On the approximation of spectra of linear operators on Hilbert spaces

Anders C. Hansen

DAMTP, University of Cambridge
email: A.Hansen@damtp.cam.ac.uk

Abstract

We present several new techniques for approximating spectra of linear operators (not necessarily bounded) on an infinite dimensional, separable Hilbert space. Our approach is to take well known techniques from finite dimensional matrix analysis and show how they can be generalized to an infinite dimensional setting to provide approximations of spectra of elements in a large class of operators. We conclude by proposing a solution to the general problem of approximating the spectrum of an arbitrary bounded operator by introducing the n-pseudospectrum and argue how that can be used as an approximation to the spectrum.

1 Introduction

This paper follows up on the ideas initiated by Arveson in [Arv94a] and [Arv91], [Arv93b], [Arv93a], [Arv94b] on how to approximate spectra of linear operators on separable Hilbert spaces. This fundamental question in operator theory goes back to Szegö [Sze20] and has received some attention throughout the history [Kat49], [Aro51], [Rid67], [Kau93], [DVV94], [Pok95], [Béd97], [Sha00], [BCN01]. The question is fundamental in the sense that our understanding of most physical phenomena in quantum mechanics, both relativistic and non-relativistic, depends on the understanding of the spectra of linear operators. However, to get a complete understanding of such physical phenomena we not only need mathematical descriptions of the behavior of spectra of linear operators, we also need a mathematical theory on how to find explicit approximations to such spectra. It is a completely open question how to compute the spectrum of an arbitrary linear operator as pointed out in [Arv94b]: "Unfortunately, there is a dearth of literature on this basic problem, and so far as we have been able to tell, there are no proven techniques." Since this observation was made, there have been new developments in the self-adjoint case [Dav00], but for the general non-self-adjoint case techniques for approximating spectra are not known. It has been questioned in [Dav05] whether or not it is possible at all to determine spectra of arbitrary non-normal operators (a suggestion to the solution to that problem is discussed in section 8). The lack of mathematical techniques for approximating spectra presents therefore a serious limitation of our possible understanding of quantum systems since non-self-adjoint operators are ubiquitous in quantum mechanics [HN96], [HN97].

We will in this article present explicit techniques on how to approximate the spectrum of different classes of linear operators on a separable Hilbert space. Throughout the article $\mathcal{H}$ will always denote a separable Hilbert space, and $\mathcal{B}(\mathcal{H})$ will be the set of bounded linear operators on $\mathcal{H}$. Also, $\mathcal{C}(\mathcal{H})$ denotes the set of densely defined, closed linear operators on $\mathcal{H}$. If $T \in \mathcal{C}(\mathcal{H})$ the domain of T will be denoted by $\mathcal{D}(T)$, and if $z \notin \sigma(T)$ then $R(z,T) = (T-z)^{-1}$. Also, $\sigma(T)$ and $\sigma_e(T)$ denotes the spectrum and the essential spectrum of T respectively.

2 Quasidiagonality and the Finite-Section Method

The finite-section method for approximating the spectrum of bounded self-adjoint operators on Hilbert spaces is a well-known technique and has been studied in several articles and monographs [Arv94a], [Bro07], [BS99], [HRS01]. The approach is to first find a sequence of finite rank projections $\{P_n\}$ such that $P_{n+1} \geq P_n$ and $P_n \to I$ strongly, and then use known techniques to find the spectrum of the compression $A_n = P_nAP_n$.

The most obvious approach is to use some orthonormal basis $\{e_n\}$ for the Hilbert space $\mathcal{H}$ and then let P_n be the projection onto $\mathrm{sp}\{e_1, \dots e_n\}$. Given a self-adjoint $A \in \mathcal{B}(\mathcal{H})$ and $\{e_n\}$ we may consider the associate infinite matrix (a_{ij})

$$a_{ij} = \langle Ae_j, e_i \rangle, \quad i,j = 1,2,\dots.$$

In this case the compression becomes $A_n \in \mathcal{B}(\mathcal{H}_n)$, where $\mathcal{H}_n = P_n\mathcal{H}$, $A_n = P_nA\lceil_{\mathcal{H}_n}$, where the matrix with respect to $\{e_1, \dots, e_n\}$ is

$$A_n = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}.$$

The operator-theoretical question is to analyze how the spectrum $\sigma(P_nA\lceil_{P_n\mathcal{H}})$ evolves as $n \to \infty$.

Definition 2.1. *Given a sequence $\{A_n\} \subset \mathcal{B}(\mathcal{H})$, define*

$$\Lambda = \{\lambda \in \mathbb{R} : \exists \lambda_n \in \sigma(A_n), \lambda_n \to \lambda\}.$$

Also, for every set S of real numbers let $N_n(S)$ (and $\tilde{N}_n(S)$) denote the number of eigenvalues counting multiplicity (and not counting multiplicity respectively) of A_n which belong to S.

Definition 2.2. *(i) A point $\lambda \in \mathbb{R}$ is called essential if, for every open set $U \subset \mathbb{R}$ containing λ, we have*

$$\lim_{n\to\infty} N_n(U) = \infty.$$

The set of essential points is denoted Λ_e

(ii) $\lambda \in \mathbb{R}$ is called transient if there is an open set $U \subset \mathbb{R}$ containing λ such that

$$\sup_{n\geq 1} N_n(U) < \infty.$$

Theorem 2.3. *(Arveson)[Arv94a] Let $A \in \mathcal{B}(\mathcal{H})$ and let $\{P_n\}$ be a sequence of projections converging strongly to the identity such that $P_{n+1} \geq P_n$. Define $A_n = P_nA\lceil_{P_n\mathcal{H}}$ and let Λ and Λ_e be as in definitions 2.1 and 2.2. Then $\sigma(A) \subset \Lambda$ and $\sigma_e(A) \subset \Lambda_e$.*

Definition 2.4. *(i) A filtration of $\mathcal{H}$ is a sequence $\mathcal{F} = \{\mathcal{H}_1, \mathcal{H}_2, \dots\}$ of finite dimensional subspaces of $\mathcal{H}$ such that $\mathcal{H}_n \subset \mathcal{H}_{n+1}$ and*

$$\overline{\bigcup_{n=1}^{\infty} \mathcal{H}_n} = \mathcal{H}$$

(ii) Let $\mathcal{F} = \{\mathcal{H}_n\}$ be a filtration of $\mathcal{H}$ and let P_n be the projection onto $\mathcal{H}_n$. The degree of an operator $A \in \mathcal{B}(\mathcal{H})$ is defined by

$$deg(A) = \sup_{n \geq 1} \operatorname{rank}(P_n A - A P_n).$$

Arveson gave in [Arv94a], [Arv94b] a complete theory of the finite-section method applied to operators of finite degree, which is an abstraction of band-limited infinite matrices. We will not discuss that theory here, but refer the reader to the original articles. We will however present the following theorem, which is a special case of Theorem 3.8 in [Arv94a], to give the reader an impression of what one can expect to get when using the finite-section method.

Theorem 2.5. *(Arveson)[Arv94a] Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint and*

$$\mathcal{F} = \{\mathcal{H}_1, \mathcal{H}_2, \dots\}$$

be a filtration with corresponding projections $\{P_n\}$. Define $A_n = P_n A\lceil_{P_n\mathcal{H}}$ and let Λ and Λ_e be as in definitions 2.1 and 2.2. Suppose that A has finite degree with respect to $\mathcal{F}$. Then

(i) $\sigma_e(A) = \Lambda_e$

(ii) Every point of Λ is either transient or essential.

In this section we will investigate how the finite section method can be applied to quasi-diagonal operators. First we recall some basic definitions as well as some well know results.

Definition 2.6. *An operator A on a separable Hilbert space is diagonal if there exists a complete orthonormal set of eigenvectors of A.*

Definition 2.7. *An operator A on a separable Hilbert space is quasi-diagonal if there exists an increasing sequence $\{P_n\}$ of finite rank projections such that $P_n\mathcal{H} \subset \mathcal{D}(A)$, $P_n \to I$, strongly, and $\|P_n A - A P_n\| \to 0$. The sequence $\{P_n\}$ is said to quasi-diagonalize A.*

Before the next definition we need to recall that an unbounded operator A is said to commute with the bounded operator T if

$$TA \subset AT.$$

This means that whenever $\xi \in \mathcal{D}(A)$, then $T\xi$ also belongs to $\mathcal{D}(A)$ and $AT\xi = TA\xi$.

Definition 2.8. *An operator A on a separable Hilbert space is said to be block diagonal with respect to an increasing sequence $\{P_n\}$ of finite-dimensional projections converging strongly to I if A commutes with $P_{n+1} - P_n$ for all n.*

Note that if A is self-adjoint and $P_n\mathcal{H} \subset \mathcal{D}(A)$ then Definition 2.8 is equivalent to each of the assertions

(i) P_n commutes with A for every n.

(ii) $AP_n\mathcal{H} \subset P_n\mathcal{H}$.

The following theorem assures us the existence of a vast set of quasi-diagonal operators.

Theorem 2.9. *(Weyl,von Neumann, Berg)[Ber71] Let A be a (not necessarily bounded) normal operator on the separable Hilbert space $\mathcal{H}$. Then for $\epsilon > 0$ there exist a diagonal operator D and a compact operator C such that $\|C\| < \epsilon$ and $A = D + C$.*

Corollary 2.10. *Every normal operator is quasi-diagonal.*

Definition 2.11. *(i) For a set $\Sigma \subset \mathbb{C}$ and $\delta > 0$ we will let $\Gamma_\delta(\Sigma)$ denote the δ-neighborhood of Σ (i.e. the union of all δ-balls centered at points of Σ).*

(ii) Given two sets $\Sigma, \Lambda \subset \mathbb{C}$ we say that Σ is δ-contained in Λ if $\Sigma \subset \Gamma_\delta(\Lambda)$.

(iii) Given two compact sets $\Sigma, \Lambda \subset \mathbb{C}$ their Hausdorff distance is

$$d_H(\Sigma, \Lambda) = \max\{\sup_{\lambda \in \Lambda} d(\lambda, \Lambda), \sup_{\lambda \in \Sigma} d(\lambda, \Sigma)\}$$

where $d(\lambda, \Lambda) = \inf_{\rho \in \Lambda} |\rho - \lambda|$.

We will need a couple of basic lemmas.

Lemma 2.12. *(Davies, Plum)[DP04] Let $A \in \mathcal{B}(\mathcal{H})$, P be a projection and $\epsilon > 0$ such that $\|PAP - AP\| \leq \epsilon$. If $\lambda \in \sigma(PAP)$ then $(\lambda - \epsilon, \lambda + \epsilon) \cap \sigma(A) \neq \emptyset$.*

Lemma 2.13. *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint and compact. Let $\{P_n\}$ be a sequence of finite-dimensional projections such that $P_n \to I$ strongly. Then $P_nAP_n \to A$ in norm.*

Proof. Since $P_n^\perp = I - P_n$ is a sequence of projections tending strongly to zero, $\|AP_n^\perp\| \to 0$. Since $P_n^\perp A$ is the adjoint of $AP_n^\perp$, its norm tends to zero as well, so that

$$\|A - P_nAP_n\| = \|P_n^\perp A + P_nAP_n^\perp\| \leq \|P_n^\perp A\| + \|AP_n^\perp\| \longrightarrow 0, \qquad n \to \infty.$$

□

Lemma 2.14. *Let A be a self-adjoint (not necessarily bounded) operator on a separable Hillbert space $\mathcal{H}$ with domain $\mathcal{D}(A)$ and a quasidiagonalizing sequence $\{P_n\}$. Then $A = D + C$ where D is self-adjoint with domain $\mathcal{D}(D) = \mathcal{D}(A)$ and block diagonal with respect to some subsequence $\{P_{n_k}\}$. Also, C is compact and self-adjoint.*

Proof. To see this we can extend Halmos' proof in [Hal70] to unbounded operators. Now, by possibly passing to a subsequence, we may assume that $\sum_n \|P_nA - AP_n\| < \infty$. The fact that $P_n \geq P_{n-1}$ assures us that $P_n - P_{n-1}$ is a projection. Thus, we may decompose $\mathcal{H} = \bigoplus_{n=1}^\infty (P_{n+1} - P_n)\mathcal{H}$ and define D on

$$\mathcal{D}(D) = \mathrm{sp}\{\xi \in \mathcal{H} : \xi \in (P_{n+1} - P_n)\mathcal{H}\}$$

in the following way. If $\xi \in (P_{n+1} - P_n)\mathcal{H}$ then $D\xi = (P_{n+1} - P_n)A(P_{n+1} - P_n)\xi$. Now D is densely defined, with $\mathcal{D}(D) \subset \mathcal{D}(A)$, and obviously (by definition) block diagonal with respect to $\{P_n\}$. Define the operator C on $\mathcal{D}(C) = \mathcal{D}(D)$ by $C = A - D$. We will show that C is compact on $\mathcal{H}$. Indeed, by letting

$$C_n = P_{n+1}(AP_n - P_nA)P_n - P_n(AP_n - P_nA)P_{n+1}$$

we can form the operator $\tilde{C} = \sum_n C_n$ since $\|C_n\| \leq 2\|AP_n - P_nA\|$ and $\sum_n \|P_nA - AP_n\| < \infty$, hence the previous sum is norm convergent. Also, since C_n is finite dimensional and therefore compact it follows that $\tilde{C}$ is compact. A straightforward calculation shows that $\tilde{C} = C$ on $\mathcal{D}(C)$ which is dense, thus we can extend C to $\tilde{C}$ on $\mathcal{H}$. It is easy to see that C_n is self-adjoint since A is self-adjoint and hence C is self-adjoint. Let $\tilde{D} = A - C$. Then $\mathcal{D}(\tilde{D}) = \mathcal{D}(A)$ and $\tilde{D}$ is a self-adjoint extension of D. Also, since $\tilde{D}$ is an extension of D (which is block diagonal with respect to $\{P_n\}$) it follows that D is block diagonal with respect to $\{P_n\}$. □

Theorem 2.15. *Let A be a self-adjoint operator (not necessary bounded) on the separable Hilbert space $\mathcal{H}$ and let $\{P_n\}$ be a sequence of projections that quasi-diagonalizes A. If $K \subset \mathbb{R}$ is a compact set such that $\sigma(A) \cap K \neq \emptyset$, then*

$$\sigma(P_nA\lceil_{P_n\mathcal{H}}) \cap K \longrightarrow \sigma(A) \cap K, \quad n \to \infty$$

in the Hausdorff distance.

Proof. To prove the assertion we need to establish the following; given $\delta > 0$ then

$$\sigma(P_nA\lceil_{P_n\mathcal{H}}) \cap K \subset \Gamma_\delta(\sigma(A) \cap K)$$

and

$$\Gamma_\delta(\sigma(P_nA\lceil_{P_n\mathcal{H}}) \cap K) \supset \sigma(A) \cap K$$

for all sufficiently large n. The second inclusion follows by Theorem VIII.24 ([RS72], p. 290) if we can show that $P_nAP_n \to A$ in the strong resolvent sense. By Theorem VIII.25 ([RS72], p. 292) it suffices to show that $P_nAP_n\xi \to A\xi$ for $\xi \in \mathcal{D}(A)$, which is a common core for $\{P_nAP_n\}$ and A, and this is easily seen.

To see the first inclusion note that it will follow if we can show that

$$\sigma(P_{n_k}A\lceil_{P_{n_k}\mathcal{H}}) \cap K \subset \Gamma_{\delta/2}(\sigma(A) \cap K) \tag{2.1}$$

when k is large, for some subsequence $\{P_{n_k}\}$. Indeed, if that is the case we only need to show that

$$\sigma(P_mA\lceil_{P_m\mathcal{H}}) \subset \Gamma_{\delta/2}(\sigma(P_{n_k}A\lceil_{P_{n_k}\mathcal{H}}))$$

for large m and n_k where $m \leq n_k$. Now this is indeed the case because we may assume, by appealing to Lemma 2.14 and possibly passing to another subsequence, that A is block diagonal with respect to $\{P_{n_k}\}$. Thus,

$$\|P_mP_{n_k}AP_{n_k}P_m - P_{n_k}AP_{n_k}P_m\| = \|P_mAP_m - AP_m\| \longrightarrow 0, \quad m \to \infty,$$

by assumption, and hence the desired inclusion follows by appealing to Lemma 2.12.

