SIMON-REED

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1 ERGODIC THEORY: AN INTRODUCION

In this section we give a brief introduction to ergodic theory. For our discussion we need several concepts not formally defined until Chapter VI: adjoint operators, projection operators, and the kernel and range of an operator. Any reader not already familiar with these concepts should consult Chapter VI. We give this discussion here because ergodic theory illustrates nicely the power and limitations of Hilbert-space methods and serves as a nice example of the main theme of these books, namely the interplay between functional analysis and mathematical physics. We will see that it is useful to reformulate the question of why macroscopic systems approach equilibrium in terms of abstract spaces, but that one must pay a price: The natural question in the abstract setting is slightly different from the original question and one may be tempted to accept weaker results.

The statement "any system approaches an equilibrium state" is sometimes known as the zeroth law of thermodynamics. From a microscopic point of view it is perhaps surprising that any system should approach equilibrium since microscopically there is no steady state and therefore no equilibrium.

Nevertheless, any attempt at a microscopic justification of thermodynamics must explain why the zeroth laws holds macroscopically. There is far from universal agreement among physicists as to what constitutes a justification of the zeroth law, but we would like to avoid a discussion of the pros and cons of the many different approaches which have been suggested (however, see the Notes). The approach that we use is generally accepted by most physicists.

The first basic idea is that thermodynamical systems undergo fluctuations (see Problem 17); put differently, by their very nature the laws of thermodynamics are not absolute statements about a system at a fixed time but are statements about measurements made ver time periods long with respect to some characteristic times such as relaxation or collision times. Thus, thermodynamics deals with average measurements of observables over a time period T. Since the collision times, etc., are dependent on the dynamics, one can only hope to prove thermodynamic statements about the limit as $T \to \infty$. How large T has to be for the average over the interval T to be approximately equal to the limit is a detailed dynamical question, but in specific cases one would hope to be able to prove something.

Let us suppose that we describe the state of a classical mechanical system by a point in some phase space Γ. For each time t; there is a map $\mathsf{T}_t : \Gamma \to \Gamma$, where $\mathsf{T}_t x$ is the state which results by taking a state x at t_0 and waiting until $t_0 + t$ (we are assuming time-translation invariance so t_0 never enters).

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Obviously, $\mathsf{T}_{t+s} = \mathsf{T}_t\mathsf{T}_s$. In classical mechanics, the observables of the system like energy or angular momentum are functions on phase discussion above suggests that we study

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(\mathsf{T}_t x)\,\mathrm{d}t\,. \tag{1}$$

We would like to show that the limit exists, at least for continuous functions. Typically Γ is a metric space, so "continuous" has a meaning. Not only would we like the limit to exist, but it should be independent of the initial point x or at least only dependent on a few "macroscopic" observables we can associate with an equilibrium state. For systems which are time-translation independent, the energy is a conserved quantity, so the average-energy is the initial energy—thus we cannot hope for measurements to be independent of the initial energy. Therefore, for each energy E we look at the constant energy surface, Ω_E, in phase space, and for each $w \in \Omega_E$ and each continuous function f on Ω_E we hope that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(\mathsf{T}_t w)\,\mathrm{d}t \tag{2}$$

exists and is a number, $\mu(f)$, independent of w. The map $f \mapsto \mu(f)$ clearly has three properties:

1. $\mu(1) = 1$.

2. μ is linear.

3. $\mu(f) \geq 0$ if $f \geq 0$.

We will eventually see (Section I[V.4]) that such a μ is always associated with a measure $\hat{\mu}$ on Ω_E with $\hat{\mu}(\Omega_E) = 1$, so that

$$\mu(f) = \int_{\Omega_E} f(w)\,\mathrm{d}\hat{\mu}(w)\,. \tag{3}$$

From now on we denote linear functional μ and the measure $\hat{\mu}$, by the same letter μ.

To summarize: We have shown that if

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(\mathsf{T}_t w)\,\mathrm{d}t \tag{4}$$

exists for each fixed w and is independent of $w \in \Omega_E$, then there is a measure μ on Ω_E so that

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T f(\mathsf{T}_t w)\,\mathrm{d}t = \int_{\Omega_E} f(w)\,\mathrm{d}\mu(w)\,. \tag{5}$$

The measure μ has a very important property. Let s be fixed and suppose χ_F is the characteristic function of a measurable set $F \subset \Omega_E$. The

$$\frac{1}{T} \int_0^T \chi_{\mathsf{T}_s^{-1}F}(\mathsf{T}_t w)\,\mathrm{d}t = \frac{1}{T} \int_0^T \chi_F(\mathsf{T}_s\mathsf{T}_t w)\,\mathrm{d}t \tag{6}$$

so if the $\lim_{T\to\infty}$ exists, then $\mu(\mathsf{T}_s^{-1}F) = \mu(F)$, that is, the measure is **invariant**. We also say that T is **measure preserving**. Classical mechanical systems come equipped with a natural invariant measure: if $\Gamma = \mathbb{R}^{6N}$ (N is the number of particles), the measure $\mathrm{d}^{3N}q\,\mathrm{d}^{3N}p$ is known to be invariant under the Hamiltonian flow (Liouville's theorem). This measure has a restriction to Ω_E given formally by

$$\mu_E(F) = \int_F \delta\left[H(p,q) - E\right]\,\mathrm{d}^{3N}p\,\mathrm{d}^{3N}q \tag{7}$$

where $H(p, q)$ is the Hamiltonian. Explicitly, if we pick a set of local coordinates at $x \in \Omega_E$, say $Q_1, \cdots, Q_{6N-1}$, which are orthogonal and normalized, then

$$d\mu_E = C d^{6N-1} Q / |\nabla H| \,, \tag{8}$$

C is picked so that $\mu_E(\Omega_E) = 1$. Thus, the goal in justifying the zeroth law is to consider

$$M_T(f)(w) = \frac{1}{T} \int_0^T f(T_t w) \, dt \tag{9}$$

and to prove that in a suitable sense the function $(M_T f)(w)$ converges as $T \to \infty$ to the constant function with value

$$\int_{\Omega_E} f(w) \, d\mu_E(w) \,. \tag{10}$$

Notice that if we can prove this, we will have proven much more; not only will we have shown that measurements over long periods of time are independent of the initial conditions (except for the energy), but we will have shown that the equilibrium state is described by a measure in phase space and this measure is

$$\int_F \delta \left[H(p, q) - E \right] d^{3N} p \, d^{3N} q \tag{11}$$

the "microcanonical ensemble".

