Computing Spectral Measures and Spectral Types:
New Algorithms and Classifications

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Abstract
Despite new results on computing the spectrum, there has been no general method able to compute spectral measures (as given by the classical spectral theorem) of infinite-dimensional normal operators. Given a matrix representation, we show that if each matrix column decays at infinity at a known asymptotic rate, then it is possible to compute spectral measures of self-adjoint and unitary linear operators on separable Hilbert spaces. The central ingredient of the new algorithm is the computation of the resolvent operator with error control. Computational spectral problems in infinite dimensions have led to the SCI hierarchy, which classifies the difficulty of a problem through the number of limits needed to numerically compute the solution. We classify the computation of measures, measure decompositions, types of spectra (pure point, absolutely continuous, singular continuous), functional calculus and Radon–Nikodym derivatives in the SCI hierarchy for such operators. The new algorithms are demonstrated to be efficient and practical on examples taken from orthogonal polynomials on the real line and the unit circle, and are also applied to evolution equations on a two-dimensional quasicrystal model.

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1 Introduction

Spectral analysis and computation forms a core part of many branches of science and mathematics, arising in diverse fields such as differential and integral equations, orthogonal polynomials, quantum mechanics, statistical mechanics, optics etc. [12,34,35,60,105,125,132]. Methods to numerically compute the spectrum, $\sigma(T)$, of an operator $T$ acting on the canonical Hilbert space $l^2(\mathbb{N})$ have attracted a large amount of interest over the last 60 years or so [6–9,15,18,19,22,23,30,31,36,39,62,68,69,88,92,93,111,117,118,120,121,137]. However, part of the richness and beauty that arises in infinite dimensions is the possibility of different spectral types. Given a normal operator $T$, there is an associated projection-valued measure (resolution of the identity), which we denote by $E_T$, whose existence is guaranteed by the spectral theorem and whose support is $\sigma(T)$ [76, 77, 109].

This allows the representation of the operator $T$ as an integral over $\sigma(T)$, analogous to the finite-dimensional case of diagonalisation:

$$Tx = \int_{\sigma(T)} \lambda dE_T(\lambda)x, \quad \forall x \in D(T),$$

(1.1)

where $D(T)$ denotes the domain of $T$. For example, if $T$ is compact then $E_T$ corresponds to projections onto eigenspaces, familiar from the finite-dimensional setting. However, in general, the situation is much more complicated with different types of continuous spectra (see §5). The computation of $E_T$, along with its various decompositions and their supports, is of great interest, both theoretically and for practical applications. An excellent and readable introduction can be found in Paul Halmos’ article “What does the spectral theorem say?” [65].

Recent work has shown how to compute the discrete part of the spectrum (isolated eigenvalues) [28, 29, 72] and essential spectra [11]. However, apart from the work of [147] (which deals with compact perturbations of tridiagonal Toeplitz operators) and methods for computing spectral density functions of Sturm–Liouville problems, there has been little work\(^1\) on the computation of the measure $E_T$ for $T$ in a given class\(^2\) of operators $\Omega$. From a numerical/computational point of view, the current state of affairs in infinite-dimensional spectral computations is thus analogous in finite dimensions to being able to compute the location of eigenvalues but not eigenvectors! It has been a long-standing open question whether the computation of spectral measures is possible, even for simple non-trivial subclasses such as discrete Schrödinger operators. We answer this question in the affirmative by providing the first set of algorithms for the computation of spectral measures for a large class of self-adjoint and unitary operators, namely, those whose matrix columns decay at a known asymptotic rate. This class covers the majority of operators, even unbounded, found in applications. In particular, those whose representation is sparse and also PDE operators, once a suitable basis has been selected.

A surprise thrown up by the infinite-dimensional spectral problem, which turns out to be quite generic, is the Solvability Complexity Index (SCI) [69]. The SCI provides a hierarchy for classifying the difficulty of computational problems. In classical numerical analysis, one hopes to construct an algorithm with one limit, $\Gamma_n$, such that for an operator $T$,

$$\Gamma_n(T) \rightarrow \sigma(T), \quad n \rightarrow \infty,$$

(1.2)

\(^1\)See §1.5 for connections with previous work.
\(^2\)For the computational problem to be existentially non-trivial, we must consider classes of operators as opposed to a single $T$.\n
preferably with some form of error control of the convergence. However, this is not always possible. For example, when considering the class of bounded $T$, the best possible alternative is an algorithm depending on three indices $n_1, n_2, n_3$ such that

$$\lim_{n_3 \to \infty} \lim_{n_2 \to \infty} \lim_{n_1 \to \infty} \Gamma_{n_3, n_2, n_1}(T) = \sigma(T).$$

Any algorithm with fewer than three limits will fail, and neither error control nor convergence rates on any of the limits are possible since these would reduce the number of limits needed. However, for self-adjoint operators, it is possible to reduce the number of limits to two, but not one [11, 69]. With more structure (such as sparsity or column decay) it is possible to compute the spectrum in one limit with a certain type of error control [31]. Hence, the only way to characterise the computational spectral problem is through a hierarchy classifying the difficulty of computing spectral properties of different subclasses of operators. The SCI classifies difficulty by considering the minimum number of limits that one must take to calculate the quantity of interest (see Appendix A for a full definition). This phenomenon also covers general numerical analysis problems, such as Smale’s question on the existence of purely iterative algorithms for polynomial root finding [11,41,95,96,128]. Extensions of the hierarchy to error control [28, 29] also have potential applications in the growing field of computer-assisted proofs [47, 48, 64] (where one must perform a computation with absolute certainty).

This paper provides classifications of spectral problems associated with $E^T$ (such as decompositions of the measure and spectrum) in the SCI hierarchy, some of which can be computed in one limit. We provide algorithms for these problems, and one of the main tools used is the computation of the resolvent operator $R(z, T) := (T - zI)^{-1}$ with error control (Proposition 2.1). We will also numerically demonstrate the algorithms.

1.1 Main contributions of the paper

Our main focus is on self-adjoint operators given as an infinite matrix whose columns (or off-diagonal elements) decay at a known asymptotic rate:

$$\| (P_{f(n)} - I)TP_n \| = O(\alpha_n)$$

for a sequence $\alpha_n \downarrow 0$ and function $f : \mathbb{N} \to \mathbb{N}$, where $P_n$ denotes the orthogonal projection onto the span of the first $n$ basis vectors. This paper contributes in three areas.

First, we consider the problem of computing spectral measures and projection-valued measures. Specifically, for operators of the form (1.3) we develop the first algorithms (and SCI classifications) for:

- **Proposition 2.1 and Corollary 2.2**: The action of the resolvent $x \mapsto R(z, T)x$ (with error control). This forms the basis of many of the algorithms constructed in this paper. The computation of the resolvent with error control also opens up potential applications in computer-assisted proofs.

- **Theorem 3.1**: The projection-valued spectral measure and, through taking inner products, the computation of the (standard) scalar spectral measures discussed in §1.3. This is done for open sets and can be extended to other types of sets such as closed intervals or singletons.

- **Theorem 3.2**: The decompositions (on a general open set) of the projection-valued and scalar-valued spectral measures into absolutely continuous, singular continuous and pure point parts.

- **Theorem 4.1**: The functional calculus of operators. In some cases, error control is possible, for instance, when considering the holomorphic functional calculus.

- **Theorem 4.2**: The Radon–Nikodym derivatives of the absolutely continuous parts of the scalar spectral measures with convergence in the $L^1$ sense on an open set. This requires a certain separation condition, without which our algorithm converges (Lebesgue) almost everywhere.

Second, we consider the computation of spectra as sets in the complex plane. Convergence is measured using the Hausdorff metric in the bounded case and using the Attouch–Wets metric in the unbounded case. Specifically, we prove in Theorem 5.1 that:

- The absolutely continuous spectrum $\sigma_{ac}(T)$ can be computed in two limits but not one limit.
- The pure point spectrum $\sigma_{pp}(T)$ can be computed in two limits but not one limit. In addition, we can set up the algorithm to ensure that we recover a portion of the eigenvalues after the first limit (i.e. this set is contained in the point spectrum).
The singular continuous spectrum $\sigma_{sc}(T)$ can be computed in three limits. If $f(n) - n \geq \sqrt{2n + 1/2}$ then the computation cannot be done in two limits. That is, if the local asymptotic bandwidth is allowed to grow sufficiently rapidly, three limits are needed, and this computational problem is exceedingly difficult. We do not know whether this growth condition on $f$ can be dropped, but without it the problem still requires at least two limits.

Our final contribution is the demonstration that the “one-limit” algorithms constructed in this paper are implementable and efficient. These provide the first set of algorithms addressing these problems, and we have provided extensive numerical experiments in §6. This includes orthogonal polynomials on the real line and unit circle, as well as transport properties of a two-dimensional model of a quasicrystal. We also develop a new collocation method for the computation of the Radon–Nikodym derivative. In the case where the derivative is regular enough, this is found to increase the performance substantially. Future work will look at extending the numerical examples to partial differential operators using state-of-the-art spectral methods.

Some brief remarks are in order.

(i) The impossibility results hold in general, even when restricted to tridiagonal operators. Furthermore, many of the impossibility results hold for structured operators such as bounded discrete Schrödinger operators. Our results (constructive algorithms and impossibility results) also carry over to a large class of normal operators, including unitary operators or skew-adjoint operators, both of which are important in applications, though, for the sake of clarity, we have stuck to the self-adjoint case in the statement of theorems and proofs.

(ii) The difficulty encountered when computing the singular continuous spectrum is partially due to the negative definition of the singular continuous part of a measure as the part that is not continuous with respect to Lebesgue measure and does not contain atoms. It is the “leftover” part of the measure. The challenge of studying $\sigma_{sc}$ analytically also reflects this difficulty - singular continuous spectra were once thought to be rather rare or exotic. However, they are quite generic; see for example [124].

(iii) The positive results hold for arithmetic algorithms and the impossibility results hold for general algorithms. We refer the reader to §1.4 and Appendix A for an explanation. Put simply, this means that the algorithms constructed can be implemented using only arithmetic operations (they can also be made to work with inexact input and restrictions to arithmetic over the rationals) and the impossibility results hold in any model of computation.

(iv) One might at first expect computational results to be independent of the function $f$ due to tridiagonalisation. However, the infinite-dimensional case is much more subtle than the finite-dimensional case. Using Householder transformations on a bounded sparse self-adjoint operator $T$ leads to a tridiagonal operator, but, in general, this operator is $T$ but restricted to a strict subspace of $l^2(N)$. Part of the operator may be lost in the strong operator limit. Instead, one must consider a sum of possibly infinitely many tridiagonal operators (see [67] chapters 2 and 8). Hence some spectral problems may have different classifications for different $f$.

1.2 A motivating example

As a motivating example, consider the case of a Jacobi operator with matrix

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \cdots \\ a_1 & b_2 & a_2 & \cdots \\ 0 & a_2 & b_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

where $a_j, b_j \in \mathbb{R}$ and $a_j > 0$. An enormous amount of work exists on the study of these operators, and the correspondence between bounded Jacobi matrices and probability measures with compact support [37, 136]. The entries in the matrix provide the coefficients in the recurrence relation for the associated orthonormal polynomials. To study the canonical measure $\mu_J$, one usually considers the principal resolvent function defined on $\mathbb{C}\backslash \sigma(J)$ via

$$G(z) := \langle R(z, J)e_1, e_1 \rangle = \int_R \frac{d\mu_J(x)}{x - z},$$

(1.4)
and then takes $z$ close to the real axis. The function $G$ is also known in the differential equations and Schrödinger communities as the Weyl $m$-function [56, 136] and one can develop the discrete analogue of what is known as Weyl–Titchmarsh–Kodaira theory for Sturm–Liouville operators. Going back to the work of Stieltjes [130] (see also [3, 145]), there is a representation of $G$ as a continued fraction:

$$G(z) := \frac{1}{-z + b_1 - \frac{a_1^2}{-z + b_2 - \ldots}}.$$  \hspace{1cm} (1.5)

One can also approximate $G$ via finite truncated matrices [136].

However, there are two major obstacles to overcome when using (1.5) and its variants as a means to compute measures. First of all, this representation of the principal resolvent function is structurally dependent. For example, (1.5) is valid for the restricted case of Jacobi operators and hence one is led to seeking different methods for different operators (such as tight binding Hamiltonians on two-dimensional lattices which have a growing bandwidth). Second, this would seem to give the wrong classification of the difficulty of the problem in the SCI hierarchy, giving rise to a tower of algorithms with two limits. One first takes a truncation parameter $n$ to infinity to compute $G(z)$ for $\text{Im}(z) > 0$, and then a second limit as $z$ approaches the real axis. One of the main messages of this paper is that both of these issues can be overcome. Measures can be computed in one limit via an algorithm $\Gamma_n$, and for a large class of operators. The only restriction is a known asymptotic decay rate of the off-diagonal entries. As a by-product, we compute the $m$-function of such operators with error control. Specific cases where this can be written explicitly do exist, such as periodic Jacobi matrices or perturbations of Toeplitz operators [43] (see also §1.5). However, there has been no general method proposed to compute the resolvent with error control. This consideration is crucial to allow the computation of measures in one limit.

To see how we might compute the measure using the resolvent, consider the Poisson kernel for the half-plane and the unit disk, defined respectively by

$$P_H(x, y) = \frac{1}{\pi} \frac{y}{x^2 + y^2}$$ and $$P_D(x, y) = \frac{1}{2\pi} \frac{1 - (x^2 + y^2)}{(x - 1)^2 + y^2} = P_D(r, \theta) = \frac{1}{2\pi} \frac{1 - r^2}{1 - 2r \cos(\theta) + r^2},$$ \hspace{1cm} (1.6)

where $(r, \theta)$ denote the usual polar coordinates. Let $T$ be a normal operator, then for $z \notin \sigma(T)$, we have from the functional calculus that

$$R(z, T) = \int_{\sigma(T)} \frac{1}{t - z} dE^T(t).$$

For self-adjoint $T$, $z = u + iv \in \mathbb{C}\setminus\mathbb{R}$, $(u, v \in \mathbb{R})$ and $x \in l^2(\mathbb{N})$ we define

$$K_H(z; T, x) := \frac{1}{2\pi i} [R(z, T) - R(\overline{z}, T)] x = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left[ \frac{1}{t - z} - \frac{1}{t - \overline{z}} \right] dE^T(t) x = \int_{-\infty}^{\infty} P_H(u - t, v) dE^T(t) x.$$

Figure 1: Smoothed approximations of the Radon–Nikodym derivative for the Jacobi operator associated to Jacobi polynomials with $\alpha = 1$, $\beta = 1/2$. Here the measure is absolutely continuous and supported on $[-1, 1]$. Left: Computation of convolutions for different $\epsilon$ using the methods of this paper. Right: The associated Poisson kernel $\pi^{-1} e/(\epsilon^2 + x^2)$ which approaches a Dirac delta distribution as $\epsilon \downarrow 0$. 

Similarly, if $T$ is unitary, $z = r \exp(i\psi) \in \mathbb{C}\setminus \mathbb{R}$ (with $z \neq 0$) and $x \in l^2(\mathbb{N})$ we define

$$K_D(z; T, x) := \frac{1}{2\pi i} [R(z, T) - R(1/\bar{z}, T)]x = \frac{1}{2\pi i} \int_{\mathbb{T}} \left[ \frac{1}{t - z} - \frac{1}{t - \frac{1}{\bar{z}}} \right] dE^T(t)x. \quad (1.8)$$

We change variables $t = \exp(i\theta)$ and with an abuse of notation, write $dE^T(t) = i \exp(i\theta)dE^T(\theta)$. A simple calculation then gives

$$K_D(z; T, x) = \int_{0}^{2\pi} P_D(r, \psi - \theta)dE^T(\theta)x. \quad (1.9)$$

Returning to our example, we see that the computation of the resolvent with error control allows the computation of $G(z)$ with error control through taking inner products. By considering $G(z) - G(\bar{z})$, this allows the computation of the convolution of the measure $\mu_j$ with the Poisson kernel $P_H$. In other words, we can compute a smoothed version of the measure $\mu_j$ with error control. Figure 1 demonstrates this for a typical example.

### 1.3 Functional analytic setup

We consider the canonical separable Hilbert space $\mathcal{H} = l^2(\mathbb{N})$, the set of square summable sequences with canonical basis $\{e_n\}_{n \in \mathbb{N}}$. Let $C(l^2(\mathbb{N}))$ be the set of closed densely defined linear operators $T$ such that span$\{e_n : n \in \mathbb{N}\}$ forms a core of $T$ and $T^*$. The spectrum of $T \in C(l^2(\mathbb{N}))$ will be denoted by $\sigma(T)$ and the point spectrum (the set of eigenvalues) by $\sigma_p(T)$. The latter set is not always closed and in general the closure of a set $S$ will be denoted by $\overline{S}$. The resolvent operator $(T - zI)^{-1}$ defined on $\mathbb{C}\setminus \sigma(T)$ will be denoted by $R(z, T)$.

This paper focusses on the subclass $\Omega_N \subset C(l^2(\mathbb{N}))$ of normal operators, that is, operators for which $D(T) = D(T^*)$ and $\|Tx\| = \|T^*x\|$ for all $x \in D(T)$. The subclasses $\subset \Omega_N$ of self-adjoint and unitary operators will be denoted by $\Omega_{SA}$ and $\Omega_U$ respectively. For $T \in \Omega_{SA}$ and $T \in \Omega_U$, $\sigma(T) \subset \mathbb{R}$ and $\sigma(T) \subset \mathbb{T}$ respectively, where $\mathbb{T}$ denotes the unit circle. Given $T \in \Omega_N$ and a Borel set $B$, $E_B^T$ will denote the projection $E^T(B)$. Given $x, y \in l^2(\mathbb{N})$, we can define a bounded (complex-valued) measure $\mu^T_{x,y}$ via the formula

$$\mu^T_{x,y}(B) = \langle E_B^T x, y \rangle. \quad (1.10)$$

Via the Lebesgue decomposition theorem [66], the spectral measure $\mu^T_{x,y}$ can be decomposed into three parts

$$\mu^T_{x,y} = \mu^T_{x,y,ac} + \mu^T_{x,y,sc} + \mu^T_{x,y,pp}, \quad (1.11)$$

the absolutely continuous part of the measure (with respect to the Lebesgue measure), the singular continuous part (singular with respect to the Lebesgue measure and atomless) and the pure point part. When considering $\Omega_{SA}$, we will consider Lebesgue measure on $\mathbb{R}$ and let

$$\mu^T_{x,y}(\lambda) = \frac{d\mu^T_{x,y,ac}}{dm}(\lambda), \quad (1.12)$$

the Radon–Nikodym derivative of $\mu^T_{x,y,ac}$ with respect to Lebesgue measure. Of course this can be extended to the unitary (and, more generally, normal) case. This naturally gives a decomposition of the Hilbert space $\mathcal{H} = l^2(\mathbb{N})$. For $I \in \{ac, sc, \text{pp}\}$, we let $H_I$ consist of vectors $x$ whose measure $\mu^T_{x,x}$ is absolutely continuous, singular continuous and pure point respectively. This gives rise to the orthogonal decomposition

$$\mathcal{H} = H_{ac} \oplus H_{sc} \oplus H_{pp} \quad (1.13)$$

whose associated projections will be denoted by $P_{ac}^T$, $P_{sc}^T$ and $P_{pp}^T$ respectively. These projections commute with $T$ and the projections obtained through the projection-valued measure. Of particular interest is the spectrum of $T$ restricted to each $H_I$, which will be denoted by $\sigma_I(T)$. These different sets and subspaces often, but not always, characterise different physical properties in quantum mechanics (such as the famous RAGE theorem [4,46,114]), where a system is modelled by some Hamiltonian $T \in \Omega_{SA}$ [32,33,53,85]. For example, pure point spectrum implies the absence of ballistic motion for many Schrödinger operators [123].

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3By a choice of basis our results extend to any separable Hilbert space. In particular, we can handle PDE operators using such a choice.
1.4 Algorithmic setup

Given an operator \( T \in C(l^2(N)) \), we can view it as an infinite matrix

\[
T = 
\begin{pmatrix}
    t_{11} & t_{12} & t_{13} & \ldots \\
    t_{21} & t_{22} & t_{23} & \ldots \\
    t_{31} & t_{32} & t_{33} & \ldots \\
    \vdots & \vdots & \vdots & \ddots
\end{pmatrix}
\]

through the inner products\(^4\) \( t_{ij} = \langle Te_j, e_i \rangle \). All of the algorithms constructed can also be adapted to operators on \( l^2(Z) \), either through the use of a suitable re-ordering of the basis, or through considering truncations of matrices in two directions, which is useful numerically since it preserves bandwidth. To be precise about the information needed to compute spectral properties, we define two classes of evaluation functions as

\[
\Lambda_1 = \{(Te_j, e_i) : i, j \in \mathbb{N}\}, \quad \Lambda_2 = \{(Te_j, e_i), (T^*e_j, T^*e_i) : i, j \in \mathbb{N}\}.
\]

These can be understood as different sets of information our algorithms are allowed to access (see Appendix A for a precise meaning). All the results proven in this paper can be easily extended to the case of inexact input. This means replacing the evaluation functions by

\[
f^{(1)}_{i,j,m}, f^{(2)}_{i,j,m} : C(l^2(N)) \rightarrow \mathbb{Q} + i\mathbb{Q}
\]

such that \( |f^{(1)}_{i,j,m}(T) - \langle Te_j, e_i \rangle| \leq 2^{-m} \) and \( |f^{(2)}_{i,j,m}(T) - \langle T^*e_j, T^*e_i \rangle| \leq 2^{-m} \), where \( \mathbb{Q} \) denotes the field of rationals. Hence, the existence results carry over to algorithms that are only allowed to perform arithmetic operations over \( \mathbb{Q} \). This could be useful for rigorous bounds using interval arithmetic and computer-assisted proofs (for those familiar with the term, our algorithms are Turing recursive), though for brevity we stick to \( \Lambda_1 \) and \( \Lambda_2 \) throughout. For discrete operators, the above information is often given to us, for example in tight binding models in physics or as a discretisation of a PDE, and hence it is natural to seek to compute spectral properties from matrix values. The set \( \Lambda_2 \) is motivated via variational problems. For PDE operators, such information is often given through inner products with a suitable basis and in this case the inexact input model is needed due to approximating the integrals (an example of this in the context of the SCI is [28]). For the classes considered in this paper, the evaluation sets \( \Lambda_1 \) and \( \Lambda_2 \) are in general different, yet the classifications in the SCI remain the same.

We will be concerned operators whose matrix representation has a known asymptotic rate of column/off-diagonal decay. Namely, let \( f : \mathbb{N} \rightarrow \mathbb{N} \) with \( f(n) > n \) and let \( \alpha = \{\alpha_n\}_{n \in \mathbb{N}}, \beta = \{\beta_n\}_{n \in \mathbb{N}} \) be null sequences\(^5\) of non-negative real numbers. We then define for \( X = \mathbb{S}A \) or \( \mathbb{U} \),

\[
\Omega_{f,\alpha,\beta}^X = \{T \in \Omega_X : \|(Pf(n) - I)TP_n\| = O(\alpha_n), \text{ as } n \rightarrow \infty\} \times \{x \in l^2(N) : \|P_n x - x\| = O(\beta_n), \text{ as } n \rightarrow \infty\},
\]

where \( P_n \) denotes the orthogonal projection onto \( \text{span}\{e_1, \ldots, e_n\} \). We will also use

\[
\Omega_{f,\alpha}^X = \{T \in \Omega_X : \|(Pf(n) - I)TP_n\| = O(\alpha_n), \text{ as } n \rightarrow \infty\}.
\]

When discussing \( \Omega_{f,\alpha,\beta}^{\mathbb{S}A} \) and \( \Omega_{f,\alpha}^{\mathbb{S}A} \) we will use the notation \( \Omega_{f,\alpha,\beta}^X \) and \( \Omega_{f,\alpha}^X \). The collection of vectors in \( l^2(N) \) satisfying \( \|P_n x - x\| = O(\beta_n) \) will be denoted by \( V_\beta \). Finally, when \( \alpha_n \equiv 0 \), we will abuse notation slightly in requiring the stronger condition that

\[
\|(Pf(n) - I)TP_n\| = 0.
\]

Thus \( \Omega_{f,\alpha} \) is the class of self-adjoint operators whose matrix sparsity structure is captured by the function \( f \). For example, if \( f(n) = n + 1 \) we recover the class of self-adjoint tridiagonal matrices, the most studied class of operators. When discussing classes that include vectors \( x \), we extend \( \Lambda_i \) to include pointwise evaluations of the coefficients of \( x \). Other additions are sometimes needed such as data regarding open sets as inputs for computations of measures but this will always be made clear. When considering the general case of \( \Omega_{f,\alpha} \), the function \( f \) and sequence \( \alpha \) can also be considered as inputs to the algorithm - in other words the same algorithm works for each class.