Now we return to the task of showing (2.1). Note that by the spectral mapping theorem, the spectra $\sigma(P_nA\lceil_{P_n\mathcal{H}})$ and $\sigma(A)$ are the images of $\sigma((P_n(A+i)\lceil_{P_n\mathcal{H}})^{-1})$ and $\sigma((A+i)^{-1})$, respectively, under the mapping $f(x) = 1/x - i$. Note that

$$f^{-1}(\sigma(P_nA\lceil_{P_n\mathcal{H}}) \cap K), \quad f^{-1}(\overline{\Gamma_\delta((\sigma(A) \cap K))})$$

are both compact and neither contain zero. Thus, by the continuity of f on $\mathbb{C} \setminus \{0\}$ and again the spectral mapping theorem, the assertion follows if we can prove that

$$\sigma((P_n(A+i)\lceil_{P_n\mathcal{H}})^{-1}) \subset \Gamma_\delta(\sigma((A+i)^{-1})) \tag{2.2}$$

for arbitrary $\delta > 0$ and large n. By Lemma 2.14 we have that $A = D + C$ where D is self-adjoint and block diagonal with respect to some subsequence $\{P_{n_k}\}$ and C is compact and self-adjoint. To simplify the notation we use the initial indexes for the subsequence. We first observe that

$$(D + P_nCP_n + i)^{-1} \to (D + C + i)^{-1} \tag{2.3}$$

in norm. Indeed, an easy manipulation gives us

$$\begin{aligned}\|(D+&C + i)^{-1} - (D + P_nCP_n + i)^{-1}\| \\ &\leq \|(D + C + i)^{-1}\|\|C - P_nCP_n\|\|(D + P_nCP_n + i)^{-1}\|,\end{aligned}$$

where $\|(D + P_nCP_n + i)^{-1}\|$ is bounded by the spectral mapping theorem since $C - P_nCP_n$ is self-adjoint. Since, by Theorem 2.13, $\|C - P_nCP_n\| \to 0$ (2.3) follows. The normality of $(D + C + i)^{-1}$ and $(D + P_nCP_n + i)^{-1}$ assures us that for any $\delta > 0$ we have

$$\sigma((D + P_nCP_n + i)^{-1}) \subset \Gamma_\delta(\sigma((D + C + i)^{-1}))$$

for sufficiently large n. Hence, to finish the proof we have to show that

$$\sigma((P_n(A + i)\lceil_{P_n\mathcal{H}})^{-1}) \subset \sigma((D + P_nCP_n + i)^{-1}).$$

In fact we have

$$\sigma((D + P_nCP_n + i)^{-1}) = \sigma((P_n(A + i)\lceil_{P_n\mathcal{H}})^{-1}) \cup \sigma(((D + i)\lceil_{P_n^\perp\mathcal{H}})^{-1}).$$

Indeed,

$$(D + P_nCP_n + i) = ((D + P_nCP_n + i)\lceil_{P_n\mathcal{H}}) \oplus (D + i)\lceil_{P_n^\perp\mathcal{H}}.$$

So

$$\begin{aligned}(D + P_nCP_n + i)^{-1} &= ((D + P_nCP_n + i)\lceil_{P_n\mathcal{H}})^{-1} \oplus ((D + i)\lceil_{P_n^\perp\mathcal{H}})^{-1} \\ &= (P_n(A + i)\lceil_{P_n\mathcal{H}})^{-1} \oplus ((D + i)\lceil_{P_n^\perp\mathcal{H}})^{-1},\end{aligned}$$

implying the assertion. □

As for the convergence of eigenvectors of the finite-section method, very little has been investigated, however we have the following:

Proposition 2.16. *Let $\{A_n\}$ be a sequence of self-adjoint bounded operators on $\mathcal{H}$ such that $A_n \to A$ strongly. Then if $\{\lambda_n\}$ is a sequence of eigenvalues of A_n such that $\lambda_n \to \lambda \in \sigma(A)$, and if $\{\xi_n\}$ is a sequence of unit eigenvectors corresponding to $\{\lambda_n\}$, such that $\{\xi_n\}$ does not converge weakly to zero, then there is a subsequence $\{\xi_{n_k}\}$ such that $\xi_{n_k} \xrightarrow{w} \xi$ where $A\xi = \lambda\xi$*

Proof. Since $\{\xi_n\}$ does not converge weakly to zero and by weak compactness of the unit ball in $\mathcal{H}$ we can find a weakly convergent subsequence such that $\xi_{n_k} \xrightarrow{w} \xi \neq 0$. To see that $A\xi = \lambda\xi$ we observe that this will follow if we can show that $\lambda_{n_k}\xi \xrightarrow{w} A\xi$. But the latter follows easily if we can show that $\lambda_{n_k}\xi_{n_k} - \lambda_{n_k}\xi \xrightarrow{w} 0$, $A_{n_k}\xi - A\xi \xrightarrow{w} 0$ and $A_{n_k}\xi - A_{n_k}\xi_{n_k} \xrightarrow{w} 0$. The first two are obvious and the last follows from the fact that for $\eta \in \mathcal{H}$ we have

$$\begin{aligned}\langle A_{n_k}(\xi - \xi_{n_k}), \eta\rangle &= \langle \xi - \xi_{n_k}, A_{n_k}\eta\rangle \\ &= \langle \xi - \xi_{n_k}, A\eta\rangle + \langle \xi - \xi_{n_k}, (A_{n_k} - A)\eta\rangle \longrightarrow 0,\end{aligned}$$

as $k \to \infty$. □

3 Divide and conquer

The divide-and-conquer technique has its origin in finite-dimensional matrix analysis. The idea was originally to divide the problem into smaller problems for simplicity reasons, a concept we will not discuss here. Since the crucial assumption for the procedure is that the operator acts on a finite dimensional space, we can not use it directly and we will not discuss its details here, but refer the reader to [Cup81]. However, one can use the concept of the method to improve the results of Theorem 2.5 for tridiagonal infinite matrices. How to reduce the original spectral problem to a spectral problem for tridiagonal operators is discussed in section 5.

Definition 3.1. *Let $A \in \mathcal{B}(\mathcal{H})$ and $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. A is said to be tridiagonal with respect to $\{e_j\}$ if $\langle Ae_j, e_i\rangle = 0$ for $|i-j| \geq 2$.*

Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint and $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. Suppose that A is tridiagonal with respect to $\{e_j\}$ and suppose that $a_{ij} = \langle Ae_j, e_i\rangle$ for $i, j = 1, 2, \ldots$ is real. It is easy to see that this is no restriction. Let P_n be the projection onto $\mathrm{sp}\{e_1, \ldots, e_n\}$. In the finite-section method one decomposes A into

$$A = P_nAP_n \oplus P_n^{\perp}AP_n^{\perp} + T, \qquad T \in \mathcal{B}(\mathcal{H}),$$

and then computes the spectrum of P_nAP_n. The idea of the divide-and-conquer approach is to decompose A into

$$A = A_{1,n} \oplus A_{2,n} + \beta\eta \otimes \eta, \qquad \eta \in \mathcal{H},$$

where $A_{1,n} \in \mathcal{B}(P_n\mathcal{H})$, $A_{2,n} \in \mathcal{B}(P_n^{\perp}\mathcal{H})$, $\eta = e_n + e_{n+1}$ and then compute $\sigma(A_{1,n})$. It is easy to see that the divide and conquer technique is very close to the finite-section method i.e. we have $\langle P_nAP_ne_j, e_i\rangle = \langle A_{1,n}e_j, e_i\rangle$ for all i, j except for $i = j = n$. The goal is to improve the results in Theorem 2.5.

In finite dimensions one has the following theorem [Cup81] which gave us the idea to a more general theorem in infinite dimensions.

Theorem 3.2. *(Cuppen) Let D be a diagonal (real) matrix,*

$$D = diag(d_1, \ldots, d_n)$$

where $n \geq 2$ and $d_1 < d_2 < \ldots < d_n$. Let $\eta \in \mathbb{R}^n$ with $\eta_i \neq 0$ for $i = 1, \ldots, n$ and $\beta > 0$ be a scalar. Then the eigenvalues $\{\lambda_1, \ldots, \lambda_n\}$ of the matrix $D + \beta\eta \otimes \eta$ satisfy

$$d_1 < \lambda_1 < d_2 < \lambda_2 < \ldots < d_n < \lambda_n < d_n + \beta\|\eta\|^2.$$

Some of the techniques in the proof of the next theorem are inspired by the proof of Theorem 3.2 which can be found in [Cup81]. Before we can state and prove the main theorem we need to introduce the concept of Householder reflections in an infinite-dimensional setting.

Definition 3.3. *A Householder reflection is an operator $S \in \mathcal{B}(\mathcal{H})$ of the form*

$$S = I - \frac{2}{\|\xi\|^2}\xi \otimes \bar{\xi}, \qquad \xi \in \mathcal{H}.$$

In the case where $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ and I_i is the identity on $\mathcal{H}_i$ then

$$U = I_1 \oplus \left(I_2 - \frac{2}{\|\xi\|^2}\xi \otimes \bar{\xi}\right) \qquad \xi \in \mathcal{H}_2.$$

will be called a Householder transformation.

A straightforward calculation shows that $S^* = S^{-1} = S$ and thus also $U^* = U^{-1} = U$. An important property of the operator S is that if $\{e_j\}$ is an orthonormal basis for $\mathcal{H}$ and $\eta \in \mathcal{H}$ then one can choose $\xi \in \mathcal{H}$ such that

$$\langle S\eta, e_j\rangle = \langle (I - \frac{2}{\|\xi\|^2}\xi \otimes \bar{\xi})\eta, e_j\rangle = 0, \qquad j \neq 1.$$

Indeed, if $\eta_1 = \langle \eta, e_1\rangle \neq 0$ one may choose $\xi = \eta \pm \|\eta\|\zeta$, where $\zeta = \eta_1/|\eta_1|e_1$ and if if $\eta_1 = 0$ choose $\xi = \eta \pm \|\eta\|e_1$, The verification of the assertion is a straightforward calculation.

Theorem 3.4. *Let $A_{1,n}$ be defined as above and let $\{d_j\}_{j=1}^k = \sigma(A_{1,n})$ be arranged such that $d_j < d_{j+1}$.*

(i) If $d_l, d_{l+1} \notin \sigma(A)$, for some $l < k$, then there is a $\lambda \in \sigma(A)$ such that $d_l < \lambda < d_{l+1}$.

(ii) If $d_j \in \sigma(A_{1,n})$ has multiplicity $m \geq 2$ then $d_j \in \sigma(A)$ and d_j is an eigenvalue. Also, $m_{A_{1,n}}(d_j) \leq m_A(d_j) + 1$, where $m_{A_{1,n}}(d_j)$ and $m_A(d_j)$ denote the multiplicity of d_j as an element of $\sigma(A_{1,n})$ and $\sigma(A)$ respectively.

Proof. We will start with (i). Suppose that $d_l, d_{l+1} \notin \sigma(A)$. We will show that $\sigma(A) \cap (d_l, d_{l+1}) \neq \emptyset$. We argue as follows. Let $\epsilon > 0$, $I_a = (-a, a]$ be an interval containing $\sigma(A_{2,n})$ and let g be a step function on I_a of the form $g = \sum_{j=1}^m \chi_{(a_j,b_j]}$ such that $\sup_{x\in I_a} |x - g(x)| < \epsilon$. Let $\tilde{A}_{2,n} = g(A_{2,n})$. Then $\sigma(\tilde{A}_{2,n})$ contains only isolated eigenvalues and $\|\tilde{A}_{2,n} - A_{2,n}\| < \epsilon$. Also, let

$$\tilde{A} = A_{1,n} \oplus \tilde{A}_{2,n} + \beta\eta \otimes \eta.$$

Then $\tilde{A}$ is self-adjoint and $\|\tilde{A} - A\| < \epsilon$ so

$$d_H(\sigma(\tilde{A}), \sigma(A)) < \epsilon$$

where d_H denotes the Hausdorff metric. Also, by choosing ϵ small enough we have $d_l, d_{l+1} \notin \sigma(\tilde{A})$. Note that, since ϵ is arbitrary and $\sigma(A)$ is closed, the assertion that $\sigma(A) \cap (d_l, d_{l+1}) \neq \emptyset$ will follow if we can show that $\sigma(\tilde{A}) \cap (d_l, d_{l+1}) \neq \emptyset$.

Let P_n be the projection onto $\mathrm{sp}\{e_j\}_{j=1}^n$. Now, choose a unitary operator Q_1 on $P_n\mathcal{H}$ such that $Q_1 A_{1,n} Q^* = D_1$ where D_1 is diagonal with respect to $\{e_j\}_{j=1}^n$. Since $\sigma(\tilde{A}_{2,n})$ contains only finitely many eigenvalues we may choose a unitary Q_2 on $\mathrm{ran}P_n^{\perp}$ such that $Q_2\tilde{A}_{2,n}Q_2^* = D_2$ is diagonal with respect to $\{e_j\}_{j=n+1}^{\infty}$. Thus,

$$(Q_1 \oplus Q_2)(A_{1,n} \oplus \tilde{A}_{2,n} + \beta\eta \otimes \eta)(Q_1^* \oplus Q_2^*) = D_1 \oplus D_2 + \beta\xi \otimes \bar{\xi},$$

where a straightforward calculation shows that $\xi = Q_1 e_n \oplus Q_2 e_{n+1}$. Let $D = D_1 \oplus D_2$.

Claim1: *There exists a unitary operator U and an integer N such that*

$$\langle U\xi, e_i\rangle = 0$$

for $i \geq N + 1$ and $\langle U\xi, e_i\rangle \neq 0$ for $i \leq N$, and also that UDU^* is diagonal with respect to $\{e_j\}$. Note that the claim will follow if we can show that there is a unitary operator V such that $\langle V\xi, e_j\rangle \neq 0$ only for finitely many js and that $VDV^* = D$. Indeed, if we have such a V then we can find a unitary operator $\tilde{V}$ that permutes $\{e_j\}$ such that $U = \tilde{V}V$ is the desired unitary operator mentioned above.

To construct V we first note that, since D is diagonal with respect to $\{e_j\}$, the spectral projections $\chi_\lambda(D)$, $\lambda \in \sigma(D)$ are also diagonal with respect to $\{e_j\}$. Note that

$$D = \bigoplus_{\lambda \in \sigma(D)} \lambda \chi_\lambda(D).$$

We will use this decomposition to construct V. Let

$$i_\lambda = \inf\{j : \chi_\lambda(D)e_j \neq 0\}.$$

If $\chi_\lambda(D)\xi = 0$ let $V_\lambda = I$ on $\chi_\lambda(D)\mathcal{H}$. If not, choose a Householder reflection on $\chi_\lambda(D)\mathcal{H}$,

$$S = I - \frac{2}{\|\zeta\|^2}\zeta \otimes \bar{\zeta}, \qquad \zeta \in \chi_\lambda(D)\mathcal{H},$$

such that

$$\langle S\chi_\lambda(D)\xi, e_{i_\lambda}\rangle \neq 0 \quad \text{and} \quad \langle S\chi_\lambda(D)\xi, e_i\rangle = 0, \quad i \geq i_\lambda + 1. \tag{3.1}$$

Let $V_\lambda = S$. The fact that $\chi_\lambda(D)$ for $\lambda \in \sigma(D)$ is diagonal with respect to $\{e_j\}$ gives $V_\lambda \chi_\lambda(D) V_\lambda^* = \chi_\lambda(D)$. Letting

$$V = \bigoplus_{\lambda \in \sigma(D)} V_\lambda \tag{3.2}$$

we get $VDV^* = D$ and thus we have constructed the desired unitary operator V whose existence we asserted. As argued above, this yields existence of the unitary operator U asserted in Claim1. Let $N = \max\{j : \langle U\xi, e_j\rangle \neq 0\}$, let P_N be the projection onto $\mathrm{sp}\{e_j\}_{j=1}^N$ and $\tilde{D} = UDU^*$.

