# WEYL THEOREMS FOR THE POLLUTED SET OF SELF-ADJOINT OPERATORS IN GALERKIN APPROXIMATIONS

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ABSTRACT. Let $A$ be a self-adjoint operator on a separable Hilbert space $\mathcal{H}$ and let $(\mathcal{L}_n)_{n\in\mathbb{N}}$ be a sequence of finite dimensional subspaces of the domain of $A$, approximating $\mathcal{H}$ in the large $n$ limit. Denote by $A_n$ the compression of $A$ to $\mathcal{L}_n$. In general the spectrum of $A$ is only a subset of the limit of the spectra of $A_n$ and the latter might differ from the former in a non-trivial "polluted set". In this paper we show that this polluted set is determined by the existence of particular Weyl sequences of singular type. This characterization allows us to identify verifiable conditions on self-adjoint perturbations $B$, ensuring that the polluted set of $B$ is identical to that of $A$. The results reported are illustrated by means of several canonical examples and they reveal the many subtleties involved in the systematic study of spectral pollution.

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## 1. CONTEXT

Computing approximations of the spectrum of a self-adjoint operator $A$ acting on an infinite dimensional Hilbert space is a subtle task, in particular when $A$ has gaps in its essential spectrum. A natural approach, which can be traced back to the beginning of the XXth Century, consists in choosing a family $(\mathcal{L}_n)_{n\in\mathbb{N}}$ of finite-dimensional subspaces of the domain and calculating the spectrum of the corresponding compressions $A_n$ of $A$ to $\mathcal{L}_n$. This is the basic idea behind the so-called Galerkin method. In general it is not guaranteed that $\sigma(A_n)$ would converge

*Date*: November 17, 2010.
*Key words and phrases.* Weyl's Theorem, generalized essential spectrum, spectral pollution, Galerkin method.

in an appropriate natural sense to $\sigma(A)$ in regions inside the convex hull of the essential spectrum, even in cases when $\mathcal{L}_n$ contains a subspace becoming increasingly close to spectral subspaces of $A$ (see the various examples below). Typically the large $n$ limit of $\sigma(A_n)$ would cover $\sigma(A)$, however the former can be much larger than the latter, giving rise to what is usually referred to as spectral pollution.

Spectral pollution is a remarkable phenomenon which is encountered in many different practical situations. It arises when approximating the spectrum of Sturm-Liouville operators [1, 32, 31], perturbations of periodic Schrödinger operators [7] and systems underlying elliptic partial differential equations [2, 4, 5]. It is a well-documented difficulty in quantum chemistry and physics, in particular regarding relativistic computations [20, 30, 17, 15]. It also plays a fundamental rôle in elasticity and magnetohydrodynamics [19, 10, 27, 3].

In recent years this phenomenon has raised a large interest in the mathematical community [23, 18, 21, 12, 13, 26, 25] and there are known alternative computational procedures capable of avoiding it. These include specialized variational formulations such as those studied at length in [16, 19, 14, 24], as well as general methods such as those proposed in [8, 6, 7, 21, 12]. Another possible approach is to derive conditions on the approximating subspaces allowing to avoid pollution in a given interval of the real line. These conditions can be found for operators with a particular structure, and they are motivated from procedures in numerical analysis [2, 5, 27] and computational physics and chemistry [22]. In the latter work an abstract framework in this respect was formulated and successfully applied to problems from relativistic and non-relativistic quantum theory.

In the present article we adopt a similar approach as that considered in [22]. We introduce the notion of relative spectrum, $\sigma(A,\mathcal{L})$, obtained from the approximating sequence of spaces $\mathcal{L} = (\mathcal{L}_n)_{n\in\mathbb{N}}$, as the limiting set in Hausdorff distance of the spectra $\sigma(A_n)$ as $n \to \infty$. Under natural conditions, $\sigma(A) \subset \sigma(A,\mathcal{L})$ (Proposition 3). We then introduce (Definition 3) the notion of relative essential spectrum associated with $\mathcal{L}$, $\sigma_{\rm ess}(A,\mathcal{L})$. This latter set contain both the true essential spectrum of $A$ and the set of all spurious (or polluted) points of the method associated with $\mathcal{L}$ (Proposition 5). These points are the ones which ought to be avoided in numerical simulations.

Once we have established elementary properties of the relative spectra $\sigma(A,\mathcal{L})$ and $\sigma_{\rm ess}(A,\mathcal{L})$, we address the following natural question: under which conditions on a perturbation $B$ is the equality

$$\sigma_{\rm ess}(B,\mathcal{L}) = \sigma_{\rm ess}(A,\mathcal{L}) \tag{1}$$

satisfied? According to our main result (Theorem 11) when $A$ and $B$ are bounded from below and

$$(A-a)^{1/2}(B-a)^{-1/2} - 1 \tag{2}$$

is a compact operator for some $a$ negative enough, then (1) holds true. Therefore, under the condition (2), an approximating sequence $\mathcal{L}$ will not pollute for $A$ in a given interval if and only if it will not pollute for $B$ in the same interval. This generalizes [22, Corollary 2.5].

The key to our present approach is to adapt to the relative spectra several classical results for the spectrum and essential spectrum. In turns, this leads to many unexpected difficulties which we will illustrate on a variety of simple examples. In particular, we establish (Theorem 7) a relative version of the spectral mapping theorem allowing to replace the unbounded operator $A$ by its (bounded) resolvent $(A-a)^{-1}$. Remarkably, this theorem fails in general (Remark 4) for operators which are not semi-bounded.

The theoretical framework that we presently establish, provides an insight on the difficulties encountered in the presence of spectral pollution and it highlights its many subtleties.

**Background notation.** We will subsequently denote by $\mathcal{B}(\mathcal{H}_1,\mathcal{H}_2)$ the space of bounded operators between two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$. We will denote by $\mathcal{K}(\mathcal{H})$ the algebra of compact operators on the Hilbert space $\mathcal{H}$. We adopt the bra-ket symbol $|x\rangle\langle y|$, to denote the rank-one operator defined as $|x\rangle\langle y|\, z = \langle y, z\rangle x$. Here $\langle\cdot,\cdot\rangle$ is the scalar product of $\mathcal{H}$.

Below $A$ denotes a densely defined self-adjoint operator acting on a separable infinite dimensional $\mathcal{H}$, with domain $\mathrm{D}(A)\subset\mathcal{H}$. By $\sigma(A)$, $\sigma_{\mathrm{ess}}(A)$ and $\sigma_{\mathrm{disc}}(A)$ we mean the spectrum, essential spectrum and discrete spectrum of $A$.

On sequences $(x_n)_{n\in\mathbb{N}}\subset\mathcal{H}$ of vectors and $(\mathcal{L}_n)_{n\in\mathbb{N}}$ of subspaces $\mathcal{L}_n\subset\mathrm{D}(A)$ we will ofter suppress the index and write $(x_n)$ and $(\mathcal{L}_n)$ instead. we will denote by $x_n \rightharpoonup x$ the fact that $x_n$ is weakly convergent to $x\in\mathcal{H}$. When the norm is not specified, $x_n\to x$ will denote the fact that $\|x_n-x\|\to 0$.

## 2. Basic definitions

We will often make the assumption that $A$ is bounded from below, however we will not require this for the moment. For $n\in\mathbb{N}$, let $\mathcal{L}=(\mathcal{L}_n)$ be a sequence of finite-dimensional subspaces of $\mathrm{D}(A)$. We assume that $\mathcal{L}_n$ approximates $\mathrm{D}(A)$ as $n\to\infty$ in the following precise sense:

**Definition 1** ($A$-regular Galerkin sequences)**.** We say that $\mathcal{L}=(\mathcal{L}_n)$ is an <u>$A$-regular Galerkin sequence</u>, or simply an $A$-regular sequence, if for all $f\in\mathrm{D}(A)$ there exists a sequence of vectors $(f_n)$ with $f_n\in\mathcal{L}_n$ such that $f_n\to f$ in the graph norm of $A$, that is:

$$\|f_n-f\|+\|Af_n-Af\|\to_{n\to\infty} 0. \tag{3}$$

Below we will always assume that $\mathcal{L}=(\mathcal{L}_n)$ is an $A$-regular sequence. The orthogonal projection in the scalar product of $\mathcal{H}$ onto $\mathcal{L}_n$ will be denoted by $\pi_n:\mathcal{H}\longrightarrow\mathcal{L}_n$ and the compression of $A$ to $\mathcal{L}_n$ by $A_n=\pi_n A\restriction_{\mathcal{L}_n}:\mathcal{L}_n\longrightarrow\mathcal{L}_n$. The compression $A_n$ will sometimes be identified with one of its matrix representation.

### 2.1. Spectrum of a self-adjoint operator relative to a Galerkin sequence.

The spectrum of $A$ relative to the $A$-regular Galerkin sequence $\mathcal{L}$, will be the set of all limit points of the spectra of $A_n$ in the large $n$ limit.