Hilbert space methods are so powerful that as soon as one has a measure, it is tempting to try to reformulate the problem in terms of $L^2(\Omega_E, d\mu_E)$. Therefore, if $f \in L^2(\Omega_E, d\mu_E)$, we define a map $f \overset{U_t}{\mapsto} f \circ T_t$, that is,

$$(U_t f)(w) = f(T_t w) \,. \tag{12}$$

Lemma 1 (Koopman's lemma). U_t is a unitary map of $L^2(\Omega_E, d\mu_E)$ onto $L^2(\Omega_E, d\mu_E)$.

Proof.

$$(U_t f, U_t g) = \int_{\Omega_E} \overline{f(T_t w)} g(T_t w) \, d\mu_E(w) = \int_{\Omega_E} \overline{f(y)} g(y) \, d\mu_E(T_t^{-1} y) = \tag{13}$$

$$= \int_{\Omega_E} \overline{f(y)} g(y) \, d\mu_E(y) = (f, g) \,,$$

where we have used the invariance of the measure μ_E. Since $U_t U_{-t} = U_0 = I$, U is invertible and thus unitary. $\qquad\square$

We want to study

$$\frac{1}{T} \int_0^T (U_1 f)(w) \, D\mu(w) \,, \tag{14}$$

but it is simpler to consider the discrete analogue

$$\frac{1}{N} \sum_{m=0}^{N-1} U^m f \,. \tag{15}$$

The following elegant result settles the convergence question in the discrete case. Problem 18 extends the discrete result to the continuous case.

Theorem 1 (Mean ergodic theorem, or von Neumann's ergodic theorem). *Let* U *be a unitary operator on a Hilbert space* $\mathcal{H}$. *Let* P *be the orthogonal projection onto* $\{\psi | \psi \in \mathcal{H}, \mathsf{U}\psi = \psi\}$. *Then, for any* $f \in \mathcal{H}$,

$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N-1} \mathsf{U}^n f = \mathsf{P} f . \tag{16}$$

We first prove an elementary technical lemma:

Lemma 2. *1. If* U *is unitary,* $\mathsf{U}f = f$ *if and only if* $\mathsf{U}^\star f = f$.

2. For any operator on a Hilbert space $\mathcal{H}$, $(\operatorname{Ran} \mathsf{A})^\perp = \operatorname{Ker} \mathsf{A}^\star$.

Proof. To prove (2), notice that both conditions are equivalent to $f = \mathsf{U}^{-1} f$. To prove (1), observe that $\psi \in \operatorname{Ker} \mathsf{A}^\star$ means that $(\phi, \mathsf{A}^\star \psi) = 0$ for all ϕ in $\mathcal{H}$. But, $\psi \in (\operatorname{Ran} \mathsf{A})^\perp$ means that $(\mathsf{A}\phi, \psi) = 0$ for all $\phi \in \mathcal{H}$. (2) now follows from the definition of adjoint. □

Proof of the mean ergodic theorem. First let $f = g - \mathsf{U}g$, that is, $f \in \operatorname{Ran} (\mathsf{I} - \mathsf{U})$. Then,

$$\left\| \frac{1}{N} \sum_{n=0}^{N-1} \mathsf{U}^n f \right\| = \left\| \frac{1}{N} (g - \mathsf{U}^N g) \right\| \le \frac{2}{N} \|g\| \overset{N \to \infty}{\Rightarrow} 0 . \tag{17}$$

By an $\varepsilon/3$ argument

$$\frac{1}{N} \sum_{n=0}^{N-1} \mathsf{U}^n f \to 0 \quad \text{for any} \quad f \in \overline{\operatorname{Ran} (\mathsf{I} - \mathsf{U})} . \tag{18}$$

By the lemma,

$$(\operatorname{Ran} (\mathsf{I} - \mathsf{U}))^\perp = \operatorname{Ker} (\mathsf{I} - \mathsf{U}^\star) = \{\psi | \mathsf{U}^\star \psi = \psi\} = \{\psi | \mathsf{U}\psi = \psi\} . \tag{19}$$

Therefore, $\mathsf{P}f = 0$ if and only if $f \in \overline{\operatorname{Ran} (\mathsf{I} - \mathsf{U})}$. Now, suppose $\mathsf{P}f = f$. Trivially,

$$\frac{1}{N} \sum_{n=0}^{N-1} \mathsf{U}^n f = f \tag{20}$$

converges to $f = \mathsf{P}f$. Thus the limit statement hold on $\overline{\operatorname{Ran} (\mathsf{I} - \mathsf{U})}$ and on $\operatorname{Ker} (\mathsf{I} - \mathsf{U}^\star)$ and therefore on $\overline{\operatorname{Ran} (\mathsf{I} - \mathsf{U})} \oplus \operatorname{Ker} (\mathsf{I} - \mathsf{U}^\star)$, which is all of $\mathcal{H}$ by the projection theorem and (2) above. □

In the continuous case $\mathsf{U}_t f = f \circ \mathsf{T}_t$, what are the functions in $L^2(\Omega_E, \mathrm{d}\mu_E)$ which satisfy $\mathsf{U}_t f = f$? Clearly, the constant functions are invariant.

Definition 1. T_t is called **ergodic** if the constant functions are the only functions on $L^2(\Omega_E, \mathrm{d}\mu_E)$ for which $f \circ \mathsf{T}_t = f$ (as L^2 function) for all t.

