

# Computing the spectrum and pseudospectrum of infinite-volume operators from local patches

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## Abstract

We show how the spectrum of normal discrete short-range infinite-volume operators can be approximated with two-sided error control using only data from finite-sized local patches. As a corollary, we prove the computability of the spectrum of such infinite-volume operators with the additional property of finite local complexity and provide an explicit algorithm. Such operators appear in many applications, e.g. as discretizations of differential operators on unbounded domains or as so-called tight-binding Hamiltonians in solid state physics. For a large class of such operators, our result allows for the first time to establish computationally also the absence of spectrum, i.e. the existence and the size of spectral gaps. We extend our results to the  $\varepsilon$ -pseudospectrum of non-normal operators, proving that also the pseudospectrum of such operators is computable.

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# 1 Introduction

The computation of spectra of linear operators is a fundamental problem that has been studied at various levels of generality. For finite-dimensional matrices, the theorem of Abel and Ruffini shows that there is no closed-form solution [1, 86], but the eigenvalues can be approximated numerically [99, 50, 88]. The approximation error can be bounded using statements such as the Gershgorin and Bauer-Fike theorems [49, 6, 93], and there are also algorithms that compute validated intervals for the eigenvalues, thus providing rigorous error control [102–104].

Operators on infinite-dimensional spaces are usually studied by restriction to a finite-dimensional subspace. Rigorous upper bounds on the eigenvalues can be derived from finite-dimensional approximations using the Rayleigh-Ritz method [85, 83]. A number of methods have been proposed over the years to compute complementary lower bounds on the eigenvalues [100, 63, 101, 7–9, 17, 18, 41]. These methods usually assume that the spectrum in a certain energy window consists of a finite number of eigenvalues [83]. Thus, they are applicable for example to differential operators on compact domains. For this setting, e.g. finite element methods with error control are available [30, 29, 79, 60].

In this paper, we consider the problem of computing spectra with rigorous and explicit error control for *short-range infinite volume operators*, a class of operators for which the known methods do not apply and which are at the same time very relevant for applications. We say that a bounded operator  $H$  on a separable Hilbert space  $\mathcal{H}$  is a short-range infinite volume operator, if there is a basis  $(e_x)_{x \in \Gamma}$  indexed by a uniformly discrete subset  $\Gamma \subset \mathbb{R}^n$  for some  $n \in \mathbb{N}$ , such that the matrix elements  $H_{xy} := \langle e_x, H e_y \rangle$  of  $H$  fulfill the *short-range* condition

$$|H_{xy}| \leq C \frac{1}{d(x, y)^{n+\varepsilon}}$$

for some  $C, \varepsilon > 0$  and all  $x, y \in \Gamma$ . Here  $d$  denotes the maximum distance on  $\mathbb{R}^n$ , cf. (8). Important examples of such short-range infinite volume operators are discretizations of differential operators on infinite domains and so-called tight-binding models from solid state physics. In Section 2.3 we briefly discuss examples of operators arising from applications for which computability of the spectrum was not previously known and to which our algorithm can be applied.

Since there is an extensive mathematical literature dealing with the spectral problem for infinite volume operators, we will briefly comment on some recent results. The easiest method to implement is probably the finite section method, which is not only widely used in practice, but has also been studied theoretically from various perspectives [4, 28, 32, 74, 75, 31]. The finite section  $H_\Lambda$  of  $H$  on a finite subset  $\Lambda \subset \Gamma$  is just the square matrix  $(H_{xy})_{x, y \in \Lambda}$ . For certain classes of operators, sequences of finite sections can be found such that their spectra are provably convergent. However, the occurrence of spectral pollution at the boundaries makes it difficult to achieve good error control for general operators using finite sections [42, 73].

Another popular approach to computing the spectrum of infinite-volume operators with strong error control is based on approximating aperiodic operators by periodic ones, e.g. [16, 15, 33]. Bounding the approximation error of such periodic approximations has motivated a number of results proving the Lipschitz or Hölder continuity of the spectrum in the coefficients for a large class of operators connected to dynamical systems [21, 14]. Because there are easily computable bounds on the Lipschitz constants, these continuity results can be used to provide error control for the convergence of the approximant spectra in Hausdorff distance.

To make practical use of these bounds, however, suitable periodic approximations are required. To use the Lipschitz continuity of the spectrum, the periodic approximant has to have the same set of local patches as the infinite-volume operator at a certain scale. While the existence of such periodic approximations for substitution systems is increasingly well-understood in one dimension [12, 38, 94] the situation in higher dimensions is more complex and under active investigation [13, 5]. In both cases, there are important examples of operators that cannot be approximated periodically, such as the jump potential in one dimension, or the two-dimensional Penrose tiling, for which the local matching rules force an aperiodic pattern [82]. Therefore, while the dynamical systems method provides strong error control, it requires the construction of periodic approximants, which is not always possible and for which no general algorithm is known.

A different way to compute spectra is the recently proposed method of *uneven sections* [36, 33], in which the operator  $H$  is approximated by a rectangular matrix  $(H_{xy})_{x \in \Lambda', y \in \Lambda}$  for some finite  $\Lambda \subset \Lambda' \subset \Gamma$ . In addition to effectively reducing spectral pollution compared to the finite section method, this method also provides one-sided error control [36].

A central object in the following discussions is the so-called *lower norm function*

$$\rho_H(\lambda) = \begin{cases} \|(H - \lambda)^{-1}\|^{-1} & \text{for } \lambda \notin \text{Spec}(H) \\ 0 & \text{otherwise.} \end{cases} \quad (1)$$

For normal operators  $H$  it satisfies  $\rho_\lambda(H) = d(\lambda, \text{Spec}(H))$  and for general operators it can serve as a definition of the  $\varepsilon$ -pseudospectrum, cf. (11).

The method from [36] implies (cf. Theorem 22 below) that for every patch size  $L > 0$  and center point  $x \in \mathbb{R}^n$  the smallest singular value  $\varepsilon_{L,\lambda,x} \geq 0$  of the rectangular matrix  $(H_{yz})_{y \in B_{L+m}(x), z \in B_L(x)}$  satisfies

$$\rho_H(\lambda) \leq \varepsilon_{L,\lambda,x} \quad (2)$$

and thus, for normal  $H$ , also

$$d(\lambda, \text{Spec}(H)) \leq \varepsilon_{L,\lambda,x}. \quad (3)$$

Here  $B_L(x) \subset \mathbb{R}^n$  denotes the hypercube around  $x$  with side length  $2L$  and  $m$  is a fixed finite number.

This form of error control is only one-sided, however, as there is no lower bound for  $\rho_H(\lambda)$ . In fact, the authors of [36] prove that no algorithm giving a lower bound on  $\rho_H(\lambda)$  can exist as long as the operator is given solely by its matrix elements [52]. The impossibility of a lower bound implies that only the existence of spectrum in a certain interval can be shown, while the absence of spectrum (a spectral gap) can not be rigorously established in this general setting. This also implies that it is not possible to give a bound on the Hausdorff distance to the infinite-volume spectrum, as for example in the periodic approximation approach of [16, 15].

However, for many applications involving infinite volume operators the existence and size of spectral gaps is of central importance. In a previous paper, we have shown that the no-go theorem which rules out a lower bound on  $\rho_H(\lambda)$  can be circumvented in most cases of physical

interest, and have given a practical algorithm to compute validated spectral gaps of an infinite-volume system by considering all subsystems of a given size [57]. In the present work, we expand on this by giving a general algorithm to compute the spectrum of operators with finite local complexity (*flc*) with full error control. The primary insight making this possible is that for finite range operators knowledge of the infimum of  $\varepsilon_{L,\lambda,x}$  over *all centers*  $x \in \mathbb{R}^n$  is sufficient to provide a quantitative lower bound on  $\rho_H(\lambda)$ . More precisely, for

$$\varepsilon_{L,\lambda} := \inf_{x \in \mathbb{R}^n} \varepsilon_{L,\lambda,x},$$

we prove the following theorem.

**Theorem 1.** *Let  $H$  be a discrete operator with finite range  $m > 0$ . Then for every  $\lambda \in \mathbb{C}$  and  $L > m$  it holds that*

$$\rho_H(\lambda) \geq \varepsilon_{L,\lambda} \sqrt{1 - \delta_L} - \|H - \lambda\| \sqrt{\delta_L}, \quad (4)$$

where  $\varepsilon_{L,\lambda} := \inf_{x \in \mathbb{R}^n} \varepsilon_{L,\lambda,x}$ , with  $\varepsilon_{L,\lambda,x}$  defined in (24), and

$$\delta_L := \frac{n}{\lfloor L/m \rfloor}. \quad (5)$$

The practical significance of Theorem 1 lies in the observation that for *flc* operators, the infimum  $\varepsilon_{L,\lambda}$  can be computed by evaluating  $\varepsilon_{L,\lambda,x}$  for a finite number of suitably chosen centres  $x \in \mathbb{R}^n$ . We show that combining (2) and (4) then leads to a general algorithm for computing the spectrum of *flc* operators with error control. That is, given any short-range, discrete, normal, *flc* operator  $H$  and  $k \in \mathbb{N}$ , our algorithm computes an approximation  $\Gamma_k(H) \subseteq \mathbb{C}$  such that

$$d_H(\text{Spec}(H), \Gamma_k(H)) \leq 2^{-k}, \quad (6)$$

where  $d_H$  is the Hausdorff distance on subsets of  $\mathbb{C}$ . Thus the algorithm is able to compute the spectrum of *flc* infinite-volume operators to any given precision in Hausdorff distance.

For non-normal operators, we can use Theorem 1 to show the computability of the  $\varepsilon$ -pseudospectrum [71, 98, 58, 96]  $\text{Spec}_\varepsilon(H)$ . Again, we provide an algorithm which computes for any  $\varepsilon > 0$  an approximation  $\Gamma_k(H, \varepsilon)$  such that

$$d_H(\text{Spec}_\varepsilon(H), \Gamma_k(H, \varepsilon)) \leq 2^{-k}. \quad (7)$$

The existence of algorithms fulfilling (6) and (7) should be viewed in the context of previous results about the computability of the general infinite-dimensional spectral problem [52]. In extending the theory of computability from discrete computations to analytical and numerical problems [97, 27, 26], the *solvability complexity index* (SCI) is a very useful classification of computational problems by the number of limits required for their solution [52]. The spectral problem for operators on infinite-dimensional spaces has been a particular focus of investigation for determining the SCI [43, 53, 54, 35, 55, 23, 34, 87].

If a general infinite-volume operator is given by its matrix entries, it has been shown that it is impossible to compute the spectrum with error control [36]. But it is possible to compute the spectrum via a series of convergent estimates (without error control), which places the general spectral problem for self-adjoint operators in the SCI = 1 class, which require one limit to solve [52]. The precise SCI has also been determined for many spectral problems differing in the conditions placed on  $H$  [22]. The possibility of one-sided error control by an upper bound on the distance to spectrum has also inspired an intermediate SCI class  $\Sigma_1$  that is in between the classes  $\Delta_1$  and  $\Delta_2$ , the classes of SCI = 1 with and without error control, respectively [35, 22].

The authors of this no-go theorem have stressed, however, that the SCI of a given computation can be lowered through additional structure and conditions on the general problem [22]. This is precisely what we achieve here by introducing the structure of finite local complexity. It turns out that by adding this requirement, the spectrum becomes computable and the *flc* spectral problem is therefore in class  $\Delta_1$  (full error control), instead of the class  $\Delta_2$  (SCI = 1) or  $\Sigma_1$  (one-sided error control), which contains the general spectral problem. This lowering of the SCI is especially interesting in light of the fact the *flc* is a rather general condition that is fulfilled by most operators that occur in practice.

## 2 Definitions of computational problems

To prove the computability of the spectrum for operators of finite local complexity, we require a clear notion of computational problems and their solvability. Following [22], we define a computational problem by the following data:

**Definition 2.** A *computational problem* is a tuple  $(\Omega, \Lambda, (\mathcal{M}, d), \Xi)$ , where

- $\Omega$  is a set (the “set of problems”);
- $\Lambda$  is a family of functions  $\Lambda = (f_i)_{i \in \mathcal{G}}$ , indexed by a countable set  $\mathcal{G}$ , where each  $f_i$  is a function  $f_i : \Omega \rightarrow \mathbb{R}$  (the “evaluation functions”);
- $(\mathcal{M}, d)$  is a metric space (the metric space of “possible solutions”);
- $\Xi$  is a function  $\Omega \rightarrow \mathcal{M}$  (the “problem function”).

In this definition, the set  $\Omega$  is the set of concrete problems that an algorithm has to be able to solve. For spectral problems, this would correspond to a certain set of operators. The exact solution of the problem is given by the function  $\Xi$ , which takes values in the metric space  $(\mathcal{M}, d)$ . For the spectral case, we would choose  $\Xi(A) = \text{Spec}(A)$  for any  $A \in \Omega$ , and  $\mathcal{M}$  would be the power set of  $\mathbb{C}$ . Because we approximate the spectrum and pseudospectrum in Hausdorff distance, we equip  $\mathcal{M}$  with the Hausdorff distance  $d_H$ . The functions  $f_i \in \Lambda$ , finally, define how the algorithm can get information about the concrete problem. For the spectral problem as defined in [36], for example, the evaluation functions would return the matrix elements of the operator in a certain basis, for example. We would like to stress that the choice of evaluation functions  $f_i \in \Lambda$  can be decisive for the solvability or unsolvability of a computational problem.

Computational problems can be solved by algorithms. The solvability of course depends on what kinds of computations one allows the algorithm to perform (for example, whether only algebraic or more general computations are allowed) [22]. Unless otherwise noted, in the following we will understand computability to refer to algorithms that can be executed by BSS machines [27, 26], a classical framework for computations with real numbers. In Appendix B, we describe our model of computation in more detail, including what it means for the BSS algorithm to sequentially access information about the computational problem via the evaluation functions  $f_i \in \Lambda$ .

In this paper, we consider the spectral and pseudospectral problem with the additional structure of finite local complexity (*flc*). We can thus circumvent the impossibility result of [36] by using a restricted set  $\Omega$ . But the resulting class of *flc* operators is still very general, and can accommodate many if not most physical situations, including all examples from [36]. We show that the spectral problem becomes computable when considering operators of finite local complexity. In addition to restricting the problem set  $\Omega$ , the set of evaluation functions  $\Lambda$  must be augmented in order to allow the algorithm to make use of the *flc* structure.

