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Published Version

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Chandler-Wilde, S. N. ORCID: <https://orcid.org/0000-0003-0578-1283>, Chonchaiya, R. and Lindner, M. (2023)
Convergent spectral inclusion sets for banded matrices.
Proceedings in Applied Mathematics and Mechanics, 23 (4).
e202300016. ISSN 1617-7061 doi: 10.1002/pamm.202300016
Available at <https://centaur.reading.ac.uk/113411/>

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To link to this article DOI: <http://dx.doi.org/10.1002/pamm.202300016>

Publisher: Wiley

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RESEARCH ARTICLE

Convergent spectral inclusion sets for banded matrices

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Abstract

We obtain sequences of inclusion sets for the spectrum, essential spectrum, and pseudospectrum of banded, in general non-normal, matrices of finite or infinite size. Each inclusion set is the union of the pseudospectra of certain submatrices of a chosen size n . Via the choice of n , one can balance accuracy of approximation against computational cost, and we show, in the case of infinite matrices, convergence as $n \rightarrow \infty$ of the respective inclusion set to the corresponding spectral set.

1 | INTRODUCTION

In many finite difference schemes or in physical or social models, where interaction between objects is direct in a finite radius only (and is of course indirect on a global level), the corresponding matrix or operator is *banded*, also called *of finite dispersion*, meaning that the matrix is supported on finitely many diagonals only. In the case of finite matrices this is of course a tautology; in that context one assumes that the *bandwidth* is not only finite but small compared to the matrix size, where the bandwidth of a matrix A is the distance from the main diagonal in which nonzeros can occur. (Precisely: it is the largest $|i - j|$ over all matrix positions (i, j) with $A_{i,j} \neq 0$.) So this is our setting: finite, semi-infinite or bi-infinite banded matrices.

We equip the underlying vector space with the Euclidian norm, so our operators act on an ℓ^2 space over $\{1, \dots, N\}$ or $\mathbb{N} = \{1, 2, \dots\}$ or $\mathbb{Z} = \{\dots, -1, 0, 1, \dots\}$. In the two latter cases (semi- and bi-infinite matrices), we assume each diagonal to be a bounded sequence, whence the matrix acts as a bounded linear operator, again denoted by A , on the corresponding ℓ^2 space.

The exact computation of the spectrum by analytical means is in general impossible (by Abel-Ruffini) if the size of the matrix is larger than four. So one is forced to resort to approximations. But for non-normal matrices and operators, also the approximation of the spectrum is extremely delicate and unreliable, hence one often substitutes for the spectrum, $\text{spec } A$, the *pseudospectrum*,

$$\text{spec}_\varepsilon A := \{\lambda \in \mathbb{C} : \|(A - \lambda I)^{-1}\| > 1/\varepsilon\}, \quad \varepsilon > 0,$$

that is much more stable to approximate, and then sends $\varepsilon \rightarrow 0$. Note that, by agreeing to say $\|B^{-1}\| = \infty$ if B is not invertible, one has $\text{spec } A \subset \text{spec}_\varepsilon A$ for all $\varepsilon > 0$. For an impressive account of pseudospectra and their applications, see the monograph [1].

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Our aim in this paper is to derive inclusion sets for $\text{spec } A$, $\text{spec}_\varepsilon A$ as well as the essential spectrum, $\text{spec}_{\text{ess}} A$, in terms of unions of pseudospectra of moderately sized (but many) finite submatrices of A of column dimension n . Moreover, if the matrix is infinite, we prove convergence, as $n \rightarrow \infty$, of the respective inclusion set to each of $\text{spec } A$, $\text{spec}_\varepsilon A$, or $\text{spec}_{\text{ess}} A$.

2 | APPROXIMATING THE LOWER NORM ON $\ell^2(\mathbb{Z})$

Our arguments are, perhaps surprisingly, tailor-made for the case of bi-infinite vectors and matrices on them. In fact, instead of $\ell^2(\mathbb{Z})$, everything also works for $\ell^2(G)$ with a discrete group G , for example, $G = \mathbb{Z}^d$, subject to Yu's so-called Property A [2, 3]. Only later, in Section 6, we manage to work around the group structure and to transfer results to $\ell^2(\mathbb{N})$ and $\ell^2(\{1, \dots, N\})$, hence: to semi-infinite and finite matrices.