Finally, we give an informal definition of the SCI hierarchy, with a detailed summary contained in Appendix A. For a given set of evaluation functions (in this case \( \Lambda_1 \) or \( \Lambda_2 \), class of objects (in this case subclasses of operators acting on \( l^2(N) \)) and model of computation \( \alpha \) (in this paper general, \( G \), or arithmetic, \( A \)) we define:

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\(^4\)Our convention throughout will be that the inner product \( \langle \cdot, \cdot \rangle \) is linear in the first component and conjugate-linear in the second.

\(^5\)We use the term “null sequence” for a sequence converging to zero.
\Delta_0^\mathbb{N}: \text{The set of problems that can be computed in finite time, the SCI} = 0.

\Delta^\mathbb{N}_1: \text{The set of problems that can be computed using one limit, the SCI} = 1, \text{however one has error control, and one knows an error bound that tends to zero as the algorithm progresses.}

\Delta^\mathbb{N}_2: \text{The set of problems that can be computed using one limit, the SCI} = 1, \text{but error control may not be possible.}

\Delta^\mathbb{N}_{m+1}: \text{For } m \in \mathbb{N}, \text{the set of problems that can be computed by using } m \text{ limits, the SCI} \leq m.

The class \( \Delta_1 \) is, of course, a highly desired class; however, non-trivial spectral problems are higher up in the hierarchy. For example, the following classifications are known \([11, 69]\):

(i) The general spectral problem is in \( \Delta_4 \setminus \Delta_3 \).

(ii) The self-adjoint spectral problem is in \( \Delta_3 \setminus \Delta_2 \).

(iii) The compact spectral problem is in \( \Delta_2 \setminus \Delta_1 \).

Here, the notation \( \setminus \) indicates the standard “setminus”. Hence, the computational spectral problem becomes an infinite classification theory to characterise the above hierarchy. In order to do so, there will, necessarily, have to be many different types of algorithms. Indeed, characterising the hierarchy will yield a myriad of different approaches, as different structures on the various classes of operators will require specific algorithms.

1.5 Connections with previous work

We have mentioned the literature on infinite-dimensional spectral problems. Our point of view in this paper is closest to the work of Olver, Townsend and Webb on practical infinite-dimensional linear algebra \([98, 99, 101, 102, 147]\). This work includes efficient codes, such as the infinite-dimensional QL (IQL) algorithm \([146]\) (see also \([30]\) for the IQR algorithm), as well as theoretical results. A PDE version of the FEAST algorithm based on contour integration of the resolvent has recently been proposed in \([72]\), which seeks to compute the discrete part of the spectrum. The set of algorithms this paper provides can be considered as a new member in the growing family of infinite-dimensional techniques.

A similar, though different, object studied in the mathematical physics literature, particularly when considering random Schrödinger operators, and related to the finite section (Galerkin) method, is the density of states \([25, 79, 82]\), which we mention for completeness and to avoid potential confusion. This object is defined via the “thermodynamic limit”, where instead of considering the infinite-dimensional operator \(T\), one considers finite truncations, say \(P_nTP_n\), and the limit \( n \to \infty \) of the measure \( \sum_{\delta_j \in \sigma(P_nTP_n)} \delta_{\delta_j}/n \). To see why the density of states is different from the spectral measure of \(T\), consider \(T\) with discrete spectra below the essential spectrum. The contribution of these eigenvalues to the density of states vanishes as \( n \to \infty \). The spectral measure, on the other hand, allows the computation of spectral decompositions, as we demonstrate in this paper. The idea of using the resolvent to approximate the density of states of finite matrices was first introduced in the method of Haydock \([70]\), which approximates the imaginary part of \(\text{Trace} [R(z, P_nTP_n)]\) for \(\text{Im}(z) > 0\). Our algorithm is similar to Haydock’s method in that it involves computation of the resolvent in the complex plane, though with three key differences. First, we seek to deal with the full, infinite-dimensional, operator directly to compute the spectral measure. Second, and as a consequence of the first, the object we are computing contains more refined spectral information of the operator. The density of states does not capture the full spectral information, such as the contribution of eigenvalues in the discrete spectrum, whereas the spectral measure does and is also dependent on the input vector since we are computing the full action of spectral projections. For an example of this, we refer the reader to §6.4 where we use these projections to compute the functional calculus as a method of solving evolution equations on a quasicrystal. Third, there is a subtlety regarding the limits as \(\text{Im}(z)\) goes to zero and the truncation parameter goes to infinity, which is not present in the finite-dimensional case. Appropriate truncations of the infinite-dimensional operator are required to compute the resolvent with error control (see Proposition 2.1).

However, the density of states is an important quantity in quantum mechanics, and there is a large literature on its computation \([42, 44, 139, 148, 149]\). We refer the reader to the excellent review article \([89]\) which discusses the most common methods. For the C∗-algebra viewpoint of the density of states, we refer the reader to \([8, 10]\) and the references therein. For connections with equilibrium measures, we refer the reader to \([84]\). Estimating the spectrum of \(T\) via \(\sigma(P_nTP_n)\) is known as the finite section method. This has often been viewed in connection with Toeplitz theory and the reader may want to consult the work by Böttcher \([14, 17]\), Böttcher
The study of spectral measures also has a rich history in the theory of orthogonal polynomials and quadrature rules for numerical integration [40, 133], briefly touched upon in §1.2. In certain cases, it is possible to recover a distribution function for the associated measure of the Jacobi operator as a limit of functions constructed using Gaussian quadrature (see [26] chapter 2).

There are several papers considering the computation of spectral density functions for Sturm–Liouville problems. A common approach is to truncate the domain and use the Levitan–Levinson formula, as implemented in the software package SLEDGE [51, 52, 106]. More sophisticated methods avoiding domain truncation are considered for special cases in [49, 50] and an application in plasma physics can be found in [151]. These make use of the additional structure present in Sturm–Liouville problems using results analogous to (1.5) in the continuous case. In this paper, we focus solely on the discrete case, and in generality, though the ideas can be extended to PDE operators much more complicated than Sturm–Liouville operators (a subject of a future paper).

Finally, we wish to highlight the work of Webb and Olver [147], which is of particular relevance to the present study. There the authors studied Jacobi operators that are compact perturbations of Toeplitz operators through connection coefficients. The use of connection coefficients between two sets of orthogonal polynomials as a means of accessing spectral measures has its roots in the work of Uvarov [140, 141] and Kautsky and Golub [78]. The results proven in [147] can be stated in terms of the SCI hierarchy:

- If the perturbation is finite rank (and known), the computation of \( \sigma_{pp} \) and \( \mu_{pp} \) lies in \( \Delta_1^G \) and the computation of the \( \mu_{ac} \) lies in \( \Delta_0^G \) (note that \( \sigma_{ac} \) is known analytically).

- If the perturbation is compact with a known rate of decay at infinity, then the computation of the full spectrum \( \sigma \) lies in \( \Delta_1^G \).

The current paper extends the work of [147] by; considering operators much more general than tridiagonal compact perturbations of Toeplitz operators, allowing operators to be unbounded and building algorithms that are arithmetic and can cope with inexact input. At the price of this greater generality, the objects we study are not computable with error control and lead to computational problems higher up in the SCI hierarchy, though still computationally useful as we shall demonstrate. Our methods are also entirely different and rely on estimating the resolvent operator with error control.

### 1.6 Organisation of the paper

The paper is organised as follows. In §2 we consider the computation of the resolvent with error control and show how this can be used to compute the full measure via generalisations of Stone’s formula. The computation of measures, their various decompositions and projections are discussed in §3. We then mention two simple applications (the functional calculus and density of measures) in §4. The computation of the different spectra as sets in the complex plane is discussed in §5, which will also rely on an auxiliary result connected to Anderson localisation proven in Appendix B. We run extensive numerical tests in §6, where we also introduce a new collocation method for computation of the Radon–Nikodym derivative. Finally, we wrap up with a discussion in §7.

### 2 The Resolvent and Generalised Stone’s Formula

The algorithms built in this paper rely on the ability to compute the action of the resolvent operator \( R(z, T) = (T - z)^{-1} \) for \( z \not\in \sigma(T) \) with error control. Given this, one can then compute the action of the projections \( E_S^E \) for a wide range of sets \( S \) (Theorem 3.1 and its generalisations), and hence the measures \( \mu_{ac,S} \). In this section we discuss the computation of the resolvent with error control and how this can be used to compute measures via generalisations of Stone’s formula.

#### 2.1 Approximating the resolvent operator

The key proposition for computing the action of the resolvent operator is the following proposition, where we use \( \sigma_1 \) to denote the injection modulus of an operator:

\[
\sigma_1(T) := \min \{ \|Tx\| : x \in \mathcal{D}(T), \|x\| = 1 \}.
\]

The proof boils down to a careful computation of a least squares solution of a rectangular linear system.
Proposition 2.1. Let $T \in \Omega_N$, $z \in \mathbb{C} \setminus \sigma(T)$ and $x \in l^2(N)$. Suppose that the following hold for constants $C_1$ and $C_2$ (that may depend on $T$ and $x$ and may be unknown), together with null sequences $\{\alpha_n\}_{n \in \mathbb{N}}$ and $\{\beta_n\}_{n \in \mathbb{N}}$ independent of $T$ and $x$:

1. For $f : \mathbb{N} \to \mathbb{N}$ with $f(n) > n$, $\| (I - P_{f(n)} )T P_n \| \leq C_1 \alpha_n$,

2. $\| P_n x - x \| \leq C_2 \beta_n$,

3. For $\delta > 0$, $\text{dist}(z, \sigma(T)) \geq \delta$.

Then there exists a sequence of arithmetic algorithms $\Gamma_n(T, x, z)$ mapping into $l^2(N)$, each of which use the evaluation functions in $\Lambda_1$, such that each vector $\Gamma_n(T, x, z)$ has finite support with respect to the canonical basis for each $n$ and $\Gamma_n(T, x, z) \to R(z, T)x$. Moreover, the following error bound holds

$$\| \Gamma_n(T, x, z) - R(z, T)x \| \leq \frac{C_2 \beta_{f(n)} + C_1 \alpha_n \| \Gamma_n(T, x, z) \| + \| P_{f(n)}(T - zI)\Gamma_n(T, x, z) - P_{f(n)}x \|}{\delta}, \quad (2.1)$$

If a bound on $C_1$ and $C_2$ are known, this error bound can be computed to arbitrary accuracy using finitely many arithmetic operations and comparisons. In the more general case for a fixed $\{\alpha_n\}$, $\{\beta_n\}$ and $f$, this gives an asymptotic error bound for all $T$, $x$ and $z$ which satisfy the above assumptions.

Proof. We have that $n = \text{rank}(P_n) = \text{rank}((T - zI)P_n) = \text{rank}(P_{f(n)}(T - zI)P_n)$ for large $n$ since $\sigma_1(T - zI) > 0$ and $\| (I - P_{f(n)})(T - zI)P_n \| \leq C_1 \alpha_n \to 0$. Hence we can define

$$\tilde{\Gamma}_n(T, x, z) := \begin{cases} 0 & \text{if } \sigma_1(P_n(T^* - zI)P_{f(n)}(T - zI)P_n) \leq \frac{1}{n} \\
\left[ P_n(T^* - zI)P_{f(n)}(T - zI)P_n \right]^{-1} P_n(T^* - zI)P_{f(n)}x & \text{otherwise.} \end{cases}$$

Suppose that $n$ is large enough so that $\sigma_1(P_n(T^* - zI)P_{f(n)}(T - zI)P_n) > 1/n$. Then $\tilde{\Gamma}_n(T, x, z)$ is a (least squares) solution of the optimization problem $\text{arg} \min_y \| P_{f(n)}(T - zI)P_n y - x \|$. The linear space span $\{e_n : n \in \mathbb{N} \}$ forms a core of $T$ and hence of $T - zI$. It follows by invertibility of $T - zI$ that given any $\epsilon > 0$, there exists an $m = m(\epsilon)$ and a $y = y(\epsilon)$ with $P_m y = y$ such that

$$\| (T - zI)y - x \| \leq \epsilon.$$

It follows that for all $n \geq m$,

$$\| (T - zI)\tilde{\Gamma}_n(T, x, z) - x \| \leq \| P_{f(n)}(T - zI)\tilde{\Gamma}_n(T, x, z) - x \| + C_1 \alpha_n \| \tilde{\Gamma}_n(T, x, z) \| \leq \| P_{f(n)}(T - zI)y - x \| + C_1 \alpha_n \| \tilde{\Gamma}_n(T, x, z) \| \leq \| P_{f(n)}(T - zI)y - P_{f(n)}x \| + C_2 \beta_{f(n)} + C_1 \alpha_n \| \tilde{\Gamma}_n(T, x, z) \| \leq \epsilon + C_2 \beta_{f(n)} + C_1 \alpha_n \| \tilde{\Gamma}_n(T, x, z) \|.$$

This implies that

$$\| \tilde{\Gamma}_n(T, x, z) - R(z, T)x \| \leq \| R(z, T) \| \| (T - zI)\tilde{\Gamma}_n(T, x, z) - x \| \leq \| R(z, T) \| \left( \epsilon + C_2 \beta_{f(n)} + C_1 \alpha_n \| \tilde{\Gamma}_n(T, x, z) \| \right).$$

In particular, since $\alpha_n$ and $\beta_n$ are null, this implies that $\| \tilde{\Gamma}_n(T, x, z) \|$ is uniformly bounded in $n$. Since $\epsilon > 0$ was arbitrary and $\beta_{f(n)} \to 0$, we also see that $\tilde{\Gamma}_n(T, x, z)$ converges to $R(z, T)x$.

Define the matrices

$$B_n = P_n(T^* - zI)P_{f(n)}(T - zI)P_n, \quad C_n = P_n(T^* - zI)P_{f(n)}.$$

Given the evaluation functions in $\Lambda_1$, we can compute the entries of these matrices to any given accuracy and hence also to arbitrary accuracy in the operator norm (say using the Frobenius norm to bound the operator norm) using finitely many arithmetic operations and comparisons. Denote the approximations of $B_n$ and $C_n$ by $\tilde{B}_n$ and $\tilde{C}_n$, respectively and assume that

$$\| B_n - \tilde{B}_n \| \leq u_n, \quad \| C_n - \tilde{C}_n \| \leq v_n,$$
for null sequences \( \{u_n\}, \{v_n\} \). Note that \( \hat{B}_n^{-1} \) can be computed using finitely many arithmetic operations and comparisons. So long as \( u_n \) is small enough, the resolvent identity implies that

\[
\|B_n^{-1} - \hat{B}_n^{-1}\| \leq \frac{\|\hat{B}_n^{-1}\|^2}{1 - u_n \|B_n^{-1}\|} =: w_n.
\]

By taking \( u_n \) and \( v_n \) smaller if necessary (so that the algorithm is adaptive and it is straightforward to bound the norm of a finite matrix from above), we can ensure that \( \|\hat{B}_n^{-1}\|v_n \leq n^{-1} \) and \( (\|\hat{C}_n\| + v_n)w_n \leq n^{-1} \). From Proposition A.7 and a simple search routine, we can also compute \( \hat{C}_n \) to arbitrary accuracy using finitely many arithmetic operations and comparisons. Suppose this is done to an accuracy \( 1/n^2 \) and denote the approximation via \( \tau_n \). We then define

\[
\Gamma_n(T, x, z) := \begin{cases} 0 & \text{if } \tau_n \leq \frac{1}{n} \\ \hat{B}_n^{-1}\hat{C}_n x_n & \text{otherwise}, \end{cases}
\]

where \( x_n = P_{f(n)} x \). It follows that \( \Gamma_n(T, x, z) \) can be computed using finitely many arithmetic operations and, for large \( n \),

\[
\|\Gamma_n(T, x, z) - \tilde{\Gamma}_n(T, x, z)\| \leq \left(\|\hat{B}_n^{-1}\|v_n + (\|\hat{C}_n\| + v_n)w_n\right)\|x\| \to 0,
\]

so that \( \Gamma_n(T, x, z) \) converges to \( R(z, T)x \).

Furthermore, the following error bound holds (which also holds if \( \tau_n \leq 1/n \))

\[
\|\Gamma_n(T, x, z) - R(z, T)x\| \leq \|R(z, T)\|\|(T - zI)\Gamma_n(T, x, z) - x\|
\leq C_2\beta f(n) + C_1\alpha_n\|\Gamma_n(T, x, z)\| + \|P_{f(n)}(T - zI)\Gamma_n(T, x, z) - P_{f(n)} x\|
\leq \frac{C_2\beta f(n) + C_1\alpha_n}{\text{dist}(z, \sigma(T))} |||T - zI||| / n^2,
\]

since \( T \) is normal so that \( \|R(z, T)\| = \text{dist}(z, \sigma(T))^{-1} \). This bound converges to 0 as \( n \to \infty \). If the \( C_1 \) and \( C_2 \) are known it can be approximated to arbitrary accuracy using finitely many arithmetic operations and comparisons.

**Remark 1.** Of course, a vast literature exists on computing \( R(z, T) \), especially for infinite matrices with structure (such as being banded) and we refer the reader to [61, 91, 107, 119].

**Remark 2.** If \( T \) corresponds to a choice of basis in a Hilbert space of functions, there is often a link between the regularity of the functions \( x \) and the decay of the terms \( \beta_n \). The bound (2.1) can often be adapted to include these asymptotics and hence give an indication of how large \( n \) needs to be to gain a given approximation.

Note that if \( T \) is banded with bandwidth \( m \), then we can take \( f(n) = n + m \) and the above computation can be done in \( O(nm^2) \) operations [57]. The following corollary of Proposition 2.1 will be used repeatedly in the following proofs.

**Corollary 2.2.** There exist a sequence of arithmetic algorithms

\[ \Gamma_n : \Omega_{f, \alpha, \beta} \times \mathbb{C} \setminus \mathbb{R} \to l^2(\mathbb{N}) \]

with the following properties:

1. For all \( (T, x) \in \Omega_{f, \alpha, \beta} \) and \( z \in \mathbb{C} \setminus \mathbb{R} \), \( \Gamma_n(T, x, z) \) converges to \( R(z, T)x \) in \( l^2(\mathbb{N}) \) as \( n \to \infty \).
2. For any \( (T, x) \in \Omega_{f, \alpha, \beta} \), there exists a constant \( C(T, x) \) such that for all \( z \in \mathbb{C} \setminus \mathbb{R} \),

\[
\|\Gamma_n(T, x, z) - R(z, T)x\| \leq \frac{C(T, x)}{\text{Im}(z)} \left[\alpha_n + \beta_n\right].
\]

**Proof.** Let \( \Gamma_n(T, x, z) = \hat{\Gamma}_{m(n, T, x, z)}(T, x, z) \) where \( \hat{\Gamma}_k \) are the algorithms from the statement of Proposition 2.1 and \( m(n, T, x, z) \) is a subsequence diverging to infinity as \( n \to \infty \). Clearly statement (1) holds so we must show how to choose the sequence \( m(n, T, x, z) \) such that (2) holds (and hence our algorithms will be adaptive). From (2.1), it is enough to show that \( m = m(n, T, x, z) \) can be chosen such that

\[
\beta f(m) + \alpha_n \hat{\Gamma}_m(T, x, z) + \|P_{f(m)}(T - zI)\hat{\Gamma}_m(T, x, z) - P_{f(m)} x\| \leq \alpha_n + \beta_n.
\]

The left-hand side can be approximated to arbitrary accuracy using finitely many arithmetic operations and comparisons and hence by repeatedly computing approximations to within \( \alpha_n + \beta_n \), we can choose the minimal \( m \) such that these approximate bounds are at most \( 2(\alpha_n + \beta_n) \).\[\square\]
2.2 Stone’s formula and Poisson kernels

We next show how the computation of the action of the resolvent with error control allows the computation of the convolution of spectral measures with Poisson kernels as mentioned in §1.2. Moreover, this can be done with a certain sense of error control. This is related to Stone’s famous formula [27, 109, 131] to compute the pointwise action of the projection-valued measures associated with an operator \( T \in \Omega_{SA} \). However, Stone’s formula can be generalised to unitary operators and a much larger class of normal operators (see Proposition 2.4). We will assume the reader is familiar with standard results from spectral theory and harmonic analysis which, for example, can be found in [45, 109]. The following proposition is the celebrated Stone’s formula, and we include a short proof for the benefit of the reader since the ideas in the proof will be used elsewhere.

**Proposition 2.3** (Stone’s formula). Recalling the definitions of \( K_H \) and \( K_D \) in §1.2, the following boundary limits hold.

(i) Let \( T \in \Omega_{SA} \). Then for any \(-\infty \leq a < b \leq \infty \) and \( x \in l^2(\mathbb{N})\),

\[
\lim_{\epsilon \downarrow 0} \int_a^b K_H(u + i\epsilon; T, x) du = \frac{1}{2} E_{(a,b)}^T x + \frac{1}{2} E_{(a,b)}^T x.
\]

(ii) Let \( T \in \Omega_U \). Then for any \( 0 \leq a < b < 2\pi \) and \( x \in l^2(\mathbb{N}) \),

\[
\lim_{\epsilon \downarrow 0} \int_a^b i \exp(i\epsilon) K_D((1 - \epsilon) \exp(i\epsilon); T, x) d\psi = \frac{1}{2} E_{(a,b)}^T x + \frac{1}{2} E_{(a,b)}^T x,
\]

where \((a,b)\) denotes the image of \((a,b)\) under the map \( \theta \to \exp(i\theta) \).

**Proof.** To prove (i), we can apply Fubini’s theorem to interchange the order of integration and arrive at

\[
\int_a^b K_H(u + i\epsilon; T, x) du = \int_{-\infty}^{\infty} \int_a^b P_H(u - t, \epsilon) du dE^T(t)x.
\]

But

\[
\int_a^b P_H(u - t, \epsilon) du = \frac{1}{\pi} \left[ \tan^{-1} \left( \frac{b - t}{\epsilon} \right) - \tan^{-1} \left( \frac{a - t}{\epsilon} \right) \right]
\]

is bounded and converges pointwise as \( \epsilon \downarrow 0 \) to \( \chi_{(a,b)}(t) + \chi_{(a,b)}(t)/2 \), where \( \chi_S \) denotes the indicator function of a set \( S \). Part (i) now follows from the dominated convergence theorem.

To prove (ii), we apply Fubini’s theorem again, now noting that

\[
\int_a^b i \exp(i\epsilon) P_D((1 - \epsilon), \psi - \theta) d\psi = \frac{i \exp(i\theta)}{2\pi} \int_{a - \theta}^{b - \theta} \frac{(2\epsilon - \epsilon^2) \exp(i\psi)}{\epsilon^2 + 2(1 - \epsilon)(1 - \cos(\psi))} d\psi. \tag{2.2}
\]

We can split the interval into small intervals of width \( O(\rho) \) \((0 < \rho < 1)\) around each point where \( 1 - \cos(\psi) = 1 \) and a finite union of intervals on which \( 1 - \cos(\psi) \) is positive, bounded away from 0. On these later intervals, the limit vanishes as \( \epsilon \downarrow 0 \). Hence by periodicity and considering odd and even parts, we are left with considering

\[
I_1(\rho, \epsilon) = \int_0^\rho \frac{(2\epsilon - \epsilon^2) \cos(\psi)}{\epsilon^2 + 2(1 - \epsilon)(1 - \cos(\psi))} d\psi, \quad I_2(\rho, \epsilon) = \int_0^\rho \frac{(2\epsilon - \epsilon^2) \sin(\psi)}{\epsilon^2 + 2(1 - \epsilon)(1 - \cos(\psi))} d\psi.
\]

Explicit integration yields \( I_2(\rho, \epsilon) = O(\epsilon \log(\epsilon)) \) and hence the contribution vanishes in the limit. We also have

\[
I_1(\rho, \epsilon) = \frac{(\epsilon^2 - 2\epsilon)\rho + 2(2 + \epsilon^2 - 2\epsilon) \tan^{-1} \left( \frac{2(\epsilon - \rho)\tan \left( \frac{\epsilon}{2} \right)}{2(\epsilon - \rho)} \right)}{2(1 - \epsilon)}.
\]

This converges to \( \pi \) as \( \epsilon \downarrow 0 \). Considering the contributions of \( I_1 \) and \( I_2 \) in (2.2), we see that (2.2) converges pointwise as \( \epsilon \downarrow 0 \) to

\[
i \exp(i\theta) \left\{ \chi_{(a,b)}(\theta) + \left[ \chi_{(a)}(\theta) + \chi_{(b)}(\theta) \right]/2 \right\}.
\]

Since the integral is also bounded, part (ii) now follows from the dominated convergence theorem and change of variables. \( \square \)
Remark 3. The line segment/cone conditions near $T_w$ for some $f$ limit principal value integral of the resolvent $R_z$ bourhood of each of the $(Generalised Stone’s formula)$

Proposition 2.4

The next proposition does this and also holds for operators whose spectrum does not necessarily lie along a curve. However, it is much more straightforward in the general case to use the analyticity properties of the resolvent.

