9 Spectral measures and Spectral Theorem

9.1 Continuous functional calculus

In the last talk we got to know the spectrum of bounded operators, which are an immensely important tool when dabbling in applications of quantum mechanics.

In this chapter, we want to further expand upon this idea and in particular prove several variations of the Spectral Theorem. This is a very important result, upon which the rest of this course rests. We start with its equivalent 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?
Before we get to that, another question arises.

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 9.4 tells us, yes.

For the proof we need a lemma:

Lemma 9.3. *Let $A \in \mathcal{B}(\mathcal{H})$ be self-adjoint, $p \in \mathbb{C}[X]$ i.e. a polynomial. Then*

$$\|p(A)\| = sup\{|p(z)| : z \in \sigma(A)\}$$

Theorem 9.4 (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.*

- $(f + g)(A) = f(A) + g(A)$
- $(\alpha f)(A) = \alpha f(A)$

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

– $(fg)(A) = f(A)g(A)$

– $(f(A))^* = \bar{f}(A)$

– $\chi_{\sigma(A)}(A) = id_{\sigma(A)}$

$\forall f, g \in C(\sigma(A))$, $\alpha \in \mathbb{C}$ 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, and thus by lemma 9.3 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 $\sigma(A)$. We then see again by 9.3 that $p_n(A) - q_n(A)$ converges in norm to the zero operator. It follows that $(q_n(A))_{n\geq 1}$ converges to $f(A)$ as well. $\square$

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 9.5. 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, if an operator $A \in \mathcal{B}(\mathcal{H})$ satisfies:

a) $\|A\| \leq 1$

b) $\sigma(A) \subset \mathbb{R}_{\geq 0}$ (e.g. when A is monotonic, i.e. if $\langle Av, v\rangle \geq 0$ $\forall v \in \mathcal{H}$)

Then $P_n(A) \rightrightarrows \sqrt{A}$, where $(\sqrt{A})^2 = A$. This is because in order to be well-defined, uniform convergence must hold (only) on the spectrum.

9.2 Spectral measures

Remark 9.6. 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 $v \in \mathbb{C}^n$, we may compute

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

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 9.7 (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.

Proof. Theorem 9.4 implies that $l : C(\sigma(A)) \to \mathbb{C}$ given by $f \mapsto \langle \phi, f(A)\psi \rangle$ defines a bounded, linear functional. The Riesz-Markov-Kakutani representation theorem guarantees the unique existence of such a complex, regular 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 $\Rightarrow \mu$ a non-negative measure. $\square$

The existence of such a measure motivates the following definition.

Definition 9.8. 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 9.9. 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 9.10. 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 $f(A)$.

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

Example 9.11. Let $\mathcal{H} = L^2([0,1],\mu)$ where μ an arbitrary measure on $\mathcal{H}$, $\phi \in \mathcal{H}$ with $\|\phi\|_2 = 1$. Now consider D as the (diagonal) multiplication operator on $\mathcal{H}$, i.e.

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

Note that D does not possess any Eigenvalues, however it's spectrum is the entire interval (more precisely the spectrum equals the support of μ, but for now let's assume that this covers the interval).
Let $f \in C(\sigma(D)) = C([0,1])$. Then we get

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

Thus we get the spectral measure associated to ϕ:

$$\mu_\phi = |\phi|^2\mu$$

The physical interpretation is as follows: ϕ represents a physical state/wave function defined on $[0,1]$. A physical example of this is an electron in a potential well of width 1. In fact, $|\phi|^2$ is the probability density of the position of this electron. So, the mean value corresponds to the expected position of the electron. Thus it is important for the wave function to be normalised, i.e. to have norm 1 in $L^2([0,1])$. In this context D is called the position operator. Then we get that the spectral measure μ_ϕ is the probability distribution of the position of the particle.

Thanks to Theorem 9.7, 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, $\forall\lambda' \in \sigma(A)$,

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

by the second Spectral Theorem 9.7.
"$\geq$": is generally true for bounded operators.
Indeed, assume by contradiction that $\|R(A,z)\| < \operatorname{dist}(z,\sigma(A))^{-1}$. Then $\exists s \in \sigma(A)$ s.t.

