Eigenvalues of Schrödinger operators perturbed by dissipative barriers

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Introduction

Let T_0 be a linear operator.
In this talk we are concerned with perturbations of T_0 of the form

$$T_n := T_0 + i\gamma s_n \tag{1}$$

where

- $\gamma > 0$,
- s_n are T_0-compact, bounded, self-adjoint operators,
- $s_n \xrightarrow{\mathrm{s}} I$ (strong convergence as $n \to \infty$).

$(i\gamma s_n)$ is called a sequence of *dissipative barriers* for T_0

Dissipative barrier for Schrödinger operators on the half-line

$$T_n = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,n]} \qquad \text{on } L^2(0,\infty) \tag{2}$$

Aim: Understand the eigenvalues of operators perturbed by dissipative barriers for *large* n.

Structure of the talk

Talk based on: Spectral Inclusion and Pollution for a Class of Dissipative Perturbations, S. (2020) arXiv:2006.10097

Part I: Dissipative Barrier Method

- Motivation from numerical analysis.

Part II: Abstract Results

- Based on enclosures for the limiting essential spectrum.

Part III: 1D Schrödinger Operators

- More precise results (convergence rates, inclusion for essential spectrum and structure of spectral pollution).

Spectral inclusion and pollution

Let H and H_n, $n \in \mathbb{N}$ be operators on a Hilbert space.

- (H_n) is said to be *spectrally inclusive* for H in some $\Omega \subseteq \mathbb{C}$

$$\forall \lambda \in \sigma(H) \cap \Omega : \exists \lambda_n \in \sigma(H_n),\ n \in \mathbb{N} : \lambda_n \to \lambda \text{ as } n \to \infty.$$

- The *limiting spectrum* of (H_n) is defined by

$$\sigma((H_n)) = \{\lambda \in \mathbb{C} : \exists I \subseteq \mathbb{N} \text{ infinite}, \exists \lambda_n \in \sigma(H_n), n \in I \text{ with } \lambda_n \to \lambda\}.$$

- The set of *spectral pollution* for (H_n) with respect to H is defined by

$$\sigma_{\mathrm{poll}}((H_n)) = \{\lambda \in \sigma((H_n)) : \lambda \notin \sigma(H)\}.$$

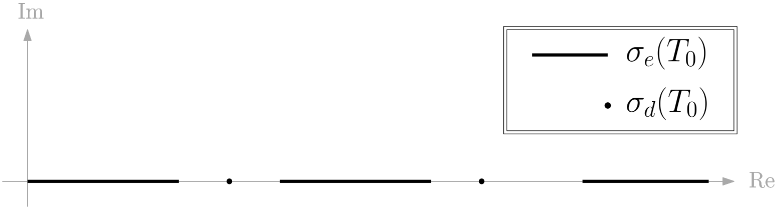
- (H_n) is *spectrally exact* for H in Ω if:
  1. (H_n) is spectrally inclusive for H in Ω,
  2. No spectral pollution in Ω, i.e. $\sigma_{\mathrm{poll}}((H_n)) \cap \Omega = \emptyset$.

Notation:

Essential spectrum: $\sigma_e(H)$, Eigenvalues of finite multiplicity: $\sigma_d(H)$.

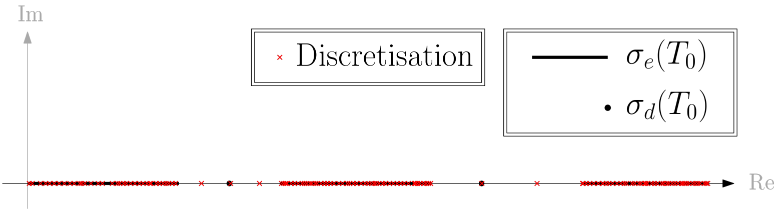
Computing eigenvalues in spectral gaps

- Consider a self adjoint, semi-bounded T_0, such that the essential spectrum $\sigma_e(T_0)$ has a band gap spectrum.
- Suppose we want to numerically compute the eigenvalues in the spectral gaps.



Computing eigenvalues in spectral gaps

- Consider a self adjoint, semi-bounded T_0, such that the essential spectrum $\sigma_e(T_0)$ has a band gap spectrum.
- Suppose we want to numerically compute the eigenvalues in the spectral gaps.
- Numerically discretise T_0 (e.g. finite section method, finite element).
- **Problem:** In general, there may be spectral pollution in the gaps.