**Definition 3.** A subset  $\Gamma \subseteq \mathbb{R}^n$  is called *uniformly discrete* if there exists a constant  $q > 0$  such that  $d(x, y) > q$  for all  $x, y \in \Gamma$  with  $x \neq y$ .

In the above definition, and for the rest of this paper, we define the distance  $d(x, y)$  on  $\mathbb{R}^n$  as the *maximum distance*

$$d((x_1, \dots, x_n), (y_1, \dots, y_n)) = \max_{k=1, \dots, n} |x_k - y_k|. \quad (8)$$

We also define  $B_r(x)$ , for  $x \in \mathbb{R}^n$  and  $r > 0$ , as the open ball using this distance; that is, the set  $B_r(x)$  is a hypercube with side length  $2r$  centered at  $x$ .

**Definition 4.** We define a *discrete operator*  $H$  in dimension  $n \in \mathbb{N}$  as a bounded operator on a separable Hilbert space  $\mathcal{H}$ , together with an orthonormal basis  $(e_i)_{i \in \Gamma}$  indexed by a uniformly discrete subset  $\Gamma \subset \mathbb{R}^n$ . We define the *matrix elements* at points  $x, y \in \Gamma$  as  $H_{xy} = \langle e_x, H e_y \rangle$ .

In the following, we will always represent discrete operators  $H$  with respect to the special basis  $(e_i)_{i \in \Gamma}$  and use the basis isomorphism to identify  $\mathcal{H}$  with  $\ell^2(\Gamma)$ . Furthermore, for any  $x \in \mathbb{R}^n$  and  $L > 0$ , the finite dimensional subspace  $\mathcal{H}_{B_L(x)} \subset \mathcal{H}$  is defined by  $\mathcal{H}_{B_L(x)} := \text{span}\{e_x \mid x \in B_L(x)\}$ , and the orthogonal projection onto  $\mathcal{H}_{B_L(x)}$  is denoted by  $\mathbf{1}_{B_L(x)}$ .

We now define our two main conditions on  $H$ , short-range and finite local complexity.

**Definition 5.** Let  $H$  be a discrete operator in dimension  $n$ . Then  $H$  is called *short-range* if there exist  $C$  and  $\varepsilon > 0$  such that

$$|H_{xy}| \leq C d(x, y)^{-(n+\varepsilon)}.$$

for all  $x, y \in \Gamma$ .  $H$  is said to have *finite range* if there is a number  $m > 0$  (the maximal hopping length) such that  $H_{xy} = 0$  whenever  $d(x, y) > m$ .

The condition of finite local complexity is usually defined for point sets [68–70, 24]. Very succinctly, a uniformly discrete set  $\Gamma \subset \mathbb{R}^n$  is defined to have *flc* iff  $\Gamma - \Gamma$  is discrete. This turns out to be equivalent to the set of finite patches  $\{\Gamma \cap B_L(x) \mid x \in \Gamma\}$ , falling into finitely many equivalence classes under translation [24] for each  $L > 0$ . To extend this concept to operators, we require that there are finitely many equivalence classes on which, additionally, the operator  $H$  acts in the same way, which we define precisely as follows.

**Definition 6.** A discrete operator  $H$  is said to have *equivalent action* on two subsets  $A, B \subseteq \Gamma$  if there is a  $t \in \mathbb{R}^n$  such that  $B = t + A$  and if there exist  $U(z) \in S^1 \subseteq \mathbb{C}$  for every  $z \in A$  such that for any  $a_1, a_2 \in A$  we have

$$H_{b_1 b_2} = U(a_1) H_{a_1 a_2} U(a_2)^*,$$

where  $b_1 = a_1 + t, b_2 = a_2 + t$ .

**Remark 7.** It is clear that for any operator  $H$ , equivalent action of  $H$  defines an equivalence relation on subsets of  $\Gamma$ . The complex phases  $U(a_1)$  and  $U(a_2)$  can often be set to unity, but they are necessary as gauge transformations for certain operators, in particular for discrete Schrödinger operators with magnetic fields.

**Definition 8.** A discrete operator  $H$  is said to have *finite local complexity* if for any  $L > 0$ , the set  $\{\Gamma \cap B_L(x) \mid x \in \mathbb{R}^n\}$  is contained in finitely many equivalence classes with respect to equivalent action of  $H$ .

**Remark 9.** More explicitly,  $H$  has finite local complexity if for any  $L > 0$  there are finitely many  $x_1, \dots, x_s \in \mathbb{R}^n$  such that for any  $y \in \mathbb{R}^n$ , there is a  $k \in \{1, \dots, s\}$  such that  $H$  has equivalent action on  $\Gamma \cap B_L(y)$  and  $\Gamma \cap B_L(x_k)$ .

We now define the spectral and pseudospectral problems for operators of finite local complexity. The main goal of this paper is to show that these problems are solvable with error control. We will consider the spectral problem only for normal operators. The spectral problem

for non-normal operators is intractable because the spectrum of non-normal operators is not Hausdorff-continuous in the matrix entries, even for *flc* operators [96]. Instead, we show that the  $\varepsilon$ -pseudospectrum is computable for non-normal operators, for all  $\varepsilon > 0$ .

To define the spectral problem for operators of finite local complexity, some work has to be done to define suitable evaluation functions which will allow the algorithm to make use of the *flc* structure. There are multiple ways to do this; for example, it would be sufficient to give the algorithm access to the *repetitivity function*, which gives a radius in which all patches of size  $L$  occur [24]. However, to stay closer to the way actual implementations are likely to operate, we here define the evaluation so as to allow the algorithm to enumerate all local patches of a given size and to access the matrix elements and site locations for any given patch. It is expected that for concrete applications, special-purpose algorithms for the enumeration of local patches will be used. We have demonstrated this for the case of cut-and-project quasicrystals in [57, 56]. Because the exact definition of the evaluation functions is a bit tedious, it is given in Appendix C. We now define the *flc* version of the spectral computational problem as follows.

**Definition 10.** The *flc spectral problem* is the computational problem  $(\Omega, \Lambda, (\mathcal{M}, d_H), \Xi)$ , where

- $\Omega$  is the set of normal discrete operators with finite local complexity and short-range;
- $\Lambda$  is a family of functions  $(f_i)_{i \in \mathcal{G}}$  satisfying Conditions 35 in Appendix C;
- $\mathcal{M}$  comprises all compact subsets of  $\mathbb{C}$ , and  $d_H$  is the Hausdorff distance;
- $\Xi$  is the function which assigns to every operator  $H$  its spectrum,  $\Xi(H) = \text{Spec}(H)$ .

One of the main results in this paper is that the *flc* spectral problem is solvable with error control in Hausdorff distance.

**Theorem 11.** *Let  $(\Omega, \Lambda, (\mathcal{M}, d_H), \Xi)$  be the flc spectral problem. Then for every  $k \in \mathbb{N}$  there exists a Blum-Shub-Smale (BSS) algorithm  $\Gamma_k : \Omega \rightarrow \mathcal{M}$ , using the family of evaluation functions  $\Lambda$ , such that*

$$d_H(\Gamma_k(H), \Xi(H)) \leq 2^{-k}$$

for all  $H \in \Omega$ .

The proof of this Theorem is given in Sections 6 and 7.

## 2.1 The pseudospectrum

For non-normal operators, we cannot compute the spectrum itself, but it is still possible to compute the  $\varepsilon$ -pseudospectrum for  $\varepsilon > 0$ . The pseudospectrum may be defined in terms of the *lower norm function*  $\rho_H : \mathbb{C} \rightarrow \mathbb{R}_+$  [77], which is defined as

$$\rho_H(\lambda) = \begin{cases} \|(H - \lambda)^{-1}\|^{-1} & \text{for } \lambda \notin \text{Spec}(H) \\ 0 & \text{otherwise.} \end{cases} \quad (9)$$

The lower norm function is not a norm, but it can be given a variational definition that is similar to the operator norm:

$$\rho_H(\lambda) = \inf_{\psi \in \mathcal{H} \setminus \{0\}} \frac{\|(H - \lambda)\psi\|}{\|\psi\|}. \quad (10)$$

Moreover,  $\rho_H$  is Lipschitz continuous with Lipschitz constant 1 (see, for example, [76], Lemma 2.1). The  $\varepsilon$ -pseudospectrum is defined as the closed  $\varepsilon$ -sublevel set of  $\rho_H$ :

$$\text{Spec}_\varepsilon(H) := \{z \in \mathbb{C} \mid \rho_H(z) \leq \varepsilon\}. \quad (11)$$

Some authors also define the pseudospectrum as the open set  $\text{Spec}_\varepsilon^\circ(H) = \{z \in \mathbb{C} \mid \rho_H(z) < \varepsilon\}$ , using a strict inequality. This has no influence on the computability, however, because  $\text{Spec}_\varepsilon(H)$  is the closure of  $\text{Spec}_\varepsilon^\circ(H)$  [96], and thus  $\text{Spec}_\varepsilon(H)$  and  $\text{Spec}_\varepsilon^\circ(H)$  have Hausdorff distance zero. Consequently, any algorithm computing  $\text{Spec}_\varepsilon(H)$  with error control, according to Equation (7), also computes  $\text{Spec}_\varepsilon^\circ(H)$  in this sense and vice versa.

For normal operators, we have

$$\rho_H(\lambda) = d(\lambda, \text{Spec}(H)), \quad (12)$$

thus the  $\varepsilon$ -pseudospectrum of a normal operator  $H$  is just the  $\varepsilon$ -fattening of its spectrum. For non-normal operators, we still have

$$\rho_H(\lambda) \leq d(\lambda, \text{Spec}(H)).$$

Thus the  $\varepsilon$ -pseudospectrum always contains the  $\varepsilon$ -fattening of  $\text{Spec}(H)$ . A computational problem for the  $\varepsilon$ -pseudospectrum can be defined similarly as for the spectrum:

**Definition 12.** The *flc pseudospectral problem* is the computational problem  $(\Omega_{\text{ps}}, \Lambda_{\text{ps}}, (\mathcal{M}, d_H), \Xi_{\text{ps}})$ , where

- $\Omega_{\text{ps}}$  is the set of all tuples  $(H, \varepsilon)$ , where  $H$  is a discrete operator with finite local complexity and short-range (but not necessarily normal), and  $\varepsilon > 0$ ;
- $\Lambda_{\text{ps}}$  consists of the same evaluation functions of Definition 10, applied to  $H$ , and one additional evaluation function which returns  $\varepsilon$ ;
- $(\mathcal{M}, d_H)$  is as in Definition 10;
- $\Xi_{\text{ps}}(H, \varepsilon) = \text{Spec}_\varepsilon(H)$ .

The following theorem states that the  $\varepsilon$ -pseudospectrum, for  $\varepsilon > 0$ , is computable with error control, just like the spectrum for normal operators.

**Theorem 13.** *Let  $(\Omega_{\text{ps}}, \Lambda_{\text{ps}}, (\mathcal{M}, d), \Xi_{\text{ps}})$  be the flc pseudospectral problem. Then for every  $k \in \mathbb{N}$  there exists a Blum-Shub-Smale (BSS) algorithm  $\Gamma_k : \Omega_{\text{ps}} \rightarrow \mathcal{M}$ , using the family of evaluation functions  $\Lambda_{\text{ps}}$ , such that*

$$d(\Gamma_k(H, \varepsilon), \Xi_{\text{ps}}(H, \varepsilon)) \leq 2^{-k}$$

for all  $H \in \Omega_{\text{ps}}$ .

The proof of Theorem 13 is given in Section 8.

**Remark 14.** The computation of the (pseudo-) spectrum in systems of finite local complexity can be performed practically by our method. In [57], we have already described an algorithm to prove spectral gaps using an edge state criterion on finite patches. For this we used Dirichlet boundary conditions and computed an edge state criterion to provably avoid spectral pollution. While this method could be used to prove the computability of the spectrum [56], here we instead use the method of uneven sections [36], which enables us to give a unified treatment of the computation of the spectrum and pseudospectrum. Although it is not as efficient as the Dirichlet-based method of [57] for higher-dimensional system, we can use this approach to compute gap bounds for the  $\varepsilon$ -pseudospectrum. Figure 1 shows a computation of the spectral inclusion and spectral gap bounds for the pseudospectrum of a non-Hermitian Hamiltonian with Fibonacci-like potential [48, 40, 61].

