

Spectral theory for unbounded self-adjoint operators

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Abstract

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The focus of this thesis is the spectral theory for unbounded self-adjoint operators. The main result of the thesis is the corresponding spectral theorem, which states that any unbounded self-adjoint operator can be written as an operator-valued integral over the spectrum of the operator. This is a generalization of the spectral decomposition for self-adjoint matrices.

The proof of the spectral theorem for unbounded self-adjoint operators follows by proving it first for bounded self-adjoint operators and then for unitary operators. From the unitary case, the spectral theorem for unbounded self-adjoint operators is proven by using the Cayley transform.

Finally, some consequences of the spectral theory are considered. Special emphasis is given to its applications to quantum mechanics where physical observables correspond to self-adjoint operators.

Tiivistelmä

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Spektraaliteoria rajoittamattomille itseadjungoiduille operaattoreille

Pro gradu -tutkielma

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Tässä tutkielmassa keskitytään rajoittamattomien itseadjungoitujen operaattorien spektraaliteoriaan. Tutkielman päätulos on tällaisten operattorien spektraalilause, jonka mukaan mikä tahansa rajoittamaton itseadjungoitu operaattori voidaan kirjoittaa operaattoriarvoisena integraalina operaattorin spektrin yli. Tämä on itseadjungoitujen matriisien spektraalihajotelman yleistys.

Rajoittamattomien itseadjungoitujen operaattorien spektraalilause seuraa johtamalla se ensin rajoitetuille itseadjungoiduille operaattoreille ja tämän jälkeen unitaarille operaattoreille. Unitaaristen operaattorien spektraalilauseesta saadaan johdettua rajoittamattomien itseadjungoitujen operaattorien tapaus Cayleyn muunnoksen avulla.

Lopuksi tarkastellaan joitain spektraaliteorian seurauksia. Erityisesti keskitytään sen sovelluksiin kvanttimekaniikassa, missä fysikaaliset suureet vastaavat itseadjungoituja operaattoreita.

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1 Introduction

Linear operators appear in many different fields of mathematics where the system can be written in terms of a Hilbert space. Thus, it is useful to have a thorough understanding of linear operators. A subset of linear operators, i.e. normal operators, can be understood via the spectral theory, which allows us to write the operator in terms of its spectral representation. The central theorem describing this is the spectral theorem. Writing an operator in terms of its spectral representation often simplifies the situation significantly as it essentially turns the operator to a simple multiplication.

While the study of the spectral theory started originally from eigenvalues of matrices and Fredholm integrals, the presentation in terms of abstract operators in a Hilbert space was started by Hilbert in the beginning of the 20th century. This was completed to the unbounded case later by von Neumann who was largely inspired by the recent developments in quantum mechanics making use of linear operators. Generalizations of the spectral theory were also considered later, where instead of working in a Hilbert space one considers a more abstract C^* -algebra. The spectral theorem for this more general case is due to Gel'fand and Naimark. [Steen 1973]

In this thesis, we focus on a special case of normal operators, namely the self-adjoint operators. The main property of these operators is that their spectrum is limited to a subset of real numbers \mathbb{R} . This is also the reason why they are one of the most common normal operators one encounters in other fields, making them of special interest. An example is given by self-adjoint operators that are mostly studied in quantum mechanics, where the self-adjoint operators correspond to physical observables. The spectral theory for self-adjoint operators thus finds lots of applications also outside pure mathematics.

The main result of this thesis is the spectral theorem for unbounded self-adjoint operators, Theorem 5.5. To prove this, we first consider the spectral theorem in the case of bounded self-adjoint operators in Section 4. This can then be used to show the unbounded case in Section 5, which follows from the spectral theorem for unitary operators by the Cayley transform. This proof of the spectral theorem follows largely [Hall 2013; Kreyszig 1978]. The spectral theorem is written in terms of the projection-valued measure associated with the corresponding operator. Projection-valued measures along with the required measure theory are explained in Section 3. We note that there are also several other versions of the spectral theorem which are written in a slightly different form, see e.g. [Hall 2013, Theorem 7.19]. Finally, we consider some applications of spectral theory to quantum mechanics in Section 6.

2 Hilbert space

The central objects of interest in this thesis are operators acting in some Hilbert space. In general, a Hilbert space is a special case of a vector space with some additional structure that allows us to talk about relations between different elements of the Hilbert space. This structure is given by the inner product.

Definition 2.1 (Inner product). An **inner product** on a vector space X over \mathbb{C} is a map $\langle \cdot, \cdot \rangle : X \times X \rightarrow \mathbb{C}$, such that for all $\phi, \psi, \chi \in X$ and $c \in \mathbb{C}$ we have:

1. $\langle \psi, \phi \rangle = \overline{\langle \phi, \psi \rangle}$.
2. $\langle \phi, \phi \rangle$ is real and non-negative, and $\langle \phi, \phi \rangle = 0$ if and only if $\phi = 0$.
3. $\langle c\phi, \psi \rangle = \bar{c}\langle \phi, \psi \rangle$ and $\langle \phi, c\psi \rangle = c\langle \phi, \psi \rangle$.
4. $\langle \phi + \psi, \chi \rangle = \langle \phi, \chi \rangle + \langle \psi, \chi \rangle$ and $\langle \phi, \psi + \chi \rangle = \langle \phi, \psi \rangle + \langle \phi, \chi \rangle$.

Here we follow the physics convention that an inner product is *conjugate linear* (or antilinear) in its first argument and *linear* in its second argument, as defined by Points 3 and 4. This property of the inner product is called **sesquilinearity**.

The inner product defines a **norm** on the vector space by

$$\|\psi\| = \sqrt{\langle \psi, \psi \rangle}. \quad (1)$$

A norm allows us to have a notion of distance on the vector space, which gives the vector space extra structure that for example allows us to talk about the convergence of sequences. A vector space is said to be complete if every Cauchy sequence converges to an element in the vector space. A complete vector space equipped with a norm is called a **Banach space**. A **Hilbert space** is a Banach space where the norm is defined in terms of the inner product by Equation (1). Throughout this thesis, we will denote the Hilbert space we are working on by **H**.

The inner product also allows us to talk about the orthogonality of vectors: vectors $\psi, \phi \in \mathbf{H}$ are called **orthogonal** if $\langle \psi, \phi \rangle = 0$. For a vector space $V \subset \mathbf{H}$ we can define its **orthogonal complement** by

$$V^\perp = \{\psi : \langle \psi, \phi \rangle = 0 \text{ for all } \phi \in V\}. \quad (2)$$

One can show that the orthogonal complement is also a vector space.

2.1 Operators on a Hilbert space

Mappings from one vector space to another are called operators. In this work, operators are taken to mean specifically *linear* operators:

Definition 2.2 (Operator). Let X, Y be vector spaces over \mathbb{C} . Then a mapping $T : X \rightarrow Y$ is an **operator** from X to Y if it is linear. The range of the operator T is denoted by $\text{Ran}(T) = T(X)$.

A special case of an operator is a linear **functional** which is a linear function from a vector space to complex numbers, $f : X \rightarrow \mathbb{C}$.

Operators can be used to define different notions of convergence in the Hilbert space.

Definition 2.3 (Convergence of sequence of vectors). Let X be a normed space. A sequence $\{\psi_n\}_{n \in \mathbb{N}}$ of vectors in X is said to be:

1. **strongly convergent** if there is a vector $\psi \in X$ such that $\lim_{n \rightarrow \infty} \|\psi_n - \psi\| = 0$.
2. **weakly convergent** if there is a vector $\psi \in X$ such that for every bounded linear functional $f : X \rightarrow \mathbb{C}$ we have $\lim_{n \rightarrow \infty} f(\psi_n) = f(\psi)$.

It is straightforward to show that strong convergence implies weak convergence, and if they both converge then the limit is the same. Different notions of convergence are sometimes useful, as some sequences may be weakly convergent but not strongly.

It is interesting to note that operators $T : X \rightarrow Y$ also form a vector space. A norm for operators can be defined in the following way.

Definition 2.4 (Norm of an operator). *Let X, Y be normed vector spaces with norms $\|\cdot\|_X, \|\cdot\|_Y$, and $T : X \rightarrow Y$ an operator. Then the **operator norm** of T is given by*

$$\|T\| = \inf \{K \in \mathbb{R} : \|T\psi\|_Y \leq K\|\psi\|_X \text{ for all } \psi \in X\}. \quad (3)$$

*In the case $\|T\| < \infty$ the operator T is called **bounded**. If an operator is not bounded, it is called **unbounded**.*

It turns out that an operator is bounded if and only if it is continuous. Bounded operators are generally well-behaved, in contrast to unbounded ones, as we will see when proving the spectral theorem for unbounded self-adjoint operators. We denote the space of bounded operators $T : \mathbf{H} \rightarrow \mathbf{H}$ in Hilbert space \mathbf{H} by $\mathcal{B}(\mathbf{H})$.

It is also useful to have a notion of convergence for a sequence of operators T_n . The simplest definition is in terms of the operator norm, but other definitions also exist.

Definition 2.5 (Convergence of sequence of operators). *Let X and Y be normed spaces. A sequence $\{T_n\}_{n \in \mathbb{N}}$ of bounded operators $T_n : X \rightarrow Y$ is said to be:*

1. **uniformly operator convergent** if $\{T_n\}_{n \in \mathbb{N}}$ converges in the operator norm.
2. **strongly operator convergent** if $\{T_n\psi\}_{n \in \mathbb{N}}$ converges strongly in Y for every $\psi \in X$.
3. **weakly operator convergent** if $\{T_n\psi\}_{n \in \mathbb{N}}$ converges weakly in Y for every $\psi \in X$.

It is straightforward to show that in terms of convergence, uniform implies strong and strong implies weak. Also, if the limit exists for different types of convergence then they converge to the same operator.

Another useful notion we can define with operators is the dual space. For a vector space X we define a **dual space** X^* that consists of all linear functionals $f : X \rightarrow \mathbb{C}$. One important theorem on Hilbert spaces is the Riesz representation theorem which allows us to associate a bounded element in the dual space \mathbf{H}^* for every element in the initial Hilbert space \mathbf{H} :

Theorem 2.6 (Riesz representation theorem). *If $f : \mathbf{H} \rightarrow \mathbb{C}$ is a bounded linear functional, then there exists a unique $\chi \in \mathbf{H}$ such that*

$$f(\psi) = \langle \chi, \psi \rangle \quad (4)$$

for all $\psi \in \mathbf{H}$. Furthermore, the operator norm of f as a linear functional is equal to the norm of χ as an element of \mathbf{H} .

Proof. See [Kreyszig 1978, Theorem 3.8-1]. \square

We also quote here the **bounded linear transformation theorem** (BLT) which can be used to extend bounded operators defined on a dense subspace of a Hilbert space to the whole Hilbert space in a continuous manner.

Theorem 2.7 (Bounded linear transformation theorem). *Let V_1 be a normed space and V_2 a Banach space. Suppose W is a dense subspace of V_1 and $T : W \rightarrow V_2$ is a bounded operator. Then there exists a unique bounded operator $\tilde{T} : V_1 \rightarrow V_2$ such that $\tilde{T}|_W = T$. Furthermore, the norm of \tilde{T} equals the norm of T .*

Proof. See [Kreyszig 1978, Theorem 2.7-11]. \square

From here on we will assume that bounded operators are defined on the whole Hilbert space \mathbf{H} , as they can always be extended continuously to the completion of their domain.

On Hilbert spaces, we can define the adjoint of an operator. For bounded operators defining the adjoint is simple.

Definition 2.8 (Adjoint of a bounded operator). *Let T be a bounded operator on \mathbf{H} . Then the **adjoint** of the operator T is an operator T^* such that for all $\psi, \phi \in \mathbf{H}$, we have*

$$\langle \psi, T\phi \rangle = \langle T^*\psi, \phi \rangle. \quad (5)$$

Theorem 2.9 (Existence of the adjoint for bounded operators). *The adjoint operator T^* of T in Definition 2.8 exists, is unique, and is a bounded operator with the norm $\|T^*\| = \|T\|$.*

Proof. This is essentially a consequence of the Riesz representation theorem 2.6. See [Kreyszig 1978, Theorem 3.9-2] for details. \square

For unbounded operators the definition of the adjoint operator is more complicated, rising from the fact that unbounded operators might not be defined on the whole Hilbert space \mathbf{H} . Instead, we will assume that they are defined on a dense subspace of \mathbf{H} . Then the following definition can be given.

Definition 2.10 (Adjoint of an unbounded operator). *For an unbounded operator T on \mathbf{H} , the adjoint T^* of T is defined as follows. A vector $\phi \in \mathbf{H}$ belongs to the domain $\text{Dom}(T^*)$ of T^* if the linear functional*

$$\langle \phi, T\cdot \rangle \quad (6)$$

defined on $\text{Dom}(T)$ is bounded. For $\phi \in \text{Dom}(T^*)$, let $T^*\phi$ be the unique vector χ such that

$$\langle \chi, \psi \rangle = \langle \phi, T\psi \rangle \quad (7)$$

for all $\psi \in \text{Dom}(T)$.

Here the existence and uniqueness of the vector $\chi = T^*\phi$ follow from the Riesz representation theorem 2.6.

Finally, we will also note the definition of a closed operator which will be needed when considering the definition of self-adjoint operators.

Definition 2.11 (Closed operator). *An operator T on \mathbf{H} is said to be **closed** if its graph,*

$$\mathcal{G}(T) = \{(\psi, T\psi) : \psi \in \text{Dom}(T)\}, \quad (8)$$

*is a closed subset of $\mathbf{H} \times \mathbf{H}$. An operator T on \mathbf{H} is said to be **closable** if the closure in $\mathbf{H} \times \mathbf{H}$ of the graph of T is the graph of a function. If T is closable, then the closure T^{cl} of T is the operator with a graph equal to the closure of the graph of T .*

The following important theorem states that closed unbounded operators cannot be defined on a closed subset of \mathbf{H} .

Theorem 2.12 (Closed graph theorem). *Let $T : \text{Dom}(T) \rightarrow \mathbf{H}$ be a closed operator on \mathbf{H} . Then if $\text{Dom}(T)$ is closed in \mathbf{H} , the operator T is bounded.*

Proof. See [Kreyszig 1978, Theorem 4.13-2]. □

2.2 Spectrum of an operator

Operators can often be studied in terms of their spectrum. For finite-dimensional Hilbert spaces the spectrum coincides with the eigenvalues of the operator. The infinite-dimensional case is a little bit more technical, and the general definition of the spectrum is more complicated.

Definition 2.13 (Spectrum of an operator). *Let T be an operator on \mathbf{H} .*

1. *One calls a **resolvent set** of T the set $\rho(T)$ of numbers $\lambda \in \mathbb{C}$ such that:*

(a) $\overline{\text{Ran}(T - \lambda I)} = \mathbf{H}$,

(b) $(T - \lambda I) : \text{Dom}(T) \rightarrow \mathbf{H}$ is injective,

(c) $(T - \lambda I)^{-1} : \text{Ran}(T - \lambda I) \rightarrow \mathbf{H}$ is bounded.

2. *If $\lambda \in \rho(T)$, the **resolvent** of T is the operator*

$$R_\lambda(T) = (T - \lambda I)^{-1} : \text{Ran}(T - \lambda I) \rightarrow \text{Dom}(T). \quad (9)$$

3. *The **spectrum** of T is the set $\sigma(T) = \mathbb{C} \setminus \rho(T)$.*

The spectrum of T can be further divided into three disjoint subsets:

1. the **point spectrum** $\sigma_p(T)$, made by the $\lambda \in \mathbb{C}$ for which $T - \lambda I$ is not injective,
2. the **continuous spectrum** $\sigma_c(T)$, made by the $\lambda \in \mathbb{C}$ for which $T - \lambda I$ is injective and $\overline{\text{Ran}(T - \lambda I)} = \mathbf{H}$, but $(T - \lambda I)^{-1}$ is not bounded,
3. the **residual spectrum** $\sigma_r(T)$, made by the $\lambda \in \mathbb{C}$ for which $T - \lambda I$ is injective but $\overline{\text{Ran}(T - \lambda I)} \neq \mathbf{H}$.

In essence, the condition for a complex number λ to belong to the resolvent set is the following: if there exists a bounded inverse $(T - \lambda I)^{-1} : \text{Ran}(T - \lambda I) \rightarrow \text{Dom}(T)$, where $\overline{\text{Ran}(T - \lambda I)} = \mathbf{H}$, then $\lambda \in \rho(T)$. Also note that if T is defined on the whole space \mathbf{H} and $\lambda \in \rho(T)$, then $\text{Ran}(T - \lambda I) = R_\lambda^{-1}(\mathbf{H})$ is closed as the preimage of the closed set \mathbf{H} for the continuous map R_λ , and we actually have $\text{Ran}(T - \lambda I) = \mathbf{H}$.

We can show that the spectrum $\sigma(T)$ of an operator is always closed. To see this, we first need the following lemma.

Lemma 2.14. *Let $T \in \mathcal{B}(\mathbf{H})$ be an operator such that $\|T\| < 1$. Then $(I - T)^{-1}$ exists as a bounded linear operator on the whole space \mathbf{H} and*

$$(I - T)^{-1} = \sum_{n=0}^{\infty} T^n \quad (10)$$

where the series converges in the operator norm sense.

