.0003	0.4408-1.9817i	1.9968

Table: The smallest three scattering poles and their convergence orders for the unit square.

	k_1	Order	k_2	Order	k_3	Order
h_1	0.8804-1.1007i		2.4388-1.0543i		2.4096-1.7587i	
h_2	0.8814-1.0972i		2.4246-1.0347i		2.4127-1.7610i	
h_3	0.8815-1.0955i	1.0990	2.4187-1.0270i	1.3179	2.4134-1.7616i	2.0810
h_4	0.8814-1.0948i	1.1870	2.4162-1.0240i	1.3211	2.4135-1.7618i	2.0736
h_5	0.8814-1.0945i	1.2454	2.4153-1.0228i	1.3256	2.4136-1.7618i	2.0562

Photonic Crystals Band Structures



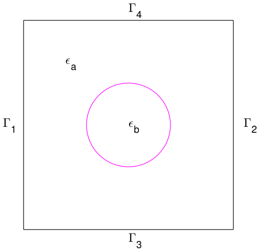


Figure: Left: Light propagation inside a photonic crystal (courtesy: IOP). Right: schematic picture for 2D PCs.

Mathematical Model

Photonic band structures are posted as the eigenvalue problems of the Maxwell's equations

$$\begin{cases} \nabla \times \dfrac{1}{\epsilon(x,\omega)} \nabla \times \mathbf{H} = \left(\dfrac{\omega}{c}\right)^2 \mathbf{H}, \\ \nabla \cdot \mathbf{H} = 0, \end{cases} \tag{16}$$

where $\mathbf{H}$ is the magnetic field satisfying quasi-periodic boundary condition, ω is the frequency, $\epsilon(x,\omega)$ is the electric permittivity, and c is the speed of light in the vacuum.

In 2D, the Maxwell's equations (16) can be reduced to the transverse electric (TE) case or the transverse magnetic (TM) case.

Consider the TE case

$$-\Delta\psi = \left(\frac{\omega}{c}\right)^2 \epsilon(x,\omega)\psi. \tag{17}$$

The Eigenvalue Problem

Assume that the photonic crystal has the unit periodicity.
Let $\mathbb{Z} = \{0, \pm 1, \pm 2, \cdots\}$ and $\Lambda = \mathbb{Z}^2$.

$$\epsilon(x + n, \omega) = \epsilon(x, \omega) \quad \text{for all } x \in \mathbb{R}^2 \text{ and } n \in \Lambda.$$

The periodic domain $D := \mathbb{R}^2/\mathbb{Z}^2$ can be identified with the unit square $D_0 := (0,1)^2$ by imposing quasi-periodic boundary conditions. Introduce the quasimomentum vector $\boldsymbol{k} \in \mathcal{K}$, where

$$\mathcal{K} = \{\boldsymbol{k} \in \mathbb{R}^2 | -\pi \le k_j \le \pi, j = 1, 2\}$$

is called the Brillouin zone.
The eigenvalue problem is equivalent to

$$-(\nabla + i\boldsymbol{k}) \cdot (\nabla + i\boldsymbol{k}) u(x) = \left(\frac{\omega}{c}\right)^2 \epsilon(x, \omega) u(x) \quad \text{in } D_0, \qquad (18)$$

where u is the Floquet transform of ψ, a periodic function.

Frequency Dependent Material

Let $H^1(D_0)$ be the Sobolev space of functions in $L^2(D_0)$ with square integrable gradients. Define the subspace of functions in $H^1(D_0)$ with periodic boundary conditions by

$$H_p^1(D_0) = \{v \in H^1(D_0)|\ v|_{\Gamma_1} = v|_{\Gamma_2}, v|_{\Gamma_3} = v|_{\Gamma_4}\}. \qquad (19)$$

Multiplying (18) by $v \in H_p^1(D_0)$ and integrating by parts, the weak formulation is to find $(\omega, u) \in \Omega \times H_p^1(D_0)$ such that

$$\int_{D_0} (\nabla + i\boldsymbol{k})u \cdot \overline{(\nabla + i\boldsymbol{k})v} dx = \left(\frac{\omega}{c}\right)^2 \int_{D_0} \epsilon(x, \omega) u\bar{v} dx \qquad (20)$$

for all $v \in H_p^1(D_0)$.

If $\epsilon(x, \omega)$ depends on ω, (20) is nonlinear in general.