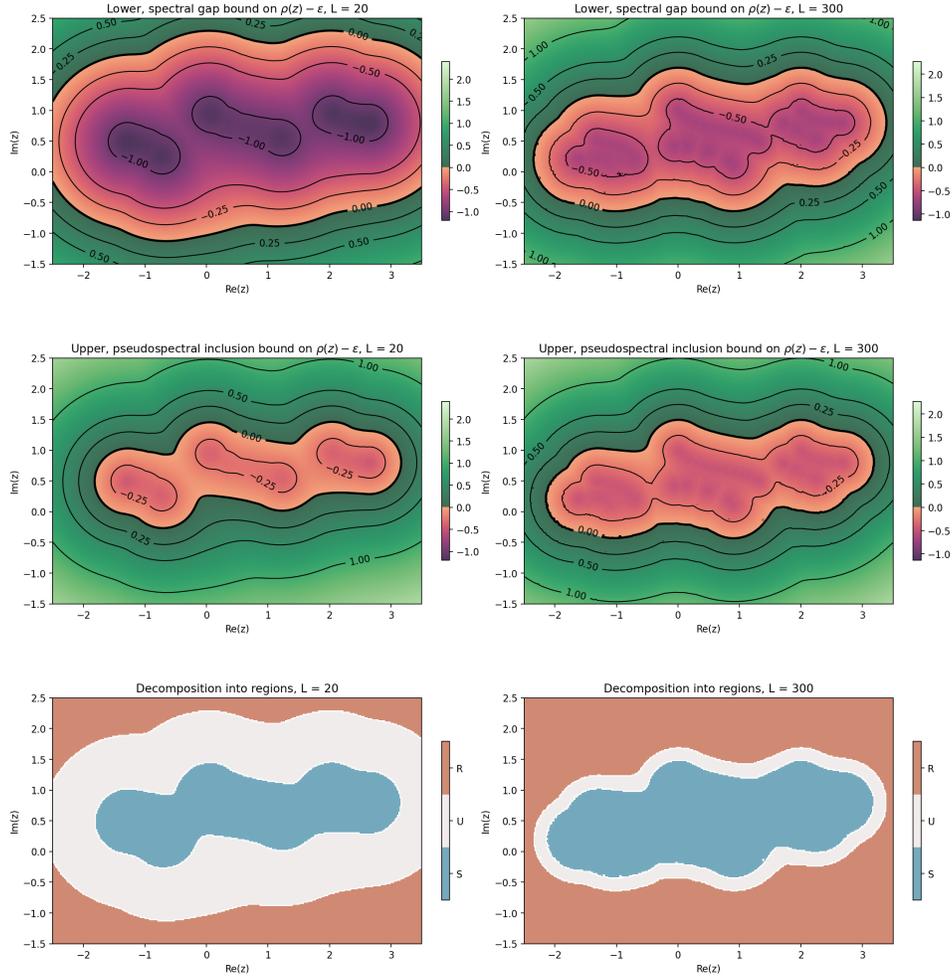


Figure 1: Exact computation of the  $\varepsilon$ -pseudospectrum of a non-Hermitian Hamiltonian with a cut-and-project potential for  $\varepsilon = 0.5$ . The Hamiltonian is defined by  $H\psi(n) = -\psi(n-1) + V(n)\psi(n) - \psi(n+1)$ . The chosen potential has the form  $V(n) = (1+i)\mathbf{1}(\alpha n < 1/\alpha)$ , where we chose  $\alpha = 1.66$  (For  $\alpha = (1+\sqrt{5})/2$ , this construction gives the Fibonacci quasicrystal, but we chose  $\alpha = 1.66$  because it creates a less uniform potential leading to a slower convergence and thus a more pronounced effect of increasing  $L$  in the pictures.). The left and right column show the same computation with  $L = 20$  and  $L = 300$ , respectively. The uppermost row shows the lower, spectral gap bound on  $\rho_H$ , while the row below shows the upper bound on  $\rho_H$  from [36]. If the lower bound is positive, the associated point is known to be in the complement of the pseudospectrum; if the upper bound is negative, the point is known to be inside the pseudospectrum. This gives a decomposition of the plane into three sets  $R, U$ , and  $S$  of points, where it is known that  $S \subseteq \text{Spec}_\varepsilon(H)$ , that  $R \cap \text{Spec}_\varepsilon(H) = \emptyset$ , and no statement can be made about  $U$ . This is very similar to the sets  $S_\tau, R_\tau$  and  $U_\tau$  in Section 8, except that here we have fixed  $L$  instead of  $\tau$  and we do not vary the spacing of the grid on which  $\tilde{\rho}_H(\lambda, \tau)$  is evaluated.

## 2.2 Proof strategy

Our proof of Theorems 11 and 13 is based on the spectral detectability result, Theorem 1. We have formulated Theorem 1 for finite-range as opposed to short-range operators because this simplifies the statement considerably. In Section 3, we show that the computational spectral and pseudospectral problems for short-range *flc* operators can be reduced to that for finite range operators.

In Section 4, we recall the upper bound  $\varepsilon_{L,\lambda,x}$  on  $\rho_H(\lambda)$  from [36], adapted to our setting and finite range interactions. The corresponding lower bound on  $\rho_H(\lambda)$  that as formulated in Theorem 1 is our most important novel contribution. The proof is given in Section 5 and combines the method of *uneven sections* with the new notion of *n-disjoint* subsets. In Section 6, we apply Theorem 1 to show that  $\rho_H(\lambda)$  is computable at every  $\lambda \in \mathbb{C}$ .

In Section 7, we show how to apply the computability of  $\rho_H(\lambda)$  at any  $\lambda \in \mathbb{C}$  to show the computability of the spectrum (Theorem 11). The computability of the  $\varepsilon$ -pseudospectrum (Theorem 13) is shown in Section 8.

## 2.3 Examples

Infinite-volume operators which are discrete and of finite local complexity, as described in Definitions 4, 5, and 8, occur frequently in physics. For example, a so-called discrete Schrödinger operator on  $\ell^2(\mathbb{Z}^n)$  [64, 95, 72] is of the form

$$(H\psi)(x) = (2n + V(x))\psi(x) - \sum_{\substack{y \in \mathbb{Z}^n \\ d(x,y)=1}} \psi(y)$$

and can be obtained as the discretization of a Schrödinger operator on  $\mathbb{R}^n$ . Here the function  $V : \mathbb{Z}^n \rightarrow \mathbb{R}$  is called the potential. Despite its simple structure, the spectral problem for discrete Schrödinger operators is an area of active research [44, 84, 78].

The spectrum of a discrete Schrödinger operator with periodic potential  $V(x)$  can be computed using the Bloch-Floquet transform. In this case, the spectrum consists of finitely many intervals separated by so called gaps. A more general class of operators is obtained when  $V(x)$  is defined via a substitution rule. Such operators are of high interest in mathematical physics due to their connection to quasicrystals. For example,  $V(x)$  may be the Fibonacci potential [66, 40, 61] or the Thue-Morse sequence [19]. Important mathematical questions about these operators concern the nature and fractal dimension of their spectrum [92, 37] and the gap labelling [20, 65].

Despite many results on the fractal nature of the spectrum, for numerical investigation the spectrum is usually approximated by reverting to periodic approximants [39]. While good error bounds on the spectrum of such approximations exist [11, 16] and can be computed in concrete cases, their application requires specialized analysis to find suitable periodic approximations and compute the constants in the bound [10]. In contrast, our method only requires the enumeration of local patches of a given size, and therefore provides the first immediately applicable algorithm to compute the spectrum of discrete Schrödinger operators with potentials given by substitution rules.

The Schrödinger operator can also be discretized when a magnetic field is present. In the case of a constant magnetic field in a two-dimensional square lattice, this leads to the Hofstadter model [59, 89], which is famous for the self-similar, fractal structure of its spectrum as a function of the magnetic field (Hofstadter butterfly). The spectrum of the Hofstadter model is usually approximated using periodic approximations; however, this is only possible for rational fluxes [59]. For general fluxes, our method is to our knowledge the first that allows

computing the spectrum with error control to arbitrary precision in the infinite Hofstadter model.

The Hofstadter model has also been investigated on quasiperiodic lattices like Ammann-Beenker and Rauzy tilings, which lead to a butterfly structure that depends on the quasiperiodicity [66, 46, 62, 47, 45]. Our method is the first to allow computing the spectrum of such systems with error control, which we have also implemented for concrete examples in [57].

A different generalization is to consider Schrödinger operators on arbitrary graphs [91, 67]. Because we do not presuppose that our operators are defined on a grid, or the existence of a groupoid structure as in [16], our algorithm can be readily applied to any Schrödinger operator on arbitrary geometrically embedded infinite graphs as long as their local structure is known.

## 2.4 Random operators

Our method can also be applied to random operators, which play an important role in physics as models of noise and impurities [3, 51, 2]. For example, choosing  $\Gamma = \mathbb{Z}^n$ , a random operator may be defined as a weakly measurable function defined on a probability space  $(\Omega, \mathcal{A}, \mathbb{P})$  which assigns to every  $\omega \in \Omega$  a bounded operator  $H_\omega$  acting on the common Hilbert space  $\mathcal{H}$ . If the action  $T$  of the translation group  $\mathbb{Z}^n$  on  $\Omega$  is measure preserving and ergodic, and such that  $H_{T_x\omega}$  is unitarily equivalent to  $H_\omega$  for every  $x \in \mathbb{Z}^n$ , then it can be shown that the spectrum  $\text{Spec}(H_\omega)$  is almost surely constant [2].

For ergodic random operators, the almost sure spectrum can be computed using our method by enumerating all local patches that occur in  $H_\omega$  with non-zero probability. The ergodicity implies that all such patches occur with probability one. We can thus compute the almost sure spectrum of random operators in a completely deterministic manner, without sampling random potentials, by enumerating all possible local patches. This procedure would have to be optimized for practical use however, because the number of local patches grows exponentially in  $L$  for most random models.

## 3 Reduction to finite range operators

In the problem statements in Definitions 10 and 12, we have assumed  $H$  to be of short range, meaning that its matrix elements  $H_{xy}$  decay with a sufficient power of the distance  $d(x, y)$ . The statements needed for the computation of the spectrum and pseudospectrum, however, are much easier to prove if we assume  $H$  to have finite range. In this section, we show that if we can compute the spectrum for operators of finite range, we can extend this to short-range operators by simply cutting off the operator  $H$  at a sufficiently large hopping length.

Let  $H$  be a discrete operator on  $\mathcal{H}$ , and let  $m > 0$ . Then we define the *trimmed operator*  $G^m$  by its matrix elements

$$G_{xy}^m = \begin{cases} H_{xy} & \text{for } d(x, y) \leq m, \\ 0 & \text{otherwise.} \end{cases} \quad (13)$$

The trimmed operator  $G^m$ , which is also an operator on  $\mathcal{H}$ , always has finite range  $m$ .

As a first step, we show that  $G^m \rightarrow H$  converges in norm for short-range operators  $H$ . We can prove this using the Schur test, which provides a bound on the operator norm of a linear operator based on its matrix elements [90]. A convenient formulation of the Schur test for discrete operators is the following Proposition [2, Proposition 10.6]:

**Proposition 15.** *Let  $B$  be a discrete operator on  $\Gamma$  satisfying*

$$\begin{aligned}\|B\|_{1,1} &:= \sup_{y \in \Gamma} \sum_{x \in \Gamma} |B_{xy}| < \infty, \\ \|B\|_{\infty,\infty} &:= \sup_{x \in \Gamma} \sum_{y \in \Gamma} |B_{xy}| < \infty.\end{aligned}$$

*Then  $B$  is bounded by  $\|B\| \leq \sqrt{\|B\|_{1,1}\|B\|_{\infty,\infty}}$ .*

We will also need the following bound of the sum of  $d(x,y)^{-(n+\varepsilon)}$ , when summing only over points with a given minimum distance  $m$  from  $x$ .

**Lemma 16.** *Let  $\varepsilon > 0$  and  $\Gamma$  be a subset of  $\mathbb{R}^n$  which is uniformly discrete with distance  $l$ . Then there is a constant  $C$ , depending only on  $n$  and  $l$ , such that*

$$\sum_{\substack{y \in \Gamma \\ d(x,y) > m}} d(x,y)^{-(n+\varepsilon)} \leq C \cdot \frac{1}{m^\varepsilon}. \quad (14)$$

*Furthermore, the constant  $C$  can be computed by a BSS algorithm from  $n, \varepsilon$  and  $l$ .*

The proof of this lemma is given in Appendix A. We can now combine Lemma 16 with Proposition 15 to prove the norm convergence  $G^m \rightarrow H$ .

**Lemma 17.** *Let  $H$  be a short-range discrete operator. Then for every  $\delta > 0$ , there exists an  $m > 0$  such that*

$$\|H - G^m\| \leq \delta. \quad (15)$$

*The number  $m$  is a computable function of  $\delta$ , the dimension  $n$ , and the decay constant  $C$  of Definition 5.*

*Proof.* Let  $B^m = H - G^m$ . The entries of  $B^m$  fulfill the opposite relation to (13):

$$B_{xy}^m = \begin{cases} H_{xy} & \text{for } d(x,y) > m, \\ 0 & \text{otherwise.} \end{cases}$$

By the short-range property of  $H$ , there is a constant  $C > 0$  such that

$$|H_{xy}| \leq C d(x,y)^{-(n+\varepsilon)}$$

for all  $x, y \in \Gamma$ . For any  $x \in \Gamma$ , we can therefore bound

$$\sum_{y \in \Gamma} |B_{xy}^m| = \sum_{\substack{y \in \Gamma \\ d(x,y) > m}} |H_{xy}| \leq C \sum_{\substack{y \in \Gamma \\ d(x,y) > m}} d(x,y)^{-(n+\varepsilon)}.$$

By Lemma 16, there is a constant  $C_2 > 0$ , which obviously does not depend on  $H$ , such that this sum is bounded by

$$\sum_{\substack{y \in \Gamma \\ d(x,y) > m}} |H_{xy}| \leq C \cdot C_2 \cdot \frac{1}{m^\varepsilon}.$$

The same bound clearly applies when summing over  $x$ . In the language of Proposition 15, this means that

$$\|B\|_{1,1} \leq C \cdot C_2 \cdot \frac{1}{m^2} \quad \text{and} \quad \|B\|_{\infty,\infty} \leq C \cdot C_2 \cdot \frac{1}{m^\varepsilon}.$$

Therefore Proposition 15 bounds the operator norm of  $B^m$  by

$$\|H - G^m\| = \|B^m\| \leq C \cdot C_2 \cdot \frac{1}{m^\varepsilon}.$$

It follows that Equation (15) is fulfilled for any  $m \geq \left(\frac{C \cdot C_2}{\delta}\right)^{1/\varepsilon}$ , proving the Lemma. It is also clear that a suitable  $m$  can be computed by a BSS algorithm, since it is given by a simple formula in  $C, C_2$  and  $\delta$ .  $\square$

Having shown the convergence  $G^m \rightarrow H$  in norm, we can now proceed to show how the spectrum of any short-range operator  $H$  may be computed from that of a suitable trimming  $G^m$ . This is quite simple in the normal case, but somewhat more involved for non-normal operators.

