43. Let M and N be subspaces of a Banach space X such that $M+N=X$ and $M\cap N=\{0\}$. Let P be the projection of X onto M. Prove that P is bounded if and only if *both* M and N are closed.

44. (a) Define the numerical range, $N(T)$, of a bounded operator, T, on a Hilbert space, $\mathscr{H}$, by $N(T)=\{(\psi, T\psi)\mid\psi\in\mathscr{H},\ \|\psi\|=1\}$. Prove that $\sigma(T)\subset\overline{N(T)}$. (Hint: First show that if λ is an eigenvalue of T or T^*, then $\lambda\in N(T)$; then show that if $\lambda\in\sigma(T)$ and λ is not an eigenvalue of T or T^*, we can find $\psi_n\in\mathscr{H}$ so that $\|(T-\lambda)\psi_n\|\to 0$.)
(b) Find an example where $N(T)$ is not closed and $\sigma(T)\not\subset N(T)$.
(c) Find an example where $\sigma(T)\neq N(T)=\overline{N(T)}$.

Remark: There is a deep result of Hausdorff that $N(T)$ is convex.

45. (a) Let $\{\phi_n\}_{n=1}^{\infty}$ be an orthonormal basis for a Hilbert space $\mathscr{H}$. Let A be an operator with

$$\sup_{\substack{\psi\in[\phi_1,\ldots,\phi_n]^{\perp}\\ \|\psi\|=1}}\|A\psi\|\to 0\qquad\text{as}\quad n\to\infty.$$

Prove that A is compact.
(b) Let $\{\phi_n\}_{n=1}^{\infty}$ be any orthonormal basis for a Hilbert space $\mathscr{H}$ and let A be compact. Prove that

$$\sup_{\psi\in[\phi_1,\ldots,\phi_n]^{\perp}}\|A\psi\|\to 0\qquad\text{as}\quad n\to\infty.$$

46. (a) Let $A\geq 0$ with A compact. Prove that $A^{1/2}$ is compact. (Hint: Use Problem 45.)
(b) Let $0\leq A\leq B$. Prove that A is compact if B is compact. (Hint: Prove that $A^{1/2}$ is compact using Problem 45 and part (a).)

47. Let $\mathscr{H}$ and $\mathscr{H}'$ be two Hilbert spaces. If T is a bounded linear map from $\mathscr{H}$ to $\mathscr{H}'$ we define $T^*:\mathscr{H}'\to\mathscr{H}$ by $(T^*\psi,\phi)_{\mathscr{H}}=(\psi, T\phi)$. T is called *Hilbert–Schmidt* if and only if $T^*T:\mathscr{H}\to\mathscr{H}$ is trace class. Let T be Hilbert-Schmidt. Prove that there are real numbers, $\lambda_n>0$, and orthonormal sets $\{\phi_n\}_{n=1}^{N}\subset\mathscr{H}$, $\{\psi_n\}_{n=1}^{N}\in\mathscr{H}'$ so that

$$T\phi=\sum_{n=1}^{N}\lambda_n(\phi_n,\phi)\psi_n$$

48. Let $\mathscr{H}$ and $\mathscr{H}'$ be the two Hilbert spaces and let $\mathscr{I}_2(\mathscr{H},\mathscr{H}')$ denote the Hilbert–Schmidt operators from $\mathscr{H}$ to $\mathscr{H}'$.
(a) Prove that $\mathscr{I}_2(\mathscr{H},\mathscr{H}')$ with the inner product

$$(S,T)=\operatorname{Tr}_{\mathscr{H}}(S^*T)$$

is a Hilbert space.
(b) Given $\psi\in\mathscr{H}$, $\phi\in\mathscr{H}'$ define $I(\psi,\phi)\in\mathscr{I}_2(\mathscr{H}^*,\mathscr{H}')$ by $I(\psi,\phi)\ell=\ell(\psi)\phi$ for any $\ell\in\mathscr{H}^*$. Prove that the map J, taking $\psi\otimes\phi$ into $I(\psi,\phi)$, is well defined and extends to an isometry of $\mathscr{H}\otimes\mathscr{H}'$ and $\mathscr{I}_2(\mathscr{H}^*,\mathscr{H}')$.
(c) Given $\eta\in\mathscr{H}\otimes\mathscr{H}'$ show that there exist reals, $\lambda_n>0$, and orthonormal sets $\{\phi_n\}_{n=1}^{N}\subset\mathscr{H}$, $\{\psi_n\}_{n=1}^{N}\subset\mathscr{H}'$ with N finite or infinite, so that

$$\sum_{n=1}^{N}|\lambda_n|^2=\|\eta\|^2\qquad\text{and}\qquad\sum_{n=1}^{N}\lambda_n\phi_n\otimes\psi_n=\eta.$$

VII: The Spectral Theorem

Mathematical proofs, like diamonds, are hard as well as clear, and will be touched with nothing but strict reasoning. John Locke in ***Second Reply to the Bishop of Worcester***

VII.1 The continuous functional calculus

In this chapter, we will discuss the spectral theorem in its many guises. This structure theorem is a concrete description of all self-adjoint operators. There are several apparently distinct formulations of the spectral theorem. In some sense they are all equivalent.

The form we prefer says that every bounded self-adjoint operator is a multiplication operator. (We emphasize the word bounded since we will deal extensively with unbounded self-adjoint operators in the next chapter; there is a spectral theorem for unbounded operators which we discuss in Section VIII.3.) This means that given a bounded self-adjoint operator on a Hilbert space $\mathscr{H}$, we can always find a measure μ on a measure space M and a unitary operator $U:\mathscr{H}\to L^2(M, d\mu)$ so that

$$(UAU^{-1}f)(x)=F(x)f(x)$$

for some bounded real-valued measurable function F on M.

This is clearly a generalization of the finite-dimensional theorem, which says any self-adjoint $n\times n$ matrix can be diagonalized, or in an abstract form: Given self-adjoint operator A on an n-dimensional complex space V, there is a unitary operator $U: V \to \mathbb{C}^n$ and real numbers $\lambda_1, \ldots, \lambda_n$ so that

$$(UAU^{-1}f)_i = \lambda_i f_i$$

for each $f = \langle f_1, \ldots, f_n \rangle$ in $\mathbb{C}^n$.