**Definition 2** (Relative spectrum)**.** The <u>spectrum of $A$ relative to</u> $\mathcal{L}=(\mathcal{L}_n)$, $\sigma(A,\mathcal{L})$, is the set of all $\lambda\in\mathbb{R}$ for which there exists a sequence $\lambda_k\in\sigma(A_{n_k})$ such that $n_k\to\infty$ and $\lambda_k\to\lambda$ as $k\to\infty$.

Since all $A_n$ are Hermitian endomorphisms in the above definition, clearly $\sigma(A,\mathcal{L})\subset\mathbb{R}$. The following lemma provides an alternative characterization of $\sigma(A,\mathcal{L})$.

**Lemma 1** ($\mathcal{L}$-Weyl sequences)**.** *The real number $\lambda\in\sigma(A,\mathcal{L})$ if and only if there exists a sequence $(x_k)\subset\mathrm{D}(A)$ such that $x_k\in\mathcal{L}_{n_k}$, $\|x_k\|=1$ and $\pi_{n_k}(A-\lambda)\,x_k\to 0$ as $k\to\infty$.*

*Proof.* According to the definition, $\lambda \in \sigma(A, \mathcal{L})$ if and only if there exists $\lambda_k \in \mathbb{R}$ and $x_k \in \mathcal{L}_{n_k}$ with $\|x_k\| = 1$ such that $\lambda_k \to \lambda$ and $\pi_{n_k}(A - \lambda_k)\, x_k = 0$. As $\pi_{n_k}(A - \lambda)\, x_k = (\lambda_k - \lambda) x_k \to 0$, one of the stated implications follows immediately.

On the other hand, if $(x_k) \subset \mathrm{D}(A)$ is as stated, then $\|(A_{n_k} - \lambda) x_k\| \to 0$. Since the $A_n$ are Hermitian, there necessarily exists $\lambda_k \in \sigma(A_{n_k})$ such that $|\lambda_k - \lambda| \le \|(A_{n_k} - \lambda) x_k\| \to 0$. Thus $\lambda \in \sigma(A, \mathcal{L})$ ensuring the complementary implication. □

We call $(x_k)$ an $\mathcal{L}$-Weyl sequence for $\lambda \in \sigma(A, \mathcal{L})$ by analogy to the classical notion of Weyl sequence [11].

**Remark 1.** Self-adjointness of the $A_n$ is crucial in Lemma 1. We illustrate this by means of a simple example. Let $\mathcal{H} = \ell^2(\mathbb{N})$ and $(e_j) \subset \mathcal{H}$ be the canonical orthonormal basis of this space. Let $A$ be the left shift operator defined by the condition $A : e_j \longmapsto e_{j-1}$ with the convention $e_0 = 0$. Let $\mathcal{L}_k = \operatorname{Span}\{e_i, i \le k\}$. For this data an analogous of Lemma 1 is no longer valid. Indeed, if $|\lambda| < 1$ and

$$x_k := \sqrt{\frac{1 - |\lambda|^2}{1 - |\lambda|^{2k-2}}} \sum_{i=1}^{k} \lambda^i e_i,$$

then $x_k \in \mathcal{L}_k$, $\|x_k\| = 1$ and

$$\|A x_k - \lambda x_k\| = \sqrt{\frac{1 - |\lambda|^2}{1 - |\lambda|^{2k-2}}}\, |\lambda|^{k+1} \to 0.$$

Therefore any point of the open unit disk is associated with an $\mathcal{L}$-Weyl sequence. However, on the other hand, $A_n$ is a Jordan block, so $\sigma(A_n) = \{0\}$ for all $n \in \mathbb{N}$ and hence necessarily $\sigma(A, \mathcal{L}) = \{0\}$. ◇

The above characterization of points in the relative spectrum combined with the minimax principle yields the following fundamental statement.

**Proposition 2** (The relative spectra and the spectrum)**.** *Let $\mathcal{L}$ be an $A$-regular Galerkin sequence. Then*

$$\sigma(A) \subset \sigma(A, \mathcal{L}) \tag{4}$$

*and*

$$\sigma(A, \mathcal{L}) \setminus \sigma(A) \subset \left(\ell^-\,,\, \ell^+\right) \tag{5}$$

*where*

$$\ell^- := \begin{cases} -\infty & \text{for } \inf \sigma(A) = -\infty \\ \inf \sigma_{\mathrm{ess}}(A) & \text{otherwise} \end{cases}$$

$$\ell^+ := \begin{cases} +\infty & \text{for } \sup \sigma(A) = +\infty \\ \sup \sigma_{\mathrm{ess}}(A) & \text{otherwise.} \end{cases}$$

*Proof.* The classical characterization of the spectrum of self-adjoint operators ensures that $\lambda \in \sigma(A)$ if and only if there is a normalized sequence $(y_k) \subset \mathrm{D}(A)$ such that $\|(A - \lambda) y_k\| \to 0$ (that is $(y_k)$ is a Weyl sequence for $\lambda$). We will now construct an $\mathcal{L}$-Weyl sequence from $(y_k)$. According to (3), we can find $(x^k_m)_{(k,m) \in \mathbb{N}^2}$ such that $x^k_m \in \mathcal{L}_m$, $(y_k - x^k_m) \to 0$ and $(A - \lambda)(y_k - x^k_m) \to 0$ as $m \to \infty$. By virtue of a diagonal process, we can extract a subsequence such that $\pi_{m_k}(A - \lambda) x^k_{m_k} \to 0$. Dividing by $\|x^k_{m_k}\|$ (which does not vanish in the $k \to \infty$ limit), gives (4) as consequence of Lemma 1.

The proof of (5) is a classical consequence of the minimax principle. It may be found, for instance, in [21, Theorem 2.1] and also [22, Theorem 1.4]. □

In [22, Theorem 1.4] the existence of an $A$-regular Galerkin sequence $\mathcal{L}$ such that $\sigma(A,\mathcal{L}) = [\ell^-, \ell^+]$ is shown. The inclusion complementary to (4) does not hold in general. This is a source of difficulties in applications as there is not known systematic procedure able to identify $A$-regular Galerkin sequences such that $\sigma(A) = \sigma(A,\mathcal{L})$. By virtue of (5), spectral pollution can only occur in "gaps" of the essential spectrum.

2.2. **Relative essential and discrete spectra.** Points in $\sigma(A,\mathcal{L}) \setminus \sigma(A)$ can be characterized in a more precise manner in terms of particular $\mathcal{L}$-Weyl sequences as we will see next.

**Definition 3** (Relative essential spectrum)**.** We denote by $\sigma_{\mathrm{ess}}(A,\mathcal{L})$ the set of all $\lambda \in \sigma(A,\mathcal{L})$ for which there exists an $\mathcal{L}$-Weyl sequence $(x_k)$ as in Lemma 1 with the additional property that $x_k \rightharpoonup 0$.

By analogy to the classical notions, we will call $\sigma_{\mathrm{ess}}(A,\mathcal{L})$ the essential spectrum of $A$ relative to $\mathcal{L}$ and the corresponding sequence $(x_k)$ a singular $\mathcal{L}$-Weyl sequence.

**Remark 2.** From the definition it follows that $\sigma_{\mathrm{ess}}(A+K,\mathcal{L}) = \sigma_{\mathrm{ess}}(A,\mathcal{L})$ for any self-adjoint operator $K \in \mathcal{K}(\mathcal{H})$. ◇

**Definition 4** (Relative discrete spectrum)**.** We call the residual set $\sigma_{\mathrm{disc}}(A,\mathcal{L}) = \sigma(A,\mathcal{L}) \setminus \sigma_{\mathrm{ess}}(A,\mathcal{L})$, the discrete spectrum of $A$ relative to $\mathcal{L}$.

We illustrate these definitions by means of various simple examples.

**Example 1** ($A$ a bounded operator)**.** Let $\mathcal{H} = \mathrm{Span}\{e_n^\pm\}_{n\in\mathbb{N}}$ where $e_n^\pm$ is an orthonormal set of vectors in a given scalar product. Define $\mathcal{L}_n = \mathrm{Span}\{e_1^\pm, \dots, e_{n-1}^\pm, f_n\}$ where $f_n = \cos\theta\, e_n^+ + \sin\theta\, e_n^-$ for $\theta \in (0,\pi/2)$. Let

$$A = \sum_{n\geq 1} |e_n^+\rangle\langle e_n^+|,$$

that is, $A$ is the orthogonal projector onto $\mathrm{Span}(e_n^+)$ and $\sigma(A) = \sigma_{\mathrm{ess}}(A) = \{0,1\}$. Then $\sigma(A_n) = \{0, 1, \cos^2\theta\}$ for all $n$ and $\sigma(A,\mathcal{L}) = \sigma_{\mathrm{ess}}(A,\mathcal{L}) = \{0,1,\cos^2\theta\}$. ◇

**Example 2** ($A$ a semi-bounded operator)**.** Let $\mathcal{H}$ be as in Example 1 and define

$$\mathcal{L}_n = \mathrm{Span}\{e_1^\pm, \dots, e_{n-1}^\pm, e_n^-\}.$$

For $f_n^\pm = \sin(\frac{1}{n})\, e_n^\mp \pm \cos(\frac{1}{n})\, e_n^\pm$, let

$$A = \sum n^2 |f_n^+\rangle\langle f_n^+| - \sum |f_n^-\rangle\langle f_n^-|$$

which has a $2\times 2$ block diagonal representation in the basis $(e_n^\pm)$. Then $\sigma_{\mathrm{ess}}(A) = \{-1\}$ and $\sigma_{\mathrm{disc}}(A) = \{n^2 : n \in \mathbb{N}\}$. On the other hand

$$\sigma(A_n) = \left\{ -1, n^2 \sin\left(\frac{1}{n}\right)^2 - \cos\left(\frac{1}{n}\right)^2, 1, \dots, (n-1)^2 \right\},$$

where $-1$ is an eigenvalue of multiplicity $n$, therefore

$$\sigma_{\mathrm{ess}}(A,\mathcal{L}) = \{-1, 0\} \qquad \text{and} \qquad \sigma_{\mathrm{disc}}(A,\mathcal{L}) = \{n^2 : n \in \mathbb{N}\}.$$

The former is a consequence of Proposition 3-(ii) while the latter follows from Proposition 5-(iii) below.