As some sort of antagonist of the operator norm, $\|A\| = \sup\{\|Ax\| : \|x\| = 1\}$, we look at the so-called *lower norm*¹

$$\nu(A) := \inf\{\|Ax\| : \|x\| = 1\}$$

of a banded and bounded operator on $\ell^2(\mathbb{Z})$. Fixing $n \in \mathbb{N}$ and limiting the selection of unit vectors x to those with a finite support of diameter less than n , further limits how small $\|Ax\|$ can get. Precisely,

$$\nu_n(A) := \inf\{\|Ax\| : \|x\| = 1, \text{diam}(\text{supp } x) < n\}, \quad n \in \mathbb{N}, \quad (2.1)$$

is typically larger than $\nu(A)$ – but (and this is remarkable) only larger by at most the amount of a certain $\varepsilon_n \sim 1/n$ that we will quantify precisely below. Let us first write this important fact down:

$$\nu_n(A) - \varepsilon_n \leq \nu(A) \leq \nu_n(A). \quad (2.2)$$

This observation can be traced back to refs. [4, 5] and, for Schrödinger operators, even to refs. [6, 7]. Extensive use has been made of (2.2), for example, in refs. [8, 9]. The statement $\text{diam}(\text{supp } x) < n$ in (2.1) translates to $\text{supp } x \subseteq k + \{1, \dots, n\}$ for some $k \in \mathbb{Z}$. Hence,

$$\nu_n(A) = \inf\{\nu(A|_{\ell^2(k+\{1, \dots, n\})}) : k \in \mathbb{Z}\}. \quad (2.3)$$

Let us write $P_{n,k}$ for the operator of multiplication by the characteristic function of $k + \{1, \dots, n\}$ and agree on writing

$$A|_{\ell^2(k+\{1, \dots, n\})} =: AP_{n,k} : \ell^2(k + \{1, \dots, n\}) \rightarrow \ell^2(\mathbb{Z}), \quad n \in \mathbb{N}, k \in \mathbb{Z}.$$

In matrix language, $AP_{n,k}$ corresponds to the matrix formed by columns number $k + 1$ to $k + n$ of A . By the band structure of A , that submatrix is supported in finitely many rows only, even reducing it to a finite $m \times n$ matrix, where m equals n plus two times the bandwidth of A . Then $\nu(AP_{n,k})$, as in (2.3), is the smallest singular value of this $m \times n$ matrix, making this a standard computation.

3 | ε_n AND THE REDUCTION TO TRIDIAGONAL FORM

Our analysis of ε_n is particularly optimized in the case of tridiagonal matrices, that is when A has bandwidth one, so that it is only supported on the main diagonal and its two adjacent diagonals. Let $\alpha, \beta, \gamma \in \ell^\infty(\mathbb{Z})$ denote, in this order, the sub-, main- and superdiagonal of A , with entries $\alpha_i = A_{i+1,i}$, $\beta_i = A_{i,i}$ and $\gamma_i = A_{i-1,i}$ with $i \in \mathbb{Z}$. In that case (see refs. [4, 12, 13]),

$$\varepsilon_n = 2(\|\alpha\|_\infty + \|\gamma\|_\infty) \sin \frac{\pi}{2(n+1)} < (\|\alpha\|_\infty + \|\gamma\|_\infty) \frac{\pi}{n+1} \sim \frac{1}{n}. \quad (3.1)$$

¹ It is not a norm! Our terminology is that of refs. [10, 11].

Although (2.2) holds with this choice of ε_n for the very general setting of all tridiagonal matrices, formula (3.1) turns out to be best possible in some nontrivial examples such as the shift operator [12].

To profit from these well-tuned parameters also in the case of larger bandwidths, note that (2.2) and (3.1) even work in the block case, that is when the entries in the ℓ^2 vectors are themselves elements of some Banach space X and the matrix entries of A are operators on X . So the trick with a band matrix B with a larger bandwidth b is to interpret B as block-tridiagonal with blocks of size $b + 1$:

$$B = \begin{pmatrix} \text{band matrix} \end{pmatrix} \cong \begin{pmatrix} A_{1,1} & A_{1,2} & A_{1,3} & A_{1,4} \\ A_{2,1} & A_{2,2} & A_{2,3} & A_{2,4} \\ A_{3,1} & A_{3,2} & A_{3,3} & A_{3,4} \\ A_{4,1} & A_{4,2} & A_{4,3} & A_{4,4} \end{pmatrix} = A.$$

Here, a matrix B with bandwidth $b = 2$ is identified with a block-tridiagonal matrix A with 3×3 blocks, noting that $3 = b + 1$.