Given the continuous analogue of the mean ergodic theorem (Problem 18) we have:

Corollary 1. *Let* T_t *be ergodic. Then for any* $f \in L^2(\Omega_E, \mathrm{d}\mu_E)$,

$$L^2 - \lim_{T \to \infty} \frac{1}{T} \int_0^T f(\mathsf{T}_t w) \, \mathrm{d}t = \int_{\Omega_E} f(y) \, \mathrm{d}\mu_E(y) . \tag{21}$$
eq:II.4

Proof. In this case $\{\psi | \mathsf{U}\psi = \psi\}$ is one dimensional. Thus $\mathsf{P}\psi$ is a constant C and

$$C = (1, \psi) = \int_{\Omega_E} \psi(w) \, \mathrm{d}\mu_E(w) \,. \tag{22}$$

$\square$

Notice that if (21) holds then $\mathsf{P}\psi$ is constant so that T_t must be ergodic; thus ergodicity is necessary and sufficient for (21) to hold. It is sometimes useful to express ergodicity in terms of the measure.

Proposition 1. T_t *is ergodic if and only if for all measurable sets* $F \in \Omega_E$.

Proof. Suppose T_t is ergodic and $\mathsf{T}_t^{-1}F = F$ for all t. Then $f = \chi_F$ is an invariant function so χ_F is constant a.e., which implies $\mu_E(F) = 0$ or $\mu_E(F) = 1$.

Conversely, suppose that the second condition holds. Then $\{w | f(w) < \alpha\}$ is invariant under T_t so $f(w) < a$ ae. or $f(w) \geq a$ a.e. Since this is true for all a, $f(w)$ is constant a.e. $\square$

The condition that $\mathsf{T}_t^{-1}F = F$ implies $\mu_E(F) = 0$ or $\mu_E(F) = 1$ is sometimes called **metric transitivity**. Let us take stock of what we have proven. We have derived a necessary and sufficient condition on the flow T_t so that

$$\lim_{T \to \infty} \frac{1}{T} \int_0^T f(\mathsf{T}_t w) \, \mathrm{d}t \tag{23}$$

is precisely what we want it to be, but not in the sense of convergence for each w; instead, we have L^2 convergence of $1T \int_0^T f(\mathsf{T}_t w) \, \mathrm{d}t$ to the constant function

$$\int_{\Omega_E} f(w) \, \mathrm{d}\mu(w) \,. \tag{24}$$

This is not surprising since pointwise convergence is not an L^2 notion. By using Hilbert space methods we have given up the chance of proving that

$$\frac{1}{T} \int_0^T f(\mathsf{T}_t w) \, \mathrm{d}t \tag{25}$$

converges pointwise for each w as $T \to \infty$. Actually, the pointwise limit does exist but this must be proven by entirely different methods. We state the result:

Theorem 2 (Individual or Birkhoff ergodic theorem)**.** *Let* T *be a measure preserving transformation on a measure space* (Ω, μ). *Them for any* $f \in L^1(\Omega, \mu)$,

$$\lim_{N \to 0} \frac{1}{N} \sum_{N=0}^{N-1} f(\mathsf{T}^n x) \tag{26}$$

exist pointwise a.e. and is some function $f^\star \in L^1(\Omega, \mathrm{d}\mu)$ *satisfying* $f^\star(\mathsf{T}x) = f^\star(x)$. *If* $\mu(\Omega) < \infty$, *then*

$$\int_\Omega f^\star(x) \, \mathrm{d}\mu(x) = \int_\Omega f(x) \, \mathrm{d}\mu(x) \,. \tag{27}$$

Furthermore, if μ *is ergodic and* $\mu(\Omega) = 1$, *then*

$$\frac{1}{N} \sum_{n=0}^{N-1} f(\mathsf{T}^n x) \overset{N \to \infty}{\to} \int_\Omega f(y) \, \mathrm{d}\mu(y) \tag{28}$$

for almost all x.

This theorem is closer to what one wants to justify statistical mechanics than the von Neumann theorem, and it is fashionable to say that the von Neumann theorem is unsuitable for statistical mechanics. We feel that this is an exaggeration. If we had only the von Neumann theorem we could probably live with it quite well. Typically, initial conditions are not precisely measurable anyway, so that one could well associate initial states with measures $f \, d\mu$ where $\int f \, d\mu = 1$, in which case the von Neumann theorem suffices. However, the Birkhoff theorem does hold and is clearly a result that we are happier to use in justifying the statement that phase-space averages and time averages are equal.

Finally, one should ask whether classical mechanical flows on constant energy surfaces are in fact ergodic. Little is known about this interesting but difficult question. However, Sinai has shown recently that a gas of hard spheres in a box is an ergodic system.

2   DOMAINS, GRAPHS, ADJOINTS AND SPECTRUM

It is a fact of life that many of the most important operators which occur in mathematical physics are not bounded. In this chapter we will introduce some of the basic definitions and theorems necessary for dealing with unbounded operators on Hilbert spaces. The Hellinger-Toeplitz theorem (see Section III.5) says that an everywhere-defined operator A which satisfies $(A\phi, \psi) = (\phi, A\psi)$ is necessarily a bounded operator suggesting that a general unbounded operator T will only be defined on a dense linear subset of the Hilbert space. Thus an **operator** on a Hilbert space $\mathcal{H}$ is a linear map from its domain, a linear subspace of $\mathcal{H}$, into $\mathcal{H}$. Unless we specify otherwise, we will always suppose that the domain is dense. This subspace, which we denote by $D(T)$, is called the **domain** of the operator T. So, to identify an unbounded operator on a Hilbert space one must first give the domain on which it acts and then specify how it acts on that subspace.

Example 1 (The position operator)**.** Let $\mathcal{H} = L^2(\mathbb{R})$ and let $D(T)$ be the set of functions ϕ in $L^2(\mathbb{R})$ which satisfy $\int_{-\infty}^{\infty} x^2 |\phi(x)|^2 \, dx < \infty$. For $\phi \in D(T)$ define $(T\phi)(x) = x\phi(x)$. It is clear that T is unbounded since if we choose ϕ to have support near plus or minus infinity, we can make $\|T\phi\|$ as large as we like while keeping $\|\phi\| = 1$. Of course, even if $\phi \notin D(T)$, $x\phi(x)$ has a well- defined meaning as a function, but it is not in $L^2(\mathbb{R})$. Thus, if we want to deal only with the Hilbert space $L^2(\mathbb{R})$ we must restrict the domain of T. The domain we have chosen is the largest one for which the range is in $L^2(\mathbb{R})$.

