9 Spectral measures and Spectral Theorem

9.1 Continuous functional calculus

We start with an important theorem for theoretical quantum mechanics in the n-dimensional case.

Theorem 9.1 (Spectral Theorem 0: Finite-dimensional case)**.** *Let $A \in Mat_n(\mathbb{C})$ be self-adjoint, i.e. $A^* = A$. Then $\exists U$ unitary, D diagonal s.t. $U^*AU = D$, where the columns of U are the normalized eigenvectors of A, and the diagonal entries of D are the corresponding eigenvalues.*

This is a well-known result from linear algebra. Can we extend this into the infinite?

Remark 9.2. Given a self-adjoint operator A and a function f continuous on the spectrum $\sigma(A)$, we'd like to properly define $f(A)$ in order to construct new operators. Let $(p_n)_{n\geq 1}$ be a sequence of polynomials converging uniformly to f. Is the notion

$$f(A) \equiv \lim_{n\to\infty} p_n(A)$$

well-defined? Indeed, Theorem 9.3 tells us, yes.

Theorem 9.3 (Spectral Theorem I: Continuous functional calculus)**.** *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint. Denote $\mathcal{A} \subseteq \mathcal{B}(\mathcal{H})$ to be the algebra*[1] *generated by A (i.e. the smallest closed subalgebra of $\mathcal{B}(\mathcal{H})$ containing A). Then:*

a) The limes $\lim_{n\to\infty} p_n(A)$ exists and does not depend on the choice of appropriate polynomials to approximate f.

b) $\|f(A)\| = \|f\|_\infty \quad \forall f \in C(\sigma(A))$

*c) The map $C(\sigma(A)) \to \mathcal{A}$ given by $f \mapsto f(A)$ is a *-homomorphism, i.e.*

- $(f+g)(A) = f(A) + g(A)$
- $(\alpha f)(A) = \alpha f(A)$
- $(fg)(A) = f(A)g(A)$
- $(f(A))^* = \bar{f}(A)$
- $\chi_{\sigma(A)}(A) = id_{\sigma(A)}$

$\forall f, g \in C(\sigma(A))$, $\alpha \in \mathbb{C}$ where χ denotes the indicator function and id the identity morphism.

Proof. a) Let $(p_n)_{n\geq 1}$ be a sequence of polynomials converging to f uniformly on $\sigma(A)$. Then $(p_n(A))_{n\geq 1}$ a Cauchy sequence in $\mathcal{B}(\mathcal{H})$ by proposition given in the last lecture. Since $\mathcal{B}(\mathcal{H})$ is Banach, it is complete, thus the limit of the Cauchy sequence $f(A)$ exists. Let now $(q_n)_{n\geq 1}$ be another sequence of polynomials converging to f uniformly on $\sigma(A)$. By the same former proposition, $(q_n(A))_{n\geq 1}$ converges to $f(A)$ as well. □

[1] Algebra over a field: A vector space equipped with a bilinear product (e.g. $\mathbb{R}^3$ with the vector product).

While polynomials of operators are always well-defined and relatively easy to compute, general functions with operators as arguments are not. For instance, the concept of the square root of an operator is easy to grasp: it is the operator, if squared (i.e. a two-fold application of itself), returns the original operator back. However, explicit computations turn out to be a nightmare. Luckily, the first Spectral Theorem is here to save the day.

Example 9.4. Let's look at the position operator x on the Hilbert space $[0,1]$. What is its square root? Define the polynomial sequence P_n as follows:

$$P_0 = 0 \quad P_{n+1}(t) = P_n(t) + \frac{1}{2}(t - P_n(t)^2)$$

This sequence is monotonously increasing and converges uniformly to $\sqrt{t}$ $\forall t \in [0,1]$. Thus this is applicable for all operators with a norm less or equal than 1.

