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# On The Solvability Complexity Index for Unbounded Selfadjoint Operators and Schrödinger Operators

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## Abstract

We study the solvability complexity index (SCI) for unbounded selfadjoint operators on separable Hilbert spaces and perturbations thereof. In particular, we show that if the extended essential spectrum of a selfadjoint operator is convex, then the SCI for computing its spectrum is equal to 1. This result is then extended to relatively compact perturbations of such operators and applied to Schrödinger operators with (complex valued) potentials decaying at infinity to obtain  $\text{SCI}=1$  in this case, as well.

## 1 Introduction

The problem of computing spectra of partial differential operators is fundamental to many problems in physics with real world applications. Perhaps one of the most prominent examples of this is quantum mechanics, where the possible bound state energies of a particle subject to a force described by a potential function  $V$  are given by the eigenvalues of the corresponding Schrödinger operator  $-\Delta + V$ . Generically, the spectral problem of such an operator cannot be solved explicitly and one has to resort to numerical methods. By practical constraints, any computer algorithm, which might be used to compute the spectrum, will only be able to handle a finite amount of information about the operator and perform a finite number of arithmetic operations on this information (in practice, this “finite amount of information” is usually given by some sort of discretisation of the domain, which approximates the infinite dimensional spectral problem by a finite dimensional one). In other words, any algorithm will always “ignore” an infinite amount of information about the operator. One might hope that by increasing the dimension of the approximation (or decreasing the step size of the discretisation), one will eventually obtain a reasonable approximation of the spectrum. Hence, it is a legitimate question to ask:

*Given a class of operators  $\Omega$ , does there exist a sequence of algorithms  $\Gamma_n$  such that  $\Gamma_n(T) \rightarrow \sigma(T)$  (in an appropriate sense) for all  $T \in \Omega$ ?*

It turns out that the answer to the above question is not always in the affirmative. Indeed, it has been shown in [BHNS15] that if  $\Omega = L(\mathcal{H})$  (the space of bounded operators on a separable Hilbert space  $\mathcal{H}$ ), then for any sequence of algorithms there exists  $T \in \Omega$  whose spectrum is not approximated by that sequence. This observation has led to the wider definition of the so-called *Solvability Complexity Index* (SCI), introduced in [Han11], of which we will now give a brief review.

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**Definition 1.1.** A *computational problem* is a quadruple  $(\Omega, \Lambda, \Xi, \mathcal{M})$ , where

- (i)  $\Omega$  is a set, called the *primary set*,
- (ii)  $\Lambda$  is a set of complex valued functions on  $\Omega$ , called the *evaluation set*,
- (iii)  $\mathcal{M}$  is a metric space,
- (iv)  $\Xi : \Omega \rightarrow \mathcal{M}$  is a map, called the *problem function*.

In the above definition,  $\Omega$  is the set of objects that give rise to the computational problem,  $\Lambda$  plays the role of providing the information accessible to the algorithm, and  $\Xi : \Omega \rightarrow \mathcal{M}$  gives the quantity that one wishes to compute numerically.

An example of a computational problem in the sense of Definition 1.1 is given by the spectral problem discussed above. Indeed, given a separable Hilbert space  $\mathcal{H}$  with orthonormal basis  $\{e_i\}$ , one can choose  $\Omega = L(\mathcal{H})$ ,  $\mathcal{M} = \{\text{compact subsets of } \mathbb{C}\}$ , equipped with the Hausdorff metric, and  $\Xi(T) = \sigma(T)$ . For the evaluation set one could choose  $\Lambda := \{f_{ij} \mid i, j \in \mathbb{N}\}$ , where  $f_{ij}(T) = \langle T e_i, e_j \rangle$  give the matrix elements of an operator with respect to the basis  $\{e_i\}$ .

**Definition 1.2.** Let  $(\Omega, \Lambda, \Xi, \mathcal{M})$  be a computational problem. An *arithmetic algorithm* is a map  $\Gamma : \Omega \rightarrow \mathcal{M}$  such that for each  $T \in \Omega$  there exists a finite subset  $\Lambda_\Gamma(T) \subset \Lambda$  such that

- (i) the action of  $\Gamma$  on  $T$  depends only on  $\{f(T)\}_{f \in \Lambda_\Gamma(T)}$ ,
- (ii) for every  $S \in \Omega$  with  $f(T) = f(S)$  for all  $f \in \Lambda_\Gamma(T)$  one has  $\Lambda_\Gamma(S) = \Lambda_\Gamma(T)$ ,
- (iii) the action of  $\Gamma$  on  $T$  consists of performing only finitely many arithmetic operations on  $\{f(T)\}_{f \in \Lambda_\Gamma(T)}$ .

We will refer to any arithmetic algorithm simply as an *algorithm* from now on. For more general concepts the reader may consult [BHNS15].

In [BHNS15] it has been shown that if  $\Omega$  is the set of compact operators on a separable Hilbert space  $\mathcal{H}$ , then there exists a sequence of algorithms  $\Gamma_n : \Omega \rightarrow \mathbb{C}$  such that  $\Gamma_n(T) \rightarrow \sigma(T)$  (in Hausdorff sense) for all  $T \in \Omega$ , while for the set of bounded selfadjoint operators  $\Omega = \{T \in L(\mathcal{H}) \mid T^* = T\}$  this is not possible.

However, it turns out that there exists a family  $\Gamma_{mn}$  of algorithms such that

$$\lim_{n \rightarrow \infty} \lim_{m \rightarrow \infty} \Gamma_{mn}(T) = \sigma(T)$$

for all bounded selfadjoint operators. Hence, it is possible to compute the spectrum of non-compact operators using algorithms, but the number of limits required may increase (this general phenomenon has first been observed by Doyle and McMullen in the context of finding zeros of polynomials, cf. [DM89]). In order to capture this phenomenon, the following definition has been made

**Definition 1.3** ([BHNS15]). Let  $(\Omega, \Lambda, \Xi, \mathcal{M})$  be a computational problem. A *tower of algorithms* of height  $k$  is a family  $\Gamma_{n_1, n_2, \dots, n_k} : \Omega \rightarrow \mathcal{M}$  of arithmetic algorithms such that for all  $T \in \Omega$

$$\Xi(T) = \lim_{n_k \rightarrow \infty} \cdots \lim_{n_1 \rightarrow \infty} \Gamma_{n_1, n_2, \dots, n_k}(T).$$

The examples above show that the number of limits required to compute the problem function  $\Xi$  is a measure for the numerical complexity of the underlying computational problem. This motivates the

**Definition 1.4** ([BHNS15]). A computational problem  $(\Omega, \Lambda, \Xi, \mathcal{M})$  is said to have *Solvability Complexity Index*  $k$  if  $k$  is the smallest integer for which there exists a tower of algorithms of height  $k$  that computes  $\Xi$ .

If a computational problem has solvability complexity index  $k$ , we write  $\text{SCI}(\Omega, \Lambda, \Xi, \mathcal{M}) = k$ .

*Remark 1.5.* In this article we are mainly interested in the spectral problem and will therefore write  $\text{SCI}(\Omega, \Lambda)$  instead of  $\text{SCI}(\Omega, \Lambda, \Xi, \mathcal{M})$ , where it is understood that  $\Xi(T) = \sigma(T)$  and  $\mathcal{M}$  is the set of closed subsets of  $\mathbb{C}$  equipped with the Attouch-Wets metric  $d_{\text{AW}}$  defined as

$$d_{\text{AW}}(A, B) = \sum_{i=1}^{\infty} 2^{-i} \min \left\{ 1, \sup_{|x| < i} |\text{dist}(x, A) - \text{dist}(x, B)| \right\}.$$

(Note that if  $A, B \subset \mathbb{C}$  are bounded, then  $d_{\text{AW}}$  coincides with the Hausdorff distance.)

In practice it is often important to have control of the error  $d(\Gamma_{n_1, \dots, n_k}(T), \Xi(T))$  for all  $T \in \Omega$ . It is straightforward to show, however, that such an estimate is impossible to obtain as soon as  $\text{SCI}(\Omega, \Lambda, \Xi, \mathcal{M}) > 1$  (cf. [BHNS15, Thm. 6.1]). Indeed, it is easy to see that if for a tower of algorithms  $\Gamma_{n_1, \dots, n_k}$  there exist subsequences  $n_1(m), \dots, n_k(m)$  such that  $\Gamma_{n_1(m), \dots, n_k(m)}(T) \rightarrow 0$  for all  $T \in \Omega$ , then  $\tilde{\Gamma}_m := \Gamma_{n_1(m), \dots, n_k(m)}$  is in fact a tower of height 1 for  $\Omega$  and hence  $\text{SCI}(\Omega) = 1$ .

For this reason, it is of particular interest to find classes  $\Omega$  of operators for which  $\text{SCI}(\Omega, \Lambda, \sigma(\cdot)) = 1$  (with appropriately chosen  $\Lambda$ ). The present article addresses precisely this question. In fact, we will show that for selfadjoint operators whose *extended essential spectrum* (see (2.2)) is convex, we have  $\text{SCI} = 1$ . This is done by explicitly constructing a sequence of arithmetic algorithms which computes the spectrum of any such operator. The result is then extended to certain relatively compact perturbations of such operators. We stress that the new aspect of our work is to consider the *shape of the essential spectrum* as a relevant criterion for reducing the numerical complexity of the spectral problem. As an application of this approach, we will show that our results apply to non-selfadjoint Schrödinger operators with certain well behaved potentials.

The problem of determining the SCI for spectral problems has previously been studied in [Han11, BHNS15] for operator in abstract Hilbert spaces, as well as for partial differential operators. Previous results include

**Bounded operators:** Let  $\mathcal{H}$ ,  $\Lambda$  be as in the example above Definition 1.2. It was shown in [BHNS15, Th. 3.3, Th. 3.7] that then

$$\begin{aligned} \text{SCI}(\Omega, \sigma(\cdot)) &= 3 && \text{if } \Omega = L(\mathcal{H}) \\ \text{SCI}(\Omega, \sigma(\cdot)) &= 2 && \text{if } \Omega = \{T \in L(\mathcal{H}) \mid T \text{ selfadjoint}\} \\ \text{SCI}(\Omega, \sigma(\cdot)) &= 1 && \text{if } \Omega = \mathcal{K}(\mathcal{H}), \end{aligned}$$

where  $\mathcal{K}(\mathcal{H})$  denotes the set of compact operators. The last bound  $\text{SCI}(\mathcal{K}(\mathcal{H}), \sigma(\cdot)) = 1$  is related to the fact that compact operators can be approximated in operator norm by finite range operators.