We can also verify the validity of the latter as follows. Assume that $(x_k)$ is a singular $\mathcal{L}$-Weyl sequence associated with $\nu^2 \in \sigma_{\rm disc}(A)$. Then $\pi_{n_k}(A-\nu^2)x_k \to 0$ and $x_k \rightharpoonup 0$. For $m < n_k$

$$p_m \pi_{n_k}(A-\nu^2)x_k = (A-\nu^2)p_m x_k$$

where $p_m = \sum_{i<m} |f_i^\pm\rangle\langle f_i^\pm|$. Then

$$\|p_{n_k-1}x_k - \langle f_\nu^+|x_k\rangle f_\nu^+\|^2 \le \left\|(A-\nu^2)p_{n_k-1}x_k\right\|^2 \to 0$$

as $k \to \infty$. Since $x_k \rightharpoonup 0$, then also $\|p_{n_k-1}x_k\|^2 + \left\|(A-\nu^2)p_{n_k-1}x_k\right\|^2 \to 0$. Therefore

$$(A-\nu^2)(x_k - \langle e_{n_k}^-, x_k\rangle e_{n_k}^-) \to 0.$$

As $\left|\langle (A-\nu^2)e_n^-, e_n^-\rangle\right| = \left|n^2\sin^2(\frac{1}{n}) + \cos^2(\frac{1}{n}) - \nu^2\right| \to \left|2-\nu^2\right| > 0$, projecting each term onto $\mathcal{L}_{n_k}$ yields $\langle e_k^-, x_k\rangle \to 0$. Thus $1 = \|x_k\| \to 0$, which is a contradiction. ◇

**Example 3** ($A$ a strongly indefinite operator)**.** Let $\mathcal{H}$ and $\mathcal{L}_n$ be as in Example 2. Let $f_n^\pm = \frac{1}{\sqrt{2}}e_n^+ \pm \frac{1}{\sqrt{2}}e_n^-$. Let

$$A = \sum n|f_n^+\rangle\langle f_n^+| - \sum n|f_n^-\rangle\langle f_n^-|.$$

Then $\sigma(A) = \{\pm n : n \in \mathbb{N}\} = \sigma_{\rm disc}(A)$. On the other hand

$$\sigma(A,\mathcal{L}) = \mathbb{Z}, \qquad \sigma_{\rm ess}(A,\mathcal{L}) = \{0\}, \qquad \text{and} \qquad \sigma_{\rm disc}(A,\mathcal{L}) = \{\pm n : n \in \mathbb{N}\}.$$

Note that the proof of the latter is similar to that of the analogous property in Example 2. ◇

## 3. The relative spectra and the behaviour of singular $\mathcal{L}$-Weyl sequences

In this section we establish various properties of the relative spectra $\sigma(A,\mathcal{L})$, $\sigma_{\rm ess}(A,\mathcal{L})$ and $\sigma_{\rm disc}(A,\mathcal{L})$. These properties can be deduced from properties of different types of $\mathcal{L}$-Weyl sequences.

**Proposition 3** (Essential and discrete relative spectra and the spectrum)**.** *Let $\mathcal{L}$ be an $A$-regular Galerkin sequence. Then*

(i) *the relative spectrum $\sigma(A,\mathcal{L})$ and the relative essential spectrum $\sigma_{\rm ess}(A,\mathcal{L})$ are closed subsets of $\mathbb{R}$;*

(ii) *moreover $\sigma_{\rm ess}(A) \subset \sigma_{\rm ess}(A,\mathcal{L})$ and $\sigma_{\rm disc}(A,\mathcal{L}) \subset \sigma_{\rm disc}(A)$.*

*Proof.* The proof of (i) involves a standard diagonal argument and it is left to the reader. For the second statement we need the following auxiliary result which will be used repeatedly below.

**Lemma 4.** *There exists $x_k \in \mathcal{L}_{n_k}$ such that $\|x_k\| = 1$, $x_k \rightharpoonup x$ and $\pi_{n_k}(A-\lambda)x_k \to 0$, only when $x \in \operatorname{Ker}(A-\lambda)$.*

*Proof of Lemma 4.* Suppose that $(x_k)$ satisfies the hypothesis. Let $f \in \mathrm{D}(A)$ and $f_n \in \mathcal{L}_n$ such that $f_n \to f$ in the norm of $\mathrm{D}(A)$. Then $\langle \pi_{n_k}(A-\lambda)x_k, f_{n_k}\rangle \to 0$. On the other hand, since $f_k \to f$ in $\mathrm{D}(A)$,

$$\langle \pi_{n_k}(A-\lambda)x_k, f_{n_k}\rangle = \langle x_k, (A-\lambda)f_{n_k}\rangle \to \langle x, (A-\lambda)f\rangle.$$

Thus $\langle x, (A-\lambda)f\rangle = 0$ for all $f \in \mathrm{D}(A)$, so that $x \in \mathrm{D}(A^*) = \mathrm{D}(A)$ and $(A-\lambda)x = 0$ as required. □

In order to prove (ii) of Proposition 3 we proceed as follows. The fact that $\sigma_{\rm ess}(A) \subset \sigma_{\rm ess}(A,\mathcal{L})$ is proved similarly to (4). It should only be noted that the $\mathcal{L}$-Weyl sequence found for $\lambda \in \sigma_{\rm ess}(A)$ additionally satisfies $x^k_{m_k} \rightharpoonup 0$.

For the inclusion $\sigma_{\rm disc}(A,\mathcal{L}) \subset \sigma_{\rm disc}(A)$ note that, if $\lambda \in \sigma_{\rm disc}(A,\mathcal{L})$, there exists $x_k \in \mathcal{L}_{n_k}$ such that $\|x_k\| = 1$, $x_k \rightharpoonup x \neq 0$ and $\pi_{n_k}(A-\lambda)x_k \to 0$. As $\lambda \notin \sigma_{\rm ess}(A)$ (by the previous part), then either $\lambda \in \sigma_{\rm disc}(A)$ or $\lambda \notin \sigma(A)$. By Lemma 4, the latter is impossible. □

**Remark 3.** If $\sigma_{\rm ess}(A) = \sigma_{\rm ess}(A,\mathcal{L})$ then automatically $\sigma_{\rm disc}(A) = \sigma_{\rm disc}(A,\mathcal{L})$ and $\sigma(A) = \sigma(A,\mathcal{L})$. ◇

We will now describe in more details the behaviour of singular $\mathcal{L}$-Weyl sequences in the particular case $\lambda \in \sigma_{\rm ess}(A,\mathcal{L}) \setminus \sigma_{\rm ess}(A)$.

**Proposition 5** (Singular $\mathcal{L}$-Weyl sequences)**.** *The real number $\lambda \in \sigma_{\rm ess}(A,\mathcal{L})$ if and only if*

(i) *either $\lambda \notin \sigma(A)$ and there exists $\lambda_k \to \lambda$ and $y_k \in \mathcal{L}_{n_k}$ such that $y_k \rightharpoonup 0$ and $\Pi_{n_k}(A-\lambda_k)y_k = 0$;*

(ii) *or $\lambda \in \sigma_{\rm ess}(A)$ and there exists $\lambda_k \to \lambda$ and $y_k \in \mathcal{L}_{n_k}$ such that $y_k \rightharpoonup 0$ and $\Pi_{n_k}(A-\lambda_k)y_k = 0$;*

(iii) *or $\lambda \in \sigma_{\rm disc}(A)$ and for any $\varepsilon > 0$*

$$\mathrm{Rank}\left(\mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(A_n)\right) \geq \mathrm{Rank}\left(\mathbb{1}_{\{\lambda\}}(A)\right) + 1$$

*for all $n$ large enough.*

In cases (i) and (iii), $\lambda$ can be regarded as an <u>$\mathcal{L}$-spurious point</u> of $A$. In case (iii) $\lambda \in \sigma(A)$, but the multiplicity of the approximated spectrum $\sigma(A_n)$ is too large for $n$ large, leading to the wrong spectral representation of $A$ in the limit $n \to \infty$. In case (ii) the singular $\mathcal{L}$-Weyl sequence $(y_k)$ behaves like a classical singular Weyl sequence.