In practice, M will be a union of copies of $\mathbb{R}$ and F will be x, so the core of the proof of the theorem will be the construction of certain measures. This will be done in Section VII.2 by using the Riesz–Markov theorem. Our goal in this section will be to make sense out of $f(A)$, for f a continuous function. In the next section, we will consider the measures defined by the functionals $f \mapsto \langle \psi, f(A)\psi \rangle$ for fixed $\psi \in \mathscr{H}$.

Given a fixed operator A, for which f can we define $f(A)$? First, suppose that A is an arbitrary bounded operator. If $f(x) = \sum_{n=1}^{N} a_n x^n$ is a polynomial, we want $f(A) = \sum_{n=1}^{N} a_n A^n$. Suppose that $f(x) = \sum_{n=0}^{\infty} c_n x^n$ is a power series with radius of convergence R. If $\|A\| < R$, then $\sum_{n=0}^{\infty} c_n A^n$ converges in $\mathscr{L}(\mathscr{H})$ so it is natural to set $f(A) = \sum_{n=0}^{\infty} c_n A^n$. In this last case, f was a function analytic in a domain including all of $\sigma(A)$. In general, one can make a reasonable definition for $f(A)$ if f is analytic in a neighborhood of $\sigma(A)$ (see the Notes).

The functional calculus we have talked about thus far works for any operator in any Banach space. The special property of self-adjoint operators (or more generally normal operators; see Problems 3, 5) is that $\|P(A)\| = \sup_{\lambda \in \sigma(A)} |P(\lambda)|$ for any polynomial P, so that one can use the B.L.T. theorem to extend the functional calculus to continuous functions. Our major goal in this section is the proof of:

Theorem VII.1 (continuous functional calculus) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Then there is a *unique* map $\phi: C(\sigma(A)) \to \mathscr{L}(\mathscr{H})$ with the following properties:

(a) ϕ is an algebraic $*$-homomorphism, that is,

$$\phi(fg) = \phi(f)\phi(g) \qquad \phi(\lambda f) = \lambda\phi(f)$$
$$\phi(1) = I \qquad \phi(\bar{f}) = \phi(f)^*$$

(b) ϕ is continuous, that is, $\|\phi(f)\|_{\mathscr{L}(\mathscr{H})} \le C\|f\|_\infty$.

(c) Let f be the function $f(x) = x$; then $\phi(f) = A$.

Moreover, ϕ has the additional properties:

(d) If $A\psi = \lambda\psi$, then $\phi(f)\psi = f(\lambda)\psi$.

(e) $\sigma[\phi(f)] = \{f(\lambda) \mid \lambda \in \sigma(A)\}$ [spectral mapping theorem].

(f) If $f \ge 0$, then $\phi(f) \ge 0$.

(g) $\|\phi(f)\| = \|f\|_\infty$ [this strengthens (b)].

We sometimes write $\phi_A(f)$ or $f(A)$ for $\phi(f)$ to emphasize the dependence on A.

The idea of the proof which we give below is quite simple. (a) and (c) uniquely determine $\phi(P)$ for any polynomial $P(x)$. By the Weierstrass theorem, the set of polynomials is dense in $C(\sigma(A))$ so the heart of the proof is showing that

$$\|P(A)\|_{\mathscr{L}(\mathscr{H})} = \|P(x)\|_{C(\sigma(A))} \equiv \sup_{\lambda \in \sigma(A)} |P(\lambda)|$$

The existence and uniqueness of ϕ then follow from the B.L.T. theorem.

To prove the crucial equality, we first prove a special case of (e) (which holds for arbitrary bounded operators):

Lemma 1 Let $P(x) = \sum_{n=0}^{N} a_n x^n$. Let $P(A) = \sum_{n=0}^{N} a_n A^n$. Then

$$\sigma(P(A)) = \{P(\lambda) \mid \lambda \in \sigma(A)\}$$

Proof Let $\lambda \in \sigma(A)$. Since $x = \lambda$ is a root of $P(x) - P(\lambda)$, we have $P(x) - P(\lambda) = (x - \lambda)Q(x)$, so $P(A) - P(\lambda) = (A - \lambda)Q(A)$. Since $(A - \lambda)$ has no inverse neither does $P(A) - P(\lambda)$, that is, $P(\lambda) \in \sigma(P(A))$.

Conversely, let $\mu \in \sigma(P(A))$ and let $\lambda_1, \ldots, \lambda_n$ be the roots of $P(x) - \mu$, that is, $P(x) - \mu = a(x - \lambda_1) \cdots (x - \lambda_n)$. If $\lambda_1, \ldots, \lambda_n \notin \sigma(A)$, then

$$(P(A) - \mu)^{-1} = a^{-1}(A - \lambda_1)^{-1} \cdots (A - \lambda_n)^{-1}$$

so we conclude that some $\lambda_i \in \sigma(A)$, that is, $\mu = P(\lambda)$ for some $\lambda \in \sigma(A)$. ∎

Lemma 2 Let A be a bounded self-adjoint operator. Then

$$\|P(A)\| = \sup_{\lambda \in \sigma(A)} |P(\lambda)|$$

Proof

$$\begin{aligned} \|P(A)\|^2 &= \|P(A)^*P(A)\| \\ &= \|(\bar{P}P)(A)\| \\ &= \sup_{\lambda \in \sigma(\bar{P}P(A))} |\lambda| \qquad \text{(by Theorem VI.6)} \\ &= \sup_{\lambda \in \sigma(A)} |\bar{P}P(\lambda)| \qquad \text{(by Lemma 1)} \\ &= \Big(\sup_{\lambda \in \sigma(A)} |P(\lambda)|\Big)^2 \end{aligned}$$ ∎

Proof of Theorem VII.1 Let $\phi(P) = P(A)$. Then $\|\phi(P)\|_{\mathscr{L}(\mathscr{H})} = \|P\|_{C(\sigma(A))}$ so ϕ has a unique linear extension to the closure of the polynomials in $C(\sigma(A))$. Since the polynomials are an algebra containing 1, containing complex conjugates, and separating points, this closure is all of $C(\sigma(A))$. Properties (a), (b), (c), (g) are obvious and if $\tilde{\phi}$ obeys (a), (b), (c) it agrees with ϕ on polynomials and thus by continuity on $C(\sigma(A))$. To prove (d), note that $\phi(P)\psi = P(\lambda)\psi$ and apply continuity. To prove (f), notice that if $f \geq 0$, then $f = g^2$ with g real and $g \in C(\sigma(A))$. Thus $\phi(f) = \phi(g)^2$ with $\phi(g)$ self-adjoint, so $\phi(f) \geq 0$. (e) is left for the reader (Problem 8). ∎

Before turning to some examples, we make several remarks:

(1) $\phi(f) \geq 0$ if and only if $f \geq 0$ (Problem 9).