Since the blocks of A can be operators on a Banach space X , one can even study $\text{spec } B$ and $\text{spec}_\varepsilon B$ by our techniques for bounded operators B on $L^2(\mathbb{R}) \cong \ell^2(\mathbb{Z}, X)$, where $X = L^2([0, 1])$, for example, for integral operators B with a banded kernel $k(\cdot, \cdot)$.

4 | THE ROLE OF THE LOWER NORM IN SPECTRAL COMPUTATIONS

If A sends a unit vector x to a vector Ax with norm $\frac{1}{4}$ then, clearly, A^{-1} , bringing Ax back to x , has to have at least norm four. The lower norm, $\nu(A)$, is pushing this observation to the extreme. By minimizing $\frac{\|Ax\|}{\|x\|}$, it minimizes $\frac{\|y\|}{\|A^{-1}y\|}$ and hence computes the reciprocal of $\|A^{-1}\|$ – with one possible exception: non-invertibility of A due to $\nu(A) = 0$ or $\nu(A^*) = 0$. Properly: since $\nu(A) > 0$ iff A is injective and has a closed range (e.g., [10, Lemma 2.32]), A is invertible iff both $\nu(A)$ and $\nu(A^*)$ are nonzero². Keeping this symmetry of A and A^* in mind,

$$1/\|A^{-1}\| = \min\{\nu(A), \nu(A^*)\} =: \mu(A),$$

(see, e.g., [2]), where, again, $\|A^{-1}\| = \infty$ signals non-invertibility and where $1/\infty := 0$. From here it is just a small step to

$$\text{spec } A = \{\lambda \in \mathbb{C} : \|(A - \lambda I)^{-1}\| = \infty\} = \{\lambda \in \mathbb{C} : \mu(A - \lambda I) = 0\}$$

and

$$\text{spec}_\varepsilon A = \{\lambda \in \mathbb{C} : \|(A - \lambda I)^{-1}\| > 1/\varepsilon\} = \{\lambda \in \mathbb{C} : \mu(A - \lambda I) < \varepsilon\}, \quad \varepsilon > 0. \quad (4.1)$$

Being able to approximate $\nu(A)$, up to $\varepsilon_n \sim \frac{1}{n}$, by $\nu_n(A)$, enables us to approximate $\text{spec } A$ and $\text{spec}_\varepsilon A$, with a controllable error, by sets built on $\nu_n(A - \lambda I)$ and $\nu_n(A^* - \lambda I)$.

5 | APPROXIMATING THE PSEUDOSPECTRUM IN THE BI-INFINITE CASE

Applying (2.2) to $A - \lambda I$ and $(A - \lambda I)^* = A^* - \lambda I$ in place of A , we see that

$$\mu_n(A - \lambda I) < \varepsilon \Rightarrow \mu(A - \lambda I) < \varepsilon \Rightarrow \mu_n(A - \lambda I) < \varepsilon + \varepsilon_n,$$

where $\mu_n(B) := \min\{\nu_n(B), \nu_n(B^*)\}$, noting that ε_n is independent of $\lambda \in \mathbb{C}$, by (3.1).

² By A^* we denote the Banach space adjoint of A . In particular, $(\lambda I)^* = \lambda I$, not $\bar{\lambda} I$.

Combining this with (2.3) and (4.1), we conclude (cf. [4, Thm. 4.3 & Cor. 4.4]):

Proposition 5.1 (Bi-infinite case). *For bounded band operators A on $\ell^2(\mathbb{Z})$ and corresponding ε_n from (3.1)³, one has*

$$\bigcup_{k \in \mathbb{Z}} \text{spec}_\varepsilon(AP_{n,k}, A^*P_{n,k}) \subseteq \text{spec}_\varepsilon A \subseteq \bigcup_{k \in \mathbb{Z}} \text{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k}, A^*P_{n,k}), \quad \varepsilon > 0, n \in \mathbb{N}, \quad (5.1)$$

where we abbreviate $\text{spec}_\varepsilon(A, B) := \text{spec}_\varepsilon A \cup \text{spec}_\varepsilon B$.