Only in cases (i) and (ii) the existence of a singular $\mathcal{L}$-Weyl sequence $(y_k)$ consisting of <u>exact eigenvectors</u> of $A_{n_k}$ such that $\Pi_{n_k}(A-\lambda_k)y_k = 0$ and $\lambda_k \to \lambda$ is guaranteed. In case (iii) it may occur that all the eigenvectors of $A_{n_k}$ whose corresponding eigenvalue converges to $\lambda$, converge weakly to a non-zero element of $\mathrm{Ker}(A-\lambda)$, and that only a linear combination of these eigenvectors converges weakly to zero. This can be illustrated by means of a simple example.

**Example 4** (Spectral point satisfying Proposition 5-(iii))**.** Let $\mathcal{H} = \mathrm{Span}\{e_0, e_n^\pm\}$ where $e_0, e_n^\pm$ form an orthonormal basis. Let

$$A = \sum_{n=1}^{\infty} |e_n^+\rangle\langle e_n^+| - \sum_{n=1}^{\infty} |e_n^-\rangle\langle e_n^-|.$$

Then $\sigma(A) = \{-1, 0, 1\}$ and $\sigma_{\rm ess}(A) = \{-1, 1\}$. The eigenvalue 0 has multiplicity one and associated eigenvector $e_0$. Let

$$\mathcal{L}_n = \mathrm{Span}\{e_1^\pm, \ldots, e_{n-1}^\pm, f_n^\pm\} \quad \text{where} \quad f_n^\pm = \frac{e_0 + \alpha_n^\pm\, e_n^+ + \beta_n^\pm\, e_n^-}{\sqrt{1 + (\alpha_n^\pm)^2 + (\beta_n^\pm)^2}}$$

for

$$\alpha_n^\pm = \pm\sqrt{\frac{1 \pm \frac{1}{n^2}}{2(1 \mp \frac{1}{n^2})}} \qquad \text{and} \qquad \beta_n^\pm = \pm\sqrt{\frac{1 \mp \frac{1}{n^2}}{2(1 \pm \frac{1}{n^2})}}.$$

Then $\sigma(A, \mathcal{L}) = \{0, \pm 1\} = \sigma_{\rm ess}(A, \mathcal{L})$. In this case $A_n$ has two eigenvalues approaching zero in the large $n$ limit, with corresponding eigenvectors $f_n^+$ and $f_n^-$. It is readily seen that $f_n^\pm \rightharpoonup e_0/\sqrt{2}$ and so only the difference $f_n^+ - f_n^-$ tends weakly to zero. ◇

*Proof of Proposition 5.* Let $\lambda \in \sigma_{\rm ess}(A, \mathcal{L}) \subset \sigma(A, \mathcal{L})$. By definition of $\sigma(A, \mathcal{L})$ there exists a normalized sequence $(y_k)$ such that $\pi_{n_k}(A - \lambda_k)y_k = 0$ and $\lambda_k \to \lambda$. The main question is whether one can ensure that $y_k \rightharpoonup 0$ weakly. Up to extraction of a subsequence we may assume that $y_k \rightharpoonup y \in \operatorname{Ker}(A - \lambda)$ (by Lemma 4). If $\lambda \notin \sigma(A)$, then $\operatorname{Ker}(A - \lambda) = \{0\}$ and necessarily $y = 0$, thus (i) follows.

We now turn to the proof of (ii). To proceed further, we require the following auxiliary result.

**Lemma 6.** *Let $\mathcal{V} \subset \mathrm{D}(A)$ be a subspace of dimension $d > 0$. Let $\varepsilon > 0$ be such that*

$$\|(A - \lambda)x\| \le \varepsilon\|x\| \qquad \forall x \in \mathcal{V}.$$

*Let $\mathcal{W}_n = \pi_n\mathcal{V}$. There exists $N > 0$ such that for all $n \ge N$,*

$$\|(A - \lambda)y\| \le 2\varepsilon\sqrt{d}\|y\| \qquad \forall y \in \mathcal{W}_n.$$

*Proof of Lemma 6.* Let $(e_j)$ be an orthonormal basis of $\mathcal{V}$. For sufficiently large $n$, $\pi_n e_j$ is a basis for $\mathcal{W}_n$. By applying the Gramm-Schmidt procedure to $\pi_n e_j$, we can construct an orthonormal basis $(f_j^n)$ of $\mathcal{W}_n$ such that

$$\|e_j - f_j^n\|_{\mathrm{D}(A)} \to 0 \qquad n \to \infty.$$

Let $N > 0$ be such that

$$\|(A - \lambda)f_j^n\| \le 2\varepsilon \qquad \forall n \ge N, \quad j = 1, \ldots, d.$$

For $y = \sum_{j=1}^d \hat{y}_j f_j^n \in \mathcal{W}_n$, we get

$$\|(A - \lambda)y\| \le 2\varepsilon\sum_{j=1}^d |\hat{y}_j| \le 2\varepsilon\sqrt{d}\|y\|,$$

which ensures the desired property. □

The proof of (ii) in Proposition 5 is achieved as follows. Assume that $\lambda \in \sigma_{\rm ess}(A)$. For all $d \in \mathbb{N}$ there exists a subspace $\mathcal{V}_d \subset \mathrm{D}(A)$, such that $\dim \mathcal{V}_d = d^2$ and

$$\|(A - \lambda)y\| \le \frac{1}{d^2}\|y\| \qquad \forall y \in \mathcal{V}_d,$$

see for instance [11, Lemma 4.1.4]. According to Lemma 6 and an inductive argument, there is a sequence $(n_d) \subset \mathbb{N}$ and $d^2$-dimensional subspaces $\mathcal{W}_d \subset \mathcal{L}_{n_d}$, such that

$$\|\pi_{n_d}(A - \lambda)y\| \le \frac{2}{d}\|y\| \qquad \forall y \in \mathcal{W}_d.$$

This ensures that $A_{n_d}$ has at least $d^2$ eigenvalues in the interval $\big[\lambda - 2/d, \lambda + 2/d\big]$.

Let $(f_j^{n_d})_{j=1}^{d^2} \subset \mathcal{L}_{n_d}$ be an orthonormal set of $d^2$ eigenvectors of $A_{n_d}$, with associated eigenvalues $(\lambda_j^{n_d})_{j=1}^{d^2}$ satisfying $|\lambda_j^{n_d} - \lambda| \le 2/d$. We inductively define the following singular $\mathcal{L}$-Weyl sequence for $\lambda$:

$$\begin{aligned}
y_1 &= f_1^{n_1} && \\
y_2 &= f_{\delta_2}^{n_2} && \text{with } 1 \le \delta_2 \le 2^2 \text{ such that } |\langle y_2, y_1\rangle| \le 1/\sqrt{2} \\
y_3 &= f_{\delta_3}^{n_3} && \text{with } 1 \le \delta_3 \le 3^2 \text{ such that } |\langle y_3, y_j\rangle| \le 1/\sqrt{3} \text{ for } j = 1,2 \\
&\vdots && \\
y_d &= f_{\delta_d}^{n_d} && \text{with } 1 \le \delta_d \le d^2 \text{ such that } |\langle y_d, y_j\rangle| \le 1/\sqrt{d} \text{ for } j = 1, \dots, d-1.
\end{aligned}$$

The existence of $\delta_d$ is guaranteed by the fact that

$$\forall k = 1, ..., d-1, \qquad 1 = \|y_k\|^2 \ge \sum_{j=1}^{d^2} |\langle y_k, f_j^{n_d}\rangle|^2.$$

Indeed, there are at most $d$ indices $j$ in the above summation, such that $|\langle y_k, f_j^{n_d}\rangle|^2 \ge 1/d$. Hence, in total, there are at most $d(d-1)$ indices $j$ such that $|\langle y_k, f_j^{n_d}\rangle|^2 \ge 1/d$ for at least one $k = 1, ..., d-1$. Since $d(d-1) < d^2$ for $d \ge 1$, we deduce that there is at least one index $j =: \delta_d$ such that $|\langle y_k, f_j^{n_d}\rangle|^2 \le 1/d$ for all $k = 1, ..., d-1$.

By construction $\|y_d\| = 1$ and $|\langle y_i, y_j\rangle| \le 1/\sqrt{\max(i,j)}$. Thus $y_k \rightharpoonup 0$ as $k \to \infty$, ensuring (ii).

Note that, conversely, if (i) or (ii) holds true, then $\lambda \in \sigma_{\text{ess}}(A, \mathcal{L})$ by Definition 3.