**Schrödinger operators:** In [BHNS15], the SCI for the spectral problem of Schrödinger operators with complex valued potentials  $V$  has been studied. It has been shown that if

$$\Omega = \{-\Delta + V \mid V \text{ is sectorial and } |V(x)| \rightarrow \infty \text{ as } |x| \rightarrow \infty\}, \quad (1.1)$$

then  $\text{SCI}(\Omega, \sigma(\cdot)) = 1$ . The proof relies on the fact that operators as in (1.1) have compact resolvent.

In the case of *bounded* potentials, one lacks compact resolvent and the situation is somewhat more difficult. It has been shown in [BHNS15, Th. 4.2] that if  $\Omega$  denotes

the set of Schrödinger operators on  $\mathbb{R}^d$  with  $V$  bounded and of bounded variation, then  $\text{SCI}(\Omega, \sigma(\cdot)) \leq 2$ . It has since then been an open problem, whether without any additional information the SCI of this problem is equal to one or two.

The SCI of certain unbounded operators in separable Hilbert spaces, whose matrix representation is banded, has been studied in [Han11].

In this article, we will take a step towards closing this gap. We will prove that if  $M > 0$  and  $\Omega$  denotes the set of all Schrödinger operators  $-\Delta + V$  with  $\text{supp}(V) \subset B_M(0)$  and  $|\nabla V| \leq M$ , then  $\text{SCI}(\Omega, \sigma(\cdot)) = 1$  (for the precise statement, see Section 4). This is done by first proving two abstract theorems about the SCI of selfadjoint operators which are of independent interest. The proofs of these abstract results rely on recent developments in the theory of essential numerical ranges for unbounded operators, cf. [BMT19]. The main theorems of this article are Theorems 2.1, 3.1 and 4.3.

The question as to whether the assumption on the decay of  $V$  is essential for having  $\text{SCI} = 1$  remains an interesting open problem and will be addressed in future work.

## 2 Selfadjoint Operators

Let  $\mathcal{H}$  be a separable Hilbert space and  $\mathcal{H}_n \subset \mathcal{H}$  be a sequence of finite dimensional subspaces such that  $\mathcal{H}_n \subset \mathcal{H}_{n+1}$  for all  $n \in \mathbb{N}$  and  $P_n \xrightarrow{s} I$ , where  $P_n$  denotes the orthogonal projection onto  $\mathcal{H}_n$ . Define

$$\Omega_1 := \left\{ T : \text{dom}(T) \rightarrow \mathcal{H} \left| \begin{array}{l} T \text{ selfadjoint, } \widehat{\sigma}_e(T) \text{ convex} \\ \text{and } \bigcup_{n \in \mathbb{N}} \mathcal{H}_n \text{ is a core of } T \end{array} \right. \right\}, \quad (2.1)$$

where

$$\widehat{\sigma}_e(T) = \sigma_{e2}(T) \cup \begin{cases} \{+\infty\}, & \text{if } T \text{ unbounded above} \\ \{-\infty\}, & \text{if } T \text{ unbounded below} \end{cases} \quad (2.2)$$

and

$$\sigma_{e2}(T) = \{\lambda \in \mathbb{C} \mid \exists (x_k) \subset \text{dom}(T) : \|x_k\| = 1 \forall k, x_k \rightarrow 0, \|(T - \lambda)x_k\| \rightarrow 0\}. \quad (2.3)$$

Furthermore, for each  $n \in \mathbb{N}$ , let  $\{e_1^{(n)}, \dots, e_{k_n}^{(n)}\}$  be an orthonormal basis of  $\mathcal{H}_n$  and define

$$\Lambda_1 := \{f_{i,j,n} \mid 1 \leq i, j \leq k_n, n \in \mathbb{N}\}, \quad (2.4)$$

where  $f_{i,j,n} : T \mapsto \langle T e_i^{(n)}, e_j^{(n)} \rangle$  are the evaluation functions producing the  $(i, j)$ th matrix elements. This is the set of information accessible to the algorithm.

**Theorem 2.1.** *We have  $\text{SCI}(\Omega_1, \Lambda_1, \sigma(\cdot)) = 1$ .*

*Remark 2.2.* (i) Note that Theorem 2.1 in particular applies to bounded selfadjoint operators with convex essential spectrum. In this sense, Theorem 2.1 can be viewed as an extension of [BHNS15, Th. 3.7], where it was shown that  $\text{SCI} = 1$  for the set of all *compact* operators (which naturally satisfy  $\sigma_e(T) \subset \{0\}$ ).

(ii) Theorem 2.1 is optimal in the sense that the selfadjointness assumption in (2.1) cannot be dropped. Indeed, counterexamples show that  $\text{SCI} \geq 2$  for non selfadjoint bounded operators with convex essential spectrum (cf. [BHNS15, Proof of Th. 3.7, Step II] for an explicit construction).

*Remark 2.3.* In addition to (2.3) we will need another version of the essential spectrum, which is sometimes denoted  $\sigma_{e5}$ . Let  $H$  be a closed, densely defined operator on  $\mathcal{H}$ . Then

$$\sigma_{e5}(H) := \mathbb{C} \setminus \Delta_5(H), \quad (2.5)$$

where  $\Delta_5(H)$  denotes the union of all components of the set  $\{\lambda \in \mathbb{C} \mid H - \lambda \text{ is semi-Fredholm}\}$  which intersect  $\rho(H)$ . Note that the definitions (2.3) and (2.5) do *not* agree in general. However, it can be shown that for *selfadjoint* operators  $T$  on  $\mathcal{H}$ , one always has  $\sigma_{e2}(T) = \sigma_{e5}(T)$  (cf. [EE87, Th. IX.1.6]). For this reason, we will simply use the notation  $\sigma_e(T)$  to denote the essential spectrum, whenever the operators in question are selfadjoint.

## 2.1 Construction of the Algorithm

Let  $T \in \Omega_1$  and define the truncated operator

$$T_n := P_n T|_{\mathcal{H}_n}. \quad (2.6)$$

This operator can be represented by a finite dimensional (square) matrix with elements  $(T_n)_{ij} = \langle T e_i^{(n)}, e_j^{(n)} \rangle$ . Moreover, let  $G_n^{\mathbb{R}} := \frac{1}{n}\mathbb{Z} \cap (-n, n) \subset \mathbb{R}$ .

**Lemma 2.4.** *Let  $\lambda \in G_n^{\mathbb{R}}$  and denote by  $s(\cdot)$  the smallest singular value of a matrix. Then*

- (i) *For all  $n$  and  $\lambda$ , we have  $s(T_n - \lambda) = \|(T_n - \lambda)^{-1}\|_{L(\mathcal{H}_n)}^{-1}$ .*
- (ii) *For any  $q > 0$ , testing whether  $s(T_n - \lambda) > q$  requires only finitely many arithmetic operations on the matrix elements of  $T_n$ .*

*with the convention that  $\|(T_n - \lambda)^{-1}\|^{-1} = 0$  for  $\lambda \in \sigma(T_n)$ .*

*Proof.* Part (i) was proved in [Han11], while part (ii) follows by noting that  $s(T_n - \lambda) > q$  is equivalent to  $(T_n - \lambda)^*(T_n - \lambda) - q^2 I$  being positive definite; see [BHNS15, Prop. 10.1] for a full proof.  $\square$

For  $n \in \mathbb{N}$  we define a map  $\Gamma_n^{(1)} : \Omega_1 \rightarrow \{\text{closed subsets of } \mathbb{C}\}$  by

$$\Gamma_n^{(1)}(T) := \left\{ \lambda \in G_n^{\mathbb{R}} \mid s(T_n - \lambda) \leq \frac{1}{n} \right\}.$$

Then, by the above lemma, each  $\Gamma_n^{(1)}$  is an arithmetic tower of height one in the sense of Definition 1.3. Clearly,  $\Gamma_n^{(1)}(T) \subset \sigma_{\frac{1}{n}}(T_n)$  for all  $n$ , where  $\sigma_{\frac{1}{n}}(\cdot)$  denotes the  $\frac{1}{n}$ -pseudospectrum, i.e.  $\sigma_{\frac{1}{n}}(T_n) = \{z \in \mathbb{C} \mid \|(T_n - z)^{-1}\| > n\}$ . Next we prove a version of the second resolvent identity for our operator approximation.

**Lemma 2.5.** *Let  $T : \text{dom}(T) \rightarrow \mathcal{H}$  be selfadjoint,  $\bigcup_n \mathcal{H}_n$  form a core of  $T$  and  $T_n$  be defined as in (2.6). Then each  $T_n$  is selfadjoint on  $\mathcal{H}_n$  and  $T_n \rightarrow T$  in strong resolvent sense.*

*Proof.* We start by showing that each  $T_n$  is selfadjoint. First note that each  $T_n$  is automatically bounded, since the  $\mathcal{H}_n$  are finite dimensional. Now let  $x, y \in \mathcal{H}_n$ . Then we have

$$\begin{aligned} \langle T_n x, y \rangle &= \langle P_n T x, y \rangle = \langle T x, P_n y \rangle = \langle T x, y \rangle \\ &= \langle x, T y \rangle = \langle P_n x, T y \rangle = \langle x, P_n T y \rangle = \langle x, T_n y \rangle. \end{aligned} \quad (2.7)$$

and hence  $T_n$  is selfadjoint. The claim now follows directly from [Wei00, Satz 9.29], since  $\bigcup_n \mathcal{H}_n$  is a core for  $T$  and  $P_n$  converges strongly to the identity.  $\square$

## 2.2 General results on spectral and pseudospectral pollution

In this subsection we collect facts about spectral and pseudospectral pollution for closed, densely defined operators  $H, H_n$  on  $\mathcal{H}$ , which are not necessarily selfadjoint. These results

will be used in later sections. The sets of spectral and pseudospectral pollution are defined, respectively, as

$$\begin{aligned}\sigma_{\text{poll}}(H) &= \{z \in \mathbb{C} \setminus \sigma(H) \mid \exists \text{ sequence } \lambda_n \in \sigma(H_n) : \lambda_n \rightarrow z\} \\ \sigma_{\varepsilon, \text{poll}}(H) &= \{z \in \mathbb{C} \setminus \sigma_{\varepsilon}(H) \mid \exists \text{ sequence } \lambda_n \in \sigma_{\varepsilon}(H_n) : \lambda_n \rightarrow z\}.\end{aligned}$$