Claim2: *If $\lambda \in \sigma(P_N\tilde{D}\lceil_{P_N\mathcal{H}})$ then λ has multiplicity one.* We argue by contradiction. Suppose that $\lambda \in \sigma(P_N\tilde{D}\lceil_{P_N\mathcal{H}})$ has multiplicity greater than one. Then $\langle \tilde{D}e_p, e_p\rangle = \langle \tilde{D}e_q, e_q\rangle = \lambda$ for some $p, q \leq N$. Also, $\langle U\xi, e_p\rangle \neq 0$ and $\langle U\xi, e_q\rangle \neq 0$. Thus, it follows from the construction of U that $\langle De_{\tilde{p}}, e_{\tilde{p}}\rangle = \langle De_{\tilde{q}}, e_{\tilde{q}}\rangle = \lambda$ for some integers $\tilde{p}$ and $\tilde{q}$, and hence $e_{\tilde{p}}, e_{\tilde{q}} \in \mathrm{ran}\chi_\lambda(D)$. Also $\langle V\xi, e_{\tilde{p}}\rangle \neq 0$ and $\langle V\xi, e_{\tilde{q}}\rangle \neq 0$ and thus it follows that

$$\langle V_\lambda \chi_\lambda(D)\xi, e_j\rangle = \langle \bigoplus_{\lambda \in \sigma(D)} V_\lambda \xi, e_j\rangle \neq 0, \qquad j = \tilde{p}, \tilde{q},$$

and this contradicts (3.1). Armed with the results from Claim1 and Claim2 we can now continue with the proof.

Let $\zeta = U\xi$. We then have

$$U(D + \beta\xi \otimes \bar{\xi})U^* = (P_N\tilde{D}P_N + \beta P_N\zeta \otimes \overline{P_N\zeta})\lceil_{P_N\mathcal{H}} \oplus P_N^\perp \tilde{D}\lceil_{P_N^\perp\mathcal{H}},$$

since $P_N^\perp(\zeta \otimes \bar{\zeta}) = (\zeta \otimes \bar{\zeta})P_N^\perp = 0$. So, with a slight abuse of notation we will denote $P_N\zeta$ just by ζ. Note that

$$\sigma(\tilde{A}) = \sigma((P_N\tilde{D}P_N + \beta\zeta \otimes \bar{\zeta})\lceil_{P_N\mathcal{H}}) \cup \sigma(P_N^\perp \tilde{D}\lceil_{P_N^\perp\mathcal{H}}) \tag{3.3}$$

and hence our primary goal to prove that $\sigma(\tilde{A}) \cap (d_l, d_{l+1}) \neq \emptyset$ has been reduced to showing that

$$\sigma((P_N\tilde{D}P_N + \beta\zeta \otimes \bar{\zeta})\lceil_{P_N^\perp\mathcal{H}}) \cap (d_l, d_{l+1}) \neq \emptyset. \tag{3.4}$$

Before continuing with that task note that

$$d_l, d_{l+1} \in \sigma(P_N \tilde{D}\lceil_{P_N\mathcal{H}}). \tag{3.5}$$

Indeed, it is true, by the construction of $\tilde{D}$, that $d_l, d_{l+1} \in \sigma(\tilde{D})$. But by (3.3) it follows that $\sigma(P_N^{\perp}\tilde{D}P_N^{\perp}) \subset \sigma(\tilde{A})$ and since $d_l, d_{l+1} \notin \sigma(\tilde{A})$ the assertion follows. This observation will be useful later in the proof.

Now returning to the task of showing (3.4), let $\hat{D} = P_N\tilde{D}\lceil_{P_N\mathcal{H}}$ and then let λ be an eigenvalue of $\hat{D} + \beta\zeta \otimes \bar{\zeta}$ with corresponding nonzero eigenvector η. Here $\zeta \otimes \bar{\zeta}$ denotes, with a slight abuse of notation, the operator $(\zeta \otimes \bar{\zeta})\lceil_{P_N\mathcal{H}}$. Then we have

$$(\hat{D} + \beta\zeta \otimes \bar{\zeta})\eta = \lambda\eta \quad \text{so} \quad (\hat{D} - \lambda I)\eta = -\beta\langle\eta, \zeta\rangle\zeta. \tag{3.6}$$

Note that $\hat{D} - \lambda I$ is nonsingular. Indeed, had it been singular, we would have had $\lambda = \hat{d}_i$ for some $i \leq N$, where $\{\hat{d}_j\}_{j=1}^N = \sigma(\hat{D})$. Hence, by (3.6), we have

$$\langle(\hat{D} - \lambda I)\eta, e_i\rangle = -\beta\langle\eta, \zeta\rangle\langle\zeta, e_i\rangle = 0.$$

But, since $\zeta = U\xi$ and by Claim1, it is true that $\langle\zeta, e_i\rangle \neq 0$, so $\langle\eta, \zeta\rangle = 0$. Thus, by (3.6), it follows that $(\hat{D} - \lambda I)\eta = 0$, so $\langle(\hat{D} - \lambda)\eta, e_j\rangle = 0$ for $j \leq N$. Note that, by Claim2, $\sigma(\hat{D})$ contains only eigenvalues with multiplicity one, thus we have $\lambda = \hat{d}_i$ only for one such i. Thus, $\langle\eta, e_j\rangle = 0$ for $j \neq i$, so

$$\langle\eta, \zeta\rangle = \langle\zeta, e_i\rangle\langle\eta, e_i\rangle = 0.$$

But we have assumed that $\eta \neq 0$ so $\langle\eta, e_i\rangle \neq 0$ and therefore $\langle\zeta, e_i\rangle = 0$, a contradiction. We therefore deduce that $\hat{D} - \lambda I$ is nonsingular and $\langle\eta, \zeta\rangle \neq 0$. Thus, by (3.6), it follows that

$$\eta = -\beta\langle\eta, \zeta\rangle(\hat{D} - \lambda I)^{-1}\zeta$$

and

$$\langle\eta, \zeta\rangle(1 + \beta\langle(D - \lambda I)^{-1}\zeta, \zeta\rangle) = \langle\eta, \zeta\rangle f(\lambda) = 0,$$

where

$$f(\lambda) = 1 + \beta\sum_{j=1}^{N}\frac{|\zeta_j|^2}{\hat{d}_j - \lambda}, \qquad \zeta_j = \langle\zeta, e_j\rangle.$$

Since $\langle\eta, \zeta\rangle \neq 0$ it follows that $f(\lambda) = 0$. Note that, by (3.5), it is true that $d_l, d_{l+1} \in \{\hat{d}_j\}_{j=1}^N$ and so by the properties of f it follows that there is at least one

$$\lambda \in \sigma(\hat{D} + \beta\zeta \otimes \bar{\zeta})$$

such that $d_l < \lambda < d_{l+1}$, proving (3.4).

To show (ii) we need to prove that if $\sigma(A_{1,n})$ has an eigenvalue d with multiplicity $m > 1$ then $d \in \sigma(A)$ and $m_{A_{1,n}}(d) \leq m_A(d) + 1$. To prove that we proceed as in the proof of (i). Let P_n be the projection onto $\mathrm{sp}\{e_j\}_{j=1}^n$. Now, choose a unitary operator Q_1 on $P_n\mathcal{H}$ such that $Q_1A_{1,n}Q_1^* = D_1$ where D_1 is diagonal with respect to $\{e_j\}_{j=1}^n$ so that

$$\begin{aligned}(Q_1 \oplus I_2)(A_{1,n} \oplus A_{2,n} + &\beta\eta \otimes \eta)(Q_1^* \oplus I_2)\\ &= D_1 \oplus A_{2,n} + \beta(\zeta \oplus e_{n+1}) \otimes (\bar{\zeta} \oplus e_{n+1}),\end{aligned}$$

where I_2 is the identity on $P_n^{\perp}\mathcal{H}$ and $\zeta = Q_1 e_n$. For any set S let $\#S$ denote the number of elements in S. Note that the assertion will follow if we can show that there is a unitary operator V on $P_n\mathcal{H}$, such that $VD_1V^* = D_1$, and that

$$\#\{e_j : \langle \chi_d(D_1)V\zeta, e_j\rangle \neq 0,\, 1 \leq j \leq n\} \leq 1. \tag{3.7}$$

Indeed, if so is true, we have that

$$D_1 \oplus A_{2,n} + \beta(\zeta \oplus e_{n+1}) \otimes (\bar{\zeta} \oplus e_{n+1})$$

is unitarily equivalent to

$$B = D_1 \oplus A_{2,n} + \beta(V\zeta \oplus e_{n+1}) \otimes (\overline{V\zeta} \oplus e_{n+1}),$$

and $\Lambda = \{e_j : \langle V\zeta, e_j\rangle = 0\}$ are all eigenvectors of B. Also, the eigenvalue corresponding to the set

$$\tilde{\Lambda} = \{e_j \in \Lambda : \chi_d(D_1)e_j \neq 0\}$$

is d. Thus, by (3.7), we get the following estimate

$$\begin{aligned} m_A(d) &\geq \#\tilde{\Lambda} \\ &\geq \dim(\mathrm{ran}\chi_d(D_1)) - \#\{e_j : \langle \chi_d(D_1)V\zeta, e_j\rangle \neq 0,\, 1 \leq j \leq n\} \\ &\geq m_{A_{1,n}}(d) - 1, \end{aligned}$$

and this proves the assertion. The existence of V follows by exactly the same construction as done in the proof of Claim1 in the proof (i) by using Householder reflections. □

Note that the following theorem is similar to Theorem 2.3 and Theorem 3.8 in [Arv94a] and the proof requires similar techniques. Since the divide-and-conquer method is different form the finite-section method, we cannot use the theorems in [Arv94a] directly. However, one should note that the following theorem gives much stronger estimates on the behavior of the false eigenvalues that may occur.

Theorem 3.5. *Let $\{A_{1,n}\}$ be the sequence obtained from A as in Theorem 3.4 (recall also definitions 2.1 and 2.2).*

(i) $\sigma(A) \subset \Lambda$.

(ii) Let $a \in \sigma_e(A)^c$. Then a is transient.

(iii) If $U \subset \mathbb{R}$ is an open interval such that $U \cap \sigma(A) = \emptyset$ then $N_n(U) \leq 1$. If $U \cap \sigma(A)$ contains only one point then $\widetilde{N}_n(U) \leq 3$.

(iv) Let λ be an isolated eigenvalue of A with multiplicity m. If $U \subset \mathbb{R}$ is an open interval containing λ such that $U \setminus \{\lambda\} \cap \sigma(A) = \emptyset$ then $N_n(U) \leq m + 3$.

(v) $\sigma_e(A) = \Lambda_e$,

(vi) Every point of $\mathbb{R}$ is either transient or essential.

Proof. Now, (i) follows from the fact that $A_{1,n} \to A$ strongly (see Theorem VIII.24 in [RS72], p. 290), which is easy to see. Also, (iii) follows immediately by Theorem 3.4 and (ii) follows by (iii) and (iv). Indeed, assuming (iv) we only have to show that if $a \in \sigma(A)^c$ then a is transient and this follows from (iii). Hence, we only have to prove (iv). Let λ be an isolated eigenvalue of A with multiplicity m. If $U \subset \mathbb{R}$ is an open interval containing λ such that $U \setminus \{\lambda\} \cap \sigma(A) = \emptyset$ then, by (iii), we have $\widetilde{N}_n(U) \leq 3$. But, by Theorem 3.4, we can have $\widetilde{N}_n(U) \leq 3$ and $N_n(U) > 3$ only if $\lambda \in \sigma(A_{1,n})$. Also, by Theorem 3.4, $m_{A_{1,n}}(\lambda) \leq m + 1$, and this yields the assertion.

To get (v) and (vi) we only have to show that $\sigma_e(A) \subset \Lambda_e$. Indeed, by (ii), we have $\sigma_e(A)^c \subset \Lambda_e^c$, so if $\sigma_e(A) \subset \Lambda_e$ then (v) follows. But then $\mathbb{R} \setminus \Lambda_e = \mathbb{R} \setminus \sigma(A)_e$ and the left hand side of the equality is, by (ii), contained in the set of transient points, thus we obtain (vi).

To show that $\sigma_e(A) \subset \Lambda_e$ we will show that $\Lambda_e^c \subset \sigma_e(A)^c$. Let $\lambda \in \Lambda_e^c$. We will show that $\lambda \in \sigma_e(A)^c$. Note that, by the definition of the essential spectrum, this follows if we can show that there is an operator $T \in \mathcal{B}(\mathcal{H})$ such that $T(A - \lambda I) = (A - \lambda I)T = I + C$, where C is compact.

Since $\lambda \in \Lambda_e^c$ there is a subsequence $\{n_k\} \subset \mathbb{N}$, an $\epsilon > 0$, and an integer K such that for $\Omega = (\lambda - \epsilon, \lambda + \epsilon)$ then $N_{n_k}(\Omega) \leq K$. Let P_k be the projection onto $sp\{e_j\}_{j=1}^{n_k}$ and $E_k = \chi_\Omega(A_{1,n_k})$. Then A_{1,n_k}, P_k and E_k all commute, so we can let $B_k = (A_{1,n_k} - \lambda I)|_{\mathcal{H}_k}$ where $\mathcal{H}_k = \mathrm{ran}(P_k E_k^\perp)$. Note that B_k must be invertible with $\|B_k^{-1}\| \leq \epsilon^{-1}$. Since $P_k E_k^\perp = P_k - E_k$, we deduce that

$$(A_{1,n_k} - \lambda I)B_k^{-1}(P_k - E_k) = B_k^{-1}(P_k - E_k)(A_{1,n_k} - \lambda I) = P_k - E_k. \tag{3.8}$$

Since $\{B_k^{-1}\}$ is bounded and norm closed, while bounded sets of $\mathcal{B}(\mathcal{H})$ are weakly sequentially compact, we may assume, by possibly passing to a new subsequence that

$$\text{WOT} \lim_{k\to\infty} B_k^{-1}(P_k - E_k) = T \in \mathcal{B}(\mathcal{H}), \quad \text{WOT} \lim_{k\to\infty} E_k = C \in \mathcal{B}(\mathcal{H}).$$

The fact that $A_{1,n} \longrightarrow A$ strongly together with the uniform boundedness of $B_k^{-1}(P_k - E_k)$ allow us to take weak limits in (3.8) and we get $T(A - \lambda I) = (A - \lambda I)T = I + C$.

Note that C is compact, in fact it is trace class. For $\dim E_k \leq K$ so $\mathrm{trace}(E_k) \leq K$ and $\{H \in \mathcal{B}(\mathcal{H}) : \mathrm{trace}(H) \leq K\}$ is weakly closed. □

Corollary 3.6. *Let $\lambda \in \sigma(A)_e$ be an isolated eigenvalue. Then $\lambda \in \sigma(A_{1,n})$ for all sufficiently large n. Moreover, $m_n(\lambda) \longrightarrow \infty$, where $m_n(\lambda)$ is the multiplicity of λ as an element of $\sigma(A_{1,n})$.*

Proof. Since, by Theorem 3.5, $\sigma_e(A) = \Lambda_e$, for any open neighborhood U around λ we have $N_n(U) \to \infty$. Let U be an open interval containing λ such that $(U \setminus \{\lambda\}) \cap \sigma(A) = \emptyset$. Then, by Theorem 3.4, $U \cap \sigma(A_{1,n})$ cannot contain more that three distinct points, and since $N_n(U) \to \infty$ it follows that $A_{1,n}$ must have eigenvalues in U with multiplicity larger than two. Using Theorem 3.4 again it follows that $\lambda \in \sigma(A_{1,n})$ for all sufficiently large n. The last assertion of the corollary follows by similar reasoning. □

4 Detecting false eigenvalues

Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint. The fact that both the finite-section method and the divide and conquer method may produce points that are not in the spectrum of A poses the question; can one detect false eigenvalues? The phenomenon of false eigenvalues is well known and is often referred to as spectral pollution.