Operator Formulation

Rewrite the sesquilinear form as

$$(u, v)_1 - b(\omega; u, v) = 0, \tag{21}$$

where

$$b(\omega; u, v) = \int_{D_0} \left(\left(\frac{\omega}{c} \right)^2 \epsilon + 1 \right) u\overline{v} - 2iu\boldsymbol{k} \cdot \nabla \overline{v} - |\boldsymbol{k}|^2 u\overline{v} dx, \ \omega \in \Omega.$$

Due to boundedness of ϵ, $b(\omega; \cdot, \cdot)$ is bounded.
By the Riesz representation theorem, define an operator function $B : \Omega \to \mathcal{L}(H_p^1(D_0), H_p^1(D_0))$ such that

$$b(\omega; u, v) = (B(\omega)u, v)_1 \quad \text{for all } v \in H_p^1(D_0). \tag{22}$$

Using (21), the weak formulation can be written as

$$(u, v)_1 - (B(\omega)u, v)_1 = 0 \quad \text{for all } v \in H_p^1(D_0). \tag{23}$$

Holomorphic Operator Function

Define an operator function $T : \Omega \to \mathcal{L}(H_p^1(D_0), H_p^1(D_0))$ by

$$T(\omega) := I - B(\omega), \tag{24}$$

where I is the identity operator.
The eigenvalue problem is to find $(\omega, u) \in \Omega \times H_p^1(D_0)$ such that

$$T(\omega)u = u - B(\omega)u = 0. \tag{25}$$

If $\epsilon(x, \omega)$ is holomorphic in ω, $T(\omega)$ is holomorphic in ω.

Lemma

The operator $B(\omega)$ is compact for all $\omega \in \Omega$.

Lemma

The operator function T is a holomorphic Fredholm operator function with index zero on Ω.

Finite Element Approximation

Let $\mathcal{T}_h$ be a regular triangular mesh for D_0. Let $V_h \subset H^1_p(D_0)$ be the Lagrange finite element space.
Let $B^h : \Omega \to \mathcal{L}(V_h, V_h)$ be given by

$$(B^h(\omega)u_h, v_h)_1 := b(\omega; u_h, v_h) \quad \text{for all } v_h \in V_h.$$

Define $T^h : \Omega \to \mathcal{L}(V_h, V_h)$ such that

$$T^h(\omega) = I^h - B^h(\omega).$$

Define the linear projection operator $p_h : H^1_p(D_0) \to V_h$ such that

$$(u, v_h)_1 = (p_h u, v_h)_1 \quad \text{for all } v_h \in V_h. \tag{26}$$

p_h is bounded and $\|p_h u - u\|_1 \to 0$ as $h \to 0$ for $u \in H^1_p(D_0)$.
Using the Aubin-Nitsche Lemma, it holds that

$$\|u - p_h u\|_{L^2(D_0)} \leq Ch\|u\|_{H^1(D_0)}. \tag{27}$$

Convergence [Karmar 96]

Lemma

There exists $h_0 > 0$ *small enough such that, for every compact set* $\Omega \subset \mathbb{C}$, $\sup_{h<h_0} \sup_{\omega\in\Omega} \|T^h(\omega)\|_{\mathcal{L}(V_h,V_h)} < \infty$. *Let* $g \in H^1_p(D_0)$ *and* $\omega \in \Omega$. *Then* $\|T^h(\omega)p_h g - p_h T(\omega)g\|_{H^1(D_0)} \le Ch\|g\|_{H^1(D_0)}$.

Theorem

Let $\omega \in \sigma(T)$ *and* h *be small enough. Then there exists a sequence* $\{\omega_h \in \sigma(T^h)\}$ *such that* $\omega_h \to \omega$ *as* $h \to 0$ *and*

$$|\omega_h - \omega| \le Ch^{\frac{1}{r_0}}. \tag{28}$$

Furthermore, if $G(\omega) \subset H^1_p(D_0) \cap H^{1+\sigma}(D_0)$, $0 < \sigma \le 1$, *then*

$$|\omega_h - \omega| \le Ch^{\frac{1+\sigma}{r_0}}. \tag{29}$$

Numerical Example

Let $\epsilon_b(\omega) = \epsilon_\infty \frac{\omega_L^2 - \omega^2}{\omega_T^2 - \omega^2}$, where ϵ_∞ is the optical frequency dielectric constant, ω_L and ω_T are the frequencies of the longitudinal and transverse optical vibration modes of infinite wavelength.