Proof. First of all, we note that $\|T^j\| \leq \|T\|^j$ for all $j \in \mathbb{N}$. This can be seen from

$$\|T^j \psi\| \leq \|T\| \|T^{j-1} \psi\| \leq \dots \leq \|T\|^j \|\psi\| \quad (11)$$

where we have used the definition of the norm 2.4. As this is true for all $\psi \in \mathbf{H}$, we must have $\|T^j\| \leq \|T\|^j$. Using this we then see that the partial sums $S_N = \sum_{n=0}^N T^n$ converge to $S = \sum_{n=0}^{\infty} T^n$ as

$$\|S - S_N\| = \left\| \sum_{n=N+1}^{\infty} T^n \right\| \leq \sum_{n=N+1}^{\infty} \|T^n\| \leq \sum_{n=N+1}^{\infty} \|T\|^n \rightarrow 0 \quad (12)$$

when $N \rightarrow \infty$ because $\|T\| < 1$. Thus the series is operator norm convergent. To show that $S = (I - T)^{-1}$, we see that by a direct calculation

$$(I - T)S_N = S_N(I - T) = I - T^{N+1}. \quad (13)$$

When $N \rightarrow \infty$, this converges to the identity operator I , showing that $S = (I - T)^{-1}$. \square

Theorem 2.15 (Closed spectrum). *The resolvent set $\rho(T)$ of an operator T is open; hence the spectrum $\sigma(T)$ is closed.*

Proof. If $\rho(T) = \emptyset$, the resolvent is trivially open. Consider then $\rho(T) \neq \emptyset$ and $\lambda_0 \in \rho(T)$. As $T - \lambda_0 I$ is invertible, we can write

$$T - \lambda I = [I - (\lambda - \lambda_0)(T - \lambda_0 I)^{-1}] (T - \lambda_0 I). \quad (14)$$

The inverse $(T - \lambda_0 I)^{-1} : \text{Ran}(T - \lambda_0 I) \rightarrow \text{Dom}(T)$ is also bounded, and thus we can extend the bounded operator $V_\lambda : \text{Ran}(T - \lambda_0 I) \rightarrow \mathbf{H}$, $V_\lambda = I - (\lambda - \lambda_0)(T - \lambda_0 I)^{-1}$ to the whole space $\overline{\text{Ran}(T - \lambda_0 I)} = \mathbf{H}$ by the BLT theorem 2.7. Let us denote this extension by $\tilde{V}_\lambda : \mathbf{H} \rightarrow \mathbf{H}$. If we choose λ such that $|\lambda - \lambda_0| < \frac{1}{\|(T - \lambda_0 I)^{-1}\|}$, by Lemma 2.14 the operator \tilde{V}_λ has a bounded inverse on the whole space \mathbf{H} , and thus also the operator V_λ has a bounded inverse defined on the space $\text{Ran}(V_\lambda)$. Then the operator $T - \lambda I = V_\lambda(T - \lambda_0 I)$ also has a bounded inverse $(T - \lambda)^{-1} : \text{Ran}(V_\lambda) \rightarrow \text{Dom}(T)$. We must also have $\overline{\text{Ran}(V_\lambda)} = \overline{\text{Ran}(\tilde{V}_\lambda)} = \mathbf{H}$, and thus $\lambda \in \rho(T)$ for all $|\lambda - \lambda_0| < \frac{1}{\|(T - \lambda_0 I)^{-1}\|}$. This proves that $\rho(T)$ is open and hence $\sigma(T) = \mathbb{C} \setminus \rho(T)$ is closed. \square

The spectrum of the operator is also related to its norm, given by the following theorem.

Theorem 2.16. *If $T \in \mathcal{B}(\mathbf{H})$, then its spectrum satisfies the following property*

$$\sup_{\lambda \in \sigma(T)} |\lambda| = \lim_{n \rightarrow \infty} \sqrt[n]{\|T^n\|}. \quad (15)$$

Proof. See [Kreyszig 1978, Theorem 7.5-5]. \square

Numbers in the point spectrum are also called the **eigenvalues** of T . If $\lambda \in \sigma_p(T)$, then $\text{Ker}(T - \lambda I) \neq \{0\}$ and there exists $\psi \in \mathbf{H}$ such that $T\psi = \lambda\psi$. Such a vector ψ is called an **eigenvector** with an eigenvalue λ . Conversely, if there exists some $\psi \in \mathbf{H}$ such that $T\psi = \lambda\psi$, then $T - \lambda I$ is not injective and $\lambda \in \sigma_p(T)$. Finite-dimensional operators have only a point spectrum which simplifies their discussion. The distinction between the continuous and residual spectra is not as clear cut, but it turns out that the continuous spectrum is in many cases more relevant. For example, normal operators do not have a residual spectrum but may have a continuous one [Moretti 2017, Proposition 8.7].

2.3 Normal operators

An important class of operators is normal operators.

Definition 2.17 (Self-adjoint, unitary and normal operators). *An operator $T \in \mathcal{B}(\mathbf{H})$ is said to be:*

1. **self-adjoint** if $T^* = T$,
2. **unitary** if T is bijective and $T^* = T^{-1}$,
3. **normal** if $TT^* = T^*T$.

Note that self-adjoint and unitary operators are special cases of normal operators. The usefulness of normal operators is that the spectral theorem can be applied to them: in the finite-dimensional case, this is given the fact that normal matrices are exactly the ones that can be unitarily diagonalizable. Self-adjoint operators are in general very common, as in a certain sense they correspond to “real-valued” operators. This will become more apparent in Section 4. One reason why unitary operators are important is that they keep the inner product invariant: $\langle U\psi, U\phi \rangle = \langle \psi, \phi \rangle$ for all $\psi, \phi \in \mathbf{H}$ when U is a unitary operator. For example, changing the basis of a vector space orthogonally corresponds to a unitary operator.

Normal and self-adjoint operators can also be defined in the unbounded case, but then one has to be careful with the domains of the operators. Essentially, the equivalences in Definition 2.17 also mean that the domains of the operators agree. This is generally not the case, which is why we make the following distinction for operators that are seemingly self-adjoint.

Definition 2.18 (Unbounded self-adjoint operator). *An unbounded operator A on \mathbf{H} is **symmetric** if*

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle \quad (16)$$

*for all $\phi, \psi \in \text{Dom}(A)$. The operator A is **self-adjoint** if it is symmetric and $\text{Dom}(A^*) = \text{Dom}(A)$. Finally, A is **essentially self-adjoint** if it is closable and its closure A^{cl} is self-adjoint.*

The difference between symmetric and self-adjoint operators is in the domain of the adjoint operator A^* . We always have $\text{Dom}(A) \subset \text{Dom}(A^*)$, but it is also possible that $\text{Dom}(A^*)$ is strictly larger than $\text{Dom}(A)$. It turns out that in this case the spectral properties of the operator might vastly differ from those of self-adjoint operators. For example, the spectrum $\sigma(A)$ might also contain complex numbers outside the real line which is not possible for self-adjoint operators as we will prove shortly [Hall 2013, Section 9.6]. For this reason, it is the self-adjoint operators that are more interesting in many cases instead of the symmetric ones, and the spectral theorem considered in this work is for self-adjoint operators. The spectral theorem also works for essentially self-adjoint operators, as we can simply consider their closure instead which is self-adjoint. The requirement of the closure being self-adjoint is reasonable in the sense that self-adjoint operators are always closed (see [Hall 2013, 9.8]). Note that (essentially) self-adjoint operators are also the ones that correspond to observables in quantum mechanics, where they are usually called Hermitian operators.

It should also be noted that in general it is not easy to prove that a symmetric operator is also self-adjoint. For example, a sum of self-adjoint operators might not be self-adjoint [Hall 2013, Section 9.10]. Some theorems for proving the self-adjointness of an operator can be found in [Hall 2013, Section 9] and [Moretti 2017, Section 5].

Self-adjoint and unitary operators have the following spectral properties.

Theorem 2.19. *Let \mathbf{H} be a Hilbert space.*

1. *If A is self-adjoint on \mathbf{H} (but not necessarily bounded, nor defined on the whole \mathbf{H} in general):*

- (a) $\sigma(A) \subset \mathbb{R}$
- (b) $\sigma_r(A) = \emptyset$

2. If $U \in \mathcal{B}(\mathbf{H})$ is unitary:

- (a) $\sigma(U)$ is a subset of the complex unit circle $S^1 = \{\lambda \in \mathbb{C} : |\lambda| = 1\}$.
- (b) $\sigma_r(U) = \emptyset$

Proof. Let $A \in \mathbf{H}$ be self-adjoint, and consider $\lambda = \mu + i\nu$ with $\mu, \nu \in \mathbb{R}$ and $\nu \neq 0$. We wish to show that $\lambda \in \rho(A)$. By a direct calculation, we see that

$$\begin{aligned} \langle (A - \lambda I)\psi, (A - \lambda I)\psi \rangle &= \langle (A - \mu I)\psi, (A - \mu I)\psi \rangle + \nu^2 \langle \psi, \psi \rangle \\ &\quad - i\nu [\langle (A - \mu I)\psi, \psi \rangle - \langle \psi, (A - \mu I)\psi \rangle] \\ &= \langle (A - \mu I)\psi, (A - \mu I)\psi \rangle + \nu^2 \langle \psi, \psi \rangle \end{aligned} \quad (17)$$

for all $\psi \in \text{Dom}(A)$. In other words,

$$\|(A - \lambda I)\psi\|^2 \geq \nu^2 \|\psi\|^2 \quad (18)$$

and thus $\text{Ker}(A - \lambda I) = \{0\}$. A similar argument shows that also $\text{Ker}(A - \bar{\lambda}I) = \{0\}$. Thus, there exists an inverse $(A - \lambda I)^{-1} : \text{Ran}(A - \lambda I) \rightarrow \mathbf{H}$ which is also bounded by

$$\|(A - \lambda I)^{-1}\|^2 \leq \frac{1}{\nu^2}. \quad (19)$$

To show that also $\overline{\text{Ran}(A - \lambda I)} = \mathbf{H}$, consider $\psi \in \overline{\text{Ran}(A - \lambda I)}^\perp \cap \text{Dom}(A)$. Then

$$0 = \langle \psi, (A - \lambda I)\phi \rangle = \langle (A - \bar{\lambda}I)\psi, \phi \rangle \quad (20)$$

for all $\phi \in \text{Dom}(A)$. As $\text{Dom}(A)$ is dense in \mathbf{H} we must have $\psi \in \text{Ker}(A - \bar{\lambda}I) = \{0\}$ which shows that $\overline{\text{Ran}(A - \lambda I)} = \mathbf{H}$. All of this means that $\lambda = \mu + i\nu \in \rho(A)$ when $\nu \neq 0$, meaning that $\sigma(A) \subset \mathbb{R}$.

To show that $\sigma_r(A) = \emptyset$, consider $\lambda \in \sigma(A) \setminus \sigma_p(A)$. This means that $A - \lambda I$ is injective. We can repeat the previous argument to show that $\overline{\text{Ran}(A - \lambda I)} = \mathbf{H}$. This means that $\lambda \notin \sigma_r(A)$ and hence the residual spectrum must be empty.

Consider then a unitary operator $U \in \mathcal{B}(\mathbf{H})$. Because

$$\|U\psi\| = \|U^*\psi\| = \|\psi\| \quad (21)$$

for all $\psi \in \mathbf{H}$, we have $\|U\| = \|U^*\| = 1$. We can then use Theorem 2.14 to show that if $|\lambda| > 1$ the operator $U - \lambda I$ has the inverse $(U - \lambda I)^{-1} : \mathbf{H} \rightarrow \mathbf{H}$,

$$(U - \lambda I)^{-1} = -\frac{1}{\lambda} \left(I - \frac{1}{\lambda} U \right)^{-1} = -\frac{1}{\lambda} \sum_{n=0}^{\infty} \left(\frac{1}{\lambda} U \right)^n, \quad (22)$$

and if $|\lambda| < 1$ then the inverse is given by

$$(U - \lambda I)^{-1} = U^*(I - \lambda U^*)^{-1} = U^* \sum_{n=0}^{\infty} (\lambda U^*)^n. \quad (23)$$

These values of λ then cannot be part of the spectrum and thus $\sigma(U) \subset S^1$.

Proving $\sigma_r(U) = \emptyset$ goes in a similar way as the self-adjoint case. Let $\lambda \in \sigma(U) \setminus \sigma_p(U)$, which means that $U - \lambda I$ is injective. Let $\psi \in \overline{\text{Ran}(U - \lambda I)}^\perp$ so that for all $\phi \in \mathbf{H}$ we have

$$0 = \langle \psi, (U - \lambda I)\phi \rangle = \langle (U^* - \bar{\lambda}I)\psi, \phi \rangle. \quad (24)$$

Thus $U^*\psi = \bar{\lambda}\psi$, which can also be written as $U\psi = \lambda\psi$ by noting that $U^* = U^{-1}$ and $\bar{\lambda} = \lambda^{-1}$ for $\lambda \in \sigma(U) \subset S^1$. But $U - \lambda I$ is injective, so we must have $\psi \in \{0\}$ which proves that $\overline{\text{Ran}(U - \lambda I)} = \mathbf{H}$. Hence $\lambda \notin \sigma_r(U)$, which means that $\sigma_r(U) = \emptyset$. \square

3 Projection-valued measure

In this section, we will go through the notion of a **projection-valued measure** that can be used to present the spectral theorem in a very general form. As the name implies, a projection-valued measure is a generalization of the notion of a measure where, instead of having values in the real numbers, the values of the measure are projection operators to subspaces of the original Hilbert space.

The need for a projection-valued measure can be motivated by first considering the spectral theorem for finite-dimensional operators $T : \mathbf{H} \rightarrow \mathbf{H}$. Then, provided that the operator T is normal, the finite-dimensional spectral theorem states that the operator can be written as the sum

$$T = \sum_i \lambda_i \mathbf{e}_i \mathbf{e}_{\lambda_i}^\dagger, \quad (25)$$

where λ_i is the i th eigenvalue and \mathbf{e}_i the corresponding eigenvector. This allows us to interpret $T\psi$ in the following way: each term in the sum can be thought of as first projecting the vector ψ onto the eigenspace and then multiplying by the corresponding eigenvalue. The problem with this approach is that it does not generalize directly to infinite-dimensional Hilbert spaces, as the existence of eigenvectors for normal operators is no longer guaranteed. Instead of writing the operator in terms of the eigenvectors, it is better to think of the terms $\mathbf{e}_i \mathbf{e}_{\lambda_i}^\dagger$ as projections to subspaces of the Hilbert space that stay invariant under T . This notion *does* generalize to infinite dimensions with the help of projection-valued measures. For example, the finite-dimensional case can then be written as

$$T = \int_{\sigma(T)} \lambda d\mu^T(\lambda) \quad (26)$$

where $\sigma(T)$ is the spectrum of the operator T and $\mu^T : \sigma(T) \rightarrow \mathcal{B}(\mathbf{H})$ is the projection-valued measure defined as

$$\mu^T(E) = \sum_{\lambda \in E} P_\lambda \quad (27)$$

with the projection operators $P_\lambda = \mathbf{e}_\lambda \mathbf{e}_\lambda^\dagger$. In the infinite-dimensional case, the projection-valued measure cannot be written in such a simple form, and the proof

of the spectral theorem boils down to finding a projection-valued measure μ^T such that Equation (26) is satisfied.

3.1 Measure and integration theory

Understanding projection-valued measures requires some familiarity with measure theory. For this reason, we briefly go through the basic definitions and most important theorems that will be needed later. First, we need the notion of a σ -algebra which defines a suitable collection of subsets for which we can define a measure.

Definition 3.1 (σ -algebra). *A collection of subsets Ω of set X is a σ -algebra provided that the following properties are satisfied.*

1. $\emptyset, X \in \Omega$.
2. $\mathcal{A} \in \Omega$ implies $X \setminus \mathcal{A} \in \Omega$.
3. If $\mathcal{A}_k \in \Omega$ for all $k = 1, 2, \dots$, then $\cup_{k=1}^{\infty} \mathcal{A}_k \in \Omega$.
4. If $\mathcal{A}_k \in \Omega$ for all $k = 1, 2, \dots$, then $\cap_{k=1}^{\infty} \mathcal{A}_k \in \Omega$.

The space X with a σ -algebra Ω is denoted by (X, Ω) .

An important case of a σ -algebra is the **Borel σ -algebra** which is the smallest σ -algebra containing the open sets of X . Sets contained in the Borel σ -algebra are called **Borel sets**. The notion of a Borel set will be useful in this work, as the projection-valued measure in the spectral theorem will be defined on the Borel σ -algebra of \mathbb{C} .

Definition 3.2 (Measure). *Let X be a set and Ω a σ -algebra over X . A set function μ from Ω to the extended real number line $[-\infty, \infty]$ is called a **measure** if it satisfies the following properties:*

1. (Non-negativity) For all $E \in \Omega$, we have $\mu(E) \geq 0$.
2. (Null empty set) $\mu(\emptyset) = 0$.
3. (Countable additivity) For all countable collections $\{E_k\}_{k=1}^{\infty}$ of pairwise disjoint sets in Ω , we have $\mu(\cup_{k=1}^{\infty} E_k) = \sum_{k=1}^{\infty} \mu(E_k)$.