**Proposition 2.4** (Generalised Stone’s formula). Let $\gamma$ be a rectifiable positively oriented Jordan curve. Suppose that $T \in \Omega_N$ is such that $\sigma(T)$ intersects $\gamma$ at finitely many points $z_1, ..., z_m$. Suppose also that in a neighbourhood of each of the $z_i$, $\gamma$ is formed of a line segment meeting $\sigma(T)$ only at $z_i$, at which point $\sigma(T)$ has a local exterior cone condition with respect to $\gamma$ (see Figure 2). Let $x \in \ell^2(N)$. We can then define the Cauchy principal value integral of the resolvent $R(z, T)x$ along $\gamma$ and have

$$
\lim_{\epsilon \to 0} \frac{-1}{2\pi i} \text{PV} \int_{\gamma} R(z, T) x dz = E_{\sigma(T; \gamma)}^T x - \frac{1}{2} \sum_{j=1}^{m} E_{\{z_j\}}^T x,
$$

(2.3)

where $\sigma(T; \gamma)$ is the closure of the intersection of $\sigma(T)$ with the interior of $\gamma$.

**Remark 3.** The line segment/cone conditions near $z_i$ may seem strong. However, this is satisfied if $\sigma(T)$ lies on a curve with a well-defined normal near each $z_i$.

**Proof.** We will argue for the case $m = 1$, and the general case follows in exactly the same manner. Let $\epsilon > 0$ be small so that in a neighbourhood of the $\epsilon$-ball around $z_1$, $\gamma$ is given by a straight line. We then decompose $\gamma$ into two disjoint parts

$$
\gamma = \gamma_1^1 \cup \gamma_2^2
$$

as shown in Figure 2. We set

$$
F_{\epsilon}(x, T) = \int_{\gamma_1^1} R(z, T) x dz = \int_{\sigma(T)} \int_{\gamma_1^1} \frac{1}{t - z} dz dE^T(t)x.
$$

We then consider the inner integral

$$
f_{\epsilon}(t) = \int_{\gamma_1^1} \frac{1}{t - z} dz.
$$

If $t$ is inside $\gamma$ then $\lim_{\epsilon \to 0} f_{\epsilon}(t) = -2\pi i$ via Cauchy’s residue theorem. Similarly, if $t$ is outside $\gamma$ then $\lim_{\epsilon \to 0} f_{\epsilon}(t) = 0$. To calculate $f_{\epsilon}(z_1)$, consider the contour integral along $\gamma_\epsilon$ in Figure 2. We see that

$$
f_{\epsilon}(z_1) - i\pi = -2i\pi
$$

and hence $f_{\epsilon}(z_1) = -i\pi$. We would like to apply the dominated convergence theorem. Clearly, away from $z_1$ $f_{\epsilon}$ is bounded as $\epsilon \downarrow 0$. Now let $0 < \delta < \epsilon$ then

$$
f_{\delta}(t) - f_{\epsilon}(t) = \int_{\delta}^{\epsilon} \frac{1}{t - z} ds + \frac{1}{t - z_1} ds = \log \left( \frac{\epsilon + \frac{t - z_1}{w}}{-\epsilon + \frac{t - z_1}{w}} \right) - \log \left( \frac{\delta + \frac{t - z_1}{w}}{-\delta + \frac{t - z_1}{w}} \right)
$$

for some $w \in T$. Taking the pointwise limit $\delta \downarrow 0$, we see that we can prove that $f_{\epsilon}(t)$ is bounded for $t \in \sigma(T)$ in a neighbourhood of $z_1$ as $\epsilon \downarrow 0$ if we can prove the same for

$$
g_{\epsilon}(t) = \log \left( \frac{\epsilon + \frac{t - z_1}{w}}{-\epsilon + \frac{t - z_1}{w}} \right).
$$
By rotating and translating, we can assume that \( w = 1 \) and \( z_1 = 0 \) without loss of generality. Let \( t_1 = \text{Re}(t) \) and \( t_2 = \text{Im}(t) \). Using the cone condition gives \( \alpha |t_1| \leq |t_2| \) for some \( \alpha > 0 \). Assume \( t_1 \neq 0 \) then
\[
\frac{\epsilon + t}{-\epsilon + t} = \frac{(\epsilon + t_1)^2 + t_2^2}{(\epsilon - t_1)^2 + t_2^2} = 1 + \frac{4x}{(x - 1)^2 + y^2},
\]
where \( x = \epsilon/t_1 \) and \( y = t_2/t_1 \). Note that \( y^2 \geq \alpha^2 \) and without loss of generality we take \( y \geq \alpha \). Define
\[
h(x, y) = \frac{4x}{(x - 1)^2 + y^2}
\]
Note that \( h(x, y) \to 0 \) as \( |x|^2 + |y|^2 \to \infty \). We must show that \( h(x, y) \) is bounded above \(-1\) for \( y \geq \alpha \). It is enough to consider points where \( \partial h/\partial x = 0 \) which occur when \( x_\pm = \pm \sqrt{1 + y^2} \). We have
\[
h(x_\pm, y) = \frac{\pm 2}{\sqrt{1 + y^2} + 1} \geq \frac{-2}{\sqrt{1 + \alpha^2} + 1} > -1,
\]
and hence we have proved the required boundedness. We then define
\[
\text{PV} \int_\gamma R(z, T)xdz = \lim_{\epsilon \downarrow 0} F_\epsilon(x, T).
\]
The relation (2.3) now follows from the dominated convergence theorem. \( \square \)

**Remark 4.** It is possible to study non-tangential limits (which avoid the need for \( \gamma \) to be a straight line in a neighbourhood of the \( z_j \)) if one assumes more regularity on the measure. This is related to non-tangential limits of Cauchy integrals [97, 138] – a discussion of which is beyond the scope of this paper.

### 3 Computation of Measures

For the sake of brevity, the rest of this paper will consider the self-adjoint case \( T \in \Omega_{SA} \), which is the case most encountered in applications. However, the algorithms built are based on Proposition 2.1 (and Corollary 2.2) and the link with Poisson kernels/Cauchy transforms. Given the relation (1.9) and Proposition 2.4, the results can be straightforwardly extended to the unitary case and more general cases where conditions similar to that of Proposition 2.4 hold. We consider examples of unitary operators in §6.3.

#### 3.1 Full spectral measure

We start by considering the computation of \( E_U^T x \) where \( U \subset \mathbb{R} \) is a non-trivial open set. The collection of these subsets will be denoted by \( \mathcal{U} \). To be precise, we assume that we have access to a finite or countable collection \( a_m(U), b_m(U) \in \mathbb{R} \cup \{\pm \infty\} \) such that \( U \) can be written as a disjoint union
\[
U = \bigcup_m (a_m(U), b_m(U)). \quad (3.1)
\]

With an abuse of notation, we add this information as evaluation functions to \( \Lambda_1 \) to form \( \tilde{\Lambda}_1 \).

**Theorem 3.1** (Computation of measures on open sets). Given the above set-up, consider the map
\[
\Xi_{\text{meas}} : \Omega_{f, \alpha, \beta} \times \mathcal{U} \to l^2(\mathbb{N})
\]
\[
(T, x, U) \to E_U^T x.
\]
Then \( \{\Xi_{\text{meas}}, \Omega_{f, \alpha, \beta} \times \mathcal{U}, \tilde{\Lambda}_1\} \in \Delta_2^F \). In other words, we can construct a convergent sequence of arithmetic algorithms for the problem.

**Remark 5.** What this theorem essentially tells us, is that if we can compute the action of the resolvent operator with asymptotic error control, then we can compute the spectral measures of open sets in one limit. In the unitary case, this can easily be extended to relatively open sets of \( \mathbb{T} \). For any \( U \in \mathcal{U} \), the approximation of \( E_U^T x \) has finite support, and hence we can take inner products to compute \( \mu_{T, x, y}^U(U) \).
Proof. Let $T \in \Omega_{SA}$ and $z_1, z_2 \in \mathbb{C}\setminus \mathbb{R}$. By the resolvent identity and self-adjointness of $T$,
\[
\|R(z_1, T) - R(z_1, T)\| \leq \|\text{Im}(z_1)\|^{-1} \|\text{Im}(z_2)\|^{-1} |z_1 - z_2|.
\]

Hence, for $z = u + i\epsilon$ with $\epsilon > 0$, the vector-valued function $K_H(u + i\epsilon; T, x)$ (considered with argument $u$) is Lipschitz continuous with Lipschitz constant bounded by $\epsilon^{-2}\|x\|/\pi$. Now consider the class $\Omega_{f,\alpha,\beta} \times \mathcal{U}$ and let $(T, x, U) \in \Omega_{f,\alpha,\beta} \times \mathcal{U}$. From Corollary 2.2, we can construct a sequence of arithmetic algorithms, $\tilde{\Gamma}_n$, such that
\[
\|\tilde{\Gamma}_n(u, z) - K_H(u + i\epsilon; T, x)\| \leq \frac{C(T, x)}{\epsilon} (\alpha_n + \beta_n)
\]
for all $(T, x) \in \Omega_{f,\alpha,\beta}$. It follows from standard quadrature rules and taking subsequences if necessary (using that $\{\alpha_n\}$ and $\{\beta_n\}$ are null), that for $-\infty < a < b < \infty$, the integral
\[
\int_a^b K_H \left(u + \frac{i}{n}; T, x\right) \, du
\]
can be approximated to an accuracy $\tilde{C}(T, x)/n$ using finitely many arithmetic operations and comparisons and the relevant set of evaluation functions $\tilde{\Lambda}_i$ (the constant $C$ now becomes $\tilde{C}$ due to not knowing the exact value of $\|x\|$).

Recall that we assumed the disjoint union
\[
U = \bigcup_m (a_m, b_m)
\]
where $a_m, b_m \in \mathbb{R} \cup \{\pm\infty\}$ and the union is at most countable. Without loss of generality, we assume that the union is over $m \in \mathbb{N}$. We then let $a_{m,n}, b_{m,n} \in \mathbb{Q}$ be such that $a_{m,n} \downarrow a_m$ and $b_{m,n} \uparrow b_m$ as $n \to \infty$ with $a_{m,n} < b_{m,n}$ and hence $(a_{m,n}, b_{m,n}) \subset (a_m, b_m)$. Let
\[
U_n = \bigcup_{m=1}^n (a_{m,n}, b_{m,n}),
\]
then the proof of Stone’s formula in Proposition 2.3 (essentially an application of the dominated convergence theorem) can be easily adapted to show that
\[
\lim_{n \to \infty} \int_{U_n} K_H \left(u + \frac{i}{n}; T, x\right) \, du = E^T_U x.
\]

Note that we do not have to worry about contributions from endpoints of the intervals $(a_m, b_m)$ since we approximate strictly from within. To finish the proof, we simply let $\Gamma_n(T, x, U)$ be an approximation of the integral
\[
\int_{U_n} K_H \left(u + \frac{i}{n}; T, x\right) \, du
\]
to within accuracy $\tilde{C}(T, x)/n$ (which by the above remarks can be computed using finitely many arithmetic operations and comparisons and the relevant set of evaluation functions $\tilde{\Lambda}_1$).

This theorem can clearly be extended to cover the more general case of Proposition 2.4 if $\gamma$ is regular enough to allow approximation of
\[
\text{PV} \int_{\gamma} R(z, T) x \, dz
\]
given the ability to compute $R(z, T)x$ with asymptotic error control. Note that when it comes to numerically computing the integrals in Propositions 2.3 and 2.4, it is advantageous to deform the contour so that most of the contour lies far from the spectrum so that the resolvent has a smaller Lipschitz constant. The proof can also be adapted to compute $E_1 x$ where $I$ is a closed interval by considering intervals shrinking to $[a, b]$ ($a, b$ finite). A special case of this is the computation of the spectral measure of singleton sets. However, for these it must be easier to directly use the formulae
\[
E^T_{(u)} x = \lim_{\epsilon \downarrow 0} \epsilon \pi K_H(u + i\epsilon; T, x), \quad E^T_{(\exp(i\theta))} x = \lim_{\epsilon \downarrow 0} \epsilon \pi i \exp(i\theta) K_D((1 - \epsilon) \exp(i\theta); T, x),
\]
for $T \in \Omega_{SA}$ and $T \in \Omega_U$ respectively.

In the setting of Theorem 3.1, it is possible to compute the convolutions with error control. One may also wonder whether it is possible to upgrade the convergence of the algorithm in Theorem 3.1 from $\Delta_2$ to $\Delta_1$. In other words, whether it is possible to compute the measure with error control. However, this is difficult because the measure may be singular. Theorem 5.3 shows this is impossible even for singleton sets and discrete Schrödinger operators acting on $l^2(\mathbb{N})$.

3.2 Measure decompositions and projections

Recall from §1.3 that $P_T$ denotes the orthogonal projection onto the space $\mathcal{H}_T$, where $\mathcal{I}$ denotes a generic type (ac, sc, pp, c or s). We have included the continuous and singular parts denoted by c or s which correspond to $\mathcal{H}_ac \oplus \mathcal{H}_sc$ and $\mathcal{H}_ac \oplus \mathcal{H}_{pp}$, respectively. In this section we prove the following theorem.

Theorem 3.2. Given the set-up in §§1.3 and 3.1, consider the map

$$\Xi_\mathcal{I} : \Omega_{f,\alpha,\beta} \times V_\beta \times U \to \mathbb{C}$$

$$(T, x, y, U) \to \langle P_T E_T^T x, y \rangle = \mu_{x,y,T}(U),$$

for $\mathcal{I} = ac, sc, pp, c$ or s. Then for $i = 1, 2$

$$\Delta^Q_2 \notin \{\Xi_\mathcal{I}, \Omega_{f,\alpha,\beta} \times V_\beta \times U, \tilde{\Lambda}_i\} \in \Delta^A_3.$$

By the polarisation identity, it is enough to consider $x = y$ (note that all the projections commute). Since $P_T = I - P_{sc}, P_T^T = I - P_{pp}$ and $P_T = P_T^T - P_{pp}^T$, it is enough to consider only $\mathcal{I} = c$ and $\mathcal{I} = s$. We will split the proof into two parts - the positive $\Delta^A_3$ inclusion (for which it is enough to consider $\tilde{\Lambda}_1$) and the negative $\Delta^Q_2$ exclusion (for which it is enough to consider $\tilde{\Lambda}_2$).

Proof of positive part of Theorem 3.2. Step 1: We first deal with $\mathcal{I} = c$, where we shall use a similar argument to the proof of Theorem 4.1 (which is more general than what we need). We recall the RAGE theorem [44,46,114] as follows. Let $Q_n$ denote the orthogonal projection onto vectors in $l^2(\mathbb{N})$ with support outside the subset \{1, ..., n\} $\subset \mathbb{N}$. Then for any $x \in l^2(\mathbb{N})$,

$$\langle P_T E_T^T x, x \rangle = \|P_T E_T^T x\|^2 = \lim_{n \to \infty} \lim_{t \to \infty} \frac{1}{t} \int_0^t \|Q_n e^{-itS} E_T^T x\|^2 \, ds$$

$$= \lim_{n \to \infty} \lim_{t \to \infty} \frac{1}{t} \int_0^t \|Q_n e^{-itS} \chi_U(T) x\|^2 \, ds. \quad (3.3)$$

The proof of Theorem 4.1 is easily adapted to show that there exists arithmetic algorithms $\tilde{\Gamma}_{n,m}$ using $\tilde{\Lambda}_1$ such that

$$\|Q_n e^{-itS} \chi_U(T) x - \tilde{\Gamma}_{n,m}(T,x,U,s)\| \leq \frac{C(T,x,U)}{m}$$

for all $(T,x,U,s) \in \Omega_{f,\alpha,\beta} \times U \times \mathbb{R}$. Note that this bound can be made independent of $s$ (as we have written above) by sufficiently approximating the function $\exp(-its)\chi_U(t)$ (it has known total variation for a given $s$ and uniform bound). We now define

$$\Gamma_{n,m}(T,x,U) = \frac{1}{m^2} \sum_{j=1}^{m^2} \|\tilde{\Gamma}_{m,n}(T,x,U,j/m)\|^2.$$

Using the fact that for $a, b \in l^2(\mathbb{N})$,

$$|\langle a, a \rangle - \langle b, b \rangle| \leq \|a - b\| (2\|a\| + \|a - b\|), \quad (3.4)$$

it follows that

$$\left|\|Q_n e^{-itS} \chi_U(T) x\|^2 - \|\tilde{\Gamma}_{n,m}(T,x,U,s)\|^2\right| \leq \frac{C(T,x,U)}{m} \left(2\|x\| + \frac{C(T,x,U)}{m}\right).$$
Hence we have shown that
\[
\left| \Gamma_{n,m}(T, x, U) - \frac{1}{m} \int_0^m \| Q_n e^{-iT_{:\chi_U}}(T)x \|^2 \, ds \right| \leq \frac{1}{m^2} m^2 \sum_{j=1}^{m^2} \frac{C(T, x, U)}{m} \left( 2\|x\| + \frac{C(T, x, U)}{m} \right) + \frac{1}{m^2} m^2 \sum_{j=1}^{m^2} g_n(j/m) - m \int_{\Omega} g_n(s)ds ,
\]
where \( g_n(s) = \| Q_n e^{-iT_{:\chi_U}}(T)x \|^2 \). Clearly the first term converges to 0 as \( m \to \infty \) so we only need to consider the second. Using (3.4), it follows that for any \( \epsilon > 0 \) that
\[
|g_n(s) - g_n(s + \epsilon)| \leq 4\| Q_n e^{-iT_{\chi_U}}(e^{-iT_{\epsilon}} - I)\chi_U(T)x \|\| x \| \leq 4\|x\|\| (e^{-iT_{\epsilon}} - I)\chi_U(T)x \|.
\]
But \( e^{-iT_{\epsilon}} - I \) converges strongly to 0 as \( \epsilon \to 0 \) and hence the quantity
\[
\left| g_n(j/m) - m \int_{\Omega} g_n(s)ds \right| \to 0
\]
as \( m \to \infty \) uniformly in \( j \). It follows that
\[
\lim_{m \to \infty} \Gamma_{n,m}(T, x, U) = \lim_{\epsilon \to \infty} \frac{1}{t} \int_0^t \| Q_n e^{-iT_{\chi_U}}E_{T}^T(x) \|^2 \, ds
\]
and hence
\[
\lim_{n \to \infty} \lim_{m \to \infty} \Gamma_{n,m}(T, x, U) = \langle P_{\epsilon}^T E_T\chi_U(x, x) \rangle.
\]

**Step 2:** Next we deal with the case \( \Omega = \delta \). Note that for \( z \in \mathbb{C} \setminus \mathbb{R} \), \( \langle R(z, T)x, x \rangle \) is simply the Stieltjes transform (also called the Borel transform) of the positive measure \( \mu_{x, x}^T \):
\[
\langle R(z, T)x, x \rangle = \int_{\mathbb{R}} \frac{1}{t - z} d\mu_{x, x}^T(t).
\]
The Hilbert transform of \( \mu_{x, x}^T \) is given by the limit
\[
H_{\mu}(t) = H_{\mu_{x, x}^T}(t) = \frac{1}{\pi} \lim_{\epsilon \to 0} \text{Re}(\langle R(t + i\epsilon, T)x, x \rangle),
\]
with the limit existing (Lebesgue) almost everywhere. This object was studied in [103, 104], where we shall use the result (since the measure is positive) that for any bounded continuous function \( f \), \( \mu_{x, x}^T \)
\[
\lim_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f(t)\chi_{\{w : |H_{\mu}(w)| > s\}} dt = \int_{\mathbb{R}} f(t) d\mu_{x, x}^T(t). \tag{3.5}
\]
Now let \( (T, x, U) \in \Omega f_{\alpha, \beta} \times U \) with
\[
U = \bigcup_m (a_m, b_m)
\]
where \( a_m, b_m \in \mathbb{R} \cup \{ \pm \infty \} \) and the union is at most countable. Without loss of generality, we assume that the union is over \( m \in \mathbb{N} \). Due to the possibility of point spectra at the endpoints \( a_m, b_m \), we cannot simply replace \( f \) by \( \chi_U \) in the above limit (3.5). However, this can be overcome by using the Hilbert transform of point measures in the following manner. Let \( \mu_{x, x}^T \) denote the measure \( \mu_{x, x}^T \) restricted to the bounded interval \( (-\infty, \infty) \) so that the measure \( \mu_{x, x}^T - \mu_{x, x}^T \) has no atomic part at the endpoints. Let \( f_s \) denote a pointwise increasing sequence of continuous functions, converging everywhere up to \( \chi_U \) such that the support of each \( f_s \) is contained in
\[
[-s, s] \cap \left( \bigcup_{m=1}^{[s]} (a_m, b_m - \sqrt{s}^{-1}) \right),
\]
\[\text{Note that this is stronger than weak* convergence which in this case means restricting to continuous functions vanishing at infinity.} \]
That the result holds for arbitrary \( f \) is due to the tightness condition that the result holds for the function identically equal to 1.
Such a sequence exists (and can be constructed) precisely because $U$ is open. We first claim that

$$
\lim_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f_s(t) \chi_{\{w \mid |\mu(w)| \geq s\}} dt = \mu^{T}_{x,x,s}(U).
$$

(3.6)

To see this note that for any $u \in \mathbb{R}$, the following inequalities hold

$$
\liminf_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f_s(t) \chi_{\{w \mid |\mu(w)| \geq s\}} dt \geq \liminf_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f_u(t) \chi_{\{w \mid |\mu(w)| \geq s\}} dt
$$

$$
= \int_{\mathbb{R}} f_u(t) d\mu^{T}_{x,x,s}(t).
$$

Taking $u \to \infty$ gives that

$$
\liminf_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f_s(t) \chi_{\{w \mid |\mu(w)| \geq s\}} dt \geq \mu^{T}_{x,x,s}(U),
$$

(3.7)

so we are left with proving a similar bound for the limit supremum. A simple calculation shows that for 
$t \notin \{a_m, b_m : m \in \mathbb{N}\}$, it holds that

$$
H^{T}_{x,x,s}(t) = \sum_{m=1}^{\infty} \left( \frac{\mu^{T}_{x,x}(\{a_m\})}{\pi(a_m - t)} + \frac{\mu^{T}_{x,x}(\{b_m\})}{\pi(b_m - t)} \right).
$$

Hence, there exists a constant $C$ (since the measure $\mu^{T}_{x,x}$ is finite) such that

$$
\left| H^{T}_{x,x,s}(t) \right| \leq C \sqrt{s}
$$

on the support of $f_s$. Now let $\epsilon \in (0, 1)$. Then, for large $s$, $s - C \sqrt{s} \geq (1 - \epsilon) s$ and hence

$$
\text{supp}(f_s) \cap \{w : |\mu(w)| \geq s\} \subseteq \text{supp}(f_s) \cap \{w : |\mu - \tilde{\mu}(w)| \geq (1 - \epsilon) s\}. \quad (3.8)
$$

Now let $f$ be any bounded continuous function such that $f \geq \chi_U$. Then using (3.8),

$$
\limsup_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f_s(t) \chi_{\{w \mid |\mu(w)| \geq s\}} dt \leq \limsup_{s \to \infty} \frac{1}{1 - \epsilon} \frac{\pi(1 - \epsilon)s}{2} \int_{\mathbb{R}} f_s(t) \chi_{\{w \mid |\mu(w)| \geq (1 - \epsilon)s\}} dt
$$

$$
\leq \limsup_{s \to \infty} \frac{1}{1 - \epsilon} \frac{\pi(1 - \epsilon)s}{2} \int_{\mathbb{R}} f(t) \chi_{\{w \mid |\mu - \tilde{\mu}(w)| \geq (1 - \epsilon)s\}} dt
$$

$$
= \frac{1}{1 - \epsilon} \int_{\mathbb{R}} f(t) d(\mu^{T}_{x,x,s} - \tilde{\mu}^{T}_{x,x,s})(t).
$$

We now take $f \downarrow \chi_U$ and use the dominated to convergence to yield

$$
\limsup_{s \to \infty} \frac{\pi s}{2} \int_{\mathbb{R}} f_s(t) \chi_{\{w \mid |\mu(w)| \geq s\}} dt \leq \frac{1}{1 - \epsilon} \mu^{T}_{x,x,s}(U).
$$

Taking $\epsilon \downarrow 0$ gives the bound for the limit supremum and together with (3.7) yields the claim (3.6).