Let $\lambda \in \mathbb{R}$. The easiest way to determine whether $\lambda \in \sigma(A)$ is to estimate

$$\operatorname{dist}(\lambda, \sigma(A)) = \inf_{\xi \in \mathcal{H}, \|\xi\|=1} \langle (A-\lambda)^2 \xi, \xi \rangle.$$

Let $\{P_n\}$ be an increasing sequence of finite-dimensional projections converging strongly to the identity. Let $\gamma(\lambda) = \operatorname{dist}(\lambda, \sigma(A))$ and

$$\gamma_n(\lambda) = \inf_{\xi \in P_n\mathcal{H}, \|\xi\|=1} \langle (A-\lambda)^2 \xi, \xi \rangle.$$

It is easy to show that γ and γ_n are Lipchitz continuous with Lipchitz constant bounded by one. This implies that $\gamma_n \to \gamma$ locally uniformly and hence one can use $\gamma_n(\lambda)$ as an approximation to $\operatorname{dist}(\lambda, \sigma(A))$. Obtaining $\gamma_n(\lambda)$ is done by finding the smallest eigenvalue of a self-adjoint (finite rank) matrix. In fact γ_n can be used alone to estimate $\sigma(A)$ and that has been investigated in [DP04]. However, it seems that a combination of the finite-section method or the divide-and-conquer method, accompanied by estimates as in the previous sections and in [Arv94a], with some computed values of γ_n will give more efficient computational algorithms, especially for detecting isolated eigenvalues.

5 Tridiagonalization

In the previous section the crucial assumption was that the operator was tridiagonal with respect to some basis. We will in this section show how we can reduce the general problem to a tridiagonal one. In the finite-dimensional case every self-adjoint matrix is tridiagonalizable. This is not the case in infinite dimensions, however, it is well known that if a self-adjoint operator $A \in \mathcal{B}(\mathcal{H})$ has a cyclic vector ξ then A is tridiagonal with respect to the basis $\{e_j\}$ constructed by using the Gram-Schmidt procedure to $\{A^n\xi\}_{n=0}^{\infty}$. The problem is that our operator may not have a cyclic vector, however the following lemma is well known.

Lemma 5.1. *Let $A \in \mathcal{B}(\mathcal{H})$ and let $\mathcal{A}$ be the complex algebra generated by A, A^* and the identity. Then there is a (finite or infinite) sequence of nonzero $\mathcal{A}$-invariant subspaces $\mathcal{H}_1, \mathcal{H}_2 \dots$ such that:*

(i) $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots$

(ii) Each $\mathcal{H}_n$ contains a cyclic vector ξ_n for $\mathcal{A}$: $\mathcal{H}_n = \overline{\mathcal{A}\xi_n}$, $n = 1, 2, \dots$.

Thus, if we knew the decomposition above we could decompose our operator A into $A = H_1 \oplus H_2 \oplus \cdots$ where H_n would have a cyclic vector and hence be tridiagonalizable. Also, we would have $\sigma(A) = \overline{\bigcup_j \sigma(H_j)}$. The problem is: how do we compute H_n? This is what we will discuss in this section.

Definition 5.2. *Let $A \in \mathcal{B}(\mathcal{H})$ and let $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. A is said to be Hessenberg with respect to $\{e_j\}$ if $\langle Ae_j, e_i \rangle = 0$ for $i \geq j+2$.*

Theorem 5.3. *Let A be a bounded operator on a separable Hilbert space $\mathcal{H}$ and let $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. Then there exists an isometry V such that $V^*AV = H$ where H is Hessenberg with respect to $\{e_j\}$. Moreover $V = \text{SOT-}\lim_{n\to\infty} V_n$ where $V_n = U_1 \cdots U_n$ and U_j is a Householder transformation. Also, the projection $P = VV^*$ satisfies $PAP = AP$.*

Proof. We will obtain H as the strong limit of a sequence $\{V_n^* A V_n\}$ where $V_n = U_1 \cdots U_n$ is a unitary operator and U_j is a Householder transformation. The procedure is as follows: Let P_n be the projection onto $\mathrm{sp}\{e_1, \ldots, e_n\}$. Suppose that we have the n elements in the sequence and that the n-th element is an operator $H_n = V_n^* A V_n$ that with respect to $\mathcal{H} = P_n\mathcal{H} \oplus P_n^\perp\mathcal{H}$ has the form

$$H_n = \begin{pmatrix} \tilde{H}_n & B_n \\ C_n & N_n \end{pmatrix}, \quad \tilde{H}_n = P_n H_n P_n,\ B_n = P_n R_n P_n^\perp,\ C_n = P_n^\perp R_n P_n,$$

where $N_n = P_n^\perp R_n P_n^\perp$, $\tilde{H}_n$ is Hessenberg and $C_n e_j = 0$ for $j < n$. Let $\zeta = C_n e_n$. Choose $\xi \in P_n^\perp\mathcal{H}$ such that the Householder reflection $S \in \mathcal{B}(P_n^\perp\mathcal{H})$ defined by

$$S = I - \frac{2}{\|\xi\|^2}\xi \otimes \bar{\xi}, \quad \text{and} \quad U_n = P_n \oplus S, \tag{5.1}$$

gives $S\zeta = \{\tilde{\zeta}_1, 0, 0, \ldots\}$, and let $R_{n+1} = U_n R_n$. Hence,

$$H_{n+1} = U_n R_n U_n = \begin{pmatrix} \tilde{R}_n & B_n S \\ SC_n & SN_nS \end{pmatrix} = \begin{pmatrix} \tilde{R}_{n+1} & B_{n+1} \\ C_{n+1} & N_{n+1} \end{pmatrix}, \tag{5.2}$$

where the last matrix is understood to be with respect to the decomposition $\mathcal{H} = P_{n+1}\mathcal{H} \oplus P_{n+1}^\perp\mathcal{H}$. Note that, by the choice of S, it is true that $\tilde{H}_{n+1}$ is Hessenberg and $C_{n+1}e_j = 0$ for $j < n+1$. Defining $H_1 = A$ and letting $V_n = U_1 \cdots U_n$ we have completed the construction of the sequence $\{V_n^* A V_n\}$.

Note that $H_n = V_n^* A V_n$ is bounded, since V_n is unitary (since U_j is unitary). And since a closed ball in $\mathcal{B}(\mathcal{H})$ is weakly sequentially compact, there is an $H \in \mathcal{B}(\mathcal{H})$ and a subsequence $\{H_{n_k}\}$ such that $H_{n_k} \xrightarrow{\text{WOT}} H$. But by (5.2) it is clear that for any j we have $H_n e_j = H_m e_j$ for sufficiently large m and n. It follows that SOT-lim$_n$ $H_n = H$. Also, by(5.2) H is Hessenberg. By similar reasoning, using the previous compactness argument (since V_n is bounded) and the fact that, by (5.1), $V_n e_j = V_m e_j$ for any j and m and n sufficiently large, we deduce that there exists a $V \in \mathcal{B}(\mathcal{H})$ such that

$$\operatorname*{SOT-lim}_{n\to\infty} V_n = V, \quad \operatorname*{WOT-lim}_{n\to\infty} V_n^* = V^*.$$

Since V is the strong limit of a sequence of unitary operators, it follows that V is an isometry. We claim that $V^*AV = H$. Indeed, since multiplication is jointly continuous in the strong operator topology on bounded sets we have $AV = VH$ and since V is an isometry the assertion follows. Note that $PAP = AP$ also follows since $PAP = VV^*AVV^* = VHV^* = PA$. □

Corollary 5.4. *Suppose that the assumptions in Theorem 5.3 are true, and suppose also that A is self-adjoint. Then there exists an isometry V such that $V^*AV = H$ where H is tridiagonal with respect to $\{e_j\}$. Moreover $V = \operatorname*{SOT-lim}_{n\to\infty} V_n$ where $V_n = U_1 \cdots U_n$ and U_j is a Householder transformation. Also, the projection $P = VV^*$ satisfies $PA = AP$.*

Proof. Follows immediately from the previous theorem. □

In the case where A is self-adjoint, by the previous corollary we have that $PA = AP$, where $P = VV^*$. Now, the "part" of A, namely $P^\perp A$, that we do not capture with the construction in the proof of Theorem 5.3 can be computed by the already constructed operators i.e. we have

$$P^\perp A = A - VHV^*.$$

Thus, we may apply Theorem 5.3 again to $P^{\perp}A$. And, of course this can be applied recursively. In other words; consider $V_1^*AV_1 = H_1$, where H_1 is tridiagonal w.r.t $\{e_j\}$. Let $P_1 = V_1V_1^*$. Then $P_1A = AP_1$ and $P_1^{\perp}A = A - V_1^*H_1V_1$. Let $H_2 = V_2^*P_1^{\perp}AV_2$. In general we have

$$H_{n+1} = V_{n+1}^*(A - V_1H_1V_1^* - \cdots - V_nH_nV_n^*)V_{n+1}.$$

Using the previous construction we can actually recover the whole spectrum of A. More precisely we have the following:

Theorem 5.5. *Let A be self-adjoint and let*

$$H_{n+1} = V_{n+1}^*(A - V_1H_1V_1^* - \cdots - V_nH_nV_n^*)V_{n+1}$$

be defined as above. Then

$$\sigma(A) = \overline{\bigcup_{n\in\mathbb{N}} \sigma(H_n)}.$$

Proposition 5.6. *Let $\{P_j\}$ be a sequence of projections described above i.e. $P_j = V_j^*V_j$. Then $\mathrm{sp}\{e_1, \dots, e_n\} \subset \mathrm{ran}(P_m)$ for $m \geq n$.*

Proof. The proof is an easy induction using the fact that $e_1 \in \mathrm{ran}(P_1)$, which follows by the construction of V_1. □

Proof. Proof of Theorem 5.5 Let $P_j = V_j^*V_j$ and recall that by the construction of H_n we have

$$H_n = V_n^*P_{n-1}^{\perp}\cdots P_1^{\perp}AV_n, \tag{5.3}$$

where we have defined recursively

$$P_{n-1}^{\perp}\cdots P_1^{\perp}A = A - V_1H_1V_1^* - \cdots - V_{n-1}H_{n-1}V_{n-1}^*,$$

and by Corollary 5.4 it follows that

$$P_nP_{n-1}^{\perp}\cdots P_1^{\perp}A = P_{n-1}^{\perp}\cdots P_1^{\perp}AP_n. \tag{5.4}$$

Note that $\sigma(H_n) = \sigma(P_{n-1}^{\perp}\cdots P_1^{\perp}A\lceil_{P_n\mathcal{H}})$. Indeed, by Corollary 5.4, V_n is an isometry onto $P_n\mathcal{H}$, thus $\{V_ne_j\}$ is a basis for $P_n\mathcal{H}$, so for

$$\tilde{A} = (P_{n-1}^{\perp}\cdots P_1^{\perp}A)\lceil_{P_n\mathcal{H}}$$

it follows, by (5.3), that

$$\langle\tilde{A}V_ne_j, V_ne_i\rangle = \langle P_{n-1}^{\perp}\cdots P_1^{\perp}AV_ne_j, V_ne_i\rangle = \langle H_ne_j, e_i\rangle,$$

yielding that $\sigma(H_n) = \sigma(P_{n-1}^{\perp}\cdots P_1^{\perp}A\lceil_{P_n\mathcal{H}})$. Let us define the projection

$$E_n = P_n \wedge P_{n-1}^{\perp} \wedge \cdots \wedge P_1^{\perp}, \quad E_1 = P_1,$$

and note that $E_j \perp E_i$ for $i \neq j$. Now the theorem will follow if we can show that $AE_n = E_nA$,

$$A = \bigoplus_{n\in\mathbb{N}} E_nA$$

and

$$P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A = E_n A.$$

We will start with the former assertion (this is immediate for $n = 1$ by Corollary 5.4). Indeed, if $\xi \in \operatorname{ran}(E_n)$ for $n \geq 2$ then, by Corollary 5.4,

$$\begin{aligned} A\xi &= AP_1^{\perp} \cdots P_{n-1}^{\perp} P_n \xi = P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A\xi = P_{n-1}^{\perp} \cdots P_1^{\perp} A P_n \xi \\ &= P_{n-2}^{\perp} \cdots P_1^{\perp} A P_{n-1}^{\perp} P_n \xi = \cdots \text{etc.} \end{aligned} \tag{5.5}$$

Thus, it follows that $A \operatorname{ran}(E_n) \subset \operatorname{ran}(E_n)$. Since A is self-adjoint we have that $AE_n = E_n A$. We can now show that $A = E_1 A \oplus E_2 A \oplus \cdots$. First, an easy induction demonstrates that for any $n \in \mathbb{N}$ we have

$$A = E_1 A \oplus \cdots \oplus E_n A \oplus P_n^{\perp} \cdots P_1^{\perp} A.$$

Note that, by Proposition 5.6 and (5.4), it follows that $P_n^{\perp} \cdots P_1^{\perp} A e_j = 0$ for $j \leq n$ thus $Ae_n = (E_1 A \oplus \cdots \oplus E_n A) e_n$. Also, $E_{n+1} A e_j = 0$ for $j \leq n$. This gives us that if $T = E_1 A \oplus E_2 \oplus \cdots$. Then

$$Te_n = E_1 A \oplus \cdots \oplus E_n A e_n = Ae_n$$

yielding the assertion.

Finally, we will show that $P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A = E_n A$. Note that in (5.5) we have also shown that $P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A\xi = A\xi$ when $\xi \in \operatorname{ran}(E_n)$. So, to show that $P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A = E_n A$, we only have to show that $P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A\eta = 0$ when $\eta \in \operatorname{ran}(E_n^{\perp})$. But, by the definition of E_n we have $\eta \in \bigcup_{j=1}^{n-1} P_j \mathcal{H} \cup P_n^{\perp} \mathcal{H}$ and an easy application of Corollary 5.4 gives

$$P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A = P_n P_{n-2}^{\perp} \cdots P_1^{\perp} A P_{n-1}^{\perp} = P_n P_{n-1}^{\perp} P_{n-3}^{\perp} \cdots P_1^{\perp} A P_{n-2}^{\perp} = \cdots \text{etc},$$

which combined with (5.5) results in $P_n P_{n-1}^{\perp} \cdots P_1^{\perp} A\eta = 0$. □

6 The QR algorithm

The crucial assumption in the previous sections has been self-adjointness of the operator. Even when detecting false eigenvalues the tools we use rely heavily on self-adjointness. When we do not have self-adjointness the finite-section method may fail dramatically, the shift operator being a well known example. In fact the finite section method can behave extremely badly as the following theorem shows. First we need to recall a definition.

Definition 6.1. *Let A be a bounded operator on a Hilbert space $\mathcal{H}$. Then the numerical range of A is defined as*

$$W(A) = \{\langle A\xi, \xi\rangle : \|\xi\| = 1\},$$

and the essential numerical range is defined as

$$W_e(A) = \bigcap_{K \text{ compact}} \overline{W(A+K)}$$

Theorem 6.2. *(Pokrzywa)[Pok79] Let $A \in \mathcal{B}(\mathcal{H})$ and $\{P_n\}$ be a sequence of finite-dimensional projections converging strongly to the identity. Suppose that $S \subset W_e(A)$ then there exists a sequence $\{Q_n\}$ of finite-dimensional projections such that $P_n < Q_n$ (so $Q_n \to I$) strongly) and*

$$d_H(\sigma(A_n) \cup S, \sigma(\tilde{A}_n)) \to 0, \quad n \to \infty,$$

where

$$A_n = P_n A\lceil_{P_n\mathcal{H}}, \qquad \tilde{A}_n = Q_n A\lceil_{Q_n\mathcal{H}}$$

and d_H denotes the Hausdorff metric.

What Theorem 6.2 says is that if the essential range of a bounded operator A contains more than just elements from the spectrum, the finite section method may produce spectral pollution. As there is no restriction on the set S in Theorem 6.2 (e.g. S could be isolated points or open sets), there is no hope that the finite section method can give any information about either the essential spectrum or isolated eigenvalues.