A property of a function $f : X \rightarrow Y$ is said to be true **almost everywhere** (or a.e.) with respect to a measure μ if it is true for all $x \in X$ except in a subset $E \subset X$ with measure zero, i.e. $\mu(E) = 0$.

The purpose of these definitions is to allow a general notion of integration, called **Lebesgue integration**. Not all functions are integrable, and first we have to consider which functions we can even consider. These are called **measurable functions**.

Definition 3.3 (Measurable function). *Let (X_1, Ω_1) and (X_2, Ω_2) be two spaces with σ -algebras. A mapping $f : X_1 \rightarrow X_2$ is called measurable with respect to the pair (Ω_1, Ω_2) if $f^{-1}(B) \in \Omega_1$ for all $B \in \Omega_2$.*

For example, all continuous functions are measurable when the σ -algebras are Borel σ -algebras. Another example of measurable functions is that of **simple functions** which are used to define the Lebesgue integral.

Definition 3.4 (Simple function). *Let Ω be a σ -algebra over X . A simple function $f : X \rightarrow \mathbb{R}$ is a function that assumes only finitely many values, that is, it can be written as the finite sum $f = \sum_{i=1}^n c_i 1_{E_i}$ where $c_i \in \mathbb{R}$ and $E_i \in \Omega$. Here $1_E : X \rightarrow \{0, 1\}$ denotes an **indicator function**:*

$$1_E(x) = \begin{cases} 1 & \text{if } x \in E \\ 0 & \text{if } x \notin E \end{cases}. \quad (28)$$

Definition 3.5 (Integration of simple functions). *Let μ be a measure on a σ -algebra Ω over X and $f : X \rightarrow \mathbb{R}$, $f = \sum_{i=1}^n c_i 1_{E_i}$ a non-negative simple function. The integral of f with respect to the measure μ is defined as $\int_X f \, d\mu = \sum_{i=1}^n c_i \mu(E_i)$.*

For a general simple function f , we can divide it into negative and non-negative parts $f = f^+ - f^-$ where

$$f^+(x) = \begin{cases} f(x) & \text{if } f(x) \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad f^-(x) = \begin{cases} -f(x) & \text{if } f(x) < 0 \\ 0 & \text{otherwise} \end{cases}. \quad (29)$$

The integral is then defined as $\int_X f \, d\mu = \int_X f^+ \, d\mu - \int_X f^- \, d\mu$.

With simple functions, it is now possible to define integration for general measurable functions.

Definition 3.6 (Integration of measurable functions). *Let $f : X \rightarrow \mathbb{R}$ be a measurable function and $f(x) \geq 0$ μ -a.e. Define*

$$\int_X f \, d\mu = \sup \left\{ \int_X \phi \, d\mu : \phi \geq 0 \text{ is a simple function and } \phi(x) \leq f(x) \text{ } \mu\text{-a.e.} \right\}. \quad (30)$$

*The function f is **integrable** if this quantity is finite.*

In the general case of a signed function we shall call f Lebesgue integrable with respect to μ if both functions f^+ and f^- are integrable. Then we set

$$\int_X f \, d\mu = \int_X f^+ \, d\mu - \int_X f^- \, d\mu. \quad (31)$$

For complex functions $f : X \rightarrow \mathbb{C}$, f is integrable if both its real and complex parts are integrable, and the integral is defined as the sum

$$\int_X f \, d\mu = \int_X \operatorname{Re} f \, d\mu + i \int_X \operatorname{Im} f \, d\mu. \quad (32)$$

Lebesgue integration is continuous in regard to taking limits of function sequences under certain conditions. One important case needed in this work is the **dominated convergence**.

Theorem 3.7 (Dominated convergence theorem). *Assume $g \geq 0$ is μ -integrable and the functions f, f_k are μ -measurable for all $k \in \mathbb{N}$. Suppose $f_k \rightarrow f$ μ -a.e. as $k \rightarrow \infty$, and $|f_k| \leq g$ for all $k \in \mathbb{N}$. Then*

$$\lim_{k \rightarrow \infty} \int |f_k - f| d\mu = 0 \quad (33)$$

which also implies

$$\lim_{k \rightarrow \infty} \int f_k d\mu = \int f d\mu. \quad (34)$$

Proof. See [Evans and Gariepy 2015, Theorem 1.19]. \square

The following property of Lebesgue integration will also turn out to be useful in this work, which can be understood as a change of variables.

Theorem 3.8 (Change of variables). *Let μ be a measure on X and f a μ -measurable function $X \rightarrow Y$. A function g on Y is integrable with respect to the measure $\mu \circ f^{-1}$ precisely when the function $g \circ f$ is integrable with respect to μ . In addition, one has*

$$\int_Y g d(\mu \circ f^{-1}) = \int_X g \circ f d\mu. \quad (35)$$

Proof. See [Bogachev 2007, Theorem 3.6.1]. \square

We will sometimes denote $\int_X f(\lambda) d\mu(\lambda) = \int_X f d\mu$ to clarify that the function defined on X . Also, if the measure $\mu_X : X \rightarrow [0, \infty]$ is defined only on the subset X of some larger space Y , we extend it to the space Y by $\mu_Y : Y \rightarrow [0, \infty]$, $\mu_Y(E) = \mu_X(E \cap X)$ where $E \subset Y$.

3.2 Properties of a projection-valued measure

A projection-valued measure is defined as a map that assigns an orthogonal projection for each set in the σ -algebra. Orthogonal projections are operators that essentially divide a Hilbert space to a vector space and its orthogonal complement.

Theorem 3.9 (Orthogonal projection). *For any closed subspace $X \subset \mathbf{H}$, there is a unique bounded operator P such that $P = I$ on X and $P = 0$ on the orthogonal complement X^\perp . This operator is called the **orthogonal projection** onto X and it satisfies $P^2 = P$ and $P^* = P$.*

Conversely, if P is any bounded operator on \mathbf{H} satisfying $P^2 = P$ and $P^ = P$, then P is the orthogonal projection onto a closed subspace X , where $X = \text{Ran}(P)$.*

Proof. See [Kreyszig 1978, Theorem 9.5-1]. \square

Definition 3.10 (Projection-valued measure). *Let X be a set and Ω a σ -algebra in X . A map $\mu : \Omega \rightarrow \mathcal{B}(\mathbf{H})$ is called a **projection-valued measure** if the following properties are satisfied.*

1. For each $E \in \Omega$, $\mu(E)$ is an orthogonal projection.
2. $\mu(\emptyset) = 0$ and $\mu(X) = I$.
3. If $E_1, E_2, E_3 \dots$ in Ω are disjoint, then for all $v \in \mathbf{H}$ we have

$$\mu \left(\bigcup_{j=1}^{\infty} E_j \right) v = \sum_{j=1}^{\infty} \mu(E_j)v, \quad (36)$$

where the convergence of the sum is in the norm topology on \mathbf{H} .

4. For all $E_1, E_2 \in \Omega$ we have $\mu(E_1 \cap E_2) = \mu(E_1)\mu(E_2)$.

The general idea of the projection-valued measure is that disjoint subsets of X are mapped to orthogonal subspaces of the Hilbert space \mathbf{H} . An example of a projection-valued measure is the mapping $\mu^T(E) = \sum_{\lambda \in E} P_\lambda$ discussed earlier, where T is a finite-dimensional normal matrix and P_λ projections to the eigenspaces corresponding to the eigenvectors λ . For example, in the case of the identity matrix $T = I$ we have

$$\mu^I(E) = \begin{cases} I & \text{if } 1 \in E \\ 0 & \text{otherwise.} \end{cases} \quad (37)$$

A projection-valued measure can be used to define an ordinary measure.

Theorem 3.11. *Let Ω be a σ -algebra in a set X and let $\mu : \Omega \rightarrow \mathcal{B}(\mathbf{H})$ be a projection-valued measure. Then for all $\psi \in \mathbf{H}$ the map $\mu_\psi : \Omega \rightarrow \mathbb{R}$,*

$$\mu_\psi(E) = \langle \psi, \mu(E)\psi \rangle, \quad (38)$$

defines a measure.

Proof. By using the properties of the projection-valued measure, one can check that the map μ_ψ satisfies the properties of the measure in Definition 3.2. \square

We will next prove some properties of the projection-valued measure. To do this we need the notion of a bounded quadratic form.

Definition 3.12 (Quadratic form). *A **quadratic form** on a Hilbert space \mathbf{H} is a map $Q : \mathbf{H} \rightarrow \mathbb{C}$ with the following properties.*

1. $Q(\lambda\psi) = |\lambda|^2 Q(\psi)$ for all $\psi \in \mathbf{H}$ and $\lambda \in \mathbb{C}$.
2. The map $L : \mathbf{H} \times \mathbf{H} \rightarrow \mathbb{C}$,

$$L(\phi, \psi) = \frac{1}{2}[Q(\phi + \psi) - Q(\phi) - Q(\psi)] - \frac{i}{2}[Q(\phi + i\psi) - Q(\phi) - Q(i\psi)], \quad (39)$$

is sesquilinear.

Furthermore, a quadratic form Q is **bounded** if there exists a constant C such that $|Q(\phi)| \leq C\|\phi\|^2$.

The quadratic form Q is essentially a generalization of the notion of a norm, and the corresponding sesquilinear form L is the generalization of the inner product associated with the norm. Note that we can also write the quadratic form in terms of the sesquilinear form, $Q(\psi) = L(\psi, \psi)$. Given an operator T the sesquilinear form $L(\phi, \psi) = \langle \phi, T\psi \rangle$ defines a quadratic form $Q(\psi) = \langle \psi, T\psi \rangle$ and vice versa. This especially means that the operator $\mu_\psi(E)$ in Theorem 3.11 is a (bounded) quadratic form when it is considered as a function of ψ .

Theorem 3.13. *If Q is a bounded quadratic form on \mathbf{H} , there is a unique $T \in \mathcal{B}(\mathbf{H})$ such that $Q(\psi) = \langle \psi, T\psi \rangle$ for all $\psi \in \mathbf{H}$. If $Q(\psi)$ belongs to \mathbb{R} for all $\psi \in \mathbf{H}$, then the operator T is self-adjoint.*

Proof. We wish to use the Riesz representation theorem 2.6 to find the required operator T . First we note that if Q is bounded, then also the associated sesquilinear map L is bounded as

$$\begin{aligned} |L(\phi, \psi)| &= \|\phi\| \|\psi\| \left| L\left(\frac{\phi}{\|\phi\|}, \frac{\psi}{\|\psi\|}\right) \right| \\ &\leq \|\phi\| \|\psi\| \left\{ \frac{1}{2} \left| Q\left(\frac{\phi}{\|\phi\|} + \frac{\psi}{\|\psi\|}\right) \right| + \frac{1}{2} \left| Q\left(\frac{\phi}{\|\phi\|} + i\frac{\psi}{\|\psi\|}\right) \right| \right. \\ &\quad \left. + \left| Q\left(\frac{\phi}{\|\phi\|}\right) \right| + \left| Q\left(\frac{\psi}{\|\psi\|}\right) \right| \right\} \\ &\leq C \|\phi\| \|\psi\| \end{aligned} \quad (40)$$

for some constant $C \geq 0$. The linear functional $\mathcal{L}_\phi(\psi) = L(\phi, \psi)$ is then also bounded, and the Riesz representation theorem asserts that there exists a unique $\chi \in \mathbf{H}$ such that $\langle \chi, \psi \rangle = \mathcal{L}_\phi(\psi)$ for all $\psi \in \mathbf{H}$. Furthermore, $\|\chi\| \leq C\|\phi\|$. This χ depends on ϕ , and let us denote this dependence by a mapping $B\phi = \chi$. From the sesquilinearity of L it follows that the map B is linear, and B is also bounded as $\|B\phi\| \leq C\|\phi\|$. As B is a bounded operator defined on \mathbf{H} , it has an adjoint operator $T = B^*$ defined also on \mathbf{H} . This allows us to write $L(\phi, \psi) = \langle B\phi, \psi \rangle = \langle \phi, T\psi \rangle$, giving us $Q(\psi) = \langle \psi, T\psi \rangle$ as was required. This operator is also unique: if we have $L(\phi, \psi) = \langle \phi, T\psi \rangle = \langle \phi, T'\psi \rangle$ for all $\phi, \psi \in \mathbf{H}$, then $T = T'$.

If $Q(\psi)$ is real for all $\psi \in \mathbf{H}$, then

$$\begin{aligned} \overline{L(\psi, \phi)} &= -i \overline{L(i\psi, \phi)} \\ &= -\frac{i}{2} [Q(\phi + i\psi) - Q(\phi) - Q(i\psi)] + \frac{1}{2} [Q(i\phi + i\psi) - Q(i\phi) - Q(i\psi)] = L(\phi, \psi). \end{aligned} \quad (41)$$

This means that $\langle T\phi, \psi \rangle = \overline{\langle \psi, T\phi \rangle} = \overline{L(\psi, \phi)} = L(\phi, \psi) = \langle \phi, T\psi \rangle$ for all $\phi, \psi \in \mathbf{H}$, meaning that T is self-adjoint. \square

Theorem 3.14 (Operator-valued integral). *Let Ω be a σ -algebra in a set X and let $\mu : \Omega \rightarrow \mathcal{B}(\mathbf{H})$ be a projection-valued measure. Then there exists a unique linear*

map, denoted $f \mapsto \int_X f \, d\mu$, from the space of bounded, measurable, complex-valued functions on Ω into $\mathcal{B}(\mathbf{H})$ with the property that

$$\left\langle \psi, \left(\int_X f \, d\mu \right) \psi \right\rangle = \int_X f \, d\mu_\psi \quad (42)$$

for all f and all $\psi \in \mathbf{H}$, where μ_ψ is given by $\mu_\psi(E) = \langle \psi, \mu(E)\psi \rangle$. This integral has the following additional properties.

1. For all $E \in \Omega$, we have

$$\int_X 1_E \, d\mu = \mu(E). \quad (43)$$

In particular, the integral of the constant function 1 is the identity operator I .

2. For all f , we have

$$\left\| \int_X f \, d\mu \right\| \leq \|f\|_\infty \quad (44)$$

where $\|f\|_\infty = \sup_{\lambda \in X} |f(\lambda)|$ is the sup norm of f .

3. Integration is multiplicative: For all f and g , we have

$$\int_X fg \, d\mu = \left(\int_X f \, d\mu \right) \left(\int_X g \, d\mu \right). \quad (45)$$

4. For all f , we have

$$\int_X \bar{f} \, d\mu = \left(\int_X f \, d\mu \right)^* \quad (46)$$

In particular, if f is real-valued, then $\int_X f \, d\mu$ is self-adjoint.

5. If the sequence of bounded measurable functions $\{f_n\}_{n \in \mathbb{N}}$ is bounded and converges to $f : X \rightarrow \mathbb{C}$ pointwise, the integral of f in the projection-valued measure μ exists and equals

$$\int_X f \, d\mu = \lim_{n \rightarrow \infty} \int_X f_n \, d\mu. \quad (47)$$

The limit is taken in the strong operator norm sense.

Proof. First we need to understand how to even define an integral over the projection-valued measure, i.e. how to define the map $f \mapsto \int_X f \, d\mu$. We do this by first considering the map $Q_f : \mathbf{H} \rightarrow \mathbb{C}$, $Q_f(\psi) = \int_X f \, d\mu_\psi$, where μ_ψ is the measure given in Theorem 3.11.

As the measure μ_ψ is a bounded quadratic form, a simple calculation shows that Q_f is also a bounded quadratic form when f is a bounded, measurable function on Ω . To prove this, let us first consider the case of simple functions $f = \sum_{i=1}^n c_i 1_{E_i}$. Then $Q_f(\psi) = \sum_{i=1}^n c_i \mu_\psi(E_i)$ and it is straightforward to show that the properties of a quadratic form are satisfied. Furthermore, Q_f is bounded, as $|Q_f(\psi)| \leq \|f\|_\infty \mu_\psi(X) = \|f\|_\infty \|\psi\|^2$. Passing the integration from simple functions to bounded

measurable functions by Definition 3.6, one can show that the mapping Q_f satisfies the properties of a bounded quadratic form also in the case of bounded measurable functions f .

As Q_f is a bounded quadratic form, Theorem 3.13 then says that there exists a unique operator A_f such that $Q_f(\psi) = \langle \psi, A_f \psi \rangle$ for all $\psi \in \mathbf{H}$. This allows us to *define* integration with respect to the projection-valued measure by setting $\int_X f \, d\mu = A_f$. We are then left with proving the additional properties of the operator-valued integration.

To prove Point 1, consider $f = 1_E$. Then $Q_f(\psi) = \int_X 1_E \, d\mu_\psi = \mu_\psi(E) = \langle \psi, \mu(E)\psi \rangle$, and by the uniqueness of A_f we find $\int_X 1_E \, d\mu = \mu(E)$.

