Computing the eigenvalues of self-adjoint operators using quadratic matrix polynomials

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Motivation

A - self-adjoint operator on a Hilbert space $\mathcal{H}$.

Projection method

$\{e_j\}_{j=1}^{\infty}$ - orthonormal basis of $\mathcal{H}$,

$\mathcal{L}_n := \mathrm{Span}\,\{e_1, \ldots, e_n\}$,

$M_n := [\langle Ae_j, e_k\rangle]_{jk=1}^{n}$ - $n \times n$ matrix approx. of A.

Question

$$\lim_{n\to\infty} \mathrm{Spec}\, M_n = \mathrm{Spec}\, A \quad ?$$

Answer

Not necessarily!

Spectral pollution

$$\lim_{n\to\infty} \operatorname{Spec} M_n = \operatorname{Spec} A \quad ?$$

"$\not\subseteq$" - *spectral pollution*.
"$\not\supseteq$" - indicates lack of approximation.

- Natural conditions on $\mathcal{L}_n \Rightarrow$ "$\supseteq$".
- Ensuring "$\subseteq$" is much harder in general.

$$\operatorname{Spec} A = \operatorname{Spec}_{\mathrm{disc}} A \cup \operatorname{Spec}_{\mathrm{ess}} A$$

- Eigenvalues outside the extrema of $\operatorname{Spec}_{\mathrm{ess}} A$ are safe.
- Portions of $\operatorname{Spec} M_n$ can accumulate in the resolvent set between any two points of $\operatorname{Spec}_{\mathrm{ess}} A$.

A concrete example

Perturbed band-gap Schrödinger operator

$\mathcal{H} = L^2(\mathbb{R}^2)$, $\qquad f \in H^2(\mathbb{R}^2)$,

$Hf(x,y) = -\Delta f(x,y) + V(x,y)f(x,y)$,

$V(x,y) = \cos(x) + \cos(y) - ke^{-(x^2+y^2)}$,

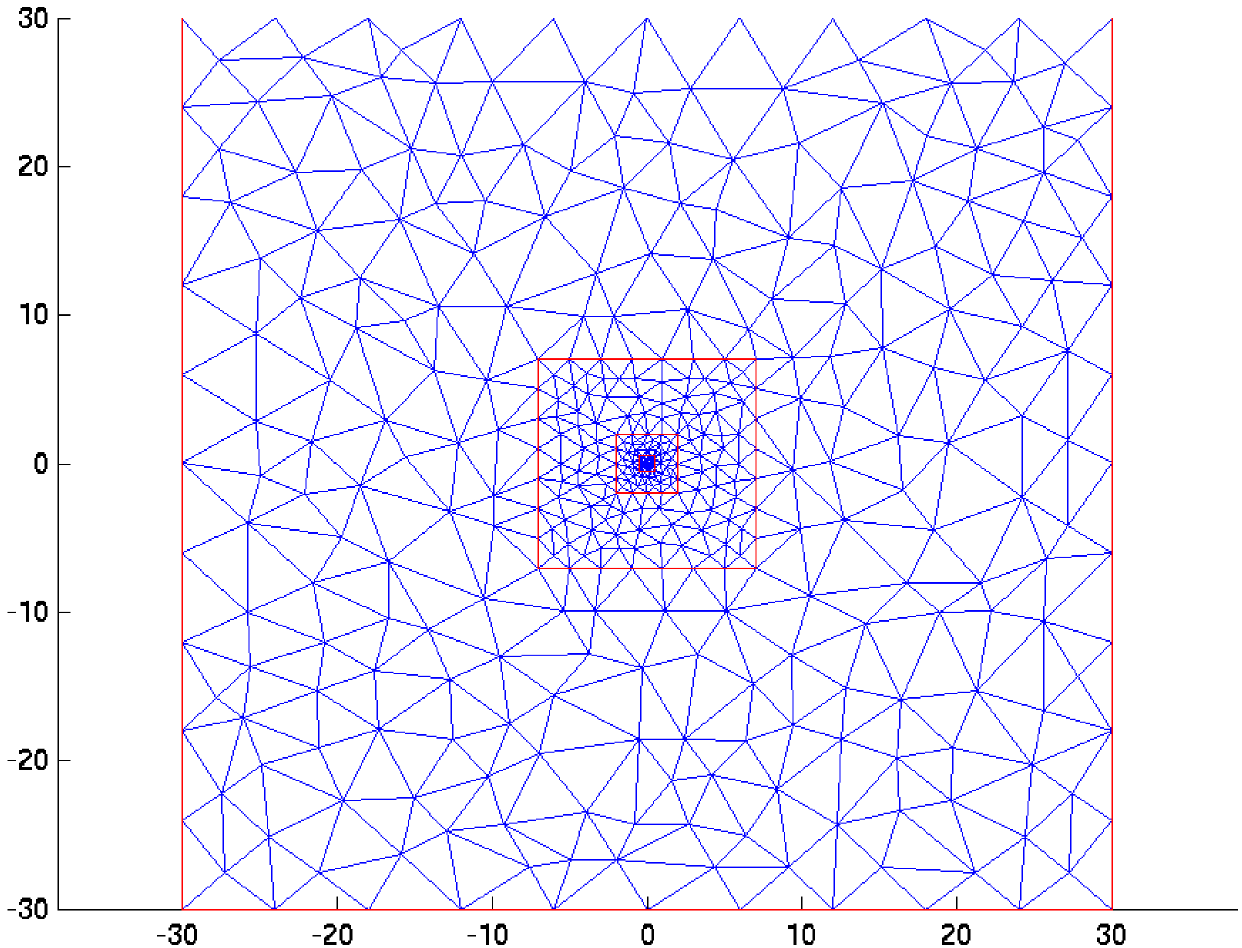
Floquet-Bloch technique $\rightsquigarrow \mathrm{Spec}_{\mathrm{ess}} H$

$$\mathrm{Spec}\, H \approx [-.75, -.69] \cup [.21, .57] \cup [.91, \infty) \cup \{\text{possibly isolated evs}\}$$

Test spaces:

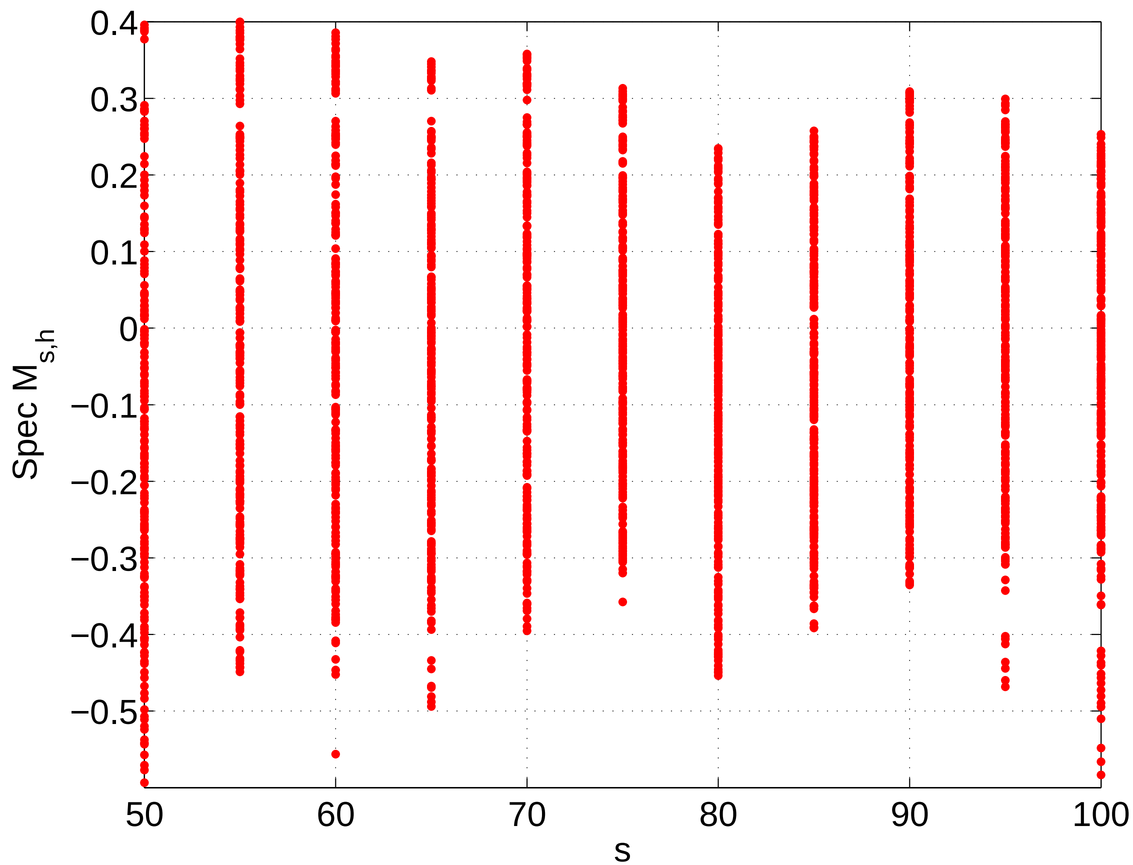
$\mathcal{L}_{s,h}$ - FEM in a mesh of max element size $h > 0$ with support in $[-s,s]^2$ and C^1 in $\mathbb{R}^2$. Adapted mesh.

A typical mesh



The Schrödinger operator

The 200 eigenvalues of $M_{s,h}$ near to -0.1 for $s = 50 : 5 : 100$.



$$\mathrm{Spec}\, H \approx [-.75, -.69] \cup [.21, .57] \cup [.91, \infty)$$

Why does pollution occur?

Π_n - orthogonal projection onto $\mathcal{L}_n$. $\quad M_n = \Pi_n A \restriction \mathcal{L}_n$.

$$\tilde{F}_n(x) := \min_{0 \neq u \in \mathcal{L}_n} \frac{\|\Pi_n(x - A)u\|}{\|u\|}.$$

$$\mu \in \operatorname{Spec} M_n \iff \tilde{F}_n(\mu) = 0,$$

$$\iff \exists\, v \in \mathcal{L}_n \text{ s.t. } (\mu - A)v \perp \mathcal{L}_n.$$

As $\|(\mu - A)v\|/\|v\|$ is not guaranteed to be small, we have no indication whether μ is close to $\operatorname{Spec} A$ or not.

Approximate spectral distances

Why not look instead at

$$F_n(x) := \min_{0 \neq u \in \mathcal{L}_n} \frac{\|(x-A)u\|}{\|u\|}.$$

$$F_n(x) \geq \inf_{\mathrm{Dom}(A)} \frac{\|(x-A)u\|}{\|u\|} = \|(x-A)^{-1}\|^{-1} = \operatorname{dist}[x, \operatorname{Spec} A].$$

Strategy:
use the profile of $F_n(x)$ for $x \in \mathbb{R}$ and n large to estimate points in $\operatorname{Spec} A$.

$$F_n(x) \underset{n\to\infty}{\longrightarrow} \operatorname{dist}[x, \operatorname{Spec} A].$$

[Davies & Plum, 2004]

How to compute $F_n(x)$?

If $\mathcal{L}_n \subset \mathrm{Dom}(A^2)$ and $Q_n(x) := \Pi_n(x - A)^2 \upharpoonright \mathcal{L}_n$,

$$\begin{aligned} F_n(x)^2 &= \min_{\mathcal{L}_n} \frac{\langle \Pi_n (x-A)^2 u, u\rangle}{\|u\|^2} \\ &= \text{least sing.val.}[Q_n(x)] \\ &=: G_n(x). \end{aligned}$$

Profile of $F_n(x)$

$\updownarrow$

finding singular values on a 1-D mesh.

N.B. For this we need the orthogonal projection associated to $\mathcal{L}$.