The following definitions from [BMT19], which are related to the essential spectrum, will be used frequently in the sequel. The *limiting essential spectrum*:

$$\sigma_e((H_n)_{n \in \mathbb{N}}) := \{\lambda \in \mathbb{C} \mid \exists x_k \in \text{dom}(H_{n_k}) : \|x_k\| = 1 \forall k, x_k \rightharpoonup 0, \|(H_{n_k} - \lambda)x_k\| \rightarrow 0\},$$

the *limiting  $\varepsilon$ -near spectrum*:

$$\Lambda_{e, \varepsilon}((H_n)_{n \in \mathbb{N}}) := \{\lambda \in \mathbb{C} \mid \exists x_k \in \text{dom}(H_{n_k}) : \|x_k\| = 1 \forall k, x_k \rightharpoonup 0, \|(H_{n_k} - \lambda)x_k\| \rightarrow \varepsilon\},$$

the *essential numerical range*

$$W_e(H) := \{\lambda \in \mathbb{C} \mid \exists x_k \in \text{dom}(H) : \|x_k\| = 1 \forall k, x_k \rightharpoonup 0, \langle Hx_k, x_k \rangle \rightarrow \lambda\}$$

and the *limiting essential numerical range*

$$W_e((H_n)_{n \in \mathbb{N}}) := \{\lambda \in \mathbb{C} \mid \exists x_k \in \text{dom}(H_{n_k}) : \|x_k\| = 1 \forall k, x_k \rightharpoonup 0, \langle H_{n_k}x_k, x_k \rangle \rightarrow \lambda\}.$$

The essential limiting spectrum was originally introduced in [BBL12] in the context of Galerkin approximation and later adapted to a more general framework in [Bög18, Bög17], where the set  $\Lambda_{e, \varepsilon}((H_n)_{n \in \mathbb{N}})$  was introduced. The essential numerical range was originally introduced by Stampfli and Williams in [SW68] for bounded operators and recently extended to unbounded operators in [BMT19]. It was shown there that the essential numerical range is a convenient tool when studying spectral and pseudospectral pollution of operator approximations. This fact will prove useful to our purpose as we shall see in the following.

In order to prove the next lemma, we need a fact about closures of pseudospectra.

**Lemma 2.6.** *For all operators  $H$  on  $\mathcal{H}$  of the form  $H = T + V$ , where  $T$  is selfadjoint and  $V$  is bounded, and all  $\varepsilon < \varepsilon'$  one has*

$$\overline{\sigma_{\varepsilon}(H)} \subset \sigma_{\varepsilon'}(H).$$

*Proof.* This follows from the fact that the resolvent norm of any such operator tends to 0 at  $i\infty$  and hence cannot be constant on an open set (cf. [BS14, Th. 3.2]). Indeed, in this case we have

$$\overline{\sigma_{\varepsilon}(H)} = \{z \mid \|(H - z)^{-1}\| \geq \varepsilon^{-1}\} \subset \{z \mid \|(H - z)^{-1}\| > \varepsilon'^{-1}\} = \sigma_{\varepsilon'}(H).$$

□

**Lemma 2.7.** (i) *For any closed, densely defined operator  $H$  on  $\mathcal{H}$  one has*

$$\bigcap_{\varepsilon > 0} \bigcup_{\delta \in (0, \varepsilon]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}}) \subset \sigma_e((H_n)_{n \in \mathbb{N}}).$$

(ii) *The above inclusion holds, if  $\bigcap_{\varepsilon > 0} \bigcup_{\delta \in (0, \varepsilon]}$  is replaced by  $\bigcap_k \bigcup_{\delta \in (0, \varepsilon_k]}$  for any sequence  $(\varepsilon_k)$  with  $\varepsilon_k \rightarrow 0$ .*

*Proof.* We first prove (i). Let  $\lambda \in \bigcap_{\varepsilon > 0} \bigcup_{\delta \in (0, \varepsilon]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}})$ . Then for all  $\varepsilon > 0$  there exists  $\delta \in (0, \varepsilon]$  and a sequence  $(x_k)$  with  $x_k \in \text{dom}(H_{n_k})$  (for some subsequence  $(n_k)$ ) such that

- $\|x_k\| = 1$  for all  $k$

- $x_k \rightarrow 0$  as  $k \rightarrow \infty$
- $\|(H_{n_k} - \lambda)x_k\| \rightarrow \delta$ .

Hence, for every  $m \in \mathbb{N}$  there exists a sequence  $(x_k^{(m)})_{k \in \mathbb{N}}$  with  $\|x_k^{(m)}\| = 1$ ,  $x_k^{(m)} \xrightarrow{k \rightarrow \infty} 0$  and

$$\lim_{k \rightarrow \infty} \|(H_{n_k(m)} - \lambda)x_k^{(m)}\| < \frac{1}{m}.$$

The notation  $n_k(m)$  indicates that the corresponding subsequence of  $(H_n)$  depends on  $m$ . Now, construct a diagonal sequence as follows. Since  $\mathcal{H}$  is separable, the weak topology is metrisable on the unit ball. Let  $d$  denote a corresponding metric. Now, for any given  $m \in \mathbb{N}$ , choose  $k_m \in \mathbb{N}$  large enough such that

$$\begin{aligned} d(x_{k_m}^{(m)}, 0) &< \frac{1}{m} \\ \|(H_{n_{k_m}(m)} - \lambda)x_{k_m}^{(m)}\| &< \frac{1}{m}. \end{aligned}$$

Then for the sequence  $y_m := x_{k_m}^{(m)}$ , one has  $\|y_m\| = 1$  for all  $m$ ,  $d(y, 0) \rightarrow 0$  and  $\|(H_{n_{k_m}(m)} - \lambda)y_m\| \rightarrow 0$  as  $m \rightarrow \infty$ . Hence  $\lambda \in \sigma_e((H_n)_{n \in \mathbb{N}})$ .

The proof of (ii) is now trivial, since the sequence of sets  $\bigcup_{\delta \in (0, \varepsilon]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}})$  is shrinking with  $\varepsilon$ .  $\square$

Finally, we prove the following characterisation of convergence of sets in the Attouch-Wets metric. We recall that  $d_{AW}(X_n, X) \rightarrow 0$  if and only if  $d_K(X_n, X) \rightarrow 0$  for all  $K \subset \mathbb{C}$  compact, where

$$d_K(X, Y) := \max \left\{ \sup_{x \in X \cap K} \text{dist}(x, Y), \sup_{y \in Y \cap K} \text{dist}(y, X) \right\}.$$

**Proposition 2.8.** *Let  $X, X_n$ ,  $n \in \mathbb{N}$  be closed subsets of  $\mathbb{C}$ . Assume that*

- (a) *If  $\lambda_n \in X_n$  and  $\lambda_n \rightarrow \lambda$ , then  $\lambda \in X$ .*
- (b) *If  $\lambda \in X$ , then there exist  $\lambda_n \in X_n$  with  $\lambda_n \rightarrow \lambda$ .*

*Then one has  $d_{AW}(X_n, X) \rightarrow 0$ .*

*Proof.* Let  $K \subset \mathbb{C}$  be compact. We will show that if (a), (b) hold, then both distances  $\sup_{z \in X_n \cap K} \text{dist}(z, X)$  and  $\sup_{w \in X \cap K} \text{dist}(w, X_n)$  converge to zero. We begin with the latter.

Let  $\varepsilon > 0$ . For all  $w \in X \cap K$ , the ball  $B_\varepsilon(w)$  contains infinitely many elements  $z_n \in X_n$ , by (b). The collection  $\{B_\varepsilon(w) \mid w \in X \cap K\}$  forms an open cover of the compact set  $X \cap K$ . Hence, there exist finitely many  $w_1, \dots, w_k \in X \cap K$  such that  $B_\varepsilon(w_1), \dots, B_\varepsilon(w_k)$  cover  $X \cap K$ . Now, any  $w \in X \cap K$  is contained in some  $B_\varepsilon(w_i)$  and hence  $\text{dist}(w, X_n) < \varepsilon$  for any  $w \in X \cap K$ , as soon as  $n = n(i)$  is large enough. But since there are only finitely many  $B_\varepsilon(w_i)$ , one will have  $\text{dist}(w, X_{n_0}) < 2\varepsilon$  for all  $w \in X \cap K$  for  $n_0 = \max\{n_i \mid i = 1, \dots, k\}$ .

To show that  $\sup_{z \in X_n \cap K} \text{dist}(z, X) \rightarrow 0$  as  $n \rightarrow \infty$ , note that since all sets  $X_n \cap K$  are compact, we can choose a sequence  $z_n \in X_n \cap K$  such that

$$\sup_{z \in X_n \cap K} \text{dist}(z, X) = \text{dist}(z_n, X).$$

Since the sequence  $(z_n)$  is obviously bounded, we can extract a convergent subsequence  $z_{n_j} \rightarrow z_0 \in K$ . Now use assertion (a) from above to conclude that in fact  $z_0 \in X \cap K$ . This readily implies

$$\sup_{z \in X_{n_j} \cap K} \text{dist}(z, X) = \text{dist}(z_{n_j}, X) \rightarrow 0.$$



Since the same reasoning can be applied to every subsequence of the sequence

$$\left( \sup_{z \in X_n \cap K} \text{dist}(z, X) \right)_{n \in \mathbb{N}},$$

we conclude that the whole sequence converges to zero.  $\square$

### 2.3 Proof of Theorem 2.1

Next, we prove convergence of the algorithm  $\Gamma_n^{(1)}$ . By the conditions in (2.1) and Lemma 2.5, we have  $T_n \rightarrow T$  in strong resolvent sense for all  $T \in \Omega$ .