Dissipative barrier method

Idea

'Pre-condition' T_0 by adding dissipative barrier:

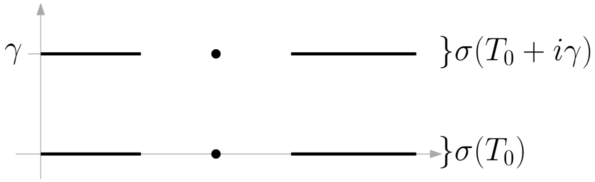
$$T_n = T_0 + i\gamma s_n$$

where $\gamma > 0$ and s_n are T_0-compact operators such that $s_n \xrightarrow{\mathrm{s}} I$.

- T_n approximates the *shifted operator* $T_0 + i\gamma$,

$$T_n \xrightarrow{\mathrm{s}} T_0 + i\gamma \quad \text{as} \quad n \to \infty.$$

- $\sigma_d(T_0)$ is encoded in $\underbrace{\sigma_d(T_0 + i\gamma)}_{\text{shifted eigenvalues}} = \sigma_d(T_0) + i\gamma$.

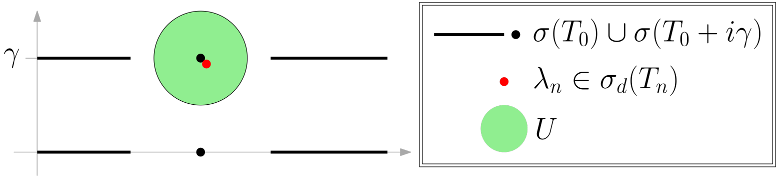


Dissipative barrier method (cont.)

- Let $\lambda_0 \in \sigma_d(T_0)$. **Assume:** (T_n) is spectrally exact for $T_0 + i\gamma$ in an open set $U \subset \mathbb{C}$ such that $U \cap \sigma(T_0 + i\gamma) = \{\lambda_0 + i\gamma\}$.

Proposed algorithm for computing $\lambda_0 \in \sigma_d(T_0)$

1. Add dissipative barrier $T_n = T_0 + i\gamma s_n$. For large n:
   - T_n has an eigenvalue λ_n near $\lambda_0 + i\gamma$.
   - All eigenvalues of T_n in U are near $\lambda_0 + i\gamma$.
2. Numerically compute $\lambda_n \in \sigma_d(T_n) \backslash \mathbb{R}$.
   - This can be done reliably since s_n is T_0-compact.[1]



[1] Essential numerical range for unbounded linear operators, Bögli, Marletta & Tretter (2020)

Expanding dissipative barriers

The dissipative barrier method motivates the question:

Question

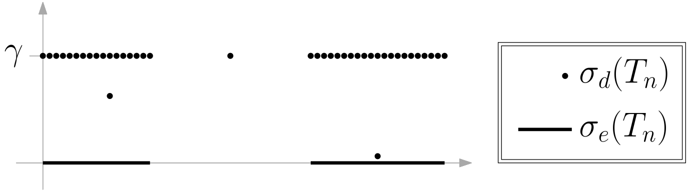
How does $\sigma(T_n)$ behave as $n \to \infty$, in relation $\sigma(T_0 + i\gamma)$?

- Since s_n are T_0-compact, by Weyl's theorem,

$$\sigma_e(T_n) = \sigma_e(T_0) \subseteq \mathbb{R}.$$

- Then, since $\sigma(T_0 + i\gamma) \subseteq i\gamma + \mathbb{R}$

$$\sigma_e(T_n) = \sigma_e(T_0) \subseteq \sigma_{\mathrm{poll}}((T_n)).$$



Limiting essential spectrum

Assumption 1

Let T_0 be self-adjoint. Let s_n such that $s_n \xrightarrow{s} I$ and $\|s_n\| \leqslant C$.
As before, $T_n := T_0 + i\gamma s_n$.

Definition (Limiting essential spectrum)

$$\sigma_e((T_n)) = \left\{ \lambda \in \mathbb{C} : \begin{array}{c} \exists I \subseteq \mathbb{N} \text{ infinite}, \exists u_n \in D(T_n), n \in I \text{ with} \\ \|u_n\| = 1,\ u_n \rightharpoonup 0,\ \|(T_n - \lambda)u_n\| \to 0 \end{array} \right\}.$$

Bad Set:

$$\mathrm{Bad}((T_n)) := \sigma_e((T_n)) \cup \sigma_e((T_n^*))^*$$

Theorem (Immediate corollary of Bögli, 2018)

Suppose Assumption 1 holds.

