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

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

where

- $\gamma > 0$,
- $s_n$ are $T_0$-compact, bounded, self-adjoint operators,
- $s_n \xrightarrow{s} I$ (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

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

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

  \[
  \sigma_{\text{poll}}((H_n)) = \{ \lambda \in \sigma((H_n)) : \lambda \notin \sigma(H) \}.
  \]

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

**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.

![Diagram showing the essential spectrum $\sigma_e(T_0)$ and the discrete spectrum $\sigma_d(T_0)$ in the complex plane with real and imaginary axes.]
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 $s_n \xrightarrow{s} I$.

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

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

- $\sigma_d(T_0)$ is encoded in $\sigma_d(T_0 + i\gamma) = \sigma_d(T_0) + i\gamma$.  

\[\begin{align*}
\gamma & \quad \bullet \quad \sigma(T_0 + i\gamma) \\
\sigma(T_0) & \quad \bullet \quad \sigma(T_0 + i\gamma)
\end{align*}\]
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 $\lambda_n$ near $\lambda_0 + i\gamma$.
   - All eigenvalues of $T_n$ in $U$ are near $\lambda_0 + i\gamma$.

2. Numerically compute $\lambda_n \in \sigma_d(T_n) \setminus \mathbb{R}$.
   - This can be done reliably since $s_n$ is $T_0$-compact.\(^1\)

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\(^1\)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 $\sigma(T_0 + i\gamma) \subseteq i\gamma + \mathbb{R}$
  $$\sigma_e(T_n) = \sigma_e(T_0) \subseteq \sigma_{\text{poll}}((T_n)).$$

![Graphical representation of dissipative barriers]

Alexei Stepanenko (Cardiff University) Dissipative Barriers Part I: Dissipative Barrier Method 7 / 20
Limiting essential spectrum

Assumption 1

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

Definition (Limiting essential spectrum)

$$\sigma_e((T_n)) = \left\{ \lambda \in \mathbb{C} : \exists I \subseteq \mathbb{N} \text{ infinite}, \exists u_n \in D(T_n), n \in I \text{ with} \right.$$

$$\|u_n\| = 1, u_n \to 0, \|(T_n - \lambda)u_n\| \to 0 \left. \right\}.$$

Bad Set:

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

Theorem (Immediate corollary of Bögli, 2018)

Suppose Assumption 1 holds.

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

2. $\sigma_{poll}((T_n)) \subseteq \text{Bad}((T_n))$
Limiting essential numerical range

**Definition (Limiting essential numerical range)**

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

**Proposition (Bögli, Marletta and Tretter, 2020)**

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

- \( W_e((T_n)) \) 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 $\text{Bad}((T_n)) \subseteq \Gamma_a$ where,

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

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 \(0 \leq s_n \leq 1\) for all \(n\) and:

\[
\forall (u_n) \subset D(T_0) \text{ s.t. } \|u_n\|, \|T_0 u_n\| \leq C, \quad \mathfrak{s}\langle s_n u_n, T_0 u_n \rangle \to 0,
\]

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

**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 $\lambda \in \sigma_d(T_0 + i\gamma)$.

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

\[ T_0 := -\frac{d^2}{d\chi^2} + i\chi[0,\chi] \]

\[ T_R := T_0 + i\chi[0,R] \]

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

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

\[ \Gamma_\gamma := [0, \infty) \times i[0, 1] \]
Schrödinger operators on the half line

- Consider
  \[ T_0 \psi = -\psi'' + q\psi \quad \text{on} \quad L^2(0, \infty) \]
  where \( q \in L^1_{\text{loc}}([0, \infty); \mathbb{C}) \) and \( T_0 \) is endowed with a Dirichlet boundary condition,
  \[ \psi(0) = 0. \]

- Fix \( \gamma \in \mathbb{C}\setminus\{0\} \). Consider the perturbed operators
  \[ T_R := T_0 + i\gamma \chi_{[0,R]} \quad (R \in \mathbb{R}_+). \]

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

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

such that

1. $k : \mathbb{C} \setminus \sigma_e(T_0) \to \mathbb{C}$ analytic with $\Im k > 0$
2. $\tilde{\psi}_{\pm}(x, \cdot)$ and $\tilde{\psi}^d_{\pm}(x, \cdot)$ analytic on $\mathbb{C} \setminus \sigma_e(T_0)$.
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': \(\text{Bad}_{1D}(\{T_{R_n}\}) \subseteq \mathbb{C}\).