A projection-type approach

$$G_n(z) = \text{least sing.val.}[Q_n(z)] = \min_{0 \neq u \in \mathcal{L}_n} \frac{\|\Pi_n (z-A)^2 u\|}{\|u\|}$$

Surface: $G_n(z)$

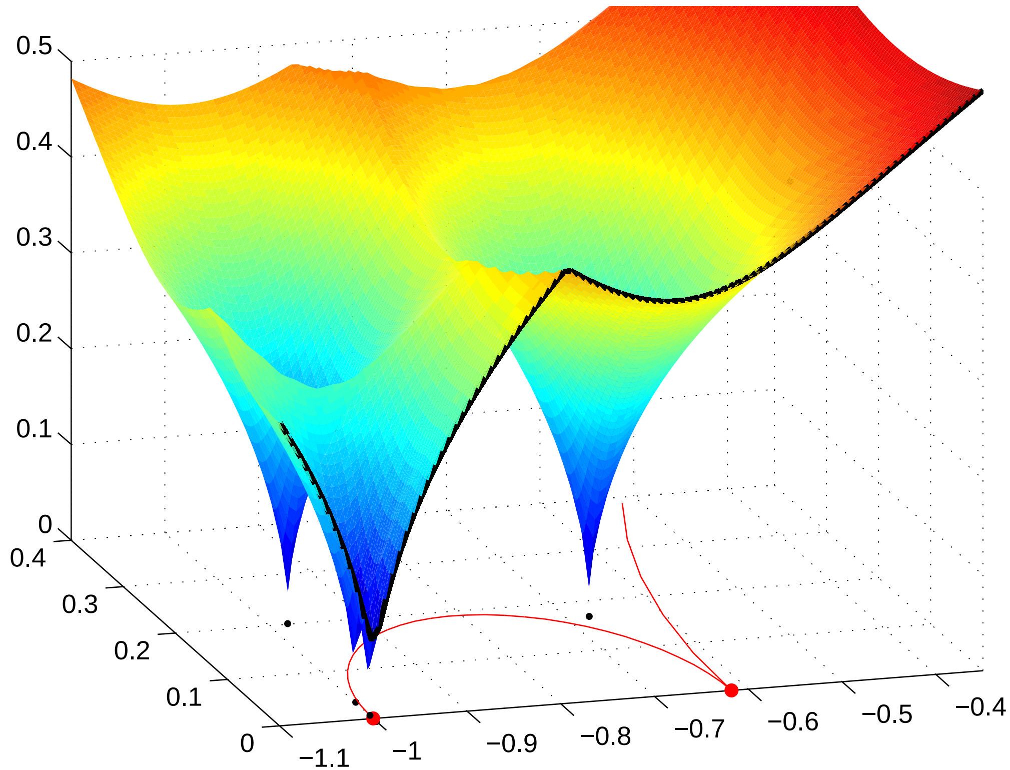
Black Line: $F_n^2(x)$

Black Dots: zeros of G_n

Red Dots: $\mathrm{Spec}\, A$

Semi-disks:

Forbidden region



$$G_n(z) = 0 \iff \det Q_n(z) = 0$$

Strategy: find the points of $\mathrm{Spec}\, Q_n$ near to $\mathbb{R}$

The quadratic projection method

$\mathcal{L} = \mathrm{Span}\{b_1, \ldots, b_n\}$, b_k - linearly independent.

$B = [\langle b_j, b_k \rangle]_1^n$, $M = [\langle Ab_j, b_k \rangle]_1^n$, $R = [\langle Ab_j, Ab_k \rangle]_1^n$.

$$Q(z) := z^2 B - 2zM + R \qquad z \in \mathbb{C}$$

- $Q(z) = Q(\overline{z})^*$,
- Typically $\mathrm{Spec}\, Q \cap \mathbb{R} = \varnothing$, unless we are lucky!

"Relative second order spectrum" of A.

[Davies, Shargorodsky, Levitin, Strauss, B]

First crucial result

$Q(z) = [\langle (z - A)^2 b_j, b_k \rangle]_1^n.$

$D(a, b) := \{w \in \mathbb{C} \,:\, |w - (a + b)/2| < (b - a)/2\}.$

Theorem A. [Shargorodsky, 2000]
Suppose that $(a, b) \cap \operatorname{Spec} A = \varnothing$. If $z \in D(a, b)$, then $Q(z)$ is non-singular.

Moreover.
Let $\zeta = \mu + i\nu$. If $G(\zeta) = 0$, then $|\nu| \geq F(\mu)$ and $F(\zeta) = \nu^2$.

Second crucial results

Theorem B. [B, 2006]

If $E \in \operatorname{Spec}_{\rm dsc} A$, (under natural conditions on $\mathcal{L}_n$)

$$\exists\, \lambda_n \in \operatorname{Spec} Q_n \; : \; \lambda_n \xrightarrow[n\to\infty]{} E.$$

Assume that $Au = Eu$ and E simple. There exists $b > 0$ and $c > 0$ independent of $\mathcal{L}$ satisfying the following. If $0 < \delta < c$ and $\mathcal{L} \subset \operatorname{Dom} A^2$ is such that

$$\exists v \in \mathcal{L}, \qquad \|A^p(v-u)\| < \delta, \qquad p = 0, 1, 2,$$

then there exists $\mu \in \operatorname{Spec} Q$ such that $|\mu - E| < b\delta^{1/2}$.

In other words...

Theorem A $\Longrightarrow$ Points in $\operatorname{Spec} Q$ which are close to $\mathbb{R}$ are *necessarily* close to $\operatorname{Spec} A$. $\Longrightarrow$ $\operatorname{Spec} Q$ does not pollute.

Theorem B $\Longrightarrow$ Under natural additional conditions, some points of $\operatorname{Spec} Q_n$ approach to eigenvalues of A.

$$\operatorname{Spec}_{\mathrm{dsc}} A \subseteq \left(\mathbb{R} \cap \lim_{n\to\infty} \operatorname{Spec} Q_n\right) \subseteq \operatorname{Spec} A.$$

For periodic Schrödinger

$$H = -\Delta + \cos(x) + \cos(y) - (5.5)e^{-(x^2+y^2)}.$$

Dots:

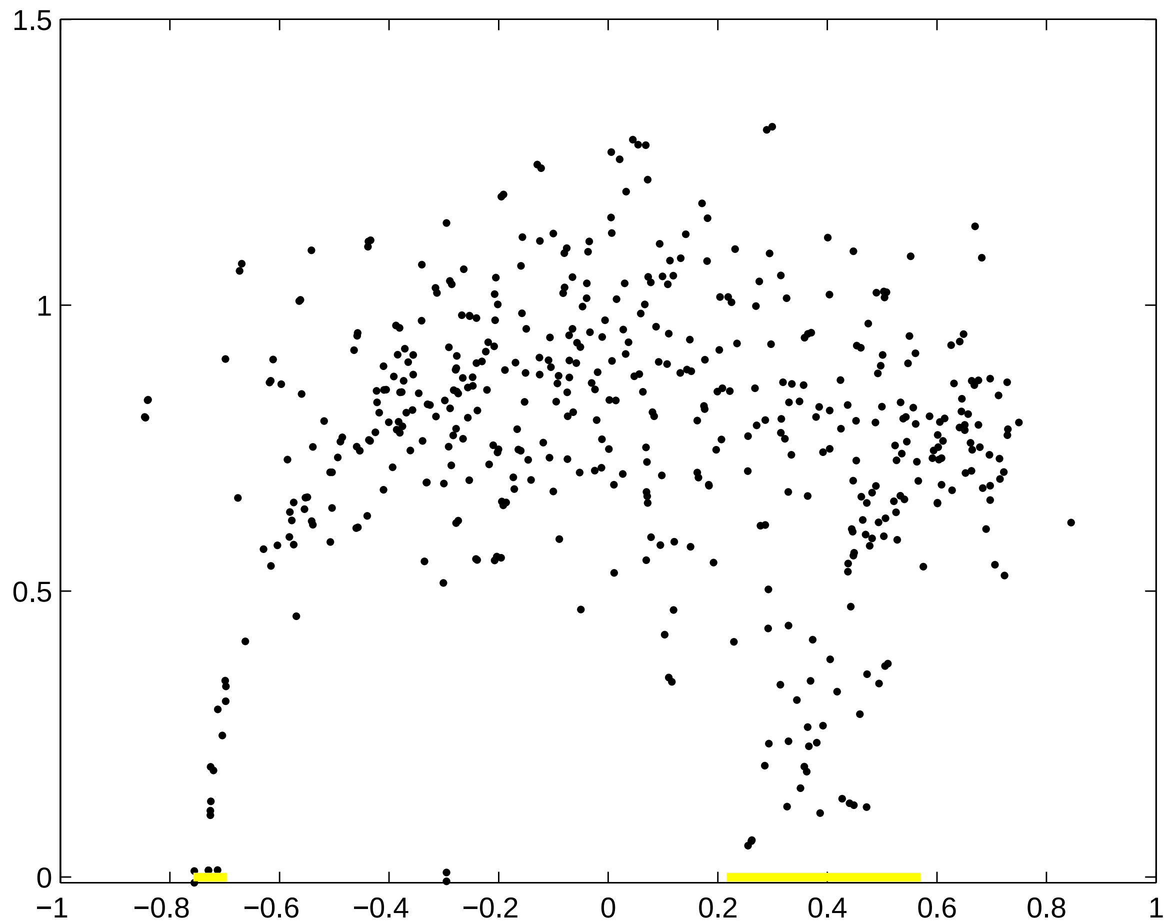
$\operatorname{Spec} Q_{s,h}$.

Here:

$s = 89$,

adapted mesh

on $[-s, s]^2$



eigenvalue at $\approx -0.295247 \pm 10^{-5}$

An open problem

Let $\Omega \subset \mathbb{R}^2$, consider the following pencil problem

$$(\mathsf{C}) \qquad \begin{cases} \lambda \Delta \underline{u} - \operatorname{grad} \operatorname{div} \underline{u} = 0 \\ \underline{u}|_{\partial\Omega} = 0 \end{cases}$$

[Cosserat 1898, Mikhlin 1973]

$$\begin{aligned} \operatorname{Spec}_{\text{ess}}(\mathsf{C}) &:= \{\lambda \in \mathbb{R} : \text{op not Fredholm}\} \\ &= \{0, 1\} \cup [1/2 - a, a + 1/2] \end{aligned}$$

Claim [Costabel-Dauge, 2000]

$$\partial\Omega = (\text{polygon}) \Rightarrow a > 0.$$

Problem.

Study $\operatorname{Spec}_{\text{disc}}(\mathsf{C})$ when $\Omega = [-1, 1] \times [-\varepsilon, \varepsilon]$.

An easier problem

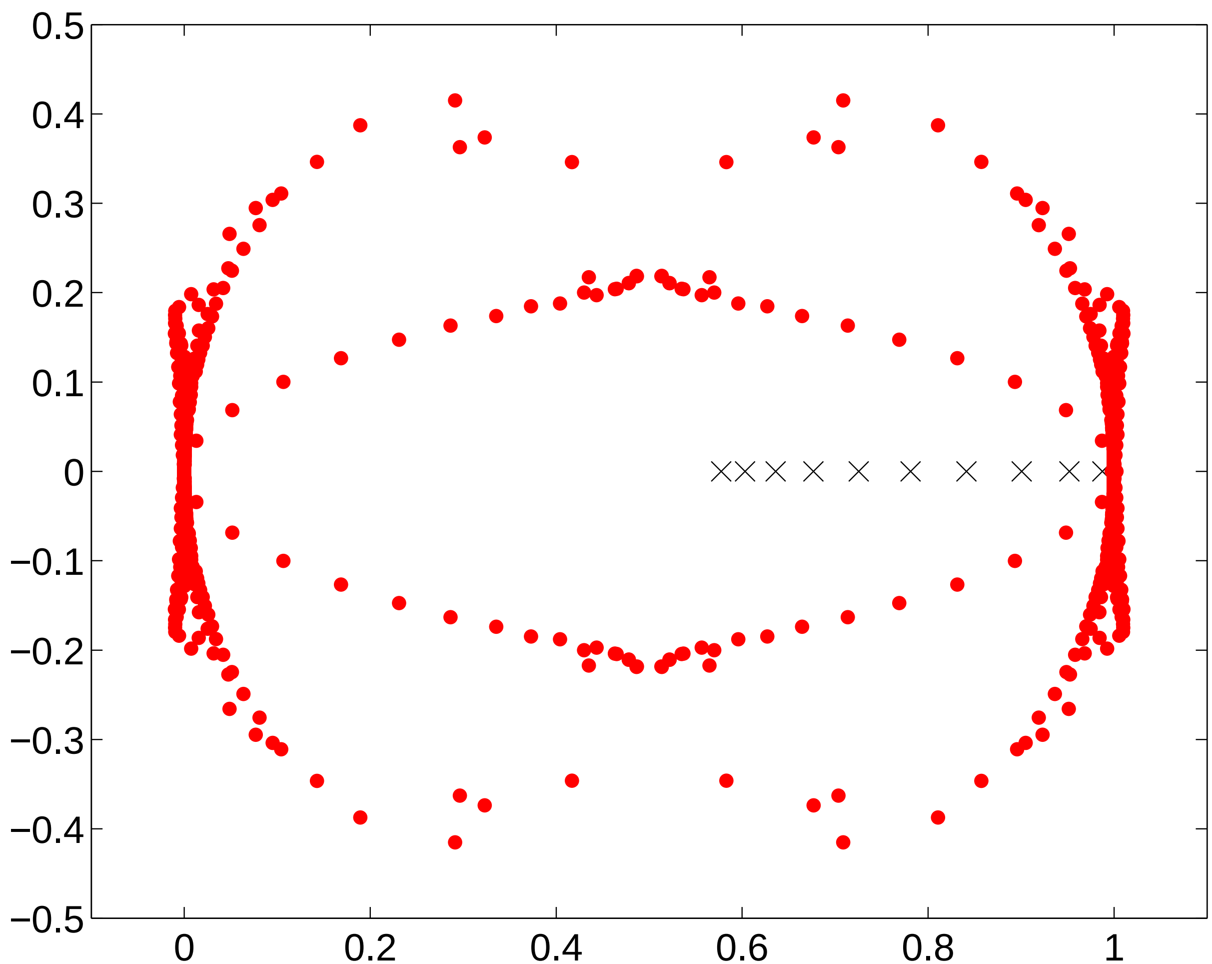
$$\underline{u}(x,y) = \begin{pmatrix} \sin(\varepsilon n\pi y)u(x) \\ \cos(\varepsilon n\pi y)v(x) \end{pmatrix}$$ u and v - DBC at 0,1