1. *If $\lambda \in \sigma_d(T_0 + i\gamma)$ is such that $\lambda \notin \mathrm{Bad}((T_n))$, then there exists $\lambda_n \in \sigma_d(T_n)$, $n \in \mathbb{N}$, such that $\lambda_n \to \lambda$.*
2. $\sigma_{\mathrm{poll}}((T_n)) \subseteq \mathrm{Bad}((T_n))$

Limiting essential numerical range

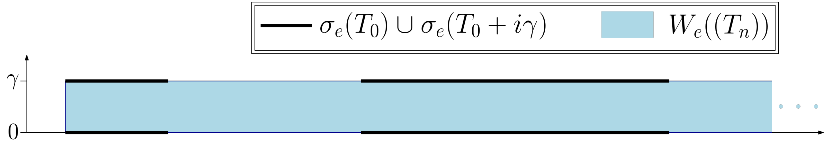
Definition (Limiting essential numerical range)

$$W_e((T_n)) := \left\{ \lambda \in \mathbb{C} : \begin{array}{c} \exists I \subseteq \mathbb{N} \text{ infinite}, \exists u_n \in D(T_n), n \in I \text{ with} \\ \|u_n\| = 1,\ u_n \rightharpoonup 0,\ \langle (T_n - \lambda) u_n, u_n \rangle \to 0 \end{array} \right\}.$$

Proposition (Bögli, Marletta and Tretter, 2020)

$W_e((T_n))$ is convex with $\mathrm{Bad}((T_n)) \subseteq W_e((T_n))$.

- $W_e((T_n))$ easily computed.
- $W_e((T_n))$ gives no info on spectral inclusion for eigenvalues of $T_0 + i\gamma$ in the gaps of $\sigma_e(T_0 + i\gamma)$.

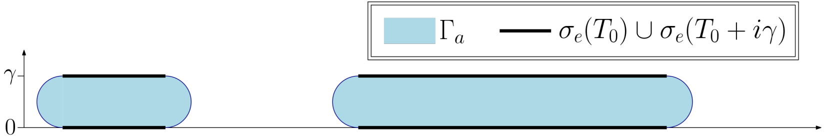


Enclosures for limiting essential spectra

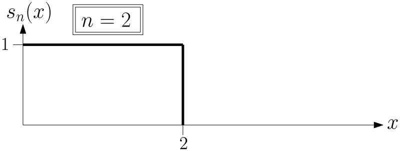
Theorem 1a (S., 2020)

Suppose Assumption 1 holds. If $s_n = s_n^2$ for all n, then $\mathrm{Bad}((T_n)) \subseteq \Gamma_a$ where,

$$\Gamma_a := \left\{\lambda \in \mathbb{C} : \Im(\lambda) \in [0,\gamma],\ \mathrm{dist}(\Re(\lambda), \sigma_e(T_0)) \leqslant \sqrt{\Im(\lambda)(\gamma - \Im(\lambda))}\right\}.$$



Example of s_n satisfying hypothesis of Th. 1a (T_0 operator on $L^2(0,\infty)$):



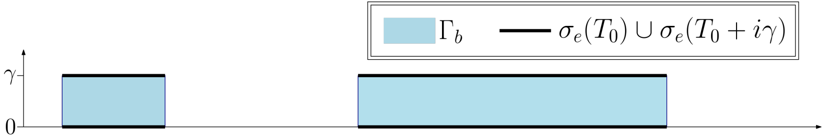
Enclosures for limiting essential spectra (cont.)

Theorem 1b (S., 2020)

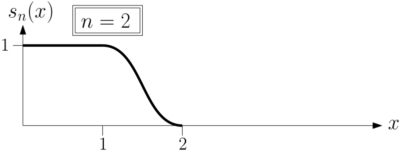
If $0 \leqslant s_n \leqslant 1$ *for all* n *and:*

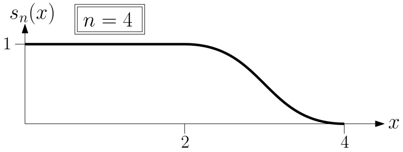
$$\forall\,(u_n) \subset D(T_0) \text{ s.t. } \|u_n\|, \|T_0 u_n\| \leqslant C, \quad \Im\langle s_n u_n, T_0 u_n\rangle \to 0,$$

then $\mathrm{Bad}((T_n)) \subseteq \Gamma_b := \sigma_e(T_0) \times i[0,\gamma]$.