9.2 Spectral measures

Remark 9.5. Motivation of spectral measures: Consider $A \in Mat_n(\mathbb{C})$ self-adjoint, with spectral decomposition

$$A = \sum_{\lambda \in \sigma(A)} \lambda P_\lambda$$

Let f continuous on $\sigma(A)$. To calculate $f(A)$ applied to any $v \in \mathbb{C}^n$, consider

$$\langle v, f(A)v \rangle = \sum_{\lambda \in \sigma(A)} f(\lambda) \|P_\lambda v\|^2$$

A constructive way to think about the underlying procedure is to integrate f against the Dirac measure[2] supported on $\sigma(A)$ (with weight at $\lambda \in \sigma(A)$ given by $\|P_\lambda v\|^2$).

To extend this notion towards an infinite-dimensional setting, we need to introduce spectral measures.

Theorem 9.6 (Spectral Theorem II: Existence of spectral measures)**.** *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint. $\forall \phi, \psi \in \mathcal{H}, \exists$ a complex Borel measure $\mu \equiv \mu^A_{\phi,\psi}$ s.t.*

$$\langle \phi, f(A)\psi \rangle = \int_{\sigma(A)} f(\lambda) d\mu(\lambda)$$

$\forall f \in C(\sigma(A))$. In particular, if $\psi = \phi$, then $\mu \equiv \mu^A_\phi \equiv \mu^A_{\phi,\phi}$ a non-negative (regular, real) measure.

[2] $\delta_x(A) = 1_A(x) = \begin{cases} 1, & x \in A \\ 0, & x \notin A \end{cases}$

Proof. Theorem 9.3 implies that $l : C(\sigma(A)) \to \mathbb{C}$ given by $f \mapsto \langle \phi, f(A)\psi \rangle$ defines a bounded, linear functional. By the Riesz-Markov representation theorem 3.19, this indeed implies the existence of such a complex Borel measure μ.
Let now $\psi = \phi$ and $f \in C(\sigma(A))$ positive. Then $\exists! g \in C(\sigma(A))$ s.t. $g^2 = f, g \geq 0$. Then

$$l(f) = \langle \phi, f(A)\phi \rangle = \langle \phi, g^2(A)\phi \rangle = \|g(A)\phi\|^2 \geq 0$$

and thus l a positive functional $\Rightarrow$ μ a non-negative measure. □

The existence of such a measure motivates the following definition.

Definition 9.7. Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint, $\phi, \psi \in \mathcal{H}$. The complex Borel measure $\mu \equiv \mu^A_{\phi,\psi}$ s.t.

$$\langle \phi, f(A)\psi \rangle = \int_{\sigma(A)} f(\lambda) d\mu(\lambda)$$

$\forall f \in C(\sigma(A))$ is called the *spectral measure* of A.

Notation 9.8. If the operator A is clear from the context, we write $\mu^A_{\phi,\psi} \equiv \mu_{\phi,\psi}$ or $\mu^A_{\phi,\phi} \equiv \mu_\phi$ resp.

Remark 9.9. This is another way to characterize $f(A)$: First, fix $\psi \in \mathcal{H}$. If we know $\langle \phi, f(A)\psi \rangle$ for all $\phi \in \mathcal{H}$, then we know $f(A)\psi$. If we know $f(A)\psi$ for all ψ, we know $f(A)$.

Example 9.10. Example of a spectral measure: Let $\mathcal{H} = L^2([0,1], \mu), \phi \in \mathcal{H}$ with $\|\phi\|_2 = 1$ and x the position operator on $\mathcal{H}$. Note that x does not possess any Eigenvalues, however it's spectrum is the entire interval.
If D an operator on $\mathcal{H}$ and

$$D\phi(x) = x\phi(x) \text{ a.e.} \quad \text{then} \quad \sqrt{D}\phi(x) = \sqrt{x}\phi(x) \text{ a.e.}$$

Let $f \in C(\sigma(A))$. Then we get

$$\begin{aligned} \langle \phi, f(D)\phi \rangle &= \int \overline{\phi(x)} f(x)\phi(x) d\mu(x) \\ &= \int_0^1 f(x)|\phi(x)|^2 d\mu(x) = \int_0^1 f(x) d\mu_\phi \end{aligned}$$

Thus we get

$$d\mu_\phi \ll d\mu \quad \frac{d\mu_\phi}{d\mu} = \phi^2$$

Absolutely continuous, probability distribution.