$$\Rightarrow \begin{cases} \lambda(u'' - \varepsilon^2 n^2 \pi^2 u) + \varepsilon^2 n^2 \pi^2 u + \varepsilon n \pi v' = 0 \\ \lambda(v'' - \varepsilon^2 n^2 \pi^2 v) - v'' - \varepsilon n \pi u' = 0 \\ u(0) = v(0) = u(1) = v(1) = 0 \end{cases}$$

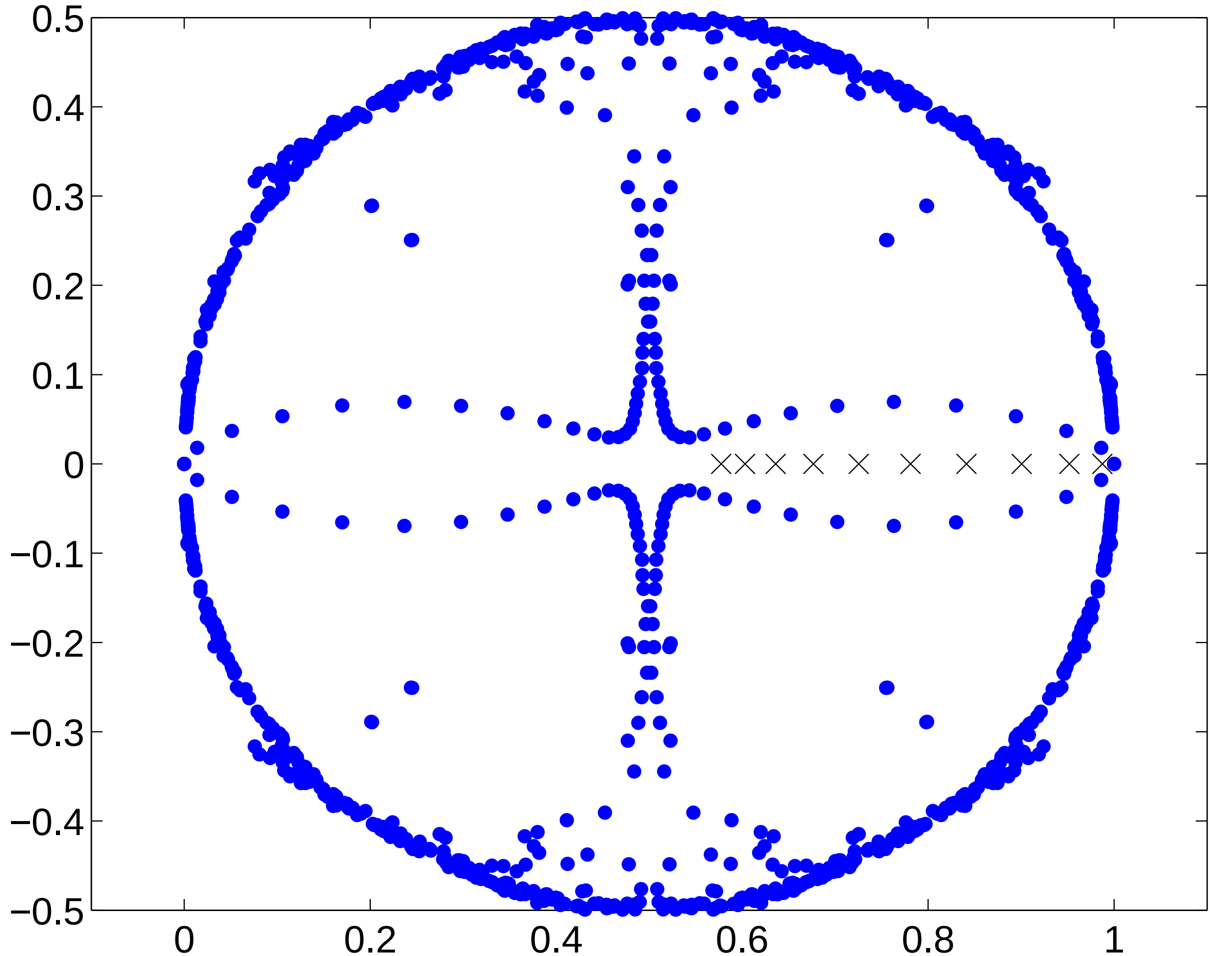
$$\Rightarrow \lambda = \frac{1}{2}\left(1 \pm \frac{n\varepsilon\pi}{\sinh(\varepsilon n\pi)}\right)$$

Perhaps the eigenvalues of (C) for $\Omega = [-1,1] \times [-\varepsilon, \varepsilon]$

Cosserat



Cosserat



Final Remarks

- Tested: multiplication operators, Stokes type systems, Schrödinger operators with band-gap spectrum.
- Stability: Theorems A and B can be extended to accommodate perturbation of the coefficients.
- Dirac (in progress with N. Boussaid, M. Levitin).
- Essential spectrum?

Proof of Theorem B

$A\phi = E\phi$, E-discrete, $\delta = \mathrm{dist}[E, \mathrm{Spec}\, A \setminus \{E\}]$.