(2) Since $fg = gf$ for all f, g, $\{f(A) \mid f \in C(\sigma(A))\}$ forms an abelian algebra closed under adjoints. Since $\|f(A)\| = \|f\|_\infty$ and $C(\sigma(A))$ is complete, $\{f(A) \mid f \in C(\sigma(A))\}$ is norm-closed. It is thus an **abelian C^* algebra** of operators.

(3) Ran ϕ is actually the **C^* algebra generated by** A, that is, the smallest C^*-algebra containing A (Problem 10).

(4) This result, that $C(\sigma(A))$ and the C^*-algebra generated by A are isometrically isomorphic, is actually a special case of the "commutative Gelfand–Naimark theorem" which we discuss in Chapter XV.

(5) (b) actually follows from (a) and abstract nonsense (Problem 11). Thus (a) and (c) alone determine ϕ uniquely.

Finally, we consider two specific examples of $\phi(f)$:

Example 1 As a corollary, we have a new proof of the existence half of the square-root lemma (Theorem VI.9) for if $A \geq 0$, then $\sigma(A) \subset [0, \infty)$ (Problem 12). If $f(x) = x^{1/2}$, then $f(A)^2 = A$.

Example 2 From (*g*) of Theorem VII.1 we see that $\|(A - \lambda)^{-1}\| = [\text{dist}(\lambda, \sigma(A))]^{-1}$ if A is bounded, self-adjoint, and $\lambda \notin \sigma(A)$.

VII.2 The spectral measures

We are now ready to introduce the measures we have anticipated so often before. Let us fix A, a bounded self-adjoint operator. Let $\psi \in \mathscr{H}$. Then $f \mapsto (\psi, f(A)\psi)$ is a positive linear functional on $C(\sigma(A))$. Thus, by the Riesz–Markov theorem (Theorem IV.14), there is a unique measure μ_ψ on the compact set $\sigma(A)$ with $(\psi, f(A)\psi) = \int_{\sigma(A)} f(\lambda)\, d\mu_\psi$.

regular Borel measure
(reg. Borel measures ⟷ Baire meas.)

Definition The measure μ_ψ is called the **spectral measure associated with the vector ψ.**

The first and simplest application of the μ_ψ is to allow us to extend the functional calculus to $\mathscr{B}(\mathbb{R})$, the bounded Borel functions on $\mathbb{R}$. Let $g \in \mathscr{B}(\mathbb{R})$. It is natural to define $g(A)$ so that $(\psi, g(A)\psi) = \int_{\sigma(A)} g(\lambda)\, d\mu_\psi(\lambda)$. The polarization identity lets us recover $(\psi, g(A)\phi)$ from the proposed $(\psi, g(A)\psi)$ and then the Riesz lemma lets us construct $g(A)$. The properties of this "measurable functional calculus" are given in (Problem 13):

Theorem VII.2 (spectral theorem—functional calculus form) Let A be a bounded self-adjoint operator on $\mathscr{H}$. There is a unique map $\hat{\phi}: \mathscr{B}(\mathbb{R}) \to \mathscr{L}(\mathscr{H})$ so that

(a) $\hat{\phi}$ is an algebraic $*$-homomorphism.

(b) $\hat{\phi}$ is norm continuous: $\|\hat{\phi}(f)\|_{\mathscr{L}(\mathscr{H})} \leq \|f\|_\infty$.

(c) Let f be the function $f(x) = x$; then $\hat{\phi}(f) = A$.

(d) Suppose $f_n(x) \to f(x)$ for each x and $\|f_n\|_\infty$ is bounded. Then $\hat{\phi}(f_n) \to \hat{\phi}(f)$ *strongly*.

Moreover $\hat{\phi}$ has the properties:

(e) If $A\psi = \lambda\psi$, then $\hat{\phi}(f)\psi = f(\lambda)\psi$.

(f) If $f \geq 0$, then $\hat{\phi}(f) \geq 0$.

(g) If $BA = AB$, then $\hat{\phi}(f)B = B\hat{\phi}(f)$.

Theorem VII.2 can be proven directly by extending Theorem VII.1; part (d) requires the dominated convergence theorem. Or, Theorem VII.2 can be proven by an easy corollary of Theorem VII.3 below. The proof of Theorem VII.3 uses only the *continuous* functional calculus. $\hat{\phi}$ extends ϕ and as before we write $\hat{\phi}(f) = f(A)$. As in the continuous functional calculus, one has $f(A)g(A) = g(A)f(A)$.

Since $\mathscr{B}(\mathbb{R})$ is the smallest family closed under limits of form (d) containing all of $C(\mathbb{R})$, we know that any $\hat{\phi}(f)$ is in the smallest C^*-algebra containing A which is also strongly closed; such an algebra is called a von Neumann or W*-algebra. When we study von Neumann algebras in Chapter XVIII we will see that this follows from (g).

The norm equality of Theorem VII.1 carries over if we define $\|f\|'_\infty$ to be the L^∞-norm with respect to a suitable notion of "almost everywhere." Namely, pick an orthonormal basis $\{\psi_n\}$ and say that a property is true a.e. if it is true a.e. with respect to *each* μ_{ψ_i}. Then $\|\hat{\phi}(f)\|_{\mathscr{L}(\mathscr{H})} = \|f\|'_\infty$.