Example of s_n satisfying hypothesis of Th. 1b (T_0 operator on $L^2(0,\infty)$):

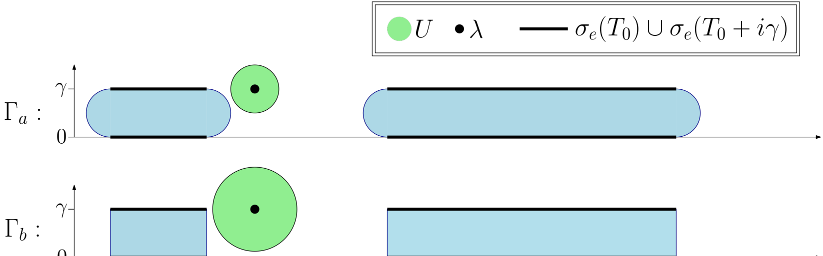




Spectral exactness near shifted eigenvalues

Corollary

If Assumption 1 and the hypothesis of either Th. 1a or Th. 1b holds then (T_n) *is spectrally exact in an open neighbourhood* U *of any* $\lambda \in \sigma_d(T_0 + i\gamma)$.



[1]Corollary for hypothesis of 1**a** is also proved in: Spectral enclosure and superconvergence for eigenvalues in gaps, Hinchcliffe and Strauss (2016)

Numerical illustration

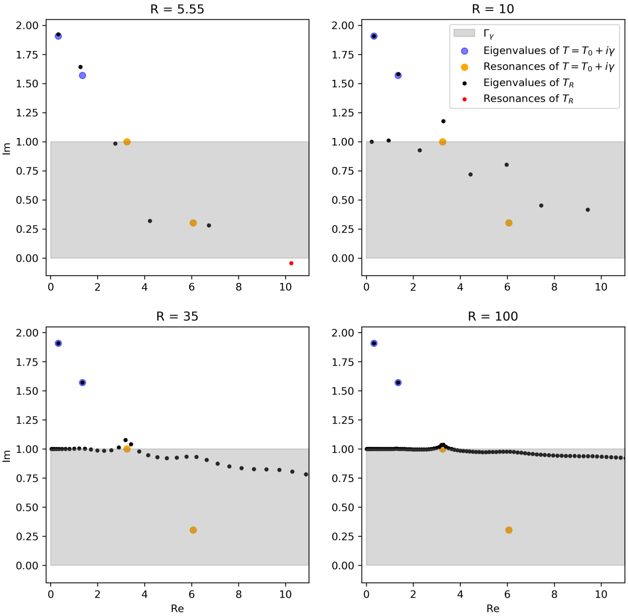
$$T_0 := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\chi_{[0,X]}$$

$$T_R := T_0 + i\chi_{[0,R]}$$

$$\sigma_e(T_R) = [0, \infty)$$

$$\sigma_e(T_0 + i\gamma) = i + [0, \infty)$$

$$\Gamma_\gamma := [0, \infty) \times i[0, 1]$$



Schrödinger operators on the half line

- Consider
$$T_0\psi = -\psi'' + q\psi \qquad \text{on} \qquad L^2(0,\infty)$$
where $q \in L^1_{\mathrm{loc}}([0,\infty);\mathbb{C})$ and T_0 is endowed with a Dirichlet boundary condition,
$$\psi(0) = 0.$$
- Fix $\gamma \in \mathbb{C}\backslash\{0\}$. Consider the perturbed operators
$$T_R := T_0 + i\gamma\chi_{[0,R]} \qquad (R \in \mathbb{R}_+).$$

Key fact: The solution space of the Schrödinger equation $-\psi'' + q\psi = \lambda\psi$ is a two-dimensional vector space.