- $G_n(z)^{-1}$ - subharmonic in $\mathrm{Spec}\, Q_n$.
- $G_n(E) \longrightarrow 0$ as $n \longrightarrow \infty$ (easy).
- Given $0 < \varepsilon < \delta/4$, $\exists N > 0$, $a > 0$:

$$G_n(z) \geq a \qquad \forall\, \varepsilon \leq |z - E| \leq \delta/4,\ n \geq N.$$

A-bdd $\|\Pi_n \phi - \phi\| \longrightarrow 0$

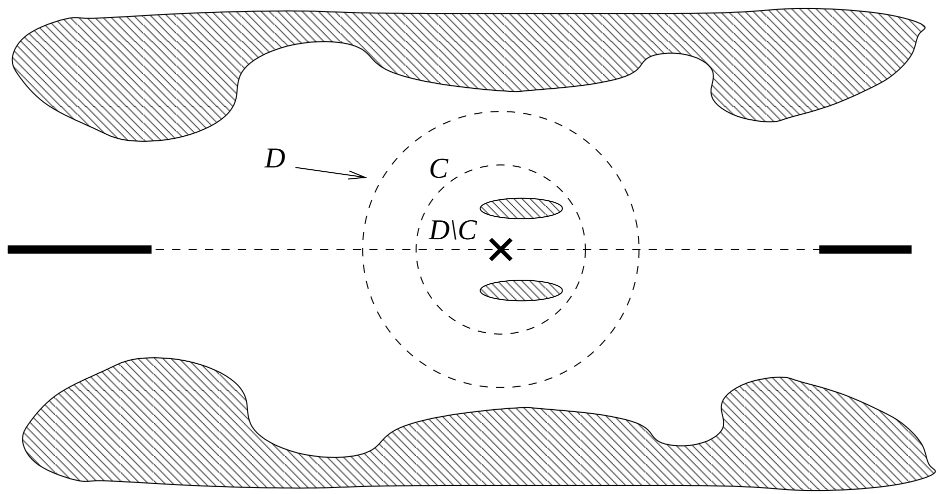
A-unbdd $\|A^p(\Pi_n \phi - \phi)\| \longrightarrow 0$, $p = 0, 1, 2$

$\Pi_n = \Pi_n^2 \neq \Pi_n^*$ additionally $\max\{\lambda_{\max}(B_n), \lambda_{\min}(B_n)^{-1}\} \leq a$

$$B_n = [\langle b_j, b_k \rangle]_{jk=1}^n \qquad \Pi_n v = \sum \alpha_k(v) b_k$$

Limit sets of pseudospectra

$$D = \{|z - E| \leq \delta/4\} \qquad C = \{\varepsilon < |z - E| \leq \delta/4\}$$



Given $\varepsilon > 0$, exists $a > 0$ and $N > 0$ such that $\forall n > N$,

- there is no a-pseudospectrum of Q_n in C

- a-pseudospectrum of Q_n intersects $D \setminus C$

Evidence

$$H = -\Delta + V$$

$$\operatorname{Spec}_{\text{ess}} H = \bigcup_1^\infty [\alpha_k, \beta_k]$$

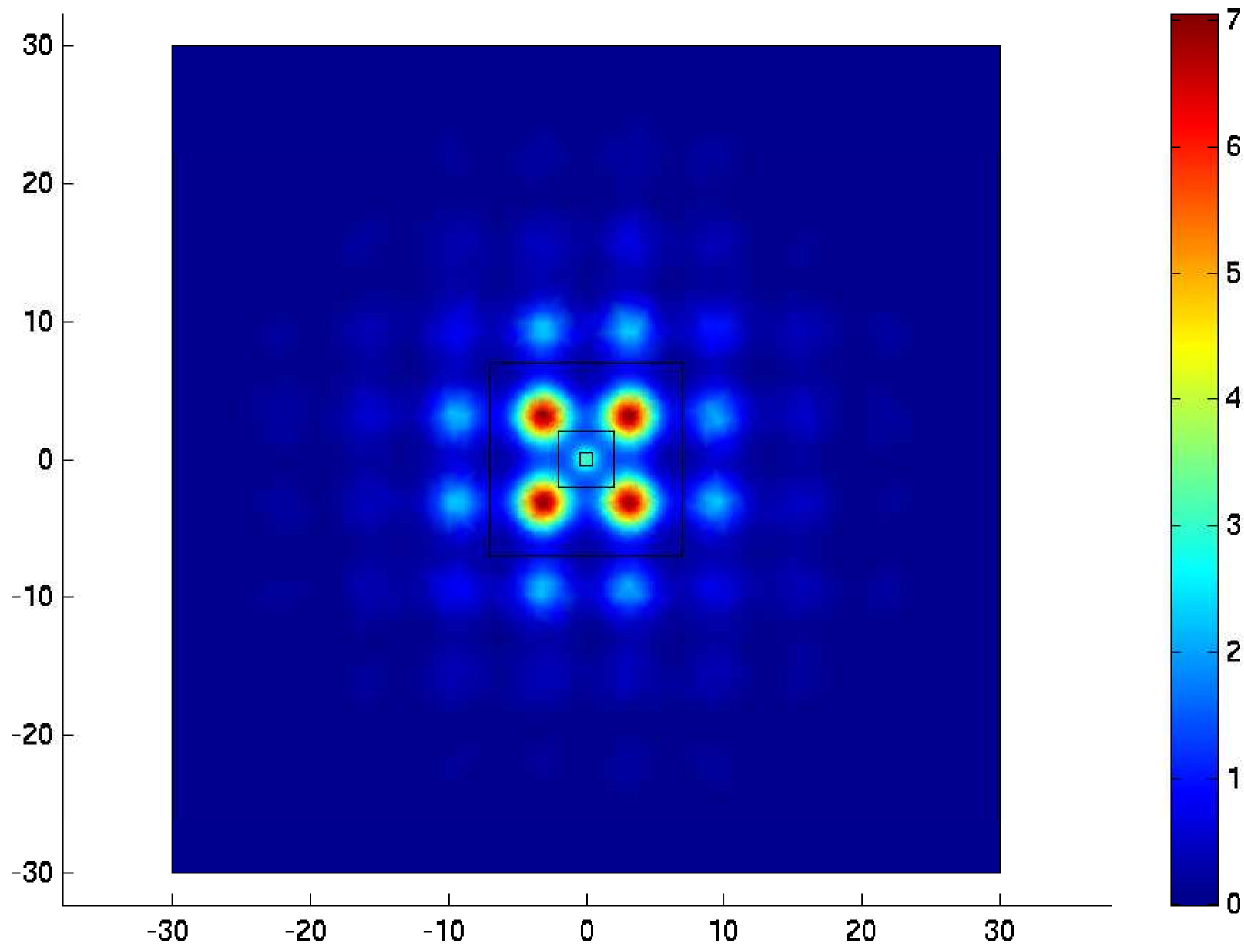
$M_{s,h}$ - matrix approximation of H in $L^2(\mathbb{R}^2)$