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

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

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

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.*

We managed to generalize theorem 9.7 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 $f(\lambda) = \langle e_\lambda, v\rangle$ for an Eigenvalue $\lambda \in \sigma(A)$). Applying the spectral theorem to the n-dimensional case yields that U is unitary and

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

for $g \in \mathcal{H}$. Thus, UAU^* becomes the multiplication operator again.

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

Note that unitary maps preserve the orthonormality of bases.

For the proof of the third spectral theorem, we need the following definition:

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. $\square$

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.
For example, as we will see, the discrete Laplacian can be expressed as a multiplication operator:

Example 9.17. Consider the discrete Laplacian Δ acting on $a \in \mathcal{H} = l^2(\mathbb{Z})$ 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. Notice that if we know two consecutive elements of a, we know all elements of Δa:

$$\begin{aligned} (\Delta a)(n) &= a(n-1) + a(n+1) \stackrel{!}{=} Ea(n) \\ \implies a(n+1) &= Ea(n) - a(n-1) \end{aligned}$$

Furthermore, if there are two elements $a, b \in \mathcal{H}$ solving the (linear) eigenvalue equation, then any linear combination of the two sequences also solve it. Putting those two findings together it becomes clear that the set of formal solutions is a vector space of dimension 2. But try as you might, you will find no sequence which will solve this equation (for example you might want to try the Ansatz $b(n) = \lambda^n$ for $\lambda \neq 0$ fixed). No matter the two starting values (apart from the case where both equal zero, which is not allowed as we disregard the zero element when searching for eigenvectors), the new series grows exponentially in at least one of the two directions. But then, Δa cannot be in $l(\mathbb{Z})$ anymore. Thus no eigenvectors exist, and therefore no eigenvalues. However, we can still compute its spectrum via diagonalisation.

Note that the Fourier series is a bijection $\mathcal{F} : L^2((-\pi, \pi)) \leftrightarrow l^2(\mathbb{Z})$. Thus we get

$$\begin{aligned}
f \xmapsto{\mathcal{F}} c_k \xmapsto{\Delta} \tilde{c}_k = c_{k-1} + c_{k+1} \xmapsto{\mathcal{F}^{-1}} \tilde{f}(x) \\
&= \sum_{k\in\mathbb{Z}} \tilde{c}_k e^{2\pi i k x} = \sum_{k\in\mathbb{Z}} (c_{k-1} + c_{k+1}) e^{2\pi i k x} \\
&= \sum_{l\in\mathbb{Z}} c_l (e^{2\pi i (l+1) x} + e^{2\pi i (l-1) x}) = 2\cos(2\pi x) \sum_{l\in\mathbb{Z}} e^{2\pi i l x} \\
&= 2\cos(2\pi x) f(x) \equiv \xi(x) f(x)
\end{aligned}$$

Then we get

$$\sigma(\Delta) = \xi((-\pi, \pi)) = [-2, 2]$$

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.

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

9.4 Characterisation of the spectrum

We want to now examine the spectrum itself a little closer. We have good reason to do so:

Example 9.18. Consider the energy operator (Hamiltonian) on the hydrogen atom:

$$H = -\Delta - \frac{q}{4\pi\varepsilon_0 |\vec{x}|}$$

where q the charge of the electron and ε_0 the vacuum permittivity constant. It has the domain $W^{1,2}(\mathbb{R}^3)$ which is the (Sobolev) space of square-integrable functions on $\mathbb{R}^3$ whose (weak) derivatives are also square-integrable. H has a discrete set of eigenvalues that can be computed via the Rydberg formula. Their corresponding eigenfunctions are exactly the bound states of the electron in the hydrogen atom.

Remark 9.19. 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 9.20. 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.

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

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

$\Rightarrow \|(A-z)\psi_n\| \geq \|R(A,z)\|^{-1}\ \forall n \geq 1 \Rightarrow (\psi_n)_{n\geq 1}$ 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. $\square$

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 $\text{dist}(z, \sigma(A)) = 0$. 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, $\text{dist}(z, \sigma(A)) = \|R(A,z)\|^{-1}$ by theorem 9.12. The quantity on the right is equal to the left hand side by a direct calculation. $\square$