Let $\chi_n$ be a sequence of non-negative continuous piecewise linear functions on $\mathbb{R}$, bounded by 1 and such that $\chi_n(t) = 0$ if $t \leq n - 1$ and $\chi_n(t) = 1$ if $t \geq n + 1$. Consider the integrals

$$
I(n, m) = \frac{\pi n}{2} \int_{\mathbb{R}} f_n(t) \chi_n(|F_m(t)|) dt,
$$

where $F_m(t)$ is an approximation of

$$
\frac{1}{\pi} \text{Re} \left( \left\langle R(t + \frac{i}{m}, T), \chi_n \right\rangle \right)
$$

to pointwise accuracy $O(m^{-1})$ over $t \in [-n, n]$. Note that a suitable piecewise linear function $f_n$ can be constructed using $\tilde{\Lambda}_1$, as can suitable $\chi_n$, and a suitable approximation function $F_m$ can be pointwise evaluated.
using \( \tilde{A}_1 \) (again by Corollary 2.2). It follows that there exists arithmetic algorithms \( \Gamma_{n,m}(T,x,U) \) using \( \tilde{A}_1 \) such that
\[
|I(n,m) - \Gamma_{n,m}(T,x,U)| \leq \frac{C(T,x,U)}{m}.
\]
The dominated convergence theorem implies that
\[
\lim_{m \to \infty} \Gamma_{n,m}(T,x,U) = \lim_{m \to \infty} I(n,m) = \frac{\pi n}{2} \int_{\mathbb{R}} f_n(t) \chi_n(|H_\mu(t)|) dt.
\]
Note that continuity of \( \chi_n \) is needed to gain convergence almost everywhere and prevent possible oscillations about the level set \( \{ H_\mu(t) = n \} \). We also have
\[
\chi_{\{ w : |H_\mu(w)| \geq n+1 \}}(t) \leq \chi_n(|H_\mu(t)|) \leq \chi_{\{ w : |H_\mu(w)| \geq n-1 \}}(t)
\]
The same arguments used to prove (3.6), therefore show that
\[
\lim_{n \to \infty} \frac{\pi n}{2} \int_{\mathbb{R}} f_n(t) \chi_n(|H_\mu(t)|) dt = \mu_{x,x,\mu}(U).
\]
Hence,
\[
\lim_{n \to \infty} \lim_{m \to \infty} \Gamma_{n,m}(T,x,U) = \mu_{x,x,\mu}(U),
\]
completing the proof of the theorem. \( \square \)

To prove the negative result, we introduce some notation which will also be used in §5.1. Consider a connected, undirected, locally finite graph \( G \), such that the degree of each vertex is bounded by some constant \( C_G \) and such that the set of vertices \( V(G) \) is countably infinite. We also assume that there exists at most one edge between two vertices and no edges from a vertex to itself and use the abuse of notation by identifying \( G \) with its canonical vector in \( \overline{I}^2(V(G)) \cong \overline{I}^2(\mathbb{N}) \). The notation \( x \sim y \) means there is an edge in \( G \) connecting vertices \( x \) and \( y \). We will use \( |x - y| \) to denote the length of a shortest path between vertices \( x, y \) (which always exists since the graph is connected), and \( \zeta(x) \) to denote the valence of \( x \). An arbitrary base vertex \( x_0 \) is chosen and we define \( |x| = |x - x_0| \).

The (negative) discrete Laplacian or free Hamiltonian \( H_0 \) acts on \( \psi \in \overline{I}^2(V(G)) \) via
\[
\{ H_0 \psi \}(x) = -\sum_{y \sim x} [\psi(y) - \psi(x)].
\]
(3.9)
Since the vertex degree being bounded, \( H_0 \) is a bounded operator. We define a Schrödinger operator on \( G \) to be an operator of the form
\[
H_v = H_0 + v,
\]
where \( v \) is a bounded (real-valued) multiplication operator
\[
\{ v \psi \}(x) = v(x) \psi(x).
\]
We will also need Theorem 5.2 from §5.1, which considers Anderson localisation under finite rank perturbations of a potential.

**Proof of negative part of Theorem 3.2.** To prove the negative result, it is enough to consider \( I = \mathbb{P}_m \) and \( s \). We begin with \( \Pi_{\mathbb{P}_m} \) and consider \( U = \mathbb{R} \). We also restrict the proof to considering bounded Schrödinger operators acting on \( \overline{I}^2(\mathbb{N}) \), which are clearly a subclass of \( \Omega_{\mathbb{P}_m} \) for \( f(n) = n+1 \). Note that since the evaluation functions in \( \tilde{A}_2 \) can be recovered from those in \( \tilde{A}_1 \) in this special case, we can assume that we are dealing with \( \tilde{A}_1 \).

Suppose for a contradiction that there does exist a sequence of general algorithms \( \Gamma_n \) such that
\[
\lim_{n \to \infty} \Gamma_n(H_v) = \langle p_{\mathbb{P}_m}^{H_v} e_1, e_1 \rangle.
\]
We will construct a potential \( v \) such that \( \Gamma_n(H_v) \) does not converge. To do this, choose \( \rho = \chi_{[-c,c]} / (2c) \) for some constant \( c \) such that the conditions of Theorem 5.2 hold. We will use Theorem 5.2 and the following well known facts:

1. If \( v \) is periodic, then \( H_v \) can be extended to a Schrödinger operator on \( \overline{I}^2(\mathbb{Z}) \) with even and periodic potential and hence the spectrum of \( H_v \) is purely absolutely continuous (see for example [136]).
2. If we are in the setting of Theorem 5.2 then the spectrum of \(H_v\) is pure point almost surely.

We will define the potential \(v\) inductively as follows. Let \(v_1\) be a potential of the form \(v_\omega\) (with the density \(\rho\)) such that \(\sigma(H_\omega)\) is pure point. Such a \(v_1\) exists by Theorem 5.2. Then \(\langle p_{pp}^{H_{\omega}}, e_1, e_1 \rangle = 1\) and hence for large enough \(n\) it must hold that \(\Gamma_n(H_{\omega}) > 3/4\). Fix \(n_1\) such that this holds. Then \(\Gamma_{n_1}(H_{v_1})\) only depends on \(\{v_1(j) : j \leq N_1\}\) for some integer \(N_1\) by (i) of Definition A.2. Define the potential \(v_2\) by \(v_2(j) = v_1(j)\) for all \(j \leq N_1\) and extending periodically to infinity otherwise. Then by fact (1) above, \(\langle p_{pp}^{H_{v_1}}, e_1, e_1 \rangle = 0\) and hence \(\Gamma_n(H_{v_1}) < 1/4\) for large \(n\), say for \(n > N_1\). But then \(\Gamma_{n_2}(H_{v_2})\) only depends on \(\{v_2(j) : j \leq N_2\}\) for some integer \(N_2\).

We repeat this process inductively switching between potentials which induce \(\Gamma_{n_k}(H_{v_k}) < 1/4\) for \(k\) even and potentials which induce \(\Gamma_{n_k}(H_{v_k}) > 3/4\) for \(k\) odd. Explicitly, if \(k\) is even then define a potential \(v_{k+1}\) by \(v_{k+1}(j) = v_k(j)\) for all \(j \leq N_k\) and \(v_{k+1}(j) = v_\omega(j)\) (with the density \(\rho\)) otherwise such that the spectrum of \(H_{v_k}\) is pure point. Such a \(\omega\) exists from Theorem 5.2 applied with the perturbation \(A\) to match the potential for \(j \leq N_k\). If \(k\) is odd then we define \(v_{k+1}\) by \(v_{k+1}(j) = v_k(j)\) for all \(j \leq N_k\) and extend periodically otherwise.

We can then choose \(n_{k+1}\) such that the above inequalities hold and \(N_{k+1}\) such that \(\Gamma_{n_{k+1}}(H_{v_{k+1}})\) only depends on \(\{v_{k+1}(j) : j \leq N_{k+1}\}\). Finally set \(v_j(j) = v_k(j)\) for \(j \leq N_k\). It is clear from (iii) of Definition A.2, that \(\Gamma_{n_k}(H_v) = \Gamma_{n_k}(H_{v_k})\). But then this implies that \(\Gamma_{n_k}(H_v)\) cannot converge, the required contradiction.

To prove the result for \(P_s^T\), note the above proof carries through since \(P_{pp}^T \leq F_s\) and \(F_s P_{ac}^T = 0\).

4 Two Simple Applications

4.1 Computation of the functional calculus

Theorem 3.1 can be extended to computing the functional calculus. Recall that given a (possibly unbounded complex-valued) Borel function \(F\), defined on \(\mathbb{C}\), and \(T \in \Omega_N\), \(F(T)\) is defined by

\[
F(T) = \int_{\sigma(T)} F(t) dE^T(t).
\]

\(F(T)\) is a densely defined closed normal operator with dense domain given by

\[
\mathcal{D}(F(T)) = \{ x \in L^2(\mathbb{N}) : \int_{\sigma(T)} |F(t)|^2 d\mu^T_x,x(t) < \infty \}.
\]

For simplicity, we will only deal with the case that \(F\) is a bounded continuous function on \(\mathbb{R}\), that is, \(F \in C_b(\mathbb{R})\). In this case \(\mathcal{D}(F(T))\) is the whole of \(L^2(\mathbb{N})\) (the measures \(\mu^T_x,x\) are finite) and we can use standard properties of the Poisson kernel. We assume that given \(F \in C_b(\mathbb{R})\) we have access to piecewise constant functions \(F_s\) supported in \([-n,n]\) such that \(\|F - F_s\|_{\infty([-n,n])} \leq n^{-1}\). Clearly other suitable data also suffices and as usual we abuse notation slightly by adding this information to \(\Lambda_1\) to define \(\tilde{\Lambda}_1\).

**Theorem 4.1 (Computation of the functional calculus).** Consider the map

\[
\Xi_{\text{fun}} : \Omega_{f,\alpha,\beta} \times C_b(\mathbb{R}) \rightarrow L^2(\mathbb{N})
\]

\((T,x,F) \rightarrow F(T)x)\).

Then \(\{\Xi_{\text{fun}} : \Omega_{f,\alpha,\beta} \times C_b(\mathbb{R}), \tilde{\Lambda}_1\} \in \Delta_3^4\).

**Proof.** Let \((T,x,F) \in \Omega_{f,\alpha,\beta} \times C_b(\mathbb{R})\) then by Fubini’s theorem,

\[
\int_{-n}^{n} K_H(u + i/n; T, x) F_s(u) du = \int_{-\infty}^{\infty} \int_{-n}^{n} P_H(u - t, 1/n) F_s(u) du \, dE^T(t)x.
\]

The inner integral is bounded since \(F\) is bounded and the Poisson kernel integrates to 1 along the real line. It also converges to \(F(t)\) everywhere. Hence by the dominated convergence theorem

\[
\lim_{n \to \infty} \int_{-n}^{n} K_H(u + i/n; T, x) F_s(u) du = F(T)x.
\]

We now use the same arguments used to prove Theorem 3.1. Using Corollary 2.2, together with \(\|K_H(u + i/n; T, x)\|_{L^2(\mathbb{R})} \leq n C_1\) and the fact that \(K_H(u + i/n; T, x)\) is Lipschitz continuous with Lipschitz constant \(n^2 C_2\) for some (possibly unknown) constants \(C_1\) and \(C_2\), we can approximate this integral with an error that vanishes in the limit \(n \to \infty\).
If \( \sigma(T) \) is bounded then with slightly more information available to our algorithms, a simpler proof holds using the Stone-Weierstrass theorem. Suppose that given \( x \), the vectors \( T^n x \) and \( (T^*)^n x \) can be computed to arbitrary precision. There exists a sequence of polynomials \( p_m(z, \bar{z}) \) converging uniformly to \( F(z) \) on \( \sigma(T) \). Assuming such a sequence can be explicitly constructed (for example using Bernstein or Chebyshev polynomials), we can take \( p_m(T, T^*) x \) as approximations of \( F(T)x \). If we can bound \( \| p_m(z, \bar{z}) - F(z) \|_{\sigma(T)} \leq \epsilon_m \) with \( \epsilon_m \) null, then the vector \( F(T)x \) can be computed with error control. However, if \( T \) is not banded, then computing \( T^n x \) and \( (T^*)^n x \) for large \( n \) (even if \( x = e_i \)) may be computationally expensive as was found in the example in §6.4. We will also see in §6.4 that if \( \sigma(T) \) is bounded and \( F \) is analytic in an open neighbourhood of \( \sigma(T) \), then \( F(T)x \) can be computed with error control by deforming the integration contour away from the spectrum. Such a deformation is useful since the resolvent does not blow up along such a contour.

### 4.2 Computation of the Radon–Nikodym derivative

Recall the definition of the Radon–Nikodym derivative in (1.12) and note that \( \mu_{x,y}^T \in L^1(\mathbb{R}) \) for \( T \in \Omega_{A} \). We consider its computation in \( L^1 \) sense in the following theorem, where, as before, we assume (3.1), adding the approximations of \( U \) to our evaluation set along with component-wise evaluations of a given vector \( y \) to form \( \tilde{\Lambda}_1 \). However, we must consider the computation away from the singular part of the spectrum.

**Theorem 4.2** (Computation of the Radon–Nikodym derivative). Consider the map

\[
\Xi_{RN} : \Omega_{f,\alpha,\beta} \times \mathbb{I}^2(\mathbb{N}) \times \mathcal{U} \to L^1(\mathbb{R})
\]

\[
(T, x, y, U) \to \mu_{x,y}^T(U).
\]

We restrict this map to the quadruples \((T, x, y, U)\) such that \( U \) is strictly separated from \( \text{supp}(\mu_{x,y,sc}^T) \cup \text{supp}(\mu_{x,y,pp}^T) \) and denote this subclass by \( \tilde{\Omega}_{f,\alpha,\beta} \). Then \( \{\Xi_{RN}, \tilde{\Omega}_{f,\alpha,\beta}, \tilde{\Lambda}_1\} \in \Delta^A_2 \). Furthermore, each output \( \Gamma_n(T, x, y, U) \) consists of a piecewise linear function, supported in \( U \) with rational knots and taking (complex) rational values at these knots.

**Remark 6.** What this theorem essentially tells us is that if we can compute the action of the resolvent operator with asymptotic error control, then we can compute the Radon–Nikodym derivative of the absolutely continuous part of the measures on open sets which are a positive distance away from the singular support of the measure. The assumption that \( U \) is separated from \( \text{supp}(\mu_{x,y,sc}^T) \cup \text{supp}(\mu_{x,y,pp}^T) \) may seem unnatural but is needed to gain \( L^1 \) convergence of the approximation. However, without it, the proof still gives almost everywhere pointwise convergence.

**Proof.** Let \((T, x, y, U) \in \tilde{\Omega}_{f,\alpha,\beta} \). For \( u \in U \) we decompose as follows

\[
\langle K_H(u + ic; T, x), y \rangle = \frac{1}{\pi} \int_{\mathbb{R}} \frac{\epsilon}{|t - u|^2 + \epsilon^2} \mu_{x,y}^T(t) dt + \frac{1}{\pi} \int_{\mathbb{R} \cup U} \frac{\epsilon}{|t - u|^2 + \epsilon^2} \left( \text{pp} \mu_{x,y,sc}^T + \text{pp} \mu_{x,y,pp}^T \right)(t).
\]

The first term converges to \( \rho_{x,y}^T u \) in \( L^1(U) \) as \( \epsilon \downarrow 0 \) since \( \rho_{x,y}^T u \in L^1(U) \). Since we assumed that \( U \) is separated from \( \text{supp}(\mu_{x,y,sc}^T) \cup \text{supp}(\mu_{x,y,pp}^T) \), it follows that the second term of (4.1) converges to 0 in \( L^1(U) \) as \( \epsilon \downarrow 0 \). Hence we are done if we can approximate \( \langle K_H(u + i/n; T, x), y \rangle \) in \( L^1(U) \) with an error converging to zero as \( n \to \infty \).

Recall that \( U \) can be written as the disjoint union

\[
U = \bigcup_m (a_m, b_m)
\]

where \( a_m, b_m \in \mathbb{R} \cup \{\pm \infty\} \) and the union is at most countable. Without loss of generality, we assume that the union is over \( m \in \mathbb{N} \). Recall that \( K_H(u + i/n; T, x) \) is Lipschitz continuous with Lipschitz constant at most \( n^2 \|x\|/\pi \). By assumption, and using Corollary 2.2, we can approximate \( K_H(u + i/n; T, x) \) to asymptotic precision with vectors of finite support. Hence the inner product \( f_n(u) := \langle K_H(u + i/n; T, x), y \rangle \) can be approximated to asymptotic precision (now with a possibly unknown constant also depending on \( \|y\| \)) and \( f_n \) is Lipschitz continuous with Lipschitz constant at most \( n^2 \|x\|/\|y\| \). Given an interval \((a_m, b_m)\), let \( a_m < z_{m,1,n} < z_{m,2,n} < \ldots < z_{m,m,n} < b_m \) such that \( z_{m,j,n} \in \mathbb{Q} \) and \( |z_{m,j,n} - z_{m,j+1,n}| \leq (b_m - a_m)^{-1} n^{-2} \). Also assume that \( |a_m - z_{m,j,n}|, |b_m - z_{m,m,n}| \leq n^{-1} \). Let \( f_{m,n} \) be a piecewise linear interpolant with knots \( z_{m,1,n}, \ldots, z_{m,m,n} \) supported on \((z_{m,1,n}, z_{m,m,n})\) with the property that \( |f_{m,n}(z_{m,j,n}) - f_n(z_{m,j,n})| < C(b_m - a_m)^{-1} n^{-1} n^{-2} \). Here \( C \) is some unknown constant which occurs from the asymptotic approximation of \( f_n \) that arises from Corollary 2.2 and we can always choose such \( f_{m,n} \).
Let $\Gamma_n(T, x, y, U)$ be the function that agrees with $f_{m,n}$ on $(a_m, b_m)$ for $m \leq n$ and is zero elsewhere. Clearly the nodes of $\Gamma_n(T, x, y, U)$ can be computed using finitely many arithmetic operations and comparisons and the relevant set of evaluation functions $\Lambda_1$. A simple application of the triangle inequality implies that

$$\int_U |\Gamma_n(T, U, x, y)(u) - \varphi^T_{x,y}(u)| \, du \leq \int_{U_{m>n}(a_m,b_m)} |\varphi^T_{x,y}(u)| \, du$$

$$+ \int_{U_{m\leq n}(a_m,b_m)}(z_{m,1,n},z_{m,r_m,n}) |\varphi^T_{x,y}(u)| \, du + \int_{U_{m\leq n}(z_{m,1,n},z_{m,r_m,n})} |\varphi^T_{x,y}(u) - f_n(u)| \, du$$

$$+ \frac{C(x,y,T)}{n} \sum_{m \leq n} \frac{1}{m^2},$$

where the last term arises due to the piecewise linear interpolant. The bound clearly converges to zero as required. \hfill \Box

5 Computing Spectra as Sets

We now turn to computing the different types of spectra as sets in the complex plane. Specifically, define the problem functions $\Xi(T) = \sigma_x(T)$ for $T = ac, sc$ or pp. Note also that $\sigma_{pp}(T) = \sigma_{pp}(T)$, the closure of the set of eigenvalues. Since we are dealing with unbounded operators we use the Attouch–Wets metric defined by

$$d_{AW}(C_1, C_2) = \sum_{n=1}^{\infty} 2^{-n} \min \{1, \sup_{|x|<n} \text{dist}(x, C_1) - \text{dist}(x, C_2)\}, \quad (5.1)$$

for $C_1, C_2 \in \text{Cl}(\mathbb{C})$, where $\text{Cl}(\mathbb{C})$ denotes the set of non-empty compact subsets of $\mathbb{C}$. When considering bounded $T$, we let $(\mathcal{M}, d)$ be the set of all non-empty compact subsets of $\mathbb{C}$ provided with the Hausdorff metric $d = d_H$:

$$d_H(X, Y) = \max \left\{ \sup_{x \in X} \inf_{y \in Y} d(x, y), \sup_{y \in Y} \inf_{x \in X} d(x, y) \right\}, \quad (5.2)$$

where $d(x, y) = |x - y|$ is the usual Euclidean distance. Note that for compact sets, the notions of convergence according to $d_H$ and $d_{AW}$ coincide. To allow the possibility that the spectral sets are empty, we add the empty set to this metric space as a separated point (the space remains metrisable).\footnote{This simply means that $F_n \to \emptyset$ if and only if $F_n = \emptyset$ eventually.}

The main theorem of this section is the following:

**Theorem 5.1.** Given the above setup, for $i = 1, 2$ it holds that

$$\Delta^G_{pp} \not\subseteq \Xi^{sc}_{pp}, \Omega_{f,\alpha}, \Lambda_i \in \Delta^A_4, \quad \Delta^G_{p} \not\subseteq \Xi^{p}_{sc}, \Omega_{f,\alpha}, \Lambda_i \in \Delta^A_4, \quad \Delta^G_{pp} \not\subseteq \Xi^{pp}_{pp}, \Omega_{f,\alpha}, \Lambda_i \in \Delta^A_4.$$

If $f(n) - n \geq \sqrt{2n} + \frac{1}{2}$ then the sharper result $\Xi^{sc}_{pp}, \Omega_{f,\alpha}, \Lambda_i \not\subseteq \Delta^G_{pp}$ also holds. Furthermore, when considering $\Xi^{p}_{pp}$, we can extend its domain to the whole of $C(l^2(N))$. In this case

$$\Delta^G_{pp} \not\subseteq \Xi^{pp}_{pp}, C(l^2(N)), \Lambda_2 \in \Delta^A_4$$

and the corresponding tower $\Gamma_{n_2,n_1}$ satisfies $\lim_{n_1 \to \infty} \Gamma_{n_2,n_1}(T) = \Gamma_{n_2}(T) \subset \sigma_p(T)$. In other words, we recover a portion of the eigenvalues after one limit.

In order to prove the first set of statements, we only need to prove the lower bounds for $\Lambda_2$ and the upper bounds for $\Lambda_1$. These results show that despite the results of $\S\S 3.2 - 4$, in general it is very hard to compute the decomposition of the spectrum in the sense of (1.13). The proof of the negative result for point spectra uses the fractional moment method to prove a certain result connected to Anderson localisation (Theorem 5.2), which was also used in $\S.3.2$. As a by-product, we also answer the question addressed in $\S.2.2$ and prove that the spectral measures, while computable in one limit, cannot be computed with error control (see Theorem 5.3). We begin with some preliminary results concerning Anderson localisation and then deal with each spectral type.
5.1 Anderson localisation and the fractional moment method

Since P. W. Anderson’s introduction of his famous model 60 years ago [5], there has been a considerable amount of work by both physicists and mathematicians aiming to understand the suppression of electron transport due to disorder (Anderson localisation). A full discussion of Anderson localisation is beyond the scope of this paper, and we refer the reader to [25, 33, 80] for broader surveys. We will use the fractional moment method [1, 2, 58] to prove Anderson localisation in the multi-dimensional setting under finite rank perturbations. The notation used is the same as that in §3.2. In particular, we consider a connected, undirected, locally finite graph $G$, such that the degree of each vertex is bounded by some constant $C_G$ and such that the set of vertices $V(G)$ is countably infinite.