Asymptotic properties of solutions

Assumption 2

For any $\lambda \in \mathbb{C} \backslash \sigma_e(T_0)$, the solution space of $-\psi'' + q\psi = \lambda\psi$ is spanned by solutions $\psi_\pm(\cdot, \lambda)$ admitting the decomposition

$$\psi_\pm(x,\lambda) = e^{\pm ik(\lambda)x}\tilde{\psi}_\pm(x,\lambda)$$
$$\psi'_\pm(x,\lambda) = e^{\pm ik(\lambda)x}\tilde{\psi}^d_\pm(x,\lambda)$$

such that

1. $k : \mathbb{C} \backslash \sigma_e(T_0) \to \mathbb{C}$ analytic with $\Im k > 0$
2. $\tilde{\psi}_\pm(x,\cdot)$ and $\tilde{\psi}^d_\pm(x,\cdot)$ analytic on $\mathbb{C} \backslash \sigma_e(T_0)$.
3. $\|\tilde{\psi}_\pm(\cdot,\lambda)\|_{L^\infty}, \|\tilde{\psi}^d_\pm(\cdot,\lambda)\|_{L^\infty} < \infty$

Example

1. $q \in L^1(0,\infty)$ - by the Levinson asymptotic theorem.
2. q eventually, real periodic - by Floquet theory.

Eigenvalue approximation and spectral pollution

- Let $(R_n) \subset \mathbb{R}_+$ be any sequence such that $R_n \to \infty$.
- We shall later introduce a '1D bad set': $\mathrm{Bad}_{1\mathrm{D}}((T_{R_n})) \subseteq \mathbb{C}$.

Theorem 2 (S., 2020)

Suppose that Assumption 2 holds. Then,

1. *Let λ be an eigenvalue of $T_0 + i\gamma$ such that $\lambda \notin \mathrm{Bad}_{1\mathrm{D}}((T_{R_n}))$. There exists $\lambda_n \in \sigma(T_n)$, $n \in \mathbb{N}$, and constants $C_0, \beta > 0$ such that*

$$|\lambda - \lambda_n| \leqslant Ce^{-\beta R_n}$$

   for large enough n.

2. *Spectral pollution of (T_{R_n}) with respect to $T_0 + i\gamma$ satisfies*

$$\sigma_{\mathrm{poll}}((T_{R_n})) \subseteq \sigma_e(T_0) \cup \mathrm{Bad}_{1\mathrm{D}}((T_{R_n})).$$

[1] Part **1** of Theorem also proved, for *small enough* γ in: Eigenvalues in spectral gaps of differential operators, Theorem 10, Marletta and Scheichl (2012)

Eigenvalues as zeros

- Eigenvalues of linear operators can be expressed as zeros of analytic functions.

Example

λ eigenvalue of $T_0 \quad \Longleftrightarrow \quad \psi_+(0,\lambda) = 0$

Lemma

$\lambda \in \mathbb{C}$ with $\lambda \notin \sigma_e(T_0) \cup \sigma_e(T_0 + i\gamma)$ is an eigenvalues of T_R if and only if

$$f_R(\lambda) := \alpha_+(R,\lambda)e^{ik(\lambda - i\gamma)R} + \psi_+(0,\lambda - i\gamma)A(R,\lambda)e^{-ik(\lambda-i\gamma)R} = 0,$$

where

$$A(R,\lambda) := \tilde{\psi}_+(R,\lambda)\tilde{\psi}_-^d(R,\lambda - i\gamma) - \tilde{\psi}_+^d(R,\lambda)\tilde{\psi}_-(R,\lambda - i\gamma)$$

$$\alpha_+(R,\lambda) := \psi_-(0,\lambda - i\gamma)\Big(\tilde{\psi}_+(R,\lambda - i\gamma)\tilde{\psi}_+^d(R,\lambda) - \tilde{\psi}_+^d(R,\lambda - i\gamma)\tilde{\psi}_+(R,\lambda)\Big).$$

- Proofs of theorems for 1D Schrödinger utilise f_R in combination with tools from complex analysis (e.g. Rouché's theorem).

The 1-D bad set

Definition (1D Bad set)

$$\mathrm{Bad}_{1\mathrm{D}}((T_{R_n})) := \left\{\lambda \in \mathbb{C}\backslash(\sigma_e(T_0) \cup \sigma_e(T_0 + i\gamma)) : \liminf_{n\to\infty}|A(R_n, \lambda)| = 0\right\}$$

Example

If $q \in L^1(0,\infty)$ then $\mathrm{Bad}_{1\mathrm{D}}((T_{R_n})) = \emptyset$.