Example 2. Let $\mathcal{H} = L^2(\mathbb{R})$ and $D(T) = \mathcal{S}(\mathbb{R})$. On $D(T)$ define $T\psi = -\psi''(x) + x^2\psi(x)$. If $\phi_n(x)$ is the n-th Hermite function (see the appendix to Section V.3), then $\phi_n \in D(T)$ and $T\phi_n(x) = (2n + 1)\phi_n(x)$. Thus T must be unbounded since it has arbitrarily large eigenvalues.

The notion of the graph of a linear transformation, introduced by von Neumann, is very useful for studying unbounded operators.

Definition 2. The **graph** of the linear transformation T is the set of pairs

$$\{[\phi, T\phi] \, | \, \phi \in D(T)\} \, . \tag{29}$$

The graph of T, denoted by $\Gamma(T)$, is thus a subset of $\mathcal{H} \times \mathcal{H}$ which is a Hilbert space with inner product

$$([\phi_1, \psi_1], [\phi_2, \psi_2]) = (\phi_1, \phi_2) + (\psi_1, \psi_2) \, . \tag{30}$$

T is called a closed operator if $\Gamma(T)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.

Definition 3. Let T_1 and T be operators on $\mathcal{H}$. If $\Gamma(T_1) \supset \Gamma(T)$, then T_1 is said to be an **extension** of T and we write $T_1 \supset T$. Equivalently, $T_1 \supset T$ if and only if $D(T_1) \supset D(T)$ and $T_1\phi = T\phi$ for all $\phi \in D(T)$.

Definition 4. An operator T is **closable** if it has a closed extension. Every closable operator has a smallest closed extension, called its **closure**, which we denote by $\overline{T}$.

A natural way to try to obtain a closed extension of an operator T, is to take the closure of its graph in $\mathcal{H} \times \mathcal{H}$. The trouble with this is that $\Gamma(T)$ may not be the graph of an operator (for example, see Problem 1). However, most operators which we deal with will be symmetric operators (introduced Section VIII.2) and we will see that they always have closed extensions.

Proposition 2. *If* T *is closable, then* $\Gamma(\overline{T}) = \overline{\Gamma(T)}$.

Proof. Suppose that S is a closed extension of T. Then $\overline{\Gamma(T)} \subset \Gamma(S)$ so if $[0, \psi] \in \overline{\Gamma(T)}$ then $\psi = 0$.

Define R with $D(R) = \left\{ \psi | [\psi, \phi] \in \overline{\Gamma(T)} \text{ for some } \phi \right\}$ by $R\psi = \phi$ where $\phi \in \mathcal{H}$ is the unique vector so that $[\psi, \phi] \in \overline{\Gamma(T)}$. Then $\Gamma(R) = \overline{\Gamma(T)}$ so R is a closed extension of T. But $R \subset S$ which is an arbitrary closed extension, so $R = \overline{T}$. $\qquad\square$

The following example illustrates the concepts we have just introduced.

Example 3. Let $\mathcal{H} = L^2(\mathbb{R})$, $D(T) = C_0^\infty(\mathbb{R})$ and $D(T_1) = C_0^1(\mathbb{R})$, the once continuously differentiable functions with compact support. Let $Tf = if'(x)$ if $f \in D(T)$ and $T_1 f = if'(x)$ if $f \in D(T_1)$. T_1 is an extension of T.

We will show that $\overline{\Gamma(T)} \supset \Gamma(T_1)$. When we prove that T is symmetric and therefore closable, it will follow that $\overline{T}$ extends T_1.

First we introduce the approximate identity, $\{j_\varepsilon(x)\}$. Let $j(x)$ be any positive, infinitely differentiable function with support in $(-1, 1)$ so that $\int_{-\infty}^{\infty} j(x)\mathrm{d}x = 1$. Define $j_\varepsilon(x) = \frac{1}{\varepsilon} j(\frac{x}{\varepsilon})$. If $\phi \in D(T_1)$, set

$$\phi_\varepsilon(x) = \int_{-\infty}^{\infty} j_\varepsilon(x - t)\phi(t)\,\mathrm{d}t\,. \tag{31}$$

Then

$$|\phi_\varepsilon(x) - \phi(x)| \leq \int_{-\infty}^{\infty} j_\varepsilon(x - t)|\phi(t) - \phi(x)|\,\mathrm{d}t \leq \tag{32}$$

$$\leq \left(\sup_{t:|x-t|<\varepsilon} |\phi(t) - \phi(x)| \right) \int_{-\infty}^{\infty} j_\varepsilon(x - t)\,\mathrm{d}t = \sup_{t:|x-t|<\varepsilon} |\phi(t) - \phi(x)|\,.$$

Since ϕ has compact support, it is uniformly continuous which implies that $\phi_\varepsilon \to \phi$ uniformly. Since the ϕ_ε have support in a fixed compact set, $\phi_\varepsilon \to \phi$ in $L^2(\mathbb{R})$.

Similarly,

$$i\frac{\mathrm{d}}{\mathrm{d}x}\phi_\varepsilon(x) = \int_{-\infty}^{\infty} i\frac{\mathrm{d}}{\mathrm{d}x}j_\varepsilon(x - t)\phi(t)\,\mathrm{d}t = \int_{-\infty}^{\infty} -i\left(\frac{\mathrm{d}}{\mathrm{d}t}j_\varepsilon(x - t) \right)\phi(t)\,\mathrm{d}t = \tag{33}$$

$$= \int_{-\infty}^{\infty} j_\varepsilon(x - t)i\frac{\mathrm{d}}{\mathrm{d}t}\phi(t)\,\mathrm{d}t \xrightarrow{L^2(\mathbb{R})} i\frac{\mathrm{d}}{\mathrm{d}x}\phi(x)\,.$$

Since $j_\varepsilon(x)$ has compact support and is infinitely differentiable, $\phi_\varepsilon \in C_0^\infty(\mathbb{R})$. Thus, $\phi_\varepsilon \in D(T)$ for each $\varepsilon > 0$. What we have shown above is that

$$\phi_\varepsilon \xrightarrow{L^2(\mathbb{R})} \phi\,, \quad T\phi_\varepsilon \xrightarrow{L^2(\mathbb{R})} T\phi\,. \tag{34}$$

Thus, the closure of the graph of T contains the graph of T_1. The notion of adjoint operator can be extended to the unbounded case.