**Theorem 2 (S., 2020)**

Suppose that Assumption 2 holds. Then,

1. Let \(\lambda\) be an eigenvalue of \(T_0 + i\gamma\) such that \(\lambda \notin \text{Bad}_{1D}(\{T_{R_n}\})\).
   There exists \(\lambda_n \in \sigma(T_n), n \in \mathbb{N}\), and constants \(C_0, \beta > 0\) such that
   \[
   |\lambda - \lambda_n| \leq C e^{-\beta R_n}
   \]
   for large enough \(n\).

2. Spectral pollution of \(\{T_{R_n}\}\) with respect to \(T_0 + i\gamma\) satisfies
   \[
   \sigma_{\text{poll}}(\{T_{R_n}\}) \subseteq \sigma_e(T_0) \cup \text{Bad}_{1D}(\{T_{R_n}\}).
   \]

\(^1\)Part 1 of Theorem also proved, for small enough \(\gamma\) 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**

\[ \lambda \text{ eigenvalue of } T_0 \iff \psi_+(0, \lambda) = 0 \]

**Lemma**

\( \lambda \in \mathbb{C} \text{ with } \lambda \notin \sigma_e(T_0) \cup \sigma_e(T_0 + i\gamma) \) 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

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

\[
\alpha_+(R, \lambda) := \psi_-(0, \lambda - i\gamma)\left(\tilde{\psi}_+(R, \lambda - i\gamma)\tilde{\psi}_d^+(R, \lambda) - \tilde{\psi}_+^d(R, \lambda - i\gamma)\tilde{\psi}_+(R, \lambda)\right).
\]

- 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)

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

Example

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

Example

If \( q \) is eventually real \( a \)-periodic and \( R_n = x_0 + na \), then \( \text{Bad}_{1D}(\{T_{R_n}\}) \) 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:

\[
\text{Bad}_{1D}(\{T_{R_n}\}) \subset \sigma_e(\{T_{R_n}\}) \subseteq \text{Bad}(\{T_{R_n}\}).
\]
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 $\int e^{ax}|q(x)| \, dx < \infty$.
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 $\mu \in \text{int} \sigma_e(T_0 + i\gamma)$ such that $\mu$ is not a resonance, then there exists $\lambda_R \in \sigma_d(T_R)$, $R > 0$, and constant $C_0 > 0$ s.t.

$$|\lambda_R - \mu| \leq \frac{C_0}{R} \quad \text{(large enough $R$)}.$$
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:

Spectral pollution

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)
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
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 $\|u_n\| = 1$, $u_n \to 0$ 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

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

$$\Rightarrow \quad \text{dist}(\Re \lambda, \sigma_e(T_0)) \leq \sqrt{\gamma - \Im(\lambda)}\Im(\lambda)$$

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

Bounds for the magnitude and number of eigenvalues

- If \( q \in L^1(0, \infty) \), then the eigenvalues of \( T_R = -\frac{d^2}{dx^2} + q + i\gamma\chi_{[0,R]} \) are contained in a ball\(^2\), \( \forall \lambda \in \sigma_d(T_R) : \sqrt{|\lambda|} \leq ||q||_{L^1} \).

- If one of the following holds:
  1. \( q \) is compactly supported
  2. \( q \) satisfies Naimark condition: \( \exists a > 0 : \int e^{ax}|q(x)|\,dx < \infty \)

  then the number of eigenvalues of \( T_R \) is finite.

Summary of results \(^3\):

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<th>( \sqrt{\cdot} ) magnitude</th>
<th>#, compact</th>
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<tbody>
<tr>
<td>Application of literature</td>
<td>( O(R) )</td>
<td>( O(R^2) )</td>
<td>( O(R^4) )</td>
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<tr>
<td>Our results</td>
<td>( O\left(\frac{R}{\log R}\right) )</td>
<td>( O\left(\frac{R^2}{\log R}\right) )</td>
<td>( O\left(\frac{R^3}{(\log R)^2}\right) )</td>
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\(^2\)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)