For Point 3, we note that for indicator functions we have

$$\begin{aligned} \left(\int_X 1_{E_1} \, d\mu \right) \left(\int_X 1_{E_2} \, d\mu \right) &= \mu(E_1)\mu(E_2) = \mu(E_1 \cap E_2) = \int_X 1_{E_1 \cap E_2} \, d\mu \\ &= \int_X 1_{E_1} 1_{E_2} \, d\mu. \end{aligned} \quad (48)$$

A direct calculation then shows that this also holds for simple functions, and by taking limits from simple functions we can prove this for bounded measurable functions.

Point 4 follows from the identity

$$\begin{aligned} Q_{\bar{f}}(\psi) &= \left\langle \psi, \left(\int_X \bar{f} \, d\mu \right) \psi \right\rangle = \int_X \bar{f} \, d\mu_\psi = \overline{\left(\int_X f \, d\mu_\psi \right)} \\ &= \overline{\left\langle \psi, \left(\int_X f \, d\mu \right) \psi \right\rangle} = \left\langle \left(\int_X f \, d\mu \right) \psi, \psi \right\rangle = \left\langle \psi, \left(\int_X f \, d\mu \right)^* \psi \right\rangle. \end{aligned} \quad (49)$$

The uniqueness of the operator corresponding to $Q_{\bar{f}}$ asserts that we must have $\int_X \bar{f} \, d\mu = \left(\int_X f \, d\mu \right)^*$.

To prove Point 2, we can use Points 3 and 4. For all $\psi \in \mathbf{H}$ we have

$$\begin{aligned} &\left| \left\langle \left(\int_X f \, d\mu \right) \psi, \left(\int_X f \, d\mu \right) \psi \right\rangle \right| = \left| \left\langle \psi, \left(\int_X f \, d\mu \right)^* \left(\int_X f \, d\mu \right) \psi \right\rangle \right| \\ &= \left| \left\langle \psi, \left(\int_X |f|^2 \, d\mu \right) \psi \right\rangle \right| = \left| \int_X |f|^2 \, d\mu_\psi \right| \leq \sup_{\lambda \in X} (|f(\lambda)|^2) \mu_\psi(X) \\ &= \left(\sup_{\lambda \in X} |f(\lambda)| \right)^2 \|\psi\|^2, \end{aligned} \quad (50)$$

and therefore $\left\| \int_X f \, d\mu \right\| \leq \sup_{\lambda \in X} |f(\lambda)|$.

Finally, for Point 5, the function f is measurable as the limit of measurable functions. It is also bounded by the same constant K that bounds the sequence $\{f_n\}_{n \in \mathbb{N}}$. For all $\psi \in \mathbf{H}$ we then have

$$\left\| \left(\int_X f \, d\mu - \int_X f_n \, d\mu \right) \psi \right\|^2 = \int |f - f_n|^2 \, d\mu_\psi. \quad (51)$$

We have $|f - f_n|^2 \rightarrow 0$ pointwise and these functions are bounded by $|f - f_n|^2 \leq (|f| + |f_n|)^2 \leq 4K^2$. Thus, the assumptions of the dominated convergence theorem 3.7 are satisfied, and we have

$$\lim_{n \rightarrow \infty} \int f_n \, d\mu_\psi = \int f \, d\mu_\psi. \quad (52)$$

This is true for all $\psi \in \mathbf{H}$, which proves that the limit is strong operator convergent. \square

Points 1, 2, 4, and 5 are extensions of similar properties for ordinary measures. Point 3, multiplicativity of operator-valued integration, is perhaps surprising when compared to integration with respect to ordinary measures as very few measures satisfy this property. For projection-valued measures this essentially follows from the projective nature of μ , $\mu(E)^2 = \mu(E)$. The multiplicativity of operator-valued integration is a very useful property that will play an important role in proving many of the theorems in this work.

Operator-valued integration can also be extended to unbounded measurable functions f , with the restriction that the operator $\int_X f \, d\mu$ is then only defined in a subspace $W_f \subset \mathbf{H}$ of elements $\psi \in W_f$ for which the integral $\int_X f \, d\mu_\psi$ is finite. This is made precise by the following theorem.

Theorem 3.15. *Suppose μ is a projection-valued measure on (X, Ω) with values in $\mathcal{B}(\mathbf{H})$ and $f : \Omega \rightarrow \mathbb{C}$ is a measurable function (not necessarily bounded). Define a subspace W_f of \mathbf{H} by*

$$W_f = \left\{ \psi \in \mathbf{H} : \int_X |f|^2 \, d\mu_\psi < \infty \right\}. \quad (53)$$

Then there exists a unique unbounded operator on \mathbf{H} with domain W_f , denoted by $\int_X f \, d\mu$, with the property that

$$\left\langle \psi, \left(\int_X f \, d\mu \right) \psi \right\rangle = \int_X f \, d\mu_\psi \quad (54)$$

for all ψ in W_f . This operator satisfies

$$\left\langle \left(\int_X f \, d\mu \right) \psi, \left(\int_X f \, d\mu \right) \psi \right\rangle = \int_X |f|^2 \, d\mu_\psi \quad (55)$$

for all $\psi \in W_f$.

Proof. The proof goes by finding the operator associated with the quadratic form $Q_f(\psi) = \int_X f \, d\mu_\psi$. This can be done in a similar way to Theorem 3.13, even though now the quadratic form Q_f is not necessarily bounded. For details, see [Hall 2013, Proposition 10.1]. \square

These theorems then define what is meant by operator-valued integration. This definition, however, is very abstract and not explicitly constructive. An equivalent definition of operator-valued integration, reminiscent of a Lebesgue integral, is given by approximating the integral of a general measurable function by simple functions. This can be made precise by the following definition [Moretti 2017, Definition 8.49].

Definition 3.16 (Operator-valued integration, second form). *Suppose μ is a projection-valued measure on (X, Ω) with values in $\mathcal{B}(\mathbf{H})$. Let us denote the vector space of simple functions $f : X \rightarrow \mathbb{C}$, $f = \sum_{i=1}^n c_i 1_{E_i}$, equipped with the sup norm $\|\cdot\|_\infty$ by $S(X)$. The integral of simple functions, $\mathcal{I} : S(X) \rightarrow \mathcal{B}(\mathbf{H})$, is defined as $\mathcal{I}(f) = \int_X f \, d\mu = \sum_{i=1}^n c_i \mu(E_i)$.*

As the map \mathcal{I} is a bounded operator and the space of simple functions $S(X)$ is dense in the Banach space of bounded measurable functions $M_b(X)$, we can use Theorem 2.7 to extend the integral \mathcal{I} to bounded measurable functions. This extension $\tilde{\mathcal{I}} : M_b(X) \rightarrow \mathcal{B}(\mathbf{H})$ is unique and defines the operator-valued integration of bounded measurable functions: $\tilde{\mathcal{I}}(f) = \int_X f \, d\mu$.

There is also a third way to understand operator-valued integration [Bogachev and Smolyanov 2020, Proposition 7.9.3].

Definition 3.17 (Operator-valued integration, third form). *Let Ω be a σ -algebra over X , μ a projection-valued measure on (X, Ω) and $f : X \rightarrow \mathbb{C}$ a bounded measurable function. For every n , one can partition X into disjoint parts $X_{n,1} \dots X_{n,n} \in \Omega$ such that for any choice of points $x_{n,k} \in X_{n,k}$ the sums $\sum_{k=1}^n f(x_{n,k}) \mu(\Omega_{n,k})$ will converge to $\int_X f \, d\mu$ in the operator norm.*

The caveat in this definition, however, is that in general one cannot choose the sets $X_{n,k}$ arbitrarily. For example, if the integration is over $X = [a, b] \subset \mathbb{R}$ and one chooses $X_{n,k}$ as a partition of the interval $[a, b]$, this definition is an extension of Riemann integration to projection-valued measures, and thus such a choice for the sets $X_{n,k}$ works only for Riemann-integrable functions. For general measurable functions, one can choose $X_{n,k} = f^{-1}(E_{n,k})$ with sets $E_{n,k}$ that partition the complex plane into smaller regions as $n \rightarrow \infty$.

4 Spectral theorem for bounded self-adjoint operators

Before considering the spectral theorem for a general self-adjoint operator, it is easier to consider the bounded case first. There are two main reasons for this. First, the bounded case is simpler, as one does not need to worry about the domain of the operator and its adjoint: the BLT theorem 2.7 guarantees that they can be extended to the whole Hilbert space \mathbf{H} . Second, the spectral theorem in the bounded case can be used to prove the theorem for general, possibly unbounded, self-adjoint operators with little effort.

The main idea of the proof is to find the projection-valued measure μ^A that satisfies the spectral theorem. This is done by defining the functional calculus of the operator

$A \in \mathcal{B}(\mathbf{H})$, that is, defining the operator $f(A)$ for Borel-measurable functions f . The reason we need this is that the required projection-valued measure can be written as $\mu^A = 1_E(A)$, where $1_E(A)$ is given by the functional calculus of the operator A . It turns out that defining the functional calculus for measurable functions is quite tricky, but this is required as indicator functions are not even continuous. Defining the functional calculus for continuous functions is a little easier and is the first step before broadening the definition to measurable functions. Finally, having found the correct projection-valued measure, the spectral theorem follows quite directly.

4.1 Proof of the spectral theorem

Lemma 4.1 (Spectral mapping theorem). *For all $A \in \mathcal{B}(\mathbf{H})$ and all polynomials p , we have*

$$\sigma(p(A)) = p(\sigma(A)). \quad (56)$$

Proof. If p is a constant polynomial, the theorem is trivial. Hence, we can assume that the degree of p is at least one.

Let us first show that $\sigma(p(A)) \subset p(\sigma(A))$. Consider $\lambda \in \sigma(p(A))$. By the fundamental theorem of algebra, we can write $p(x) - \lambda = a(x - x_1) \dots (x - x_n)$ where x_i are the zeros of $p(x) - \lambda$. It is clear then that the operator $p(A) - \lambda I$ can be written as

$$p(A) - \lambda I = a(A - x_1 I) \dots (A - x_n I). \quad (57)$$

If $x_i \in \rho(A)$ for all i , the operator $p(A) - \lambda I$ would have a bounded inverse $(p(A) - \lambda I)^{-1} = a^{-1}(A - x_1 I)^{-1} \dots (A - x_n I)^{-1}$. As $\lambda \in \sigma(p(A))$, this is not possible, and thus $x_i \in \sigma(A)$ for some i . On the other hand, $p(x_i) = \lambda$ and thus $\lambda \in p(\sigma(A))$, which proves this part of the theorem.

Let us then show that $p(\sigma(A)) \subset \sigma(p(A))$. Consider $\lambda \in \sigma(A)$, and we wish to show that then $p(\lambda) \in \sigma(p(A))$. Using again the fundamental theorem of algebra, we can write

$$p(x) - p(\lambda) = (x - \lambda)q(x) \quad (58)$$

where q is some polynomial. The corresponding identity in the operator case can be written as

$$p(A) - p(\lambda)I = (A - \lambda I)q(A). \quad (59)$$

As $\lambda \in \sigma(A)$, the operator $A - \lambda I$ does not have a bounded inverse and so does not $p(A) - p(\lambda)I$. This shows that $p(\lambda) \in \sigma(p(A))$, which proves the final part of the theorem. □

Before defining the functional calculus for continuous functions, we need the following lemmas.

Lemma 4.2 (Weierstrass approximation theorem). *The polynomials with real coefficients are dense in the space of continuous real-valued functions on X , $\mathcal{C}(X; \mathbb{R})$, where $X \subset \mathbb{R}$ is compact and the norm is defined by the sup norm $\|f\|_\infty$.*

Proof. See [Folland 1999, Section 4.7]. □

Lemma 4.3. *If $A \in \mathcal{B}(\mathbf{H})$ is self-adjoint we have*

$$\|A\| = \sup_{\lambda \in \sigma(A)} |\lambda|. \quad (60)$$

Proof. Let us first show that $\|A^2\| = \|A\|^2$ when $A \in \mathcal{B}(\mathbf{H})$ and A is self-adjoint. By the Cauchy-Schwarz inequality

$$|\langle \chi, \psi \rangle|^2 \leq \|\chi\|^2 \|\psi\|^2, \quad (61)$$

we see that for all $\psi \in \mathbf{H}$ the equality

$$\sup_{\|\chi\|=1} |\langle \chi, \psi \rangle|^2 = \|\psi\|^2 \quad (62)$$

holds. For $\|\psi\| = 1$, this gives us

$$\begin{aligned} \|A^2\psi\|^2 &= \sup_{\|\chi\|=1} |\langle \chi, A^2\psi \rangle|^2 = \sup_{\|\chi\|=1} |\langle A\chi, A\psi \rangle|^2 = \left(\sup_{\|\chi\|=1} |\langle A\chi, A\psi \rangle| \right)^2 \\ &\geq (\|A\psi\|^2)^2 = \|A\psi\|^4 \end{aligned} \quad (63)$$

and thus $\|A^2\| \geq \|A\|^2$. On the other hand, in proving Lemma 2.14 we showed that $\|A^2\| \leq \|A\|^2$. Together these imply

$$\|A^2\| = \|A\|^2, \quad (64)$$

and a repeated use of this equation shows that $\|A^{2^n}\| = \|A\|^{2^n}$.

We can now use Theorem 2.16, which tells us that

$$\sup_{\lambda \in \sigma(A)} |\lambda| = \lim_{n \rightarrow \infty} \sqrt[n]{\|A^n\|} = \lim_{n \rightarrow \infty} \sqrt[2^n]{\|A^{2^n}\|} = \lim_{n \rightarrow \infty} \sqrt[2^n]{\|A\|^{2^n}} = \|A\| \quad (65)$$

which was to be proven. □

Theorem 4.4 (Functional calculus). *Suppose $A \in \mathcal{B}(\mathbf{H})$ is self-adjoint. Then there exists a unique bounded linear map from $\mathcal{C}(\sigma(A); \mathbb{R})$ into $\mathcal{B}(\mathbf{H})$, denoted by $f \mapsto f(A)$, such that when $f(\lambda) = \lambda^m$, we have $f(A) = A^m$. The map $f \mapsto f(A)$, $f \in \mathcal{C}(\sigma(A); \mathbb{R})$, is called the (real-valued) **functional calculus** for A .*

Proof. The idea is to show that the mapping $\mathcal{F} : \mathcal{P}(\sigma(A); \mathbb{R}) \rightarrow \mathcal{B}(\mathbf{H}), p \mapsto p(A)$ of the functional calculus is bounded as an operator from the space of real polynomials $\mathcal{P}(\sigma(A); \mathbb{R})$ to operators in the Hilbert space. Thus, we can use the BLT theorem 2.7 to extend it uniquely to the space $\overline{\mathcal{P}(\sigma(A); \mathbb{R})}$. The Weierstrass approximation theorem 4.2 then shows that this is the vector space of continuous functions $\mathcal{C}(\sigma(A); \mathbb{R})$.

We note that

$$\|\mathcal{F}(p)\| = \|p(A)\| = \sup_{\lambda \in \sigma(p(A))} |\lambda| = \sup_{\lambda \in p(\sigma(A))} |\lambda| = \|p\|_\infty \quad (66)$$

where we used Theorems 4.1 and 4.3 as $p(A)$ is a self-adjoint operator. This shows that the functional calculus mapping is bounded (with norm 1), and thus the BLT theorem can be used to extend the functional calculus to $\mathcal{C}(\sigma(A); \mathbb{R})$ uniquely. \square

With the existence and uniqueness of the functional calculus proven, the notation $f(A)$ is from now on to be understood as defined by mapping the function $f \in \mathcal{C}(\sigma(A); \mathbb{R})$ by the functional calculus corresponding to a self-adjoint operator $A \in \mathcal{B}(\mathbf{H})$. The functional calculus satisfies the following properties.

Theorem 4.5. *If $A \in \mathcal{B}(\mathbf{H})$ is self-adjoint, the (real-valued) continuous functional calculus for A , mapping $\mathcal{C}(\sigma(A); \mathbb{R})$ into $\mathcal{B}(\mathbf{H})$, has the following properties.*

1. *Multiplicativity: For all $f, g \in \mathcal{C}(\sigma(A); \mathbb{R})$, we have*

$$(fg)(A) = f(A)g(A), \quad (67)$$

where fg denotes the pointwise product of f and g .

2. *Self-adjointness: For all $f \in \mathcal{C}(\sigma(A); \mathbb{R})$, the operator $f(A)$ is self-adjoint.*
3. *Non-negativity: For all $f \in \mathcal{C}(\sigma(A); \mathbb{R})$, if f is non-negative, then $f(A)$ is a non-negative operator.*
4. *Norm and spectrum properties: For all $f \in \mathcal{C}(\sigma(A); \mathbb{R})$, we have*

$$\|f(A)\| = \sup_{\lambda \in \sigma(A)} |f(\lambda)| \quad (68)$$

and

$$\sigma(f(A)) = \{f(\lambda) : \lambda \in \sigma(A)\}. \quad (69)$$

Proof. For Point 1, first note that the product $fg \in \mathcal{C}(\sigma(A); \mathbb{R})$ if $f, g \in \mathcal{C}(\sigma(A); \mathbb{R})$. If f and g are polynomials, this property is true, and by the continuity of the functional calculus the multiplicativity then is also extended to the space $\mathcal{C}(\sigma(A); \mathbb{R})$.