Remark 9.11. Multiplication operator: extend matrix to infinite dimensional

Thanks to Theorem 9.6, we can now compute the norm of resolvent operators less cumbersomely.

Theorem 9.12. *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint, $z \in \rho(A)$. Then*

$$\|R(A,z)\| = \frac{1}{dist(z,\sigma(A))} \equiv \frac{1}{\inf_{\lambda\in\sigma(A)} |z-\lambda|}$$

Proof. "$\leq$": Let $\lambda \in \sigma(A)$ s.t. $\operatorname{dist}(z,\sigma(A)) = |\lambda - z|, \psi$ a unit vector. Then, $\forall \lambda' \in \sigma(A)$,

$$\|R(A,z)\|^2 = \|R(A,z)\psi\|^2 = \int \frac{d\mu_\psi(\lambda')}{|\lambda'-z|^2} \leq \int \frac{d\mu_\psi(\lambda')}{|\lambda-z|^2} = \frac{1}{|\lambda-z|^2} = \frac{1}{\operatorname{dist}(z,\sigma(A))^2}$$

by theorem 9.6.
"$\geq$": is generally true for bounded operators.
Indeed, assume by contradiction that $\|R(A,z)\| > \operatorname{dist}(z,\sigma(A))$. Then $\exists s \in \sigma(A)$ s.t.

$$\|(s-z)\mathbf{1}\| = |s-z| < \|R(A,z)\|^{-1} = \|(A-z)^{-1}\|^{-1}$$

As $(A-z)$ is invertible, this means that by theorem 4.14, $(A-z)+(z-s) = A-s$ is invertible. But this is a contradiction, as $s \in \sigma(A)$ by definition means the opposite. Thus,

$$\|R(A,z)\| \leq \operatorname{dist}(z,\sigma(A)) \implies \|R(A,z)\| \geq \frac{1}{\operatorname{dist}(z,\sigma(A))}$$

Notice how we didn't require A to be self-adjoint, only bounded. □

As we shall see, f needs not to be continuous in order for the notion of spectral measures to make sense, bounded and Borel measurable suffices.

Theorem 9.13. *Let $A \in \mathcal{B}(\mathcal{H})$ self-adjoint, $f \in \mathcal{B}(\sigma(A))$. Then*

$$\langle \phi, f(A)\psi \rangle = \int_{\sigma(A)} f(\lambda) d\mu^A_{\phi,\psi}(\lambda)$$

*defines an element $f(A) \in \mathcal{B}(\mathcal{H})$. In particular, the mapping $\mathcal{B}(\sigma(A)) \to \mathcal{B}(\mathcal{H})$ given by $f \mapsto f(A)$ is a *-homomorphism.*

O joy! We managed to generalize theorem 9.6 and the definition of the spectral measure to a much broader class of functions.

9.3 Equivalence to multiplication operators

Remark 9.14. The spectral theorem is truly versatile and highly useful in applications. Thanks to this, we can frame any self-adjoint operator as a simple multiplication operator. What does this mean?
Again, consider $A \in Mat_n(\mathbb{C})$ self-adjoint. For simplicity we may assume that A has n distinct eigenvalues λ (i.e. the spectrum $\sigma(A)$ is not degenerate) with corresponding normalized eigenvectors e_λ. Consider the space

$$\mathcal{H} = l^2(\sigma(A)) = \{f : \sigma(A) \to \mathbb{C}\}$$

and the map $U : \mathbb{C}^n \to \mathcal{H}$ given by $v \mapsto f(-) \equiv \langle e_-, v\rangle$ (i.e. then $f(\lambda) = \langle e_\lambda, v\rangle$). Applying the spectral theorem to the n-dimensional case yields that U is unitary and

$$(UAU^* g)(\lambda) = \lambda g(\lambda)$$

for $g \in \mathcal{H}$. Note that unitary maps preserve the orthonormality of bases.

$$\begin{tikzcd}
\mathbb{C}^n \arrow[r, "A"] \arrow[d, "U"'] & \mathbb{C}^n \arrow[d, "U"] \\
L^2(\sigma(A)) \arrow[r, "UAU^\dagger"] & L^2(\sigma(A))
\end{tikzcd}$$

To establish the framework for the proof, a definition up front is needed.