**Lemma 2.9.** *If  $\lambda_n \in \Gamma_n^{(1)}(T)$ ,  $n \in \mathbb{N}$  and  $\lambda_n \rightarrow \lambda$ , then*

$$\lambda \in \sigma(T) \cup \sigma_e((T_n)_{n \in \mathbb{N}}).$$

*Proof.* By definition of  $\Gamma_n^{(1)}$ , one has that

$$\frac{1}{n} \geq \|(\lambda_n - T_n)^{-1}\|^{-1} \geq \text{dist}(\lambda_n, \sigma(T_n))$$

for all  $n \in \mathbb{N}$ . Hence, there exists a sequence  $z_n \in \sigma(T_n)$  such that  $|z_n - \lambda_n| \rightarrow 0$  and consequently  $z_n \rightarrow \lambda$ . We conclude from [Bög18, Th. 2.3] that  $\lambda \in \sigma(T) \cup \sigma_e((T_n)_{n \in \mathbb{N}})$ .  $\square$

To conclude, we apply [BMT19, Th. 6.1] to show that spectral pollution is in fact absent for  $T \in \Omega_1$ . Indeed, let  $\lambda_n \in \Gamma_n^{(1)}(T)$  with  $\lambda_n \rightarrow \lambda$ . Then by Lemma 2.9 and [BMT19, Prop. 5.6, Th. 6.1], we get

$$\begin{aligned} \lambda &\in \sigma(T) \cup \sigma_e((T_n)_{n \in \mathbb{N}}) \\ &\subset \sigma(T) \cup W_e(T) \\ &= \sigma(T) \cup \text{conv}(\widehat{\sigma}_e(T)) \setminus \{\pm\infty\} \\ &= \sigma(T) \cup \sigma_e(T) \\ &= \sigma(T). \end{aligned}$$

It remains to prove spectral inclusion, i.e. nothing is missed by  $\Gamma_n^{(1)}(T)$ .

**Lemma 2.10.** *For every  $\lambda \in \sigma(T)$  there exist  $\lambda_n \in \Gamma_n^{(1)}(T)$  such that  $\lambda_n \rightarrow \lambda$ .*

*Proof.* Let  $\lambda \in \sigma(T)$ . A simple adaption of the proof of [RS80, Th. VIII.24] shows that there exists a sequence  $(\mu_n)$  with  $\mu_n \in \sigma(T_n)$  and  $\mu_n \rightarrow \lambda$ .

For each  $n$ , there exists  $\lambda_n \in G_n^{\mathbb{R}}$  such that  $|\mu_n - \lambda_n| < \frac{1}{n}$  and hence  $\|(T_n - \lambda_n)^{-1}\|_{L(\mathcal{H}_n)} \geq n$  which implies  $\lambda_n \in \Gamma_n^{(1)}(T)$ . Since  $|\mu_n - \lambda_n| \rightarrow 0$  and  $\mu_n \rightarrow \lambda$ , it follows that  $\lambda_n \rightarrow \lambda$ .  $\square$

**Conclusion.** We have shown that

- (a) If  $\lambda_n \in \Gamma_n^{(1)}(T)$  and  $\lambda_n \rightarrow \lambda$ , then  $\lambda \in \sigma(T)$ .
- (b) If  $\lambda \in \sigma(T)$ , then there exist  $\lambda_n \in \Gamma_n^{(1)}(T)$  with  $\lambda_n \rightarrow \lambda$ .

By Proposition 2.8, this implies Attouch-Wets convergence.

### 3 Relatively Compact Perturbations

In this section we show that Theorem 2.1 remains true for certain relatively compact, bounded perturbations of selfadjoint operators. More precisely, we have

**Theorem 3.1.** *Define a computational problem by*

$$\Omega_2 := \left\{ H = T + V : \text{dom}(T) \rightarrow \mathcal{H} \left| \begin{array}{l} T \text{ selfadjoint, semibounded, } \bigcup_{n \in \mathbb{N}} \mathcal{H}_n \text{ core for } T, \\ \sigma(T) = \sigma_e(T), \widehat{\sigma}_e(T) \text{ convex,} \\ V \in L(\mathcal{H}) \text{ and } V, V^* \text{ are } T\text{-compact.} \end{array} \right. \right\}$$

*For every  $H \in \Omega_2$ , choose a decomposition  $H = T + V$  as in the definition of  $\Omega_2$  and define the maps  $s_T(H) := T$  and  $s_V(H) := V$ . Then let*

$$\Lambda_2 := \{f_{i,j,n} \circ s_T \mid 1 \leq i, j \leq n, n \in \mathbb{N}\} \cup \{f_{i,j,n} \circ s_V \mid 1 \leq i, j \leq n, n \in \mathbb{N}\},$$

*where  $f_{i,j,n}$  are the evaluation functions producing the  $(i, j)$ th matrix elements (see (2.4)). Then one has  $\text{SCI}(\Omega_2, \Lambda_2, \sigma(\cdot)) = 1$ .*

*Remark 3.2.* Note that the information provided to the algorithm in  $\Lambda_2$  includes the decomposition of  $H \in \Omega_2$  into a selfadjoint part  $T$  and a perturbation  $V$ . This means, that the algorithm *does not have to compute this decomposition*. It gets it for free. This is a reasonable assumption in many applications as we will see in Section 4.

Note the additional assumption  $\sigma(T) = \sigma_e(T)$  in the selfadjoint part  $T$ . This will be needed later in order to exclude spectral pollution of the algorithm.

#### 3.1 Proof of Theorem 3.1

**Spectrum of  $H$ .** The proof of Theorem 3.1 is via perturbation theory. We first focus on the spectrum of an operator  $H \in \Omega_2$ . Recall the definitions of the essential spectra  $\sigma_{e2}, \sigma_{e5}$  from Section 2. In the proof, we will need the following results, which are classical.

**Theorem 3.3** ([EE87, Th. IX.1.5]). *For any closed, densely defined operator  $H$  on  $\mathcal{H}$ , one has  $\lambda \notin \sigma_{e5}(H)$  if and only if  $H - \lambda$  is Fredholm with  $\text{ind}(H - \lambda) = 0$  and a deleted neighbourhood of  $\lambda$  lies in  $\rho(H)$ .*

In other words, if  $\lambda \notin \sigma_{e5}(H)$ , then  $\lambda$  is an isolated eigenvalue of finite multiplicity. Furthermore, the following perturbation result is known.

**Theorem 3.4** ([RS80, XIII.4, Cor. 2]). *Let  $T$  be a selfadjoint operator on  $\mathcal{H}$  and  $V$  relatively compact w.r.t.  $T$ . Then*

- (i)  $H := T + V$  is closed on  $\text{dom}(T)$  and
- (ii)  $\sigma_{e5}(H) = \sigma_e(T)$ .

From Theorems 3.3 and 3.4 we immediately conclude that for all  $H \in \Omega_2$  the spectrum of  $\mathcal{H}$  is of the form

$$\sigma(H) = \sigma(T) \cup \{\lambda_1, \lambda_2, \dots\},$$

with isolated eigenvalues  $\lambda_i \in \mathbb{C}$ .

**Strong resolvent convergence.** Let  $P_n : \mathcal{H} \rightarrow \mathcal{H}_n$  be defined as in Section 2 and set  $V_n := P_n V|_{\mathcal{H}_n}$ .

**Lemma 3.5.** *For  $V_n$  defined as above, we have the following*

- (i)  $(V_n)^* = (V^*)_n$  (i.e. compression to  $\mathcal{H}_n$  commutes with taking the adjoint) and

(ii)  $V_n P_n \rightarrow V$  strongly in  $\mathcal{H}$ .

(iii)  $V_n^* P_n \rightarrow V^*$  strongly in  $\mathcal{H}$ .

*Proof.* Assertion (i) is easily shown by an analogous calculation to (2.7).

To see assertion (ii), let  $u \in \mathcal{H}$  and note that then  $P_n u \rightarrow u$  strongly. By continuity of  $V$ , it immediately follows that  $V P_n u \rightarrow V u$  in  $\mathcal{H}$ . Hence, from the definition of  $V_n$  we conclude that

$$V_n P_n u = P_n V|_{\mathcal{H}_n} P_n u = \underbrace{P_n}_{\rightarrow I \text{ strongly}} \underbrace{V P_n u}_{\rightarrow V u} \rightarrow V u.$$

Assertion (iii) now immediately follows by combining (i) and (ii).  $\square$

The next lemma shows that even the perturbed operators  $H_n$  converge in strong resolvent sense.

**Lemma 3.6.** *For  $H \in \Omega_2$  and  $H_n = P_n H|_{\mathcal{H}_n}$ , one has  $H_n \rightarrow H$  and  $H_n^* \rightarrow H^*$  in strong resolvent sense.*

*Proof.* This follows from [Bög17, Cor. 3.5], since  $\|(T - z)^{-1}\|^{-1}, \|(T_n - z)^{-1}\|^{-1} \geq \text{dist}(z, \mathbb{R})$ , which tends to  $\infty$  as  $z \rightarrow i\infty$ , and  $\|V\|, \|V_n\|$  are uniformly bounded.  $\square$

**The algorithm.** The algorithm for  $\Omega_2, \Lambda_2$  is defined analogously to that in Section 2. Namely, we define  $G_n^{\mathbb{C}} := \frac{1}{n}(\mathbb{Z} + i\mathbb{Z}) \cap B_n(0) \subset \mathbb{C}$ .

$$\Gamma_n^{(2)}(H) := \left\{ \lambda \in G_n^{\mathbb{C}} \mid \min \{s(H_n - \lambda), s(H_n^* - \bar{\lambda})\} \leq \frac{1}{n} \right\} \cup \Gamma_n^{(1)}(T). \quad (3.1)$$

Note that we have  $\min \{s(M - \lambda), s(M^* - \bar{\lambda})\} = \|(M - \lambda)^{-1}\|^{-1}$  for any  $n \times n$  matrix  $M$  (cf. [Han11]). Since we have already shown that  $\Gamma_n^{(1)}$  approximates  $\sigma(T)$  correctly and that  $\sigma(T) = \sigma_e(T) = \sigma_{e5}(H)$ , we know that  $\Gamma_n^{(2)}$  will not miss anything in  $\sigma_{e5}(H)$ . Thus, it only remains to prove absence of spectral pollution and spectral inclusion for the discrete set  $\sigma(H) \setminus \sigma_{e5}(H)$  for the algorithm

$$\tilde{\Gamma}_n(H) := \left\{ \lambda \in G_n^{\mathbb{C}} \mid \min \{s(H_n - \lambda), s(H_n^* - \bar{\lambda})\} \leq \frac{1}{n} \right\}$$

This will be done in the remainder of this section.