Definition 5. Let T be a densely defined linear operator on a Hilbert space $\mathcal{H}$. Let $D(\mathsf{T}^\star)$ be the set of $\phi \in \mathcal{H}$ for which there is an $\eta \in \mathcal{H}$ with

$$(\mathsf{T}\psi, \phi) = (\psi, \eta) \quad \text{for all } \psi \in D(\mathsf{T}). \tag{35}$$

For each such $\phi \in D(\mathsf{T}^\star)$ we define $\mathsf{T}^\star \phi = \eta$. $\mathsf{T}^\star$ is called the **adjoint** of T. By the Riesz lemma, $\phi \in D(\mathsf{T}^\star)$ if and only if $|(\mathsf{T}\psi, \phi)| \le C\,\|\psi\|$ for all $\psi \in D(\mathsf{T})$.

We note that $\mathsf{S} \subset \mathsf{T}$ implies $\mathsf{T}^\star \subset \mathsf{S}^\star$. Notice that for η to be uniquely determined by (35) we need the fact that $D(\mathsf{T})$ is dense. Unlike the case of bounded operators, the domain of $\mathsf{T}^\star$ may not be dense as the following example shows. As a matter of fact it is possible to have $D(\mathsf{T}^\star) = \{0\}$.

Example 4. Suppose that f is a bounded measurable function, but that $f \notin L^2(\mathbb{R})$. Let $D(\mathsf{T}) = \left\{ \psi \in L^2(\mathbb{R})\,|\, \int_{-\infty}^{\infty} f(x)\psi(x)\,\mathrm{d}x < \infty \right\}$. $D(\mathsf{T})$ certainly contains all the L^2 functions with compact support so $D(\mathsf{T})$ is dense in $L^2(\mathbb{R})$. Let ψ_0 be some fixed vector in $L^2(\mathbb{R})$ and define $\mathsf{T}\psi = (f, \psi)\psi_0$ for $\psi \in D(\mathsf{T})$. Suppose that $\phi \in D(\mathsf{T}^\star)$, then for all $\psi \in D(\mathsf{T})$

$$(\psi, \mathsf{T}^\star \phi) = (\mathsf{T}\psi, \phi) = ((f, \psi)\psi_0, \phi) = \overline{(f, \psi)}(\psi_0, \phi) = (\psi, (\psi_0, \phi)f). \tag{36}$$

Thus $\mathsf{T}^\star \phi = (\psi_0, \phi)f$. Since $f \notin L^2(\mathbb{R})$, $(\psi_0, \phi) = 0$. Thus any $\phi \in D(\mathsf{T}^\star)$ is orthogonal to ψ_0, so $D(\mathsf{T}^\star)$ is not dense. In fact, $D(\mathsf{T}^\star)$ is just the vectors perpendicular to ψ_0, and on that domain $\mathsf{T}^\star$ is the zero operator.

If the domain of $\mathsf{T}^\star$ is dense, then we can define $\mathsf{T}^{\star\star} = (\mathsf{T}^\star)^\star$. There is a simple relationship between the notions of adjoint and closure.

Theorem 3. *Let T be a densely defined operator on a Hilbert space $\mathcal{H}$. Then:*

- $\mathsf{T}^\star$ *is closed.*

- T *is closable if and only if $D(\mathsf{T}^\star)$ is dense in which case $\overline{\mathsf{T}} = \mathsf{T}^{\star\star}$.*

- *If T is closable, then $(\overline{\mathsf{T}})^\star = \mathsf{T}^\star$.*

Proof. We define a unitary operator V on $\mathcal{H} \times \mathcal{H}$ by

$$\mathsf{V}[\phi, \psi] = [-\psi, \phi]. \tag{37}$$

Since V is unitary, $\mathsf{V}[E^\perp] = (\mathsf{V}[E])^\perp$ for any subspace E. Let T be a linear operator on $\mathcal{H}$ and suppose $[\phi, \eta] \subset \mathcal{H} \times \mathcal{H}$. Then $[\phi, \eta] \in \mathsf{V}[\Gamma(\mathsf{T})]^\perp$ if and only if $([\phi, \eta], [-\mathsf{T}\psi, \psi]) = 0$ for all $\psi \in D(\mathsf{T})$ which holds if and only if $(\phi, \mathsf{T}\psi) = (\eta, \psi)$ for all $\psi \in D(\mathsf{T})$, that is, if and only if $[\phi, \eta] \in \Gamma(\mathsf{T}^\star)$. Thus $\Gamma(\mathsf{T}^\star) = \mathsf{V}\,[\Gamma(\mathsf{T})]^\perp$. Since $\mathsf{V}[\Gamma(\mathsf{T})]^\perp$ is always a closed subspace of $\mathcal{H} \times \mathcal{H}$, this proves (1).

To prove (2), observe that $\Gamma(\mathsf{T})$ is a linear subset of $\mathcal{H} \times \mathcal{H}$ so

$$\overline{\Gamma(\mathsf{T})} = \left[\Gamma(\mathsf{T})^\perp\right]^\perp = \left[\mathsf{V}^2 \Gamma(\mathsf{T})^\perp\right]^\perp = \left[\mathsf{V}(\mathsf{V}\Gamma(\mathsf{T}))^\perp\right]^\perp. \tag{38}$$

MB: If M is an subspace of $\mathcal{H}$, then $M^\perp$ is always closed. If $\{y_n\}_n \subset M^\perp$ which $y_n \to y$, then $(y_n, x) = 0$ for all $x \in M$ and so $(y, x) = 0$ for all $x \in M$, therefore $y \in \mathcal{H}$. Also $(M^\perp)^\perp = \overline{M}$.