The first part of Point 4, $\|f(A)\| = \sup_{\lambda \in \sigma(A)} |f(\lambda)|$, is essentially shown in proving Theorem 4.4, as one can extend this property from polynomials to functions in $\mathcal{C}(\sigma(A); \mathbb{R})$ by taking limits. To show the second part $\sigma(f(A)) = \{f(\lambda) : \lambda \in \sigma(A)\}$, let us first consider $\lambda_0 \notin \{f(\lambda) : \lambda \in \sigma(A)\}$. Then the function $g(\lambda) = 1/(f(\lambda) - \lambda_0)$ is continuous on $\sigma(A)$, and the operator $g(A)$ is the inverse of $f(A) - \lambda_0 I$. This means that $\lambda_0 \notin \sigma(f(A))$, and thus $\sigma(f(A)) \subset \{f(\lambda) : \lambda \in \sigma(A)\}$.

For the direction $\{f(\lambda) : \lambda \in \sigma(A)\} \subset \sigma(f(A))$, consider $\lambda_0 = f(\mu)$ for some $\mu \in \sigma(A)$. The idea then is that we can find a sequence of polynomials $(p_n)_{n \in \mathbb{N}}$ that converges to f in sup norm. By the spectral mapping theorem 4.1, the operator

$p_n(A) - p_n(\mu)I$ is not invertible, and by taking the limit $n \rightarrow \infty$ it can be shown that also $f(A) - f(\mu)I$ is not invertible, proving this side of the theorem. For details, see [Hall 2013, Proposition 8.4].

Point 2 can also be proven in a similar way to Points 1 and 4, as $p(A)$ is self-adjoint for all polynomials p . By continuity of the functional calculus we then have

$$\langle f(A)\psi, \phi \rangle = \langle \psi, f(A)\phi \rangle \quad (70)$$

for all $\psi, \phi \in \mathbf{H}$. Note that $f(A)$ is also defined in the whole Hilbert space \mathbf{H} , as by Point 4 it is bounded.

Non-negativity in Point 3 means that $\langle \psi, f(A)\psi \rangle \geq 0$ for all $\psi \in \mathbf{H}$. This follows from the fact that if $f \in \mathcal{C}(\sigma(A); \mathbb{R})$ is non-negative, then there exists $g \in \mathcal{C}(\sigma(A); \mathbb{R})$ such that $f = g^2$ and $g = \sqrt{f}$ is real-valued. This means that $g(A)$ is self-adjoint by Point 2, and we have

$$\langle \psi, f(A)\psi \rangle = \langle \psi, g(A)^2\psi \rangle = \langle g(A)\psi, g(A)\psi \rangle \geq 0 \quad (71)$$

which proves Point 3. □

We will now go on to define the projection-valued measure associated with the operator A . First, we need the Riesz-Markov-Kakutani representation theorem which allows us to write a linear functional in terms of a unique measure.

Theorem 4.6 (Riesz-Markov-Kakutani representation theorem). *Let X be a compact metric space. Suppose $\Lambda : \mathcal{C}(X; \mathbb{R}) \rightarrow \mathbb{R}$ is a linear functional with the property that $\Lambda(f)$ is non-negative whenever all the values of f are non-negative. Then there exists a unique measure μ on the Borel σ -algebra in X for which*

$$\Lambda(f) = \int_X f \, d\mu \quad (72)$$

for all $f \in \mathcal{C}(X; \mathbb{R})$.

Proof. See [Folland 1999, Theorems 7.2 and 7.8]. □

This, combined with the functional calculus, allows us to find a measure associated with $\langle \psi, A\psi \rangle$.

Corollary 4.7. *Let $A \in \mathcal{B}(\mathbf{H})$ be self-adjoint and $\Lambda_\psi : \mathcal{C}(\sigma(A); \mathbb{R}) \rightarrow \mathbb{R}$ be the linear functional such that $\Lambda_\psi(f) = \langle \psi, f(A)\psi \rangle$. Then there exists a unique measure μ_ψ on the Borel σ -algebra of $\sigma(A)$ such that*

$$\Lambda_\psi(f) = \int_{\sigma(A)} f(\lambda) \, d\mu_\psi(\lambda). \quad (73)$$

Proof. First note that $\sigma(A)$ is compact if A is bounded, and as a subset of \mathbb{R} it is also a metric space. By the non-negativity property of the functional calculus $f(A)$ in Theorem 4.5, the map Λ_ψ satisfies the requirements in Theorem 4.6 and thus the unique measure μ_ψ can be found. □

We can then use the measure μ_ψ to define the integral $\int_{\sigma(A)} f(\lambda) d\mu_\psi(\lambda)$ for general bounded measurable functions f .

Definition 4.8. *If f is a bounded measurable (complex-valued) function on $\sigma(A)$, define a map $Q_f : \mathbf{H} \rightarrow \mathbb{C}$ by the formula*

$$Q_f(\psi) = \int_{\sigma(A)} f(\lambda) d\mu_\psi(\lambda), \quad (74)$$

where μ_ψ is the measure in Theorem 4.7.

Theorem 4.9. *For any bounded measurable function f on $\sigma(A)$, the map Q_f in Definition 4.8 is a bounded quadratic form.*

Proof. See the proof of Theorem 3.14. □

Definition 4.10. *For a bounded measurable function f on $\sigma(A)$, let $f(A)$ be the operator associated with the quadratic form Q_f by Theorem 3.13. This means that $f(A)$ is the unique operator such that*

$$\langle \psi, f(A)\psi \rangle = Q_f(\psi) = \int_{\sigma(A)} f d\mu_\psi \quad (75)$$

for all $\psi \in \mathbf{H}$.

The uniqueness of the operator $f(A)$ in this definition follows from the uniqueness in Theorem 3.13. The operator $f(A)$ agrees with the operator in the functional calculus by the definition of Λ_ψ and Q_f when $f \in \mathcal{C}(\sigma(A); \mathbb{R})$. The power of Definition 4.10 is that it allows us to extend the functional calculus from continuous functions to bounded measurable functions and especially to the indicator functions. From the indicator functions we can then build the projection-valued measure associated with the operator A . Before that, we need the following proposition that simply extends the multiplicativity of the functional calculus to bounded measurable functions:

Theorem 4.11. *For any two bounded measurable functions f and g , we have*

$$(fg)(A) = f(A)g(A). \quad (76)$$

Proof. See [Hall 2013, Proposition 8.9]. □

Theorem 4.12. *Suppose $A \in \mathcal{B}(\mathbf{H})$ is self-adjoint. For any Borel set $E \subset \sigma(A)$, define an operator $\mu^A(E)$ by*

$$\mu^A(E) = 1_E(A), \quad (77)$$

where 1_E is the indicator function, and $1_E(A)$ is given by Definition 4.10. Then μ^A is a projection-valued measure on $\sigma(A)$ and satisfies

$$f(A) = \int_{\sigma(A)} f d\mu^A(\lambda) \quad (78)$$

where $f : \mathbb{R} \rightarrow \mathbb{C}$ is a bounded measurable function and $f(A)$ is defined by the functional calculus of A .

Proof. Let us first prove that μ^A is a projection-valued measure, i.e. it satisfies the four properties in Definition 3.10.

For Point 1, we have to prove that $\mu^A(E)^2 = \mu^A(E)$ and $\mu^A(E)$ is self-adjoint for all $E \subset \sigma(A)$. As $(1_E)^2 = 1_E$, by Theorem 4.11 we have $\mu^A(E)^2 = 1_E(A)1_E(A) = (1_E)^2(A) = 1_E(A) = \mu^A(E)$. The self-adjointness follows from Definition 4.10 and the real-valuedness of the function 1_E .

Point 2 follows from the fact that $1_\emptyset(x) = 0$ and $1_{\sigma(A)}(x) = 1$ for all $x \in \sigma(A)$. Thus, by the definition of functional calculus for polynomials 4.4, we have $\mu^A(\emptyset) = 0$ and $\mu^A(\sigma(A)) = I$.

Point 4 follows from Theorem 4.11, as $\mu^A(E_1 \cap E_2) = 1_{E_1 \cap E_2}(A) = (1_{E_1}1_{E_2})(A) = 1_{E_1}(A)1_{E_2}(A) = \mu^A(E_1)\mu^A(E_2)$.

Finally, to prove Point 3, consider disjoint sets E_i . Let us define $\mu_N^A = \sum_{i=1}^N \mu^A(E_i)$ and $E = \bigcup_{i=1}^\infty E_i$. Let us first consider the convergence of the infinite series $\sum_{i=1}^\infty \mu^A(E_i)$. If the sets E_i are non-empty, the sum $\sum_{i=1}^\infty \mu^A(E_i)$ does not converge in the uniform operator sense, as $\|\sum_{i=1}^n \mu^A(E_i) - \sum_{i=1}^m \mu^A(E_i)\| = 1$ for all $n > m$. It does, however, converge in the strong sense. To see this, we note that

$$\begin{aligned} \lim_{N \rightarrow \infty} \langle \psi, \mu_N^A \psi \rangle &= \lim_{N \rightarrow \infty} \int_{\sigma(A)} \sum_{i=1}^N 1_{E_i} d\mu_\psi = \int_{\sigma(A)} \lim_{N \rightarrow \infty} 1_{\bigcup_{i=1}^N E_i} d\mu_\psi = \int_{\sigma(A)} 1_E d\mu_\psi \\ &= \langle \psi, \mu^A(E) \psi \rangle. \end{aligned} \tag{79}$$

The limit can be taken inside the integral by the dominated convergence theorem 3.7 as $\sum_{i=1}^N 1_{E_i} \leq 1$ for all $N \in \mathbb{N}$, and the third equivalence follows from the pointwise convergence $\lim_{N \rightarrow \infty} \sum_{i=1}^N 1_{E_i}(x) = 1_E(x)$. As μ_N^A and $\mu^A(E)$ are orthogonal projections satisfying $P^2 = P$, from this it follows that $\|\mu_N^A \psi\| \xrightarrow{\text{strong}} \|\mu^A(E) \psi\|$. Thus, we can understand the series $\sum_{i=1}^\infty \mu^A(E_i)$ converging in the strong operator sense, and the limit is given by $\mu^A(E)$. This proves Point 3.

We have then proven that μ^A is a projection-valued measure. Also note that $\langle \psi, \mu^A(E) \psi \rangle = \int_X 1_E d\mu_\psi^A = \mu_\psi^A(E)$, so that the measure μ_ψ^A in Theorem 4.7 agrees with the one used for defining operator-valued integration in Theorem 3.14. This means that for all bounded measurable functions f , the operator $f(A)$ given by the functional calculus can be written as $f(A) = \int_{\sigma(A)} f d\mu^A$. \square

Having found the required projection-valued measure μ^A , we are ready to prove the spectral theorem for bounded self-adjoint operators.

Theorem 4.13 (Spectral theorem for bounded self-adjoint operators). *If $A \in \mathcal{B}(\mathbf{H})$ is self-adjoint, then there exists a unique projection-valued measure μ^A on the Borel σ -algebra in $\sigma(A)$, with values in projections on \mathbf{H} , such that*

$$A = \int_{\sigma(A)} \lambda d\mu^A(\lambda). \tag{80}$$

Proof. The existence of the measure is guaranteed by Theorem 4.12, and also setting $f(\lambda) = \lambda$ we see that Equation (80) is satisfied.

For the uniqueness of the measure μ^A , suppose that there is another projection-valued measure ν^A with the property $A = \int_{\sigma(A)} \lambda d\nu^A(\lambda)$. By Corollary 4.7 the measure μ_ψ^A is unique, so we must have $\mu_\psi^A = \nu_\psi^A$ for all $\psi \in \mathbf{H}$. Operator-valued integration is defined in Theorem 3.14 using the measure μ_ψ and thus $\int_{\sigma(A)} f d\mu^A = \int_{\sigma(A)} f d\nu^A$ for all measurable bounded functions f . For every set E in the Borel σ -algebra of $\sigma(A)$ we see that $\mu^A(E) = \int_{\sigma(A)} 1_E d\mu^A = \int_{\sigma(A)} 1_E d\nu^A = \nu^A(E)$. Therefore the projection-valued measures μ^A and ν^A have to be the same, and the projection-valued measure in the spectral theorem is unique. \square

The spectral theorem allows us to write the functional calculus in terms of operator-valued integration. From now on we will *define* the functional calculus in this way for an operator that can be written in the form of the spectral theorem. The functional calculus defined in this way satisfies the following properties which will be needed later.

Theorem 4.14. *Let T be an operator on \mathbf{H} such that there is a unique projection-valued measure μ^T which satisfies*

$$T = \int_{\sigma(T)} \lambda d\mu^T(\lambda). \quad (81)$$

Then the functional calculus for the operator T is defined as

$$f(T) = \int_{\sigma(T)} f d\mu^T \quad (82)$$

where $f : \sigma(T) \rightarrow \mathbb{C}$ is a measurable function. The functional calculus satisfies the following properties:

1. *For all polynomials p we have*

$$p(f(T)) = (p \circ f)(T) \quad (83)$$

where $p(f(T))$ is defined as the polynomial p of the operator $f(T)$ and $(p \circ f)(T)$ by the functional calculus on the function $p \circ f$.

2. *If $f(T)$ is invertible and the function $g(x) = \frac{1}{f(x)}$ is bounded in $\sigma(T)$, the inverse $f(T)^{-1}$ can be written as*

$$f(T)^{-1} = \int_{\sigma(T)} g d\mu^T. \quad (84)$$

3. *If the function f can be written as a power series $f(\lambda) = \sum_{n=0}^{\infty} c_n \lambda^n$ that is absolutely convergent for all $\lambda \leq k$ and the operator T is bounded with the norm $\|T\| \leq k$, then*

$$f(T) = \sum_{n=0}^{\infty} c_n T^n \quad (85)$$

where the series is norm operator convergent.

4. Let T be bounded and $W \in \mathcal{B}(\mathbf{H})$ an operator that commutes with T , $WT = TW$. If the function f is a bounded measurable function, then W also commutes with $f(T)$.

Proof. First note that operator-valued integration is linear and multiplicative according to Theorem 3.14.

To prove Point 1, let us consider a polynomial $p(x) = \sum_{i=1}^n a_i x^i$. A direct calculation shows that

$$(p \circ f)(T) = \int_{\sigma(T)} \sum_{i=1}^n a_i f^i \, d\mu^T = \sum_{i=1}^n a_i \left(\int_{\sigma(T)} f \, d\mu^T \right)^i = \sum_{i=1}^n a_i f(T)^i = p(f(T)). \quad (86)$$

For Point 2, suppose that the inverse $f(T)^{-1}$ exists and the function $g(x) = \frac{1}{f(x)}$ is measurable. Then we have

$$f(T) \left(\int_{\sigma(T)} g \, d\mu^T \right) = \int_{\sigma(T)} fg \, d\mu^T = \int_{\sigma(T)} d\mu^T = 1 \quad (87)$$

and similarly

$$\left(\int_{\sigma(T)} g \, d\mu^T \right) f(T) = 1. \quad (88)$$

The uniqueness of the inverse proves Point 2.

For Point 3, suppose $f(\lambda) = \sum_{n=0}^{\infty} c_n \lambda^n$ is absolutely convergent for all $|\lambda| \leq k$ and $\|T\| \leq k$. Let us denote $f_N(\lambda) = \sum_{i=1}^N c_n \lambda^n$. Then

$$\begin{aligned} \|f(T) - f_N(T)\| &= \left\| \int_{\sigma(T)} (f - f_N) \, d\mu^T \right\| \leq \sup_{\lambda \in \sigma(T)} |f(\lambda) - f_N(\lambda)| \\ &\leq \sup_{\lambda \in \sigma(T)} \sum_{n=N+1}^{\infty} |c_n| |\lambda|^n \leq \sum_{n=N+1}^{\infty} |c_n| k^n \rightarrow 0 \end{aligned} \quad (89)$$

as $N \rightarrow \infty$ because the series $\sum_{n=0}^{\infty} c_n \lambda^n$ is absolutely convergent for all $|\lambda| \leq k$. This proves Point 3.

For Point 4, see [Hall 2013, 7.16]. It essentially follows from the fact that if $WT = TW$ then all polynomials $p(T)$ commute with W , and by taking limits suitably this is true for all $f \in \mathcal{C}(\sigma(T); \mathbb{R})$. It is then possible to extend this property to all bounded measurable functions f . □

It is important to assume the uniqueness of the projection-valued measure μ^T here for if there were two different projection-valued measures for which Equation (81) holds, it would be possible that the functional calculus depends on the chosen measure. Although we will not prove it here, it turns out that normal operators are the only ones that can be written in the form of Equation (81), and the associated projection-valued measure is unique [van Neerven 2022, Theorem 10.54]. Thus, if an operator can be written in the form of the spectral theorem, the associated projection-valued measure is always unique.

5 Unbounded self-adjoint operators

The purpose of this section is to expand the spectral theorem from bounded self-adjoint operators to the unbounded case. While the form of the spectral theorem is similar, the proof requires a few extra steps that come from the unboundedness of the operators. One also has to be careful when considering the domain of unbounded operators. For example, unbounded self-adjoint operators cannot be defined on the whole Hilbert space, which is a direct consequence of the closed graph theorem 2.12 as self-adjoint operators are also closed [Moretti 2017, Theorem 5.18]. Instead, we will assume that the operators are defined on some dense subset of the Hilbert space.