In the next section, we will return to the operators $\chi_\Omega(A)$ where χ_Ω is a characteristic function; this is the most important set of operators in the measurable but not in the continuous functional calculus. For the time being, we turn to using the spectral measures to form L^2 spaces. We first define:

Definition A vector $\psi \in \mathscr{H}$ is called a **cyclic vector** for A if finite linear combinations of the elements $\{A^n\psi\}_{n=0}^{\infty}$ are dense in $\mathscr{H}$.

Not all operators have cyclic vectors (Problem 14), but if they do:

Lemma 1 Let A be a bounded self-adjoint operator with cyclic vector ψ. Then, there is a unitary operator $U: \mathscr{H} \to L^2(\sigma(A), d\mu_\psi)$ with

$$(UAU^{-1}f)(\lambda) = \lambda f(\lambda)$$

Equality is in the sense of elements of $L^2(\sigma(A), d\mu_\psi)$.

Proof Define U by $U\phi(f)\psi \equiv f$ where f is continuous. U is essentially the inverse of the map ϕ of Theorem VII.1. To show that U is well defined we compute

$$\|\phi(f)\psi\|^2 = (\psi, \phi^*(f)\phi(f)\psi) = (\psi, \phi(\bar{f}f)\psi)$$
$$= \int |f(\lambda)|^2 \, d\mu_\psi$$

Therefore, if $f = g$ a.e. with respect to μ_ψ, then $\phi(f)\psi = \phi(g)\psi$. Thus U is well defined on $\{\phi(f)\psi \mid f \in C(\sigma(A))\}$ and is norm preserving. Since ψ is cyclic $\overline{\{\phi(f)\psi \mid f \in C(\sigma(A))\}} = \mathscr{H}$, so by the B.L.T. theorem U extends to an isometric map of $\mathscr{H}$ into $L^2(\sigma(A), d\mu_\psi)$. Since $C(\sigma(A))$ is dense in L^2, Ran $U = L^2(\sigma(A), d\mu_\psi)$. Finally, if $f \in C(\sigma(A))$,

$$(UAU^{-1}f)(\lambda) = [UA\phi(f)](\lambda)$$
$$= [U\phi(xf)](\lambda)$$
$$= \lambda f(\lambda)$$

By continuity, this extends from $f \in C(\sigma(A))$ to $f \in L^2$. ∎

To extend this lemma to arbitrary A, we need to know that A has a family of invariant subspaces spanning $\mathscr{H}$ so that A is cyclic on each subspace:

Lemma 2 Let A be a self-adjoint operator on a separable Hilbert space $\mathscr{H}$. Then there is a direct sum decomposition $\mathscr{H} = \bigoplus_{n=1}^{N} \mathscr{H}_n$ with $N = 1, 2, \ldots$, *or* ∞ so that:

(a) A leaves each $\mathscr{H}_n$ **invariant**, that is, $\psi \in \mathscr{H}_n$ implies $A\psi \in \mathscr{H}_n$.
(b) For each n, there is a $\phi_n \in \mathscr{H}_n$ which is cyclic for $A \restriction \mathscr{H}_n$, i.e. $\mathscr{H}_n = \overline{\{f(A)\phi_n \mid f \in C(\sigma(A))\}}$.

Proof A simple Zornication (Problem 15).

We can now combine Lemmas 1 and 2 to prove the form of the spectral theorem which we regard as the most transparent:

Theorem VII.3 (spectral theorem—multiplication operator form) Let A be a bounded self-adjoint operator on $\mathscr{H}$, a separable Hilbert space. Then, there exist measures $\{\mu_n\}_{n=1}^{N}$ ($N = 1, 2, \ldots$ or ∞) on $\sigma(A)$ and a unitary operator

$$U: \mathscr{H} \to \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n)$$

so that

$$(UAU^{-1}\psi)_n(\lambda) = \lambda\psi_n(\lambda)$$

where we write an element $\psi \in \bigoplus_{n=1}^{N} L^2(\mathbb{R}, d\mu_n)$ as an N-tuple $\langle\psi_1(\lambda), \ldots, \psi_N(\lambda)\rangle$. This realization of A is called a **spectral representation**.

Proof Use Lemma 2 to find the decomposition and then use Lemma 1 on each component. ∎

This theorem tells us that every bounded self-adjoint operator is a multiplication operator on a suitable measure space; what changes as the operator changes are the underlying measures. Explicitly:

Corollary Let A be a bounded self-adjoint operator on a separable Hilbert space $\mathscr{H}$. Then there exists a *finite* measure space $\langle M, \mu\rangle$, a bounded function F on M, and a unitary map, $U: \mathscr{H} \to L^2(M, d\mu)$, so that

$$(UAU^{-1}f)(m) = F(m)f(m)$$

Proof Choose the cyclic vectors ϕ_n so that $\|\phi_n\| = 2^{-n}$. Let $M = \bigcup_{n=1}^{N}\mathbb{R}$, i.e. the union of N copies of $\mathbb{R}$. Define μ by requiring that its restriction to the nth copy of $\mathbb{R}$ be μ_n. Since $\mu(M) = \sum_{n=1}^{N}\mu_n(\mathbb{R}) < \infty$, μ is finite. ∎

We also notice that this last theorem is essentially a rigorous form of the physicists' Dirac notation. If we write $\psi_n(x) = \psi(x; n)$, we see that in the "new representation defined by U" one has

$$(\psi, \phi) = \sum_n \int d\mu_n \overline{\psi(\lambda; n)}\phi(\lambda; n)$$

$$(\psi, A\phi) = \sum_n \int d\mu_n \overline{\psi(\lambda; n)}\lambda\phi(\lambda; n)$$

These are the Dirac type formulas familiar to physicists except that the formal sums of Dirac are replaced with integrals over spectral measures, where we define:

Definition The measures $d\mu_n$ are called **spectral measures**; they are just $d\mu_\psi$ for suitable ψ.