### 3.1 Normal case

Lemma 17 is sufficient to reduce the computational problem for short-range operators to that for finite range operators. Define the *finite range flc spectral problem* as tuples  $(\Omega \cap \Omega_{\text{fr}}, \Lambda \cup \Lambda_{\text{fr}}, (\mathcal{M}, d_H), \Xi)$  and the *finite range flc pseudospectral problem* as  $(\Omega_{\text{ps}} \cap \Omega_{\text{fr}}, \Lambda_{\text{ps}} \cup \Lambda_{\text{fr}}, (\mathcal{M}, d_H), \Xi_{\text{ps}})$ , where  $\Omega_{\text{fr}}$  is the set of all operators with finite range and  $\Lambda_{\text{fr}}$  contains just one additional evaluation function that associates to any finite-range operator  $H$  the minimal  $m$  such that  $H_{xy} = 0$  whenever  $d(x, y) > m$ . Then we have the following proposition:

**Proposition 18.** *If the finite range flc spectral problem  $(\Omega \cap \Omega_{\text{fr}}, \Lambda \cup \Lambda_{\text{fr}}, (\mathcal{M}, d_H), \Xi)$  is solvable, then so is the short-range flc spectral problem  $(\Omega, \Lambda, (\mathcal{M}, d_H), \Xi)$ .*

*Proof.* Suppose that the finite range flc spectral problem is solvable. To solve the short-range flc spectral problem, let  $H \in \Omega$  be given, and let  $k \in \mathbb{N}$  be arbitrary. Then by Lemma 17, we can find a cutoff distance  $m$  such that  $\|H - G^m\| \leq 2^{-(k+1)}$ . Because we have a solution of the finite range flc spectral problem, we can then apply that solution to the finite range operator  $G^m$  to produce an approximation  $A$  to the spectrum of  $G^m$  such that

$$d_H(A, \text{Spec}(H)) < 2^{-(k+1)}.$$

But because  $\|H - G^m\| \leq 2^{-(k+1)}$ , we also have

$$d_H(\text{Spec}(H), \text{Spec}(G^m)) \leq 2^{-(k+1)}.$$

The triangle inequality then implies that  $d_H(A, \text{Spec}(H)) \leq 2^{-k}$ . Thus, we can always compute a set  $A$  such that  $d_H(A, \text{Spec}(H)) \leq 2^{-k}$ , solving the short-range flc spectral problem.  $\square$

### 3.2 Non-normal case

For normal operators, we have used that a perturbation of size  $\delta$  only changes the spectrum by at most  $\delta$  in Hausdorff distance in order to prove that the spectral problem can be reduced to the case of finite range. For non-normal operators, however, a small perturbation can cause arbitrarily large changes in the  $\varepsilon$ -pseudospectrum. However, we still have for any perturbation  $R$  of norm  $\|R\| \leq \tau < \varepsilon$  the inclusions

$$\text{Spec}_{\varepsilon-\tau}(H) \subseteq \text{Spec}_\varepsilon(H + R) \subseteq \text{Spec}_{\varepsilon+\tau}(H). \quad (16)$$

Equation (16) follows immediately from the following equivalent characterization of the  $\varepsilon$ -pseudospectrum as union of perturbed spectra [96, Equation 4.4]:

$$\text{Spec}_\varepsilon(H) = \bigcup_{\substack{B \in \mathcal{L}(\mathcal{H}) \\ \|B\| \leq \varepsilon}} \text{Spec}(H + B).$$

To show that the inclusions (16) are sufficient to bound the pseudospectrum of  $H + R$  arbitrarily well, we need the following lemma, which shows the continuity of the  $\varepsilon$ -pseudospectrum in the level  $\varepsilon$ .

**Lemma 19.** *Let  $H$  be a bounded operator and  $\varepsilon > 0$ . Then for every  $\delta > 0$ , there exists a  $\tau > 0$  so that*

$$d_{\text{H}}(\text{Spec}_{\varepsilon-\tau}(H), \text{Spec}_{\varepsilon+\tau}(H)) \leq \delta. \quad (17)$$

*In other words, the function  $\varepsilon \rightarrow \text{Spec}_\varepsilon(H)$  is continuous in  $\varepsilon$  if the codomain is equipped with the Hausdorff distance.*

*Proof.* Because  $\text{Spec}_{\varepsilon-\tau}(H)$  is a subset of  $\text{Spec}_{\varepsilon+\tau}(H)$ , the Hausdorff distance is just

$$d_{\text{H}}(\text{Spec}_{\varepsilon-\tau}(H), \text{Spec}_{\varepsilon+\tau}(H)) = \sup_{x \in \text{Spec}_{\varepsilon+\tau}(H)} d(x, \text{Spec}_{\varepsilon-\tau}(H)).$$

Equation (17) is therefore fulfilled if and only if for every  $x \in \text{Spec}_{\varepsilon+\tau}(H)$ , there is a  $y \in \text{Spec}_{\varepsilon-\tau}(H)$  with  $|x - y| < \delta$ .

Suppose for the sake of contradiction that there is no  $\tau > 0$  fulfilling the conditions of the Lemma. Then for every  $\tau_j = 1/j$ ,  $j \in J_{\varepsilon, \delta} := \{n \in \mathbb{N} \mid n \geq \max\{\lceil \frac{2}{\varepsilon} \rceil, \lceil \frac{2}{\delta} \rceil\}\}$ , we can find an  $x_j \in \text{Spec}_{\varepsilon+1/j}(H)$  such that

$$B_\delta(x_j) \cap \text{Spec}_{\varepsilon-1/j}(H) = \emptyset. \quad (18)$$

Because all the  $x_j$  are contained in  $\text{Spec}_{\varepsilon+1}(H)$ , which is a compact set (see [96], Theorem 2.4), the sequence  $(x_j)_{j \in J_{\varepsilon, \delta}}$  has a convergent subsequence. Without loss of generality, we can assume that  $x_j$  converges, say to  $x_* \in \mathbb{C}$ , and that  $|x_j - x_*| < 1/j$ . The latter then implies  $|x_j - x_*| < \delta/2$  for all  $j \in J_{\varepsilon, \delta}$ . Combined with (18), this implies that

$$B_{\delta/2}(x_*) \cap \text{Spec}_{\varepsilon-1/j}(H) = \emptyset \quad (19)$$

for all  $j \in J_{\varepsilon, \delta}$ . Since all sets  $\text{Spec}_{\varepsilon+1/j}(H)$  are closed sets, we also have that

$$x_* \in \text{Spec}_{\varepsilon+1/j}(H) \quad (20)$$

for all  $j \in J_{\varepsilon, \delta}$ . In terms of the function  $\rho_H$ , condition (20) means that

$$\rho_H(x_*) \leq \varepsilon + 1/j$$

for all for all  $j \in J_{\varepsilon, \delta}$ , while condition (19) is equivalent to

$$\rho_H(z) > \varepsilon - 1/j$$

for all  $z \in B_{\delta/2}(x_*)$  and all for all  $j \in J_{\varepsilon, \delta}$ . Taking  $j \rightarrow \infty$ , we conclude that  $x_*$  must be a strict local minimum of  $\rho_H$  and thus a strict local maximum of  $\rho_H^{-1}$ . This is impossible, however, because  $\rho_H^{-1}$  is subharmonic and therefore fulfills a maximum principle [96, Theorem 4.2].  $\square$

Lemma 19 will also be useful to prove the computability of the pseudospectrum for finite range operators in Section 8. Here we use it to prove that the computation of the pseudospectrum can be reduced to the case of finite range operators instead of short-range ones using the inclusions (16).

**Proposition 20.** *If the finite range frc pseudospectral problem  $(\Omega_{\text{ps}} \cap \Omega_{\text{fr}}, \Lambda_{\text{ps}} \cup \Lambda_{\text{fr}}, (M, d), \Xi_{\text{ps}})$  is solvable, then the short-range problem  $(\Omega_{\text{ps}}, \Lambda_{\text{ps}}, (M, d), \Xi_{\text{ps}})$  is solvable.*

*Proof.* Assume that the finite range problem is solvable. Let  $(H, \varepsilon) \in \Omega_{\text{ps}} \cap \Omega_{\text{fr}}$  be a concrete short-range spectral problem and fix the allowed margin of error  $\delta := 2^{-k}$ . In order to approximate the  $\varepsilon$ -pseudospectrum of  $H$ , we proceed as follows: Iterate over  $\tau = 1, \frac{1}{2}, \frac{1}{4}, \dots$ . For each  $\tau$ , trim  $H$  to an operator  $G^m$  such that  $\|H - G^m\| \leq \tau$ . A cut-off length  $m$  fulfilling that inequality can be found in a computable way by Lemma 17. We have assumed that the finite range problem has a solution, so we can now apply that solution to construct subsets  $A$  and  $B$  such that

$$d_{\text{H}}(A, \text{Spec}_{\varepsilon-\tau}(G^m)) \leq \delta/6 \quad (21)$$

$$d_{\text{H}}(B, \text{Spec}_{\varepsilon+\tau}(G^m)) \leq \delta/6. \quad (22)$$

Then, if we have  $d_{\text{H}}(A, B) \leq \delta/2$ , we terminate with  $A$  as our approximation to  $\text{Spec}_{\varepsilon}(H)$ , otherwise we continue with the next  $\tau$  in our sequence.

Now if the algorithm terminates because the condition  $d_{\text{H}}(A, B) \leq \delta/2$  is fulfilled, then the result  $A$  will be an approximation of  $\text{Spec}_{\varepsilon}(H)$  with Hausdorff distance less than  $\delta$ . We can show this using the triangle inequality and the inclusions (16) as follows:

$$\begin{aligned} d_{\text{H}}(A, \text{Spec}_{\varepsilon}(H)) &\leq d_{\text{H}}(A, \text{Spec}_{\varepsilon-\tau}(G^m)) + d_{\text{H}}(\text{Spec}_{\varepsilon-\tau}(G^m), \text{Spec}_{\varepsilon}(H)) \\ &\leq d_{\text{H}}(A, \text{Spec}_{\varepsilon-\tau}(G^m)) + d_{\text{H}}(\text{Spec}_{\varepsilon-\tau}(G^m), \text{Spec}_{\varepsilon+\tau}(G^m)) \\ &\leq d_{\text{H}}(A, \text{Spec}_{\varepsilon-\tau}(G^m)) + d_{\text{H}}(\text{Spec}_{\varepsilon-\tau}(G^m), A) \\ &\quad + d_{\text{H}}(A, B) + d_{\text{H}}(B, \text{Spec}_{\varepsilon+\tau}(G^m)) \\ &\leq 3\frac{\delta}{6} + \frac{\delta}{2} = \delta. \end{aligned}$$

In the last step, we have combined the cut-off bounds (21) and (22) with the condition  $d_{\text{H}}(A, B)$ .

It remains to show that the described algorithm does always terminate. That is, we need to show that the condition  $d_{\text{H}}(A, B) \leq \delta/2$  will be fulfilled for  $\tau$  small enough and  $A, B$  as above. According to Lemma 19 there exists a  $\tau' > 0$  such that

$$d_{\text{H}}(\text{Spec}_{\varepsilon-\tau'}(H), \text{Spec}_{\varepsilon+\tau'}(H)) \leq \delta/6.$$

This does not imply a way of computing  $\tau'$ , but because our algorithm descends to arbitrarily small  $\tau$ , it will eventually come to a  $\tau$  such that  $\tau < \tau'/2$ . Assuming this, the algorithm will then choose  $G^m$  such that  $\|G^m - H\| < \tau$ , and we can use (16) to conclude

$$\text{Spec}_{\varepsilon-\tau'}(H) \subseteq \text{Spec}_{\varepsilon-\tau}(G^m) \subseteq \text{Spec}_{\varepsilon}(H) \subseteq \text{Spec}_{\varepsilon+\tau}(G^m) \subseteq \text{Spec}_{\varepsilon+\tau'}(H), \quad (23)$$

where we have used  $2\tau < \tau'$ . We can now apply Lemma 33 twice to the inclusions in (23) to see that

$$\begin{aligned} d_{\text{H}}(\text{Spec}_{\varepsilon+\tau}(G^m), \text{Spec}_{\varepsilon-\tau}(G^m)) &\leq d_{\text{H}}(\text{Spec}_{\varepsilon+\tau}(G^m), \text{Spec}_{\varepsilon-\tau'}(H)) \\ &\leq d_{\text{H}}(\text{Spec}_{\varepsilon-\tau'}(H), \text{Spec}_{\varepsilon+\tau'}(H)) \\ &\leq \delta/6. \end{aligned}$$

It then follows from (21) and (22) that

$$\begin{aligned} d_H(A, B) &\leq d_H(A, \text{Spec}_{\varepsilon-\tau}(G^m)) + d_H(\text{Spec}_{\varepsilon-\tau}(G^m), \text{Spec}_{\varepsilon+\tau}(G^m)) + d_H(\text{Spec}_{\varepsilon+\tau}(G^m), B) \\ &\leq 3\frac{\delta}{6} = \delta/2. \end{aligned}$$

We have thus shown that the algorithm terminates at the latest when  $\tau$  becomes smaller than  $\tau'/2$ .  $\square$

We have thus established the reduction of the spectral and pseudospectral problems to finite range operators. In the rest of the paper, we restrict ourselves to finite range operators when describing how to solve the *flc* spectral and pseudospectral problems, since by Propositions 18 and 20, the same algorithms can then also be applied to the short-range *flc* problems by using a suitable cut-off.

## 4 The pseudospectral inclusion bound

In this section, we formulate and prove the pseudospectral inclusion bound from [36] for our setting. Moreover, we also show that the bound is computable.

### 4.1 Formulation of the pseudospectral inclusion bound

A bound showing the inclusion of a complex number in the  $\varepsilon$ -pseudospectrum for a certain  $\varepsilon$ , or in other words an upper bound on  $\rho_H$ , has been described in [36]. In the following we describe the bound using the singular value decomposition (SVD) of a rectangular matrix  $A$ , while in [36], the eigenvalues of  $A^T A$  are used, which are just the squares of the singular values of  $A$ .

**Definition 21.** Let  $H$  be a discrete operator with finite range  $m$ , let  $x \in \mathbb{R}^n$  be any point and  $L > 0$ ,  $\lambda \in \mathbb{C}$ . The *uneven section* for these data is the linear operator

$$\begin{aligned} Q_{L,\lambda,x} &: \mathcal{H}_{B_L(x)} \rightarrow \mathcal{H}_{B_{L+m}(x)} \\ Q_{L,\lambda,x}(\psi) &= \mathbf{1}_{B_{L+m}(x)}(H - \lambda)\mathbf{1}_{B_L(x)}\psi. \end{aligned}$$

Recall that  $\mathcal{H}_{B_L(x)} := \text{span}\{e_y \mid y \in B_L(x) \cap \Gamma\}$  and  $\mathbf{1}_{B_L(x)}$  denotes the orthogonal projection onto  $\mathcal{H}_{B_L(x)}$ . Because  $\Gamma$  is uniformly discrete,  $\mathcal{H}_{B_L(x)}$  and  $\mathcal{H}_{B_{L+m}(x)}$  are finite dimensional, so that  $Q_{L,\lambda,x}$  can be represented as a rectangular matrix.