Let us now prove that if $\lambda \in \sigma_{\text{ess}}(A, \mathcal{L}) \cap \sigma_{\text{disc}}(A)$, then (iii) holds true. Let $x_k \in \mathcal{L}_{n_k}$ be a singular $\mathcal{L}$-Weyl sequence: $\pi_{n_k}(A - \lambda)x_k \to 0$, $\|x_k\| = 1$ and $x_k \rightharpoonup 0$. Let $\mathcal{V} = \text{Ker}(A - \lambda) \ne \{0\}$ and $d = \dim(\mathcal{V})$. For $n$ sufficiently large $\mathcal{W}_n := \pi_n \mathcal{V} \subset \mathcal{L}_n$ is of dimension $d$. Also, for all $\varepsilon > 0$, there exists $N > 0$ such that

$$\|\pi_n(A - \lambda)y\| \le \varepsilon \|y\| \qquad \forall y \in \mathcal{W}_n$$

whenever $n \ge N$. Let $\mathcal{S}_k = \text{Span}\{\mathcal{W}_{n_k}, x_k\}$. Since $x_k \rightharpoonup 0$ and $\mathcal{W}_{n_k}$ does not increase in dimension in the large $k$ limit, necessarily $\dim(\mathcal{S}_k) = d+1$ for all $k$ large enough. For all $\varepsilon > 0$ there exists $M > 0$ such that

$$\|\pi_{n_k}(A - \lambda)y\| \le \varepsilon \|y\| \qquad \forall y \in \mathcal{S}_k$$

whenever $k \ge M$. This ensures that $\sigma(A_{n_k}) \cap (\lambda - \varepsilon, \lambda + \varepsilon)$ contains at least $d+1$ points counting multiplicity and hence the claimed conclusion is achieved.

It only remains to prove that (iii) implies $\lambda \in \sigma_{\text{ess}}(A, \mathcal{L})$. Each individual eigenvector of $A_{n_k}$ might not converge weakly to 0, however there is a linear combination of them that does it. We prove this as follows. Let $(f_j^k)_{j=1}^{d+1}$ be an orthonormal set of $d+1$ eigenvectors

$$A_{n_k} f_j^k = \lambda_j^k f_j^k \qquad j = 1, \dots, d+1.$$

Up to extraction of subsequences we may assume that $f_j^k \rightharpoonup f_j \in \text{Ker}(A - \lambda)$ for all $j = 1, \dots, d+1$. If $f_j = 0$ for some $j$, then the desired conclusion follows. Otherwise, since $\dim \text{Ker}(A - \lambda) = d$, there exist coefficients $(a_j) \in \mathbb{C}^{d+1} \setminus \{0\}$ such that $\sum_{j=1}^{d+1} a_j f_j = 0$. Therefore, we may take

$$y_k := \frac{\sum_{j=1}^{d+1} a_j f_j^k}{\sqrt{\sum_{j=1}^{d+1} |a_j|^2}}$$

as singular $\mathcal{L}$-Weyl sequence for $\lambda$. This ends the proof of Proposition 5. □

## 4. Mapping of relative spectra

In this section we establish mapping theorems for the different relative spectra. They are a natural generalization of the analogous well-known result for $\sigma(A)$ and $\sigma_{\rm ess}(A)$ (see for example [29, Section XIII.4]).

**Theorem 7** (Mapping of the relative spectra)**.** *Let $A$ be semi-bounded from below and let $a < \inf \sigma(A)$. Then*

$$\lambda \in \sigma(A, \mathcal{L}) \iff (\lambda - a)^{-1} \in \sigma\left((A-a)^{-1}, \mathcal{G}\right) \tag{6}$$

*and*

$$\lambda \in \sigma_{\rm ess}(A, \mathcal{L}) \iff (\lambda - a)^{-1} \in \sigma_{\rm ess}\left((A-a)^{-1}, \mathcal{G}\right) \tag{7}$$

*where $\mathcal{G} = \left((A-a)^{1/2}\mathcal{L}_n\right)_{n\in\mathbb{N}}$.*

**Remark 4.** Recall that a self-adjoint operator $A$ is unbounded ($\mathrm{D}(A) \subsetneq \mathcal{H}$) if and only if $0 \in \sigma((A-a)^{-1})$ for one (hence for all) $a \notin \sigma(A)$. As it turns out, $A$ is unbounded if and only if $0 \in \sigma_{\rm ess}((A-a)^{-1}, \mathcal{L})$ for one (and hence all) $a < \min \sigma(A)$ and $A$-regular sequence $\mathcal{L}$. Formally in Theorem 7 this corresponds to the case $+\infty \in \sigma(A)$ and $(+\infty - a)^{-1} = 0$. ⋄

Evidently a result analogous to Theorem 7 can be established when $A$ is semi-bounded from above. Here $A$ is required to be semi-bounded, in order to be able to define the square root $(A-a)^{1/2}$, see for example [11, Section 4.3], and also for a more fundamental reason. When $a$ is in a gap of the essential spectrum, it would be natural to expect an extension of the above result by considering, for example, $\mathcal{G} = \left(|A-a|^{1/2}\mathcal{L}_n\right)_{n\in\mathbb{N}}$. The following shows that this extension is not possible in general.

**Example 5** (Impossibility of extending Theorem 7 for $A$ strongly indefinite)**.** Let $\mathcal{H}$ be as in Example 2. Define $\mathcal{L}_n = \mathrm{Span}\{e_1^\pm, \dots, e_{n-1}^\pm, \cos(\theta_n)\, e_n^+ + \sin(\theta_n)\, e_n^-\}$ with $\theta_n := \pi/4 - \lambda/(2n)$ for a fixed $\lambda \in (0,1)$. Let

$$A = \sum n|e_n^+\rangle\langle e_n^+| - \sum n|e_n^-\rangle\langle e_n^-|.$$

Then $\sigma(A) = \{\pm n : n \in \mathbb{N}\} = \sigma_{\rm disc}(A)$. On the other hand

$$\sigma(A,\mathcal{L}) = \sigma(A) \cup \{\lambda\}, \qquad \sigma_{\rm ess}(A,\mathcal{L}) = \{\lambda\} \quad \text{and} \quad \sigma_{\rm disc}(A,\mathcal{L}) = \sigma(A).$$

Now

$$A^{-1} = \sum n^{-1}|e_n^+\rangle\langle e_n^+| - n^{-1}|e_n^-\rangle\langle e_n^-|$$

and $\mathcal{G} = \sqrt{|A|}\mathcal{L} = \mathcal{L}$. Since $A^{-1}$ is compact we have

$$\sigma(A^{-1},\mathcal{G}) = \sigma(A^{-1}) \quad \text{and} \quad \sigma_{\rm ess}(A^{-1},\mathcal{G}) = \sigma_{\rm ess}(A^{-1}) = \{0\}.$$

Thus $\lambda \in \sigma_{\rm ess}(A,\mathcal{L})$ whereas $1/\lambda \notin \sigma(A^{-1},\mathcal{G})$. ⋄

In fact the following example shows that no general extension of this theorem is possible whenever $a$ lies in the convex hull of the essential spectrum, even for $A \in \mathcal{B}(\mathcal{H})$.

**Example 6** (Impossibility of extending Theorem 7 for $a \in \mathrm{Conv}\{\sigma_{\mathrm{ess}}(A)\}$)**.** Let $\mathcal{H} = L^2(-\pi, \pi)$ and $Af(x) = \mathrm{sgn}(x)f(x)$ for all $f \in \mathcal{H}$. Then $\sigma(A) = \{\pm 1\}$. If $\mathcal{L}$ is any $A$-regular sequence, then $\sigma(A, \mathcal{L}) \subset [-1, 1]$. Fixing $a = 0$ yields $(A-a)^{-1} = A$. Thus also $\sigma((A-a)^{-1}, \mathcal{G}) \subset [-1, 1]$ for any $A$-regular sequence $\mathcal{G}$. Therefore a general extension of Theorem 7 to $a$ in a gap of the essential spectrum would be impossible. ◇

*Proof of Theorem 7.* Statement (6) will follow immediately from the next result.

**Lemma 8** (Mapping for the spectrum of compressions)**.** *Let $A$ be semi-bounded from below, let $a < \inf \sigma(A)$ and $\mathcal{L}_n \subset \mathrm{D}(A)$. Then*

$$\lambda \in \sigma(\pi_n A \restriction_{\mathcal{L}_n}) \quad \Longleftrightarrow \quad (\lambda - a)^{-1} \in \sigma(p_n (A-a)^{-1} \restriction_{\mathcal{G}_n})$$

*where $\mathcal{G}_n = (A-a)^{1/2}\mathcal{L}_n$ and $p_n$ is the associated orthogonal projector.*

*Proof.* Note that $\lambda \in \sigma(A_n)$ if and only if there exists $x \in \mathcal{L}_n \setminus \{0\}$ such that

$$\pi_n (A-a)^{1/2} \left((\lambda - a)^{-1} - (A-a)^{-1}\right)(A-a)^{1/2} x = \frac{1}{\lambda - a}\pi_n (A - \lambda)x = 0.$$

By fixing $y = (A-a)^{1/2}x \in \mathcal{G}_n \setminus \{0\}$, it is readily seen that $\lambda \in \sigma(A_n)$ if and only if there exist $y \in \mathcal{G}_n \setminus \{0\}$ such that

$$\left\langle (A-a)^{1/2}u,\ \left((\lambda - a)^{-1} - (A-a)^{-1}\right) y \right\rangle = 0$$

for all $u \in \mathcal{L}_n$. Therefore, the statement $\lambda \in \sigma(A_n)$ is equivalent to the existence of $y \in \mathcal{G}_n \setminus \{0\}$ such that $\left((\lambda - a)^{-1} - (A-a)^{-1}\right) y \perp \mathcal{G}_n$ which, in turns, is equivalent to $p_n \left((\lambda - a)^{-1} - (A-a)^{-1}\right) y = 0$. □

We now turn to the proof of (7). We begin by providing an alternative characterization of the relative essential spectrum and then establishing a stability result for the relative spectra with respect to compact perturbations of the $A$-regular sequence.