These measures are *not* uniquely determined and we will eventually discuss this nonuniqueness question. First, let us consider a few examples:

Example 1 Let A be an $n \times n$ self-adjoint matrix. The "usual" finite-dimensional spectral theorem says that A has a complete orthonormal set of eigenvectors, $\psi_1, \ldots, \psi_n$, with $A\psi_i = \lambda_i \psi_i$. Suppose first that the eigenvalues are distinct. Consider the sum of Dirac measures, $\mu = \sum_{i=1}^n \delta(x - \lambda_i)$. $L^2(\mathbb{R}, d\mu)$ is just $\mathbb{C}^n$ since $f \in L^2$ is determined by $f = \langle f(\lambda_1), \ldots, f(\lambda_n)\rangle$. Clearly, the function λf corresponds to the n-tuple $\langle \lambda_1 f(\lambda_1), \ldots, \lambda_n f(\lambda_n)\rangle$, so A is multiplication by λ on $L^2(\mathbb{R}, d\mu)$. If we take $\tilde{\mu} = \sum_{i=1}^n a_i \delta(x - \lambda_i)$ with $a_1, \ldots, a_n > 0$, A can also be represented as multiplication by λ on $L^2(\mathbb{R}, d\tilde{\mu})$. Thus, we explicitly see the nonuniqueness of the measure in this case. We can also see when more than one measure is needed: one can represent a finite-dimensional self-adjoint operator as multiplication on $L^2(\mathbb{R}, d\mu)$ with only one measure if and only if A has no repeated eigenvalues.

Example 2 Let A be compact and self-adjoint. The Hilbert–Schmidt theorem tells us there is a complete orthonormal set of eigenvectors $\{\psi_n\}_{n=1}^\infty$ with $A\psi_n = \lambda_n \psi_n$. If there is no repeated eigenvalue, $\sum_{n=1}^\infty 2^{-n}\delta(x - \lambda_n)$ works as a spectral measure.

Example 3 Let $\mathscr{H} = \ell^2(-\infty, \infty)$, that is, the set of sequences, $\{a_n\}_{n=-\infty}^\infty$ with $\sum_{n=-\infty}^\infty |a_n|^2 < \infty$. Let $L: \mathscr{H} \to \mathscr{H}$ by $(La)_n = a_{n+1}$, that is, L shifts to the left. $L^* = R$ with $(Ra)_n = a_{n-1}$. Let $A = R + L$ which is self-adjoint. Can we represent A as a multiplication operator? Map $\mathscr{H}$ into $L^2[0, 1]$ by $U: \{a_n\} \to \sum_{n=-\infty}^\infty a_n e^{2\pi i n x}$. Then ULU^{-1} is multiplication by $e^{-2\pi i x}$ and URU^{-1} is multiplication by $e^{+2\pi i x}$ so UAU^{-1} is multiplication by $2\cos(2\pi x)$. The necessary transformations needed to represent A as multiplication by x on $L^2(\mathbb{R}, d\mu_1) \oplus L^2(\mathbb{R}, d\mu_2)$ are left for the problems. μ_1 and μ_2 have support in $[-2, 2]$.

Example 4 Consider $i^{-1}d/dx$ on $L^2(\mathbb{R}, dx)$. This is an unbounded operator and thus not strictly within the context of this section, but we will prove an analogue of Theorem VII.3 in Section VIII.3. We thus seek an operator U and a measure $d\mu$ (it turns out that only one μ is needed) with $U: L^2(\mathbb{R}, dx) \to L^2(\mathbb{R}, d\mu(k))$ so that

$$U\left(\frac{1}{i}\frac{d}{dx} f\right)(k) = kUf(k)$$

The Fourier transform $(Uf)(k) = (2\pi)^{-1/2} \int f(x)e^{-ikx}\, dx$ which we study in Chapter IX precisely does the trick. Thus, the Fourier transform is one example of a spectral representation.

We now investigate the connection between spectral measures and the spectrum.

Definition If $\{\mu_n\}_{n=1}^N$ is a family of measures, the **support** of $\{\mu_n\}$ is the complement of the largest open set B with $\mu_n(B) = 0$ for all n; so

$$\operatorname{supp}\{\mu_n\} = \overline{\bigcup_{n=1}^N \operatorname{supp} \mu_n}$$

Proposition Let A be a self-adjoint operator and $\{\mu_n\}_{n=1}^N$ a family of spectral measures. Then

$$\sigma(A) = \operatorname{supp}\{\mu_n\}_{n=1}^N$$

There is also a simple description of $\sigma(A)$ in terms of the more general multiplication operators discussed after Theorem VII.3:

Definition Let F be a real-valued function on a measure space $\langle M, \mu\rangle$. We say λ is in the **essential range** of F if and only if

$$\mu\{m \mid \lambda - \varepsilon < F(m) < \lambda + \varepsilon\} > 0$$

for all $\varepsilon > 0$.

√ **Proposition** Let F be a bounded real-valued function on a measure space $\langle M, \mu\rangle$. Let T_F be the operator on $L^2(M, d\mu)$ given by

$$(T_F g)(m) = F(m)g(m)$$

Then $\sigma(T_F)$ is the essential range of F.

Proof See Problem 17b.

We can now see exactly what information is contained in the spectrum. A unitary invariant of a self-adjoint operator A is a property P so that $P(A) = P(UAU^{-1})$ for all unitary operators U. Thus, unitary invariants are "intrinsic" properties of self-adjoint operators, that is, properties independent of "representation." An example of such a **unitary invariant** is the spectrum $\sigma(A)$. However, the spectrum is a poor invariant: for example, multiplication by x on $L^2([0, 1], dx)$ and an operator with a complete set of eigenfunctions having all rationals in $[0, 1]$ as eigenvalues are very different even though both have spectrum $[0, 1]$.