**Theorem 22.** Let  $H$  be a discrete operator with finite range  $m > 0$ , and let  $\lambda \in \mathbb{R}$ ,  $L > 0$ , and  $x \in \mathbb{R}^n$  be arbitrary. Let

$$\varepsilon_{L,\lambda,x} = s_1(Q_{L,\lambda,x}) \tag{24}$$

be the smallest singular value of  $Q_{L,\lambda,x}$ . Then  $\lambda$  is contained in the  $\varepsilon_{L,\lambda,x}$ -pseudospectrum of  $H$ :

$$\rho_H(\lambda) \leq \varepsilon_{L,\lambda,x}. \tag{25}$$

*Proof.* The singular value decomposition (SVD) of  $Q_{L,\lambda,x}$  decomposes  $Q_{L,\lambda,x}$  as a product

$$Q_{L,\lambda,x} = USV^*$$

where  $U$  and  $V$  are unitary and  $S$  is a rectangular diagonal matrix. We can also write this matrix product as

$$Q_{L,\lambda,x} = \sum_{i=1}^n |u_i\rangle s_i \langle v_i|$$

where  $(u_i)_{i=1,\dots,n}$  are the first  $n$  columns of  $U$ ,  $(v_i)_{i=1,\dots,n}$  are the columns of  $V$ , and  $(s_i)_{i=1,\dots,n}$  are the diagonal elements of  $S$ . We assume that the  $(s_i)_{i=1,\dots,n}$  are sorted in ascending order so that  $s_1 = \varepsilon_{L,\lambda,x}$ .

Then  $v_1$ , considered as a vector in  $\mathcal{H}$  via the canonical inclusion  $\iota : \mathcal{H}_{B_L(x)} \rightarrow \mathcal{H}$ , is an  $\varepsilon_{L,\lambda,x}$ -quasimode for  $H$ . Indeed, we have

$$\begin{aligned} (H - \lambda)v_1 &= (H - \lambda)\mathbf{1}_{B_L(x)}v_1 && \text{(since } v_1 \text{ is supported on } B_L(x)) \\ &= \mathbf{1}_{B_{L+m}(x)}(H - \lambda)\mathbf{1}_{B_L(x)}v_1 && \text{(by the finite range of } H) \\ &= Q_{L,\lambda,x}v_1 \\ &= s_1u_1 \end{aligned}$$

and therefore  $\|(H - \lambda)v_1\| = s_1\|u_1\| = s_1$ . We conclude that  $\|(H - \lambda)v_1\| \leq s_1 = \varepsilon_{L,\lambda,x}$ , and thus  $v_1$  is an  $\varepsilon_{L,\lambda,x}$ -quasimode, which implies  $\lambda \in \text{Spec}_{\varepsilon_{L,\lambda,x}}(H)$  by definition of the pseudospectrum [96].  $\square$

For normal operators, Equation (25) corresponds to an upper bound on the distance to the spectrum of  $H$ .

## 4.2 Computability of the pseudospectral inclusion bound

In order to derive statements about computability from the existence of the pseudospectral inclusion bound, we need to relate it to our model of computation and show that the bound is actually computable from our problem definition. The following Lemma shows the computability of  $\varepsilon_{L,\lambda,x}$  for a fixed  $x \in \mathbb{R}^n$ . We recall that a short review on BSS algorithms is given in Appendix B.

**Lemma 23.** *For every  $k \in \mathbb{N}$  and  $\varepsilon > 0$  there exists a BSS algorithm  $\Gamma_{\varepsilon,k}$  such that  $\Gamma_{\varepsilon,k}(Q_{L,\lambda,x}) \in \mathbb{R}$  and*

$$d(\Gamma_{\varepsilon,k}(Q_{L,\lambda,x}), \varepsilon_{L,\lambda,x}) \leq 2^{-k}. \quad (26)$$

*Proof.* First, let us note that in [36] the authors describe a method for approximating  $\varepsilon_{L,\lambda,x}$  using finitely many arithmetic operations. In short, to compute a bound on the distance to the spectrum using Proposition 22, one can use that  $\varepsilon_{L,\lambda,x}$  is the square root of the smallest eigenvalue of  $Q_{L,\lambda,x}^T Q_{L,\lambda,x}$ . This implies that, for any  $t \in \mathbb{R}$ ,

$$t < \varepsilon_{L,\lambda,x} \iff Q_{L,\lambda,x}^T Q_{L,\lambda,x} - t^2 \text{ is positive definite.}$$

Whether a symmetric matrix is positive definite can be decided using finitely many rational computations using the Cholesky decomposition. Recall that the Cholesky decomposition is a method of factorizing positive semidefinite matrices  $A$  in the form  $L^*L$ , where  $L$  is a lower triangular matrix. If the matrix is not positive semidefinite, this will lead to the square root of a negative number being computed in the algorithm. Thus, we can approximate  $\varepsilon_{L,\lambda,x}$  with finitely many operations.

In view of this, the formulation of the BSS method  $\Gamma_{\varepsilon,k}$  is simple because for every  $t$ , testing whether  $t < \varepsilon_{L,\lambda,x}$  is computable using a finite number of additions, multiplications

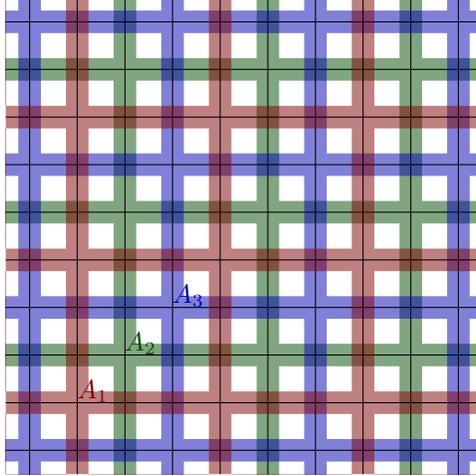


Figure 2: In dimension  $n = 2$ , the sets  $A_1$  to  $A_3$ , which are defined as the edges of three overlapping grids, form a 2-disjoint grid, meaning that every intersection of three of the sets is empty. In general, we need  $(n + 1)$  grids in  $n$  dimensions to construct a similar set out of boxes. A decomposition like this can be used to show the detectability of bulk  $\varepsilon$ -quasimodes.

and divisions. To define  $\Gamma_{\varepsilon,k}$ , let  $S = \{2^{-j} \mid j \in \mathbb{N}\}$ . The algorithm  $\Gamma_{\varepsilon,k}$  can then simply check for each  $t \in S$  successively whether  $Q_{L,\lambda,x}^T Q_{L,\lambda,x} - t^2$  is positive definite or not, terminating with the smallest  $t \in S$  for which this is not the case. (Since  $\varepsilon_{L,\lambda,x}$  is a real number, there must certainly be a  $t \in S$  with  $t \geq \varepsilon_{L,\lambda,x}$ .) We take this  $t$  as the result of the BSS algorithm  $\Gamma_{\varepsilon,k}$ . Since  $t - 1/k < \varepsilon_{L,\lambda,x} \leq t$ , we know that  $|t - \varepsilon_{L,\lambda,k}| < \varepsilon$ , proving that (26) is satisfied.  $\square$

## 5 Spectral gap bound

It was proven in [36] that the pseudospectral inclusion bound  $\varepsilon_{L,\lambda,x}$  always converges to  $\rho_H(\lambda)$  as  $L \rightarrow \infty$ , at least for normal, short-range operators. However, the convergence is not uniform in the operator  $H$ , and thus cannot be used to provide a lower bound on  $\rho_H(\lambda)$ . As described in the introduction, we can work around this by instead using  $\varepsilon_{L,\lambda}$ , which is defined as the infimum of  $\varepsilon_{L,\lambda,x}$  over all  $x \in \mathbb{R}^n$ . In this section, we prove Theorem 1, which is restated below for convenience.

**Theorem 1.** *Let  $H$  be a discrete operator with finite range  $m > 0$ . Then for every  $\lambda \in \mathbb{C}$  and  $L > m$  it holds that*

$$\rho_H(\lambda) \geq \varepsilon_{L,\lambda} \sqrt{1 - \delta_L} - \|H - \lambda\| \sqrt{\delta_L}, \quad (4)$$

where  $\varepsilon_{L,\lambda} := \inf_{x \in \mathbb{R}^n} \varepsilon_{L,\lambda,x}$ , with  $\varepsilon_{L,\lambda,x}$  defined in (24), and

$$\delta_L := \frac{n}{\lfloor L/m \rfloor}. \quad (5)$$

Theorem 1 is a general statement about the locality of the (pseudo-)spectrum. It says that any (pseudo-)spectrum can be detected in some local patch of a size  $L$ , where  $L$  can be explicitly determined from the following data: the range  $m$  of  $H$ , an upper bound on the norm

of  $\|H - \lambda\|$ , and the desired accuracy. We will show in Corollary 28 how this statement can be used to compute  $\rho_H(\lambda)$  to any desired accuracy for *flc* operators.

To prove Theorem 1, we tile the space  $\mathbb{R}^n$  with disjoint boxes  $\{B_{L+m}(x) \mid x \in Z\}$ , where  $Z$  is some discrete subset of  $\mathbb{R}^n$ . For the boxes to be disjoint,  $Z$  must be uniformly discrete with length  $2(L+m)$ . In each of the boxes, we can then compute  $\varepsilon_{L,\lambda,x}$  to approximate  $\rho_H(\lambda)$ .

However, this simple decomposition approach might fail for quasimodes of  $H$  that have a large part of their  $\ell^2$  mass concentrated in the edges of the boxes  $B_{L+m}(x) \setminus B_L(x)$ . Such states  $\psi$  can be quasimodes of the infinite-volume operator  $H$ , while none of their restrictions  $\psi_{B_L(x)}$  for  $x \in Z$  are quasimodes.

We overcome this problem by considering several overlapping disjoint decompositions of  $\mathbb{R}^n$  into boxes, corresponding to different uniformly discrete subsets  $Z_i \subseteq \mathbb{R}^n$ . It is possible to choose a set of such overlapping decompositions in such a way that no quasimode  $\psi$  can have a large part of its  $\ell^2$  mass near the edges for *every* decomposition. An example with three overlapping decompositions is shown in Figure 2. Because, in that figure, no point is in the edges of all three decompositions simultaneously, no state  $\psi$  can have more than  $2/3$  of its  $\ell^2$  mass concentrated in the colored edges for all three grids.

To implement this approach in general, we will first, in Section 5.1, give the exact condition which the overlapping decompositions have to fulfill to guarantee that at least one of the decompositions has low  $\ell^2$  mass in the edges for any  $\psi \in H$ . We will also show how to construct decompositions of  $\mathbb{R}^n$  which fulfill this condition, and detail how the mass in the edges can be lowered arbitrarily by increasing  $L$ . In Section 5.2, we then apply this result to prove Theorem 1, by showing that if the  $\ell^2$  mass of a quasimode  $\psi$  in the edges of a decomposition is small enough, the restriction of this bulk quasimode to one of the  $B_L(x)$  must again be a quasimode. This then implies that the bounds  $\varepsilon_{L,\lambda,x}$  can be used to bound  $\rho_H(\lambda)$  from below, as in inequality (4).

## 5.1 Construction of $n$ -disjoint grids

We will now construct a set of  $r$   $n$ -dimensional grids, similar to the one shown in Figure 2, such that no function  $\psi$  can have a large part of its mass concentrated in all the  $r$  grids simultaneously.

We start by defining the notion of  $n$ -disjoint sets.

**Definition 24.** A set  $(A_i)_{i=1,\dots,r}$  of subsets  $A_i \subseteq \mathbb{R}^n$  is called  *$n$ -disjoint* if every point  $x \in \mathbb{R}^n$  is contained in at most  $n$  of the sets.

As one can see from Figure 2, the tree grids  $A_1$ ,  $A_2$  and  $A_3$  are 2-disjoint: even though they have nonempty pairwise intersections, the intersection of all three is empty. The next Lemma shows that any set of grid-shaped sets is actually  $n$ -disjoint.

**Lemma 25.** Let  $n \in \mathbb{N}$  and  $r \in \mathbb{N}$ . Let  $(J_i)_{i=1,\dots,r}$  be a set of mutually disjoint subsets of  $\mathbb{R}$ . Define

$$A_i := \bigcup_{j=1}^n \left( \mathbb{R}^{j-1} \times J_i \times \mathbb{R}^{n-j} \right) \subset \mathbb{R}^n. \quad (27)$$

Then the sets  $A_i$ ,  $i \in \{1, \dots, r\}$  are  $n$ -disjoint.

*Proof.* For any point  $p \in \mathbb{R}^n$  to be in  $A_i$ , at least one of its  $n$  coordinates must lie in  $J_i$ , but then that coordinate cannot lie in any other  $J_j$ . Thus,  $p$  can lie in at most  $n$  different  $A_i$ .  $\square$

If  $r$ , the number of subsets, is large enough,  $n$ -disjointness is already sufficient to bound the minimum of the  $\ell^2$  masses in any  $A_i$ , which is shown in the following Lemma. To simplify notation, in the following we denote by  $\|\psi\|_X = \|\psi \mathbf{1}_{X \cap \Gamma}\|$  the  $\ell^2$  mass of  $\psi$  in  $X$ , for any subset  $X \subseteq \mathbb{R}^n$ .