By iterated application of (5.1), one can extend (5.1) to the left and right as follows:

$$\text{spec}_{\varepsilon-\varepsilon_n} A \subseteq \bigcup_{k \in \mathbb{Z}} \text{spec}_\varepsilon(AP_{n,k}, A^*P_{n,k}) \subseteq \text{spec}_\varepsilon A \subseteq \bigcup_{k \in \mathbb{Z}} \text{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k}, A^*P_{n,k}) \subseteq \text{spec}_{\varepsilon+\varepsilon_n} A.$$

And now, sending $n \rightarrow \infty$, we have $\varepsilon_n \rightarrow 0$, by (3.1), and then Hausdorff-convergence $\text{spec}_{\varepsilon+\varepsilon_n} A \rightarrow \text{spec}_\varepsilon A$ as well as $\text{spec}_{\varepsilon-\varepsilon_n} A \rightarrow \text{spec}_\varepsilon A$, see for example, [14]⁴. We conclude (cf. [4, Sec. 4.3]):

Proposition 5.2. *The subsets and supersets of $\text{spec}_\varepsilon A$ in (5.1) both Hausdorff-converge to $\text{spec}_\varepsilon A$ as $n \rightarrow \infty$.*

6 | APPROXIMATING THE PSEUDOSPECTRA OF SEMI-INFINITE AND FINITE MATRICES

Now take a bounded and banded operator A on $\ell^2(\mathbb{N})$. In ref. [13] we show how to reduce this case (via embedding A into a bi-infinite matrix plus some further arguments) to the bi-infinite result:

Proposition 6.1 (Semi-infinite case). *For bounded band operators A on $\ell^2(\mathbb{N})$ and corresponding ε_n from (3.1), one has*

$$\bigcup_{k \in \mathbb{N}_0} \text{spec}_\varepsilon(AP_{n,k}, A^*P_{n,k}) \subseteq \text{spec}_\varepsilon A \subseteq \bigcup_{k \in \mathbb{N}_0} \text{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k}, A^*P_{n,k}), \quad \varepsilon > 0, n \in \mathbb{N},$$

where again $\text{spec}_\varepsilon(A, B) := \text{spec}_\varepsilon A \cup \text{spec}_\varepsilon B$. Also here the sub- and supersets Hausdorff-converge to $\text{spec}_\varepsilon A$ as $n \rightarrow \infty$.

The technique that helps to deal with one endpoint on the axis can essentially be repeated for a second endpoint:

Proposition 6.2 (Finite case). *For finite band matrices A on $\ell^2(\{1, \dots, N\})$ with some $N \in \mathbb{N}$, one has*

$$\bigcup_{k=0}^{N-n} \text{spec}_\varepsilon(AP_{n,k}, A^*P_{n,k}) \subseteq \text{spec}_\varepsilon A \subseteq \bigcup_{k=0}^{N-n} \text{spec}_{\varepsilon+\varepsilon_n}(AP_{n,k}, A^*P_{n,k}), \quad \varepsilon > 0, 1 \leq n \leq N,$$

where again $\text{spec}_\varepsilon(A, B) := \text{spec}_\varepsilon A \cup \text{spec}_\varepsilon B$.

This time, of course, there is no way of sending $n \rightarrow \infty$, hence no Hausdorff-convergence result.

7 | APPROXIMATING SPECTRA

So far we have convergent subsets and supersets of $\text{spec}_\varepsilon A$ for $\varepsilon > 0$. The spectrum, $\text{spec} A$, can now be Hausdorff-approximated via sending $\varepsilon \rightarrow 0$. However, there is a more direct approach: introducing closed-set versions of

³ Note that ε_n , if using (3.1), has to be computed for the block-tridiagonal representation of A , see Section 3.