When considering Anderson localisation, we will assume that $v = v_{\omega}$ is a random potential where $\omega = \{v_x\}_{x \in V(G)}$ is a collection of independent identically distributed random variables. Following [58], we assume that the single-site probability distribution has a density $\rho \in L^1(\mathbb{R})$ with $\|\rho\|_1 = 1$ (with respect to the standard Lebesgue measure). For such a potential, a measure of disorder is given by the quantity $\|\rho\|_\infty^{-1}$. The following theorem generalises the results of [58] to certain finite rank perturbations and more general graphs and is used in the proof of Theorem 5.1. We have included a short proof in Appendix B since the result may be of independent interest.

**Theorem 5.2** (Anderson Localisation for Perturbed Operator). There exists a constant $\delta(C_G) > 0$ such that if $\|\rho\|_\infty \leq \delta(C_G)$ and $\rho$ has compact support, then the operator $H_v + A$ has only pure point spectrum with probability 1 for any fixed self-adjoint operator $A$ of the form

$$A = \sum_{j=1}^{M} \alpha_j |x_{n_j} \rangle \langle x_{n_j}|.$$  (5.3)

In other words, the operator $A$’s matrix with respect to the canonical basis has only finitely many non-zeros.

**Remark 7.** We do not discuss the property of exponentially localised eigenfunctions. For this and cases such as less regular probability distributions, dependent potential sites, slowly decaying off-diagonal terms, off-diagonal randomness etc. we refer the reader to the seminal paper [1].

5.2 Point spectra

**Proof** that $\{\Xi_{pp}^{C}, \Omega_{f,0}, \Lambda_2\} \notin \Delta^G_v$. To prove this, it is enough to consider bounded Schrödinger operators acting on $l^2(\mathbb{N})$, which are clearly a subclass of $\Omega_{f,0}$ for $f(n) = n+1$. Note that since the evaluation functions in $\Lambda_2$ can be recovered from those in $\Lambda_1$ in this special case, we can assume that we are dealing with $\Lambda_1$. Suppose for a contradiction that there does exist a sequence of general algorithms, $\Gamma_n$, with

$$\lim_{n \to \infty} \Gamma_n(H_v) = \Xi_{pp}^C(H_v).$$

We will construct a potential $v$ such that $\Gamma_n(H_v)$ does not converge. To do this, choose $\rho = \chi_{[-c, c]}/(2c)$ for some constant $c$ such that the conditions of Theorem 5.2 hold. We will use Theorem 5.2 and the following well known facts:

1. If $v$ has compact support then $\sigma_{pp}(H_v) \cap (0, 4) = \emptyset$ [110].

2. If we are in the setting of Theorem 5.2 with $A = 0$ then $\sigma(H_v) = [-c, 4 + c]$ almost surely (see for example [81]). If $A \neq 0$ then since compact perturbations preserve the essential spectrum, we still have $[-c, 4 + c] \subset \sigma(H_v + A)$ almost surely.

We will define the potential $v$ inductively as follows. Let $v_1$ be a potential of the form $v_{\omega}$ (with density $\rho$) such that $[-c, 4 + c] \subset \sigma(H_{v_1})$ and $\sigma(H_{v_1})$ is pure point. Such a $v_1$ exists by Theorem 5.2 and fact (2) above. Then for large enough $n$ there exists $z_n \in \Gamma_n(H_{v_1})$ such that $|z_n - 2| \leq 1$. Fix $n_1$ such that this holds. Then $\Gamma_{n_1}(H_{v_2})$ only depends on $\{v_1(j) : j \leq N_1\}$ for some integer $N_1$ by (i) of Definition A.2. Define the potential $v_2$ by $v_2(j) = v_1(j)$ for all $j \leq N_1$ and $v_2(j) = 0$ otherwise. Then by fact (1) above $\Gamma_{n_1}(H_{v_2}) \cap [1/2, 7/2] = \emptyset$ for large $n$, say for $n_2$. But then $\Gamma_{n_2}(H_{v_3})$ only depends on $\{v_2(j) : j \leq N_2\}$ for some integer $N_2$.

We repeat this process inductively switching between potentials which induce $\Gamma_{n_1}(H_{v_1}) \cap [1/2, 7/2] = \emptyset$ for $k$ even and potentials which induce $\Gamma_{n_1}(H_{v_2}) \cap [1/2, 7/2] = \emptyset$ for $k$ odd. Explicitly, if $k$ is even then define a potential $v_{k+1}$ by $v_{k+1}(j) = v_k(j)$ for all $j \leq N_k$ and $v_{k+1}(j) = v_{k}(j)$ (with the density $\rho$) otherwise such that $[-c, 4 + c] \subset \sigma(H_{v_{k+1}})$ and $\sigma(H_{v_{k+1}})$ is pure point. Such a $\omega$ exists from Theorem 5.2 and fact (2).
above applied with the perturbation $A$ to match the potential for $j \leq N_k$. If $k$ is odd then we define $v_{k+1}$ by $v_{k+1}(j) = v_k(j)$ for all $j \leq N_k$ and $v_{k+1}(j) = 0$ otherwise. We can then choose $n_{k+1}$ such that the above intersections hold and $N_{k+1}$ such that $\Gamma_{n_{k+1}}(H_{v_{k+1}})$ only depends on $\{v_{k+1}(j) : j \leq N_{k+1}\}$. Finally set $v(j) = v_k(j)$ for $j \leq N_k$. It is clear from (iii) of Definition A.2, that $\Gamma_{n_k}(H_v) = \Gamma_{n_k}(H_{v_k})$. But then this implies that $\Gamma_{n_k}(H_v)$ cannot converge, the required contradiction. \hfill \Box

**Remark 8.** The result can be extended to Schrödinger operators on $\mathbb{Z}^d$ or much more general lattices. This result can be extended to Schrödinger operators acting on $L^2(\mathbb{R}^d)$ via Kato’s famous theorem regarding potentials decaying faster than $O(1/|x|)$ (see for example [108]) and recent results on Anderson localisation for Bernoulli random variables [20].

A similar argument gives the following theorem, where $\mathbb{V}$ is used to denote bounded real-valued potentials on $\mathbb{N}$ and $\Lambda_3$ denotes the pointwise evaluations of such potentials.

**Theorem 5.3 (Impossibility of computing spectral measures with error control).** Consider the problem function

$$\hat{\Xi} : \mathbb{V} \times \mathbb{N} \to \mathbb{R}_{\geq 0}$$

$$(v, j) \to (E_{1}^{H_{j}}e_{j}, e_{j})$$

Then $\{\hat{\Xi}, \mathbb{V} \times \mathbb{N}, \Lambda_3\} \in \Delta_3^4$ but $\{\hat{\Xi}, \mathbb{V} \times \mathbb{N}, \Lambda_3\} \notin \Delta_2^4$. In other words, $\hat{\Xi}$ can be computed in one limit, but it cannot be computed with error control.

**Proof.** The positive result $\{\hat{\Xi}, \mathbb{V} \times \mathbb{N}, \Lambda_3\} \in \Delta_3^4$ follows directly from the remarks after Theorem 3.1 and Proposition 2.1. Suppose for a contradiction that $\{\hat{\Xi}, \mathbb{V} \times \mathbb{N}, \Lambda_3\} \in \Delta_2^4$ and that $\Gamma_n$ is a sequence of general algorithms solving the problem with error control. It follows that for each $j \in \mathbb{N}$, there exists a sequence of general algorithms $\Gamma'_n$ such that

$$\lim_{n \to \infty} \Gamma'_n(v) = \begin{cases} 1, & \text{if } \hat{\Xi}(v, j) > 0 \\ 0, & \text{otherwise} \end{cases}$$

Informally, these are described as follows. Fix $j$ and consider the lower bound on $\Xi(v, j)$ computed by $\{\Gamma_m(v, j) : m \leq n\}$. If this is greater than 0 then set $\Gamma'_n(v) = 1$, otherwise set $\Gamma'_n(v) = 0$. It follows that $\Gamma'_n(v)$ also converges from below. It holds that $1 \in \sigma_p(H_v)$ if and only if $\hat{\Xi}(v, j) > 0$ for some $j \in \mathbb{N}$. Now define

$$\hat{\Gamma}_n(v) = \sup_{j \leq n} \Gamma'_n(v).$$

It is clear that this is a general algorithm using $\Lambda_3$. Furthermore,

$$\lim_{n \to \infty} \hat{\Gamma}_n(v) = \begin{cases} 1, & \text{if } 1 \in \sigma_p(H_v) \\ 0, & \text{otherwise} \end{cases}$$

with convergence from below.

Now we may choose a $v$ such that $1 \in \sigma_p(H_v)$ (this can be achieved for example by taking a potential which induces pure point spectrum and shifting the operator accordingly). It follows that for large $n$ it holds that $\hat{\Gamma}_n(v) = 1$. But the computation of $\hat{\Gamma}_n(v)$ is only dependent on $v(j)$ for $j < N$ for some $N \in \mathbb{N}$. Define $v_0 \in \mathbb{V}$ by $v_0(j) = v(j)$ if $j < N$ and $v_0(j) = 0$ otherwise. It follows that $\hat{\Gamma}(v_0) = 1$. But since the potential has compact support, $1 \notin \sigma_p(H_{v_0})$ and hence $\hat{\Gamma}(v_0) = 0$, the required contradiction. \hfill \Box

We now shift our attention to proving that $\Xi_{pp}^c$ can be computed using a height two arithmetical tower. The first step is the following technical lemma, whose proof will also be used later when considering $\Xi_{\infty}^c$.

**Lemma 5.4.** Let $a < b$ with $a, b \in \mathbb{R}$ and consider the decision problem

$$\Xi_{a,b,pp} : \Omega_{f.a} \to \{0, 1\}$$

$$T \to \begin{cases} 1 & \text{if } \sigma_{pp}(T) \cap [a, b] \neq \emptyset \\ 0 & \text{otherwise.} \end{cases}$$

Then there exists a height two arithmetical tower $\Gamma_{n_2,n_1}$ (with evaluation functions $\Lambda_1$) for $\Xi_{a,b,pp}$. Furthermore, the final limit is from below in the sense that $\Gamma_{n_2}(T) \leq \Xi_{a,b,pp}(T)$. 

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Proof. Step 1 of the proof of Theorem 3.2 yields a height two arithmetical tower $\tilde{\Gamma}_{n_2,n_1}^j(T)$ for the computation of $\mu_{g_{e_j,c_j}}^T((a,b))$. Note that the final limit is from above and using the fact that $\mu_{g_{e_j,c_j}}^T((a,b)) = 0$ we obtain a height two tower for $\mu_{g_{e_j,c_j}}^T((a,b))$. We can then use the height one tower $\tilde{\Gamma}_{n_1}^j(T)$ for $\mu_{g_{e_j,c_j}}^T((a,b))$ (constructed in §2.2) and define

$$a_{j,n_2,n_1} = \tilde{\Gamma}_{n_1}^j(T) - \tilde{\Gamma}_{n_2,n_1}^j(T).$$

This provides a height two arithmetical tower for $\mu_{g_{e_j,c_j}}^T((a,b))$ with the final limit from below. Without loss of generality (by taking successive maxima) we can assume that these towers are non-decreasing in $n_2$. Now set

$$\mathcal{T}_{n_2,n_1}(T) = \max_{1 \leq j \leq n_2} a_{j,n_2,n_1}.$$

Then it is clear that the limit $\lim_{n_2 \to \infty} \mathcal{T}_{n_2,n_1}(T) = \mathcal{T}_{n_2}(T)$ exists. Furthermore, the monotonicity of the limit $a_{j,n_2,n_1}$ in $n_2$ implies that

$$\lim_{n_2 \to \infty} \mathcal{T}_{n_2}(T) = \sup_{n \in \mathbb{N}} \mu_{\Omega_{a,b,pp}}^T([a,b]),$$

with monotonic convergence from below. This limiting value is zero if $\Xi_{a,b,pp}(T) = 0$, otherwise it is a positive finite number.

To convert this to a height two tower for the decision problem $\Xi_{a,b,pp}$ (that maps to the discrete space $\{0, 1\}$) we use the following trick. Consider the intervals $J_k^{12} = [0, 1/n_2]$, and $J_k^{12} = [2/n_2, \infty)$. Let $k(n_2, n_1) \leq n_1$ be maximal such that $\mathcal{T}_{n_2,n_1}(T) \in J_k^{12}$ or $J_k^{21}$ If no such $k$ exists or $\mathcal{T}_{n_2,n_1}(T) \in J_k^{12}$ then set $\Gamma_{n_2,n_1}(T) = 0$. Otherwise set $\Gamma_{n_2,n_1}(T) = 1$. These can be computed using finitely many arithmetic operations and comparisons using $A_1$. The point of the intervals $J_k^{12}$ and $J_k^{21}$ is that we can show $\lim_{n_1 \to \infty} \Gamma_{n_2,n_1}(T) = \mathcal{T}_{n_2}(T)$ exists. This is because $\lim_{n_1 \to \infty} \mathcal{T}_{n_2,n_1}(T) = \mathcal{T}_{n_2}(T)$ exists and hence we cannot oscillate infinitely often between the separated intervals $J_k^{12}$ and $J_k^{21}$. Now suppose that $\Xi_{a,b,pp}(T) = 0$, then $\lim_{n_1 \to \infty} \Gamma_{n_2,n_1}(T) = 0$ and hence $\lim_{n_1 \to \infty} \Gamma_{n_2,n_1}(T) = 0$ for all $n_2$. Now suppose that $\Xi_{a,b,pp}(T) = 1$, then for large enough $n_2$ we must have that $\mathcal{T}_{n_2}(T) > 2/n_2$ and hence $\Gamma_{n_2}(T) = 1$. Together, these prove the convergence and that $\Gamma_{n_2}(T) \leq \Xi_{a,b,pp}(T)$. □

Proof that $\{\Xi_{pp}, \Omega_{f,a}, \Lambda_1\} \in \Delta^A$. To construct a height two arithmetical tower for $\Xi_{pp}$ we will use Lemma 5.4 repeatedly. Let $\hat{\Gamma}_{n_2,n_1}(T)$ denote the height two tower constructed in the proof of Lemma 5.4 for the closed interval $I$ ($I = [a,b]$), where without loss of generality by taking successive maxima in $n_2$, we assume that this tower is non-decreasing in $n_2$ (this is where we use convergence from below in the final limit in the statement of the lemma). For a given $n_1$ and $n_2$, we construct $\Gamma_{n_2,n_1}(T)$ as follows (we will use some basic terminology from graph theory).

Define the intervals $I_{n_2,n_1,j} = [j,j+1]$ for $j = -n_2, ..., n_2 - 1$ so that these form a cover of the interval $[-n_2,n_2]$. Now suppose that $\Gamma_{n_2,n_1,j}$ are defined for $j = 1, ..., r_k(n_2,n_1,T)$. Compute each $\Gamma_{n_2,n_1}(T, I_{n_2,n_1,j})$ and if this is 1, bisect $I_{n_2,n_1,j}$ via its midpoint into two equal halves consisting of closed intervals. We then take all these bisected intervals and label them as $I_{n_2,n_1,j}^{k+1}$ for $j = 1, ..., r_{k+1}(n_2,n_1,k,T)$. This is repeated until the intervals $I_{n_2,n_1,j}^{k}$ have been computed. By adding the interval $[-n_2,n_2]$ as a root with children $I_{n_2,n_1,j}^{0}$, this creates a finite tree structure where a non-root interval $I$ is a parent of two intervals precisely if those two intervals are formed from its bisection and $\Gamma_{n_2,n_1}(T,I) = 1$. We then prune this tree by discarding all leaves $I$ which have $\hat{\Gamma}_{n_2,n_1}(T,I) = 0$ to form the tree $\tilde{\Gamma}_{n_2,n_1}(T)$. Finally, we let $\Gamma_{n_2,n_1}(T)$ be the union of all the leaves of $\tilde{\Gamma}_{n_2,n_1}(T)$. Clearly this can be computed using finitely many arithmetic operations and comparisons using $A_1$. The construction is shown visually in Figure 3.

In the above construction, the number of intervals considered (including those not in the tree $\tilde{\Gamma}_{n_2,n_1}(T)$) for a fixed $n_2$ is $2^{2n_2+1} + 1$ and hence independent of $n_1$. It follows that $\tilde{\Gamma}_{n_2,n_1}(T)$ and $\Gamma_{n_2,n_1}(T)$ are constant for large $n_1$ (due to the convergence of the $\Gamma_{n_2,n_1}(T,I)$ in $\{0, 1\}$). We denote these limiting values by $\Gamma_{n_2}(T)$ and $\Gamma_{n_2}(T)$ respectively and also denote the corresponding intervals in the construction at the $m$-th level of this limit by $I_{n_2,m}$. Note also that if $\Xi_{pp}(T) = 0$ then $\Gamma_{n_2}(T) = 0$.

Now suppose that $z \in \Xi_{pp}(T)$, then there exists a sequence of nested intervals $I_m = I_{n_2,a_0,a_2}$ containing $z$ for $m = 0, ..., n_2$ (where the notation means that these intervals are independent of $n_2$). Fix $m$, then for large $n_2$ we must have that $\hat{\Gamma}_{n_2}(T,I_j) = 1$ for $j = 1, ..., m$. It follows that $I_m$ has a descendent interval $I_{n_2,m}$ contained in $\Gamma_{n_2}(T)$ and hence we must have

$$\text{dist}(z, \Gamma_{n_2}(T)) \leq 2^{-m}.$$ 

Since $m$ was arbitrary it follows that $\text{dist}(z, \Gamma_{n_2}(T))$ converges to 0 as $n_2 \to \infty$. 

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Conversely, suppose that $z_{m_j} \in \Gamma_{m_j}(T)$ with $m_j \to \infty$, then we must show that all limit points of $\{z_{m_j}\}$ lie in $\Xi_{\text{pp}}^c(T)$. Suppose this were false, then by taking a subsequence if necessary, we can assume that $z_{m_j} \to z$ and $\text{dist}(z_{m_j}, \Xi_{\text{pp}}^c(T)) \geq \delta$ for some $\delta > 0$. We claim that it is sufficient to prove that the maximum length of the leaves of $\mathcal{T}_{n_2}(T)$ intersecting a fixed compact subset of $\mathbb{R}$ converges to zero as $n_2 \to \infty$. Suppose this has been shown, then $z_{m_j} \in \Gamma_{m_j}$ for some leaf $\Gamma_{m_j}$ of $\mathcal{T}_{m_j}(T)$. It follows that $I_{m_j} \cap \Xi_{\text{pp}}^c(T) \neq \emptyset$ and $\|I_{m_j}\| \to 0$. But this contradicts $z_{m_j}$ being positively separated from $\Xi_{\text{pp}}^c(T)$.

We are thus left with proving the claim regarding the lengths of leaves. Suppose this were false, then there exists a compact set $K \subset \mathbb{R}$ and leaves $I_j$ in $\mathcal{T}_{n_j}(T)$ such that the lengths of $I_j$ do not converge to zero and $I_j$ intersect $K$. By taking subsequences if necessary, we can assume that the lengths of each $I_j$ are constant. Then by compactness of $K$ and taking subsequences if necessary again, we can assume that each of the $I_j$ are equal to a common interval $I$. It follows that $\hat{\Gamma}_{b_j}(T, I) = 1$ but that $\hat{\Gamma}_{b_j}(T, I_1) = \hat{\Gamma}_{b_j}(T, I_2) = 0$ since $I$ is a leaf, where $I_1$ and $I_2$ form the bisection of $I$. Taking $b_j \to \infty$, this implies that $I \cap \Xi_{\text{pp}}^c(T) \neq \emptyset$ but $I_1 \cap \Xi_{\text{pp}}^c(T) = I_2 \cap \Xi_{\text{pp}}^c(T) = 0$ which is absurd. Hence we have shown the required contradiction, and we have finished the proof.

The final statement of Theorem 5.1 regarding pure point spectra of general closed operators is proven in Appendix C using different techniques.

### 5.3 Absolutely continuous spectra

We will first prove the lower bound and recall the following result from [83] which will be crucial for the proof.

**Theorem 5.5 (Krutikov and Remling).** Consider discrete Schrödinger operators acting on $l^2(\mathbb{N})$. Let $v$ be a (real-valued and bounded) potential of the following form:

$$v(n) = \sum_{j=1}^{\infty} g_j \delta_{n,m_j}, \quad m_{j-1}/m_j \to 0.$$ 

Then $[0,4] \subset \sigma_{\text{ess}}(H_0 + v)$ and the following dichotomy holds:

(a) If $\sum_{j \in \mathbb{N}} g_j^2 < \infty$ then $H_0 + v$ is purely absolutely continuous on $(0,4)$.

(b) If $\sum_{j \in \mathbb{N}} g_j^2 = \infty$ then $H_0 + v$ is purely singular continuous on $(0,4)$.

To prove the lower bound (that one limit will not suffice) our strategy will be to reduce a certain decision problem to the computation of $\Xi_{\text{ac}}^c$. Let $(\mathcal{M}', \mathcal{d}')$ be the discrete space $\{0,1\}$, let $\Omega'$ denote the collection of all infinite sequence $\{a_j\}_{j \in \mathbb{N}}$ with entries $a_j \in \{0,1\}$ and consider the problem function

$$\Xi'(\{a_j\}) : \text{‘Does } \{a_j\} \text{ have infinitely many non-zero entries?’}$$

In [11], it was shown that $\text{SCI}(\Xi', \Omega')_G = 2$ (where the evaluation functions consist in component-wise evaluation of the array $\{a_j\}$).

![Figure 3: Example of tree structure used to compute the point spectrum for $n_2 = 3$. Each tested interval is shown in green ($\hat{\Gamma}_{n_2,n_1}(T, I) = 1$) or red ($\hat{\Gamma}_{n_2,n_1}(T, I) = 0$). The arrows show the bisections and the final output is shown in blue.](image-url)
Proof that $\{\Xi_{ac}, \Omega_{f,\alpha}, \Lambda_2\} \not \in \Delta^A_0$. We are done if we prove the result for $f(n) = n + 1$ and $\alpha = 0$. In this case $\Lambda_1$ and $\Lambda_2$ are equivalent so we can restrict the argument to $\Lambda_1$. Suppose for a contradiction that $\Gamma_n$ is a height one tower of general algorithms solving $\{\Xi_{ac}, \Omega_{f,0}, \Lambda_2\}$. We will gain a contradiction by using the supposed tower to solve $\{\Xi^t, \Omega^t\}$.

Given $\{a_j\} \in \Omega^t$, consider the operator $H = H_0 + v$ where the potential is of the following form:

$$v(m) = \sum_{k=1}^{\infty} a_k \delta_{m,k}.$$  

Then by Theorem 5.5, $[0, 4] \subset \sigma_{ac}(H)$ if $\sum a_k < \infty$ (that is, if $\Xi(\{a_j\}) = 0$) and $\sigma_{ac}(H) \cap (0, 4) = \emptyset$ otherwise. Given $N$ we can evaluate any matrix value of $H$ using only finitely many evaluations of $\{a_j\}$ and hence the evaluation functions $\Lambda_1$ can be computed using component-wise evaluations of the sequence $\{a_j\}$.

We now set

$$\hat{\Gamma}_n(\{a_j\}) = \begin{cases} 0 & \text{if } \text{dist}(2, \Gamma_n(H)) < 1 \\ 1 & \text{otherwise.} \end{cases}$$  

The above comments show that each of these is a general algorithm and it is clear that it converges to $\Xi(\{a_j\})$ as $n \to \infty$, the required contradiction.

To construct the height two (arithmetical) tower for $\Xi_{ac}^t$ we will need the following lemma.

**Lemma 5.6.** Let $a < b$ with $a, b \in \mathbb{R}$ and consider the decision problem

$$\Xi_{a,b,ac} : \Omega_{f,\alpha} \to \{0, 1\}$$

$$T \to \begin{cases} 1 & \text{if } \sigma_{ac}(T) \cap [a, b] \neq \emptyset \\ 0 & \text{otherwise.} \end{cases}$$

Then there exists a height two arithmetical tower $\Gamma_{n_2,n_1}$ (with evaluation functions $\Lambda_1$) for $\Xi_{a,b,ac}$. Furthermore, the final limit is from below in the sense that $\Gamma_{n_2}(T) \leq \Xi_{a,b,ac}(T)$.