Thus, by the proof of (1), if $\mathsf{T}^\star$ is densely defined, $\Gamma(\mathsf{T})$ is the graph of $\mathsf{T}^{\star\star}$.

Conversely, suppose that $D(\mathsf{T}^\star)$ is not dense and that $\psi \in D(\mathsf{T}^\star)^\star$. A simple computation shows that $[\psi, 0] \in [\Gamma(\mathsf{T}^\star)]^\perp$ so $\mathsf{V}[\mathsf{T}(\mathsf{T}^\star)]^\perp$ is not the graph of a (single-valued) operator. Since $\overline{\Gamma(\mathsf{T})} = \mathsf{V}[\mathsf{T}(\mathsf{T}^\star)]^\perp$, we see that T is not closable.

To prove (3), notice that if T is closable,

$$\mathsf{T}^\star = \overline{(\mathsf{T}^\star)} = \mathsf{T}^{\star\star\star} = (\overline{\mathsf{T}})^\star . \tag{39}$$

$\square$

Definition 6. Let T be a closed operator on a Hilbert space 9. A complex number λ is in the resolvent set $\rho(\mathsf{T})$, if $\lambda \mathsf{I} - \mathsf{T}$ is a bijection of $D(\mathsf{T})$ onto $\mathcal{H}$ with a bounded inverse. If $\lambda \in \rho(\mathsf{T})$, operator $\mathsf{R}_\lambda(\mathsf{T}) = (\lambda \mathsf{I} - \mathsf{T})^{-1}$ is called the **resolvent** of T at λ.

For a point to be in the resolvent set of T, several conditions must be satisfied. These conditions are not all independent. For example, if $\lambda \mathsf{I} - \mathsf{T}$ is a bijection of $D(\mathsf{T})$ onto $\mathcal{H}$, by the closed-graph theorem, its inverse is automatically bounded. For other relationships, see Problem 2.

The definitions of **spectrum**, **point spectrum**, and **residual spectrum** are the same for unbounded operators as they are for bounded operators. We will sometimes refer to the spectrum of nonclosed, but closable operators. In this case we always mean the spectrum of the closure.

Theorem 4. *Let* T *be a closed densely defined linear operator. Then the resolvent set of* T *is an open subset of the complex plane on which the resolvent is an analytic operator-valued function. Furthermore,*

$$\{\mathsf{R}_\lambda(\mathsf{T}) | \lambda \in \rho(\mathsf{T})\} \tag{40}$$

is a commuting family of bounded operators satisfying

$$\mathsf{R}_\lambda(\mathsf{T}) - \mathsf{R}_\mu(\mathsf{T}) = (\mu - \lambda)\mathsf{R}_\mu(\mathsf{T})\mathsf{R}_\lambda(\mathsf{T}) . \tag{41}$$

The proof of this theorem is exactly the same as the proof of the bounded case (Theorem VI.5). It may seem to the reader that many of the questions about domains and closures of unbounded operators are just a technical inconvenience; that one need only choose any dense domain which is small enough so that the unbounded operator makes sense and that is good enough. However, the choice of an appropriate domain is often intimately connected with the physics of the situation being described; see, for example, the discussion in Section X.1. Further, many of the properties of operators which are important are very sensitive to the choice of domain. The following example shows that the spectrum is such a property. In the example we use the notion of "absolutely continuous function" and the corresponding fundamental theorem of calculus. The reader who is unfamiliar with the definition and theorem can find them in the notes.

Example 5. We denote by $AC[0,1]$ the set of absolutely continuous functions on $[0,1]$ whose derivatives are in $L^2([0,1])$. Let T_1, and T_2, be the operation $\mathsf{i}\dfrac{\mathsf{d}}{\mathsf{d}x}$ with domains

$$D(\mathsf{T}_1) = \{\phi | \phi \in AC[0,1]\} , \tag{42}$$

$$D(\mathsf{T}_2) = \{\phi | \phi \in AC[0,1] \text{ and } \phi(0) = 0\} . \tag{43}$$

Both $D(\mathsf{T}_1)$ and $D(\mathsf{T}_2)$ are dense in $L^2([0,1])$ and both of the operators are closed. But:

1. The spectrum of T_1 is $\mathbb{C}$.

2. The spectrum of T_2 is empty.

The proof that T_1 and T_2 are closed is left as an exercise (Problem 3). To see that the spectrum of T_1 is the whole plane we observe that

$$(\lambda\mathsf{I} - \mathsf{T}_1)e^{-i\lambda x} = 0 \quad \text{and} e^{-i\lambda x} \in D(\mathsf{T}_1) \tag{44}$$

for all $\lambda \in \mathbb{C}$. As for the T_2, the operator

$$(\mathsf{S}_\lambda g)(x) = i \int_0^x e^{-i\lambda(x-s)} g(s)\, ds \tag{45}$$

satisfies $(\lambda I - \mathsf{T}_2)\mathsf{S}_\lambda = \mathsf{I}$ and $\mathsf{S}_\lambda(\lambda\mathsf{I} - \mathsf{T}_2)$ is the identity on $D(\mathsf{T}_2)$. Moreover,

$$\|\mathsf{S}_\lambda g\|_2^2 = \int_0^1 |(\mathsf{S}_\lambda g)(x)|^2\, dx \le \left(\sup_{x\in[0,1]} |(\mathsf{S}_\lambda g)(x)| \right)^2 \le \tag{46}$$

$$\le \left(\sup_{x\in[0,1]} \int_0^x |e^{-i\lambda(x-s)} g(s)|\, ds \right)^2 \le$$

$$\le \left(\sup_{x\in[0,1]} \int_0^x \left| e^{-i\lambda(x-s)} g(s) \right|^2 ds \right) \left(\sup_{x\in[0,1]} \int_0^x |g(s)|^2\, ds \right) \le C(\lambda)\, \|g\|_2^2\, ,$$

so S_λ is bounded. By the remark immediately after the definition of resolvent set, we need only have shown that $\lambda\mathsf{I} - \mathsf{T}_2$ is a bijection to conclude that S_λ is bounded. So, we could have avoided the above computation.