Definition 9.15. Let $A \in \mathcal{B}(\mathcal{H})$, $\phi \in \mathcal{H}$. The *cyclic subspace* generated by A and ϕ is the smallest closed subspace of $\mathcal{H}$ containing $A^n\phi$ $\forall n \geq 0$. ϕ is called *cyclic* for A if the corresponding cyclic subspace is all of $\mathcal{H}$.

We are now ready to tackle this application for the infinite-dimensional case.

Theorem 9.16 (Spectral Theorem III: Equivalence to multiplication operators)**.** *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint. Then there exist at most countably many $\phi_n \in \mathcal{H}$ s.t. with $\mu_n \equiv \mu_{\phi_n}$, s.t. there is a unitary map*

$$U : \mathcal{H} \to \bigoplus_n L^2(\mathbb{R}, \mu_n)$$

such that

$$(UAU^* h)_n(E) = Eh_n(E)$$

where we write $h(E) \equiv \{h_n(E)\}_n$ for $h \in \bigoplus_n L^2(\mathbb{R}, \mu)$.

Proof. Let ϕ be cyclic. Define the map U s.t. $U(f(A)\phi) = f$. Since $f(A)\phi = g(A)\phi$ for $f, g \in C(\sigma(A))$ implies $f = g$, U is well-defined on the dense set $C(\sigma(A))$. Furthermore, U preserves norms, with the additional property $(UAU^{-1}f)(E) = Ef(E), \forall f \in C(\sigma(A))$. Thus we can extend the definition of U to the closure of $C(\sigma(A))$, which is $\mathcal{H}$. In the cyclic case,

we can thus conclude.
Let now ϕ arbitrary, not necessarily cyclic. By Zornification, we can decompose $\mathcal{H} = \bigoplus_n \mathcal{H}_n$ where $\forall n \exists \phi_n \in \mathcal{H}$ s.t. $\mathcal{H}_n$ is the cyclic subspace generated by A and ϕ_n. Note that the index set of n is at most countable. Denote $\mu_n \equiv \mu^A_{\phi_n}$ the spectral measure and $U_n : \mathcal{H} \to L^2(\mathbb{R}, \mu_n)$ given by $f(A)\phi_n \mapsto f$. It can be checked that U_n is unitary. Then $U \equiv \bigoplus_n U_n$ is the desired unitary map. $\square$

Spectral Theorem III is somewhat equivalent to Spectral Theorems I and II combined. If applied to the n-dimensional case, they all fall back to Spectral Theorem 0.

Remark 9.17. ((Put this into perspective of theoretical quantum mechanics)) By theorem 9.16, we can diagonalize (i.e. change coordinates in the physical space $\mathcal{H}$) any observable s.t. we can express them as a multiplication operator. If we now take the square of a state function $\psi \in L^2$, we obtain the probability distribution of outputs of the measure corresponding to the observable (under a suitable representation), s.t. the wave function perfectly describes the observable..

The rest of the chapter can be viewed as an in-depth discussion for interested readers.

9.4 Characterisation of the spectrum

Remark 9.18. We want to now examine the spectrum itself a little closer. We know that all eigenvalues (if they exist, that is) are contained in the spectrum of an operator. There are however also operators, that have no eigenvalues at all. One notable example is the Laplacian Δ. But not all hope is lost. If the operator is self-adjoint, we can characterize its spectrum as the values z for which there is a sequence of "approximate eigenvectors". We shall now build this notion on solid mathematical ground.