**Proof.** Fix such an $a$ and $b$ and let $\chi_n$ be a sequence of non-negative, continuous piecewise linear functions on $\mathbb{R}$, bounded by 1 and of compact support such that $\chi_n$ converge pointwise monotonically up to the constant function 1. Define also the function

$$v_{m,n}(u; T) = \langle K_H(u + i/n, T, e_m), e_m \rangle$$

and set

$$a_{m,n_2,n_1} = \int_{a}^{b} v_{m,n_1}(u,T)\chi_{n_2}(v_{m,n_2}(u,T))du.$$  

Since each $\chi_n$ is continuous and has compact support, and since $v_{m,n}(u; T)$ converges almost everywhere to $\rho_{e_m,e_m}^T(u)$ (the Radon–Nikodym derivative of the absolutely continuous part of the measure $\mu_{e_m,e_m}$), it follows by the dominated convergence theorem that

$$\lim_{n_1 \to \infty} a_{m,n_2,n_1} = a_{m,n_2} := \int_{a}^{b} \rho_{e_m,e_m}^T(u)\chi_{n_2}(\rho_{e_m,e_m}^T(u))du.$$  

We now use the fact that the $\chi_n$ are increasing and the dominated convergence theorem again to deduce that

$$\lim_{n_2 \to \infty} a_{m,n_2} = \mu_{e_m,e_m,ac}([a,b]),$$  

with monotonic convergence from below.

Using Corollary 2.2 (and the now standard argument of Lipschitz continuity of the resolvent), we can compute approximations of $a_{m,n_2,n_1}$ to accuracy $1/n_1$ in finitely many arithmetic operations and comparisons. Call these approximations $\tilde{a}_{m,n_2,n_1}$ and set

$$\Upsilon_{n_2,n_1}(T) = \max_{1 \leq j \leq n_2} \tilde{a}_{j,n_2,n_1}.$$  

The proof now follows that of Lemma 5.4 exactly.

**Proof**. This is exactly the same construction as in the above proof of the inclusion $\{\Xi_{ac}, \Omega_{f,\alpha}, \Lambda_1\} \in \Delta^A_0$. We simply replace the tower constructed in the proof of Lemma 5.4 by the tower constructed in the proof of Lemma 5.6.
5.4 Singular continuous spectra

We will first prove the lower bound for the singular continuous spectrum via Theorem 5.5. Note that the impossibility result \( \{ \Xi_{\text{sc}}, \Omega_{f,0}, \Lambda_2 \} \notin \Delta_2^C \) follows from the same argument that was used to show \( \{ \Xi_{\text{sc}}, \Omega_{f,0}, \Lambda_2 \} \notin \Delta_2^C \). To show that two limits will not suffice for \( f(n) - n \geq \sqrt{2n} + 1/2 \), our strategy will be to again reduce a certain decision problem to the computation of \( \Xi_{\text{sc}} \). Let \((\mathcal{M}', d')\) be the discrete space \([0, 1]\), let \(\Omega'\) denote the collection of all infinite matrices \(\{a_{i,j}\}_{i,j \in \mathbb{N}}\) with entries \(a_{i,j} \in \{0, 1\}\) and consider the problem function

\[ \Xi'\left(\{a_{i,j}\}\right) : \text{‘Does } a_{i,j} \text{ have a column containing infinitely many non-zero entries?’} \]

In [11], a Baire category argument was used to prove that \(\text{SCI}(\Xi', \Omega') \bigcap \mathcal{C} = 3\) (where the evaluation functions consist in component-wise evaluation of the array \(\{a_{i,j}\}\)).

**Proof that** \(\{\Xi_{\text{sc}}, \Omega_{f,0}, \Lambda_2\} \notin \Delta_2^C\)** if** \(f(n) - n \geq \sqrt{2n} + 1/2\). Assume that the function \(f\) satisfies \(f(n) - n \geq \sqrt{2n} + 1/2\). The proof will use a direct sum construction. Given \(\{a_{i,j}\} \in \Omega'\), consider the operators \(H_j = H_0 + v(j)\) where the potential is of the following form:

\[ v(j)(n) = \sum_{k=1}^{\infty} a_{k,j} \delta_{n,k}. \]

Using Theorem 5.5, \([0, 4] \subset \sigma_{\text{sc}}(H_j)\) if \(\sum_k a_{k,j} = \infty\) (that is, if the \(j\)-th column has infinitely many 1s) and \(\sigma_{\text{sc}}(H_j) \cap (0, 4) = \emptyset\) otherwise. Now consider an effective bijection (with effective inverse) between the canonical bases of \(l^2(\mathbb{N})\) and \(\bigoplus_{\mathbb{N}} l^2(\mathbb{N})\):

\[ \phi : \{e_n : n \in \mathbb{N}\} \to \{e_k : k \in \mathbb{N}^N, \|k\|_0 = 1\}. \]

Set \(H(\{a_{i,j}\}) = \bigoplus_{n=1}^{\infty} H_j\). Then through \(\phi\), we view \(H = H(\{a_{i,j}\})\) as a self-adjoint operator acting on \(l^2(\mathbb{N})\). Explicitly, we consider the matrix

\[ H_{m,n} = (H e_{\phi(n)}, e_{\phi(m)}). \]

We choose the following bijection (where \(m\) lists the canonical basis in each Hilbert space):

\[ j = 1 \quad j = 2 \quad j = 3 \quad \ldots \]

\[ m = 1 \quad \phi(1) \quad \phi(3) \quad \phi(6) \quad \ldots \]

\[ m = 2 \quad \phi(2) \quad \phi(3) \quad \phi(4) \quad \ldots \]

\[ m = 3 \quad \phi(4) \quad \ldots \]

A straightforward computation shows that \(H \in \Omega_{f,0}\). We also observe that if \(\Xi'(\{a_{i,j}\}) = 1\) then \([0, 4] \subset \sigma_{\text{sc}}(H)\), otherwise \(\sigma_{\text{sc}}(H) \cap (0, 4) = \emptyset\).

Suppose for a contradiction that \(\Gamma_{n_2,n_1}\) is a height two tower of general algorithms solving \(\{\Xi_{\text{sc}}, \Omega_{f,0}, \Lambda_1\}\).

We will gain a contradiction by using the supposed height two tower to solve \(\Xi', \Omega'\). We now set

\[ \tilde{\Gamma}_{n_2,n_1}(\{a_{i,j}\}) = 1 - \min\{1, \text{dist}(3, \Gamma_{n_2,n_1}(A(\{a_{i,j}\}))\}), \]

where we use the convention \(\text{dist}(3, \emptyset) = 1\). The comments above show that each of these is a general algorithm. Furthermore, the convergence of \(\Gamma_{n_2,n_1}\) implies that

\[ \lim_{n_2 \to \infty} \lim_{n_1 \to \infty} \tilde{\Gamma}_{n_2,n_1}(\{a_{i,j}\}) = 1 - \min\{1, \text{dist}(3, \sigma_{\text{sc}}(H(\{a_{i,j}\}))\}) = \Xi'(\{a_{i,j}\}). \]

We are not quite done since the convergence here takes place on the interval \([0, 1]\) with the usual metric as opposed to \([0, 1]\) with the discrete metric. To get round this we use the following, now familiar, trick.

Consider the intervals \(J_1 = [0, 1/2]\), and \(J_2 = [3/4, 1]\). Let \(k(n_2, n_1) \leq n_1\) be maximal such that \(\tilde{\Gamma}_{n_2,k}(\{a_{i,j}\}) \in J_1 \cup J_2\). If no such \(k\) exists or \(\tilde{\Gamma}_{n_2,k}(\{a_{i,j}\}) \in J_1\) then set \(\Gamma_{n_2,n_1}(\{a_{i,j}\}) = 0\). Otherwise set \(\Gamma_{n_2,n_1}(\{a_{i,j}\}) = 1\). Again, the point of the intervals \(J_1, J_2\) is that we can show \(\lim_{n_2 \to \infty} \Gamma_{n_2,n_1}(\{a_{i,j}\}) = \Gamma_{n_2}(\{a_{i,j}\})\) exists. If \(\Xi'(\{a_{i,j}\}) = 0\) then for large \(n_2\) it holds that \(\lim_{n_1 \to \infty} \tilde{\Gamma}_{n_2,k}(A) < 1/2\) and hence \(\lim_{n_2 \to \infty} \Gamma_{n_2}(\{a_{i,j}\}) > 3/4\) and hence \(\lim_{n_2 \to \infty} \Gamma_{n_2}(\{a_{i,j}\}) = 1\). Hence \(\Gamma_{n_2,n_1}^\prime\) is a height two tower of general algorithms solving \(\{\Xi', \Omega'\}\), a contradiction. \(\square\)
Finally, we will use the following lemma to prove that the singular continuous spectrum can be computed in three limits.

**Lemma 5.7.** Let $a < b$ with $a, b \in \mathbb{R}$ and consider the decision problem

$$\Xi_{a,b,sc} : \Omega_{f,\alpha} \rightarrow \{0, 1\}$$

$$T \rightarrow \begin{cases} 1 & \text{if } \sigma_{ac}(T) \cap [a, b] \neq \emptyset \\ 0 & \text{otherwise.} \end{cases}$$

Then there exists a height three arithmetical tower $\Gamma_{n_2,n_3,n_1}$ (with evaluation functions $\Lambda_1$) for $\Xi_{a,b,sc}$. Furthermore, the final limit is from below in the sense that $\Gamma_{n_2}(T) \leq \Xi_{a,b,sc}(T)$.

Once this is proven, we can use the same construction that was used to prove $\{\Xi_{pp}, \Omega_{f,\alpha}, \Lambda_1\}, \{\Xi_{ac}, \Omega_{f,\alpha}, \Lambda_1\} \in \Delta_4^1$ to show that $\{\Xi_{ac}, \Omega_{f,\alpha}, \Lambda_1\} \in \Delta_4^1$, but with an additional limit. Namely, we replace $(n_2, n_1)$ by $(n_3, n_2)$ in the proof and use the tower constructed in the proof of Lemma 5.6 instead of $\Gamma_{n_2,n_1}(T,I)$ for an interval $I$. We still gain the required convergence since the only change is an additional limit in the finite number of decision problems that decide the appropriate tree.

**Proof of Lemma 5.7.** Note that we can write

$$\hat{\mu}^T_{e_m,e_m,sc}([a,b]) = \mu^T_{e_m,e_m,pp}([a,b]) - \mu^T_{e_m,e_m,ac}([a,b]).$$

From this and the proofs of Lemmas 5.4 and 5.6, it is clear that we can construct a height two arithmetical tower, $\alpha_{n_2,n_1}(T)$, for $\mu^T_{e_m,e_m,sc}([a,b])$ where the final limit is from above. Now set

$$\Upsilon_{n_2,n_3,n_1}(T) = \max_{1 \leq j \leq n_3} \alpha_{j,n_2,n_1}.$$  

We see that each successive limit converges, with the second from above and the final from below. By taking successive maxima, minima of our base algorithms, we can assume that the second and final limits are monotonic and that $\Upsilon_{n_2,n_3,n_1}(T)$ is monotonic in both $n_2$ and $n_3$. Define $\Upsilon_{n_2,n_3,n_1}(T) = \lim_{n_2 \to \infty} \Upsilon_{n_2,n_3,n_1}(T)$, $\Upsilon_{n_3}(T) = \lim_{n_3 \to \infty} \Upsilon_{n_3,n_2}(T)$ and $\Upsilon(T) = \lim_{n_3 \to \infty} \Upsilon_{n_3}(T)$. Then $\Upsilon(T)$ is zero if $\Xi_{a,b,sc}(T) = 0$, otherwise it is a positive finite number.

With a slight change to the previous argument (the monotonicity in $n_2$ and $n_3$ is crucial for this to work), consider the intervals $J^m_1 = [0, 1/m]$, and $J^m_2 = [2/m, \infty)$. Let $k(m,n,n_1) \leq n_2$ be maximal such that $\Upsilon_{m,n,n_1}(T) \in J^m_1 \cup J^m_2$. If no such $k$ exists or $\Upsilon_{m,n,k}(T) \in J^m_1$ then set $\hat{\Gamma}_{m,n,n_1}(T) = 0$. Otherwise set $\hat{\Gamma}_{m,n,n_1}(T) = 1$. We then define

$$\Gamma_{n_2,n_3,n_1} = \max_{1 \leq m \leq n_3} \min_{1 \leq n \leq n_2} \hat{\Gamma}_{m,n,n_1}(T).$$

These can be computed using finitely many arithmetic operations and comparisons using $\Lambda_1$, and, as before, the first limit exists with

$$\Gamma_{n_2,n_3}(T) = \lim_{n_1 \to \infty} \Gamma_{n_2,n_3,n_1}(T) = \max_{1 \leq m \leq n_3} \min_{1 \leq n \leq n_2} \hat{\Gamma}_{m,n}(T).$$

Note also by construction that the second and third sequential limits exist through the use of maxima and minima.

Now suppose that $\Xi_{ac}(T) = 0$ and fix $n_3$. Then for large $n_2$, we must have that $\Upsilon_{m,n_2}(T) < 1/(2n_3)$ for all $m \leq n_3$ due to the monotonic convergence of $\Upsilon_p$ as $p \to \infty$. It follows in this case that

$$\lim_{n_2 \to \infty} \Gamma_{n_2,n_3}(T) = 0, \quad \text{for all } n_3.$$  

Now suppose that $\Xi_{ac}(T) = 1$. It follows in this case that there exists $M \in \mathbb{N}$ such that if $m \geq M$ then $\Upsilon_{m}(T) > 3/m$. Due to the monotonic convergence of $\Upsilon_{m,p}$ as $p \to \infty$ it follows that for all $p$ we must have $\Upsilon_{m,p} > 3/m$ and hence there exists $N(m,p) \in \mathbb{N}$ such that if $n_1 \geq N(m,p)$ then we must have $\Upsilon_{m,p,n_1} \geq 2/m$. It follows that if $n_3 \geq M$ then we must have $\hat{\Gamma}_{n_3,p}(T) = 1$ for all $p$ and hence that

$$\lim_{n_3 \to \infty} \Gamma_{n_3}(T) = 1.$$  

The conclusion of the Lemma now follows.
6 Numerical Examples

Here we will demonstrate the applicability of the new algorithms constructed which have SCI = 1. In particular, these are the first algorithms that compute their respective spectral properties for $\Omega_f, \alpha$, and even for the restricted case of tridiagonal self-adjoint matrices. It should be mentioned that these algorithms are also parallelisable (allowing large scale computations). Although we have focused in this paper on the case of discrete operators, many of the results extend to operators in the continuum, such as PDEs, and this will be the focus of future work.

6.1 Jacobi matrices and orthogonal polynomials

A wealth of test examples\footnote{We found the table in [26] to be particularly useful in this regard.} arises from the natural link between Jacobi operators and orthogonal polynomials (on $\mathbb{R}$). Let $J$ be a Jacobi matrix

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \cdots \\ a_1 & b_2 & a_2 & \cdots \\ 0 & a_2 & b_3 & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

with $a_j, b_j \in \mathbb{R}$ and $a_j > 0$. In this case, under suitable conditions, which hold in particular if $J$ is bounded, the probability measure $\mu : = \mu_J$ is exactly the probability measure associated with the orthonormal polynomials defined by

$$xP_k(x) = a_{k+1}P_{k+1}(x) + b_{k+1}P_k(x) + a_kP_{k-1}(x),$$

$$P_0(x) = 1,$$

and the spectral measure that appears in the (multiplicative version of the) spectral theorem (see for example [37, 131, 136]).

Classically, one usually first considers the measure and then constructs the orthogonal polynomials (and the corresponding $J$). Hence this gives us a large class of examples with known analytic solutions to test the new algorithms (clearly any such $J$ lies in $\Omega_{n \rightarrow n+1, 0}$), and in some sense, the algorithms constructed in this paper compute the inverse problem. In other words, we compute the measure $\mu_J$ given the recurrence coefficients defining the orthogonal polynomials - a problem which, until now, there has been no method of computation in general.

We begin with the well-known class of Jacobi polynomials defined for $\alpha, \beta > -1$ which have

$$a_k = 2 \sqrt{\frac{k(\alpha + k + \beta)(k + \alpha + \beta)}{(2k + \alpha + \beta - 1)(2k + \alpha + \beta)^2(2k + \alpha + \beta)}}, \quad b_k = \frac{\beta^2 - \alpha^2}{(2k + \alpha + \beta)(2k - 2 + \alpha + \beta)}$$

and measure on the interval $[-1, 1]$ given by

$$d\mu_J = \frac{(1-x)^\alpha(1+x)^\beta}{N(\alpha, \beta)}dx = f_{\alpha, \beta}(x)dx,$$  \hspace{0.5cm} (6.1)

where $N(\alpha, \beta)$ is a normalising constant, ensuring the measure is a probability measure. To assess the convergence of the algorithm in §4.2, we have plotted the convergence in $L^1([-1, 1])$ as a function of $n$ (matrix size) for various $\alpha$ and $\beta$ in Figure 4. In this case the method seems to converge algebraically. Whilst smoother density functions (larger $\alpha$, $\beta$) have smaller errors, there appears to be no real difference in the rate of convergence, suggesting that the rate of convergence is determined by the amount of spectral information in the first $(n + 1) \times n$ block of the matrix. The method is also fast, taking about a minute for $n = 10^6$ and evaluation at 199 points on a standard desktop computer with four cores. The algorithms developed in this paper are all parallelisable and hence faster results are likely to be possible given access to more cores. The absolute errors of estimates are also shown in Figure 4, demonstrating smaller errors near smoother parts of the density function. Here we took a uniform value $\epsilon(n)$ over the whole interval, however $\epsilon$ can also be a function of the position $x$, allowing it to be smaller for points where the resolvent is estimated more accurately for a given $n$. Finally the computation of the approximation of $f_{\alpha, \beta}$ at a given point can be computed in $O(n)$ operations and requires the computation of a least squares solution of a banded (in this case tridiagonal) linear system.
To demonstrate the algorithm on unbounded operators, we next consider the class of generalised Laguerre polynomials for $\alpha > -1$ which have

$$a_k = \sqrt{k(k + \alpha)}, \quad b_k = 2k + \alpha - 1$$

and measure on the interval $[0, \infty)$ given by

$$d\mu_J = \frac{x^\alpha e^{-x}}{\Gamma(\alpha + 1)} dx. \quad (6.2)$$

The results are shown in Figure 5 where we have plotted the $L^1$ error over the interval $[0, 1]$. Similar conclusions can be drawn as before, with an algebraic rate of convergence and smaller errors for larger $\alpha$. We have also shown the absolute errors. Convergence in this case was a lot slower than for the Jacobi polynomials. However, we will present a method to considerably speed up convergence in §6.2.

We also consider a class of orthogonal polynomials related to Bernoulli numbers [26]. For $-1 < \alpha < 1$, these have

$$a_k = k \sqrt{\frac{k^2 - \alpha^2}{4k^2 - 1}}, \quad b_k = 0$$

and measure on the interval $(-\infty, \infty)$ given by

$$d\mu_J = \frac{\pi \sin(\pi \alpha)}{4 \tan^{-1}\left(\frac{1 - \cos(\pi \alpha)}{\sin(\pi \alpha)}\right)} \frac{1}{\cos(\pi \alpha) + \cosh(\pi x)} dx. \quad (6.4)$$
For further properties in the $\alpha = 0$ case, we refer the reader to [21, 152]. The results are shown in Figure 6 measured over the interval $[-3, 3]$ with similar behaviour for the Laguerre polynomials. Convergence in this case is extremely slow owing to the need for large $n$ to approximate the resolvent accurately, and becomes slower for larger $\alpha$ as the measure becomes more peaked around 0.

Finally, we demonstrate the computation of measures for a Jacobi operator with discrete spectrum. The Charlier polynomials are generated by

$$a_k = \sqrt{\alpha k}, \quad b_k = k + \alpha - 1$$

for $\alpha > 0$ and have measure

$$d\mu_J = \exp(-\alpha) \sum_{m=0}^{\infty} \frac{\alpha^m}{m!} \delta_m,$$

where $\delta_x$ denotes a Dirac measure located at the point $x$. Figure 7 shows plots of $\epsilon \pi K_H(x + i\epsilon)$ for $\epsilon = 10^{-7}$ and $n = 1000$. The peaks clearly coincide with the atoms of the measure. The difference between the peak values and the weight $\exp(-\alpha)\alpha^m/m!$ was of the order $10^{-13}$ for both examples. This highlights the fact that if the solutions of the resolvent equation $(T - zI)y = x$ for a given $x$ are localised, that is, they have fast decaying tails, then in general smaller $n$ are needed to gain a given accuracy.

### 6.2 A new collocation method

To improve the rate of convergence of the above algorithm, we now present a new collocation method for the computation of Radon–Nikodym derivatives. Suppose that we know the spectral measure of an operator $T$ has
an interval $I$ (finite or infinite) as its support and is absolutely continuous. A natural way to approximate the Radon–Nikodym derivative is through a formal basis expansion

$$\rho_{x,y}^T(\lambda) = \sum_{m=1}^{\infty} a_m \phi_m(\lambda)$$

where $\phi_m$ are functions with support $I$ whose Cauchy’s transforms are easy to compute. To approximate the coefficients $a_m$ we collocate in the complex plane as follows. Let $C$ be a finite collection of complex points in the upper half plane and truncate the approximation of $\rho_{x,y}^T$ to $M$ terms. To generate a linear system for $\{a_m\}_{m=1}^M$, we evaluate the Cauchy transform at points $z \in C$. The Cauchy transform satisfies

$$\int_{\mathbb{R}} \frac{\rho_{x,y}^T(\lambda)}{\lambda - z} d\lambda = \langle R(z,T)x,y \rangle$$

which can be computed with error control using the results of §2.1. Call this approximation $b_{x,y,n}(z)$ (where $n$ denotes the size of the matrix used for the approximation). Define

$$\tilde{\phi}_m(z) = \int_{\mathbb{R}} \frac{\phi_m(\lambda)}{\lambda - z} d\lambda,$$

then for each $z \in C$, an approximate linear relation can be written as

$$\sum_{m=1}^{M} a_m \tilde{\phi}_m(z) = b_{x,y,n}(z).$$

Evaluating at $\geq M$ points in $C$ gives rise to a linear system which can be inverted in the least squares sense for the approximation of the coefficients $\{a_m\}_{m=1}^M$. In what follows, we preconditioned the linear system so that each row has $l_1$ norm equal to one. If $x = y$, and the basis functions are real, we know that the coefficients are real. Hence taking real and imaginary parts of the linear system gives further linear relations. We will consider basis functions which obey recursion relations of the form

$$\phi_{m+1}(\lambda) = \alpha_m \phi_m(\lambda) + \beta_m \phi_{m-1}(\lambda) + \gamma_m \phi_{m-2}(\lambda).$$

Such a relation allows computation of the associated Cauchy transforms through recursion relations as outlined in Appendix D. We found that by far the most computationally expensive part of the proposed collocation method is the computation of $b_{x,y,n}(z)$ (which if needed can be done in parallel).

Figure 8 shows the collocation method in the case of Legendre or Chebyshev polynomials as basis functions (taking the first $M = 1501$ - similar results were found for much smaller $M$, but we have shown this to demonstrate the stability of the method) for the considered cases of Jacobi polynomials. For collocation points, we took $M$ Chebyshev nodes offset by an additional $n^{-1/2}$ to lie just above the interval $[-1,1]$ in the complex plane. Both sets of polynomials behaved similarly, and the collocation method converges much faster with smaller errors than the method in §6.1 (at the price of there being no proof of convergence). Figure 9 shows similar results for the Laguerre polynomials and polynomials defined by (6.3). For these, we took Laguerre and Hermite functions (the polynomials multiplied by the square root of the weight function) as basis functions with $M = 501$ and $M = 301$ respectively. The collocation points where $\{1^2/(M + 1)^2, 2^2/(M + 1)^2, ..., 1\} + 50n^{-1/2}$ and $\{\pm 1^2/M^2, \pm 2^2/M^2, ..., 1\} + i/2$ respectively. Again, this method converges much faster than that in §6.1. For the Laguerre case, the method converges faster for smoother measures (see the $\alpha = 0, 1, 2$ cases).