**Lemma 26.** *Let  $(A_i)_{i=1,\dots,r}$  be a set of  $r$  subsets of  $\mathbb{R}^n$  which are  $n$ -disjoint. Then for any  $\psi \in \mathcal{H}$  there exists an  $i \in \{1, \dots, r\}$  such that*

$$\|\psi\|_{A_i}^2 \leq \frac{n}{r} \|\psi\|^2.$$

*Proof.* Consider what happens if we take the sum over all  $\|\psi\|_{A_i}^2$ , for  $1 \leq i \leq r$ . Each squared norm can be written as a sum over points in  $\Gamma$ :

$$\sum_{i=1}^r \|\psi\|_{A_i}^2 = \sum_{i=1}^r \sum_{x \in \Gamma \cap A_i} |\psi(x)|^2.$$

Because the  $A_i$  are  $n$ -disjoint, every  $x \in \Gamma$  is contained in at most  $n$  of the sets  $A_i$ . Thus, every term  $|\psi(x)|^2$ , for  $x \in \Gamma$ , occurs at most  $n$  times in the above double sum. Thus we have

$$\sum_{i=1}^r \|\psi\|_{A_i}^2 \leq \sum_{x \in \Gamma} n |\psi(x)|^2 = n \|\psi\|^2.$$

Dividing this inequality by  $r$ , we obtain that the average of all the  $\|\psi\|_{A_i}^2$  is at most  $\frac{n}{r} \|\psi\|^2$ . Because at least one of the numbers must be smaller or equal to the average, there is an  $i \in \{1, \dots, r\}$  such that

$$\|\psi\|_{A_i}^2 \leq \frac{n}{r} \|\psi\|^2. \quad \square$$

For our purposes we use grid-shaped sets, as the ones in (27), that form a regular mesh in  $\mathbb{R}^n$ . Moreover, we also need to control the "thickness" of the grid. Let us be more explicit. Consider  $r \in \mathbb{N}$ ,  $L > 0$  and  $m > 0$ . For every  $i \in \{1, \dots, r\}$  we define the set

$$J_i := [-m, m] + 2(L + m) \left( \mathbb{Z} + \frac{i}{r} + \frac{1}{2} \right) \subset \mathbb{R}. \quad (28)$$

If  $L > (r-1)m$ , the sets  $J_i$ , with  $i = 1, \dots, r$ , are mutually disjoint, thus, by using (27), we get a set of  $n$ -disjoint sets  $(A_i)_{i=1,\dots,r}$ . Furthermore, the mesh formed by each of the  $A_i$ , namely  $A_i^c$ , is just the union of the boxes  $B_L(x)$  with centers

$$x \in Z_i := 2(L + m) \left( \mathbb{Z}^n + \frac{i}{r} (1, 1, \dots, 1) \right). \quad (29)$$

In other words, we have

$$A_i^c = \bigcup_{x \in Z_i} B_L(x). \quad (30)$$

## 5.2 Proof of Theorem 1

Let  $L$ ,  $M$ ,  $m$ , and  $n$  be given, and define

$$r := \left\lfloor \frac{L}{m} \right\rfloor.$$

Consider the set of  $r$  sets  $(J)_{i=1,\dots,r}$  defined in (28). Since  $L \geq rm > (r-1)m$ , the sets  $(A_i)_{i=1,\dots,r}$  defined in (27) are  $n$ -disjoint. It then follows from Lemma 26 that for any  $\psi \in \mathcal{H}$ , there exists an  $i \in \{1, \dots, r\}$  such that

$$\|\psi_{A_i}\|^2 \leq \frac{n}{r} \|\psi\|^2.$$

Hence, for the orthogonal decomposition

$$\psi = \mathbf{1}_{A_i}\psi + \mathbf{1}_{A_i^c}\psi =: \psi_{A_i} + \psi_{A_i^c}$$

and writing  $\delta_L := n/r$ , we have

$$\|\psi_{A_i}\|^2 \leq \delta_L \|\psi\|^2 \quad \text{and} \quad \|\psi_{A_i^c}\|^2 \geq (1 - \delta_L) \|\psi\|^2. \quad (31)$$

The inverse triangle inequality implies

$$\|(H - \lambda)\psi\| \geq \|(H - \lambda)\psi_{A_i^c}\| - \|(H - \lambda)\psi_{A_i}\|. \quad (32)$$

For the  $A_i$  term, we find with (31) that

$$\|(H - \lambda)\psi_{A_i}\| \leq \|H - \lambda\| \|\psi_{A_i}\| \leq \sqrt{\delta_L} \|H - \lambda\| \|\psi\|. \quad (33)$$

To obtain a lower bound for the  $A_i^c$  term, we note that the decomposition

$$A_i^c = \bigcup_{x \in Z_i} B_L(x),$$

described in (30) is disjoint and hence

$$(H - \lambda)\psi_{A_i^c} = \sum_{x \in Z_i} (H - \lambda)\psi_{B_L(x)}.$$

For each  $x \in Z_i$ , we have by definition

$$\|(H - \lambda)\psi_{B_L(x)}\| = \|Q_{L,\lambda,x}\psi_{B_L(x)}\| \geq \varepsilon_{L,\lambda,x} \|\psi_{B_L(x)}\| \geq \varepsilon_{L,\lambda} \|\psi_{B_L(x)}\|. \quad (34)$$

Because  $H$  has finite range  $m$ , every vector  $(H - \lambda)\psi_{B_L(x)}$  is supported in  $B_{L+m}(x)$ . Because the sets  $Z_i$  are uniformly discrete with distance  $2(L + m)$ , the hypercubes  $B_{L+m}(x)$  for  $x \in Z_i$  are pairwise disjoint. Hence, by summing Equation (34) over all  $x \in Z_i$ , and combining it with (31), we obtain that

$$\|(H - \lambda)\psi_{A_i^c}\| \geq \varepsilon_{L,\lambda} \|\psi_{A_i^c}\| \geq \varepsilon_{L,\lambda} \sqrt{1 - \delta_L} \|\psi\|. \quad (35)$$

Now, we can insert the bounds (35) and (33) into the inverse triangle inequality (32), and obtain

$$\|(H - \lambda)\psi\| \geq \left( \varepsilon_{L,\lambda} \sqrt{1 - \delta_L} - \|H - \lambda\| \sqrt{\delta_L} \right) \|\psi\|. \quad (36)$$

Recalling the definition of the lower norm function (10), this proves the theorem.

## 6 Computability of $\rho_H$

In this section, we show that the lower norm function  $\rho_H(\lambda)$  can be computed with error control, for any *flc* operator  $H$  and  $\lambda \in \mathbb{C}$ . We prove this by combining Theorem 1 and Theorem 22. We will need the following Lemma:

**Lemma 27.** *Let  $H$  be a finite range discrete operator. For any fixed  $\lambda \in \mathbb{C}$ , the value of  $\varepsilon_{L,\lambda}$  is nonincreasing in  $L$ . Similarly, for any fixed  $\lambda \in \mathbb{C}$  and  $x \in \mathbb{R}^n$ , the value of  $\varepsilon_{L,\lambda,x}$  is nonincreasing in  $L$ .*

The proof of Lemma 27 is given in Appendix A. The computability of  $\rho_H(\lambda)$  is encapsulated in the following Corollary, which shows the existence of a computable approximation  $\tilde{\rho}_H(\lambda, \tau)$  with guaranteed error control.

**Corollary 28.** Let  $H$  be any  $flc$  discrete operator with finite range  $m$ . Define the function

$$\tilde{\rho}_H(\lambda, \tau) := \varepsilon_{L_H(\tau), \lambda}, \quad (37)$$

using the quantities  $\varepsilon_{L, \lambda}$  from Theorem 1, for any  $\lambda \in \mathbb{C}$  and  $\tau > 0$ . Here the function  $L_H(\tau)$  determines a patch size sufficient to approximate  $\rho_H(\cdot)$  to precision  $\tau$ . Its value at any given  $\tau > 0$  can be computed from  $H$  via the evaluation functions  $\Lambda$  of Definition 10 by a BSS algorithm. Then the function  $\tilde{\rho}_H(\lambda, \tau)$  fulfills

$$|\rho_H(\lambda) - \tilde{\rho}_H(\lambda, \tau)| \leq \tau. \quad (38)$$

for any  $\lambda \in \mathbb{C}, \tau > 0$ .

**Remark 29.** Because  $\tilde{\rho}_H(\lambda, \tau)$  can be computed from  $H$  via the evaluation functions  $\Lambda$  of Definition 10 by a BSS algorithm, the function  $\tilde{\rho}(\lambda, \tau)$  is also computable in this sense.

*Proof of Corollary 28.* Recall from Theorems 1 and 22 that, for any  $L > m$ , we have

$$\varepsilon_{L, \lambda} \sqrt{1 - \delta_L} - M \sqrt{\delta_L} \leq \rho_H(\lambda) \leq \varepsilon_{L, \lambda}, \quad (39)$$

where  $\delta_L$  is defined as

$$\delta_L = \frac{n}{\lfloor L/m \rfloor},$$

and  $M := \|H - \lambda\|$ .

We write the difference between upper and lower bounds in formula (39) using the function

$$f(\varepsilon, \delta) = \varepsilon(1 - \sqrt{1 - \delta}) + M\sqrt{\delta}. \quad (40)$$

for general  $\varepsilon > 0$  and  $\delta \in (0, 1)$ . Then formula (39) implies that

$$|\varepsilon_{L, \lambda} - \rho_H(\lambda)| < f(\varepsilon_{L, \lambda}, \delta_L) \quad (41)$$

for all  $L > m$ .

As a first step, set  $L_0 = m + 1$  and compute  $\varepsilon_0 = \varepsilon_{L_0, \lambda}$ . Lemma 23 shows that computing  $\varepsilon_0$  is possible using a BSS algorithm from the evaluation functions  $\Lambda$  of Definition 10. Then by Lemma 27, we have

$$f(\varepsilon_{L, \lambda}, \delta_L) \leq f(\varepsilon_0, \delta_L) \quad (42)$$

for all  $L \geq L_0$ , because  $\varepsilon_{L, \lambda} \leq \varepsilon_0$ , and  $f(\varepsilon, d)$  is increasing in  $\varepsilon$ .

Now for any  $\tau > 0$ , because  $f(\varepsilon, \delta)$  is increasing in  $\delta$  for  $\delta \in (0, 1)$  and  $\lim_{\delta \rightarrow 0} f(\varepsilon, \delta) = 0$ , a value  $\delta'_\tau > 0$  can be computed, for example using the bisection method, such that

$$f(\varepsilon_0, \delta'_\tau) < \tau. \quad (43)$$

We now choose our value of  $L_H(\tau)$  such that

$$L_H(\tau) > \max(L_0, m \lceil n/\delta'_\tau \rceil). \quad (44)$$

This definition of  $L_H(\tau)$  fulfills the computability requirements because the right hand side of the inequality is computable. Furthermore, we have  $\delta_{L_H(\tau)} \leq \delta'_\tau$ . Then, by using (41), (42) and (43), we get

$$|\varepsilon_{L_H(\tau), \lambda} - \rho_H(\lambda)| < f(\varepsilon_{L_H(\tau), \lambda}, \delta_{L_H(\tau)}) \leq f(\varepsilon_{L_H(\tau), \lambda}, \delta'_\tau) \leq f(\varepsilon_0, \delta'_\tau) < \tau,$$

thus (38) holds.  $\square$

Our algorithms for computing the spectrum and  $\varepsilon$ -pseudospectrum of  $flc$  operators  $H$  will be based on approximating  $\rho_H(\lambda)$  at different points  $\lambda \in \mathbb{C}$ . In fact, the computability of approximations  $\tilde{\rho}_H(\lambda, \tau)$  fulfilling (38) are all that we use about the operator  $H$  in showing the computability of the (pseudo-) spectrum. The same methods could therefore also be applied to show the computability of the (pseudo-) spectrum with Hausdorff error control for any other class of operators where the lower norm function  $\rho_H(\lambda)$  can be approximated with error control.

## 7 Computability of the spectrum for normal operators

In this section, we will prove Theorem 11, the computability of the spectrum for normal operators. Our proof will be based on Corollary 28, the computability of  $\rho_H(\lambda)$ . Note that the normal spectral problem is not a special case of the pseudospectral problem because we can only compute the  $\varepsilon$ -pseudospectrum for  $\varepsilon > 0$ . In addition to normal operators, the method described below could easily be extended, as in [36], to classes of operators fulfilling a bound of the form

$$\rho_H(\lambda) \geq g(d(\lambda, \text{Spec}(H))) \quad (45)$$

for some strictly increasing continuous function  $g$ .

*Proof of Theorem 11.* Let the operator  $H$  and  $k \in \mathbb{N}$  be given. We define the desired accuracy as  $\tau := 2^{-k}$ .

We know that  $H$  is bounded, and the algorithm can access a bound on the norm of  $H$  via the evaluation function  $f_5 \in \Lambda$  (see Definition 35). Let  $M := f_5(H)$  be this bound and define the restricted square grid

$$T_\tau := B_M(0) \cap \left( \frac{\tau}{4} \sqrt{2} \cdot \mathbb{Z}^2 \right) \subseteq \mathbb{C}, \quad (46)$$

where we use the natural identification  $\mathbb{R}^2 \simeq \mathbb{C}$ . The side length of the rectangular grid is chosen such that  $T_\tau$  has covering radius  $\tau/4$  inside  $B_M(0)$ . We will approximate the spectrum by a subset of  $T_\tau$ .

For every  $\lambda \in T_\tau$ , we can use the algorithm of Corollary 28 to compute an approximation  $\tilde{\rho}_H(z, \tau/4)$  to  $\rho_H(z)$ . We define our approximation  $\tilde{\Gamma}(H, \tau)$  of the spectrum as

$$\tilde{\Gamma}(H, \tau) := \left\{ \lambda \in T_\tau \mid \tilde{\rho}_H(\lambda, \tau/4) < \tau/2 \right\}. \quad (47)$$

We will now show that  $d_H(\tilde{\Gamma}(H, \tau), \text{Spec}(H)) \leq \tau$  in Hausdorff distance.

First, let  $\lambda \in \text{Spec}(H)$ . Then  $\rho_H(\lambda) = 0$ . Because we have chosen  $T_\tau$  to have covering radius  $\tau/4$  inside  $B_M(0)$ , there exists a point  $\lambda' \in T_\tau$  with  $|\lambda - \lambda'| < \tau/4$ . Because  $\rho_H$  is Lipschitz continuous with Lipschitz constant 1 (see, for example, [76], Lemma 2.1), it follows that  $|\rho_H(\lambda) - \rho_H(\lambda')| < \tau/4$ . By Corollary 28, we have  $|\rho_H(\lambda') - \tilde{\rho}_H(\lambda', \tau/4)| < \tau/4$ . The triangle inequality thus implies

$$\tilde{\rho}_H(\lambda', \tau/4) \leq |\tilde{\rho}_H(\lambda', \tau/4) - \rho_H(\lambda')| + |\rho_H(\lambda') - \rho_H(\lambda)| + \rho_H(\lambda) < \tau/2,$$

where we have used  $\rho_H(\lambda) = 0$ . Hence,  $\lambda' \in \tilde{\Gamma}(H, \tau)$ . Because  $\lambda$  was arbitrary, we have  $d(\lambda, \tilde{\Gamma}(H, \tau)) \leq \tau/2$  for any  $\lambda \in \text{Spec}(H)$ .