⁴ In the case of a Banach space-valued ℓ^2 , that Banach space should be finite-dimensional or subject to the conditions in Theorem 2.5 of ref. [14].

pseudospectra,

$$\text{Spec}_\varepsilon A := \{\lambda \in \mathbb{C} : \|(A - \lambda I)^{-1}\| \geq 1/\varepsilon\} = \{\lambda \in \mathbb{C} : \mu(A - \lambda I) \leq \varepsilon\}, \quad \varepsilon \geq 0,$$

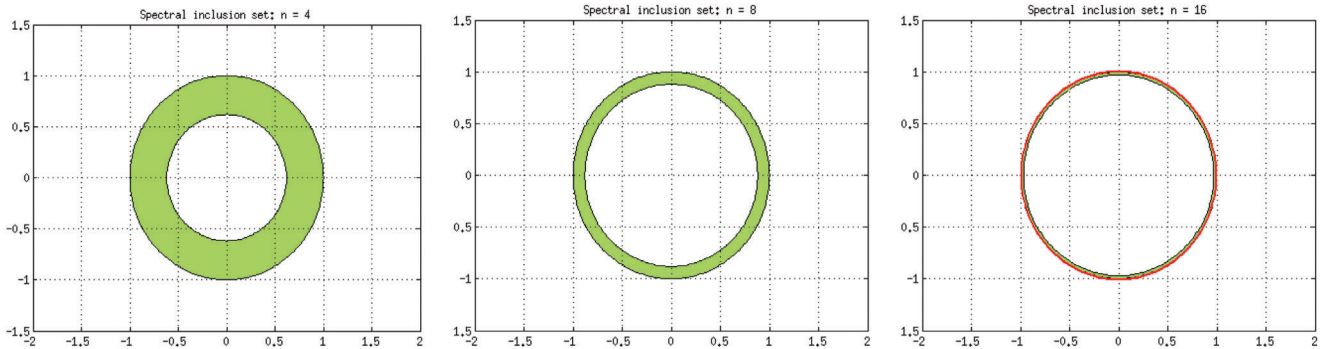
we can prove identical copies of Propositions 5.1, 6.1 and 6.2 with upper-case (i.e., closed) instead of lower-case (i.e., open) pseudospectra everywhere – and including the case $\varepsilon = 0$, see ref. [13]. The latter brings convergent supersets for $\text{spec } A = \text{Spec}_0 A$ right away, without the need for a further limit $\varepsilon \rightarrow 0$. Here is the new formula for the bi-infinite case, evaluated for $\varepsilon = 0$.

$$\bigcup_{k \in \mathbb{Z}} \text{spec}(AP_{n,k}, A^*P_{n,k}) \subseteq \text{spec } A \subseteq \bigcup_{k \in \mathbb{Z}} \text{Spec}_{\varepsilon_n}(AP_{n,k}, A^*P_{n,k}), \quad n \in \mathbb{N}. \quad (7.1)$$

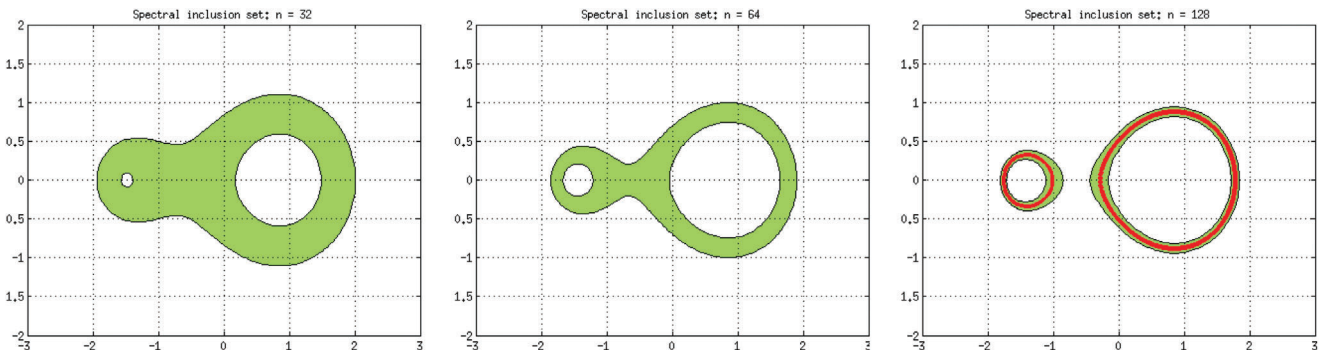
8 | EXAMPLES

For three selected operator examples, we show the Hausdorff-convergent (as $n \rightarrow \infty$) superset bounds on $\text{spec } A$ from (7.1). All three operators are given by tridiagonal bi-infinite matrices. Moreover, all three matrices are periodic, so that we can analytically compute the spectrum by Floquet-Bloch; that is, treating the 3-periodic matrix as a 3×3 -block convolution on $\ell^2(\mathbb{Z}, \mathbb{C}^3)$ and turning that, via the corresponding block-valued Fourier-transform, into a 3×3 -block multiplication on $L^2(\mathbb{T}, \mathbb{C}^3)$, whose spectrum is obvious, see, for example, Theorem 4.4.9 in ref. [15]. For comparison, the exact spectrum is superimposed in each example as a red curve in the last column.