The next question is therefore; is there an alternative to the finite-section method in the case where the operator is not self-adjoint? Another important question is; can one find eigenvectors? These are the issues we will address when introducing the QR algorithm in infinite dimensions.

6.1 The QR decomposition

The QR algorithm is the standard tool for finding eigenvalues and eigenvectors in finite dimensions. We will discuss the method in detail, but first we need to extend the well known QR decomposition in finite dimensions to infinite dimensions.

Theorem 6.3. *Let A be a bounded operator on a separable Hilbert space $\mathcal{H}$ and let $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. Then there exist an isometry Q such that $A = QR$ where R is upper triangular with respect to $\{e_j\}$. Moreover*

$$Q = \underset{n\to\infty}{\text{SOT-lim}}\ V_n$$

where $V_n = U_1 \cdots U_n$ and U_j is a Householder transformation.

Proof. We will obtain R as the weak limit of a sequence $\{V_n^* A\}$ where V_n is unitary and the unitary operator is $Q = \text{SOT-lim}_{n\to\infty} V_n$. The procedure is as follows: Let P_n be the projection onto $\{e_1, \ldots, e_n\}$ and suppose that we have the n elements in the sequence and that the n-th element is an operator $R_n = V_n^* A$ such that, with respect to the decomposition $\mathcal{H} = P_n\mathcal{H} \oplus P_n^{\perp}\mathcal{H}$, we have

$$R_n = \begin{pmatrix} \tilde{R}_n & B_n \\ C_n & N_n \end{pmatrix}, \quad \tilde{R}_n = P_n R_n P_n,\ B_n = P_n R_n P_n^{\perp},\ C_n = P_n^{\perp} R_n P_n,$$

where $N_n = P_n^{\perp} R_n P_n^{\perp}$ and $\tilde{R}$ is upper triangular and $Ce_j = 0$ for $j \leq n-1$. Let $\zeta = Ce_n$. Choose $\xi \in P_n^{\perp}\mathcal{H}$ and define the Householder reflection $S \in \mathcal{B}(P_n^{\perp}\mathcal{H})$,

$$S = I - \frac{2}{\|\xi\|^2}\xi \otimes \bar{\xi}, \quad \text{and} \quad U_n = P_n \oplus S, \tag{6.1}$$

such that $S\zeta = \{\tilde{\zeta}_1, 0, 0, \ldots\}$. Finally let $R_{n+1} = U_n R_n$. Hence,

$$R_{n+1} = U_n R_n = \begin{pmatrix} \tilde{R}_n & B_n \\ SC_n & SN_n \end{pmatrix} = \begin{pmatrix} \tilde{R}_{n+1} & B_{n+1} \\ C_{n+1} & N_{n+1} \end{pmatrix}, \tag{6.2}$$

where the last matrix is understood to be with respect to the decomposition $\mathcal{H} = P_{n+1}\mathcal{H} \oplus P_{n+1}^{\perp}\mathcal{H}$. Note that, by the choice of S it is true that $\tilde{R}_{n+1}$ is upper triangular and $C_{n+1}e_j = 0$

for $j \leq n$. Defining $R_1 = A$ and letting $V_n = U_1 \dots U_n$, we have completed the construction of the sequence $\{V_n^* A\}$.

Note that $R_n = V_n^* A$ is bounded, since V_n is unitary (since U_j is unitary). And since a closed ball in $\mathcal{B}(\mathcal{H})$ is weakly sequentially compact, there is an $R \in \mathcal{B}(\mathcal{H})$ and a subsequence $\{R_{n_k}\}$ such that $R_{n_k} \xrightarrow{\text{WOT}} R$. But by (6.2) it is clear that for any integer j we have $P_j R_n P_j = P_j R_m P_j$ for sufficiently large n and m. Hence WOT-lim$_n R_n = R$. Now, by (6.2) R is upper triangular with respect to $\{e_j\}$ and also $Re_j = R_n e_j$ for large n, thus SOT-lim$_n R_n = R$. By similar reasoning, using the previous compactness argument (since V_n is bounded) and the fact that, by (6.1), for any integer j we have $V_n e_j = V_m e_j$ for sufficiently large m and n, it follows that there is a $V \in \mathcal{B}(\mathcal{H})$ such that $V_n \xrightarrow{\text{SOT}} V$ and, being a strong limit of unitary operators; V is an isometry. Let $Q = V$. Therefore, $A = QR$ since $A = V_n R_n$ and multiplication is jointly strongly continuous on bounded sets. □

6.2 The QR algorithm

Let $A \in \mathcal{B}(\mathcal{H})$ be invertible and let $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. By Theorem 6.3 we have $A = QR$, where Q is unitary and R is upper triangular with respect to $\{e_j\}$. Consider the following construction of unitary operators $\{\hat{Q}_k\}$ and upper triangular (w.r.t. $\{e_j\}$) operators $\{\hat{R}_k\}$. Let $A = Q_1 R_1$ be a QR decomposition of A and define $A_2 = R_1 Q_1$. Then QR factorize $A_2 = Q_2 R_2$ and define $A_3 = R_2 Q_2$. The recursive procedure becomes

$$A_{m-1} = Q_m R_m, \quad A_m = R_m Q_m. \tag{6.3}$$

Now define

$$\hat{Q}_m = Q_1 Q_2 \dots Q_m, \quad \hat{R}_m = R_m R_{m-1} \dots R_1. \tag{6.4}$$

Definition 6.4. *Let $A \in \mathcal{B}(\mathcal{H})$ be invertible and let $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. Sequences $\{\hat{Q}_j\}$ and $\{\hat{R}_j\}$ constructed as in (6.3) and (6.4) will be called a Q-sequence and an R-sequence of A with respect to $\{e_j\}$.*

The following observation will be useful in the later developments. From the construction in (6.3) and (6.4) we get

$$A = Q_1 R_1 = \hat{Q}_1 \hat{R}_1,$$
$$A^2 = Q_1 R_1 Q_1 R_1 = Q_1 Q_2 R_2 R_1 = \hat{Q}_2 \hat{R}_2,$$
$$A^3 = Q_1 R_1 Q_1 R_1 Q_1 R_1 = Q_1 Q_2 R_2 Q_2 R_2 R_1 = Q_1 Q_2 Q_3 R_3 R_2 R_1 = \hat{Q}_3 \hat{R}_3.$$

An easy induction gives us that

$$A^m = \hat{Q}_m \hat{R}_m.$$

Note that $\hat{R}_m$ must be upper triangular with respect to $\{e_j\}$ since R_j, $j \leq m$ is upper triangular with respect to $\{e_j\}$. Also, by invertibility of A, $\langle Re_i, e_i \rangle \neq 0$. From this it follows immediately that

$$\text{sp}\{A^m e_j\}_{j=1}^N = sp\{\hat{Q}_m e_j\}_{j=1}^N, \quad N \in \mathbb{N}. \tag{6.5}$$

In finite dimensions we have the following theorem:

Theorem 6.5. *Let $A \in \mathbb{C}^{N \times N}$ be a normal matrix with eigenvalues satisfying $|\lambda_1| > \ldots > |\lambda_N|$. Let $\{\hat{Q}_m\}$ be a Q-sequence of unitary operators. Then $\hat{Q}_m A \hat{Q}_m^* \to D$, as $m \to \infty$, where D is diagonal.*

We will prove an analogue of this theorem in infinite dimensions, but first we need to state some presumably well-known results.

6.3 The distance and angle between subspaces

We follow the notation in [Kat95]. Let $M \subset \mathcal{B}$ and $N \subset \mathcal{B}$ be closed subspaces of a Banach space $\mathcal{B}$. Define

$$\delta(M,N) = \sup_{\substack{x \in M \\ \|x\|=1}} \inf_{y \in M} \|x-y\|$$

and

$$\hat{\delta}(M,N) = \max[\delta(M,N), \delta(M,N)].$$

Given subspaces M and $\{M_k\}$ such that $\hat{\delta}(M_k, M) \to 0$ as $k \to \infty$, we will sometimes use the notation

$$M_k \xrightarrow{\hat{\delta}} M, \qquad k \to \infty.$$

If we replace $\mathcal{B}$ with a Hilbert space H we can express δ and $\hat{\delta}$ conveniently in terms of projections and operator norms. In particular, if E and F are the projections onto subspaces $M \subset \mathcal{H}$ and $N \subset \mathcal{H}$ respectively then

$$\delta(M,N) = \sup_{\substack{x \in M \\ \|x\|=1}} \inf_{y \in M} \|x-y\| = \sup_{\substack{x \in M \\ \|x\|=1}} \inf_{y \in M} \|F^{\perp}x\| = \|F^{\perp}E\|.$$

Since the operator $E - F = F^{\perp}E - FE^{\perp}$ is essentially the direct sum of operators $F^{\perp}E \oplus (-FE^{\perp})$, its norm is $\hat{\delta}(M,N)$, i.e.

$$\hat{\delta}(M,N) = \max(\|F^{\perp}E\|, \|E^{\perp}F\|) = \max(\|F^{\perp}E\|, \|FE^{\perp}\|) = \|E-F\|. \tag{6.6}$$

These observations come in handy in the proof of the next proposition.

Proposition 6.6. *Let $\{A_n\}$ be a sequence of N-dimensional subspaces of a Hilbert space $\mathcal{H}$ and let $B \subset \mathcal{H}$ be an N-dimensional subspace. If $\delta(A_n, B) \to 0$ or $\delta(B, A_n) \to 0$ then $\hat{\delta}(A_n, B) \to 0$.*

Proof. Suppose that $\delta(A_n, B) \to 0$. Let E_n and F be the projections onto onto A_n and B respectively. We need to show that $\|E_n - F\| \to 0$ as $n \to \infty$. Now E_n and F are N-dimensional projections such that $\|E_n^{\perp}F\| \to 0$ as $n \to \infty$. Thus, in view of (6.6), it suffices to show that $\|F^{\perp}E_n\| \to 0$. For the proof, note that

$$\|F - FE_nF\| = \|FE^{\perp}F\| \le \|E^{\perp}F\| \longrightarrow 0, \qquad n \to \infty.$$

Since $FE_n^{\perp}F$ can be viewed as a sequence of positive contractions acting on the finite dimensional space $F\mathcal{H}$, it follows that $\mathrm{trace}(F - FE_nF) \to 0$. Hence

$$\begin{aligned}\|F^{\perp}E_n\|^2 &= \|E_n - E_nFE_n\| \le \mathrm{trace}(E_n - E_nFE_n) \\ &= N - \mathrm{trace}(E_nFE_n) = N - \mathrm{trace}(FE_nF) \\ &= \mathrm{trace}(F - FE_nF) \to 0, \qquad n \to \infty.\end{aligned}$$

The proof that if $\delta(B, A_n) \to 0$ then $\hat{\delta}(A_n, B) \to 0$ is similar to the previous argument. □

Proposition 6.7. *Let $E = E_1 \oplus \ldots \oplus E_M$ where the E_js are finite-dimensional subspaces of a Hilbert space $\mathcal{H}$. Let $F_k = E_{1,k} + \ldots + E_{M,k}$ where $\hat{\delta}(E_{j,k}, E_j) \to 0$ as $k \to \infty$. Then $F_k \xrightarrow{\hat{\delta}} E$.*

Proof. Note that for projections P and Q on a Hilbert space where $\|P - Q\| < 1$ implies that $\dim P = \dim Q$. So writing E_j for the projection onto the space E_j etc., the hypothesis $\|E_{j,k} - E_j\| = \hat{\delta}(E_{j,k}, E_j) \to 0$ implies that $\dim E_{j,k} = \dim E_j$ for large k. The assertion now follows by Proposition 6.6 and the fact that

$$\delta(E, F_k) \leq \sum_{j=1}^{M} \|E_j - E_{j,k}\| \longrightarrow 0, \qquad k \to \infty.$$

□

Theorem 6.8. *Let $A \in \mathcal{B}(\mathcal{H})$ be an invertible normal operator. Suppose that $\sigma(A) = \omega \cup \Omega$ is a disjoint union such that $\omega = \{\lambda_i\}_{i=1}^N$ and the λ_is are isolated eigenvalues of finite multiplicity satisfying $|\lambda_1| > \ldots > |\lambda_N|$. Suppose further that $\sup\{|\gamma| : \gamma \in \Omega\} < |\lambda_N|$. Let $\{\xi_i\}_{i=1}^M$ be a collection of linearly independent vectors in $\mathcal{H}$ such that $\{\chi_\omega(A)\xi_i\}_{i=1}^M$ are linearly independent. The following observations are true.*

(i) There exists an M-dimensional subspace $B \subset \mathrm{ran}\chi_\omega(A)$ such that

$$\mathrm{sp}\{A^k\xi_i\}_{i=1}^M \stackrel{\hat{\delta}}{\longrightarrow} B, \quad k \to \infty.$$

(ii) If

$$\mathrm{sp}\{A^k\xi_i\}_{i=1}^{M-1} \stackrel{\hat{\delta}}{\longrightarrow} D \subset \mathcal{H}, \quad k \to \infty,$$

where D is an $(M-1)$-dimensional subspace, then

$$\mathrm{sp}\{A^k\xi_i\}_{i=1}^M \stackrel{\hat{\delta}}{\longrightarrow} D \oplus \mathrm{sp}\{\xi\}, \quad k \to \infty,$$

where $\xi \in \mathrm{ran}\chi_\omega(A)$ is an eigenvector of A.

Proof. We will first prove (i). Consider the following construction of B: Let $\tilde{\lambda}_1 \in \{\lambda_i\}_{i=1}^N$ be the largest (in absolute value) element such that

$$\{\chi_{\tilde{\lambda}_1}(A)\xi_i\}_{i=1}^M \neq \{0\}.$$

If $\{\chi_{\tilde{\lambda}_1}(A)\xi_i\}_{i=1}^M$ are linearly independent let $B = \{\chi_{\tilde{\lambda}_1}(A)\xi_i\}_{i=1}^M$. If not, then $\{\chi_{\tilde{\lambda}_1}(A)\xi_i\}_{i=1}^M$ are linearly dependent spanning a space of dimension $k_1 < M$. By taking linear combinations of elements in $\{\xi_i\}_{i=1}^M$ we can find a new basis $\{\xi_{1,i}\}_{i=1}^M$ for $\mathrm{sp}\{\xi_i\}_{i=1}^M$ such that $\mathrm{sp}\{\chi_{\tilde{\lambda}_1}(A)\xi_{1,i}\}_{i=1}^{k_1} = \mathrm{sp}\{\chi_{\tilde{\lambda}_1}(A)\xi_i\}_{i=1}^M$ and $\chi_{\tilde{\lambda}_1}(A)\xi_{1,i} = 0$, for $k_1 + 1 \leq i \leq M$. Let $\tilde{\lambda}_2 \in \{\lambda_i\}_{i=1}^N \backslash \{\tilde{\lambda}_1\}$ be the largest element such that $\{\chi_{\tilde{\lambda}_2}(A)\xi_{1,i}\}_{i=k_1+1}^M \neq \{0\}$. If $\{\chi_{\tilde{\lambda}_2}(A)\xi_{1,i}\}_{i=k_1+1}^M$ are linearly independent let

$$B = \mathrm{sp}\{\chi_{\tilde{\lambda}_1}(A)\xi_{1,i}\}_{i=1}^{k_1} \oplus \mathrm{sp}\{\chi_{\tilde{\lambda}_2}(A)\xi_{1,i}\}_{i=k_1+1}^M.$$