- matrix approximation of $H_s = H$, Dbc in $L^2(-s,s)^2$

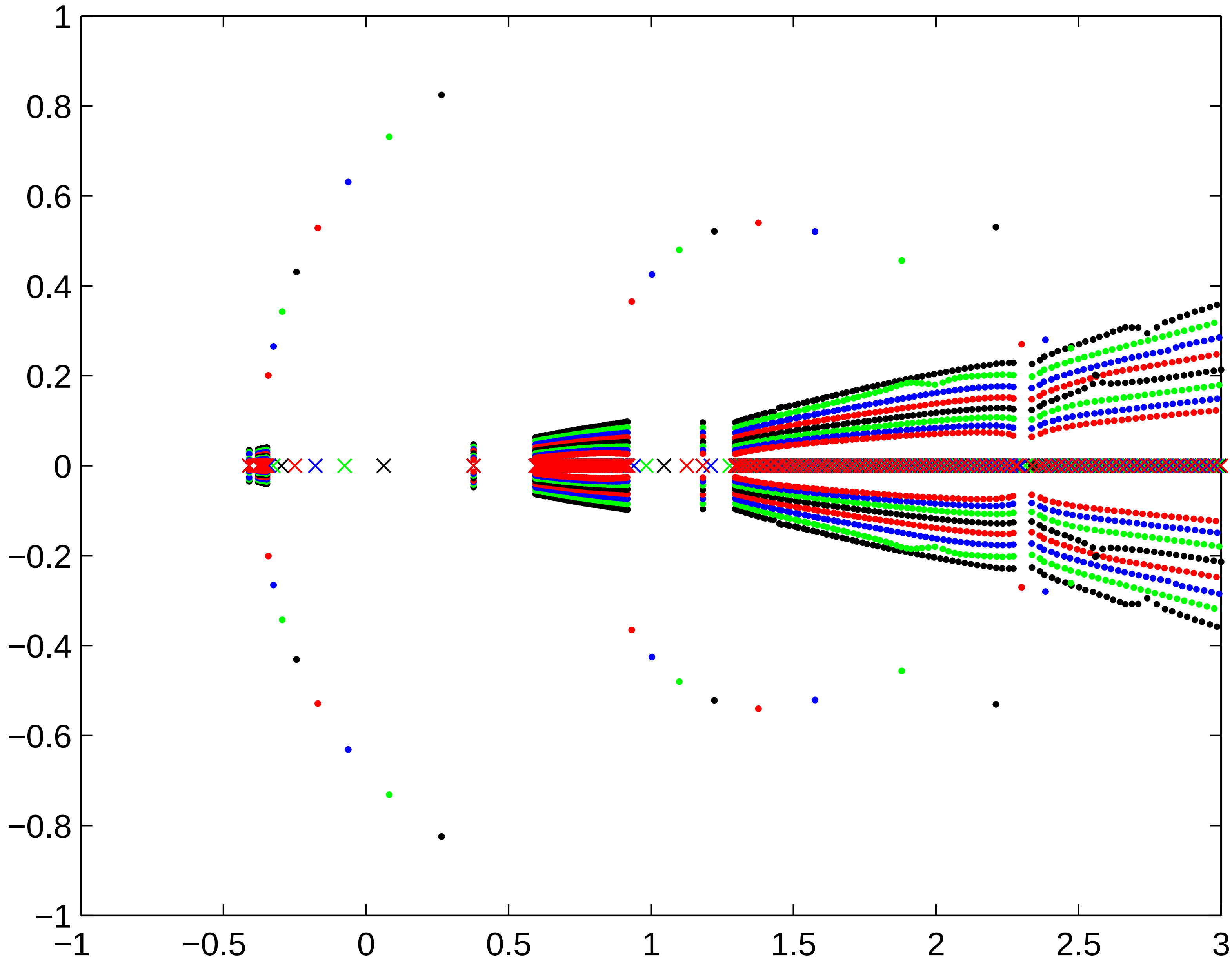
$\operatorname{Spec} M_{s,h}$ "$\longrightarrow$" $\operatorname{Spec} H_s$ as $h \to 0$.

$\operatorname{Spec} H_s$ "$\longrightarrow$" $\operatorname{Spec} H$ from above $s \to \infty$.