On the other hand, for any  $\lambda \in \tilde{\Gamma}(H, \tau)$ , the condition  $\tilde{\rho}_H(\lambda, \tau/4) < \tau/2$  in (47) implies that  $\rho_H(\lambda) < \tau$  by Corollary 28. But for normal operators,  $\rho_H(\lambda) = d(\lambda, \text{Spec}(H))$ , so we have  $d(\lambda, \text{Spec}(H)) \leq \tau$ .

Summing up, for any  $\lambda \in \text{Spec}(H)$  we have  $d(\lambda, \tilde{\Gamma}(H, \tau)) \leq \tau/2$  and for any  $\lambda' \in \tilde{\Gamma}(H, \tau)$  we have  $d(\lambda', \text{Spec}(H)) \leq \tau$ . Thus, we have shown that  $d_H(\tilde{\Gamma}(H, \tau), \text{Spec}(H)) \leq \tau$ . The proof of Theorem 11 then follows simply by choosing  $\Gamma_k(H) := \tilde{\Gamma}(H, 2^{-k})$ .  $\square$

## 8 Computability of the pseudospectrum

In this section, we will prove Theorem 13, the computability of the  $\varepsilon$ -pseudospectrum for potentially non-normal operators and for  $\varepsilon > 0$ . A related result about pseudospectra is [76], in which it is shown that the pointwise convergence of the lower norm and the lower norm of the adjoint implies the convergence of the  $\varepsilon$ -pseudospectrum in Hausdorff distance. In the following, we show an analogous result about computability, namely that the  $\varepsilon$ -pseudospectrum can be computed in Hausdorff distance if arbitrarily exact estimates of the lower norm are possible. We do not require computation of the lower norm of the adjoint. In another related result [14], the constancy of the spectrum in minimal dynamical systems has also been extended to pseudospectra, which might provide an alternative avenue for computing pseudospectra rigorously.

As in the proof of Theorem 11, we will choose a sufficiently fine grid  $T_\tau$  on which to compute the approximations  $\tilde{\rho}_H(\lambda, \tau)$ . However, in the non-normal case, the scale  $\tau$  cannot be determined *a priori*. Instead, we will simultaneously decrease the maximum error  $\tau$  of the approximation  $\tilde{\rho}_H(\lambda, \tau)$  and the spacing of the grid  $T_\tau$  on which it is computed until a certain condition is met.

As a first step, Proposition 30 in Subsection 8.1 will show that a certain easily computable criterion is sufficient to guarantee that the spectrum is approximated well enough for a given  $\tau$ .

### 8.1 Approximating the pseudospectrum

To compute the  $\varepsilon$ -pseudospectrum, we will evaluate  $\tilde{\rho}_H(\lambda, \tau)$  for all  $\lambda \in T_\tau$ , where  $T_\tau$  is the following lattice:

$$T_\tau := \tau\sqrt{2}\mathbb{Z}^2 \cap B_{M+\varepsilon}(0) \subseteq \mathbb{C}. \quad (48)$$

This definition is very close to (46), except that the factor  $\frac{1}{4}$  is not necessary in the present case. We then decompose  $T_\tau$  into the following three disjoint sets:

$$S_\tau := \{ \lambda \in T_\tau \mid \tilde{\rho}_H(\lambda, \tau) < \varepsilon - \tau \}, \quad (49)$$

$$R_\tau := \{ \lambda \in T_\tau \mid \tilde{\rho}_H(\lambda, \tau) > \varepsilon + 2\tau \}, \quad (50)$$

$$U_\tau := T_\tau \setminus (S_\tau \cup R_\tau). \quad (51)$$

It is easy to see, using Corollary 28, that all points  $S_\tau$  are certainly in  $\text{Spec}_\varepsilon(H)$ , while all points in  $R_\tau$  are certainly not in  $\text{Spec}_\varepsilon(H)$ . The following proposition shows a simple condition on  $S_\tau$ ,  $R_\tau$  and  $U_\tau$  that, if fulfilled, guarantees that  $S_\tau$  will be a good approximation of the spectrum.

**Proposition 30.** *Let  $H$  be an fnc operator and  $\delta, \tau > 0$ . Let  $S_\tau$  and  $U_\tau$  be the sets defined in (49) and (51). Then, if*

$$d(\lambda, S_\tau) < \delta - \tau \quad \text{for all } \lambda \in U_\tau, \quad (52)$$

*we have*

$$d_H(S_\tau, \text{Spec}_\varepsilon(H)) < \delta.$$

*Proof.* By definition of  $S_\tau$ , we have  $S_\tau \subseteq \text{Spec}_\varepsilon(H)$ . Thus, the inequality for the Hausdorff distance reduces to showing that  $d(\lambda, S_\tau) \leq \delta$  for all  $\lambda \in \text{Spec}_\varepsilon(H)$ .

Let  $\lambda \in \text{Spec}_\varepsilon(H)$  be given. It is easy to show that  $\lambda \in B_{M+\varepsilon}(0)$ . The lattice  $T_\tau$  was chosen to have covering radius  $\tau$  in  $B_{M+\varepsilon}(0)$ , so we can find a  $\lambda' \in T_\tau$  with  $d(\lambda, \lambda') \leq \tau$ . Consider now the additional set  $R_\tau$  defined in (50). It is clear from the definitions of  $S_\tau$ ,  $R_\tau$  and  $U_\tau$ ,

(49), (50) and (51) respectively, that they are a disjoint decomposition of  $T_\tau$ . Thus,  $\lambda'$  must be in exactly one of these sets.

Of the three options,  $\lambda' \in R_\tau$  is actually impossible. That is because we have  $\lambda \in \text{Spec}_\varepsilon(H)$ , so  $\rho_H(\lambda) \leq \varepsilon$ . The Lipschitz continuity of  $\rho_H$  implies that  $\rho_H(\lambda') \leq \varepsilon + \tau$ . From Corollary 28, we then get  $\tilde{\rho}_H(\lambda', \tau) \leq \varepsilon + 2\tau$ . This means  $\lambda' \notin R'_\tau$ .

If we have  $\lambda' \in S_\tau$ , then  $d(\lambda, S_\tau) \leq \tau$ . But the algorithm always chooses  $\tau \leq \delta$ , so we have  $d(\lambda, S_\tau) \leq \delta$  in this case.

Finally, suppose that  $\lambda' \in U_\tau$ . By the hypothesis (52), we have  $d(\lambda', S_\tau) < \delta - \tau$ . Moreover  $d(\lambda, \lambda') \leq \tau$ , thus we have  $d(\lambda, S_\tau) \leq \delta$  also in this case. Therefore  $d(\lambda, S_\tau) \leq \delta$  is fulfilled for every  $\lambda \in \text{Spec}_\varepsilon(H)$ .  $\square$

## 8.2 The computational algorithm

Because the sets  $S_\tau$  and  $U_\tau$  are always finite, condition (52) from Proposition 30 can be checked in finite time, given the sets. Because this condition is sufficient to show that  $S_\tau$  is within distance  $\delta$  of  $\text{Spec}_\varepsilon(H)$ , we can compute the  $\varepsilon$ -pseudospectrum by simply checking smaller and smaller  $\tau > 0$ , as in the following algorithm.

**Algorithm 31** (Approximate the  $\varepsilon$ -pseudospectrum of  $H$  with maximum error  $\delta$ ).

```

Compute an upper bound  $M$  on the norm of  $H$ 
Compute the lattice  $T_\tau := \tau\sqrt{2}\mathbb{Z}^2 \cap B_{M+\varepsilon}(0)$ 
for  $j \leftarrow 1, 2, 3, \dots$  do
  Set  $\tau = 2^{-j} \cdot \delta$ 
  compute  $S_\tau$  and  $U_\tau$  according to Equations (49) and (51)
  if condition (52) holds then
    return  $S_\tau$ 
  end if
end for

```

Proposition 30 shows that if Algorithm 31 terminates, the result fulfills  $d_H(S_\tau, \text{Spec}_\varepsilon(H)) < \delta$ . To complete the proof of Theorem 13 it remains to show that Algorithm 31 always terminates. In other words, we need to show that for any *flc* operator  $H$ , as well as  $\varepsilon$  and  $\delta$ , condition (52) is fulfilled for  $\tau$  small enough. This will be proven in the following subsection.

## 8.3 Proof that the algorithm terminates

**Lemma 32.** *Let an flc operator  $H$  and  $\varepsilon, \delta > 0$  be given. Then there exists a  $\tau' > 0$  such that for all  $0 < \tau < \tau'$ , the sets  $S_\tau$  and  $U_\tau$  defined in equations (49) and (51) fulfill the condition (52) in Proposition 30.*

*Proof.* By Lemma 19, there exists a  $\tau' > 0$  such that for all  $0 < \tau < \tau'$ ,

$$d_H(\text{Spec}_{\varepsilon-3\tau'}(H), \text{Spec}_{\varepsilon+3\tau'}(H)) < \delta. \quad (53)$$

(We can choose a smaller  $\delta$  in Lemma 19 to obtain the strict inequality.)

Now let  $\lambda \in U_\tau$  be arbitrary. By definition of  $U_\tau$ , we have

$$\tilde{\rho}_H(\lambda, \tau) \leq \varepsilon + 2\tau, \quad (54)$$

because otherwise we would have  $\lambda \in R_\tau$ . From Corollary 28, we can deduce

$$\rho_H(\lambda) < \varepsilon + 3\tau. \quad (55)$$

Now by (53), we know that there exists a  $\lambda'' \in \text{Spec}_{\varepsilon-3\tau}(H)$  with  $d(\lambda, \lambda'') < \delta$ . This  $\lambda''$  hence fulfills

$$\rho_H(\lambda'') \leq \varepsilon - 3\tau. \quad (56)$$

Now we will set

$$\lambda' = \lambda'' + \tau \frac{\lambda - \lambda''}{|\lambda - \lambda''|}. \quad (57)$$

The point  $\lambda'$  lies on the line connecting  $\lambda$  and  $\lambda''$ , at a distance  $\tau$  from  $\lambda''$  in the direction of  $\lambda$ . Clearly, we have

$$d(\lambda', \lambda) < \delta - \tau, \quad (58)$$

because  $d(\lambda, \lambda'') < \delta$ . On the other hand, because  $\rho_H$  is Lipschitz continuous with constant  $\leq 1$  and  $d(\lambda', \lambda'') = \tau$ , we have

$$\rho_H(\lambda') \leq \rho_H(\lambda'') + \tau \leq \varepsilon - 2\tau. \quad (59)$$

where we used (56) in the second inequality. Corollary 28 again gives

$$\tilde{\rho}_H(\lambda', \tau) \leq \varepsilon - \tau. \quad (60)$$

It follows that  $\lambda' \in S_\tau$ . We have shown  $d(\lambda', \lambda) < \delta - \tau$  in (58), so  $d(\lambda, S_\tau) < \delta - \tau$ . But  $\lambda \in U_\tau$  was arbitrary, proving the Lemma.  $\square$

*Proof of Theorem 13.* The solution to the computational problem  $(\Omega_{\text{ps}}, \Lambda_{\text{ps}}, (m, d), \Xi_{\text{ps}})$  is given by the BSS algorithm  $\Gamma_k(H, \varepsilon)$  that is just the application of Algorithm 31 to the given  $H$ ,  $\varepsilon$  and  $\delta = 2^{-k}$ .

By Lemma 32, there exists a  $\tau' > 0$  such that condition (52) is fulfilled for all  $0 < \tau < \tau'$ . Thus, Algorithm 31 will terminate after at most  $\log_2(\max(1, \delta/\tau'))$  iterations. After the algorithm has terminated, the sets  $S_\tau$  and  $U_\tau$  fulfill condition (52), and therefore, by Proposition 30, we have

$$d_H(\Gamma_k(H, \varepsilon), \Xi_{\text{ps}}(H, \varepsilon)) = d_H(S_\tau, \text{Spec}_\varepsilon(H)) < \delta = 2^{-k}.$$

This completes the proof of Theorem 13.  $\square$

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## A Elementary lemmas

This Appendix collects several Lemmas with simple proofs that have been moved here to shorten the main text.

In proving the reduction to finite range in Section 3, we used the following lemma, which provides a bound on the sum of polynomially decaying hoppings starting at a given distance.

**Lemma 16.** *Let  $\varepsilon > 0$  and  $\Gamma$  be a subset of  $\mathbb{R}^n$  which is uniformly discrete with distance  $l$ . Then there is a constant  $C$ , depending only on  $n$  and  $l$ , such that*

$$\sum_{\substack{y \in \Gamma \\ d(x,y) > m}} d(x,y)^{-(n+\varepsilon)} \leq C \cdot \frac{1}{m^\varepsilon}. \quad (14)$$

Furthermore, the constant  $C$  can be computed by a BSS algorithm from  $n, \varepsilon$  and  $l$ .

*Proof.* Without loss of generality, we can assume that  $m > l$ . To compute the sum in (14), we use the Cauchy-Maclaurin criterion adapted to our setting in same spirit as in [80]. The main idea is to estimate the sum from above by using an integral. First, notice that  $d(x,y) \leq \|x-y\|_2 \leq d(x,y)\sqrt{n}$  where  $\|\cdot\|_2$  denotes the usual Euclidean norm in  $\mathbb{R}^n$ . Then, the function  $\mathbb{R}^n \ni y \mapsto d(x,y)^{-(n+\varepsilon)}$  is such that  $d(x,y)^{-(n+\varepsilon)} \leq n^{(n+\varepsilon)/2} \|x-y\|_2^{-(n+\varepsilon)}$ . For every  $y \in \Gamma$  such that  $d(x,y) > m$ , let  $\tilde{B}_{l/4}^{(x)}(y)$  be a closed (possibly rotated) hypercube of side length  $l/2$  such that  $y$  sits on one of its corner and for every  $z \in \tilde{B}_{l/4}^{(x)}(y)$  it holds that  $\|x-z\|_2 \leq \|x-y\|_2$ . Furthermore, by hypothesis on the uniform discreteness of  $\Gamma$  we have that  $\tilde{B}_{l/4}^{(x)}(y) \cap \Gamma = \{y\}$  for every  $y \in \Gamma$  and  $\tilde{B}_{l/4}^{(x)}(y) \cap \tilde{B}_{l/4}^{(x)}(z) = \emptyset$  if  $y \neq z$ . Thus we have

$$\begin{aligned} \sum_{\substack{y \in \Gamma \\ d(x,y) > m}} d(x,y)^{-(n+\varepsilon)} &\leq n^{(n+\varepsilon)/2} (l/2)^{-n} \sum_{\substack{y \in \Gamma \\ d(x,y) > m}} (l/2)^n \|x-y\|_2^{-(n+\varepsilon)} \\ &\leq n^{(n+\varepsilon)/2} (l/2)^{-n} \sum_{\substack{y \in \Gamma \\ d(x,y) > m}} \int_{\tilde{B}_{l/4}^{(x)}(y)} d^n z \|x-z\|_2^{-(n+\varepsilon)} \\ &\leq n^{(n+\varepsilon)/2} (l/2)^{-n} \int_{\|y-x\|_2 > \frac{m}{4}} d^n z \|x-z\|_2^{-(n+\varepsilon)} \\ &\leq n^{(n+\varepsilon)/2} (l/2)^{-n} (2\pi)^{n-1} \int_{\frac{m}{4}}^{+\infty} dr r^{n-1} r^{-(n+\varepsilon)}. \end{aligned}$$

where in the last integral we used the  $n$ -spherical coordinates. By explicit integration, the proofs is concluded.  $\square$

We also needed the following Lemma, which shows that  $\varepsilon_{L,\lambda,x}$  is nonincreasing in  $L$ .