If $\{\chi_{\tilde{\lambda}_2}(A)\xi_{1,i}\}_{i=k_1+1}^M$ are linearly dependent, spanning a space of dimension k_2, we proceed exactly as in the previous step. Repeating this process until $\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^M$ is linearly independent (note that this is possible by the assumption that $\{\chi_\omega(A)\xi_i\}_{i=1}^M$ are linearly independent) we get

$$B = \bigoplus_{j=1}^{n} \mathrm{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \oplus \mathrm{sp}\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^M, \quad n \leq N-1,$$

where $k_0 = 0$. We claim that $\mathrm{sp}\{A^k\xi_i\}_{i=1}^M \xrightarrow{\hat{\delta}} B$ as $k \to \infty$. Since

$$\dim(\mathrm{sp}\{A^k\xi_i\}_{i=1}^M) = M = \dim(B),$$

(recall that A is invertible) and

$$\mathrm{sp}\{A^k\xi_i\}_{i=1}^M = \sum_{j=1}^n \mathrm{sp}\{A^k\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} + \mathrm{sp}\{A^k\xi_{n,i}\}_{i=k_n+1}^M$$

by Proposition 6.7, we only have to demonstrate that

$$\mathrm{sp}\{A^k\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \xrightarrow{\hat{\delta}} \mathrm{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j}, \quad k \to \infty, \quad j \leq n, \tag{6.7}$$

and

$$\mathrm{sp}\{A^k\xi_{n,i}\}_{i=k_n+1}^M \xrightarrow{\hat{\delta}} \mathrm{sp}\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^M. \tag{6.8}$$

To prove (6.7), by Proposition 6.6, we only need to show that

$$\begin{aligned} &\sup_{\substack{\zeta\in E\\ \|\zeta\|=1}} \inf_{\eta\in E_k} \|\zeta - \eta\| = \delta(E, E_k) \longrightarrow 0, \quad k \to \infty, \\ &E_k = \mathrm{sp}\{A^k\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j},\ E = \mathrm{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j}, \end{aligned} \tag{6.9}$$

since $\dim E = \dim E_k$. It is easy to see that (6.9) will follow if for any sequence $\{\zeta_k\} \subset E$ of unit vectors there exists a sequence $\{\eta_k\}$, where $\eta_k \in E_k$, such that $\|\zeta_k - \eta_k\| \to 0$. To show this, note that by compactness of the unit ball in E we can assume, possibly passing to a subsequence, that $\zeta_k \to \zeta$. Thus, the task is reduced to showing that we can find $\{\eta_k\}$ such that $\|\zeta - \eta_k\| \to 0$. Now, $\zeta = \sum_i \alpha_i \chi_{\tilde{\lambda}_j}(A)\xi_{j,i}$, for some complex numbers $\{\alpha_i\}$, and we claim that the right choice of $\{\eta_k\}$ is

$$\eta_k = \sum_i \alpha_i A^k \xi_{j,i}/\tilde{\lambda}_j^k.$$

Indeed, by the previous construction, $\xi_{j,i} \perp \mathrm{ran}\chi_{\tilde{\lambda}_l}(A)$ for $l > j$. Thus,

$$\xi_{j,i} = (\chi_{\tilde{\lambda}_j}(A) + \chi_\theta(A))\xi_{j,i}, \qquad \theta = \{\lambda \in \sigma(A) : |\lambda| < |\tilde{\lambda}_j|\}.$$

This gives $A^k\xi_{j,i} = \tilde{\lambda}_j^k \chi_{\tilde{\lambda}_j}(A)\xi_{j,i} + A^k\chi_\theta(A)\xi_{j,i}$. Now, by the assumption on $\sigma(A)$, we have

$$\rho = \sup\{|z| : z \in \theta\} < |\tilde{\lambda}_j|.$$

Thus, since

$$\|A^k\chi_\theta(A)\xi_{j,i}\|/|\tilde{\lambda}_j^k| < |\rho/\tilde{\lambda}_j|^k \|\chi_\theta(A)\xi_{j,i}\|,$$

we have

$$A^k\xi_{j,i}/\tilde{\lambda}_j^k = (\tilde{\lambda}_j^k\chi_{\tilde{\lambda}_j}(A)\xi_{j,i} + A^k\chi_\theta(A)\xi_{j,i})/\tilde{\lambda}_j^k \longrightarrow \chi_{\tilde{\lambda}_j}(A)\xi_{j,i}, \quad k \to \infty,$$

which yields our claim. Now (6.8) follows by a similar argument.

To show (ii), note that, by the argument in the proof of (i) and our assumption, we have

$$\begin{aligned} \mathrm{sp}\{A^k\xi_i\}_{i=1}^{M-1} \xrightarrow{\hat{\delta}} D = &\bigoplus_{j=1}^n \mathrm{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \\ &\oplus \mathrm{sp}\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^{M-1}, \quad k \to \infty, \end{aligned} \tag{6.10}$$

for $n \leq N-2$, where $k_0 = 0$, $\{\tilde{\lambda}_j\}$ and $\{\xi_{j,i}\}$ are constructed as in the proof of (i). Now, there are two possibilities:

(1) There exists $\lambda \in \Lambda = \omega \setminus \{\tilde{\lambda}_j\}_{j=1}^{n+1}$ such that $\chi_\lambda(A)\xi_M \neq 0$.

(2) We have that $\chi_\Lambda(A)\xi_M = 0$.

Starting with Case 1 we may argue as in the proof of (i) to deduce that

$$\operatorname{sp}\{A^k\xi_i\}_{i=1}^M \xrightarrow{\hat{\delta}} \bigoplus_{j=1}^{n} \operatorname{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \oplus \operatorname{sp}\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^{M-1} \oplus \operatorname{sp}\{\chi_{\tilde{\lambda}_{n+2}}(A)\xi_M\}, \quad k \to \infty,$$

where $\tilde{\lambda}_{n+2} \in \omega \setminus \{\tilde{\lambda}_j\}_{j=1}^{n+1}$ is the largest element such that $\chi_{\tilde{\lambda}_{n+2}}(A)\xi_M \neq 0$, (note that the existence of $\tilde{\lambda}_{n+2}$ is guaranteed by the assumption that $\{\chi_\omega(A)\xi_i\}_{i=1}^M$ are linearly independent) and this yields the assertion.

Note that Case 2 has two subcases, namely,

(I) $\chi_\Lambda(A)\xi_M = 0$, but $\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n+1,i}\}_{i=k_n+1}^{M-1}$ and $\chi_{\tilde{\lambda}_{n+1}}(A)\xi_M$ are linearly independent.

(II) $\chi_\Lambda(A)\xi_M = 0$ and $\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n+1,i}\}_{i=k_n+1}^{M-1}$ and $\chi_{\tilde{\lambda}_{n+1}}(A)\xi_M$ are linearly dependent, but there exists a $\tilde{\lambda}_l$, the largest eigenvalue in $\{\tilde{\lambda}_j\}_{j=1}^{n+1}$ such that $\{\chi_{\tilde{\lambda}_l}(A)\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l}$ and $\chi_{\tilde{\lambda}_l}(A)\xi_M$ are linearly independent.

Note that we cannot have $\chi_\Lambda(A)\xi_M = 0$ and also have that

$$\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \quad \text{and} \quad \chi_{\tilde{\lambda}_j}(A)\xi_M, \quad j \leq n,$$

are linearly dependent as well as $\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^{M-1}$ and $\chi_{\tilde{\lambda}_{n+1}}(A)\xi_M$ are linearly dependent at the same time because that would violate the linear independence assumption on $\{\chi_\omega(A)\xi_i\}_{i=1}^M$.

To prove (II) we may argue as in the proof of (i) and deduce that

$$\operatorname{sp}\{A^k\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l} \xrightarrow{\hat{\delta}} \operatorname{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l}, \quad k \to \infty$$

and

$$\operatorname{sp}\{A^k\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l} + \operatorname{sp}\{A^k\chi_\Gamma(A)\xi_M\} \xrightarrow{\hat{\delta}} \operatorname{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l} + \operatorname{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_M\}, \quad k \to \infty$$

where $\Gamma = \omega \setminus \{\tilde{\lambda}_j\}_{j=1}^{l-1}$. Thus, using (6.10), it is easy to see that this gives

$$\operatorname{sp}\{A^k\xi_i\}_{i=1}^M \xrightarrow{\hat{\delta}} \bigoplus_{j=1}^{l-1} \operatorname{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \oplus \Big(\operatorname{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l} + \operatorname{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_M\Big)\} \bigoplus_{j=l+1}^{n} \operatorname{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \oplus \operatorname{sp}\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^{M-1}.$$

Thus, letting P be the projection onto $\mathrm{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l}$, it follows that

$$\begin{aligned}\mathrm{sp}\{A^k\xi_i\}_{i=1}^M \xrightarrow{\hat{\delta}} & \bigoplus_{j=1}^{l-1}\mathrm{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \\ & \oplus \mathrm{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_{l,i}\}_{i=k_{l-1}+1}^{k_l} \oplus P^{\perp}\mathrm{sp}\{\chi_{\tilde{\lambda}_l}(A)\xi_M\} \\ & \bigoplus_{j=l+1}^{n}\mathrm{sp}\{\chi_{\tilde{\lambda}_j}(A)\xi_{j,i}\}_{i=k_{j-1}+1}^{k_j} \oplus \mathrm{sp}\{\chi_{\tilde{\lambda}_{n+1}}(A)\xi_{n,i}\}_{i=k_n+1}^{M-1}.\end{aligned}$$

Now Case (I) follows by similar reasoning. □

Theorem 6.9. *Let $A \in \mathcal{B}(\mathcal{H})$ be an invertible normal operator and let $\{e_j\}$ be an orthonormal basis for $\mathcal{H}$. Let $\{Q_k\}$ and $\{R_k\}$ be a Q- and R-sequences of A with respect to $\{e_j\}$. Suppose also that $\sigma(A) = \omega \cup \Omega$ such that $\omega \cap \Omega = \emptyset$ and $\omega = \{\lambda_i\}_{i=1}^N$, where the λ_is are isolated eigenvalues with finite multiplicity satisfying $|\lambda_1| > \ldots > |\lambda_N|$. Suppose further that $\sup\{|\theta| : \theta \in \Omega\} < |\lambda_N|$. Then there is a subset $\{\hat{e}_j\}_{j=1}^M \subset \{e_j\}$ such that $\mathrm{sp}\{Q_k\hat{e}_j\} \to \mathrm{sp}\{\hat{q}_j\}$ where $\hat{q}_j$ is an eigenvector of A and $M = \dim(\mathrm{ran}\chi_\omega(A))$. Moreover, $\mathrm{sp}\{\hat{q}_j\}_{j=1}^M = \mathrm{ran}\chi_\omega(A)$. Also, if $e_j \notin \{\hat{e}_j\}_{j=1}^M$, then $\chi_\omega(A)Q_ke_j \to 0$.*

The theorem will be proven in several steps. First we need a definition.

Definition 6.10. *Suppose that the hypotheses in Theorem 6.9 are true and let K be the smallest integer such that $\dim(\mathrm{sp}\{\chi_\omega(A)e_j\}_{j=1}^K) = M$. Define*

$$\Lambda_\omega = \{e_j : \chi_\omega(A)e_j \neq 0, j \leq K\} \quad \Lambda_\Omega = \{e_j : \chi_\omega(A)e_j = 0, j \leq K\}$$

and $\tilde{\Lambda}_\omega = \{e_j \in \Lambda_\omega : \chi_\omega(A)e_j \in \mathrm{sp}\{\chi_\omega(A)e_i\}_{i=1}^{j-1}\}$.

The decomposition of A into

$$A = \left(\sum_{j=1}^M \lambda_j\, \xi_j \otimes \bar{\xi}_j\right) \oplus \chi_\Omega(A)A, \quad \lambda_j \in \omega.$$

where $\{\xi_j\}_{j=1}^m$ is an orthonormal set of eigenvectors of A as well as the following two technical lemmas will be useful in the proof.

Lemma 6.11. *Let $\{\hat{e}_1, \ldots, \hat{e}_M\} = \Lambda_\omega \setminus \tilde{\Lambda}_\omega$. If $e_m \in \Lambda_\Omega \cup \tilde{\Lambda}_\omega$, then*

$$\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^m = \mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=1}^{s(m)}, \quad q_{k,j} = Q_ke_j, \quad \hat{q}_{k,j} = Q_k\hat{e}_j,$$

where $s(m)$ is the largest integer such that $\{\hat{e}_j\}_{j=1}^{s(m)} \subset \{e_j\}_{j=1}^m$.

Proof. We will show this by induction on the set $\{\tilde{e}_1, \ldots, \tilde{e}_p\} = \Lambda_\Omega \cup \tilde{\Lambda}_\omega$. Consider $\tilde{e}_\mu \in \{\tilde{e}_1, \ldots, \tilde{e}_p\}$. Then $\tilde{e}_\mu = e_{\tilde{m}}$ for some integer $\tilde{m}$. Suppose that $\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{\tilde{m}} = \mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=1}^{s(\tilde{m})}$. We will show that

$$\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^m = \mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=1}^{s(m)},$$

where $e_m = \tilde{e}_{\mu+1}$.

First, note that $\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m-1} = \mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=1}^{s(m)}$ follows from the induction hypothesis. Indeed, let β be the largest integer such that $\beta < m$ and $e_\beta \in \Lambda_\omega \setminus \tilde{\Lambda}_\omega$ i.e. if $\hat{e}_t = e_\beta$

then $t = s(m)$. Observe that since $e_{\tilde{m}} = \tilde{e}_\mu$ and $e_m = \tilde{e}_{\mu+1}$, it follows that if $\tilde{m} < \alpha < m$ then $e_\alpha \in \Lambda_\omega \setminus \tilde{\Lambda}_\omega$. So if $\beta < m-1$ then there is no $e_\alpha \in \Lambda_\omega \setminus \tilde{\Lambda}_\omega$ such that $\tilde{m} < \alpha < m$. Thus, $\tilde{m} = m-1$ and so $t = s(m) = s(\tilde{m})$, yielding the assertion.

If $\beta = m-1$ then for every e_j where $\tilde{m} < j \leq m-1$ we have $e_j \in \Lambda_\omega \setminus \tilde{\Lambda}_\omega$. So $e_{\tilde{m}+\nu} = \hat{e}_{s(\tilde{m})+\nu}$ for $\tilde{m}+\nu \leq m-1$ and $\nu \geq 1$, hence, $q_{k,\tilde{m}+\nu} = \hat{q}_{k,s(\tilde{m})+\nu}$ for $\tilde{m}+\nu \leq m-1$. Also, $e_{m-1} = \hat{e}_{s(m)}$ so $q_{k,m-1} = \hat{q}_{k,s(m)}$. Thus,

$$\begin{aligned}\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m-1} &= \mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{\tilde{m}} + \mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=\tilde{m}+1}^{m-1} \\ &= \mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{\tilde{m}} + \mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=s(\tilde{m})+1}^{s(m)},\end{aligned}$$

and by recalling the induction hypothesis this yields the assertion. Thus, we only need to prove that $\chi_\omega(A)q_{k,m} \in \mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m-1}$. To show this, note that

$$\chi_\omega(A)A^k e_m = \sum_{j=1}^{m} r_{k,j}\chi_\omega(A)q_{k,j}, \quad r_{k,j} = \langle R_k e_m, e_j\rangle.$$

Note further that, since A is invertible, we have $r_{k,m} \neq 0$. In the case $e_m \in \Lambda_\Omega$ we have $\chi_\omega(A)A^k e_m = 0$. So, since $r_{k,m} \neq 0$, it follows that $\chi_\omega(A)q_{k,m}$ is a linear combination of elements in $\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m-1}$. In the case $e_m \in \tilde{\Lambda}_\omega$ note that, by again using the fact that $\chi_\omega(A)A^k e_m = \sum_{j=1}^m r_{k,j}\chi_\omega(A)q_{k,j}$ and $r_{k,m} \neq 0$, we only have to show that $\chi_\omega(A)A^k e_m \in \mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m-1}$. Now, this is indeed the case. Since $e_m \in \tilde{\Lambda}_\omega$ we have that $\chi_\omega(A)e_m \in \mathrm{sp}\{\chi_\omega(A)e_j\}_{j=1}^{m-1}$. Thus, since A is invertible

$$\chi_\omega(A)A^k e_m \in \mathrm{sp}\{\chi_\omega(A)A^k e_j\}_{j=1}^{m-1}.$$

Also, observe that, by (6.5),

$$\mathrm{sp}\{A^k e_j\}_{j=1}^{m-1} = \mathrm{sp}\{q_{k,j}\}_{j=1}^{m-1}.$$

Hence,

$$\mathrm{sp}\{\chi_\omega(A)A^k e_j\}_{j=1}^{m-1} = \mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m-1},$$

and this yields the assertion.