Example

If q is eventually real a-periodic and $R_n = x_0 + na$, then $\mathrm{Bad}_{1\mathrm{D}}((T_{R_n}))$ consists of isolated points that can only accumulate to the band ends of $\sigma_e(T_0)$ or $\sigma_e(T_0 + i\gamma)$.
Furthermore, in this case we can prove:

$$\mathrm{Bad}_{1\mathrm{D}}((T_{R_n})) \subset \sigma_e((T_{R_n})) \subseteq \mathrm{Bad}((T_{R_n})). \tag{3}$$

Inclusion for the essential spectrum

Assumption 3

One of the following holds (ensuring analytic cont. of $\lambda \mapsto \psi_+(0,\lambda)$):

1. $q \in L^1(0,\infty)$. q is dilation analytic with power decay for continuation.
2. $q \in L^1(0,\infty)$. There exists $a > 0$ such that $\int e^{ax}|q(x)|\,\mathrm{d}x < \infty$.
3. T_0 is self-adjoint and q is eventually periodic.

Definition

Zeros of the analytic continuation of $\lambda \mapsto \psi_+(0,\lambda)$ are called *resonances* of T_0.

Theorem 3 (S., 2020)

Suppose Assumptions 2 and 3 hold. If $\mu \in \mathrm{int}\,\sigma_e(T_0 + i\gamma)$ such that μ is not a resonance, then there exists $\lambda_R \in \sigma_d(T_R)$, $R > 0$, and constant $C_0 > 0$ s.t.

$$|\lambda_R - \mu| \leqslant \frac{C_0}{R} \qquad (\textit{large enough } R).$$

Numerical illustration (again)

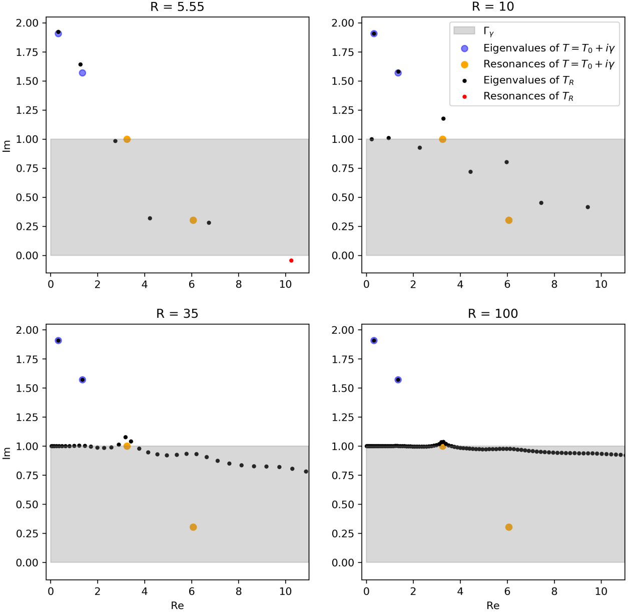
$$T_0 := -\frac{d^2}{dx^2} + i\chi_{[0,X]}$$

$$T_R := T_0 + i\chi_{[0,R]}$$

$$\sigma_e(T_R) = [0,\infty)$$

$$\sigma_e(T_0+i\gamma) = i+[0,\infty)$$

$$\Gamma_\gamma := [0,\infty) \times i[0,1]$$



Thanks for listening!

References

Talk based on:

1. Spectral inclusion and pollution for a class of dissipative perturbations, S. (2020) arXiv:2006.10097

Spectral pollution

1. Spectral pollution, Davies and Plum (2004)
2. Spectral pollution and second-order relative spectra for self-adjoint operators, Levitin and Shargorodsky (2004)

Other works on dissipative barriers

1. Eigenvalues in spectral gaps of differential operators, Marletta and Scheichl (2012)
2. Spectral enclosure and superconvergence for eigenvalues in gaps, Hinchcliffe and Strauss (2016)
3. Bounds for Schrödinger operators on the half-line perturbed by dissipative barriers, S. (2020) arXiv:2010.05663
4. On the eigenvalues of spectral gaps of matrix-valued Schrödinger operators, Aljawi and Marletta (2020)