**Lemma 9** (Alternative characterization of $\sigma_{\mathrm{ess}}(A, \mathcal{L})$)**.** *Let*

$$\mathcal{F}(A) := \left\{ f(A) \ :\ f \in C_c\big(\mathbb{R} \setminus \sigma_{\mathrm{ess}}(A), \mathbb{R}\big) \right\}$$
$$\mathcal{F}^{\pm}(A) := \left\{ f(A) \ :\ f \in C_c\big(\mathbb{R} \setminus \sigma_{\mathrm{ess}}(A), \mathbb{R}^{\pm}\big) \right\}.$$

*Then*

$$\begin{aligned} \sigma_{\mathrm{ess}}(A, \mathcal{L}) &= \bigcap_{B \in \mathcal{F}(A)} \sigma(A + B, \mathcal{L}) \\ &= \bigcap_{B \in \mathcal{F}^{+}(A)} \sigma(A + B, \mathcal{L}) = \bigcap_{B \in \mathcal{F}^{-}(A)} \sigma(A + B, \mathcal{L}). \end{aligned} \tag{8}$$

Here $C_c(\Omega, \mathbb{R})$ denotes the set of all real-valued continuous functions of compact support in the open set $\Omega$. Note that $\mathcal{F}(A)$ is a real vector space and $\mathcal{F}^{\pm}(A)$ are cones, all spanned by projectors onto the eigenspaces of $A$ associated with isolated eigenvalues of finite multiplicity. At the end of this section it will become clear the reason why we highlight the right hand side characterization in (8).

*Proof of Lemma 9.* We only prove the first equality of (8) as the proof of the other ones follows exactly the same pattern. It is well-known that

$$\sigma_{\rm ess}(A) = \bigcap_{B\in\mathcal{F}(A)} \sigma(A+B). \tag{9}$$

Since all the operators in $\mathcal{F}(A)$ are of finite rank, then $\sigma_{\rm ess}(A+B) = \sigma_{\rm ess}(A)$ for all $B \in \mathcal{F}(A)$. Hence (9) is equivalent to

$$\bigcap_{B\in\mathcal{F}(A)} \sigma_{\rm disc}(A+B) = \emptyset. \tag{10}$$

From Remark 2, it follows that $\sigma_{\rm ess}(A+B,\mathcal{L}) = \sigma_{\rm ess}(A,\mathcal{L})$ for all $B \in \mathcal{F}(A)$. On the other hand, $\sigma(A+B,\mathcal{L}) = \sigma_{\rm disc}(A+B,\mathcal{L}) \cup \sigma_{\rm ess}(A,\mathcal{L})$ and $\sigma_{\rm disc}(A+B,\mathcal{L}) \subseteq \sigma_{\rm disc}(A+B)$, by Proposition 3. Hence, by (10),

$$\bigcap_{B\in\mathcal{F}(A)} \sigma_{\rm disc}(A+B,\mathcal{L}) \subset \bigcap_{B\in\mathcal{F}(A)} \sigma_{\rm disc}(A+B) = \emptyset$$

and the result is proved. □

**Lemma 10.** *Let $T = T^*$ be such that $\|T\| < \infty$ and let $\mathcal{L}$ be a $T$-regular sequence. Let $K \in \mathcal{K}(\mathcal{H})$. If $-1 \notin \sigma(K)$, then*

$$\sigma_{\rm ess}(T,\mathcal{L}) = \sigma_{\rm ess}(T,(1+K)\mathcal{L}) \quad \textit{and} \quad \sigma_{\rm disc}(T,\mathcal{L}) = \sigma_{\rm disc}(T,(1+K)\mathcal{L}).$$

*Proof of Lemma 10.* We firstly prove that

$$\sigma_{\rm ess}(T,\mathcal{L}) \setminus \sigma_{\rm disc}(T) = \sigma_{\rm ess}(T,(1+K)\mathcal{L}) \setminus \sigma_{\rm disc}(T). \tag{11}$$

Since

$$\mathcal{L} = (1+K)^{-1}(1+K)\mathcal{L} = (1 - K(1+K)^{-1})(1+K)\mathcal{L}, \tag{12}$$

it suffices to show that the left hand side of (11) is contained in the right hand side. Let $\lambda \in \sigma_{\rm ess}(T,\mathcal{L}) \setminus \sigma_{\rm disc}(T)$. If $\lambda \in \sigma_{\rm ess}(T)$, Proposition 3-(iii) ensures that $\lambda$ lies also in the right hand side, so we can assume that $\lambda \notin \sigma(A)$. According to Proposition 5-(i), there exists $\lambda_k \to \lambda$ and $x_k \in \mathcal{L}_{n_k}$ such that $\|x_k\| = 1$, $x_k \rightharpoonup 0$ and $\pi_{n_k}(T-\lambda_k)x_k = 0$. For all $v_k \in \mathcal{L}_{n_k}$, and hence for all $w_k = (1+K)v_k \in (1+K)\mathcal{L}_{n_k}$, we have

$$\begin{aligned} 0 &= \langle (T-\lambda_k)x_k, v_k\rangle = \langle (1+K^*)^{-1}(T-\lambda_k)x_k, (1+K)v_k\rangle \\ &= \langle (1+K^*)^{-1}(T-\lambda_k)x_k, w_k\rangle. \end{aligned}$$

Let $q_k$ be the orthogonal projection onto $(1+K)\mathcal{L}_{n_k}$. Then

$$q_k(1+K^*)^{-1}(T-\lambda_k)x_k = 0.$$

Now $(1+K^*)^{-1} = 1 - \tilde{K}$ where $\tilde{K} = K^*(1+K^*)^{-1} \in \mathcal{K}(\mathcal{H})$. Hence

$$q_k(1-\tilde{K})(T-\lambda)x_k \to 0.$$

But, since $\|T\| < \infty$ and $x_k \rightharpoonup 0$, $\tilde{K}(T-\lambda)x_k \to 0$, so that also $q_k(T-\lambda)x_k \to 0$. Thus $q_k(T-\lambda)y_k \to 0$ for $y_k = (1+K)x_k \rightharpoonup 0$. By renormalizing $y_k$ in the obvious manner, we obtain a singular $\mathcal{L}$-Weyl sequence for $\lambda \in \sigma(T,(1+K)\mathcal{L})$, ensuring (11).

To complete the proof of the first identity in the conclusion of the lemma, suppose that $\lambda \in \sigma_{\rm ess}(T,\mathcal{L}) \cap \sigma_{\rm disc}(T)$. For any $\mu \neq \lambda$ let $\tilde{T} = T + (\mu-\lambda)\mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(T)$

where $\varepsilon > 0$ is sufficiently small. Then $\lambda \in \sigma_{\rm ess}(\tilde{T}, \mathcal{L}) \setminus \sigma_{\rm disc}(\tilde{T})$. By virtue of (11) and Remark 2, $\lambda \in \sigma_{\rm ess}(\tilde{T}, (1+K)\mathcal{L}) = \sigma_{\rm ess}(T, (1+K)\mathcal{L})$.

We now show the second identity. By virtue of (12) and the first identity, it is enough to verify

$$\sigma_{\rm disc}(T, \mathcal{L}) \subset \sigma(T, (1+K)\mathcal{L}).$$

This, in turns, follows from Proposition 3-(ii) and (4), since

$$\sigma_{\rm disc}(T, \mathcal{L}) \subset \sigma_{\rm disc}(T) \text{ and } \sigma(T) \subset \sigma(T, (1+K)\mathcal{L})$$

taking into account that $(1+K)\mathcal{L}$ is a $T$-regular sequence. □

We now complete the proof of Theorem 7 by showing (7). Let $\lambda \in \sigma_{\rm ess}(A, \mathcal{L})$. By virtue of Lemma 9, this is equivalent to the statement

$$\forall B \in \mathcal{F}^+(A), \qquad \lambda \in \sigma(A+B, \mathcal{L}).$$

Since $B \geq 0$ and $a < \min[\sigma(A+B)]$, according to (6) the latter is equivalent to

$$\forall B \in \mathcal{F}^+(A), \qquad (\lambda - a)^{-1} \in \sigma((A+B-a)^{-1}, \mathcal{G}_B)$$

where $\mathcal{G}_B = (A+B-a)^{-1/2}\mathcal{L}$. Since $B$ has finite rank and is therefore compact, Lemma 10 ensures that the above in turns is equivalent to

$$\forall B \in \mathcal{F}^+(A), \qquad (\lambda - a)^{-1} \in \sigma((A+B-a)^{-1}, \mathcal{G}_0).$$

Note that $0 \notin \sigma((A+B-a)^{1/2}(A-a)^{-1/2})$ as the corresponding operator is an invertible function of $A$. Now $(A+B-a)^{-1} = (A-a)^{-1} + \tilde{B}$, where $\tilde{B} = -(A-a)^{-1}B(A+B-a)^{-1}$ runs over all of $\mathcal{F}^-\left((A-a)^{-1}\right)$ as $B$ runs over all $\mathcal{F}^+(A)$ and conversely. For the latter note that $f \in \mathcal{F}^+(A)$ if and only if $-f((\cdot - a)^{-1}) \in \mathcal{F}^-((A-a)^{-1})$. Thus, once again by Lemma 9, $\lambda \in \sigma_{\rm ess}(A, \mathcal{L})$ turns out to be equivalent to

$$(\lambda - a)^{-1} \in \sigma_{\rm ess}((A-a)^{-1}, \mathcal{G}).$$

□

**Remark 5.** The proof of the above theorem mimics the proof of the classical Mapping Theorem for the essential spectrum, that can be deduced from the characterization

$$\sigma_{\rm ess}(A) = \bigcap_{B \in \mathcal{K}(\mathcal{H})} \sigma(A+B),$$

see, e.g., [28]. ◇

## 5. Stability properties of the relative essential spectrum

In this final section we present the main result of this paper, which strongly depend on the validity of Theorem 7.