However, let us first take a moment to assure that  $\Gamma_n^{(2)}$  defines a reasonable algorithm. Clearly, each  $\Gamma_n^{(2)}$  depends only on  $\langle T e_i^{(n)}, e_j^{(n)} \rangle$  and  $\langle V e_i^{(n)}, e_j^{(n)} \rangle$ ,  $1 \leq i, j \leq k_n$ . Moreover, by Lemma 2.4 it only requires finitely many algebraic operations on these numbers to determine whether  $\lambda \in G_n^{\mathbb{C}}$  belongs to the set  $\{\lambda \mid \min \{s(H_n - \lambda), s(H_n^* - \bar{\lambda})\} \leq \frac{1}{n}\}$ . Finally, since  $\Lambda_2$  contains all matrix elements  $\langle T e_i^{(n)}, e_j^{(n)} \rangle$ , it follows from the comments made in Section 2 that  $\Gamma_n^{(1)}$  is an admissible algorithm as well.

*Remark 3.7.* We note that the choice  $\frac{1}{n}$  as an upper bound for  $s(H_n - \lambda)$  in (3.1) is arbitrary. The proof below will show that one could equally well have chosen

$$\Xi_n(H) := \left\{ \lambda \in G_n^{\mathbb{C}} \mid \min \{s(H_n - \lambda), s(H_n^* - \bar{\lambda})\} \leq \frac{3}{n} \right\} \cup \Gamma_n^{(1)}(T)$$

instead of  $\Gamma_n^{(2)}(H)$ . This fact will be used in Section 4.

**Spectral pollution.** Let us prove that the approximation  $\Gamma_n^{(2)}(H)$  does not have spectral pollution for  $H \in \Omega_2$ . To this end, note that again  $\tilde{\Gamma}_n(H) \subset \sigma_\varepsilon(H_n)$  for  $\varepsilon > 0$  fixed and  $n$  large enough. According to [Bög18, Th. 3.6 ii)],  $\varepsilon$ -pseudospectral pollution of the approximation  $H_n \rightarrow H$  is confined to

$$\sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^* \cup \bigcup_{\delta \in (0, \varepsilon]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}}).$$

Hence, for any sequence  $\lambda_n \in \tilde{\Gamma}_n(H)$  with  $\lambda_n \rightarrow \lambda \in \mathbb{C}$  we have

$$\lambda \in \bigcap_{\varepsilon > 0} \left( \sigma_\varepsilon(H) \cup \sigma_e(H_n)_{n \in \mathbb{N}} \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^* \cup \bigcup_{\delta \in (0, \varepsilon]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}}) \right). \quad (3.2)$$

We conclude with the following

**Lemma 3.8.** *It follows from (3.2) that*

$$\lambda \in \sigma(H) \cup \sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^*.$$

*Proof.* Let (3.2) hold. Then

- Either there exists  $\varepsilon_0 > 0$  such that  $\lambda \in \sigma_\varepsilon(H) \cup \sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^*$  for all  $\varepsilon \in (0, \varepsilon_0)$ , or
- there exists a sequence  $\varepsilon_k$  with  $\varepsilon_k \searrow 0$  and  $\lambda \in \bigcup_{\delta \in (0, \varepsilon_k]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}})$  for all  $k$ .

In the first case, it follows that

$$\begin{aligned} \lambda &\in \bigcap_{\varepsilon > 0} \left( \sigma_\varepsilon(H) \cup \sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^* \right) \\ &= \left( \bigcap_{\varepsilon > 0} \sigma_\varepsilon(H) \right) \cup \sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^* \\ &= \sigma(H) \cup \sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^*. \end{aligned}$$

In the second case, we have

$$\begin{aligned} \lambda &\in \bigcap_{k \in \mathbb{N}} \bigcup_{\delta \in (0, \varepsilon_k]} \Lambda_{e, \delta}((H_n)_{n \in \mathbb{N}}) \\ &\subset \sigma_e((H_n)_{n \in \mathbb{N}}), \end{aligned}$$

by Lemma 2.7 (ii). □

Next, by [BMT19, Th. 6.1] we have  $\sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^* \subset W_e(H)$  and hence  $\lambda \in \sigma(H) \cup W_e(H)$ . In order to exclude spectral pollution it only remains to prove  $W_e(H) \subset \sigma(H)$ .

**Lemma 3.9.** *For  $H = T + V \in \Omega_2$  one has  $W_e(H) \subset \sigma_e(H)$ .*

*Proof.* Let  $H = T + V$  with  $T$  selfadjoint, semibounded and  $V \in L(\mathcal{H})$  such that  $V, V^*$  are  $T$ -compact. Then denoting  $\operatorname{Re}(V) := \frac{1}{2}(V + V^*)$  and  $\operatorname{Im}(V) := \frac{1}{2i}(V - V^*)$  we have that  $V = \operatorname{Re}(V) + i \operatorname{Im}(V)$  with  $\operatorname{Re}(V), \operatorname{Im}(V)$  relatively compact w.r.t.  $T$ . Applying [BMT19, Th. 4.5] we conclude that  $W_e(H) = W_e(T)$ .

But now by our assumptions on  $T$ , we can see from [BMT19, Th. 3.8] that

$$W_e(T) = \operatorname{conv}(\hat{\sigma}_e(T)) \setminus \{\pm\infty\} = \sigma_e(T) = \sigma_e(H).$$

□

Note that the previous lemma is the only place in which we need the semiboundedness assumption in the definition of  $\Omega_2$ . Overall we have shown that for any sequence  $\lambda_n \in \tilde{\Gamma}_n(H)$  which converges to some  $\lambda \in \mathbb{C}$  we necessarily have  $\lambda \in \sigma(H)$ , in other words, spectral pollution does not exist.

**Spectral inclusion.** It remains to show that the approximation  $(\Gamma_n^{(2)}(H))$  is spectrally inclusive, i.e. that for any  $\lambda \in \sigma(H)$  there exists a sequence  $\lambda_n \in \Gamma_n^{(2)}(H)$  such that  $\lambda_n \rightarrow \lambda$ . As explained above, the existence of such a sequence is already guaranteed for all  $\lambda \in \sigma_{e5}(H)$ .

**Lemma 3.10.** *For every  $\lambda \in \sigma(H) \setminus \sigma_{e5}(H)$  there exists a sequence  $\lambda_n \in \tilde{\Gamma}(H)$  with  $\lambda_n \rightarrow \lambda$ .*

*Proof.* First note that by Theorem 3.3  $\lambda$  is an isolated point. Moreover, we have seen in the proof of Lemma 3.9 that  $\sigma_e((H_n)_{n \in \mathbb{N}}) \cup \sigma_e((H_n^*)_{n \in \mathbb{N}})^* \subset \sigma_e(H)$  and hence  $\lambda$  does not belong to this set either. From Lemma 3.6 and [Bög18, Th. 2.3 i)] we conclude that there exists a sequence  $\mu_n \in \sigma(H_n)$  with  $\mu_n \rightarrow \lambda$ .

Now, by definition of  $G_n^{\mathbb{C}}$ , for each  $n$  there exists  $\lambda_n \in G_n^{\mathbb{C}}$  such that  $|\mu_n - \lambda_n| < \frac{1}{n}$  and hence  $\|(H_n - \lambda_n)^{-1}\|_{L(\mathcal{H}_n)} \geq n$  which implies  $\lambda_n \in \tilde{\Gamma}_n(H)$ . Since  $|\mu_n - \lambda_n| \rightarrow 0$  and  $\mu_n \rightarrow \lambda$ , it follows that  $\lambda_n \rightarrow \lambda$ .  $\square$

**Conclusion.** Overall we have shown that

(a') If  $\lambda_n \in \Gamma_n^{(2)}(H)$  and  $\lambda_n \rightarrow \lambda$ , then  $\lambda \in \sigma(H)$ .

(b') If  $\lambda \in \sigma(H)$ , then there exist  $\lambda_n \in \Gamma_n^{(2)}(H)$  with  $\lambda_n \rightarrow \lambda$ .

By Proposition 2.8 this implies  $d_{\text{AW}}(\Gamma_n^{(2)}(H), \sigma(H)) \rightarrow 0$ .

## 4 Application to Schrödinger Operators

In this section we will apply the results of Sections 2 and 3 to Schrödinger operators on  $L^2(\mathbb{R}^d)$ . More specifically, fix a continuous, monotone decreasing function  $g : [0, \infty) \rightarrow [0, \infty)$  with  $g(t) \rightarrow 0$  as  $t \rightarrow \infty$  and let  $M > 0$ . We define

$$\Omega_3 := \{-\Delta + V \mid V \in \mathcal{C}^1(\mathbb{R}, \mathbb{C}), \|\nabla V\|_\infty \leq M, |V(x)| \leq g(|x|)\}. \quad (4.1)$$

By the above definition, every  $H \in \Omega_3$  is a relatively compact perturbation of the free Laplacian with domain  $H^2(\mathbb{R}^d)$  (cf. e.g. [Kat95, Ch. V, Lemma 5.8]). In fact, our assumptions on  $V$  have been chosen such that every  $H \in \Omega_3$  even satisfies all conditions formulated in the set  $\Omega_2$  in Theorem 3.1.

In order to define the computational problem, we choose a finite lattice in  $\mathbb{R}^d$

$$L_n := \left\{ \frac{i}{n} \mid i \in \mathbb{Z}^d, |i| < n \right\}.$$

Moreover, let  $\mathcal{H}_n$  denote the subspace of  $L^2(\mathbb{R}^d)$  spanned by all characteristic functions of cubes of edge length  $\frac{1}{n}$  with centres inside a ball of radius  $n$ :

$$\hat{\mathcal{H}}_n := \text{span} \left\{ \chi_{i+[0, \frac{1}{n})^d} \mid i \in L_n \right\}$$

It is easily seen by smooth approximation that  $P_{\hat{\mathcal{H}}_n} \rightarrow I$  strongly in  $L^2(\mathbb{R}^d)$ . However, none of the basis functions  $\chi_{i+[0, \frac{1}{n})^d}$  are contained in the domain of  $-\Delta$ . In order to circumvent this, the space we will actually work with will be

$$\mathcal{H}_n := \text{span} \left\{ \hat{\chi}_{i+[0, \frac{1}{n})^d} \mid i \in L_n \right\}, \quad (4.2)$$

where the hat denotes the Fourier transform in  $L^2(\mathbb{R}^d)$ . For any enumeration  $i_k$  of the set  $L_n$ , we define

$$e_k^{(n)} := n^{\frac{d}{2}} \cdot \hat{\chi}_{i_k+[0, \frac{1}{n})^d},$$

where the normalisation constant  $n^{\frac{d}{2}}$  is chosen such that  $\|e_k^{(n)}\|_{L^2(\mathbb{R}^d)} = 1$  for all  $n \in \mathbb{N}$ . These are smooth functions in  $L^2(\mathbb{R}^d)$  and it is easily checked that their first and second derivatives are again in  $L^2(\mathbb{R}^d)$ .