The initial induction step follows from a similar argument and we are done. □

Lemma 6.12. *Let* $\{\hat{e}_1, \ldots, \hat{e}_M\} = \Lambda_\omega \setminus \tilde{\Lambda}_\omega$. *Suppose that* $\mathrm{sp}\{\hat{q}_{k,j}\} \to \mathrm{sp}\{\hat{q}_j\}$ *for all* $j \leq \mu$ *for some* $\mu < M$, *where* $\hat{q}_{k,j} = Q_k\hat{e}_j$ *and* $\hat{q}_j$ *is an eigenvector of* $\sum_{j=1}^M \lambda_j\, \xi_j \otimes \bar{\xi}_j$. *Let* $e_l = \hat{e}_{\mu+1}$. *If* $e_m \in \Lambda_\Omega \cup \tilde{\Lambda}_\omega$, *where* $m < l$ *then*

$$\chi_\omega(A)q_{k,m} \to 0, \qquad k \to \infty, \quad q_{k,m} = Q_k e_m.$$

Proof. Arguing by contradiction, suppose that $\chi_\omega(A)q_{k,m} \nrightarrow 0$. Since $\chi_\omega(A)$ has finite rank we may assume that $\chi_\omega(A)q_{k,m} \to q$. Note that by using the assumptions stated and the fact that Q_k is unitary (since A is invertible) it is straightforward to show that

$$\mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=1}^{\mu} \xrightarrow{\hat{\delta}} \mathrm{sp}\{\chi_\omega(A)\hat{q}_j\}_{j=1}^{\mu}, \qquad k \to \infty.$$

Also, by using the notation and results from Lemma 6.11 we have that $s(m) = \mu$ and

$$\mathrm{sp}\{\chi_\omega(A)q_{k,j}\}_{j=1}^{m} = \mathrm{sp}\{\chi_\omega(A)\hat{q}_{k,j}\}_{j=1}^{s(m)},$$

and thus it follows that

$$q \in \mathrm{sp}\{\chi_\omega(A)\hat{q}_j\}_{j=1}^{\mu}.$$

Now

$$|\langle \chi_\omega(A)q_{k,m}, \hat{q}_{k,j}\rangle| \to |\langle \chi_\omega(A)q, \hat{q}_j\rangle|, \quad k \to \infty, \quad j \le \mu.$$

Also, observe that

$$\langle \chi_\omega(A)q_{k,m}, \hat{q}_{k,j}\rangle \to 0, \qquad k \to \infty, \quad j \le \mu.$$

Indeed, this is true by the facts that $q_{k,m} \perp \hat{q}_{k,j}$ and $\langle \chi_\Omega(A)q_{k,m}, \hat{q}_{k,j}\rangle \to 0$ for all $j \le \mu$, where the latter follows since $\mathrm{sp}\{\hat{q}_{k,j}\} \to \mathrm{sp}\{\hat{q}_j\}$ and $\chi_\Omega(A)\hat{q}_j = 0$. Hence, it follows that $\langle \chi_\omega(A)q, \hat{q}_j\rangle = 0$ for $j \le \mu$. So since $q \in \mathrm{sp}\{\chi_\omega(A)\hat{q}_j\}_{j=1}^{\mu}$, we have that $q = 0$, and we have reached the contradiction. □

Proof. Proof of Theorem 6.9 Let $\{\hat{e}_1, \dots, \hat{e}_M\} = \Lambda_\omega \setminus \tilde{\Lambda}_\omega$. We claim that this is the desired subset of $\{e_j\}$ described in the theorem, i.e. we claim that for $\hat{e}_j \in \Lambda_\omega \setminus \tilde{\Lambda}_\omega$ it is true that $\mathrm{sp}\{\hat{q}_{k,j}\} \to \mathrm{sp}\{\hat{q}_j\}$, where $\hat{q}_{k,j} = Q_k\hat{e}_j$ and $\hat{q}_j$ is an eigenvector of $\sum_{j=1}^{M} \lambda_j\, \xi_j \otimes \bar{\xi}_j$. We will prove this by induction.

Suppose that $\mathrm{sp}\{\hat{q}_{k,j}\} \to \mathrm{sp}\{\hat{q}_j\}$ for $j \le \mu$. Suppose also that

$$\mathrm{sp}\{A^k\hat{e}_i\}_{i=1}^{\mu} \xrightarrow{\hat{\delta}} \mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu}, \qquad k \to \infty. \tag{6.11}$$

We will show that $\mathrm{sp}\{\hat{q}_{k,\mu+1}\} \to \mathrm{sp}\{\hat{q}_{\mu+1}\}$ and $\mathrm{sp}\{A^k\hat{e}_i\}_{i=1}^{\mu+1} \xrightarrow{\hat{\delta}} \mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu+1}$ where $\hat{q}_{\mu+1}$ is the desired eigenvector of $\sum_{j=1}^{M} \lambda_j\, \xi_j \otimes \bar{\xi}_j$. By using (6.11) and appealing to Theorem 6.8 it follows that

$$\mathrm{sp}\{A^k\hat{e}_i\}_{i=1}^{\mu+1} \xrightarrow{\hat{\delta}} \mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu} \oplus \mathrm{sp}\{\xi\}, \quad \xi \in \mathrm{ran}\chi_\omega(A), \tag{6.12}$$

where ξ is an eigenvector of A. Hence, to prove the induction assertion we need to show that $\mathrm{sp}\{\hat{q}_{\mu+1,k}\} \to \mathrm{sp}\{\xi\}$.

Let $e_l = \hat{e}_{\mu+1}$. Note that $\hat{\delta}(\mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu} \oplus \mathrm{sp}\{\xi\}, \mathrm{sp}\{A^k\hat{e}_i\}_{i=1}^{\mu+1}) \to 0$ implies

$$\delta(\mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu} \oplus \mathrm{sp}\{\xi\}, \mathrm{sp}\{A^k e_i\}_{i=1}^{l}) \to 0,$$

since $\mathrm{sp}\{A^k\hat{e}_i\}_{i=1}^{\mu+1} \subset \mathrm{sp}\{A^k e_i\}_{i=1}^{l}$. Thus, it follows that

$$\begin{aligned}\delta(\mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu} &\oplus \mathrm{sp}\{\xi\}, \mathrm{sp}\{q_{k,i}\}_{i=1}^{l}) \\ &= \delta(\mathrm{sp}\{\hat{q}_i\}_{i=1}^{\mu} \oplus \mathrm{sp}\{\xi\}, \mathrm{sp}\{A^k e_i\}_{i=1}^{l}) \longrightarrow 0, \quad k \to \infty,\end{aligned} \tag{6.13}$$

since A is invertible, $A^k = Q_kR_k$ and R_k is upper triangular with respect to $\{e_j\}$. We will use this to prove that $\mathrm{sp}\{\hat{q}_{\mu+1,k}\} = \mathrm{sp}\{q_{l,k}\} \to \mathrm{sp}\{\xi\}$. Note that this, by Proposition 6.6, is equivalent to proving $\delta(\mathrm{sp}\{\xi\}, \mathrm{sp}\{q_{l,k}\}) \to 0$, which we henceforth do. Note also that

$$\sup_{\substack{\zeta \in \mathrm{sp}\{\xi\} \\ \|\zeta\|=1}} \inf_{\eta \in \mathrm{sp}\{q_{l,k}\}} \|\zeta - \eta\| = \delta(\mathrm{sp}\{\xi\}, \mathrm{sp}\{q_{l,k}\}),$$

thus the latter assertion follows if we can show that for any sequence $\{\zeta_k\}$ of unit vectors in $\mathrm{sp}\{\xi\}$ there exists a sequence $\{\eta_k\}$ of vectors in $\mathrm{sp}\{q_{l,k}\}$ such that $\|\zeta_k - \eta_k\| \to 0$. We will demonstrate this. It is easy to see that we can, without loss of generality, assume that $\zeta_k = \zeta$

where $\zeta \in \mathrm{sp}\{\xi\}$ is a unit vector. Let $\epsilon > 0$. By (6.13) we can find $\tilde{\eta}_k \in \mathrm{sp}\{q_{i,k}\}_{i=1}^{l}$ such that $\|\zeta - \tilde{\eta}_k\| < \epsilon/2$ for sufficiently large k. Now, $\tilde{\eta}_k = \sum_{i=1}^{l} \alpha_{i,k} q_{i,k}$ where $\sum_{i=1}^{l} |\alpha_{i,k}|^2 = 1$. So

$$\begin{aligned}\|\zeta - \tilde{\eta}_k\|^2 &= \|\zeta - \alpha_{l,k} q_{l,k}\|^2 - 2\mathrm{Re}\langle \zeta - \alpha_{l,k} q_{l,k}, \sum_{i=1}^{l-1} \alpha_{i,k} q_{i,k}\rangle + \sum_{i=1}^{l-1} |\alpha_{i,k}|^2 \\ &= \|\zeta - \alpha_{l,k} q_{l,k}\|^2 - 2\mathrm{Re}\langle \zeta, \sum_{i=1}^{l-1} \alpha_{i,k} q_{i,k}\rangle + \sum_{i=1}^{l-1} |\alpha_{i,k}|^2.\end{aligned}$$

Now $\zeta \perp \hat{q}_i$ for $i \leq \mu$ and also $\zeta \in \mathrm{ran}\chi_\omega(A)$. These observations together with the induction hypothesis $\mathrm{sp}\{\hat{q}_{k,i}\} \to \mathrm{sp}\{\hat{q}_i\}$ for $i \leq \mu$ and the fact that, by Lemma 6.12, if $e_m \in \Lambda_\Omega \cup \tilde{\Lambda}_\omega$, where $m < l$ then $\chi_\omega(A) q_{k,m} \to 0$, imply that $\langle \zeta, \sum_{i=1}^{l-1} \alpha_{i,k} q_{i,k}\rangle$ becomes arbitrarily small for large k. Thus for sufficiently large k we have

$$\|\zeta - \alpha_{l,k} q_{l,k}\|^2 + \sum_{i=1}^{l-1} |\alpha_{i,k}|^2 < \epsilon^2.$$

By choosing $\eta_k = \alpha_{l,k} q_{k,l} \in \mathrm{sp}\{q_{k,l}\}$, we have proved the assertion and hence the induction hypothesis. The initial step is straightforward.

We are left with two things to prove. Firstly we demonstrate that $\mathrm{sp}\{\hat{q}_j\}_{j=1}^{M} = \mathrm{sp}\{\xi_j\}_{j=1}^{M}$. It is easily seen, from orthonormality of $\{\hat{q}_{k,i}\}_{i=1}^{M}$, that $\{\hat{q}_i\}_{i=1}^{M}$ are all orthonormal. Hence, since they are eigenvectors of $\sum_{j=1}^{M} \lambda_j \, \xi_j \otimes \bar{\xi}_j$ it follows that $\mathrm{sp}\{\hat{q}_j\}_{j=1}^{M} = \mathrm{sp}\{\xi_j\}_{j=1}^{M} = \mathrm{ran}\chi_\omega(A)$. Finally, we need to show that $e_j \notin \{\hat{e}_j\}_{j=1}^{M}$, then $\chi_\omega(A) Q_k e_j \to 0$, and this follows easily from Lemma 6.12. □

The infinite dimensional QR algorithm occurred first in the paper "Toda Flows with Infinitely Many Variables" [DLT85] by Deift, Li and Tomei, and the author is indebted to Percy Deift for pointing out the connection. Theorem 6.9 is related to Theorem 1 in section 4 of [DLT85], however, the techniques used in [DLT85] deviate quite substantially from the framework used in this paper. This is natural since one considers only self-adjoint operators in [DLT85]. Further connections between our results and [DLT85] are currently being investigated.

7 Convergence of Densities

We finish by extending some of the results in [Arv94a] from bounded to unbounded operators. In this section we change the point of view from single operators to algebras of operators. Let us recall some basics and useful facts.

By a state τ on a C^*-algebra $\mathcal{A}$ with identity we mean a positive linear functional on the positive elements of $\mathcal{A}$ such that $\tau(I) = 1$ (I denoting the identity). The state τ is tracial if $\tau(BB^*) = \tau(B^*B)$ for all positive $B \in \mathcal{A}$ and faithful if $B = 0$ when $\tau(B) = 0$.

If $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ is a C^*-algebra and τ is a state on $\mathcal{A}$, then each self-adjoint element $A \in \mathcal{A}$ induces a unique Borel probability measure μ_A^τ on $\mathbb{R}$ with the property that

$$\int_{-\infty}^{\infty} f(x) d\mu_A^\tau(x) = \tau(f(A)), \qquad f \in C_0(\mathbb{R}). \tag{7.1}$$

Also, if τ is a faithful tracial state we have $\mathrm{supp}(\mu_A^\tau) = \sigma(A)$. Thus, if $\{A_n\}$ is a sequence of self-adjoint elements in $\mathcal{A}$ converging in some sense to a self-adjoint element $A \in \mathcal{A}$ and we are interested in determining the behavior of $\sigma(A_n)$ as $n \to \infty$, the behavior of $\mu^\tau_{A_n}$ is of great interest. In particular, we consider under which conditions can we guarantee that

$$\int_{-\infty}^{\infty} f(x)d\mu^\tau_{A_n}(x) \longrightarrow \int_{-\infty}^{\infty} f(x)d\mu^\tau_A(x),$$

for all $f \in C_0(\mathbb{R})$.

As our goal is to extend some of the theorems in [Arv94a] from bounded to unbounded operators, the C^*-algebra framework sketched above must be modified slightly. Since collections of unbounded operators can never form a C^*-algebra we have to look at C^*-algebras affiliated with unbounded operators.

Definition 7.1. *Let A be a self-adjoint, unbounded operator on $\mathcal{H}$. The operator A is affiliated with the C^*-algebra $\mathcal{A}$ if and only if $\mathcal{A} \supset \{f(A) : f \in C_0(\mathbb{R})\}$.*

Note that (7.1) can be extended to unbounded operators. In particular if $\mathcal{A}$ is a C^*-algebra with a state τ and if A is a self-adjoint operator affiliated with $\mathcal{A}$ then there is a probability measure μ^τ_A on $\mathbb{R}$ such that (7.1) is valid. Before we can prove the results we need some preliminary theory.

Definition 7.2. *Let $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ be a C^*-algebra. An $\mathcal{A}$-filtration is a filtration (recall Definition 2.4) of $\mathcal{H}$ such that the $*$-subalgebra of all finite degree operators in $\mathcal{A}$ is norm dense in $\mathcal{A}$.*

Proposition 7.3. *(Arveson) Let $\mathcal{A} \subset \mathcal{B}(\mathcal{H})$ be a C^*-algebra with a unique tracial state τ and suppose that $\{\mathcal{H}_n\}$ is an $\mathcal{A}$-filtration. Let τ_n be the state of $\mathcal{A}$ defined by*

$$\tau_n(A) = \frac{1}{d_n}\mathrm{trace}(P_nA), \qquad d_n = \dim(\mathcal{H}_n).$$

Then

$$\tau_n(A) \to \tau(A), \qquad \textit{for all} \quad A \in \mathcal{A}.$$

The next theorem will be crucial in the sequel. Firstly, some notation. We let trace denote the trace on the set of trace class operators and $\|\cdot\|_2$ denote the Hilbert-Schmidt norm. Let also W^2_∞ denote the Sobolev space of measurable functions on $\mathbb{R}$ with second derivative (in the distributional sense) being L^∞.

Theorem 7.4. *(Laptev, Safarov)[LS96] Let A be a self-adjoint, unbounded operator on $\mathcal{H}$ and let P be projection such that PA is a Hilbert-Schmidt operator. Then for any $\psi \in W^2_\infty$ we have that*

$$|\mathrm{tr}(P\psi(A)P - P\psi(PAP)P)| \leq \|\psi''\|_\infty \|PA(I-P)\|_2^2.$$

The next theorem is an extension of Theorem 4.5 in [Arv94a] to unbounded operators.