### 6.3 CMV matrices

Here we will briefly demonstrate that the algorithms extend to the unitary case through use of the functions $K_D$ (convolution with Poisson kernel of the unit disk). We will consider the class of CMV matrices (named after Cantero, Moral and Velázquez [24]) linked with orthogonal polynomials on the unit circle. A full discussion of this subject is beyond this paper and instead we refer the reader to the excellent monographs of Simon [126, 127].
Figure 8: Left: Convergence of collocation method using Legendre polynomials. Right: Convergence of collocation method using Chebyshev polynomials.

Figure 9: Left: Convergence of collocation method using Laguerre functions on \([0, \infty)\). Right: Convergence of collocation method using Hermite functions on \((-\infty, \infty)\).
However, the background for this example is as follows. Given a probability measure \( \mu \) on the unit circle \( \mathbb{T} \), whose support is not a finite set, we can define a system of orthogonal polynomials \( \{ \Phi_n \}_{n=0}^{\infty} \) by applying the Gram-Schmidt process to \( \{1, z, z^2, \ldots \} \). Given a polynomial \( Q_n(z) \) of degree \( n \), we define the reversed polynomial \( Q_n^*(z) \) via \( Q_n^*(z) = z^nQ_n(1/z) \). Szegő’s recurrence relation [133] is then

\[
\Phi_{n+1}(z) = z\Phi_n(z) - \alpha_n\Phi_n^*(z),
\]

where the \( \alpha_n \) are known as Verblunsky coefficients [144] and satisfy \( |\alpha_j| < 1 \). Verblunsky’s theorem [143] sets up a one-to-one correspondence between \( \mu \) and the coefficients \( \{\alpha_j\}_{j=0}^{\infty} \). Define also

\[
\rho_j = \sqrt{1 - |\alpha_j|^2} > 0.
\]

The CMV matrix associated with \( \{\alpha_j\}_{j=0}^{\infty} \) is then given as

\[
C = \begin{pmatrix} 
\tau_0 & \tau_1\rho_0 & \rho_1\rho_0 & 0 & 0 & \cdots \\
0 & \tau_0\rho_0 & -\rho_0\rho_0 & 0 & 0 & \cdots \\
0 & \rho_0\rho_1 & -\rho_0\rho_1 & \tau_2\rho_2 & \rho_2\rho_2 & \cdots \\
& & \cdots & \cdots & \cdots & \cdots & \cdots 
\end{pmatrix}
\]

(6.6)

This matrix is unitary and banded (so clearly lies in \( \Omega_{U_{n=\infty},n=0}^{\infty} \)). This last property does not hold for the so-called GGT representation [54, 59, 135] (which uses the basis \( \{ \Phi_n \}_{n=0}^{\infty} \), whereas the CMV representation obtains a basis via applying Gram-Schmidt to \( \{1, z, z^2, \ldots\} \) which have infinitely many entries in each row. The key result is that \( \mu_C := \mu_{\alpha}^{(j)} \) precisely is the measure \( \mu \) on the unit circle. Hence our new algorithms can be considered as a computational tool for the correspondence

\[
\{\alpha_j\}_{j=0}^{\infty} \rightarrow \mu.
\]

The first example we consider are the Rogers-Szegő polynomials [113] given by

\[
\alpha_j = (-1)^jq^{(j+1)/2},
\]

where \( q \in (0, 1) \). In this case,

\[
d\mu_C = \frac{1}{\sqrt{2\pi \log(q^{-1})}} \sum_{m \in \mathbb{Z}} \exp \left( -\frac{(\theta - 2\pi m)^2}{2\log(q^{-1})} \right) d\theta,
\]

which can be expressed in terms of the theta function. Figure 10 shows the convergence of the new algorithm for various \( q \) and we see algebraic convergence as before. We can also use a similar spectral method as before using the standard Fourier basis \( \{ e^{im\theta} \}_{m \in \mathbb{Z}} \). Note that the relevant Cauchy transforms can be computed explicitly using Cauchy’s residue theorem. Collocation points inside and outside the unit disk are needed (collocating inside the unit disk cause the Cauchy transforms of the basis functions with negative \( n \) to vanish). This is also shown in Figure 10, where we used basis functions for \( m = -20, 19, \ldots, 20 \) and collocation points at \( \{ (1 \pm \epsilon)2\pi/41, (1 \pm \epsilon)2\pi \cdot 2/41, \ldots, (1 \pm \epsilon)2\pi \} \) for \( \epsilon = 0.1 \). Owing to the smoothness of the density functions, the collocation method converges exponentially to machine precision for \( n \approx 400 \).

The next example we consider are the Geronimus polynomials [55] which have \( \alpha_j = a \) with \( |a| < 1 \). In this case, for \( |a + 1/2| \leq 1/2 \),

\[
d\mu_C = \chi_{|\theta|>\theta_a} \sqrt{\frac{\cos^2(\theta/2) - \cos^2(b/2)}{2\pi |1 + a||\sin((\theta - b)/2)|}}
\]

where \( \theta \in [-\pi, \pi], b = 2\arccos(1 + \sqrt{\theta_a}) \) and \( \theta_a = 2\sin^{-1}|a| \). Figure 11 shows some typical examples and note that these density functions are not smooth. When \( |a + 1/2| > 1/2 \), there is also a singular part of the measure (see [126] for the exact formula). Figure 11 also shows the convergence of the algorithm and the spectral method with 2001 basis functions and collocation points \( \{ (1 \pm \epsilon)2\pi/2001, (1 \pm \epsilon)2\pi \cdot 2/2001, \ldots, (1 \pm \epsilon)2\pi \} \) for \( \epsilon = 0.1 \). In this case the collocation method struggles to gain an accuracy beyond \( 10^{-5} \) owing to discontinuity in the derivative of the Radon–Nikodym derivative and the algorithm based on convolutions is able to gain more accurate results. Finally, a typical example is shown in Figure 12 for \( a = 0.8 \) (there is now a singular part located at \( \theta = 0 \), where we have shown the output of the algorithm for \( n = 1000 \) and the exact convolution with the Poisson kernel (both for \( \epsilon = 0.01 \), as well as the collocation method using 21 basis functions and collocation points \( \{ (1 \pm 0.1)2\pi/21, (1 \pm 0.1)2\pi \cdot 2/21, \ldots, (1 \pm 0.1)2\pi \} \). Here, we see exact agreement between the algorithm and convolution. Unsurprisingly in the presence of point spectra, the collocation method is unstable.
Figure 10: Left: Convergence of algorithm for Rogers-Szegö polynomials. Right: Convergence of spectral method for Rogers-Szegö polynomials.

Figure 11: Left: Convergence of algorithm (Alg) and spectral method (Spec) for Geronimus polynomials. Note in this case that the algorithm can obtain more accurate results owing to the non-smoothness of the density functions. Right: Example density functions for the cases considered.

Figure 12: The smooth part of the density function (black) for the case of an additional point mass at $\theta = 0$. Note that the algorithm’s output agrees almost perfectly with the exact convolution of the measure. We have also shown the output of the spectral method, which is unstable in the presence of the point mass.
6.4 Fractional diffusion and localisation in a 2D quasicrystal model

In this example we will consider operators acting on the graph of a Penrose tile - the canonical model of a two-dimensional quasicrystal [38, 134, 142] (aperiodic crystals which typically have anomalous spectra/transport properties). Quasicrystals were discovered in 1982 by Shechtman [122] who was awarded the Nobel prize in 2011 for his discovery. Since then, they have generated considerable interest due to their often exotic physical properties [129], with a vast literature on the physics and spectral properties of such aperiodic systems. Unlike the one-dimensional case, little is known about the spectral properties of two-dimensional quasicrystals. A finite portion of the infinite tile is shown in Figure 13, and we consider the natural graph whose vertices are the vertices of the tiling and edges correspond to the edges of the rhombi. Such a graph posses no periodic structure, making it impossible with current methods to study spectral properties analytically. The free Hamiltonian $H_0$ (Laplacian) is given by

$$\langle H_0 \psi \rangle_i = \sum_{i,j} (\psi_j - \psi_i),$$

(6.8)

with summation over nearest neighbour sites (vertices). We chose a natural ordering of the vertices as in Figure 13, which leads to an operator $H_0$ acting on $L^2(\mathbb{N})$. The local bandwidth grows for this operator (our ordering is asymptotically optimal) and hence computation of powers $H_0^n$ is infeasible for $n \gtrsim 50$, rendering polynomial approximations of the functional calculus intractable. In the above notation, $H_0 \in \Omega_{f,0}$ with $f(n) - n = O(\sqrt{n})$ and so this example provides a demonstration of the algorithm for a non-banded matrix. Throughout we will generally take $u_0 = e_1$, though different initial conditions are handled in the same manner and will be used when we study localisation.

The ability to compute the functional calculus allows the solution of linear evolution equations. Given $A \in \Omega_N$, a function $F$ (continuous and bounded on $\sigma(N)$) and $u_0 \in L^2(\mathbb{N})$, consider the evolution equation

$$\frac{du}{dt} = F(A)u, \quad u_{t=0} = u_0.$$  

(6.9)

The solution of this equation is

$$u(t) = \exp(F(A)t)u_0$$

and can be computed via the algorithm outlined in §4.1.

First, we consider fractional diffusion governed by

$$\frac{du}{dt} = -(-H_0)^\alpha u, \quad u_{t=0} = u_0,$$

for $\alpha > 0$. If $\alpha$ is an integer, then the solution can be represented via contour deformation as

$$u(t) = \int_\gamma \exp(-z^\alpha t) R(z, -H_0)u_0 dz,$$

(6.10)

where $\gamma$ is a closed contour looping once around the spectrum. Typically we took the rectangular contour shown in Figure 13 and approximated the integral via Gaussian quadrature. This allows us to compute the solution with error control (we known the minimal distance between $\gamma$ and $\sigma(-H_0)$) and clearly, this holds for other functions $F$, holomorphic on a neighbourhood of $\sigma(-H_0)$. Note that other methods, such as direct diagonalisation of finite square truncations or discrete time stepping (which is difficult if $\alpha \notin \mathbb{N}$), do not give error control and are slower. When $\alpha \notin \mathbb{N}$, we can still deform the contour but not away from 0 since $0 \in \sigma(-H_0)$. This can cause numerical difficulty, so we deform the contour to that shown in Figure 13. For a discussion of contour methods applied to finite matrices (whose spectrum is strictly positive), we refer the reader to [63]. Unfortunately, such methods cannot be applied here since $0 \in \sigma(-H_0)$.

Figure 14 shows the convergence of the algorithm for $\alpha = 1/2$ and $\alpha = 1$. For $\alpha = 1/2$, error control is not given by our algorithm so we computed an error by comparing to a “converged” solution using larger $n$. The $L^2$ error refers to the error in $L^2(\mathbb{N})$. The method converges algebraically for $\alpha = 1/2$ (owing to the contour touching the spectrum at 0) but converges exponentially for $\alpha = 1$ with similar convergence observed over a large range of times $t$. Figure 15 shows the magnitude (log scale) of the computed solution for various times. As expected, a smaller $\alpha$ corresponds to more spreading out of the initial wavepacket. Similar results were found for other $\alpha$. Note that the techniques presented here can be applied to any evolution equation of the form (6.9) on infinite-dimensional Hilbert spaces. The new method may also be useful for splitting methods/exponential integrators which require fast computation of matrix/operator exponentials (see [71, 94] and the references therein) and more generally in the field of infinite-dimensional ODE/PDE systems.
Figure 13: Left: Finite portion of Penrose tile showing the fivefold rotational symmetry. We labelled vertices from the centre in a spiral outwards in increasing distance from the origin. Right: Contours used for the fractional diffusion on the Penrose tile ($\alpha \in \mathbb{N}$ top, $\alpha \notin \mathbb{N}$ bottom). The red line represents the interval containing the spectrum, the branch cut for $z^\alpha$ is taken to be $\mathbb{R}_{\leq 0}$.

Figure 14: Left: Convergence for $\alpha = 1/2$. Right: Convergence for $\alpha = 1$. 
We now consider the effect of disorder on the transport properties of the quasicrystal. Typically, introducing disorder or random potentials suppresses transport [13, 86, 112, 115, 150], an effect known as Anderson localisation [5] (and used theoretically in §5.1). However, recent remarkable experimental results reported in *Science* [87] show that in a photonic 2D quasicrystal, disorder can enhance transport. Namely, disorder enhances the transport of wave packets associated with eigenstates in the proximity of a pseudogap (a sharp reduction in the density of states). For further results and discussion of the physical process, we refer the reader to [116,142].

Our aim in this final example is to demonstrate the same phenomenon by studying a theoretical model numerically, and due to the addition of a random potential as opposed to disorder of the system. We will consider the Hamiltonian

$$H = -H_0 + \eta V$$

where $\eta \geq 0$. Here $V$ is a potential given by

$$(V\psi)_i = w_i \psi_i,$$

where $\{w_i\}_{i \in \mathbb{N}}$ are independent uniform random variables in $[-1/2, 1/2]$. The Schrödinger equation is then

$$\frac{du}{dt} = -iH u, \quad u_{t=0} = u_0.$$ 

As before, we can choose a suitable contour so that we can compute the solution at any time with error control. As a measure of localisation of the wave-vector $\psi$, we will consider the inverse participation ratio defined by

$$P(\psi)^{-1} = \frac{\sum |\psi_i|^4}{\sum |\psi_i|^2}.$$

We considered the case of an “eigenstate” in the vicinity of a pseudogap smeared with a local Gaussian as our initial condition. Figure 16 shows typical results as we increase the parameter $\eta$. We first observe a region of

Figure 15: Evolution of initial wavepacket under fractional diffusion.
Figure 16: The difference in inverse participation ratio as $\eta$ is increased. We have taken the average over 100 realisations and $\Delta P^{-1}$ denotes the value of $P^{-1}$ divided by the value at $\eta = 0$.

Figure 17: Top row: Typical profiles for $t = 5$ and various $\eta$ for $u_0$ equal to the smeared pseudogap state. Note the increase in transport followed by suppression of transport as we increase $\eta$. Bottom row: Typical profiles for $t = 5$ and various $\eta$ for $u_0 = e_1$. Note the suppression of transport as we increase $\eta$. 
increased transport due to the randomness, followed by a decrease in spreading due to Anderson localisation. This is shown visually in Figure 17, where we have also shown the generic suppression of transport for the initial condition \( u_0 = e_1 \). These numerical results provide evidence that randomness can increase transport in quasiperiodic systems.

7 Discussion

In this paper, we classified the problem of computing problems related to spectral measures and spectral decompositions. In essence, we provided the first algorithm for computing the measure, and associated properties such as the functional calculus and Radon–Nikodym derivative, in one limit for a large class of operators. However, once one wants to compute the decomposition of measures and spectra into pure point, absolutely continuous and singular continuous parts, it becomes impossible to do so in one limit, even for tridiagonal bounded self-adjoint operators with structure such as discrete Schrödinger operators. The algorithms we construct are arithmetic and can work with inexact input over \( \mathbb{Q} \), however the negative impossibility results hold for any model of computation. This is made precise in the SCI hierarchy, where we showed computing the singular continuous spectrum is harder than the pure point or absolutely continuous spectrum. We also demonstrated that those algorithms with SCI=1 are implementable.

Future research will study the following themes:

- **Collocation method** - we introduced a new collocation method for computing the Radon–Nikodym derivative. Many questions remain such as the choice of optimal collocation points. Would such a choice be related to approximation properties of rational functions? Are there better choices of basis functions to capture the expected behaviour of the measure? It was noted that the collocation behaved badly in the presence of singular behaviour (unlike the algorithm constructed for the SCI classification). Is there a way to somehow subtract off the singular part of the measure to make it behave better? Numerical methods for computing Hilbert transforms [100] may also be useful in developing a collocation approach.

- **PDE operators** - Though we deal entirely with the discrete case in this paper, the results easily carry over to the continuous case (for instance partial differential operators) with a suitable choice of basis functions allowing us to represent the operator in matrix form. From the point of view of computing the spectrum as a set, this has been explored in [11, 29]. However, it is expected that a more direct approach may be numerically beneficial, as was found in [72]. In this direction it would be useful to develop a fast and stable spectral method for domains such as the real line or half line, mirroring available methods for a bounded interval [101]. Promising work in this direction can be found in [73–75].

- **Evolution PDEs** - Examples were given of evolution equations (6.9) that can be solved using contour integration of the resolvent. Future work will explore the use of Proposition 2.1 and rectangular systems to construct stable solvers.

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A The SCI hierarchy - a framework for computation

The cornerstone in the SCI hierarchy is the definition of a computational problem, a general algorithm and towers of algorithms. The basic objects in a computational problem are as follows:

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

The set $\Omega$ is some set, called the **domain**. For example, when considering the decomposition (3.1):

The set $\mathcal{M}$ is a metric space with metric $d_\mathcal{M}$. These seemingly more complicated objects can be effectively encoded by functions that map into evaluation functions consisting of intervals exhausting a set, piecewise constant functions of compact support etc. These seemingly more complicated objects can be effectively encoded by functions that map into $\mathbb{C}$. For example, when considering the decomposition (3.1):

$$U = \bigcup_m (a_m(U), b_m(U))$$

of an open set $U$, we consider $\xi_1(U), \xi_2(U)$ with $\xi_1(U) = a_m$ and $\xi_2(U) = b_m$. For the sake of clarity of presentation of the proofs, such encodings will be used implicitly throughout the paper.

This leads to the following definition.

**Definition A.1** (Computational Problem). Given a primary set $\Omega$, an evaluation set $\Lambda$, a metric space $\mathcal{M}$ and a problem function $\Xi : \Omega \to \mathcal{M}$ we call the collection $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ a computational problem.

The goal is to find algorithms that approximate the function $\Xi$. More generally, the main pillar of our framework is the concept of a tower of algorithms, which is needed to describe problems that need several limits in the computation. However, first one needs the definition of a general algorithm.

**Definition A.2** (General Algorithm). Given a computational problem $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a general algorithm is a mapping $\Gamma : \Omega \to \mathcal{M}$ such that for each $A \in \Omega$

(i) there exists a finite subset of evaluations $\Lambda_{\Gamma}(A) \subset \Lambda$,
(ii) the action of $\Gamma$ on $A$ only depends on $\{A_f\}_{f \in \Lambda_{\Gamma}(A)}$ where $A_f := f(A)$,
(iii) for every $B \in \Omega$ such that $B_f = A_f$ for every $f \in \Lambda_{\Gamma}(A)$, it holds that $\Lambda_{\Gamma}(B) = \Lambda_{\Gamma}(A)$.

Note that the definition of a general algorithm is more general than the definition of a Turing machine or a RAM machine. A general algorithm has no restrictions on the operations allowed. The only restriction is that it can only take a finite amount of information, though it is allowed to adaptively choose the finite amount of information it reads depending on the input. Condition (iii) assures that the algorithm consistently reads the information. Note that the purpose of such a general definition is to get strong lower bounds. In particular, the more general the definition is, the stronger a lower bound will be.

With a definition of a general algorithm, we can define the concept of towers of algorithms.

**Definition A.3** (Tower of Algorithms). Given a computational problem $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$, a tower of algorithms of height $k$ for $\{\Xi, \Omega, \mathcal{M}, \Lambda\}$ is a family of sequences of functions

$$\Gamma_{n_k} : \Omega \to \mathcal{M}, \Gamma_{n_k, n_{k-1}} : \Omega \to \mathcal{M}, \ldots, \Gamma_{n_k, \ldots, n_1} : \Omega \to \mathcal{M},$$

where $n_k, \ldots, n_1 \in \mathbb{N}$ and the functions $\Gamma_{n_k, \ldots, n_1}$ at the “lowest level” of the tower are general algorithms in the sense of Definition A.2. Moreover, for every $A \in \Omega$,

$$\Xi(A) = \lim_{n_k \to \infty} \Gamma_{n_k}(A), \quad \Gamma_{n_k, \ldots, n_{j+1}}(A) = \lim_{n_j \to \infty} \Gamma_{n_k, \ldots, n_j}(A) \quad j = k - 1, \ldots, 1.$$
In addition to a general tower of algorithms (defined above), we will focus on arithmetic towers. The definition of a general algorithm allows for strong lower bounds; however, to produce upper bounds we must add structure to the algorithm and towers of algorithms. An arithmetic tower allows for arithmetic operations and comparisons.

**Definition A.4** (Arithmetic Towers). Given a computational problem \( \{ \Xi, \Omega, M, \Lambda \} \), an Arithmetic Tower of Algorithms of height \( k \) for \( \{ \Xi, \Omega, M, \Lambda \} \) is a tower of algorithms where the lowest level functions
\[
\Gamma = \Gamma_{n_k, \ldots, n_1} : \Omega \rightarrow M
\]
satisfy the following: For each \( A \in \Omega \) the action of \( \Gamma \) on \( A \) consists of only finitely many arithmetic operations and comparisons on \( \{ A_f \}_{f \in \Lambda_r(A)} \), where we remind that \( A_f = f(A) \).

In other words one may say that for the finitely many steps of the computation of the lowest functions \( \Gamma = \Gamma_{n_k, \ldots, n_1} : \Omega \rightarrow M \) only the four arithmetic operations \( +, -, \cdot, / \) within the smallest (algebraic) field which is generated by the input \( \{ A_f \}_{f \in \Lambda_r(A)} \) are allowed. We implicitly assume that any complex number can be decomposed into a real and an imaginary part, and moreover we can determine whether \( a = b \) or \( a > b \) for all real numbers \( a, b \) which can occur during the computations. Though as mentioned in \(|\Omega|, \) all of the results/algorithms in this paper can be easily modified to the case of arithmetic operations on \( \mathbb{Q} \) and inexact input. Given the definitions above we can now define the key concept, namely, the Solvability Complexity Index.

**Definition A.5** (Solvability Complexity Index). A computational problem \( \{ \Xi, \Omega, M, \Lambda \} \) is said to have Solvability Complexity Index \( \text{SCI}(\Xi, \Omega, M, \Lambda)_\alpha = k \), with respect to a tower of algorithms of type \( \alpha \), if \( k \) is the smallest integer for which there exists a tower of algorithms of type \( \alpha \) of height \( k \). If no such tower exists then \( \text{SCI}(\Xi, \Omega, M, \Lambda)_\alpha = \infty \). If there exists a tower \( \{ \Gamma_n \}_{n \in \mathbb{N}} \) of type \( \alpha \) and height one such that \( \Xi = \Gamma_{n_1} \) for some \( n_1 < \infty \), then we define \( \text{SCI}(\Xi, \Omega, M, \Lambda)_\alpha = 0 \). We may sometimes write \( \text{SCI}(\Xi, \Omega, \Lambda) \) to simplify notation when \( M \) and \( \Lambda \) are obvious.

The definition of the SCI immediately induces the SCI hierarchy:

**Definition A.6** (The Solvability Complexity Index Hierarchy). Consider a collection \( \mathcal{C} \) of computational problems and let \( \mathcal{T} \) be the collection of all towers of algorithms of type \( \alpha \) for the computational problems in \( \mathcal{C} \). Define
\[
\Delta_0^\alpha := \{ \Xi, \Omega \} \in \mathcal{C} \mid \text{SCI}(\Xi, \Omega) = 0 \}
\[
\Delta_m^\alpha := \{ \Xi, \Omega \} \in \mathcal{C} | \text{SCI}(\Xi, \Omega) \leq m \}, \quad m \in \mathbb{N},
\]
as well as
\[
\Delta^\alpha := \{ \Xi, \Omega \} \in \mathcal{C} | \exists \{ \Gamma_n \}_{n \in \mathbb{N}} \in \mathcal{T} \text{ s.t. } \forall A d(\Gamma_n(A), \Xi(A)) \leq 2^{-n} \}.
\]

We will also need the following result.

**Proposition A.7**. Given a matrix \( B \in \mathbb{C}^{m \times n} \) and a number \( \epsilon > 0 \) one can test with finitely many arithmetic operations on the entries of \( B \) whether the smallest singular value \( \sigma_1(B) \) of \( B \) is greater than \( \epsilon \).