**Lemma 4.1.** *We have  $P_{\mathcal{H}_n} \rightarrow I$  strongly in  $L^2(\mathbb{R}^d)$  and for any  $n \in \mathbb{N}$  the set  $\{e_k^{(n)}\}_{k=1}^{\#L_n}$  form an orthonormal basis of  $\mathcal{H}_n$ .*

*Proof.* This follows immediately from the unitarity of the Fourier transform and the equality

$$\left\| \sum_k \left\langle f, n^{\frac{d}{2}} \chi_{i_k + [0, \frac{1}{n}]^d} \right\rangle n^{\frac{d}{2}} \chi_{i_k + [0, \frac{1}{n}]^d} - f \right\|_{L^2(\mathbb{R}^d)} = \left\| \sum_k \left\langle \hat{f}, e_k^{(n)} \right\rangle e_k^{(n)} - \hat{f} \right\|_{L^2(\mathbb{R}^d)}.$$

□

We note that the functions  $e_k^{(n)}$  can be calculated explicitly. Indeed, one has

$$e_k^{(n)}(\xi) = \left( \frac{n}{2\pi} \right)^{\frac{d}{2}} \prod_{j=1}^d \frac{e^{i\xi_j((i_k)_j + \frac{1}{n})} - e^{i\xi_j(i_k)_j}}{\xi_j},$$

where  $(i_k)_j$  denotes the  $j$ 'th component of the vector  $i_k$  and  $\xi = (\xi_1, \dots, \xi_d) \in \mathbb{R}^d$ . Using this explicit representation, it can be easily seen that we have the following.

**Lemma 4.2.** *For each  $n \in \mathbb{N}$  one has*

$$\|e_k^{(n)}\|_{\infty}, \|\nabla e_k^{(n)}\|_{\infty} \leq (2\pi)^{-\frac{d}{2}} dn^{3-\frac{d}{2}}$$

for all  $k \in \{1, \dots, n\}$ .

*Proof.* From the definition of  $e_k^{(n)}$  it follows by direct calculation that

$$\begin{aligned} \|e_k^{(n)}\|_{\infty} &< (2\pi n)^{-\frac{d}{2}}, \\ \|\partial_j e_k^{(n)}\|_{\infty} &< (2\pi)^{-\frac{d}{2}} \frac{n^{-\frac{d}{2}+1}}{2} \left( ((i_k)_j + \frac{1}{n})^2 - (i_k)_j^2 \right) \end{aligned}$$

from which the assertion follows. Note that the bound in the second equation can be made independent of  $k$ , because  $i_k \in L_n \subset B_n(0)$  for all  $k$ . □

The information accessible to the algorithm will be the set

$$\Lambda_3 := \Lambda_3^{(1)} \cup \Lambda_3^{(2)} \cup \Lambda_3^{(3)} \cup \Lambda_3^{(4)}, \quad (4.3)$$

with

$$\begin{aligned} \Lambda_3^{(1)} &= \{\rho_x \mid x \in \mathbb{R}^d\} \\ \Lambda_3^{(2)} &= \left\{ e_k^{(n)}(i) \mid i \in l^{-1}\mathbb{Z}^d, l \in \mathbb{N}, k \in \{1, \dots, n\}, n \in \mathbb{N} \right\} \\ \Lambda_3^{(3)} &= \left\{ \frac{n\delta_{mk}}{3} \sum_{j=1}^d \left( ((i)_j + \frac{1}{n})^3 - (i)_j^3 \right) \mid i \in L_n, m, k \in \{1, \dots, \#L_n\}, n \in \mathbb{N} \right\} \\ \Lambda_3^{(4)} &= \left\{ g(l^{\frac{1}{2d}}) \mid l \in \mathbb{N} \right\} \end{aligned}$$

where  $\rho_x(V) = V(x)$  are the evaluation functionals and  $e_k^{(n)}(i)$  denote constant functions that map  $V$  to the number  $e_k^{(n)}(i)$ . The meaning of the constants  $\frac{n\delta_{mk}}{3} \sum_{j=1}^d \left( ((i)_j + \frac{1}{n})^3 - (i)_j^3 \right)$  will become clear later on.

Together,  $\Omega_3$  and  $\Lambda_3$  define a computational problem  $(\Omega_3, \Lambda_3, \sigma(\cdot))$ . The main result of this section is the following.

**Theorem 4.3.** For  $\Omega_3$  and  $\Lambda_3$  defined as above, we have  $\text{SCI}(\Omega_3, \Lambda_3, \sigma(\cdot)) = 1$ .

The proof of Theorem 4.3 will be by reduction to Theorem 3.1. In order to accomplish this, we need to be able to compute the matrix elements  $\langle (-\Delta + V)e_i, e_j \rangle$  by performing only a finite number of algebraic operations on a finite number of values of  $V$ . This will be the main difficulty.

#### 4.1 Proof of Theorem 4.3

We first show that the spaces  $\mathcal{H}_n$  defined in (4.2) are indeed a reasonable choice for the problem at hand. More precisely, we have

**Lemma 4.4.** The union  $\bigcup_{n \in \mathbb{N}} \mathcal{H}_n$  is a core for  $-\Delta$ .

*Proof.* By means of the Fourier transform the assertion is equivalent to the space  $\bigcup_{n \in \mathbb{N}} \widehat{\mathcal{H}}_n$  being a core for the multiplication operator  $u \mapsto |\xi|^2 u$  in  $L^2(\mathbb{R}^d)$ . To verify this, we have to show that for every  $u \in \text{dom}(|\xi|^2)$  there exists a sequence  $u_n \in \mathcal{H}_n$  such that

- (i)  $\|u_n - u\|_{L^2(\mathbb{R}^d)} \rightarrow 0$ ,
- (ii)  $\| |\xi|^2(u_n - u) \|_{L^2(\mathbb{R}^d)} \rightarrow 0$

Point (i) is easily shown by choosing

$$u_n := \sum_{i \in L_n} \left\langle u, n^{\frac{d}{2}} \chi_{i+[0, \frac{1}{n})^d} \right\rangle n^{\frac{d}{2}} \chi_{i+[0, \frac{1}{n})^d}. \quad (4.4)$$

Indeed, for smooth  $u$  the  $L^2$ -convergence of  $u_n$  to  $u$  is standard, while the general case follows by a density argument. We omit the technical details. To show point (ii), let  $R > 0$  and decompose the norm in (ii) as

$$\| |\xi|^2(u_n - u) \|_{L^2(\mathbb{R}^d)}^2 = \int_{B_R} | |\xi|^2(u_n - u) |^2 d\xi + \int_{\mathbb{R}^d \setminus B_R} | |\xi|^2(u_n - u) |^2 d\xi, \quad (4.5)$$

where  $B_R$  denotes the ball of radius  $R$  centered at 0. We first estimate the second term on the right hand side. To this end, we let  $u_n$  be defined by (4.4) and employ the shorthand notation  $\chi_i := n^{\frac{d}{2}} \chi_{i+[0, \frac{1}{n})^d}$ . On the whole space we have

$$\begin{aligned} \| |\xi|^2 u_n \|_{L^2(\mathbb{R}^d \setminus B_R)}^2 &= \left\| |\xi|^2 \sum_{i \in L_n} \langle u, \chi_i \rangle \chi_i \right\|_{L^2(\mathbb{R}^d \setminus B_R)}^2 \\ &\leq \sum_{i \in L_n \setminus B_R} |\langle u, \chi_i \rangle|^2 \| |\xi|^2 \chi_i \|_{L^2(\mathbb{R}^d)}^2 \\ &\leq \sum_{i \in L_n \setminus B_R} \|u\|_{L^2(i+[0, \frac{1}{n})^d)}^2 \left\| n^{\frac{d}{2}} |\xi|^2 \right\|_{L^2(i+[0, \frac{1}{n})^d)}^2, \end{aligned}$$

where we have used the fact that  $\text{supp}(\chi_i) \cap \text{supp}(\chi_j) = \emptyset$  for  $i \neq j$ . The factor  $\| n^{\frac{d}{2}} |\xi|^2 \|_{L^2(i+[0, \frac{1}{n})^d)}$  on the right hand side is clearly bounded by  $\sup_{\xi \in i+[0, \frac{1}{n})^d} |\xi|^2$ . Thus, if we define a function  $F_n$  by

$$F_n(\xi) := \sum_{i \in \frac{1}{n}\mathbb{Z}^d} \left( \sup_{\eta \in i+[0, \frac{1}{n})^d} |\eta|^2 \right) \chi_i,$$

then we will have (note that  $F_n$  is constant on each of the cubes  $i + [0, \frac{1}{n})^d$ )

$$\| |\xi|^2 u_n \|_{L^2(\mathbb{R}^d \setminus B_R)}^2 \leq \sum_{i \in L_n \setminus B_R} \|u\|_{L^2(i+[0, \frac{1}{n})^d)}^2 F_n(\xi)^2$$

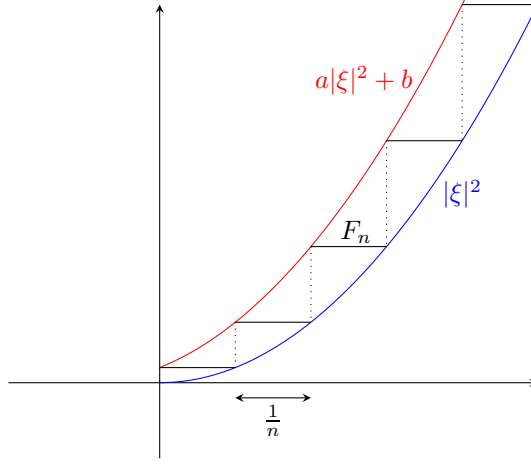


Figure 1: Sketch of function  $F_n$ .