Theorem 7.5. *Let A be a self-adjoint, unbounded operator with domain $\mathcal{D}(A)$ and let $\mathcal{A}$ be a C^*-algebra with a unique tracial state τ. Suppose that $\{\mathcal{H}_n\}$ is an $\mathcal{A}$-filtration, where $\mathcal{H}_n \subset \mathcal{D}(A)$, and that $\mathcal{A}$ is affiliated with A. Let $d_n = \dim(\mathcal{H}_n)$ and $\lambda_1, \lambda_2, \ldots, \lambda_{d_n}$ be the eigenvalues of $A_n = P_nA\lceil_{\mathcal{H}_n}$, repeated according to multiplicity. Suppose that one of the following is true.*

(i) $\|P_nA(I-P_n)\|_2/\sqrt{d_n} \to 0$, *as* $n \to \infty$.

(ii) $A = D + C$, *where D commutes with P_n and $C \in \tilde{\mathcal{A}} \subset \mathcal{B}(\mathcal{H})$ and $\tilde{\mathcal{A}}$ is a C^*-algebra such that $\{\mathcal{H}_n\}$ is also an $\tilde{\mathcal{A}}$-filtration.*

Then for every $f \in C_0(\mathbb{R})$,

$$\lim_{n\to\infty} \frac{1}{d_n}(f(\lambda_1) + f(\lambda_2) + \ldots + f(\lambda_{d_n})) = \int_{\mathbb{R}} f(x)\, d\mu_A(x),$$

where μ_A denotes the Borel measure induced by τ.

Proof. Define

$$\tau_n(T) = \frac{1}{d_n}\mathrm{trace}(P_n T), \quad T \in \mathcal{A}.$$

Since τ_n restricts to the normalized trace on $P_n\mathcal{B}(\mathcal{H})P_n$ and since, by Proposition 7.3

$$\tau_n(B) \longrightarrow \tau(B), \qquad n \to \infty, \quad B \in \mathcal{A}$$

it follows that, in both cases (i) and (ii), it suffices to show that

$$\tau_n(f(A)) - \tau_n(f(P_nAP_n)) \to 0, \quad n \to \infty. \tag{7.2}$$

To show this for (i), note that we can approximate f in the L^∞ norm by elements from W^2_∞. Combining that fact with the observation that the linear functional

$$f \mapsto \tau_n(f(A)) - \tau_n(f(P_nAP_n))$$

has norm less than two, we reduce the problem to showing (7.2) when $f \in W^2_\infty$. Now, by Theorem 7.4,

$$\begin{aligned}|\tau_n(f(A)) - \tau_n(f(P_nAP_n))| &= \frac{1}{d_n}|\mathrm{trace}(P_nf(A)P_n) - \mathrm{trace}(P_nf(P_nAP_n)P_n)| \\ &\le \frac{1}{2d_n}\|f''\|_\infty\|P_nA(I-P_n)\|_2^2,\end{aligned}$$

where the right hand side of the inequality tends to zero by assumption.

To prove the theorem when (ii) is assumed, note that, by the Stone-Weierstrass theorem, polynomials in $(x+i)^{-1}$ and $(x-1)^{-1}$ are dense in $C_0(\mathbb{R})$. Thus, by arguing as above, we can assume that $f(x) = (x+i)^{-k}(x-i)^{-l}$ for some positive integers k, l. It is not too hard to show that $(D+C\pm i)^{-1} - (D+B\pm i)^{-1}$ is small when $\|C-B\|$ is small and $B \in \mathcal{B}(\mathcal{H})$ is self-adjoint. Thus, for $\epsilon > 0$ we have

$$\|f(P_n(D+C)P_n) - f(P_n(D+B)P_n)\| \le \epsilon, \quad \|f(D+C) - f(D+B)\| \le \epsilon,$$

for $B \in \tilde{\mathcal{A}}$ and when $\|C-B\|$ is sufficiently small. Hence, since τ_n is uniformly bounded, we can assume that C has finite degree. Arguing as above we get

$$\begin{aligned}|\tau_n(f(A)) - \tau_n(f(P_nAP_n))| &\le \frac{1}{2d_n}\|f''\|_\infty\|P_n(D+C)(I-P_n)\|_2^2 \\ &\le \frac{1}{2d_n}\|f''\|_\infty \deg(C)\|C\|^2,\end{aligned}$$

and this yields the assertion. The proof of the fact that $\|P_nC(I-P_n)\|_2^2 \le \deg(C)\|C\|^2$ can be found in the proof of Lemma 3.6 in [Arv94a]. □

8 The General Problem

So far in this article we have considered approximations of spectra of self-adjoint and normal operators. We will in this section sketch some ideas on how to approach the task in general. To approximate the spectrum of an arbitrary operator $T \in \mathcal{B}(\mathcal{H})$ one has to take care of a slightly unpleasant problem, namely the fact that the spectrum is very sensitive to perturbations. The well known example is if we let $A_\epsilon : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$ be defined by

$$(A_\epsilon f)(n) = \begin{cases} \epsilon f(n+1) & n = 0 \\ f(n+1) & n \neq 0. \end{cases}$$

Now for $\epsilon \neq 0$ we have $\sigma(A_\epsilon) = \{z : |z| = 1\}$ but for $\epsilon = 0$ then $\sigma(A_0) = \{z : |z| \leq 1\}$. In fact, because of this example, Davies questions in [Dav05] whether one can actually compute the spectrum of a bounded operator with the existing model of a computer we have today. The problem is that due to the inexact arithmetic one may actually compute the spectrum of a slightly perturbed problem. And as shown, that can have dramatic consequences. We therefore suggest that instead of approximating the spectrum one should approximate a set which is close to (here close means in the Hausdorff metric) the spectrum and also has nice continuity properties.

Definition 8.1. *Let $T \in \mathcal{B}(\mathcal{H})$, $n \in \mathbb{Z}_+$ and $\epsilon > 0$. The (n, ϵ)-pseudospectrum of T is defined as the set*

$$\sigma_{n,\epsilon}(T) = \sigma(T) \cup \{z \notin \sigma(T) : \|R(z,T)^{2^n}\|^{1/2^n} > \epsilon^{-1}\}.$$

As the following theorem shows the n-pseudospectrum is an excellent approximation to the spectrum and in the same time it has the desired continuity properties.

Theorem 8.2. *Let $T \in \mathcal{B}(\mathcal{H})$ and $n \in \mathbb{Z}_+$. Then the following is true.*

(i) The n-pseudospectra are nested i.e.

$$\sigma_{n+1,\epsilon}(T) \subset \sigma_{n,\epsilon}(T).$$

(ii) Also,

$$d_H\left(\overline{\sigma_{n,\epsilon}(T)}, \overline{\Gamma_\epsilon(\sigma(T))}\right) \longrightarrow 0, \quad n \to \infty,$$

where $\Gamma_\epsilon(\sigma(T))$ denotes the ϵ-neighborhood around $\sigma(T)$.

(iii) If $\{T_k\} \subset \mathcal{B}(\mathcal{H})$ and $T_k \to T$ in norm, it follows that

$$d_H\left(\overline{\sigma_{n,\epsilon}(T_k)}, \overline{\sigma_{n,\epsilon}(T)}\right) \longrightarrow 0, \quad k \to \infty,$$

where d_H denotes the Hausdorff metric.

Hence, the previous theorem suggests that to approximate the spectrum it is enough to approximate the n-pseudospectrum. The following theorem gives an idea on how to do that.

Theorem 8.3. *Let $T \in \mathcal{B}(\mathcal{H})$ and define for $z \in \mathbb{C}$ and $n \in \mathbb{Z}_+$*

$$\gamma_n(z) = \min\Big(\big(\inf_{\|\xi\|=1,\xi\in\mathcal{H}} \langle((T-z)^*)^{2^n}(T-z)^{2^n}\xi,\xi\rangle\big)^{1/2^{n+1}},$$
$$\big(\inf_{\|\xi\|=1,\xi\in\mathcal{H}} \langle(T-z)^{2^n}((T-z)^{2^n})^*\xi,\xi\rangle\big)^{1/2^{n+1}}\Big).$$

Let $\{P_j\}$ be an increasing sequence of projections converging strongly to the identity, and define

$$\begin{aligned}&\gamma_{n,m}(z)\\ &\quad = \min\Big(\min\{\lambda^{1/2^{n+1}} : \lambda \in \sigma\left(P_m((T-z)^*)^{2^n}(T-z)^{2^n}\lceil_{P_m\mathcal{H}}\right)\},\\ &\qquad\quad \min\{\lambda^{1/2^{n+1}} : \lambda \in \sigma\left(P_m(T-z)^{2^n}((T-z)^*)^{2^n}\lceil_{P_m\mathcal{H}}\right)\}\Big).\end{aligned}$$

Then the following is true.

(i) $\sigma_{n,\epsilon}(T) = \{z \in \mathbb{C} : \gamma_n(z) < \epsilon\}$.

(ii) $\{z : \gamma_{n,m}(z) \leq \epsilon\} \cap K \longrightarrow \overline{\sigma_{n,\epsilon}(T)} \cap K, \quad m \to \infty,$

for any compact set $K \supset \sigma_{n,\epsilon}(T)$, where the convergence is understood to be in the Hausdorff metric.

Proofs of the previous theorems can be found in [Han] as well as a more comprehensive analysis of properties of the n-pseudospectra.

9 Acknowledgments

The author would like to thank Bill Arveson, Erik Bédos, Brian Davies, Percy Deift, Arieh Iserles, Barry Simon and Nick Trefethen for useful discussions and comments as well as the referee for useful suggestions and improvements.

References

[Aro51] N. Aronszajn, *Approximation methods for eigenvalues of completely continuous symmetric operators*, Proceedings of the Symposium on Spectral Theory and Differential Problems, Oklahoma Agricultural and Mechanical College, Stillwater, Okla., 1951, pp. 179–202. MR MR0044736 (13,469b)

[Arv91] William Arveson, *Discretized CCR algebras*, J. Operator Theory **26** (1991), no. 2, 225–239. MR MR1225515 (94f:46069)

[Arv93a] ———, *Improper filtrations for C^*-algebras: spectra of unilateral tridiagonal operators*, Acta Sci. Math. (Szeged) **57** (1993), no. 1-4, 11–24. MR MR1243265 (94i:46071)

[Arv93b] ———, *Noncommutative spheres and numerical quantum mechanics*, Operator algebras, mathematical physics, and low-dimensional topology (Istanbul, 1991), Res. Notes Math., vol. 5, A K Peters, Wellesley, MA, 1993, pp. 1–10. MR MR1259055

[Arv94a] ———, *C^*-algebras and numerical linear algebra*, J. Funct. Anal. **122** (1994), no. 2, 333–360. MR MR1276162 (95i:46083)

[Arv94b] ______, *The role of C^*-algebras in infinite-dimensional numerical linear algebra*, C^*-algebras: 1943–1993 (San Antonio, TX, 1993), Contemp. Math., vol. 167, Amer. Math. Soc., Providence, RI, 1994, pp. 114–129. MR MR1292012 (95i:46084)

[BCN01] A. Böttcher, A. V. Chithra, and M. N. N. Namboodiri, *Approximation of approximation numbers by truncation*, Integral Equations Operator Theory **39** (2001), no. 4, 387–395. MR MR1829276 (2002b:47035)

[Béd97] Erik Bédos, *On Følner nets, Szegő's theorem and other eigenvalue distribution theorems*, Exposition. Math. **15** (1997), no. 3, 193–228. MR MR1458766 (98h:47065a)

[Ber71] I. David Berg, *An extension of the Weyl-von Neumann theorem to normal operators*, Trans. Amer. Math. Soc. **160** (1971), 365–371. MR MR0283610 (44 #840)

[Bro07] Nathanial P. Brown, *Quasi-diagonality and the finite section method*, Math. Comp. **76** (2007), no. 257, 339–360.

[BS99] Albrecht Böttcher and Bernd Silbermann, *Introduction to large truncated Toeplitz matrices*, Universitext, Springer-Verlag, New York, 1999. MR MR1724795 (2001b:47043)

[Cup81] J. J. M. Cuppen, *A divide and conquer method for the symmetric tridiagonal eigenproblem*, Numer. Math. **36** (1980/81), no. 2, 177–195. MR MR611491 (82d:65038)

[Dav00] E. B. Davies, *A hierarchical method for obtaining eigenvalue enclosures*, Math. Comp. **69** (2000), no. 232, 1435–1455. MR MR1710648 (2001a:34148)

[Dav05] ______, *A defence of mathematical pluralism*, Philos. Math. (3) **13** (2005), no. 3, 252–276. MR MR2192174 (2006m:00005)

[DLT85] P. Deift, L. C. Li, and C. Tomei, *Toda flows with infinitely many variables*, J. Funct. Anal. **64** (1985), no. 3, 358–402. MR MR813206 (87a:58076)

[DP04] E. B. Davies and M. Plum, *Spectral pollution*, IMA J. Numer. Anal. **24** (2004), no. 3, 417–438. MR MR2068830 (2005c:47027b)

[DVV94] Trond Digernes, V. S. Varadarajan, and S. R. S. Varadhan, *Finite approximations to quantum systems*, Rev. Math. Phys. **6** (1994), no. 4, 621–648. MR MR1290691 (96e:81028)

[Hal70] P. R. Halmos, *Ten problems in Hilbert space*, Bull. Amer. Math. Soc. **76** (1970), 887–933. MR MR0270173 (42 #5066)

[Han] A.C. Hansen, *On the complexity index, the n-pseudospectrum and approximations of spectra of operators*, In preparation.

[HN96] Naomichi Hatano and David R. Nelson, *Localization transitions in non-hermitian quantum mechanics*, Phys. Rev. Lett. **77** (1996), no. 3, 570–573.

[HN97] ______, *Vortex pinning and non-hermitian quantum mechanics*, Phys. Rev. B **56** (1997), no. 14, 8651–8673.

[HRS01] Roland Hagen, Steffen Roch, and Bernd Silbermann, *C^*-algebras and numerical analysis*, Monographs and Textbooks in Pure and Applied Mathematics, vol. 236, Marcel Dekker Inc., New York, 2001. MR MR1792428 (2002g:46133)

[Kat49] Tosio Kato, *On the upper and lower bounds of eigenvalues*, J. Phys. Soc. Japan **4** (1949), 334–339. MR MR0038738 (12,447b)

[Kat95] ______, *Perturbation theory for linear operators*, Classics in Mathematics, Springer-Verlag, Berlin, 1995, Reprint of the 1980 edition. MR MR1335452 (96a:47025)

[Kau93] Robert M. Kauffman, *Finite eigenfunction approximations for continuous spectrum operators*, Internat. J. Math. Math. Sci. **16** (1993), no. 1, 1–22. MR MR1200106 (94e:47030)

[LS96] A. Laptev and Yu. Safarov, *Szegő type limit theorems*, J. Funct. Anal. **138** (1996), no. 2, 544–559. MR MR1395969 (97k:58166)

[Pok79] Andrzej Pokrzywa, *Method of orthogonal projections and approximation of the spectrum of a bounded operator*, Studia Math. **65** (1979), no. 1, 21–29. MR MR554538 (81m:47022)

[Pok95] ______, *Spectra of approximating operators*, Mat. Stos. **38** (1995), 87–100. MR MR1372862 (97a:47023)

[Rid67] R. C. Riddell, *Spectral concentration for self-adjoint operators*, Pacific J. Math. **23** (1967), 377–401. MR MR0220081 (36 #3148)

[RS72] Michael Reed and Barry Simon, *Methods of modern mathematical physics. I. Functional analysis*, Academic Press, New York, 1972. MR MR0493419 (58 #12429a)

[Sha00] Eugene Shargorodsky, *Geometry of higher order relative spectra and projection methods*, J. Operator Theory **44** (2000), no. 1, 43–62. MR MR1774693 (2001f:47004)

[Sze20] G. Szegő, *Beiträge zur Theorie der Toeplitzschen Formen*, Math. Z. **6** (1920), no. 3-4, 167–202. MR MR1544404