**Lemma 27.** *Let  $H$  be a finite range discrete operator. For any fixed  $\lambda \in \mathbb{C}$ , the value of  $\varepsilon_{L,\lambda}$  is nonincreasing in  $L$ . Similarly, for any fixed  $\lambda \in \mathbb{C}$  and  $x \in \mathbb{R}^n$ , the value of  $\varepsilon_{L,\lambda,x}$  is nonincreasing in  $L$ .*

*Proof.* It is clear that the statement about  $\varepsilon_{L,\lambda}$  directly follows from the statement about  $\varepsilon_{L,\lambda,x}$ , because the infimum of a set of nonincreasing functions is again nonincreasing.

Let  $0 < L_1 < L_2$  be two values of  $L$ . Now the bound  $\varepsilon_{L_1,\lambda,x}$  is defined as the lower norm of  $Q_{L_1,\lambda,x}$ , which is the rectangular section of  $H$  going from  $\mathcal{H}_{B_{L_1}(x)}$  to  $\mathcal{H}_{B_{L_1+m}(x)}$ . It follows that we can find a sequence  $(\psi_n)_{n \in \mathbb{N}}$  with  $\psi_n \in \mathcal{H}_{B_{L_1}(x)}$  and  $\|\psi_n\| = 1$ , such that  $\|Q_{L_1,\lambda,x} \psi_n\| \rightarrow \varepsilon_{L_1,\lambda,x}$ .

Because  $B_{L_1}(x) \subseteq B_{L_2}(x)$ , we have canonical inclusions

$$\iota : \mathcal{H}_{B_{L_1}(x)} \rightarrow \mathcal{H}_{B_{L_2}(x)} \quad \text{and} \quad \iota_m : \mathcal{H}_{B_{L_1+m}(x)} \rightarrow \mathcal{H}_{B_{L_2+m}(x)} .$$

Clearly, we have the commutation relation

$$\iota_m Q_{L_1, \lambda, x} \psi_n = Q_{L_2, \lambda, x} \iota \psi_n ,$$

because  $H$  has finite range  $m$ . Furthermore,  $\|\iota \phi\|_{B_{L_2}(x)} = \|\phi\|_{B_{L_1}(x)}$  for all  $\phi \in \mathcal{H}_{B_{L_1}(x)}$ . Thus, we obtain

$$\|Q_{L_1, \lambda, x} \iota \psi_n\| = \|Q_{L_2, \lambda, x} \psi_n\| .$$

Thus  $\iota \psi_n$  is a sequence of states in  $\mathcal{H}_{B_{L_2}(x)}$  with  $\|Q_{L_1, \lambda, x} \iota \psi_n\| \rightarrow \varepsilon_{L_1, \lambda, x}$ . Because  $\varepsilon_{L_2, \lambda, x}$  is defined as the lower norm of  $Q_{L_2, \lambda, x}$ , this implies that

$$\varepsilon_{L_2, \lambda, x} \leq \varepsilon_{L_1, \lambda, x} . \quad \square$$

The following is a sort of ‘‘Sandwich Lemma’’ for the Hausdorff distance. It proves that if a set  $B$  is sandwiched between two sets  $A$  and  $C$ , then from the perspective of any reference set  $X$ , the intermediate set  $B$  cannot be farther away than both of the extremal sets  $A$  and  $C$ .

**Lemma 33.** *Let  $A, B, C, X$  be four subsets of a metric space  $(M, d)$  such that  $A \subseteq B \subseteq C$ . Then the Hausdorff distance  $d_H$  fulfills*

$$d_H(X, B) \leq \max(d_H(X, A), d_H(X, C)) .$$

*Proof.* By definition, we have

$$d_H(X, B) = \max \left( \sup_{x \in X} d(x, B), \sup_{b \in B} d(b, X) \right) .$$

Now because  $A \subseteq B$ , we have

$$d(x, B) \leq d(x, A) \leq d_H(X, A),$$

and from  $B \subseteq C$ , we get

$$\sup_{b \in B} d(b, X) \leq \sup_{c \in C} d(c, X) \leq d_H(C, X) .$$

Thus we obtain  $d_H(X, B) \leq \max(d_H(X, A), d_H(X, C)) = M$ . □

## B Definition of BSS algorithms

Computational problems can be solved by algorithms. One can define classes of algorithms corresponding to different models of computation [22]. In the following, we will use Blum-Shub-Smale (BSS) machines to define the computational steps of our algorithms [27, 26, 25, 81]. BSS machines are similar to Turing machines [97] but can store arbitrary real numbers (or elements of any other ring) on their tape. A BSS machine is characterized by a certain set of states and rules. Any such machine defines a mapping

$$f_{\text{BSS}} : \mathbb{R}^\infty \rightarrow \{ \boxed{\text{no-halt}} \} \cup \mathbb{R}^\infty ,$$

where  $\mathbb{R}^\infty = \mathbb{R}^0 \dot{\cup} \mathbb{R}^1 \dot{\cup} \mathbb{R}^2 \dot{\cup} \dots$  is the set of finite real sequences and  $\boxed{\text{no-halt}}$  is a special symbol. To determine the value of the function  $f_{\text{BSS}}$  at a specific  $x \in \mathbb{R}^\infty$ , the elements of  $x$  are written on the tape, and the value of the function  $f_{\text{BSS}}$  will be the numbers on the tape after the machine halts, or  $\boxed{\text{no-halt}}$  if the machine does not halt on the given inputs. We say that a BSS machine *always halts* if  $f(A) \neq \boxed{\text{no-halt}}$  for all  $A \in \mathbb{R}^\infty$ .

**Definition 34.** Let  $(\Omega, \Lambda, (M, d), \Xi)$  be a computational problem and let  $F_{\text{embed}} : \mathbb{R}^\infty \rightarrow M$  be a function with dense image. (The function  $F_{\text{embed}}$  is used to parameterize the solution space.) Furthermore, suppose that  $\Lambda$  is countable and  $(f_i)_{i \in \mathbb{N}}$  is an enumeration of  $\Lambda$ .

A *BSS algorithm*  $\Gamma$  for the problem  $(\Omega, \Lambda, (M, d), \Xi)$  can be described by a sequence of BSS functions  $(c_k)_{k \in \mathbb{N}_0} : \mathbb{R}^k \rightarrow \mathbb{R}^\infty$ , all of which halt on any input. Furthermore, we require that for any  $x \in \mathbb{R}^k$ , the vector  $a := c_k(x)$  has at least one element, and furthermore

- If  $a_0 \neq 0$ , then  $a \in \mathbb{R}^2$ , and  $a_1$  is an integer.
- If  $a_0 = 0$ , then  $a$  has an odd number of elements.

The purpose of these conditions on  $a$  is that we wish to reserve the first number of the result  $a_0$  to indicate whether the algorithm has terminated in step  $k$  or whether a further evaluation is requested. If  $a_0 \neq 0$ , then  $a_1 \in \mathbb{Z}$  shall determine the evaluation function that is requested. If  $a_0 = 0$ , then the execution terminates, and the following pairs of numbers shall determine the endpoints of the intervals whose union is the result of the computation, parameterized via  $F_{\text{embed}}$ .

To evaluate a BSS algorithm on a value  $x \in \Omega$ , we define a series of functions

$$d_k : \Omega \rightarrow M \dot{\cup} \mathbb{R}^{k+1}, \quad k \in \mathbb{N}.$$

which follow the instructions given by  $c_k(x)$ . As a first step, we let

$$d_0(A) = c_0,$$

where  $c_0 \in \mathbb{R}^\infty$  since  $c_0$  has zero arguments.

Now for all  $k > 0$ , the value of  $d_k(A)$  depends on the value of  $d_{k-1}(A)$ . If  $d_{k-1}(A) \in \mathbb{R}^k$ , then the algorithm has not terminated yet, but has evaluated  $(k+1)$  evaluation functions. To decide how to proceed in the next step, we then use the function  $c_k$ . Let

$$a = (a_0, \dots, a_m) = c_k(d_{k-1}(A)).$$

If  $a_0 \neq 0$ , then  $c_k$  has determined that another evaluation is necessary. In that case,  $m = 1$ , and  $a_1$  contains the index of the function to be evaluated. Therefore, in this case, we let

$$d_k(A) = (b_1, \dots, b_k, f_{a_1}(A)).$$

where  $(b_0, \dots, b_{k-1}) = d_{k-1}(A)$ , thus appending the result of the requested evaluation to the previous ones.

If on the other hand  $a_0 = 0$ , then  $c_k$  has determined that the previous evaluations were sufficient to estimate the result, and the values  $a_1, \dots, a_N$  contain a representation of the result. In this case, therefore, we let

$$d_k(A) = F_{\text{embed}}(a_1, \dots, a_N).$$

Finally, if  $d_{k-1}(A) \in M$ , then a result has already been found in a previous step, so that we have to perform no further computation and can simply define

$$d_k(A) = d_{k-1}(A).$$

Again, we say that the algorithm *terminates* for an argument  $A \in \Omega$  if  $d_k(A) \in M$  for some  $k \in \mathbb{N}$ . If an algorithm terminates for all  $A \in \Omega$ , we can define a map  $\Gamma : \Omega \rightarrow M$  by mapping  $A$  to  $d_k(A)$  for the first  $k \in \mathbb{N}$  for which  $d_k(A) \in M$ . If we speak of an *algorithm*  $\Omega \rightarrow M$  in the following, we always mean an algorithm that terminates for all  $A \in \Omega$ , and we will usually identify the algorithm with its associated map  $\Gamma : \Omega \rightarrow M$ .

## C Evaluation functions for *flc* operators

In this section, we will describe how to augment the set of evaluation functions  $\Lambda$  in a way that allows algorithms to make use of the *flc* structure for the *flc* spectral and pseudospectral problems defined in Definitions 10 and 12.

The evaluation functions have to represent a given *flc* operator by a set of real functions. Let  $H$  be an *flc* discrete operator. As a first step, for every  $L \in \mathbb{N}$ , let  $(x_{L,i})_{i=1,\dots,n_{\text{patch}}(L)}$  be an enumeration of the local patches at scale  $L$ , so that for every  $y \in \mathbb{R}^n$ , there is exactly one  $n \in \{1, \dots, n_{\text{patch}}(L)\}$  such that  $H$  has equivalent action on  $B_L(y)$  and  $B_L(x_{L,i})$ .

Now for every local patch  $B_L(x_m)$ , since  $\Gamma$  is uniformly discrete, the set  $B_L(x_m) \cap \Gamma$  is finite. For any  $L > 0$ ,  $m \in \{1, \dots, n_{\text{patch}}(L)\}$ , let  $(p_{L,m,k})$  be the  $k$ -th point in  $B_L(x_m)$ , according to some enumeration of the points. Using these definitions, we can now define our conditions on a set of evaluation functions that captures the finite local complexity structure.

**Condition 35.** Let

$$\mathcal{G} := (\{1\} \times \mathbb{N}) \dot{\cup} (\{2\} \times \mathbb{N} \times \mathbb{N}) \dot{\cup} (\{3\} \times \mathbb{N} \times \mathbb{N} \times \mathbb{N}) \\ \dot{\cup} (\{4\} \times \mathbb{N} \times \mathbb{N} \times \mathbb{N} \times \mathbb{N}).$$

Then a family of functions  $(f_i)_{i \in \mathcal{G}}$  fulfills our conditions for a set of evaluation functions if:

- $f_{1,L}(H)$  is the number of local patches, up to equivalent action, of  $H$  at scale  $L$ , defined above as  $n_{\text{patch}}(L)$ .
- $f_{2,L,m}(H)$  is the number of points in  $\Gamma \cap B_L(x_m)$ , defined above as  $n_{\text{point}}(L, m)$ .
- $f_{3,L,m,k,l}(H)$  is the matrix element  $\langle p_k, H_{B_L(x_m)} p_l \rangle$ , where  $p_k$  and  $p_l$  are the points in  $\Gamma \cap B_L(x_m)$  according to the above enumeration.
- $f_{4,L,n,k,i}(H)$  is  $i$ -th coordinate of  $p_{L,n,k}$ , defined above as the  $k$ -th point in the  $m$ -th patch at scale  $L$ , or zero if  $n > n_{\text{patch}}(L)$  or  $i > n$  or  $k > n_{\text{patch}}(L)$ .
- $f_5(H)$  is a bound on the norm of  $H$ .
- $f_6(H) =: C$  and  $f_7(H) =: \varepsilon$  are real numbers such that

$$|H_{xy}| \leq C d(x, y)^{-(n+\varepsilon)},$$

for all  $x, y \in \Gamma$ , as in Definition 5.

The evaluation functions  $f_{2,L,m}(H)$ ,  $f_{3,L,m,k,l}(H)$ , and  $f_{4,L,m,k,i}(H)$  are defined to be zero if any index is out of bounds, that is if  $m > n_{\text{patch}}(L)$  or  $k > n_{\text{point}}(L, m)$  or  $l > n_{\text{point}}(L, m)$  or  $i > n$ .

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