$\epsilon_\infty = 10.9$, $\omega_T = 8.12$THz, $\omega_L = 8.75$THz, and $\frac{\omega_T a}{2\pi c} = 1$.

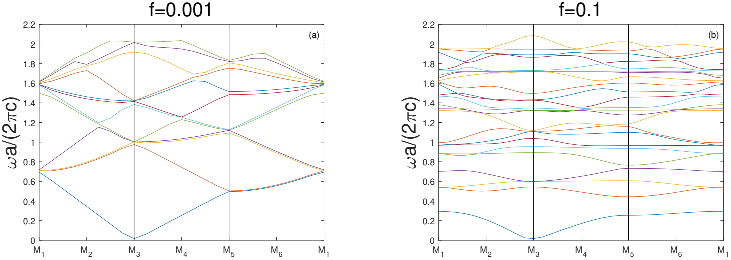


Figure: Band structures of square lattice of GaAs cylinders in vacuum. The result is consistent with [Kuzmiak 1997]

Convergence Rate

$\Omega = [0.1, 13.9] \times [-6.9, 6.9]$.

h	$\omega/(2\pi c)$	ξ	order
1/10	0.3038	-	-
1/20	0.2949	0.0301	-
1/40	0.2925	0.0080	1.9074
1/80	0.2919	0.0021	1.9679

Table: First eigenvalue, relative error, convergence order ($\boldsymbol{k} = (\pi, \pi)$).

References:

- W. Xiao, B. Gong, J. Sun and Z. Zhang, A new finite element approach for the Dirichlet eigenvalue problem. Appl. Math. Lett. 105, 106295, 2020.
- W. Xiao, B. Gong, J. Sun and Z. Zhang, *Finite element calculation of photonic band structures for frequency dependent materials.* J. Sci. Comput. 87(1), 1-16, 2021.
- W. Xiao and J. Sun, *Band structure calculation of photonic crystals with frequency-dependent permittivities.* J. Opt. Soc. Am. A 38(5), 628-633, 2021.
- X Pang, J Sun, Z Zhang *FE-holomorphic operator function method for nonlinear plate vibrations with elastically added masses.* J. Comput. Appl. Math. 410, 114156, 2022.
- W. Xiao, B. Gong, J. Lin and J. Sun, *Band structure calculations of dispersive photonic crystals in 3D using holomorphic operator functions.* submitted, 2021.

Conclusions and Future Work

A general framework to compute scattering resonances:

FEM+DtN+pmSIM.

Convergence analysis - abstract approximation theory for holomorphic Fredholm operator functions.

- Ma and S., Computation of scattering poles using boundary integrals. AML. 2023.
- Xi, Lin and S., A finite element contour integral method for computing the resonances of metallic grating structures with sub-wavelength holes. accepted.
- Xi and S., Parallel Multi-step Spectral Indicator Method for Nonlinear Eigenvalue Problems. submitted.
- Xi, Gong and S., Analysis of a finite element DtN method for scattering resonances of sound hard obstacles. submitted.
- Liu, S. and Zhang, Accurate computation of scattering poles of acoustic obstacles with impedance boundary conditions. submitted.

Future Work:

- Inhomogeneous media
- Periodic structures
- Electromagnetic waves, elasticity waves, optics, fluid-solid interaction, etc.

Conclusions and Future Work

A general framework to compute scattering resonances:

FEM+DtN+pmSIM.

Convergence analysis - abstract approximation theory for holomorphic Fredholm operator functions.

- Ma and S., Computation of scattering poles using boundary integrals. AML. 2023.
- Xi, Lin and S., A finite element contour integral method for computing the resonances of metallic grating structures with sub-wavelength holes. accepted.
- Xi and S., Parallel Multi-step Spectral Indicator Method for Nonlinear Eigenvalue Problems. submitted.
- Xi, Gong and S., Analysis of a finite element DtN method for scattering resonances of sound hard obstacles. submitted.
- Liu, S. and Zhang, Accurate computation of scattering poles of acoustic obstacles with impedance boundary conditions. submitted.

Future Work:

- Inhomogeneous media
- Periodic structures
- Electromagnetic waves, elasticity waves, optics, fluid-solid interaction, etc.

Thank you!