$$\begin{aligned}
&= \sum_{i \in L_n \setminus B_R} \|F_n(\xi)u\|_{L^2(i+[0, \frac{1}{n})^d)}^2 \\
&\leq \|F_n(\xi)u\|_{L^2(\mathbb{R}^d \setminus B_{R-\frac{\sqrt{d}}{n}})}^2
\end{aligned}$$

Next, we note that it is easy to see that there exist constants  $a, b > 0$  such that  $F_n(\xi) \leq a|\xi|^2 + b$  uniformly in  $n$  (see Figure 1). Overall we conclude that

$$\begin{aligned}
\| |\xi|^2 u_n \|_{L^2(\mathbb{R}^d \setminus B_R)}^2 &\leq \|F_n(\xi)u\|_{L^2(\mathbb{R}^d \setminus B_{R-\frac{\sqrt{d}}{n}})}^2 \\
&\leq \| (a|\xi|^2 + b)u \|_{L^2(\mathbb{R}^d \setminus B_{R-1})}^2,
\end{aligned}$$

where the last term on the right hand side is finite because by assumption  $u \in \text{dom}(|\xi|^2)$ . In fact, from this last inequality we can see immediately that

$$\| |\xi|^2 u_n \|_{L^2(\mathbb{R}^d \setminus B_R)}^2 \rightarrow 0$$

as  $R \rightarrow \infty$  uniformly in  $n$ . Estimating the second term on the right hand side of eq. (4.5) is now straightforward. We get

$$\begin{aligned}
\int_{\mathbb{R}^d \setminus B_R} \| |\xi|^2 (u_n - u) \|^2 d\xi &\leq \| |\xi|^2 u_n \|^2_{L^2(\mathbb{R}^d \setminus B_R)} + \| |\xi|^2 u \|^2_{L^2(\mathbb{R}^d \setminus B_R)} \\
&\leq \| (a|\xi|^2 + b)u \|^2_{L^2(\mathbb{R}^d \setminus B_{R-1})} + \| |\xi|^2 u \|^2_{L^2(\mathbb{R}^d \setminus B_R)}.
\end{aligned}$$

Now let  $\varepsilon > 0$  and choose  $R$  so large that  $\| (a|\xi|^2 + b)u \|^2_{L^2(\mathbb{R}^d \setminus B_{R-1})} + \| |\xi|^2 u \|^2_{L^2(\mathbb{R}^d \setminus B_R)} < \varepsilon$ . From eq. (4.5) we then see that

$$\begin{aligned}
\limsup_{n \rightarrow \infty} \| |\xi|^2 (u_n - u) \|^2_{L^2(\mathbb{R}^d)} &\leq \limsup_{n \rightarrow \infty} \int_{B_R} \| |\xi|^2 (u_n - u) \|^2 d\xi + \varepsilon \\
&\leq \limsup_{n \rightarrow \infty} R^2 \int_{B_R} |u_n - u|^2 d\xi + \varepsilon \\
&= \varepsilon,
\end{aligned}$$

because  $u_n \rightarrow u$  in  $L^2(\mathbb{R}^d)$ . Since  $\varepsilon$  was arbitrary, it follows that

$$\limsup_{n \rightarrow \infty} \| |\xi|^2 (u_n - u) \|^2_{L^2(\mathbb{R}^d)} = 0,$$

which concludes the proof.  $\square$



Our strategy for proving Theorem 4.3 is as follows. By the assumptions on  $V$  stated in the definition of  $\Omega_3$  and Lemma 4.4 we know that we have  $\Omega_3 \subset \Omega_2$ , if we choose  $\mathcal{H} = L^2(\mathbb{R}^d)$  and  $\mathcal{H}_n$  as in (4.2). Hence, we already know from Theorem 3.1 that  $\Gamma_n^{(2)}(H) \rightarrow \sigma(H)$  for all  $H \in \Omega_3$ . However,  $\Gamma_n^{(2)}$  uses the matrix elements  $\langle He_k^{(n)}, e_j^{(n)} \rangle$ , which we are not allowed to access in Theorem 4.3. Therefore, we will define a new algorithm  $\Gamma_n^{(3)}$  which only accesses the information provided in  $\Lambda_3$  and which satisfies  $\Gamma_n^{(3)}(H) \approx \Gamma_n^{(2)}(H)$  for  $H \in \Omega_3$  in an appropriate sense.

**The algorithm.** As described above, we need to approximate the matrix elements  $\langle -\Delta e_k^{(n)}, e_m^{(n)} \rangle$  and  $\langle Ve_k^{(n)}, e_m^{(n)} \rangle$  using only a finite amount of information provided in the set  $\Lambda_3$ . We start with the Laplacian, which is the simpler case. Indeed, we have

$$\begin{aligned} \langle -\Delta e_k^{(n)}, e_m^{(n)} \rangle &= \left\langle |\xi|^2 n^{\frac{d}{2}} \chi_{i_k + [0, \frac{1}{n})^d}, n^{\frac{d}{2}} \chi_{i_m + [0, \frac{1}{n})^d} \right\rangle \\ &= n^d \delta_{mk} \int_{i_k + [0, \frac{1}{n})^d} |\xi|^2 d\xi \\ &= \frac{n \delta_{mk}}{3} \sum_{j=1}^d \left( \left( (i_k)_j + \frac{1}{n} \right)^3 - (i_k)_j^3 \right). \end{aligned}$$

Note that these are precisely the terms in the third factor in eq. (4.3).

Next, we will compute the matrix elements  $\langle Ve_k^{(n)}, e_m^{(n)} \rangle$ . Since any algorithm can only use finitely many values of  $V$ , we will have to perform an approximation procedure. To this end, let  $l \in \mathbb{N}$  and define a lattice  $P_l \subset \mathbb{R}^d$  by

$$P_l := \frac{1}{l} \mathbb{Z}^d \cap Q_l,$$

where  $Q_l$  denotes the cube of edge length  $l^{\frac{1}{2d}}$  centered at 0. Next, let

$$V_l(x) := \sum_{i \in P_l} V(i) \chi_{i + [0, \frac{1}{l})^d}.$$

**Lemma 4.5.** *For any function  $f \in C^1(\mathbb{R}^d)$  one has*

$$\left\| f - \sum_{i \in P_l} f(i) \chi_{i + [0, \frac{1}{l})^d} \right\|_{L^\infty(Q_l)} \leq \frac{\|\nabla f\|_\infty}{l},$$

*Proof.* This follows immediately from the identity

$$f(x) - f(i) = \int_{[i, x]} \nabla f(t) \cdot dt,$$

where  $i \in P_l$  and  $[i, x]$  denotes a line segment connecting  $i$  to  $x \in i + [0, \frac{1}{l})^d$ .  $\square$

In order to define our approximation of  $\langle Ve_k^{(n)}, e_m^{(n)} \rangle$ , we additionally introduce the step function approximation

$$E_{k,l}(x) := \sum_{i \in P_l} e_k^{(n)}(l) \chi_{i + [0, \frac{1}{l})^d}.$$

**Lemma 4.6.** *For  $-\Delta + V \in \Omega_3$  one has*

$$\left| \langle Ve_k^{(n)}, e_m^{(n)} \rangle - \langle V_l E_{k,l}, E_{m,l} \rangle \right| \leq \frac{3}{l^{\frac{1}{2}}} (M + g(0)) (2\pi)^{-\frac{d}{2}} n^{3-\frac{d}{2}} d + g(l^{\frac{1}{2d}}),$$

for all  $l \in \mathbb{N}$ , where  $M$  is as in eq. (4.1).

*Proof.* We calculate the error

$$\begin{aligned}
& \left| \left\langle V e_k^{(n)}, e_m^{(n)} \right\rangle - \langle V_l E_{k,l}, E_{m,l} \rangle \right| \\
&= \left| \sum_{i \in P_l} \int_{i+[0, \frac{1}{l})} V e_k^{(n)} e_m^{(n)} dx - \sum_{i \in P_l} \int_{i+[0, \frac{1}{l})} V_l E_{k,l} E_{m,l} dx + \int_{\mathbb{R}^d \setminus Q_l} V e_k^{(n)} e_m^{(n)} dx \right| \\
&\leq \sum_{i \in P_l} \int_{i+[0, \frac{1}{l})} \left| V e_k^{(n)} e_m^{(n)} - V_l E_{k,l} E_{m,l} \right| dx + \int_{\mathbb{R}^d \setminus Q_l} |V e_k^{(n)} e_m^{(n)}| dx \\
&\leq \sum_{i \in P_l} \int_{i+[0, \frac{1}{l})} l^{-1} \left\| \nabla (V e_k^{(n)} e_m^{(n)}) \right\|_{\infty} dx + g(l^{\frac{1}{2d}}) \int_{\mathbb{R}^d \setminus Q_l} |e_k^{(n)} e_m^{(n)}| dx \\
&= l^{-1} |Q_l| \left\| \nabla (V e_k^{(n)} e_m^{(n)}) \right\|_{\infty} + g(l^{\frac{1}{2d}}) \|e_k^{(n)}\|_{L^2(\mathbb{R}^d)} \|e_m^{(n)}\|_{L^2(\mathbb{R}^d)} \\
&\leq l^{-1} l^{\frac{1}{2}} \left( \left\| \nabla V e_k^{(n)} e_m^{(n)} \right\|_{\infty} + \left\| V \nabla e_k^{(n)} e_m^{(n)} \right\|_{\infty} + \left\| V e_k^{(n)} \nabla e_m^{(n)} \right\|_{\infty} \right) + g(l^{\frac{1}{2d}}) \\
&\leq \frac{3}{l^{\frac{1}{2}}} (M + g(0)) (2\pi)^{-\frac{d}{2}} n^{3-\frac{d}{2}} d + g(l^{\frac{1}{2d}}),
\end{aligned}$$

where we have used Lemma 4.5 in the third line and Lemma 4.2 and the fact that  $\|V\|_{C^1} \leq M$  in the last line.  $\square$

**Corollary 4.7.** *If we denote  $H_n := P_n(-\Delta + V)|_{\mathcal{H}_n}$  and  $H_n^l := P_n(-\Delta)|_{\mathcal{H}_n} + W^l$ , where  $W^l$  denotes the operator on  $\mathcal{H}_n$  defined by the  $n \times n$  matrix with elements  $(W^l)_{km} = \langle V_l E_{k,l}, E_{m,l} \rangle$  in the basis  $\{e_k^{(n)}\}_{k=1}^{\#L_n}$ , then*

$$\|H_n - H_n^l\|_{L(\mathcal{H}_n)} \leq \frac{3d(M + g(0))(2\pi n^4)^{-\frac{d}{2}}}{l^{\frac{1}{2}}} + ng(l^{\frac{1}{2d}}).$$