3 SYMMETRIC AND SELF-ADJOINT OPERATORS: THE BASIC CRITERION FOR SELF-ADJOINTNESS

Definition 7. A densely defined operator T on a Hilbert space is called **symmetric** (or **Hermitian**) if $\mathsf{T} \subset \mathsf{T}^\star$, that is, if $D(\mathsf{T}) < D(\mathsf{T}^\star)$ and $\mathsf{T}\phi = \mathsf{T}^\star\phi$ for all $\phi \in D(\mathsf{T})$. Equivalently, T is symmetric if and only if

$$(\mathsf{T}\phi, \psi) = (\phi, \mathsf{T}\psi) \quad \text{for all } \phi, \psi \in D(\mathsf{T})\,. \tag{47}$$

Definition 8. T is called **self-adjoint** if $\mathsf{T} = \mathsf{T}^\star$, that is, if and only if T is symmetric and $D(\mathsf{T}) = D(\mathsf{T}^\star)$.

A symmetric operator is always closable, since $D(\mathsf{T}^\star) \supset D(\mathsf{T})$ is dense in $\mathcal{H}$. If T is symmetric, $\mathsf{T}^\star$ is a closed extension of T, so the smallest closed extension $T^{\star\star}$ of T must be contained in $\mathsf{T}^\star$. Thus for symmetric operators, we have

$$\mathsf{T} \subset \mathsf{T}^{\star\star} \subset \mathsf{T}^\star\,. \tag{48}$$

For closed symmetric operators,

$$\mathsf{T} = \mathsf{T}^{\star\star} \subset \mathsf{T}^\star\,. \tag{49}$$

And, for self-adjoint operators,

$$\mathsf{T} = \mathsf{T}^{\star\star} = \mathsf{T}^{\star} . \tag{50}$$

From this one can easily see that a closed symmetric operator T is self-adjoint if and only if $\mathsf{T}^{\star}$ is symmetric. The distinction between closed symmetric operators and self-adjoint operators is very important. It is only for self-adjoint operators that the spectral theorem holds (see Section VIII.3) and it is only self-adjoint operators that may be exponentiated to give the one-parameter unitary groups (see Section VII1.4) which give the dynamics in quantum mechanics. Chapter X is mainly devoted to studying methods for proving that operators are self adjoint. We content ourselves here with proving the basic criterion for self-adjointness. First, we introduce the useful notion of essential self-adjointness.

Definition 9. A symmetric operator T is called **essentially self-adjoint** if its closure $\overline{\mathsf{T}}$ is self-adjoint. If T is closed, a subset $D \subset D(\mathsf{T})$ is called a **core** for T if $\overline{\mathsf{T}|_D} = \mathsf{T}$.

If T is essentially self-adjoint, then it has one and only one self-adjoint extension, for suppose that S is a self-adjoint extension of T. Then, S is closed and thereby, since $\mathsf{S} \supset \mathsf{T}$, $\mathsf{S} \supset \mathsf{T}^{\star\star}$. Thus, $\mathsf{S} = \mathsf{S}^{\star} \subset (\mathsf{T}^{\star\star})^{\star} = \mathsf{T}^{\star\star}$, and so $\mathsf{S} = \mathsf{T}^{\star\star}$. The converse is also true; namely, if T has one and only one self-adjoint extension, then T is essentially self-adjoint (see Section X.1). Since $\mathsf{T}^{\star} = \overline{\mathsf{T}}^{\star} = \mathsf{T}^{\star\star\star}$, T is essentially self-adjoint if and only if

$$\mathsf{T} \subset \mathsf{T}^{\star\star} = \mathsf{T}^{\star} . \tag{51}$$

The importance of essential self-adjointness is that one is often given a nonclosed symmetric operator T. If T can be shown to be essentially self-adjoint, then there is uniquely associated to T a self-adjoint operator $\mathsf{T} = \mathsf{T}^{\star\star}$. Another way of saying this is that if A is a self-adjoint operator, then to specify A uniquely one need not give the exact domain of A (which is often difficult), but just some core for A. Now, suppose that T is a self-adjoint operator and that there is a $\phi \in D(\mathsf{T}^{\star}) = D(\mathsf{T})$ so that $\mathsf{T}^{\star}\phi = i\phi$. Then $\mathsf{T}\phi = i\phi$ and

$$-i(\phi,\phi) = (i\phi,\phi) = (\mathsf{T}\phi,\phi) = (\phi,\mathsf{T}^{\star}\phi) = (\phi,\mathsf{T}\phi) = i(\phi,\phi) , \tag{52}$$

so $\phi = 0$. A similar proof shows that $\mathsf{T}^{\star}\phi = -i\phi$ can have no solutions.

The converse statement, that if T is a closed symmetric operator and $\mathsf{T}^{\star}\phi = \pm i\phi$ has no solutions, then T is self-adjoint, is the basic criterion of self-adjointness.

Theorem 5 (The basic criterion for self-adjointness)**.** *Let T be a symmetric operator on a Hilbert space $\mathcal{H}$. Then the following three statements are equivalent:*

1. *T is self-adjoint.*

2. *T is closed and $\mathrm{Ker}\left(\mathsf{T}^{\star} \pm i\right) = \{0\}$.*

3. *$\mathrm{Ran}\left(\mathsf{T} \pm i\right) = \mathcal{H}$.*

Proof. We have just seen that (1) implies (2). Suppose that (2) holds; we will prove (3). Since $\mathsf{T}^{\star}\phi = -i\phi$ has no solutions, $\mathrm{Ran}\left(\mathsf{T} - i\right)$ must be dense. Otherwise, if $\psi \in \mathrm{Ran}\left(\mathsf{T} - i\right)^{\perp}$, we would have $((\mathsf{T} - i)\phi, \psi) = 0$ for all $\phi \in D(\mathsf{T})$, so $\psi \in D(\mathsf{T}^{\star})$ and $(\mathsf{T} - i)^{\star}\psi = (\mathsf{T}^{\star} + i)\psi = 0$ which is impossible since $\mathsf{T}^{\star} = -i\psi$ has no solutions. (Reversing this last argument we can show that if $\mathrm{Ran}\left(\mathsf{T} - i\right)$ is dense, the kernel of $\mathsf{T}^{\star} + i$ is $\{0\}$.) Since $\mathrm{Ran}\left(\mathsf{T} - i\right)$ is dense, we need only prove it is closed to conclude that $\mathrm{Ran}\left(\mathsf{T} - i\right) = \mathcal{H}$. But for all $\phi \in D(\mathsf{T})$