Fortunately, we can use the spectral theorem for the bounded self-adjoint operators to also prove the unbounded case. The idea is that by choosing a proper mapping we can get a correspondence between unitary and self-adjoint operators which extends to the spectral theorem. We first prove the spectral theorem for unitary operators which can then be used to prove the spectral theorem for unbounded self-adjoint operators. In total, the idea is that we map the spectrum of an unbounded self-adjoint operator A to a compact subset of the real numbers. Essentially, this is done with the function $f : \mathbb{R} \rightarrow [-\pi, \pi]$, $f(x) = 2 \operatorname{arccot}(x)$, and heuristically the idea is that the operator $f(A)$ is a bounded self-adjoint operator for which we can use the spectral theorem 4.13. The problem here is, however, that it is not clear how to even define $f(A)$ when A is unbounded. It turns out that it is easier to divide f into two maps. The first maps the unbounded self-adjoint operator A to a unitary operator U by the Cayley transform, and the second allows us to write $U = \exp(iS)$ where S is a bounded self-adjoint operator. Together, these imply that the unbounded self-adjoint operator A can be written as $A = \cot(\frac{1}{2}S)$ where S is a bounded self-adjoint operator. We will start by showing the existence of the second mapping and also prove the spectral theorem for unitary operators as a consequence.

5.1 Spectral theorem for unitary operators

The spectral theorem for unitary operators follows quite directly from the bounded self-adjoint case. First we need, however, the following lemma.

Lemma 5.1 (Wecken's lemma). *Let W and A be bounded self-adjoint operators on \mathbf{H} . Suppose that $WA = AW$ and $W^2 = A^2$. Let P be the orthogonal projection of \mathbf{H} onto $\operatorname{Ker}(W - A)$. Then:*

1. *If a bounded linear operator commutes with $W - A$, it also commutes with P .*
2. *$W\psi = 0$ implies $P\psi = \psi$ for all $\psi \in \mathbf{H}$.*
3. *We have $W = (2P - I)A$.*

Proof. Let $B \in \mathcal{B}(\mathbf{H})$ be an operator that commutes with $W - A$. This allows us to write

$$0 = B(W - A)P\psi = (W - A)BP\psi \tag{90}$$

and

$$0 = B^*(W - A)P\psi = [(W - A)B]^*P\psi = [B(W - A)]^*P\psi = (W - A)B^*P\psi. \quad (91)$$

This shows that $BP\psi \in \text{Ker}(W - A)$ and $B^*P\psi \in \text{Ker}(W - A)$ for all $\psi \in \mathbf{H}$. Consequently, $PBP = BP$ and $PB^*P = B^*P$, which allows us to write $BP = PBP = (PB^*P)^* = (B^*P)^* = PB$, where we also used the fact that P is self-adjoint as an orthogonal projection. This proves Point 1.

For Point 2, let $\psi \in \mathbf{H}$ be such that $W\psi = 0$. Then

$$\|A\psi\|^2 = \langle A\psi, A\psi \rangle = \langle \psi, A^2\psi \rangle = \langle \psi, W^2\psi \rangle = \langle W\psi, W\psi \rangle = 0 \quad (92)$$

so that $A\psi = 0$. This means that $\psi \in \text{Ker}(W - A)$ and thus $P\psi = \psi$.

Finally, for Point 3, note that $(W - A)(W + A) = W^2 - A^2 = 0$ and thus $(W + A)\psi \in \text{Ker}(W - A)$ for all $\psi \in \mathbf{H}$. This implies

$$(W + A)\psi = P(W + A)\psi = P(W - A + 2A)\psi = 2PA\psi \quad (93)$$

for all $\psi \in \mathbf{H}$, where we used Point 1 to write $P(W - A) = (W - A)P = 0$. Solving for W we have $W = (2P - I)A$ as was required. \square

Theorem 5.2 (Spectral theorem for unitary operators). *Suppose U is a unitary operator on \mathbf{H} . Then there exists a unique projection-valued measure μ^U on $\sigma(U)$ with values in $\mathcal{B}(\mathbf{H})$ such that*

$$\int_{\sigma(U)} \lambda d\mu^U(\lambda) = U. \quad (94)$$

Proof. The main idea of the proof is that we need to find a bounded self-adjoint operator S such that $U = e^{iS} = \cos S + i \sin S$. After that the projection-valued measure can be found using the spectral theorem for bounded self-adjoint operators 4.13.

Let us write $U = V + iW$, where $V = \frac{1}{2}(U + U^*)$ and $W = \frac{1}{2i}(U - U^*)$. The operators V and W are bounded with norms $\|V\|, \|W\| \leq 1$ as

$$\|V\| \leq \frac{1}{2} (\|U\| + \|U^*\|) = 1 \quad (95)$$

and similarly for W . They are also self-adjoint, which is easy to check as $(U \pm U^*)^* = (U^* \pm U)$. This means that the spectra of V and W are closed subsets of $[-1, 1]$. Additionally, a direct calculation shows that

$$V^2 + W^2 = I. \quad (96)$$

The idea is to find the required operator S using V and W . Note that if we were considering just numbers in the complex plane, constructing $s \in (-\pi, \pi]$ using $v = \cos s$ and $w = \sin s$ would work by $s = (2 \times 1_{[0,1]}(w) - 1) \arccos v$. Here the factor in front of $\arccos v$ corrects for the fact that $\arccos(\cos s) = |s|$ instead of s . A

similar idea can be used to construct the operator S with V and W , but the problem is showing that this operator satisfies $V = \cos S$ and $W = \sin S$.

Let us denote $g : [-1, 1] \rightarrow (-\pi, \pi]$,

$$g(\lambda) = \arccos \lambda. \quad (97)$$

Using the functional calculus for bounded self-adjoint operators 4.4 we are allowed to write $g(V)$. Let us also define the operator

$$A = \sin g(V) \quad (98)$$

which is again defined using the functional calculus for V . Using the integral form of the functional calculus from Theorem 4.12 it is also possible to prove that

$$\begin{aligned} V^2 + A^2 &= \int_{\sigma(V)} (\lambda^2 + \sin^2 g(\lambda)) d\mu^V(\lambda) = \int_{\sigma(V)} (\cos^2 g(\lambda) + \sin^2 g(\lambda)) d\mu^V(\lambda) \\ &= \int_{\sigma(V)} 1 d\mu^V(\lambda) = I \end{aligned} \quad (99)$$

where μ^V is the projection-valued measure from the spectral theorem for the operator V . Comparing this with Equation (96) we see that $A^2 = W^2$. As V commutes with W , by Theorem 4.14 so does also A . Thus the assumptions of Wecken's lemma 5.1 are satisfied and we conclude that

$$W = (2P - I)A. \quad (100)$$

where P is the orthogonal projection to the subspace $\text{Ker}(W - A)$. Note that P commutes with V and $g(V)$ according to Wecken's lemma, as V commutes with $W - A$. The projection P is connected to our schematic idea of writing $S = (2 \times 1_{[0,1]}(W) - 1) \arccos V$ as we could also write $P = 1_{[0,1]}(W)$. This fact is not needed to show this theorem, and it can be shown afterward using the functional calculus for the operator S .

We now proceed to define $S = (2P - I)g(V) = g(V)(2P - I)$ and show that this operator S is self-adjoint, bounded, and satisfies $U = e^{iS}$. The self-adjointness and boundedness follow from the fact that P and V are bounded and self-adjoint and the function g is bounded and real. To show that $V = \cos(S)$ and $W = \sin(S)$, we first note that $S^2 = (2P - I)^2 g(V)^2 = g(V)^2$ as $(2P - I)^2 = 4P^2 - 4P + I = I$. According to Theorem 4.14, we can write the operator e^{iS} as the Maclaurin series

$$\begin{aligned} e^{iS} &= \sum_{n=0}^{\infty} \frac{i^n}{n!} S^n = \sum_{l=0}^{\infty} \frac{i^{2l}}{(2l)!} S^{2l} + \sum_{l=0}^{\infty} \frac{i^{2l+1}}{(2l+1)!} S^{2l+1} \\ &= \sum_{l=0}^{\infty} \frac{i^{2l}}{(2l)!} g(V)^{2l} + (2P - I) \sum_{l=0}^{\infty} \frac{i^{2l+1}}{(2l+1)!} g(V)^{2l+1} \\ &= \cos g(V) + i(2P - I) \sin g(V) = V + iW = U. \end{aligned} \quad (101)$$

Thus, we have found a bounded self-adjoint operator S such that $U = e^{iS}$. Also note that $\|S\| \leq \|g(V)\| \leq \pi$, and thus $\sigma(S) \subset [-\pi, \pi]$.

Using the spectral theorem for S we can now write

$$U = \int_{[-\pi, \pi]} e^{i\lambda} d\mu^S(\lambda). \quad (102)$$

This is not yet in the form of the spectral theorem. We would like to change the integration variable to $\xi = e^{i\lambda}$, but the problem is that this map is not bijective. Let us define $f : [-\pi, \pi] \rightarrow S^1$, $f(\lambda) = e^{i\lambda}$. Note that this is not injective as $f(-\pi) = f(\pi)$, but it allows us to define the projection-valued measure $\mu^U(E) = \mu^S(f^{-1}(E))$ where $E \subset S^1$ is a Borel set. Then we note that

$$U = \int_{[-\pi, \pi]} e^{i\lambda} d\mu^S(\lambda) = \int_{[-\pi, \pi]} f d\mu^S = \int_{S^1} \lambda d\mu^U(\lambda). \quad (103)$$

This integral is defined over S^1 , not $\sigma(U)$. If we can show $\mu^U(S^1 \setminus \sigma(U)) = 0$ then we can restrict the integral to the set $\sigma(U)$ so that we have the form in the spectral theorem. For simplicity, let us define $\mu^U(\mathbb{C} \setminus S^1) = 0$ so that we can write $U = \int_{\mathbb{C}} \lambda d\mu^U(\lambda)$. Consider then some $\lambda_0 \in \rho(U)$. The resolvent $\rho(U)$ is open so $\lambda \in \rho(U)$ for all $\lambda \in B(\lambda_0, \varepsilon)$ for small enough $\varepsilon > 0$, where $B(\lambda_0, \varepsilon)$ is an open ball with a radius ε . The operator $\mu^U(B(\lambda_0, \varepsilon))$ is a projection operator to some subspace $V(\lambda_0, \varepsilon)$, and let us choose $\phi \in V(\lambda_0, \varepsilon)$. Then

$$(U - \lambda_0 I)\phi = (U - \lambda_0 I)\mu^U(B(\lambda_0, \varepsilon))\phi = \int_{B(\lambda_0, \varepsilon)} (\lambda - \lambda_0) d\mu^U(\lambda) \phi \quad (104)$$

so that

$$\|(U - \lambda_0 I)\phi\|^2 \leq \|\phi\|^2 \|\mu^U(B(\lambda_0, \varepsilon))\|^2 \sup_{\lambda \in B(\lambda_0, \varepsilon)} |\lambda - \lambda_0|^2 = \|\phi\|^2 \|\mu^U(B(\lambda_0, \varepsilon))\|^2 \varepsilon^2. \quad (105)$$

If $V(\lambda_0, \varepsilon) \neq \{0\}$, we have $\|\mu^U(B(\lambda_0, \varepsilon))\| = 1$ and we can choose $\phi \neq 0$ so that

$$\|(U - \lambda_0 I)^{-1}\|^2 \geq \frac{\|(U - \lambda_0 I)^{-1}(U - \lambda_0 I)\phi\|^2}{\|(U - \lambda_0 I)\phi\|^2} \geq \frac{\|\phi\|^2}{\|\phi\|^2 \|\mu^U(B(\lambda_0, \varepsilon))\|^2 \varepsilon^2} = \frac{1}{\varepsilon^2}. \quad (106)$$

Note that $(U - \lambda_0 I)\phi \neq 0$ as $U - \lambda_0 I$ is injective. Now if $\mu^U(B(\lambda_0, \varepsilon)) \neq 0$ for all $\varepsilon > 0$, we see that the operator $(U - \lambda_0 I)^{-1}$ is unbounded which contradicts the assumption $\lambda_0 \in \rho(U)$. Thus $\mu^U(B(\lambda_0, \varepsilon)) = 0$ for some $\varepsilon > 0$. This shows that for all $\lambda_0 \in \rho(U)$ there exists a ball $B(\lambda_0, \varepsilon)$ where $\mu^U(B(\lambda_0, \varepsilon)) = 0$, and hence we must have $\mu^U(\rho(U)) = 0$. We can then restrict the integral to the spectrum $\sigma(U)$ and write

$$U = \int_{\sigma(U)} \lambda d\mu^U(\lambda). \quad (107)$$

We are then left to prove the uniqueness of the projection-valued measure μ^U . Suppose that there is another projection-valued measure ν^U such that

$$U = \int_{S^1} \lambda d\nu^U(\lambda). \quad (108)$$

Then we can write the operators V and W as

$$V = \int_{S^1} \frac{1}{2} (\lambda + \bar{\lambda}) d\mu^U(\lambda) = \int_{S^1} \frac{1}{2} (\lambda + \bar{\lambda}) d\nu^U(\lambda), \quad (109)$$

$$W = \int_{S^1} \frac{1}{2i} (\lambda - \bar{\lambda}) d\mu^U(\lambda) = \int_{S^1} \frac{1}{2i} (\lambda - \bar{\lambda}) d\nu^U(\lambda). \quad (110)$$

On the other hand, they are self-adjoint, and thus there are unique projection-valued measures μ^V and μ^W such that

$$V = \int_{[-1,1]} \lambda d\mu^V(\lambda), \quad (111)$$

$$W = \int_{[-1,1]} \lambda d\mu^W(\lambda). \quad (112)$$

By Theorem 3.8 this suggests that

$$\mu^V(E) = \mu^U(f^{-1}(E)) = \nu^U(f^{-1}(E)) \quad (113)$$

and

$$\mu^W(E) = \mu^U(g^{-1}(E)) = \nu^U(g^{-1}(E)) \quad (114)$$

for all Borel sets $E \subset [-1, 1]$, where $f(\lambda) = \frac{1}{2}(\lambda + \bar{\lambda}) = \operatorname{Re} \lambda$ and $g(\lambda) = \frac{1}{2i}(\lambda - \bar{\lambda}) = \operatorname{Im} \lambda$. This is not enough to show that the measures μ^U and ν^U are the same as the functions $f : S^1 \rightarrow [-1, 1]$ and $g : S^1 \rightarrow [-1, 1]$ are not bijections; instead,

$$f^{-1} \circ f(E) = \{\lambda : \lambda \in E \text{ or } \bar{\lambda} \in E\} \quad (115)$$

and

$$g^{-1} \circ g(E) = \{\lambda : \lambda \in E \text{ or } -\bar{\lambda} \in E\}. \quad (116)$$

We note, however, that $[f^{-1} \circ f(E)] \cap [g^{-1} \circ g(E)] = E$ for all $E \subset S^1$, and thus

$$\begin{aligned} \mu^U(E) &= \mu^U([f^{-1} \circ f(E)] \cap [g^{-1} \circ g(E)]) = \mu^U(f^{-1} \circ f(E)) \mu^U(g^{-1} \circ g(E)) \\ &= \nu^U(f^{-1} \circ f(E)) \nu^U(g^{-1} \circ g(E)) = \nu^U([f^{-1} \circ f(E)] \cap [g^{-1} \circ g(E)]) = \nu^U(E). \end{aligned} \quad (117)$$

This proves the uniqueness of the projection-valued measure. □

5.2 Cayley transform

To prove the spectral theorem for unbounded self-adjoint operators we need a function that maps them to unitary operators. This is provided by the **Cayley transform**.

Theorem 5.3 (Cayley transform). *If A is a self-adjoint operator on \mathbf{H} , let U be the operator defined by*

$$U\psi = (A + iI)(A - iI)^{-1}\psi \quad (118)$$

Then the following results hold:

1. The operator U is a unitary operator on \mathbf{H} .
2. The operator $U - I$ is injective.
3. The range of the operator $U - I$ is equal to $\text{Dom}(A)$ and for all $\psi \in \text{Ran}(U - I)$ we have

$$A\psi = i(U + I)(U - I)^{-1}\psi. \quad (119)$$

Proof. As A is self-adjoint, its spectrum is real, and therefore the maps $A + iI : \text{Dom}(A) \rightarrow \mathbf{H}$ and $A - iI : \text{Dom}(A) \rightarrow \mathbf{H}$ are bijective with bounded inverses. Thus the map U is well-defined.

To prove Point 1, we need to show that U is bijective and $U^* = U^{-1}$. As a composition of two bijective maps, it is also bijective. To show $U^* = U^{-1}$ we first note that for any $\psi, \phi \in \text{Dom}(A)$,

$$\langle (A + iI)\psi, (A + iI)\phi \rangle = \langle (A - iI)\psi, (A - iI)\phi \rangle \quad (120)$$

which can be shown by a direct calculation. Thus for any $\xi, \chi \in \mathbf{H}$,

$$\begin{aligned} \langle U\xi, U\chi \rangle &= \langle (A + iI)(A - iI)^{-1}\xi, (A + iI)(A - iI)^{-1}\chi \rangle \\ &= \langle (A - iI)(A - iI)^{-1}\xi, (A - iI)(A - iI)^{-1}\chi \rangle = \langle \xi, \chi \rangle \end{aligned} \quad (121)$$

from which we see that $U^*U = UU^* = I$ and hence $U^* = U^{-1}$.