Limiting essential spectra and essential numerical range

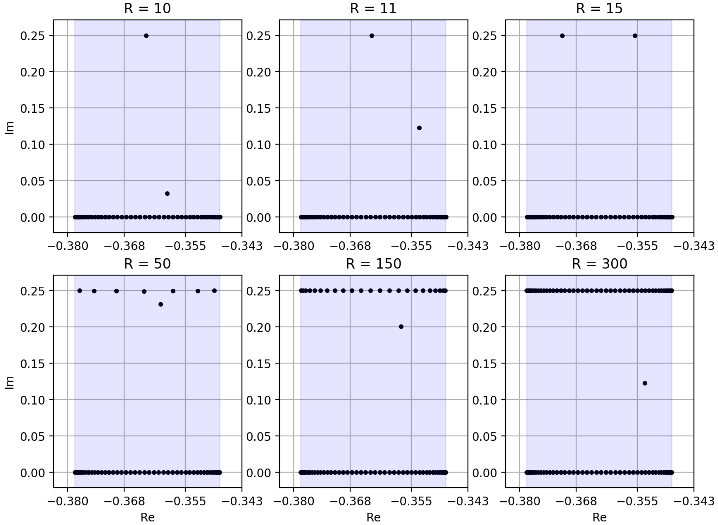
1. Local convergence of spectra and pseudospectra, Bögli (2018)
2. The essential numerical range for unbounded linear operators, Bögli, Marletta and Tretter (2020)

Computing resonances with non-self-adjoint perturbations

1. Scattering Resonances as Viscosity Limits, Zworski (2018)

Extra Slides

Numerical illustration 2: $T_R = -\frac{d^2}{dx^2} + \sin(x) + \frac{1}{4}\chi_{[0,R]}(x)$



Black dots: Finite difference approximation of $\sigma(T_R)$.

First band: $B \approx [-0.3785, -0.3477]$. Shaded region: $B \times i\mathbb{R}$.

Sketch of proof of Theorem 1 (for real part)

- Let $\lambda \in \sigma_e((T_n))$. Focus on enclosing $\Re\lambda$.
- There exists $(u_n) \subset D(T_0)$ such that $\|u_n\| = 1$, $u_n \rightharpoonup 0$ and $\|(T_n - \lambda)u_n\| = o(1)$.
- By direct computation,

$$\|(T_0 - \Re\lambda)u_n\|^2 = \gamma\Im\langle s_n u_n, T_0 u_n\rangle + o(1).$$

- If hypothesis **1** holds then

$$\begin{aligned} s_n^2 = s_n \quad &\Rightarrow \quad \gamma\Im\langle s_n u_n, T_0 u_n\rangle = (\gamma - \Im(\lambda))\Im(\lambda) + o(1) \\ &\overset{(*)}{\Longrightarrow} \quad \operatorname{dist}(\Re\lambda, \sigma_e(T_0)) \leqslant \sqrt{(\gamma - \Im(\lambda))\Im(\lambda)} \end{aligned}$$

- If hypothesis **2** holds then $\Im\langle s_n u_n, T_n u_n\rangle = o(1)$ so $\Re\lambda \in \sigma_e(T_0)$.

(*) Holds by *Direct Methods of Qualitative Spectral Analysis of Singular Differential Operators*, Glazman, Th. I.10.

Bounds for the magnitude and number of eigenvalues

- If $q \in L^1(0,\infty)$, then the eigenvalues of $T_R = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q + i\gamma\chi_{[0,R]}$ are contained in a ball[2], $\forall\lambda \in \sigma_d(T_R) : \sqrt{|\lambda|} \leqslant \|q\|_{L^1}$.
- If one of the following holds:
  1. q is compactly supported
  2. q satisfies Naimark condition: $\exists a > 0 : \int e^{ax}|q(x)|\,\mathrm{d}x < \infty$

  then the number of eigenvalues of T_R is finite.
- Summary of results [3]:

	$\sqrt{\cdot}$ magnitude	$\#$, compact	$\#$, Naimark
Application of literature	$O(R)$	$O(R^2)$	$O(R^4)$
Our results	$O\left(\frac{R}{\log R}\right)$	$O\left(\frac{R^2}{\log R}\right)$	$O\left(\frac{R^3}{(\log R)^2}\right)$

[2] A sharp bound on eigenvalues of Schrödinger operators on the half-line with complex-valued potentials, Frank, Laptev and Seiringer (2011)

[3] Bounds for Schrödinger operators on the half-line perturbed by dissipative barriers, S. (2020)