At the conclusion of this section, we will see that there is a canonical choice of "spectral measures" which forms a complete set of unitary invariants, that is, a set of properties which distinguish two self-adjoint operators A and B unless $A = UBU^{-1}$ for some unitary operator U. This explains why $\sigma(A)$ is such a bad invariant for different sorts of measures can have the same support. If we wish to find better invariants which are, however, simpler than measures, it is reasonable to first decompose spectral measures in some natural way and then pass to supports. Recall Theorem I.13 which says that any measure μ on $\mathbb{R}$ has a unique decomposition into $\mu = \mu_{pp} + \mu_{ac} + \mu_{sing}$ where μ_{pp} is a pure point measure, μ_{ac} is absolutely continuous with respect to Lebesgue measure, and μ_{sing} is continuous and singular with respect to Lebesgue measure. These three pieces are mutually singular so

$$L^2(\mathbb{R}, d\mu) = L^2(\mathbb{R}, d\mu_{pp}) \oplus L^2(\mathbb{R}, d\mu_{ac}) \oplus L^2(\mathbb{R}, d\mu_{sing})$$

It is easy to see (Problem 18) that any $\psi \in L^2(\mathbb{R}, d\mu)$ has an absolutely continuous spectral measure $d\mu_\psi$ if and only if $\psi \in L^2(\mathbb{R}, d\mu_{ac})$, and similarly for pure point and singular measures. If $\{\mu_n\}_{n=1}^N$ is a family of spectral measures, we can sum $\bigoplus_{n=1}^N L^2(\mathbb{R}, d\mu_{n;\,ac})$ by defining:

Definition Let A be a bounded self-adjoint operator on $\mathscr{H}$. Let $\mathscr{H}_{pp} = \{\psi \mid \mu_\psi \text{ is pure point}\}$, $\mathscr{H}_{ac} = \{\psi \mid \mu_\psi \text{ is absolutely continuous}\}$, $\mathscr{H}_{sing} = \{\psi \mid \mu_\psi \text{ is continuous singular}\}$.

We have thus proven:

Theorem VII.4 $\mathscr{H} = \mathscr{H}_{pp} \oplus \mathscr{H}_{ac} \oplus \mathscr{H}_{sing}$. Each of these subspaces is invariant under A. $A \restriction \mathscr{H}_{pp}$ has a complete set of eigenvectors, $A \restriction \mathscr{H}_{ac}$ has only absolutely continuous spectral measures and $A \restriction \mathscr{H}_{sing}$ has only continuous singular spectral measures.

Definition
$$\sigma_{pp}(A) = \{\lambda \mid \lambda \text{ is an eigenvalue of } A\}$$
$$\sigma_{cont}(A) = \sigma(A \restriction \mathscr{H}_{cont} \equiv \mathscr{H}_{sing} \oplus \mathscr{H}_{ac})$$
$$\sigma_{ac}(A) = \sigma(A \restriction \mathscr{H}_{ac})$$
$$\sigma_{sing}(A) = \sigma(A \restriction \mathscr{H}_{sing})$$

These sets are called the **pure point, continuous, absolutely continuous,** and **singular** (or **continuous singular) spectrum** respectively.

While it may happen that $\sigma_{ac} \bigcup \sigma_{sing} \bigcup \sigma_{pp} \neq \sigma$, this is only true because we did not define σ_{pp} as $\sigma(A \restriction \mathscr{H}_{pp})$ but rather as the actual set of eigenvalues. One always has

Proposition
$$\sigma_{cont}(A) = \sigma_{ac}(A) \bigcup \sigma_{sing}(A)$$
$$\sigma(A) = \overline{\sigma_{pp}(A)} \bigcup \sigma_{cont}(A)$$

The sets need not be disjoint, however. The reader should be warned that $\sigma_{sing}(A)$ may have nonzero Lebesgue measure (Problem 7). For many purposes, breaking up the spectrum in this way gives useful information. In Section VII.3, we introduce another breakup which is also useful.

As we discussed in the notes to Section VI.3, some authors use a notion of "continuous spectrum" which is distinct from the above, namely they define the continuous spectrum to be the set of $\lambda \in \sigma(T)$ which are neither in the point spectrum nor in the residual spectrum. To illustrate the difference between the two definitions we let $\mathscr{H} = \mathbb{C} \oplus L^2[0, 1]$ and define $A: \langle \alpha, f(x) \rangle \to \langle \frac{1}{2}\alpha, xf(x) \rangle$. With our definition, the point $\lambda = \frac{1}{2}$ is in both the pure point and the continuous spectrum. The other authors assign $\lambda = \frac{1}{2}$ to the point spectrum and their continuous spectrum is $[0, \frac{1}{2}) \cup (\frac{1}{2}, 1]$.

Finally, we turn to the question of making canonical choices for the spectral measures, a subject which goes under the title of "multiplicity theory." We will describe the basic results without proof:

1. Multiplicity free operators

We must first ask when A is unitarily equivalent to multiplication by x on $L^2(\mathbb{R}, d\mu)$, that is, when only one spectral measure is needed. A look at Example 1 tells us this happens in the finite-dimensional case only when A has no repeated eigenvalues, so we define:

Definition A bounded self-adjoint operator A is called **multiplicity free** if and only if A is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\mu)$ for some measure μ.

One is interested in intrinsic characterizations of "multiplicity free" and there are several:

Theorem VII.5 The following are equivalent:

(a) A is multiplicity free.
(b) A has a cyclic vector.
(c) $\{B \mid AB = BA\}$ is an abelian algebra.

2. Measure classes

Next we must ask about the nonuniqueness of the measure in the multiplicity free case. The situation in the finite-dimensional multiplicity free case was seen in Example 1: the "acceptable" measures were $\sum_{n=1}^{N} \alpha_n \delta(\lambda - \lambda_n)$ with each $\alpha_n \neq 0$. There is a natural generalization. Suppose $d\mu$ on $\mathbb{R}$ is given and let F be a measurable function which is positive and nonzero a.e. with respect to μ and locally $L^1(\mathbb{R}, d\mu)$, that is, $\int_C |F| \, d\mu < \infty$ for every compact set $C \subset \mathbb{R}$. Then $d\nu = F \, d\mu$ is a Borel measure and the map, U,

$$U: L^2(\mathbb{R}, d\nu) \to L^2(\mathbb{R}, d\mu)$$

given by $(Uf)(\lambda) = \sqrt{F(\lambda)} f(\lambda)$ is unitary (onto since $F \neq 0$ a.e.) and $\lambda(Uf) = U(\lambda f)$. Thus, an operator A with a spectral representation in terms of μ could just as well be represented in terms of ν. By the Radon–Nikodym theorem, $d\nu = F \, d\mu$ with F a.e. nonzero if and only if ν and μ have the same sets of measure zero. This suggests the definition:

Definition Two Borel measures μ and ν are called **equivalent** if and only if they have the same sets of measure zero. An equivalence class $\langle \mu \rangle$ is called a **measure class**.