For Point 2, consider $\psi \in \text{Ker}(U - I)$. Then

$$0 = (U - I)\psi = (A + iI)(A - iI)^{-1}\psi - \psi = 2i(A - iI)^{-1}\psi. \quad (122)$$

But $(A - iI)^{-1}$ is injective, so we must have $\psi = 0$ and hence $\text{Ker}(U - I) = \{0\}$ which proves Point 2.

As $U - I = 2i(A - iI)^{-1}$ is injective and $\text{Ran}(U - I) = \text{Ran}((A - iI)^{-1}) = \text{Dom}(A)$, it has an inverse $(U - I)^{-1} : \text{Dom}(A) \rightarrow \mathbf{H}$. For all $\psi \in \text{Dom}(A)$ we then have

$$i(U + I)(U - I)^{-1}\psi = i[2A(A - iI)^{-1}][2i(A - iI)^{-1}]^{-1}\psi = A\psi \quad (123)$$

as was required for Point 3. \square

We can understand how the Cayley transform works by considering complex numbers instead of operators. The corresponding map $C : \mathbb{C} \setminus \{i\} \rightarrow \mathbb{C}$,

$$C(x) = \frac{x + i}{x - i}, \quad (124)$$

is a Möbius transform that maps the real line to the unit circle, which means that in the Cayley transform the spectrum of a self-adjoint operator is mapped onto the spectrum of a unitary operator. The inverse Möbius transformation, $C^{-1} : \mathbb{C} \setminus \{1\} \rightarrow \mathbb{C}$,

$$C^{-1}(x) = i\frac{x + 1}{x - 1}, \quad (125)$$

maps the unit circle to the real line. It should be noted here that if U is a unitary operator such that the inverse $(U - I)^{-1}$ exists, the operator $C^{-1}(U)$ defined with the functional calculus coincides with the inverse Cayley transform

$$C^{-1}(U) = i(U + I)(U - I)^{-1} \quad (126)$$

according to Theorem 4.14.

5.3 Spectral theorem for unbounded self-adjoint operators

With all of these prerequisite results, proving the spectral theorem for unbounded self-adjoint operators is very straightforward. Let us first prove the existence of the required projection-valued measure.

Theorem 5.4. *Let A be a self-adjoint operator on \mathbf{H} . Define a projection-valued measure μ^A on \mathbb{R} by*

$$\mu^A(E) = \mu^U(C(E)), \quad (127)$$

where C is the map given by Equation (124) and μ^U is the projection-valued measure from the spectral theorem for the unitary operator $U = (A + iI)(A - iI)^{-1}$. Then

$$A = \int_{\sigma(A)} \lambda d\mu^A(\lambda). \quad (128)$$

Proof. Let us define measures $\mu_\psi^U(E) = \langle \psi, \mu^U(E)\psi \rangle$ and $\mu_\psi^A(E) = \langle \psi, \mu^U(C(E))\psi \rangle$. Using the change of variables $\lambda = C^{-1}(\xi)$ according to Theorem 3.8, we can write

$$\begin{aligned} \int_{\mathbb{R}} \lambda d\mu_\psi^A(\lambda) &= \int_{S^1 \setminus \{1\}} C^{-1}(\xi) d\mu_\psi^A(C^{-1}(\xi)) = \int_{S^1 \setminus \{1\}} C^{-1}(\xi) d\mu_\psi^U(\xi) \\ &= \langle \psi, C^{-1}(U)\psi \rangle = \langle \psi, A\psi \rangle. \end{aligned} \quad (129)$$

As this holds for all $\psi \in \mathbf{H}$, we must have

$$A = \int_{\mathbb{R}} \lambda d\mu^A. \quad (130)$$

The integral can be restricted to $\sigma(A)$ by the same argument as when proving the spectral theorem for unitary operators 5.2. □

We are finally ready to prove the main theorem of this thesis:

Theorem 5.5 (Spectral theorem for self-adjoint operators). *Suppose A is a self-adjoint operator on \mathbf{H} . Then there is a unique projection-valued measure μ^A on $\sigma(A)$ with values in $\mathcal{B}(\mathbf{H})$ such that*

$$\int_{\sigma(A)} \lambda d\mu^A(\lambda) = A. \quad (131)$$

Proof. The existence of the projection-valued measure μ^A is given by Theorem 5.4 so we only have to prove the uniqueness.

Suppose that there is another projection-valued measure ν^A such that $\int_{\sigma(A)} \lambda d\nu^A(A) = A$. Then we can show that the unitary operator given by the Cayley transform, $U = (A + iI)(A - iI)^{-1}$, can be written as

$$U = C(A) = \int_{\mathbb{R}} C(\lambda) d\nu_\psi^A(\lambda) = \int_{S^1 \setminus \{1\}} \xi d\nu_\psi^A(C^{-1}(\xi)). \quad (132)$$

On the other hand, we can write

$$U = C(A) = \int_{\mathbb{R}} C(\lambda) d\mu_{\psi}^A(\lambda) = \int_{S^1 \setminus \{1\}} \xi d\mu_{\psi}^A(C^{-1}(\xi)). \quad (133)$$

From the uniqueness of the projection-valued measure for unitary operators, we see that $\nu_{\psi}^A(C^{-1}(E)) = \mu_{\psi}^A(C^{-1}(E))$ for all E in the Borel σ -algebra of $S^1 \setminus \{1\}$. As $C^{-1} : S^1 \setminus \{1\} \rightarrow \mathbb{R}$ is a bijection, this means that we must have $\nu^A = \mu^A$ and thus the projection-valued measure is unique. \square

5.4 Consequences of the spectral theorem

We will now consider a few properties that can be proven with the help of the spectral theorem.

Definition 5.6 (Spectral subspaces). *For a self-adjoint operator A on \mathbf{H} , let μ^A be the associated projection-valued measure, extended to be a measure on \mathbb{R} by setting $\mu^A(\mathbb{R} \setminus \sigma(A)) = 0$. Then for each Borel set $E \subset \mathbb{R}$, define the **spectral subspace** V_E of \mathbf{H} by*

$$V_E = \text{Ran}(\mu^A(E)). \quad (134)$$

Theorem 5.7. *Let A be a self-adjoint operator on \mathbf{H} . Then the spectral subspaces V_E associated with the operator A have the following properties.*

1. *For disjoint sets $E_1, E_2 \subset \mathbb{R}$ the spectral subspaces V_{E_1} and V_{E_2} are orthogonal.*
2. *If E is bounded, the spectral subspace V_E belongs to the domain of A and V_E is invariant under A .*
3. *The spectrum of $A|_{V_E}$ is contained in the closure of E . In particular, if E is bounded, then $A|_{V_E}$ is a bounded operator.*
4. *If E is contained in $(\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$, then for all $\psi \in V_E$ we have*

$$\|(A - \lambda_0 I)\psi\| \leq \varepsilon \|\psi\|. \quad (135)$$

Vectors ψ satisfying this condition are called approximate eigenvectors.

5. *If λ_0 is in the spectrum of A , then for every neighborhood U of λ_0 , we have $V_U \neq \{0\}$, or, equivalently, $\mu^A(U) \neq 0$.*

Proof. For Point 1, consider sets $E_1, E_2 \subset \mathbb{R}$ such that $E_1 \cap E_2 = \emptyset$. Let $\psi_1 \in V_{E_1}$ and $\psi_2 \in V_{E_2}$, which means that there exist $\phi_1, \phi_2 \in \mathbf{H}$ such that $\psi_1 = \mu^A(E_1)\phi_1$ and $\psi_2 = \mu^A(E_2)\phi_2$. Then we have

$$\begin{aligned} \langle \psi_1, \psi_2 \rangle &= \langle \mu^A(E_1)\phi_1, \mu^A(E_2)\phi_2 \rangle = \langle \phi_1, \mu^A(E_1)\mu^A(E_2)\phi_2 \rangle \\ &= \langle \phi_1, \mu^A(E_1 \cap E_2)\phi_2 \rangle = \langle \phi_1, \mu^A(\emptyset)\phi_2 \rangle = 0 \end{aligned} \quad (136)$$

so the spectral subspaces V_{E_1} and V_{E_2} are orthogonal.

For Point 2, it is easy to see from the multiplicativity of the operator-valued integration that $A\mu^A(E) = \int_E \lambda d\mu^A$. The function $f(\lambda) = \lambda$ is bounded on E if E is bounded, and thus the operator $A\mu^A(E)$ is bounded and defined on the whole \mathbf{H} . Any $\psi \in V_E$ can be written as $\psi = \mu^A(E)\phi$ for some $\phi \in \mathbf{H}$, allowing us to write $A\psi = A\mu^A(E)\phi$ which is defined and thus $\psi \in \text{Dom}(A)$. This proves that $V_E \subset \text{Dom}(A)$. Also note that $A\mu^A(E) = \mu^A(E)A\mu^A(E)$, which means that $A\psi = \mu^A(E)A\phi \in V_E$ and thus V_E is invariant under A .

For Point 3, consider $\lambda_0 \notin \overline{E}$. Then the function $g : \mathbb{C} \rightarrow \mathbb{C}$, $g(\lambda) = \frac{1_E(\lambda)}{\lambda - \lambda_0}$ is bounded, and thus the operator $g(A)$ is also bounded and satisfies

$$g(A)(A - \lambda_0 I) = (A - \lambda_0 I)g(A) = 1_E(A) = \mu^A(E). \quad (137)$$

This is the identity operator in the subspace V_E , and thus $(A - \lambda_0 I)|_{V_E}$ has a bounded inverse. This means that $\lambda_0 \notin \sigma(A|_{V_E})$, proving Point 3.

To prove Point 4, suppose that $\psi \in V_E$ where $E \subset (\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$. Then ψ is in the range of $\mu^A(E)$, and

$$(A - \lambda_0 I)\psi = (A - \lambda_0 I)\mu^A(E)\psi. \quad (138)$$

This allows us to write

$$\begin{aligned} \|(A - \lambda_0 I)\psi\|^2 &= \langle (A - \lambda_0 I)\mu^A(E)\psi, (A - \lambda_0 I)\mu^A(E)\psi \rangle \\ &= \left\langle \psi, \int_E (\lambda - \lambda_0)^2 d\mu^A(\lambda) \psi \right\rangle = \int_E (\lambda - \lambda_0)^2 d\mu_\psi^A(\lambda) \\ &\leq \sup_{\lambda \in E} (\lambda - \lambda_0)^2 \times \|\psi\|^2 = \varepsilon^2 \|\psi\|^2 \end{aligned} \quad (139)$$

as was required.

Finally, let us consider Point 5. Let $\lambda_0 \in \sigma(A)$ and assume that there exists $\varepsilon > 0$ such that for $U = (\lambda_0 - \varepsilon, \lambda_0 + \varepsilon)$ we have $\mu^A(U) = 0$. Consider then the bounded function f defined by

$$f(\lambda) = \begin{cases} \frac{1}{\lambda - \lambda_0} & \text{when } |\lambda - \lambda_0| \geq \varepsilon \\ 0 & \text{when } |\lambda - \lambda_0| < \varepsilon. \end{cases} \quad (140)$$

The function $f(\lambda) \times (\lambda - \lambda_0)$ then agrees with the constant function 1 except in the set U . But $\mu^A(U) = 0$ so this agreement is μ_ψ^A -almost everywhere for all $\psi \in \mathbf{H}$ and thus its operator-valued integral agrees with the identity operator, i.e.

$$f(A)(A - \lambda_0 I) = (A - \lambda_0 I)f(A) = I \quad (141)$$

where the operators are defined in $\text{Dom}(A)$. As $\overline{\text{Dom}(A)} = \mathbf{H}$, we must have $\lambda_0 \in \rho(A)$. This is a contradiction with the assumption $\lambda_0 \in \sigma(A)$, proving Point 5. \square

Points 1, 2, and 3 are in a certain sense generalizations of similar properties for operators in finite-dimensional Hilbert spaces, as in that case we can divide the operator into orthogonal eigenspaces corresponding to different eigenvectors. In the general case, we also need to consider the continuous spectrum for which we do not have eigenvectors, but even then we can divide the Hilbert space into orthogonal subspaces corresponding to different subsets of the spectrum.

Point 5 says that the measure assigns non-zero values to sets that contain some λ_0 in the spectrum. The converse of this was actually proven as a part of the spectral theorem unitary operators 5.2, where it was shown that for $\lambda_0 \in \rho(A)$ there exist neighborhoods U with zero measure $\mu^A(U) = 0$.

Point 4 says that even though in general we cannot find eigenvectors for each $\lambda_0 \in \sigma(A)$, we can find vectors that are arbitrarily close to being an eigenvector. One might try to find an actual eigenvector by taking a sequence of vectors ψ_n such that Equation (135) is satisfied for $\varepsilon = \frac{1}{n}$. However, there is no guarantee that such a sequence will converge to an element in the Hilbert space, and indeed it can converge only for values in the point spectrum $\lambda_0 \in \sigma_p(A)$. In Section 6.3 we will consider a somewhat generalized case, in which a different notion of convergence is defined, such that it is possible for the limit of approximate eigenvectors to exist outside the Hilbert space.

6 Applications of the spectral theory in quantum mechanics

Since the formulation of quantum mechanics at the beginning of the 20th century, physicists noticed that understanding functional analysis is crucial for understanding the physical reality at small length scales. In quantum mechanics, physical observables are defined as self-adjoint operators on the Hilbert space describing physical states. Thus, a proper understanding of self-adjoint operators is necessary for quantum mechanics, and it is not surprising that spectral theory plays a central role. In fact, one major motivation for developing spectral theory for unbounded self-adjoint operators came from [von Neumann 1933] when it was realized that quantum mechanics can be written in terms of self-adjoint operators which are generally unbounded. The purpose of this section is to give the reader a brief introduction to how spectral theory is used in relation to quantum physics.

6.1 Introduction to quantum mechanics

The basic assumption of quantum mechanics is that physical systems are given by states $|\Psi\rangle$ which are defined as vectors in a separable Hilbert space. This is a very abstract notion, and usually the Hilbert space is left undefined as separable Hilbert spaces are isomorphic up to the dimension of the space [Moretti 2017, Theorem 3.30]. Perhaps the simplest non-trivial example of a physical state is a system with two possible states, denoted by g and e , which can for example correspond to the *ground*

state and the *excited* state of a particle. The most general form for this state is then

$$|\Psi\rangle = \alpha |g\rangle + \beta |e\rangle \quad (142)$$

where $\alpha, \beta \in \mathbb{C}$, written in Dirac's bra-ket notation. States are also generally normalized to one, as states differing by scalar multiplication are considered to correspond to the same physical state. The norm in this simple case is given by

$$\langle\Psi|\Psi\rangle = |\alpha|^2 \langle g|g\rangle + |\beta|^2 \langle e|e\rangle = |\alpha|^2 + |\beta|^2 = 1. \quad (143)$$

The numbers $|\alpha|^2$ and $|\beta|^2$ then correspond to probabilities for the state to be in the states g and e . This is called the **Born rule** of quantum mechanics.

Different states are related to each other by operators. A very important class of operators is the (essentially) self-adjoint operators, as they correspond to physical quantities that can be measured. Examples of these are position, momentum, energy, angular momentum, and electric charge of a particle, with each having a corresponding self-adjoint operator. The spectral theorem then allows us to study these properties in terms of the spectral representation of the operator. For example, one may ask what is the probability that a state $|\Psi\rangle$ has a physical property A in the set of possible values E when observed. If the property has the corresponding self-adjoint operator \hat{A} , then this probability is given by

$$\langle\Psi|\mu^A(E)|\Psi\rangle = \int_E d\mu_{\Psi}^A = \mu_{\Psi}^A(E) \quad (144)$$

where μ^A is the projection-valued measure associated with the operator \hat{A} . Essentially, this means that the state $|\Psi\rangle$ is projected onto the spectral subspace V_E , and the probability is given by the norm of the projected state. A special case of this is the position operator, where this is usually written in terms of the **wave function** of the state, $\psi : \mathbb{R}^3 \rightarrow \mathbb{C}$, as

$$\langle\Psi|\mu^X(E)|\Psi\rangle = \int_E |\psi(x)|^2 d^3x. \quad (145)$$

The wave function gives the probability density for a particle to be at the position x . Each state has a corresponding wave function, and the inner product between different states is defined as

$$\langle\Phi|\Psi\rangle = \int_{\mathbb{R}^3} \overline{\phi(x)}\psi(x) d^3x. \quad (146)$$

For this quantity to be finite the wave functions then have to belong to the Hilbert space $L^2(\mathbb{R}^3)$.