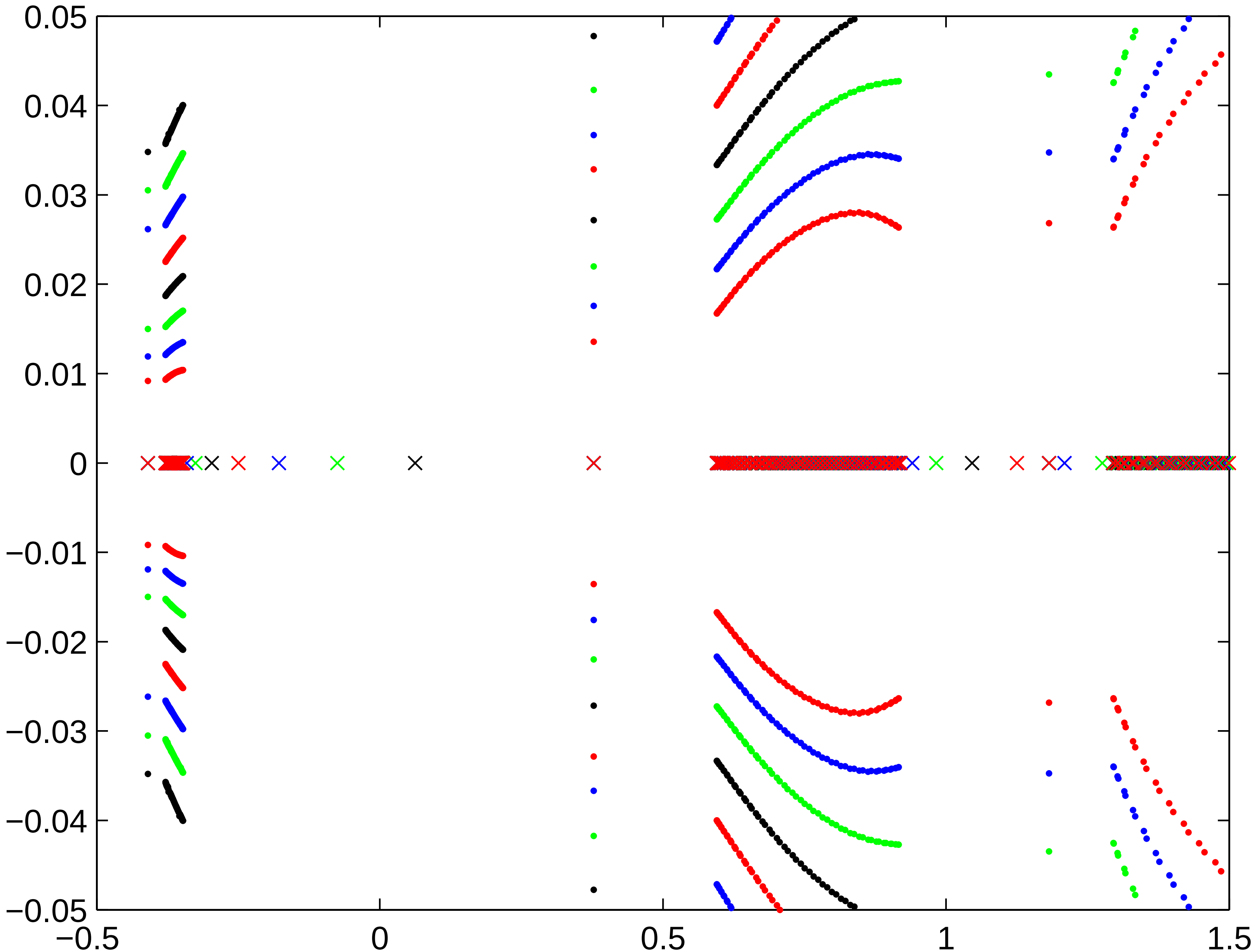
Let $E > \alpha_1$. There exist $s_n \to \infty$ and $h_n \to 0$, such that $E \in \operatorname{Spec} M_{s_n,h_n}$ for all $n \in \mathbb{N}$.

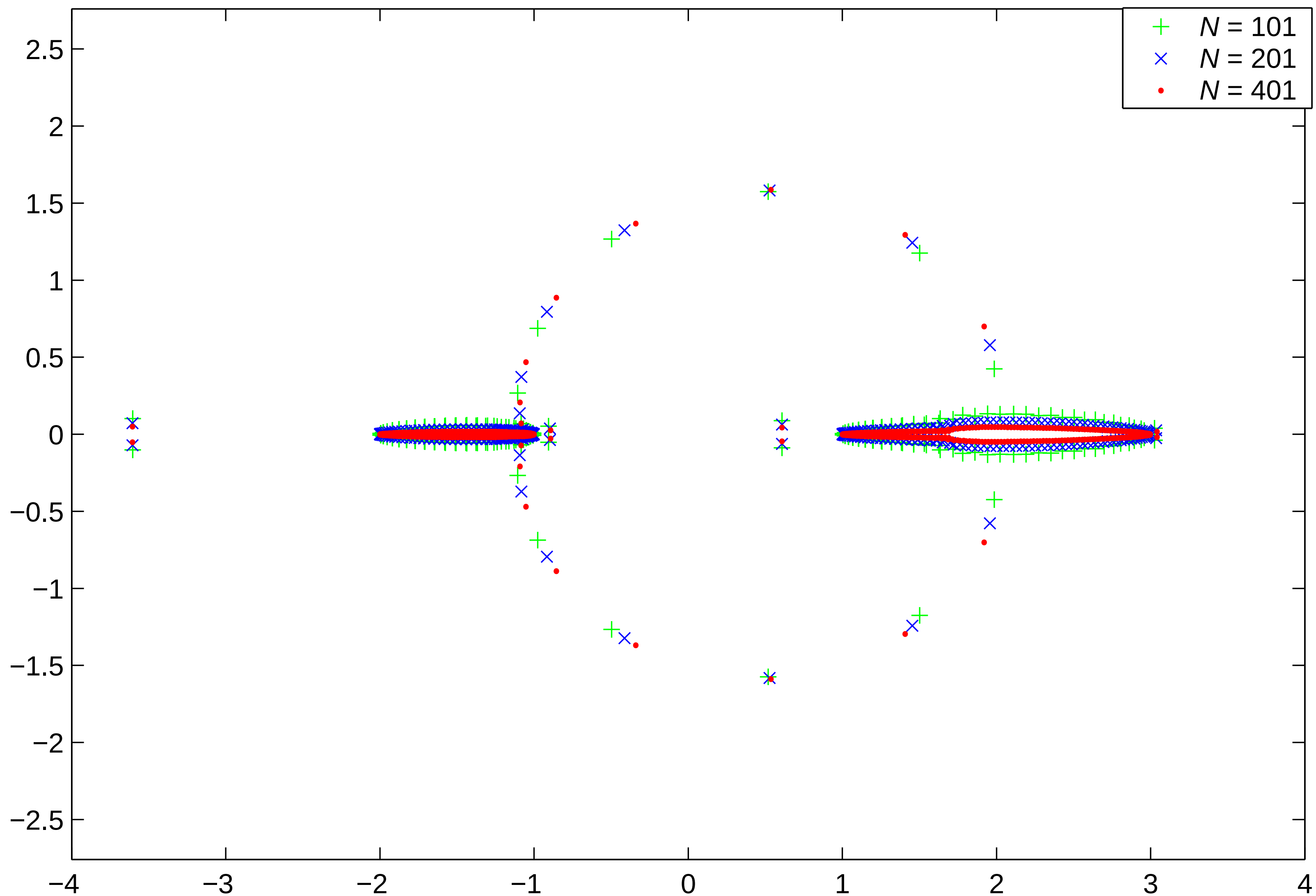


30
20
10
0
-10
-20
-30
-30
-20
-10
0
10
20
30
7
6
5
4
3
2
1
0



1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1
−1
−0.5
0
0.5
1
1.5
2
2.5
3


0.05
0.04
0.03
0.02
0.01
0
−0.01
−0.02
−0.03
−0.04
−0.05
−0.5
0
0.5
1
1.5



N = 101
N = 201
N = 401
2.5
2
1.5
1
0.5
0
−0.5
−1
−1.5
−2
−2.5
−4
−3
−2
−1
0
1
2
3
4