*Proof.* By Lemma 4.6 the matrix elements of  $H_n$  and  $H_n^l$  satisfy  $|(H_n)_{km} - (H_n^l)_{km}| \leq \frac{3}{l^{\frac{1}{2}}} (M + g(0)) (2\pi)^{-\frac{d}{2}} n^{3-\frac{d}{2}} d + g(l^{\frac{1}{2d}})$ . Now note that for any two matrices  $A = (A_{km})$  and  $B = (B_{km})$  one has

$$\begin{aligned}
\|(A - B)x\|_{\mathcal{H}_n}^2 &= \sum_{k=1}^n \left| \sum_{m=1}^n (A_{km} - B_{km}) x_m \right|^2 \\
&\leq \left( \sup_{k,m} |A_{km} - B_{km}| \right) \sum_{k,m=1}^n |x_m|^2 \\
&= n \left( \sup_{k,m} |A_{km} - B_{km}| \right) \|x\|_{\mathcal{H}_n}^2.
\end{aligned}$$

This immediately implies the assertion.  $\square$

We are finally ready to define our algorithm. Let  $n \in \mathbb{N}$  and choose  $l(n) \in \mathbb{N}$  large enough such that  $\frac{3}{l(n)^{\frac{1}{2}}} (M + g(0)) (2\pi)^{-\frac{d}{2}} n^{3-\frac{d}{2}} d + g(l(n)^{\frac{1}{2d}}) < \frac{1}{2n}$  (note that this can be done by a computer in finite time). Define for  $H = -\Delta + V \in \Omega_3$

$$\Lambda_{\Gamma_n^{(3)}}(H) := \Lambda_{\Gamma_n^{(3)}}^{(1)} \cup \Lambda_{\Gamma_n^{(3)}}^{(2)} \cup \Lambda_{\Gamma_n^{(3)}}^{(3)} \cup \Lambda_{\Gamma_n^{(3)}}^{(4)}$$

where

$$\begin{aligned}
\Lambda_{\Gamma_n^{(3)}}^{(1)} &= \{\rho_i \mid i \in P_{l(n)}\} \\
\Lambda_{\Gamma_n^{(3)}}^{(2)} &= \left\{ e_k^{(n)}(i) \mid i \in P_{l(n)}, k \in \{1, \dots, n\} \right\}
\end{aligned}$$

$$\Lambda_{\Gamma_n^{(3)}}^{(3)} = \left\{ \frac{n\delta_{mk}}{3} \sum_{j=1}^d \left( \left( (i)_j + \frac{1}{n} \right)^3 - (i)_j^3 \right) \mid i \in L_n, m, k \in \{1, \dots, \#L_n\} \right\}$$

$$\Lambda_{\Gamma_n^{(3)}}^{(4)} = \left\{ g(l^{\frac{1}{2d}}) \mid l = 0 \dots l(n) \right\}$$

and let

$$\Gamma_n^{(3)}(H) := \left\{ \lambda \in G_n^{\mathbb{C}} \mid \left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} \leq \frac{2}{n} \right\} \cup \Gamma_n^{(1)}(-\Delta)$$

with the convention that  $\left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} = 0$  when  $\lambda \in \sigma(H_n^{l(n)})$ . Note that  $\Lambda_{\Gamma_n^{(3)}}(H)$  is a finite set for each  $H \in \Omega_3$  and by Lemma 2.4 determining whether  $\left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} \leq \frac{2}{n}$  requires only finitely many algebraic operations on the matrix elements of  $H_n^{l(n)}$  (which are contained in  $\Lambda_{\Gamma_n^{(3)}}(H)$ ). Moreover, since  $\Lambda_3$  contains all matrix elements of the Laplacian, we conclude that computing  $\Gamma_n^{(1)}(-\Delta)$  can also be done by performing a finite amount of algebraic operations on the information provided. Overall, we conclude that each  $\Gamma_n^{(3)}$  is an arithmetic algorithm in the sense of Definition 1.2.

**Convergence.** It remains to prove that  $\Gamma_n^{(3)}(H) \rightarrow \sigma(H)$  in the Attouch-Wets metric. To this end, let  $\lambda \in G_n^{\mathbb{C}}$  and note that by the second resolvent identity we have

$$(H_n^{l(n)} - \lambda)^{-1} - (H_n - \lambda)^{-1} = (H_n^{l(n)} - \lambda)^{-1} (H_n - H_n^{l(n)}) (H_n - \lambda)^{-1}. \quad (4.6)$$

From (4.6) we conclude that

$$\left| \left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} - \left\| (H_n - \lambda)^{-1} \right\|^{-1} \right| \leq \|H_n - H_n^{l(n)}\|. \quad (4.7)$$

Indeed if  $\lambda \in \rho(H_n) \cap \rho(H_n^{l(n)})$ , this just follows by taking norms on both sides and using the reverse triangle inequality, while for  $\lambda \in \sigma(H_n) \cup \sigma(H_n^{l(n)})$  it can be seen by the following argument. W.l.o.g. assume that  $\lambda \in \sigma(H_n) \setminus \sigma(H_n^{l(n)})$ . Then  $\left\| (H_n - \lambda)^{-1} \right\|^{-1} = 0$  and  $\left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} > 0$ . Assume for contradiction that (4.7) is false, i.e.

$$\|H_n - H_n^{l(n)}\| < \left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1}.$$

Then by a standard Neumann series argument (cf. [Kat95, Sec. I.4.4]) it follows that  $H_n$  is boundedly invertible, which contradicts the assumption  $\lambda \in \sigma(H_n)$ . This argument is obviously symmetric in  $H_n$  and  $H_n^{l(n)}$ .

Going back to (4.7) and recalling our specific choice of  $l(n)$ , we conclude that for all  $\lambda \in G_n^{\mathbb{C}}$  one has

$$\begin{aligned} \left| \left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} - \left\| (H_n - \lambda)^{-1} \right\|^{-1} \right| &\leq \|H_n - H_n^{l(n)}\| \\ &\leq \frac{3d(M + g(0))(2\pi n^4)^{-\frac{d}{2}}}{l(n)^{\frac{1}{2}}} + ng(l(n)^{\frac{1}{2d}}) \\ &\leq \frac{1}{2n}, \end{aligned}$$

Now, if  $\lambda \in \Gamma_n^{(3)}(H)$  the above inequality implies that

$$\begin{aligned} \left\| (H_n - \lambda)^{-1} \right\|^{-1} &\leq \left\| (H_n^{l(n)} - \lambda)^{-1} \right\|^{-1} + \frac{1}{2n} \\ &\leq \frac{2}{n} + \frac{1}{2n} \end{aligned}$$

$$\leq \frac{3}{n}$$

and hence  $\lambda \in \Xi_n(H)$  (cf. Remark 3.7). Similarly, if  $\lambda \in \Gamma_n^{(2)}(H)$  then

$$\begin{aligned} \|(H_n^{l(n)} - \lambda)^{-1}\|^{-1} &\leq \|(H_n - \lambda)^{-1}\|^{-1} + \frac{1}{n} \\ &\leq \frac{1}{n} + \frac{1}{2n} \\ &\leq \frac{2}{n} \end{aligned}$$

and hence  $\lambda \in \Gamma_n^{(3)}(H)$ . Thus, we have the inclusions

$$\Gamma_n^{(2)}(H) \subset \Gamma_n^{(3)}(H) \subset \Xi_n(H).$$

Since  $\Gamma_n^{(2)}(H) \rightarrow \sigma(H)$  and  $\Xi_n(H) \rightarrow \sigma(H)$  by Theorem 3.1 and Remark 3.7, we conclude that  $\Gamma_n^{(3)}(H) \rightarrow \sigma(H)$  as well. This completes the proof of Theorem 4.3.

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## References

- [BBL12] L. Boulton, N. Boussaid, and M. Lewin. Generalised Weyl theorems and spectral pollution in the Galerkin method. *J. Spectr. Theory*, 2(4):329–354, 2012.
- [BHNS15] J. Ben-Artzi, A. C. Hansen, O. Nevanlinna, and M. Seidel. Can everything be computed? - On the solvability complexity index and towers of algorithms. *CoRR*, abs/1508.03280, 2015.
- [BMT19] S. Bögli, M. Marletta, and C. Tretter. The essential numerical range for unbounded operators. *arXiv preprint*, 1907.09599, 2019.
- [Bög17] S. Bögli. Convergence of sequences of linear operators and their spectra. *Integral Equations Operator Theory*, 88(4):559–599, 2017.
- [Bög18] S. Bögli. Local convergence of spectra and pseudospectra. *J. Spectr. Theory*, 8(3):1051–1098, 2018.
- [BS14] S. Bögli and P. Siegl. Remarks on the convergence of pseudospectra. *Integral Equations Operator Theory*, 80(3):303–321, 2014.
- [DM89] P. Doyle and C. McMullen. Solving the quintic by iteration. *Acta Math.*, 163(3-4):151–180, 1989.
- [EE87] D. E. Edmunds and W. D. Evans. *Spectral Theory and Differential Operators (Oxford Mathematical Monographs)*. Oxford University Press, 1987.
- [Han11] A. C. Hansen. On the solvability complexity index, the  $n$ -pseudospectrum and approximations of spectra of operators. *J. Amer. Math. Soc.*, 24(1):81–124, 2011.
- [Kat95] T. Kato. *Perturbation Theory for Linear Operators (Classics in Mathematics)*. Springer, reprint of the corr. 2nd edition, 1995.

- [RS80] M. Reed and B. Simon. *Methods of Modern Mathematical Physics I: Functional Analysis*. Academic Press, Inc., 1980.
- [SW68] J. G. Stampfli and J. P. Williams. Growth conditions and the numerical range in a Banach algebra. *Tôhoku Math. J. (2)*, 20:417–424, 1968.
- [Wei00] J. Weidmann. *Lineare Operatoren in Hilberträumen. Teil 1*. Mathematische Leitfäden. [Mathematical Textbooks]. B. G. Teubner, Stuttgart, 2000. Grundlagen. [Foundations].