Then, the nonuniqueness question is answered by:

Proposition Let μ and ν be Borel measures on $\mathbb{R}$ with bounded support. Let A_μ be the operator on $L^2(\mathbb{R}, d\mu)$ given by $(A_\mu f)(\lambda) = \lambda f(\lambda)$ and similarly for A_ν on $L^2(\mathbb{R}, d\nu)$. Then A_μ and A_ν are unitarily equivalent if and only if μ and ν are equivalent measures.

3. Operators of uniform multiplicity

If one wants a canonical listing of the eigenvalues of a matrix, it is natural to list all eigenvalues of multiplicity one, all eigenvalues of multiplicity two, etc. We thus need a way of saying that A is an operator of uniform multiplicity two, three, etc. It is natural to take:

Definition A bounded self-adjoint operator A is said to be of **uniform multiplicity** m if A is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\mu) \oplus \cdots \oplus L^2(\mathbb{R}, d\mu)$ where there are m terms in the sum and μ is a fixed Borel measure.

That this is a good definition is shown by

Proposition If A is unitarily equivalent to multiplication by λ on $L^2(\mathbb{R}, d\mu) \oplus \cdots \oplus L^2(\mathbb{R}, d\mu)$ (m times) and on $L^2(\mathbb{R}, d\nu) \oplus \cdots \oplus L^2(\mathbb{R}, d\nu)$ (n times), then $m = n$ and μ and ν are equivalent measures.

4. Disjoint measure classes

In listing eigenvalues of multiplicity one, two, three, etc. in the finite-dimensional case, we must add a requirement that prevents us from counting an eigenvalue of multiplicity three once as an eigenvalue of multiplicity one and once as an eigenvalue of multiplicity two. In the finite-dimensional case, we avoid this "error" by requiring the lists to be disjoint. The analogous notion for measures is:

Definition Two measure classes $\langle \mu \rangle$ and $\langle \nu \rangle$ are called **disjoint** if any $\mu_1 \in \langle \mu \rangle$ and $\nu_1 \in \langle \nu \rangle$ are mutually singular.

5. The multiplicity theorem

We can now state the basic theorem:

Theorem VII.6 (commutative multiplicity theorem) Let A be a bounded self-adjoint operator on a Hilbert space $\mathcal{H}$. Then there is a decomposition $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \cdots \oplus \mathcal{H}_\infty$ so that

(a) A leaves each $\mathcal{H}_m$ invariant.
(b) $A \restriction \mathcal{H}_m$ has uniform multiplicity m.

(c) The measure classes $\langle \mu_m \rangle$ associated with the spectral representation of $A \restriction \mathscr{H}_m$ are mutually disjoint.

Moreover, the subspaces $\mathscr{H}_1, \ldots, \mathscr{H}_m, \ldots, \mathscr{H}_\infty$ (some of which may be zero) and the *measure classes* $\langle \mu_1 \rangle, \ldots, \langle \mu_m \rangle, \ldots, \langle \mu_\infty \rangle$ are uniquely determined by (a)–(c).

The spectral theorem with the multiplicity theory just described is thus one of those gems of mathematics: a structure theorem, that is, a theorem that describes all objects of a certain sort up to a natural equivalence. Each bounded self-adjoint operator A is described by a family of mutually disjoint measure classes on $[-\|A\|, \|A\|]$; two operators are unitarily equivalent if and only if their spectral multiplicity measure classes are *identical*.

VII.3 Spectral projections

In the last section, we constructed a functional calculus, $f \mapsto f(A)$ for any Borel function f and any bounded self-adjoint operator A. The most important functions gained in passing from the continuous functional calculus to the Borel functional calculus are the characteristic functions of sets.

Definition Let A be a bounded self-adjoint operator and Ω a Borel set of $\mathbb{R}$. $P_\Omega \equiv \chi_\Omega(A)$ is called a **spectral projection** of A.

As the definition suggests, P_Ω is an orthogonal projection since $\chi_\Omega^2 = \chi_\Omega = \bar{\chi}_\Omega$ pointwise. The properties of the family of projections $\{P_\Omega \mid \Omega \text{ an arbitrary Borel set}\}$ is given by the following elementary translation of the functional calculus (Problem 22).

Proposition The family $\{P_\Omega\}$ of spectral projections of a bounded self-adjoint operator, A, has the following properties:

(a) Each P_Ω is an orthogonal projection.
(b) $P_\varnothing = 0$; $P_{(-a,a)} = I$ for some a.
(c) If $\Omega = \bigcup_{n=1}^\infty \Omega_n$ with $\Omega_n \cap \Omega_m = \varnothing$ for all $n \neq m$, then

$$P_\Omega = \operatorname*{s-lim}_{N\to\infty} \left(\sum_{n=1}^N P_{\Omega_n} \right)$$

(d) $P_{\Omega_1} P_{\Omega_2} = P_{\Omega_1 \cap \Omega_2}$

Condition (c) is very reminiscent of the condition defining a measure and in fact one defines:

Definition A family of projections obeying (a)–(c) is called a (bounded) **projection-valued measure** (p.v.m.).

We remark that (d) follows from (a) and (c) by abstract considerations (Problem 22).

As one might guess, one can integrate with respect to a p.v.m. If P_Ω is a p.v.m., then $(\phi, P_\Omega \phi)$ is an ordinary measure for any ϕ. We will use the symbol $d(\phi, P_\lambda \phi)$ to mean integration with respect to this measure. By standard Riesz lemma methods, there is a unique operator B with $(\phi, B\phi) = \int f(\lambda)\, d(\phi, P_\lambda \phi)$. Thus:

Theorem VII.7 If P_Ω is a p.v.m. and f a bounded Borel function on supp P_Ω, then there is a unique operator B which we denote $\int f(\lambda)\, dP_\lambda$ so that

$$(\phi, B\phi) = \int f(\lambda)\, d(\phi, P_\lambda \phi), \qquad \forall \phi \in \mathscr{H}$$

Example If A is a bounded self-adjoint operator and $\{P_\Omega\}$ its associated p.v.m., it is easy to see (Problem 23) that $f(A) = \int f(\lambda)\, dP_\lambda$. In particular $A = \int \lambda\, dP_\lambda$.