**Proof.** The matrix \( B^*B \) is self-adjoint and positive semidefinite, hence has its eigenvalues in \([0, \infty)\). The singular values of \( B \) are the square roots of these eigenvalues of \( B^*B \). The smallest singular value is greater than \( \epsilon \) if and only if the smallest eigenvalue of \( B^*B \) is greater than \( \epsilon^2 \), which is the case if and only if \( C := B^*B - \epsilon^2 I \) is positive definite. The matrix \( C \) is positive definite if and only if the pivots left after Gaussian elimination (without row exchange) are all positive. Thus, if \( C \) is positive definite, Gaussian elimination leads to pivots that are all positive, and this requires finitely many arithmetic operations. If \( C \) is not positive definite, then at some point a pivot is zero or negative, at this point the algorithm aborts. An alternative is the Cholesky decomposition. Although forming the lower triangular \( L \in \mathbb{C}^{n \times n} \) (if it exists) such that \( C = LL^* \) requires the use of radicals, the existence of \( L \) can be determined using finitely many arithmetic operations. This follows from the standard Cholesky algorithm, and we omit the details. 

\( \square \)
B Proof of Theorem 5.2

Throughout this section we will fix a graph $G$ as discussed in §5.1 and an operator $A$ of the form (5.3). Recall that there exists some $N \in \mathbb{N}$ such that $(Ax, y) = 0$ if $|x| \geq N$ or $|y| \geq N$. Given a (bounded) self-adjoint operator $h$ acting on $l^2(V(G))$ we recall the following definition of the Green’s function for $x, y \in V(G)$ and $z \in \mathbb{C}\setminus \sigma(h)$:

$$\mathcal{G}(x, y; z) = ((h - z)^{-1} \delta_y, \delta_x),$$

(B.1)

where $\delta_x(y) = \delta_{xy}$. We will use a subscript $\mathcal{G}_\omega$ when referring to a particular sampled operator $h = H_0 + v_\omega + A$. As mentioned in §5.1, our proof strategy will use the fractional moment method.

We follow the setup and notation of Graf [58] closely but highlight the key differences. We recall Ruelle’s criterion (or the RAGE theorem) as follows. Let $P_h$ be the projection onto the continuous spectral subspace of the operator $h$ and let $P_D$ denote the orthogonal projection onto wave functions with support inside the subset $D \subset V(G)$. Then for any $\psi \in l^2(V(G))$

$$\left\| P_h \psi \right\|^2 = \lim_{R \to \infty} \lim_{t \to \infty} \frac{1}{t} \int_0^t \left\| P_x \right\| \geq R e^{-\text{Im}(\delta_h) s} ds$$

(B.2)

The strategy is to bound the fractional moments of the Green’s function (which can be used to prove dynamical localisation) via the following series of technical lemmas.

Lemma B.1. Let $0 < s < 1$. Then there exists some constant $C_1 = C_1(s, G)$ such that

$$\mathbb{E}_\omega(\left| \mathcal{G}_\omega(x, y; z)^s \right|) \leq C_1 \| \rho \|_\infty^s$$

for all $z \in \mathbb{C}\setminus \mathbb{R}$ and $x, y \in V(G)$ with $|x|, |y| \geq N$.

Proof. The proof is virtually identical to that of Lemma 5 from [58]. The only difference is that we need $|x|, |y| \geq N$ to apply the argument in order to avoid the perturbation caused by $A$.

We also recall the following decoupling Lemma from [58]:

Lemma B.2. Let $0 < s < 1$. Then there exists some constant $c > 0$ such that

$$\int_{\mathbb{R}} \rho(\nu) (|\nu - \eta|^s / |\nu - \beta|^s) d\nu \leq c \| \rho \|_\infty^s$$

for all $\rho \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$, $0 \not= \rho \geq 0$ and all $\beta, \eta \in \mathbb{C}$.

Lemma B.3. Let $0 < s < 1$. Then if $\| \rho \|_\infty$ is sufficiently small (independent of $A$ and only dependent on $C_G$) then there exists some constant $c_{1} > 0$ such that

$$\mathbb{E}_\omega(\left| \mathcal{G}_\omega(x, y; z)^s \right|) \leq C_1 \| \rho \|_\infty^s \exp(-m \min\{|x - y|, |y| - N\})$$

for all $z \in \mathbb{C}\setminus \mathbb{R}$ and $x, y \in V(G)$ with $|x|, |y| \geq N$.

Proof. The proof is easier and similar if $x = y$ so we assume that $x \not= y$. Let $\hat{\omega}$ be obtained from $\omega$ by setting $v_x = v_y = 0$. Then we can write

$$H^{\hat{\omega}} := H_0 + v_\omega + A = H_0 + v_\omega + A + v_x P_x + v_y P_y = H^{\omega} + v_x P_x + v_y P_y,$$

that is, we consider the final two terms as a rank two perturbation. Let $P = P_x + P_y = P_{(x, y)}$. Then an application of the second resolvent identity yields Krein’s formula:

$$P(H^{\omega} - z)^{-1} P = (B + v_x P_x + v_y P_y)^{-1},$$

(B.6)

where $B = [P(H^{\omega} - z)^{-1} P]^{-1}$ if it exists acts on $\mathcal{R}(P)$ and is independent of $v_x, v_y$. The inverse exists since $\text{Im}(z)^{-1} \text{Im}((H^{\omega} - z)^{-1})$ is positive definite. Explicitly, with respect to the basis $\{\delta_x, \delta_y\}$ of $\mathcal{R}(P)$, write

$$B = \begin{pmatrix} b_{xx} & b_{xy} \\ b_{yx} & b_{yy} \end{pmatrix},$$

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then from (B.6),
\[
\mathcal{G}_\omega(x, y; z) = -\frac{b_{xy}}{(v_x + b_{xx})(v_y + b_{yy}) - b_{xy}b_{yx}} = \frac{\alpha}{v_y - \beta}
\]  
(B.7)
where \(\alpha, \beta\) are independent of \(v_y\).

Assume that \(|y| > N\) then we also have by considering the matrix elements of \((H^\omega - z)^{-1}(H^\omega - z) = I\) that
\[
\sum_{e \sim y} \mathcal{G}_\omega(x, e; z) = (v_y + \zeta(y) - z)\mathcal{G}_\omega(x, y; z)
\]
which implies that
\[
\sum_{e \sim y} |\mathcal{G}_\omega(x, e; z)|^2 \geq |v_y + \zeta(y) - z|^2 |\mathcal{G}_\omega(x, y; z)|^2.
\]
Using (B.7) and Lemma B.2, this implies
\[
\mathbb{E}_\omega\left(\sum_{e \sim y} |\mathcal{G}_\omega(x, e; z)|^2\right) \geq \mathbb{E}_\omega(|v_y + \zeta(y) - z|^2 |\mathcal{G}_\omega(x, y; z)|^2)
\]
\[
\geq c\rho\|\omega\|^2 \mathbb{E}_\omega(|\mathcal{G}_\omega(x, y; z)|^2).
\]
We assumed that any vertex degree of the graph \(G\) is bounded by \(C_G\). We can iterate the above argument at least \(\min\{\|x - y\|, |y| - N\}\) times where we iterate at most \(|y| - N\) times to be able to apply Lemma B.1. In particular, this implies that
\[
\mathbb{E}_\omega(|\mathcal{G}_\omega(x, y; z)|^2) \leq (C_Gc^{-1})^m \mathbb{E}_\omega(|\mathcal{G}_\omega(x, y; z)|^2)
\]
\[
= C_1\mathbb{E}_\omega(|\mathcal{G}_\omega(x, y; z)|^2) \exp(-m \min\{|x - y|, |y| - N\}),
\]
where \(e^{-m} = C_Gc^{-1}\|\rho\|_\infty^2\). If \(\|\rho\|_\infty\) is small enough then \(m > 0\).

**Lemma B.4.** Let \(\rho\) be as in Lemma B.3 and also of compact support. Then there exists some constant \(C_2(C_G)\) and \(m > 0\) independent of \(A\) such that
\[
\|\Im(z)\| \mathbb{E}_\omega(|\mathcal{G}_\omega(x, y; z)|^2) \leq C_2 \exp(-m \min\{|x - y|, |y| - N\})
\]
for all \(z \in \mathbb{C} \setminus \mathbb{R}\) and \(x, y \in V(G)\) with \(|x|, |y| \geq N\).

**Proof.** The proof is virtually identical to that of the proof of Lemma 3 in [58]. The only difference is that the proof uses the estimate in Lemma B.3 instead of the analogous estimate in [58].

**Proof of Theorem 5.2.** Fix \(A\) of the form (5.3) and let \(\delta(C_G) > 0\) be such that if \(\|\rho\|_\infty \leq \delta(C_G)\) then Lemma B.4 holds. We also need the constant \(m\) to be large enough (by making \(\delta(C_G)\) smaller if necessary) such that \(e^{-m}C_G < 1\). Suppose that the compact interval \(I\) contains the spectrum of \(H^\omega\) in its interior. Then
\[
\epsilon \int_{R \setminus I} \|P_x^y\| R(H^\omega - E - i\epsilon)^{-1}\psi|^2 dE \leq \epsilon \|\psi\|^2 \sup_{\lambda \in \sigma(H^\omega)} \int_{R \setminus I} R(H^\omega - E - i\epsilon)^{-1}\|\psi\|^2 dE \to 0.
\]
(B.9)
as \(\epsilon \downarrow 0\). Since \(\rho\) has compact support, \(\|H^\omega\|\) is bounded independent of \(\omega\) almost surely, so we can fix any interval \(I\) such that the above holds almost surely. Let \(x \in V(G)\) have \(|x| \geq N\) then (B.9) and (B.2) imply that
\[
\|P_x^y\delta_x\|^2 = \lim_{R \to \infty} \lim_{\epsilon \downarrow 0} \frac{\epsilon}{\pi} \int_{|y| \geq R} \|P_x^y\|^2 R(H^\omega - E - i\epsilon)^{-1}\delta_x|^2 dE
\]
\[
= \lim_{R \to \infty} \lim_{\epsilon \downarrow 0} \frac{\epsilon}{\pi} \sum_{|y| \geq R} |\mathcal{G}(x, y; E - i\epsilon)|^2 dE,
\]
(B.10)
almost surely, where we have used \(\mathcal{G}(x, y; z) = \overline{\mathcal{G}(y, x; \overline{z})}\) in the last line. From Fatou’s lemma and (B.8) we obtain
\[
\mathbb{E}_\omega(\|P_x^y\delta_x\|^2) \leq C \lim_{R \to \infty} \inf_{|y| \geq R} \exp(-m \min\{|x - y|, |y| - N\})
\]
\[
\leq C \exp(m \max\{N, |x|\}) \lim_{R \to \infty} \inf_{j = R} \sum_{j = R}^\infty \|\mathcal{G}e^{-m}\|^j = 0,
\]
where the second line is obtained by summing over \(|y| = j\) and since \(e^{-m}C_G < 1\). It follows that \(P_x^y\delta_x = 0\) almost surely. But this then implies that \(P_x^y\delta_x\) has finite rank almost surely (recall we assumed \(|x| \geq N\) and hence is 0 almost surely since a finite rank self-adjoint operator has pure point spectrum.)
C An algorithm for point spectra of operators $\mathcal{C}(l^2(\mathbb{N}))$

We now prove that the computation of $\Xi^{C}_{P_n}$ can be done in two limits for $T \in \mathcal{C}(l^2(\mathbb{N}))$ given access to the evaluation set $A_2$. Since $T$ is closed and densely defined, a point $z$ lies in the point spectrum of $T$ if and only if the closure of the range $\mathcal{R}(T^* - zI)$ is not the whole of $l^2(\mathbb{N})$. This occurs if and only if $\mathcal{F}(T, z) > 0$ where

$$\mathcal{F}(T, z) := \sup_{n \in \mathbb{N}} \text{dist}(e_n, \mathcal{R}(T^* - zI))$$

(C.1)

(which is always bounded by 1) and dist($v, S$) = inf$_{e \in S} \|v - s\|$ for a subspace $S$ and vector $v$. The point spectrum is difficult to compute precisely because $\mathcal{F}(T, \cdot)$ is highly discontinuous. However, we can approximate $\mathcal{F}(T, \cdot)$ via two limits in the following manner (where the base level algorithms are stable). Because of the inherent instabilities, extra care is taken and we will replace $A_2$ by the evaluation functions

$$f^{(1)}_{i,j,m}, f^{(2)}_{i,j,m} : \mathcal{C}(l^2(\mathbb{N})) \to \mathbb{Q} + i\mathbb{Q}$$

such that $|f^{(1)}_{i,j,m}(T) - \langle Te_j, e_i \rangle| \leq 2^{-m}$ and $|f^{(2)}_{i,j,m}(T) - \langle T^* e_j, T^* e_i \rangle| \leq 2^{-m}$. This collection will be denoted by $\tilde{A}_2$

It is straightforward to construct a sequence of vectors $\{x_j\}_{j \in \mathbb{N}} = S \subset l^2(\mathbb{N})$ with the following properties:

1. Each vector $x_j$ is constructed using only finitely many arithmetic operations, has components in $\mathbb{Q} + i\mathbb{Q}$ and has only finitely many non-zero components.

2. The full sequence $\{x_j\}_{j \in \mathbb{N}}$ is dense in $l^2(\mathbb{N})$.

Namely, we can construct a sequence with the property (1) which is dense in the unit ball of $\mathcal{R}(P_m)$, for each $m$ via approximation of simple trigonometric functions. We then combine these over $m \in \mathbb{N}$ and balls of increasing (rational) radii. Define the functions

$$\mu_{j,k}(T, z) := \|e_k - (T^* - zI)x_j\|.$$  

(C.2)

Clearly these are continuous in $z$ and the following Lemma states that they can be approximated using finitely many arithmetic operations and comparisons and the evaluation set $A_2$.

**Lemma C.1.** For any $j, k \in \mathbb{N}$ and $z \in \mathbb{Q} + i\mathbb{Q}$ and $\epsilon > 0$, $\mu_{j,k}(T, z)$ can be approximated within accuracy $\epsilon$ using finitely many arithmetic operations and comparisons over $\mathbb{Q}$ and the evaluation set $A_2$.

**Proof.** Fix $j, k \in \mathbb{N}$. There exists some (known) integer $M$ such that $\|x_j\| \leq M$ and $\langle e_i, x_j \rangle = 0$ if $i > M$. We first expand the square of (C.2) as

$$\mu_{j,k}(T, z)^2 = 1 + |z|^2 \|x_j\|^2 + 2\Re\{\overline{z}(x_j, e_k)\} + \|T^* x_j\|^2 - 2\Re\{T^* x_j, e_k + \overline{z}x_j\}$$

Clearly, the first three terms can be computed (without error) using finitely many arithmetic operations and comparisons over $\mathbb{Q}$. Since $x_j$ has finite support, the fourth term can be computed to arbitrary accuracy using the evaluation functions $f^{(2)}_{i,j,m}$ and similarly the last term can be computed to arbitrary accuracy using the evaluation functions $f^{(1)}_{i,j,m}$. We can therefore approximate $\mu_{j,k}(T, z)^2$ to accuracy $\epsilon^2/4$. We then approximate the square root of this approximation to accuracy $\epsilon/2$ using finitely many arithmetic operations and comparisons (say using the Babylonian algorithm).

Each $\mu_{j,k}(T, \cdot)$ is Lipschitz continuous with Lipschitz constant $\|x_j\|$, which we assume to have a known upper bound $M_j$. Now define the functions

$$\mathcal{F}_{n,m}(T, z) := \max_{k=1, \ldots, n} \min_{j=1, \ldots, m} \mu_{j,k}(T, z).$$

(C.3)

For $z \in \mathbb{Q} + i\mathbb{Q}$ it is clear that Lemma C.1 holds with replacing $\mu_{j,k}$ by $\mathcal{F}_{n,m}$. We assume that we approximate each $\mathcal{F}_{n,m}$ from above to within an accuracy $1/m$ via Lemma C.1 and assume without loss of generality by taking successive minima that these approximations, denoted $\tilde{\mathcal{F}}_{n,m}$, are non-increasing in $m$. We can also compute, in finitely many arithmetic operations and comparisons, a Lipschitz constant $L_{n,m} \in \mathbb{Q}_+$ for each $\tilde{\mathcal{F}}_{n,m}$. The next proposition states the approximation properties of the functions $\tilde{\mathcal{F}}_{n,m}$. Define the functions

$$\mathcal{F}_n(T, z) := \max_{k=1, \ldots, n} \text{dist}(e_k, \mathcal{R}(T^* - zI)).$$

(C.4)

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Suppose for a contradiction that \( F_{n,m}(T, z) < F_n(T, z) \) and define \( F_{n,m}(T, z) = F_n(T, z) \). The first limit is monotonically from above whereas the second is monotonically from below. Moreover, these limits hold (with \( F_{n,m} \) replaced by \( F_{n,m} \) in the first limit) for \( z \in \mathbb{C} \).

Proof. Fix \( z \in \mathbb{Q} + i\mathbb{Q} \). Then \( F_{n,m}(T, z) \) are non-increasing in \( m \) and non-negative so converge to a limit. We also clearly have that \( F_{n,m}(T, z) \geq F_n(T, z) \).

Given \( \delta > 0 \) let \( x_j \in S \) and \( k \in \{1, \ldots, n\} \) be such that

\[
\|e_k - (T^* - zI)x_j\| \leq F_n(T, z) + \delta.
\]

Such an \( x_j \) exists precisely because \( S \) forms a core of \( T^* \). But this implies for \( j \geq m \) that

\[
F_{n,m}(T, z) \leq \frac{1}{m} + \delta + F_n(T, z).
\]

Since \( \delta > 0 \) was arbitrary, the first part of the proposition is proven. The last part follows immediately from the definition of \( F \) in (C.1).

\[\square\]

Remark 10. Note that this shows that each \( F_n(T, \cdot) \) is upper semi-continuous.

Theorem C.3. Given the above setup, \( \{\Xi_{pp}, \mathcal{C}(\mathbb{P}(\mathbb{N})), \tilde{\Lambda}_2\} \in \Delta^4 \). Moreover, the constructed arithmetic tower of algorithms \( \{\Gamma_{n_1, n_2}\}_{n_1, n_2 \in \mathbb{N}} \) for this problem has \( \lim_{n_1 \to \infty} \Gamma_{n_2, n_1}(T) \subset \sigma_p(T) \).

Proof. Let

\[
G_{n,\delta'} = B_n(0) \cap \delta'(\mathbb{Z} + i\mathbb{Z})
\]

and define

\[
\Gamma_{n_2, n_1}(T) = \{ z \in G_{n_2, 2n_1, L_{n_1, n_2}} : \tilde{F}_{n_2, n_1}(T, z) \geq \frac{1}{n_2} - \frac{1}{n_1} \}.
\]

The above remarks and Lemma C.1 imply that \( \Gamma_{n_2, n_1}(T) \) can be computed using finitely many arithmetic operations and comparisons over \( \mathbb{Q} \) given the evaluation set \( \tilde{\Lambda}_2 \). Hence we only need to prove convergence of this height two tower and the fact that the first limit is contained in the point spectrum.

Suppose first that \( z \in B_{n_2}(0) \) such that \( F_{n_2}(T, z) \geq 1/n_2 \). Then there exists \( n_1 \in G_{n_2, 2n_1, L_{n_1, n_2}} \) with \( |z - z_{n_1}| \leq 1/(n_1 L_{n_1, n_2}) \). But then, since \( L_{n_1, n_2} \) is a Lipschitz constant for \( \tilde{F}_{n_2, n_1}(T, \cdot) \), we must have

\[
\tilde{F}_{n_2, n_1}(T, z_{n_1}) \geq \tilde{F}_{n_2, n_1}(T, z) - \frac{1}{n_1} \geq F_{n_2}(T, z) - \frac{1}{n_1} \geq \frac{1}{n_2} - \frac{1}{n_1}.
\]

Hence \( z_{n_1} \in \Gamma_{n_2, n_1}(T) \). Conversely, suppose that there is a subsequence \( z_{n_j} \in \Gamma_{n_2, n_1}(T) \) with \( m_j \to \infty \). By considering a subsequence if necessary we can assume that the \( z_{n_j} \) converge to some point \( z \in B_{n_2}(0) \). Suppose for a contradiction that \( z \) is not contained in the set

\[
F_{n_2}(T) := \{ w : B_{n_2}(0) : F_{n_2}(T, w) \geq \frac{1}{n_2} \}.
\]

Note that \( F_{n_2}(T) \) is closed (even though the \( F_{n_2}(T, \cdot) \) need not be continuous) since it can be written as

\[
F_{n_2}(T) = \bigcap_{m \in \mathbb{N}} \{ w : B_{n_2}(0) : F_{n_2,m}(T, w) \geq \frac{1}{n_2} \}
\]

and each \( F_{n,m}(T, \cdot) \) is continuous. Alternatively, we can use the fact that each \( F_n(T, \cdot) \) is upper semi-continuous. We can replace \( 1/n_2 \) by any positive quantity and the statement about level sets being closed still holds. It follows that there exists an open neighbourhood \( U \) of \( z \) such that for any \( \eta \in U \) it holds that \( F_{n_2}(T, w) < 1/n_2 - \epsilon \) for some \( \epsilon > 0 \). Take a small ball \( B_{\eta}(z) \) centred at \( z \) with \( \eta > 0 \) and contained in \( U \) then the functions \( \max\{1/n_2 - \epsilon, \tilde{F}_{n_2,n_1}(T, \cdot)\} \) are continuous and converge pointwise to (the continuous constant function) \( 1/n_2 - \epsilon \) monotonically from above on \( B_{\eta}(z) \). Dini’s theorem implies that this convergence must be uniform on \( B_{\eta}(z) \). In other words, there exists \( N \) such that if \( n_1 \geq N \) and \( w \in B_{\eta}(z) \) then

\[
\tilde{F}_{n_2,n_1}(T, w) \leq \frac{1}{n_2} - \frac{\epsilon}{2}.
\]

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But for large \( m_j \), it holds that \( z_{m_j} \in B_\eta(z) \) and
\[
\tilde{F}_{n_2,m_1}(T, z_{m_j}) \geq \frac{1}{n_2} - \frac{1}{m_j} > \frac{1}{n_2} - \epsilon/2,
\]
the required contradiction. The above arguments show that
\[
\lim_{n_1 \to \infty} \Gamma_{n_2,n_1}(T) = F_{n_2}(T),
\]
and this includes the empty-set cases.

Proposition C.2 implies that \( F_{n_2}(T) \) is contained in the point spectrum and that the sets are increasing in \( n_2 \). Suppose that \( z \in \text{Sp}_{pp}(T) \) and let \( \epsilon > 0 \). Then there exists \( z_\epsilon \in \sigma_p(T) \) with \( |z - z_\epsilon| \leq \epsilon \). For large \( n_2 \) we must have that \( \mathcal{F}_{n_2}(T, z_\epsilon) \geq \mathcal{F}(T, z_\epsilon)/2 > 0 \) and hence, for large \( n_2 \), \( z_\epsilon \in F_{n_2}(T) \). Since \( \epsilon > 0 \) was arbitrary, it follows that \( \lim_{n_1 \to \infty} \lim_{n_2 \to \infty} \Gamma_{n_2,n_1}(T) = \Xi_{pp}(T) \).

\[\square\]

D Computation of the Cauchy transform of basis functions

Here we will discuss for the benefit of the reader, a fast and accurate way to compute the Cauchy transform of basis functions (supported on \( I \)) that satisfy a recurrence relationship of the form
\[
\phi_{m+1}(\lambda) = \alpha_m \lambda \phi_m(\lambda) + \beta_m \phi_m(\lambda) + \gamma_m \phi_m-1(\lambda).
\]
Such a recurrence relationship holds for many common bases such as Legendre and Chebyshev polynomials, Hermite functions or Laguerre functions. We then have that
\[
\hat{\phi}_{m+1}(z) = \alpha_m \int_I \frac{\lambda \phi_m(\lambda)}{\lambda - z} d\lambda + \beta_m \hat{\phi}_m(z) + \gamma_m \hat{\phi}_{m-1}(z)
\]
\[
= \alpha_m \int_I \phi_m(\lambda)d\lambda + z \alpha_m \hat{\phi}_m(z) + \beta_m \hat{\phi}_m(z) + \gamma_m \hat{\phi}_{m-1}(z).
\]
Hence, given the values of the integrals
\[
\int_I \phi_m(\lambda)d\lambda, \quad \hat{\phi}_1(z),
\]
we can compute \( \hat{\phi}_m(z) \) for all \( m \in \mathbb{N} \). The integrals in (D.1) have simple forms for all the bases used in this paper. This method of computation of \( \hat{\phi}_m \) is fast, meaning that the most expensive part of the collocation method in §6.2 is the computation of the right hand side of the linear system, that is, computing the resolvent.