6.2 Schrödinger equation

Perhaps the most important equation in quantum mechanics is the **Schrödinger equation** which describes the time-evolution of the state:

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle. \quad (147)$$

Here \hat{H} is the **Hamiltonian operator** and \hbar is the reduced Planck constant. In the non-relativistic case, where the particles are moving at velocities much smaller than the speed of light, the single-particle Hamiltonian reads

$$\hat{H} = \frac{1}{2m} \hat{P}^2 + \hat{V} = -\frac{\hbar^2}{2m} \nabla^2 + V(x) \quad (148)$$

where ∇^2 is the Laplace operator, $\hat{V} = V(x)$ is the potential acting on the particle and m is the particle's mass. For physical reasons, the potential is often a real-valued function so that the Hamiltonian operator is symmetric. On the other hand, the Hamiltonian is not necessarily self-adjoint: an example of this is the Hamiltonian with the potential $V(x) = -x^4$ which does not correspond to a physical situation [Hall 2013, Section 9.10]. These cases where the Hamiltonian is not self-adjoint are often pathological or unphysical, which is the reason why we will from now assume that the Hamiltonian \hat{H} is a self-adjoint operator.

The Schrödinger equation (147) is formally solved by

$$|\Psi(t)\rangle = e^{-i\hat{H}t/\hbar} |\Psi(0)\rangle = \int_{E \in \mathbb{R}} d\mu^H(E) e^{-iEt/\hbar} |\Psi(0)\rangle \quad (149)$$

where we used the functional calculus of the Hamiltonian to write the operator $e^{-i\hat{H}t/\hbar}$ in terms of the projection-valued measure $\mu^{\hat{H}}$. The fact that this solves the Schrödinger equation is given by the **Stone's theorem** [Moretti 2017, Theorem 9.33] which essentially states that the derivative of the unitary operator $U_t = e^{-i\hat{H}t/\hbar}$ is well-defined and

$$\frac{d}{dt} U_t = -\frac{i}{\hbar} \hat{H} U_t. \quad (150)$$

The solution (149) to the Schrödinger equation is in practice quite complicated. A simpler form is obtained if one is restricted to solutions that are given as a linear combination of the eigenvectors of the Hamiltonian, i.e. solutions of the form

$$|\Psi(t)\rangle = \sum_{\substack{n \\ E_n \in \sigma_p(\hat{H})}} c_n(t) |\Psi_n\rangle \quad (151)$$

where the states $|\Psi_n\rangle$ satisfy the time-independent Schrödinger equation

$$\hat{H} |\Psi_n\rangle = E_n |\Psi_n\rangle. \quad (152)$$

One can then show that the coefficients have the form $c_n(t) = c_n e^{-iE_n t/\hbar}$ where c_n are constants determined by the initial condition. This reduces solving the Schrödinger equation to finding the eigenvalues and eigenvectors of the Hamiltonian which is a lot simpler than constructing the projection-valued measure μ^H .

It is then important to ask how one should understand the solutions of the Schrödinger equation corresponding to the eigenvectors of the Hamiltonian, as in general the Hamiltonian can also have a non-empty continuous spectrum. The spectrum of the Hamiltonian is dependent on the potential $V(x)$, and hence it should be

possible to study the spectrum from the form of the potential. Perhaps surprisingly, one can often relate the physical situations of bounded and unbounded particles to the simple distinction between **discrete** and **essential** spectra. The discrete spectrum $\sigma_d(\hat{H})$ consists of the isolated points in the spectrum $\sigma(\hat{H})$, and the essential spectrum is the rest of the spectrum $\sigma_{\text{ess}}(\hat{H}) = \sigma(\hat{H}) \setminus \sigma_d(\hat{H})$. Points in the discrete spectrum also correspond to eigenvalues with finite-dimensional eigenspaces [Moretti 2017, Remark 9.15-1]. Bounded and unbounded particles are, roughly speaking, characterized by the energy of the particle. If the energy is less than the bounds of the potential, the particle is considered bounded – this means that it does not have enough energy to escape the potential well.

In the simplest case of an infinitely bounded continuous potential, there are only bounded particles and hence one would expect the Hamiltonian to have only a discrete spectrum. This is indeed the case.

Theorem 6.1 ([Hislop and Sigal 1996, Theorem 10.7]). *Assume that $V \geq 0$, V is continuous and $V(x) \rightarrow \infty$ as $\|x\| \rightarrow \infty$. Then the Hamiltonian \hat{H} has a purely discrete spectrum.*

Another theorem relating bounded particles to the discrete spectrum deals with **Kato potentials**.

Definition 6.2. *A potential function $V(x)$ is called a Kato potential if V is real and $V \in L^2(\mathbb{R}^n) + L^\infty(\mathbb{R}^n)_\varepsilon$, where the ε indicates that for any $\varepsilon > 0$ we can decompose $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^n)$ and $V_2 \in L^\infty(\mathbb{R}^n)$ with $\|V_2\|_\infty < \varepsilon$.*

Theorem 6.3 ([Hislop and Sigal 1996, Corollary 14.10]). *If V is a Kato potential, then $\sigma_{\text{ess}}(\hat{H}) = [0, \infty)$.*

The definition of the Kato potential means that the potential has to approach zero as $\|x\| \rightarrow \infty$, and it also cannot have singularities that are too steep. For example, in the 3-dimensional case the Coulomb potential $V(x) = -\kappa \frac{1}{\|x\|}$ is a Kato potential, but potential $V(x) = -\kappa' \frac{1}{\|x\|^2}$ is not. Particles with the energy $E > 0$ are then unbounded, and Theorem 6.3 states that these correspond to the essential spectrum. These theorems provide some intuition to the physical correspondence between bounded particles and eigenvectors of the Schrödinger equation.

As a concrete example of this distinction between bounded and unbounded particles, consider the one-dimensional bounded potential well

$$V(x) = \begin{cases} -V_0 & \text{if } -a < x < a, \\ 0 & \text{otherwise,} \end{cases} \quad (153)$$

where $V_0 > 0$ is the depth of the well and $a > 0$ its width. Let us simply state the results here; for a more thorough study the reader is referred to [Griffiths 1995, Section 2.6]. For each interval $(-\infty, -a)$, $(-a, a)$, (a, ∞) , the solutions of the time-independent Schrödinger equation $\hat{H}\psi(x) = E\psi(x)$ have to satisfy

$$\psi(x) = \begin{cases} A_1 e^{ix\sqrt{2mE}/\hbar} + B_1 e^{-ix\sqrt{2mE}/\hbar} & \text{if } x < -a, \\ A_2 e^{ix\sqrt{2m(E+V_0)}/\hbar} + B_2 e^{-ix\sqrt{2m(E+V_0)}/\hbar} & \text{if } -a < x < a, \\ A_3 e^{ix\sqrt{2mE}/\hbar} + B_3 e^{-ix\sqrt{2mE}/\hbar} & \text{if } x > a, \end{cases} \quad (154)$$

where A_i and B_i are constants. It turns out that the solutions and their derivatives also have to be continuous, which sets constraints for the solutions at $x = -a$ and $x = a$. We immediately notice that if $E \geq 0$ the solutions do not belong to the Hilbert space $L^2(\mathbb{R}^3)$ unless $A_1 = B_1 = A_2 = B_2 = 0$. Taking into account the continuity requirements, this is only satisfied by the zero function $\Psi(x) = 0$, meaning that the values $E \geq 0$ cannot correspond to eigenvalues. They still belong to the continuous spectrum $\sigma_c(\hat{H})$, as the bounded potential well is a Kato potential and Theorem 6.3 states that $\sigma_{\text{ess}}(\hat{H}) = [0, \infty)$. A similar analysis shows that values $E_n \leq -V_0$ do not yield solutions to the Schrödinger equation, and they also do not correspond to the spectrum of the Hamiltonian. We are then left to consider values $-V_0 < E < 0$. It turns out that these values belong to the spectrum if they satisfy the transcendental equation

$$\tan\left(\frac{a}{\hbar}\sqrt{2m(E+V_0)}\right) = \sqrt{\frac{-E}{E+V_0}} \quad (155)$$

or

$$\cot\left(\frac{a}{\hbar}\sqrt{2m(E+V_0)}\right) = -\sqrt{\frac{-E}{E+V_0}}. \quad (156)$$

These equations are solved by a finite amount of values $E \in (-V_0, 0)$, and they correspond to the point spectrum of the Hamiltonian. Thus, we have found that $\sigma_d(\hat{H}) \subset (-V_0, 0)$ and $\sigma_{\text{ess}}(\hat{H}) = [0, \infty)$, i.e. the bounded states correspond to the discrete spectrum and unbounded to the essential spectrum.

Even if $E > 0$, it is still possible for a function to seemingly satisfy the time-independent Schrödinger equation. For example, in the free-particle case, $V_0 = 0$, these are simply given by

$$\Psi(x) = Ae^{ix\sqrt{2mE}/\hbar} + Be^{-ix\sqrt{2mE}/\hbar} \quad (157)$$

where $E \in (-\infty, \infty)$ and A, B are constants. One can, however, check that these functions are not square integrable, meaning that they do not belong to the Hilbert space $L^2(\mathbb{R})$ and thus do not correspond to eigenvectors of the Schrödinger equation. It is possible to generalize the notion of eigenvectors such that for all values in the spectrum we have a notion similar to the eigenvectors, called generalized eigenvectors. It is then possible to show that the values $E \geq 0$ in the finite potential well admit generalized eigenvectors, whereas the case $E < -V_0$ does not correspond to the spectrum and hence cannot be described in such a way. Generalizing the notion of eigenvectors is the topic of the next section.

6.3 Rigged Hilbert spaces and generalized eigenvectors

A crucial difference between the point spectrum σ_p and the continuous spectrum σ_c is that for the point spectrum we can find eigenvectors of the operator. In the finite-dimensional case, a normal matrix can be described entirely by how it acts on its eigenvectors as given by the finite-dimensional spectral theorem. Writing matrices in terms of their eigenvectors turns out to be a very useful way to study the properties of the matrix and thus one would like to do the same for infinite-dimensional operators.

In general, however, this is not possible as normal operators can have a non-empty continuous spectrum, in which case it is not possible to find corresponding eigenvectors. To extend the notion of an eigenvector to the continuous spectrum, one can define **generalized eigenvectors**. These are objects that in a certain sense satisfy $AF = \lambda F$ for $\lambda \in \sigma_c(A)$. The catch is that these objects do not belong to the Hilbert space \mathbf{H} , as in a sense they have an infinite norm $\|F\| = \infty$. Instead, they can be considered as functionals defined on some dense subspace $\Omega \subset \mathbf{H}$, so that they belong to the dual space Ω^* . This leads to the definition of a **rigged Hilbert space**.

Definition 6.4 (Rigged Hilbert space). *Let \mathbf{H} be a Hilbert space and $\Omega \subset \mathbf{H}$ a dense subspace such that Ω is given a topological vector space structure for which the inclusion map $i : \Omega \rightarrow \mathbf{H}$, $i(\psi) = \psi$, is continuous. The pair (\mathbf{H}, Ω) is called a rigged Hilbert space.*

Essentially, topological vector spaces are vector spaces equipped with topologies that make vector addition and scalar multiplication continuous. See [Trèves 1967, Section 3] for the exact definition. For example, normed spaces are topological vector spaces.

The usefulness of rigged Hilbert spaces is that one can now write the spectral theorem in a form that is closer to the finite-dimensional case where the operator is decomposed into eigenvalues and eigenvectors. In the infinite-dimensional case one has to consider generalized eigenvectors instead.

Definition 6.5 (Generalized eigenvector). *Let A be an operator on a rigged Hilbert space (\mathbf{H}, Ω) which maps the space Ω into itself. A generalized eigenvector of A is a linear functional $F \in \Omega^*$ such that for all $\psi \in \Omega$ the equation*

$$F(A\psi) = \lambda F(\psi) \quad (158)$$

holds. The number $\lambda \in \mathbb{C}$ is the eigenvalue corresponding to the generalized eigenvector F .

Theorem 6.6 (Spectral theorem for self-adjoint operators in rigged Hilbert spaces [Bogolubov et al. 1975, Theorem 1.3]). *A self-adjoint operator in a rigged Hilbert space possesses a complete set of generalized eigenvectors corresponding to real eigenvalues.*

Proof. See [Gel'fand and Vilenkin 1964, Section 1.4]. □

Here the completeness of generalized eigenvectors F_λ , $\lambda \in X$, means that for any vectors $\psi, \phi \in \Omega$ we can write

$$\langle \phi, \psi \rangle = \int_X \overline{F_\lambda(\phi)} F_\lambda(\psi) d\mu(\lambda) \quad (159)$$

where μ is an ordinary measure associated with the generalized eigenvectors F_λ . Note that if the functionals F_λ are bounded, then by the Riesz theorem 2.6 we can find a vector $\xi_\lambda \in \mathbf{H}$ such that $F_\lambda(\psi) = \langle \xi_\lambda, \psi \rangle$. Equation (159) then reduces to

$$\langle \phi, \psi \rangle = \sum_\lambda \frac{1}{\|\xi_\lambda\|^2} \langle \phi, \xi_\lambda \rangle \langle \xi_\lambda, \psi \rangle \quad (160)$$

which can be understood as the completeness of the basis $\{\xi_\lambda\}$.

As a concrete example, consider the one-dimensional momentum operator in quantum mechanics, $\hat{P} = -i\hbar\partial_x$, in the Hilbert space $L^2(\mathbb{R})$. It is a self-adjoint operator with the spectrum $\sigma(\hat{P}) = \sigma_c(\hat{P}) = \mathbb{R}$, $\sigma_p(\hat{P}) = \emptyset$. Thus, it does not have any eigenvectors but with a suitably chosen subset Ω , the Schwartz space [Hall 2013, Definition A.15], it has generalized eigenvectors that form a complete set. These generalized eigenvectors can be written as $\psi_p(x) = e^{ipx/\hbar}$ and they satisfy $\hat{P}\psi_p(x) = p\psi_p(x)$. Note that their norm is infinite with respect to the inner product $\langle f, g \rangle = \int_{\mathbb{R}} f(x)g(x) dx$ and thus they do not belong to $L^2(\mathbb{R})$. They can, however, be constructed from functions in $L^2(\mathbb{R})$ by using approximate eigenvectors. To see this, note that for functions $\psi_p^\varepsilon(x) = \exp\left(\frac{i}{\hbar}px - \frac{1}{\hbar^2}\varepsilon^2x^2\right)$ with $\varepsilon > 0$ we have

$$\left\|(\hat{P} - pI)\psi_p^\varepsilon\right\| = \varepsilon\|\psi_p^\varepsilon\|. \quad (161)$$

These functions converge pointwise $\psi_p^\varepsilon(x) \rightarrow \psi_p(x)$ when $\varepsilon \rightarrow 0$. The functions ψ_p are also complete in the sense that for any $\phi \in \Omega$ we have

$$\phi = \int_{\mathbb{R}} \langle \psi_p, \phi \rangle \psi_p \frac{dp}{2\pi\hbar} = \int_{\mathbb{R}} \tilde{\phi}(p) e^{ipx/\hbar} \frac{dp}{2\pi\hbar} \quad (162)$$

where

$$\tilde{\phi}(p) = \langle \psi_p, \phi \rangle = \int_{\mathbb{R}} e^{-ipx/\hbar} \phi(x) dx \quad (163)$$

is the Fourier transform of ϕ . This allows us to write Equation (159) as

$$\langle \phi, \psi \rangle = \int_{\mathbb{R}} \overline{\phi(x)} \psi(x) dx = \int_{\mathbb{R}} \overline{(\tilde{\phi}(p))} \tilde{\psi}(p) \frac{dp}{2\pi\hbar} \quad (164)$$

which is just Plancherel's theorem from Fourier analysis. Here the functional F_p corresponding to ψ_p has been written as

$$F_p(\phi) = \langle \psi_p, \phi \rangle = \tilde{\phi}(p). \quad (165)$$

There are also other ways to write the completeness that are more common in the physics literature. The completeness can be understood in terms of distributions, as it is possible to show that

$$\langle \psi_p, \psi_q \rangle = 2\pi\hbar\delta(p - q) \quad (166)$$

where $\delta(p - q)$ is the delta distribution that is formally defined on the Schwartz space in terms of the functional

$$\delta_p(\phi) = \tilde{\phi}(p) \equiv \int_{\mathbb{R}} 2\pi\hbar\delta(p - q)\tilde{\phi}(q) \frac{dq}{2\pi\hbar}. \quad (167)$$

In terms of Dirac's bra-ket notation, Equation (166) is often referred as the normalization of the momentum states

$$\langle p|q \rangle = 2\pi\hbar\delta(p - q), \quad (168)$$

and the corresponding completeness relation is written as

$$I = \int_{\mathbb{R}} |p\rangle\langle p| \frac{dp}{2\pi\hbar}. \quad (169)$$

This notation is often very convenient, as operators common in physics have generalized eigenvectors that can be written in a simple form, usually as linear combinations of delta distributions and standard functions. If these generalized eigenvectors – and the associated measure – can be solved, the spectral decomposition of the operator can be written in terms of the generalized eigenvectors, which often simplifies the situation tremendously. As a concrete example, this gives a precise definition for the wave function of the state: in terms of the position eigenstates $|x\rangle$, the wave function of the state $|\Psi\rangle$ is given by

$$\langle x|\Psi\rangle = \psi(x). \quad (170)$$

Thus, generalized eigenvectors allow one to treat states in terms of functions, making calculations easier. This is the reason why quantum mechanics is, often implicitly, defined in terms of rigged Hilbert spaces instead of ordinary ones.

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