Now, suppose a bounded p.v.m. P_Ω is given and we form $A = \int \lambda\, dP_\lambda$. Not surprisingly (Problem 23), P_Ω is just the p.v.m. associated with A. Summarizing:

Theorem VII.8 (spectral theorem—p.v.m. form) There is a one–one correspondence between (bounded) self-adjoint operators A and (bounded) projection valued measures $\{P_\Omega\}$ given by:

$$A \mapsto \{P_\Omega\} = \{\chi_\Omega(A)\}$$

$$\{P_\Omega\} \mapsto A = \int \lambda\, dP_\lambda$$

It is through this theorem and its generalization to unbounded operators that self-adjoint operators arise in quantum mechanics, for the observables occur most naturally as projection-valued measures (see Section VIII.3 for the generalization and the notes to Section VIII.11 for the quantum-mechanical explanation).

Spectral projections can be used to investigate the spectrum of A:

Proposition $\lambda \in \sigma(A)$ if and only if $P_{(\lambda-\varepsilon,\,\lambda+\varepsilon)}(A) \neq 0$ for any $\varepsilon > 0$.

The essential element of the proof is that $\|(A-\lambda)^{-1}\| = [\mathrm{dist}(\lambda, \sigma(A))]^{-1}$ The details are left to Problem 24.

This suggests that we distinguish between two types of spectrum:

Definition We say $\lambda \in \sigma_{\mathrm{ess}}(A)$, the **essential spectrum** of A, if and only if $P_{(\lambda-\varepsilon,\,\lambda+\varepsilon)}(A)$ is infinite dimensional for all $\varepsilon > 0$. If $\lambda \in \sigma(A)$, but $P_{(\lambda-\varepsilon,\,\lambda+\varepsilon)}(A)$ is finite dimensional for some $\varepsilon > 0$, we say $\lambda \in \sigma_{\mathrm{disc}}(A)$, the **discrete spectrum** of A. P is infinite dimensional means Ran P is infinite dimensional.

Thus, we have a second decomposition of $\sigma(A)$. Unlike the first, it is a decomposition into two necessarily disjoint subsets. We note that σ_{disc} is not necessarily closed, but:

Theorem VII.9 $\sigma_{\mathrm{ess}}(A)$ is always closed.

Proof Let $\lambda_n \to \lambda$ with each $\lambda_n \in \sigma_{\mathrm{ess}}(A)$. Since any open interval I about λ contains an interval about some λ_n, $P_I(A)$ is infinite dimensional. ∎

The following three theorems give alternative descriptions of σ_{disc} and σ_{ess}; their proofs are left to the reader (Problem 26).

Theorem VII.10 $\lambda \in \sigma_{\mathrm{disc}}$ if and only if *both* the following hold:

(a) λ is an isolated point of $\sigma(A)$, that is, for some ε, $(\lambda-\varepsilon, \lambda+\varepsilon) \cap \sigma(A) = \{\lambda\}$.

(b) λ is an eigenvalue of finite multiplicity, i.e., $\{\psi \mid A\psi = \lambda\psi\}$ is finite dimensional.

Theorem VII.11 $\lambda \in \sigma_{\mathrm{ess}}$ if and only if *one* or more of the following holds:

(a) $\lambda \in \sigma_{\mathrm{cont}}(A) \equiv \sigma_{\mathrm{ac}}(A) \cup \sigma_{\mathrm{sing}}(A)$.
(b) λ is a limit point of $\sigma_{\mathrm{pp}}(A)$.
(c) λ is an eigenvalue of infinite multiplicity.

Theorem VII.12 (Weyl's criterion) Let A be a bounded self-adjoint operator. Then $\lambda \in \sigma(A)$ if and only if there exists $\{\psi_n\}_{n=1}^{\infty}$ so that $\|\psi_n\| = 1$ and $\lim_{n\to\infty} \|(A-\lambda)\psi_n\| = 0$. $\lambda \in \sigma_{\mathrm{ess}}(A)$ if and only if the above $\{\psi_n\}$ can be chosen to be orthogonal.

As one might guess, the essential spectrum cannot be removed by essentially finite dimensional perturbations. In Section XIII.4, we will prove a general theorem which implies that $\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(B)$ if $A - B$ is compact.

Finally, we discuss one useful formula relating the resolvent and spectral projections. It is a matter of computation to see that

$$f_\varepsilon(x) \to \begin{cases} 0 & x \notin [a,b] \\ \frac{1}{2} & x = a \text{ or } x = b \\ 1 & x \in (a,b) \end{cases}$$

if $\varepsilon \downarrow 0$ where

$$f_\varepsilon(x) = \frac{1}{2\pi i} \int_a^b \left(\frac{1}{x - \lambda - i\varepsilon} - \frac{1}{x - \lambda + i\varepsilon} \right) d\lambda$$

Moreover, $|f_\varepsilon(x)|$ is bounded uniformly in ε, so by the functional calculus, one has:

√ **Theorem VII.13** (Stone's formula) Let A be a bounded self-adjoint operator. Then

$$\operatorname*{s-lim}_{\varepsilon\downarrow 0}\, (2\pi i)^{-1} \int_a^b [(A - \lambda - i\varepsilon)^{-1} - (A - \lambda + i\varepsilon)^{-1}]\, d\lambda = \tfrac{1}{2}[P_{[a,b]} + P_{(a,b)}]$$

VII.4 Ergodic theory revisited: Koopmanism

In Section II.4 we defined ergodicity for a measure preserving bijective map, $T\colon \Omega \to \Omega$ where Ω is a measure space with a finite measure μ, and $\mu(T^{-1}(M)) = \mu(M)$ for any measurable set $M \subset \Omega$. Koopman's lemma told us that the map U defined by $(Uf)(w) = f(Tw)$, is a unitary operator on $L^2(\Omega, d\mu)$. T was called ergodic if and only if 1 was a simple eigenvalue of U (that is, an eigenvalue of multiplicity one). In this section, we wish to examine in detail the idea of Koopman that interesting properties of T can be described in terms of spectral properties of U.