**Theorem 11** (Weyl-type stability theorem for the relative spectra)**.** *Let $A$ and $B$ be two self-adjoint operators which are bounded below. Assume that for some $a < \inf\{\sigma(A), \sigma(B)\}$,*

$$\mathrm{D}((B-a)^{1/2}) = \mathrm{D}((A-a)^{1/2}) \tag{13}$$

*and*

$$(A-a)^{1/2}((B-a)^{-1/2} - (A-a)^{-1/2}) \in \mathcal{K}(\mathcal{H}). \tag{14}$$

*Then*

$$\sigma_{\rm ess}(A, \mathcal{L}) = \sigma_{\rm ess}(B, \mathcal{L})$$

*for all sequences $\mathcal{L} = (\mathcal{L}_n)$ which are simultaneously $A$-regular and $B$-regular.*

Under Assumption (13), (14) is equivalent to the same condition with the rôles of $A$ and $B$ reversed:

$$(B-a)^{1/2}((A-a)^{-1/2} - (B-a)^{-1/2}) \in \mathcal{K}(\mathcal{H}). \tag{15}$$

**Remark 6.** The KLMN theorem [29] ensures that if $B - A$ is a densely defined symmetric $A$-form-bounded operator with bound less than 1, then (13) holds for $a$ sufficiently negative. ⋄

The following example taken from [22] shows that Theorem 11 cannot be easily generalized to operators which are not semi-bounded.

**Example 7** (Relatively compact perturbations of the Dirac operator)**.** Let $A = D^0$ and $B = D^0 + V$ where $D^0$ denotes the free Dirac operator with mass 1 [33] and $V \in C_c^\infty(\mathbb{R}^3)$ is a smooth non-negative function of compact support. The ambient Hilbert space here is $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. Under the additional assumption that $\sup V = \|V\|_{L^\infty(\mathbb{R}^3)} < 1$, it is guaranteed that $0 \notin \sigma(B)$. Furthermore it can be verified that

$$D\left(|A|^{1/2}\right) = D\left(|B|^{1/2}\right) = H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$$

and that

$$|A|^{1/2}\left(|B|^{-1/2} - |A|^{-1/2}\right) \in \mathcal{K}(\mathcal{H}).$$

As a consequence of [22, Theorem 2.7], it is known that there exists a $B$-regular Galerkin sequence $\mathcal{L} = (\mathcal{L}_n)$ such that

$$\sigma_{\rm ess}(B, \mathcal{L}) \supset \big[0\,;\sup V\big]. \tag{16}$$

These Galerkin spaces comprise upper and lower spinors, meaning that

$$\mathcal{L}_n = \mathrm{Span}\left\{\begin{pmatrix} f_1^n \\ 0\end{pmatrix}, ..., \begin{pmatrix} f_{d_n}^n \\ 0\end{pmatrix}, \begin{pmatrix} 0 \\ g_1^n\end{pmatrix}, ..., \begin{pmatrix} 0 \\ g_{d_n'}^n\end{pmatrix}\right\}$$

for suitable $(f_j^n)$, $(g_j^n) \subset L^2(\mathbb{R}^3, \mathbb{C}^2)$. This basis is known to be free of pollution if the external field $V = 0$, that is

$$\sigma(A, \mathcal{L}) = \sigma(D^0) = (-\infty, -1] \cup [1, \infty) = \sigma_{\rm ess}(A, \mathcal{L}).$$

Hence $\sigma_{\rm ess}(A, \mathcal{L}) \neq \sigma_{\rm ess}(B, \mathcal{L})$ so Theorem 11 fails for operators which are strongly indefinite. ⋄

*Proof of Theorem 11.* Denote by $K$ the operator on the left side of (14). Then

$$(B-a)^{-1} - (A-a)^{-1} = (A-a)^{-1/2} K (B-a)^{-1/2} + (A-a)^{-1} K \tag{17}$$

is a compact operator. Let $\mathcal{G} := (A-a)^{1/2}\mathcal{L}$. According to (7),

$$\lambda \in \sigma_{\rm ess}(A, \mathcal{L}) \quad \Longleftrightarrow \quad (\lambda - a)^{-1} \in \sigma_{\rm ess}\left((A-a)^{-1}, \mathcal{G}\right).$$

By Remark 2,

$$\sigma_{\rm ess}\left((B-a)^{-1}, \mathcal{G}\right) = \sigma_{\rm ess}\left((A-a)^{-1}, \mathcal{G}\right).$$

Let $\mathcal{G}' = (B-a)^{1/2}\mathcal{L}$. Then

$$\mathcal{G} = (A-a)^{1/2}\mathcal{L} = (A-a)^{1/2}(B-a)^{-1/2}\mathcal{G}' = (1+K)\mathcal{G}'.$$

Note that $K = (A-a)^{1/2}(B-a)^{-1/2} - 1$ and $-1 \notin \sigma(K)$ as a consequence of the fact that $0 \notin \sigma((A-a)^{1/2}(B-a)^{-1/2})$ by (13). According to Lemma 10,

$$\sigma_{\rm ess}\left((B-a)^{-1}, \mathcal{G}\right) = \sigma_{\rm ess}\left((B-a)^{-1}, \mathcal{G}'\right) \tag{18}$$

The conclusion follows by applying Theorem 7 again, this time to operator $B$. □

**Corollary 12.** *Let $A$ and $B$ be two bounded-below self-adjoint operators such that (13) holds true for some $a < \inf\{\sigma(A), \sigma(B)\}$. Assume that $C := B - A$ is a densely defined symmetric operator such that*

$$C \in \mathcal{B}(\mathrm{D}((B-a)^{\beta}), \mathcal{H}) \tag{19}$$

*and*

$$(A-a)^{-\alpha} C (B-a)^{-\beta} \in \mathcal{K}(\mathcal{H}) \tag{20}$$

*for some $0 \le \alpha, \beta < 1$ with $\alpha + \beta \le 1$. Then*

$$\sigma_{\rm ess}(A, \mathcal{L}) = \sigma_{\rm ess}(B, \mathcal{L})$$

*for all sequences $\mathcal{L} = (\mathcal{L}_n)$ which are simultaneously $A$-regular and $B$-regular.*

**Remark 7.** Let $A$ be a given bounded-below self-adjoint operator and assume that $A$ has a gap $(a, b)$ in its essential spectrum in the following precise sense,

$$\sigma_{\rm ess}(A) \cap (a,b) = \emptyset, \qquad \mathrm{tr}\left(\mathbb{1}_{(-\infty,a)}(A)\right) = \mathrm{tr}\left(\mathbb{1}_{(b,\infty)}(A)\right) = +\infty.$$

Let $\Pi := \mathbb{1}_{(c,\infty)}(A)$ where $a < c < b$. Results shown in [22] ensure that, when the Galerkin spaces $\mathcal{L}_n$ are compatible with the decomposition $\mathcal{H} = \Pi\mathcal{H} \oplus (1-\Pi)\mathcal{H}$ (i.e. when $\Pi$ and $\pi_n$ commute for all $n$), there is no pollution in the gap: $\sigma_{\rm ess}(A, \mathcal{L}) \cap (a, b) = \emptyset$. According to [22, Corollary 2.5], when

$$(B-a)^{-1} C (A-a)^{-1/2} \in \mathcal{K}(\mathcal{H}), \tag{21}$$

then $\sigma_{\rm ess}(B, \mathcal{L}) = \emptyset$ as well.