Definition 9.19. Let $A \in \mathcal{B}(\mathcal{H}), z \in \mathbb{C}$. A *Weyl sequence* for A at z is a sequence $(\psi_n)_{n\geq 1}$ in $\mathcal{H}$ with $\|\psi_n\| = 1$, $\forall n$ and

$$\lim_{n\to\infty} \|(A - z)\psi_n\| = 0$$

A very peculiar construct. Notice that if z is an eigenvalue, there exists a corresponding eigenvector ψ_z. Then we can set $\psi_n = \psi_z \ \forall n$. However, z here need not be an eigenvector in order for a Weyl sequence to exist. This convergence in norm thus gives us a sense of what an approximation of eigenvectors might look like, even when in reality there are none.

Example 9.20. Consider the discrete Laplacian Δ acting on $a \in l^2(\mathbb{Z})$ in the following way:

$$(\Delta a)(n) = a(n-1) + a(n+1) \quad \forall n \in \mathbb{Z}$$

Then, Δ has no eigenvalues at all. Indeed, notice that if we know two elements of a, we know all elements of Δa. This new series grows exponentially in at least one of the two directions

for any $a \neq 0$. But then, Δa cannot be in $l(\mathbb{Z})$ anymore.
However, we can still construct a Weyl sequence to find a point in the spectrum of Δ. The discrete Laplacian is an interesting operator in the term that it isn't really relevant to applications, but it is didactically useful for exemplary behaviour.

To gather points on the spectrum, the following theorem might be useful.

Theorem 9.21. *Let $A \in \mathcal{B}(\mathcal{H}), (\psi_n)_{n\geq 1}$ a Weyl sequence for A at $z \in \mathbb{C}$. Then $z \in \sigma(A)$. Let A additionally be self-adjoint. Then: $\exists$ a Weyl sequence for A at $z \iff z \in \sigma(A)$.*

Proof. Contraposition: Assume $z \notin \sigma(A)$. Then $(A - z)$ invertible, thus

$$1 = \|\psi_n\| = \|(A-z)^{-1}(A-z)\psi_n\| \leq \|(A-z)^{-1}\|\|(A-z)\psi_n\| = \|R(A,z)\|\|(A-z)\psi_n\|$$

$\Rightarrow \|(A-z)\psi_n\| \geq \|R(A,z)\|^{-1} \Rightarrow (\psi_n)_{n\geq 1}$ not a Weyl sequence for A at z. This shows the general statement.
Now, let A adjoint, $\lambda \in \sigma(A)$. Then $\lambda \in \mathbb{R}$ and $(\lambda + i\varepsilon) \in \rho(A), \forall \varepsilon > 0$. Choose a sequence $\varepsilon_n \downarrow 0$. By theorem 9.12, $\exists (\phi_n)_{n\geq 1}$ with $\|\phi_n\| = 1$ s.t. $\|(A - \lambda - i\varepsilon_n)^{-1}\phi_n\| \overset{n\to\infty}{\longrightarrow} \infty$. Defining

$$\psi_n = \frac{(A - \lambda - i\varepsilon_n)^{-1}\phi_n}{\|(A - \lambda - i\varepsilon_n)^{-1}\phi_n\|}$$

we obtain that $(A - \lambda)\psi_n \to 0$. Thus, $(\psi_n)_{n\geq 1}$ is a Weyl sequence for A at λ. □

We conclude with a neat way to calculate the operator norm of the resolvent as in theorem 9.12.

Corollary 9.22. *Let $A \in \mathcal{B}(\mathcal{H})$ self-adjoint, $z \in \mathbb{C}$. Then*

$$dist(z, \sigma(A)) = \inf_{\|v\|=1} \|(A - z)v\|$$

Proof. At first assume $z \in \sigma(A)$. Then $\mathrm{dist}(z, \sigma(A)) = 0$. On the other hand, $\inf_{\|v\|=1} \|(A - z)v\| = 0$ by theorem 9.21. Thus equality holds.
Now, assume $z \in \rho(A)$. Then, $\mathrm{dist}(z, \sigma(A)) = \|R(A,z)\|^{-1}$ by theorem 9.12. The quanity on the right is equal to the left hand side by a direct calculation. □