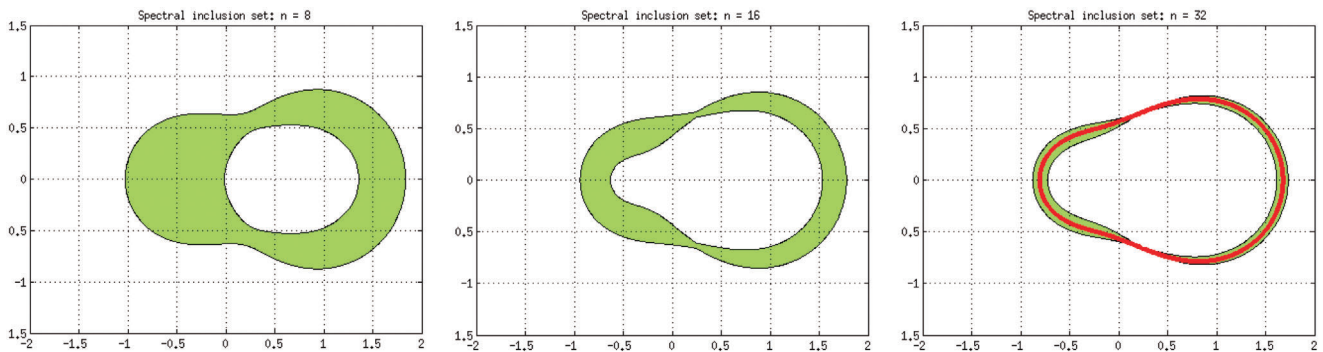
- a) We start with the right shift, where the subdiagonal is $\alpha = (\dots, 1, 1, 1, \dots)$ and the main and superdiagonal are $\beta = \gamma = (\dots, 0, 0, 0, \dots)$. The spectrum is the unit circle, and here are our supersets for $n \in \{4, 8, 16\}$:



- b) Our next example is 3-periodic with subdiagonal $\alpha = (\dots, \mathbf{0}, 0, 0, \dots)$, main diagonal $\beta = (\dots, -\frac{3}{2}, \mathbf{1}, 1, \dots)$ and superdiagonal $\gamma = (\dots, \mathbf{1}, 2, 1, \dots)$, where α_0 , β_0 and γ_0 are highlighted in boldface. The spectrum consists of two disjoint loops, and we depict our supersets for $n \in \{32, 64, 128\}$:



- c) Our third example is also 3-periodic with subdiagonal $\alpha = (\dots, \mathbf{0}, 0, 0, \dots)$, main diagonal $\beta = (\dots, -\frac{1}{2}, \mathbf{1}, 1, \dots)$ and superdiagonal $\gamma = (\dots, \mathbf{1}, 2, 1, \dots)$, where α_0 , β_0 and γ_0 are highlighted in boldface. The spectrum consists of one loop, and we depict our supersets for $n \in \{8, 16, 32\}$:



Another effect of the 3-periodicity of the diagonals in A is that there are only three distinct submatrices $AP_{n,k}$ and $A^*P_{n,k}$ each for $k \in \mathbb{Z}$. In fact, for many operator classes, the infinite unions in (5.1), (7.1) and so on, reduce to finite unions. For example, for a $\{0, 1\}$ -valued aperiodic diagonal [16], there are only $n + 1$ different subwords of length n , and for a $\{0, 1\}$ -valued random diagonal, there are 2^n (again, finitely many) different subwords of length n . Also, for non-discrete diagonal alphabets, the infinite union can be reduced to a finite one via compactness arguments, see our discussion in ref. [12].