In this respect, Theorem 11 can be seen as a generalization of these results. Although condition (20) is stronger than (21), the statement guarantees that the whole polluted spectrum will not move irrespectively of the $A$-regular Galerkin family $\mathcal{L}$ and not only for those satisfying $[\Pi, \pi_n] = 0$ for all $n$. ⋄

**Example 8** (Periodic Schrödinger operators)**.** Let $A = -\Delta + V_{\rm per}$ where $V_{\rm per}$ is a periodic potential with respect to some fixed lattice $\mathcal{R} \subset \mathbb{R}^d$ (for instance $\mathcal{R} = \mathbb{Z}^3$). Let $C = W(x)$ be a perturbation. Assume that

$$V_{\rm per} \in L^p_{\rm loc}(\mathbb{R}^d) \;\text{ where } \begin{cases} p = 2 & \text{if } d \le 3 \\ p > 2 & \text{if } d = 4 \\ p = d/2 & \text{if } d \ge 5 \end{cases}$$

and that

$$W \in L^q(\mathbb{R}^d) \cap L^p_{\rm loc}(\mathbb{R}^d) + L^\infty_\epsilon(\mathbb{R}^d)$$

for $\max(d/2, 1) < q < \infty$. Then (20) holds true and therefore

$$\sigma_{\rm ess}\left(-\Delta + V_{\rm per} + W, \mathcal{L}\right) = \sigma_{\rm ess}\left(-\Delta + V_{\rm per}, \mathcal{L}\right) \tag{22}$$

for all $A$-regular Galerkin sequence $\mathcal{L}$. See [22, Section 2.3.1].

A Galerkin sequence $\mathcal{L}$ which does not yield any pollution in a given gap can be found by localized Wannier functions, [22, 9]. In practice, these functions can only be calculated numerically, so it is natural to ask what would be the polluted spectrum when they are known only approximately. According to (22), the polluted spectrum will not increase in size more than that of the unperturbed operator $-\Delta + V_{\rm per}$. ◇

**Example 9** (Optimality of the constants in Corollary 12)**.** Let $\mathcal{H}$, $\mathcal{L}$, $e_n^\pm$ and $f_n^\pm$ be as in Example 2. Let

$$A = \sum_n n^\ell |f_n^+\rangle\langle f_n^+| + \sum |f_n^-\rangle\langle f_n^-| \quad \text{and} \quad B = \sum_n n^r |e_n^+\rangle\langle e_n^+| + \sum |e_n^-\rangle\langle e_n^-|.$$

The matrix representation of $A$ and $B$ in the basis $e_n^\pm$ is made out of $2\times 2$ blocks placed along the diagonal. More precisely $A = \mathrm{diag}[A_n]$, $B = \mathrm{diag}[B_n]$ and $C = \mathrm{diag}[C_n]$ where

$$A_n = R_{-n} \begin{pmatrix} n^\ell & 0 \\ 0 & 1 \end{pmatrix} R_n, \qquad B_n = \begin{pmatrix} n^r & 0 \\ 0 & 1 \end{pmatrix}$$

and $C_n = A_n - B_n$ for

$$R_n = \begin{pmatrix} \cos(1/n) & \sin(1/n) \\ -\sin(1/n) & \cos(1/n) \end{pmatrix}.$$

Fix $a = 0$ and let $L = A^{-\alpha} C B^{-\beta}$. The matrix representation of $L$ in the basis $e_k^\pm$ is $L = \mathrm{diag}[L_n]$ where we can calculate explicitly the entries as

$$\begin{aligned}(L_n)_{11} &= -n^{-\beta r - \alpha\ell + r}\cos^2(1/n) + n^{-\beta r}\sin^2(1/n) \\ &\qquad\qquad - n^{-r(\beta-1)}\sin^2(1/n) + n^{-\beta r - \alpha\ell + \ell}\cos^2(1/n) \\ (L_n)_{12} &= \cos(1/n)\sin(1/n)\left(n^{-\ell(\alpha-1)} - n^{-\alpha\ell}\right) \\ (L_n)_{21} &= \cos(1/n)\sin(1/n)\left(n^{-\beta r - \alpha\ell + \ell} - n^{-\beta r - \alpha\ell + r} - n^{-\beta r} + n^{-r(\beta-1)}\right) \\ (L_n)_{12} &= \sin^2(1/n)\left(n^{-\ell(\alpha-1)} - n^{-\alpha\ell}\right).\end{aligned}$$

Therefore $L$ is compact, given the following

$$\begin{gathered}\ell = 2, \quad 0 < \beta, \alpha < 1, \quad 0 < r < 2, \\ -\beta r - 2\alpha + 2 < 0, \quad \alpha > 1/2, \quad \beta > 1 - \frac{1}{r}.\end{gathered} \tag{23}$$

On the other hand, for $\ell = 2$,

$$\sigma_{\rm ess}(A, \mathcal{L}) = \{1\} \qquad \text{and} \qquad \sigma_{\rm ess}(B, \mathcal{L}) = \{1, 0\}.$$

This example shows that condition (20) in Corollary 12 is quasi-optimal for the stated range of $\beta$ and $\alpha$ as illustrated by Figure 1. ◇

*Proof of Corollary 12.* Assume firstly that $0 \le \alpha \le 1/2$. The proof reduces to showing that the operator $K$ defined by expression (14) is compact. Let $L = (A-a)^{-\alpha} C (B-a)^{-\beta}$ be the operator given by (20). Since $\beta \le 1$, we have $\mathrm{D}(B - a) \subset \mathrm{D}(B-a)^\beta$, [11, Theorem 4.3.4]. Then, by (19), $L\mathcal{H} \subset \mathrm{D}((A-a)^\alpha)$ and $Cx = (A-a)^\alpha L (B-a)^\beta x$ for all $x \in \mathrm{D}(B-a)$. By virtue of (20),

$$(A-a)^{1/2}(A-a+s)^{-1} C (B-a+s)^{-1} \in \mathcal{K}(\mathcal{H})$$

for all $s \ge 0$. Moreover

$$(A-a)^{1/2}((A-a+s)^{-1} - (B-a+s)^{-1})x = (A-a)^{1/2}(A-a+s)^{-1}C(B-a+s)^{-1}x$$

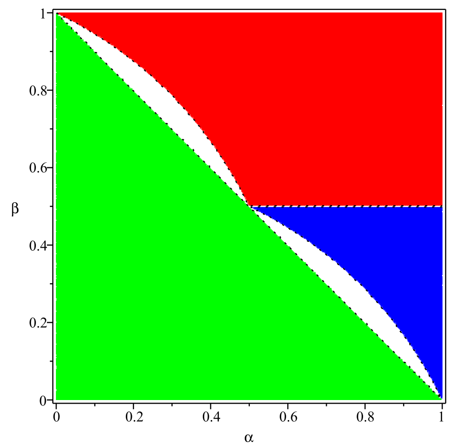


FIGURE 1. The region in green colour for the parameters $\beta$ and $\alpha$ is covered by the conditions of Corollary 12. If $A$ and $B$ satisfy (20) for $(\beta,\alpha)$ in this region, then the relative essential spectrum is preserved. The region in red shows the parameters $\beta$ and $\alpha$ in condition (23) of Example 9. The region in blue is generated by exchanging the rôles of $\beta$ and $\alpha$. It is not enough for $A$ and $B$ to satisfy (20) for $(\beta,\alpha)$ in these two regions, to guarantee preservation of the the relative essential spectrum.

for all $x \in \mathcal{H}$, as this identity is satisfied in a dense subspace of $\mathcal{H}$. Thus

$$\begin{aligned} K &= -\frac{1}{\pi}\int_0^\infty (A-a)^{1/2}(A-a+s)^{-1}C(B-a+s)^{-1}\frac{\mathrm{d}s}{\sqrt{s}} \\ &= -\frac{1}{\pi}\int_0^\infty \left\{(A-a)^{1/2}(A-a+s)^{-1}(A-a)^{\alpha}\right\} L\left\{(B-a)^{\beta}(B-a+s)^{-1}\right\}\frac{\mathrm{d}s}{\sqrt{s}}. \end{aligned}$$

Both terms in brackets multiplying $L$ are bounded operators, then the integrand in the second expression is also a compact operator. Moreover, the integral converges in the Bochner sense as its norm is $O(s^{\beta+\alpha-2})$ for $s \to \infty$ and $O(s^{-1/2})$ for $s \to 0$. Thus $K \in \mathcal{K}(\mathcal{H})$ in this case and Theorem 11 implies the desired conclusion.

Now suppose that $1/2 < \alpha \leq 1$, so that $0 \leq \beta \leq 1/2$. Since

$$\mathrm{D}(A-a)^{\alpha} \subset \mathrm{D}(A-a)^{1/2} = \mathrm{D}(B-a)^{1/2} \subset \mathrm{D}(B-a)^{\beta},$$

then $C \in \mathcal{B}(\mathrm{D}(A-a)^{\alpha},\mathcal{H})$. Hence the operator $(B-a)^{-\beta}C(A-a)^{-\alpha}$ is bounded and $(B-a)^{-\beta}C(A-a)^{-\alpha}x = L^*x$ for all $x \in \mathcal{H}$. The proof is then completed by exchanging the roles of $A$ and $B$. □

**Acknowledgement.** The authors would like to acknowledge financial support from the British-French project PHC Alliance no. 22817YA. Partial support from the ANR grant NoNAP of the French Ministry of Research is also acknowledged.

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