9 | APPROXIMATING ESSENTIAL SPECTRA

In the case where A is an infinite matrix there is large interest also in the approximation of the *essential spectrum*, $\text{spec}_{\text{ess}} A$, which is the spectrum in the Calkin algebra, that is, the set of all $\lambda \in \mathbb{C}$ where $A - \lambda I$ is not a Fredholm operator, that is, is not invertible modulo compact operators.

Our results in this section apply when each $A_{i,j} \in \mathbb{C}$, but also when each $A_{i,j}$ is a bounded linear operator on a Banach space X , as long as X is finite-dimensional or the operators $\{A_{i,j}\}$ are collectively compact in the sense of refs. [17, 18].

As for the spectrum (see Section 3) it is enough to consider the case when A is tridiagonal. The bi-infinite case is easily reduced to the semi-infinite case: Indeed, modulo compact operators,

$$A \cong \begin{pmatrix} \ddots & & & \\ & \ddots & & \\ & & A_{-2,-2} & A_{-2,-1} \\ & & A_{-1,-2} & A_{-1,-1} \\ \hline & & & 0 \\ \hline & & & A_{1,1} & A_{1,2} \\ & & & A_{2,1} & A_{2,2} & \ddots \\ & & & & \ddots & \ddots \end{pmatrix} =: \begin{pmatrix} A_- & & \\ & 0 & \\ & & A_+ \end{pmatrix},$$

so that

$$\text{spec}_{\text{ess}} A = \text{spec}_{\text{ess}} A_- \cup \text{spec}_{\text{ess}} A_+.$$

It remains to look at semi-infinite banded matrices A . Modulo compact operators, for every $m \in \mathbb{N}$,

$$A = \begin{pmatrix} A_{11} & A_{12} & & \\ A_{21} & A_{22} & \ddots & \\ & & \ddots & \ddots \end{pmatrix} \cong \begin{pmatrix} 0 & & & \\ & \ddots & & \\ & & 0 & \\ \hline & & & A_{m+1,m+1} & A_{m+1,m+2} \\ & & & A_{m+2,m+1} & A_{m+2,m+2} & \ddots \\ & & & & \ddots & \ddots \end{pmatrix},$$

so that, with

$$\begin{pmatrix} A_{m+1,m+1} & A_{m+1,m+2} & & \\ A_{m+2,m+1} & A_{m+2,m+2} & \ddots & \\ & & \ddots & \ddots \end{pmatrix} =: A_{>m},$$

we have

$$\operatorname{spec}_{\text{ess}} A = \operatorname{spec}_{\text{ess}} A_{>m} \subseteq \operatorname{spec} A_{>m} \subseteq \bigcup_{k \geq m} \operatorname{Spec}_{\varepsilon_n}(AP_{n,k}, A^*P_{n,k}), \quad m, n \in \mathbb{N},$$

using the semi-infinite version of (7.1) in the last step. Taking the intersection over all $m, n \in \mathbb{N}$ gives

$$\operatorname{spec}_{\text{ess}} A \subseteq \bigcap_{n \in \mathbb{N}} \bigcap_{m \in \mathbb{N}} \bigcup_{k \geq m} \operatorname{Spec}_{\varepsilon_n}(AP_{n,k}, A^*P_{n,k}). \quad (9.1)$$

In ref. [13], using results from ref. [2], we prove the following:

Proposition 9.1 (Semi-infinite). *For bounded band operators A on $\ell^2(\mathbb{N})$, formula (9.1) holds in fact with “ $\subseteq$ ” replaced by equality. In addition, after this replacement,*

- a) *the intersection sign “ $\bigcap_{n \in \mathbb{N}}$ ” in (9.1) can be replaced by a Hausdorff-limit $\lim_{n \rightarrow \infty}$;*
- b) *the two intersection signs “ $\bigcap_{n \in \mathbb{N}} \bigcap_{m \in \mathbb{N}}$ ” in (9.1) can be replaced by a single Hausdorff-limit $\lim_{m=n \rightarrow \infty}$.*

ACKNOWLEDGMENTS

Open access funding enabled and organized by Projekt DEAL.

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How to cite this article: Chandler-Wilde, S. N., Chonchaiya, R., & Lindner, M. (2023). Convergent spectral inclusion sets for banded matrices. *Proceedings in Applied Mathematics and Mechanics*, e202300016.

<https://doi.org/10.1002/pamm.202300016>