$$\|(\mathsf{T} - i)\phi\|^2 = \|\mathsf{T}\phi\|^2 + \|\phi\|^2 . \tag{53}$$

Thus if $\phi_n \in D(\mathsf{T})$ and $(\mathsf{T} - i)\phi_n \to \psi_0$, we conclude that ϕ_n converges to some vector ϕ_0 and $\mathsf{T}\phi_n$ converges too. Since T is closed, $\phi_0 \in D(\mathsf{T})$ and $(\mathsf{T} - i)\phi_0 = \psi_0$. Thus, Ran $(\mathsf{T} - i)$ is closed, so Ran $(\mathsf{T} - i) = \mathcal{H}$. Similarly, Ran $(T + i) = \mathcal{H}$.

Finally, we will show that (3) implies (1). Let $\phi \in D(\mathsf{T}^\star)$. Since Ran $(\mathsf{T} - i) = \mathcal{H}$, there is an $\eta \in D(\mathsf{T})$ so that $(\mathsf{T} - i)\eta = (\mathsf{T}^\star - i)\phi$. $D(\mathsf{T}) \subset D(\mathsf{T}^\star)$, so $\phi - \eta \in D(\mathsf{T}^\star)$ and

$$(\mathsf{T}^\star - i)(\phi - \eta) = 0. \tag{54}$$

Since Ran $(\mathsf{T} + i)) = \mathcal{H}$, Ker $(\mathsf{T}^\star - i) = \{0\}$, so $\phi = \eta \in D(\mathsf{T})$. This proves that $D(\mathsf{T}^\star) = D(\mathsf{T})$, so T is self-adjoint.

$\square$

Corollary 2. *Let* T *be a symmetric operator on a Hilbert space. Then the following are equivalent:*

1. T *is essentially self-adjoint.*

2. Ker $(\mathsf{T}^\star \pm i) = \{0\}$.

3. Ran $(\mathsf{T} \pm i)$ *are dense.*

We conclude with an example which shows that a symmetric operator may have many self-adjoint extensions. Lest the reader be misled we remark that a symmetric operator may have no self-adjoint extensions (see Problem 4 and Section X.1).

Example 6. Let $\mathsf{T} = i\dfrac{\mathrm{d}}{\mathrm{d}x}$ with

$$D(\mathsf{T}) = \{\phi | \phi \in AC[0,1], \, \phi(0) = 0 = \phi(1)\}. \tag{55}$$

A simple integration by parts shows that as an operator on $L^2([0,1])$, T is symmetric. We begin by determining $\mathsf{T}^\star$. Let j_ε be the function defined in Example 3 of Section VIII.1. Fix $0 < \alpha < \beta < 1$ and define

$$f_\varepsilon^{\alpha,\beta}(x) = j_\varepsilon(x - \beta) - j_\varepsilon(x - \alpha), \tag{56}$$

$$g_\varepsilon^{\alpha,\beta}(x) = \int_0^x f_\varepsilon^{\alpha,\beta}(t) \, \mathrm{d}t. \tag{57}$$

Let $\psi \in D(\mathsf{T}^\star)$. For ε small enough, $g_\varepsilon^{\alpha,\beta} \in D(\mathsf{T})$ so

$$(\mathsf{T}g_\varepsilon^{\alpha,\beta}, \psi) = (g_\varepsilon^{\alpha,\beta}, \mathsf{T}^\star\psi). \tag{58}$$

As $\varepsilon \to 0$, $-g_\varepsilon^{\alpha,\beta}$ converges to the characteristic function of (α, β) in $L^2((0,1))$ so

$$(g_\varepsilon^{\alpha,\beta}, \mathsf{T}^\star\psi) \to -\int_\alpha^\beta (\mathsf{T}^\star\psi)(x) \, \mathrm{d}x. \tag{59}$$

The basic estimate of Example 3 shows that

$$J_\varepsilon\phi = \int_0^1 j_\varepsilon(x - t)\phi(t) \, \mathrm{d}t \tag{60}$$

converges in $L^2(\mathbb{R})$ to ϕ if ϕ is continous. Moreover, each J_ε is a bounded operator of norm not greater than one. For if $\psi \in L^2((0,1))$, then

$$|(\psi, J_\varepsilon\phi)| \leq \int_{[0,1]\times[0,1]} j_\varepsilon(x-t)|\phi(t)||\psi(x)|\,\mathrm{d}x\mathrm{d}t = \int_{[0,1]\times[0,1]} j_\varepsilon(y)|\phi(t)||\psi(y+t)|\,\mathrm{d}y\mathrm{d}t \leq \quad (61)$$

$$\leq \|\phi\|\,\|\psi\| \int_{[0,1]} j_\varepsilon(y)\,\mathrm{d}y = \|\phi\|\,\|\psi\| \ . \tag{62}$$

By an $\varepsilon/3$ argument, $J_\varepsilon\phi \xrightarrow{L^2} \phi$ for all $\phi \in L^2([0,1])$. Thus, the left side of (VIII.3) converges to $-[\psi(\beta) - \psi(\alpha)]$ in mean square as $\varepsilon \to 0$. So, for almost all α, β

$$-\mathrm{i}[\psi(\beta) - \psi(\alpha)] = \int_\alpha^\beta (T^\star\psi)(x)\,\mathrm{d}x\ . \tag{63}$$

This mean that ψ is absolutely continous (see the Notes for Section VIII.1) and

$$\mathrm{i}\frac{\mathrm{d}\psi}{\mathrm{d}x} = (T^\star\psi)(x)\ . \tag{64}$$

Thus, $\psi \in AC[0,1]$ and $T^\star\psi = \mathrm{i}\dfrac{\mathrm{d}\psi}{\mathrm{d}x}$. Conversely, integration by parts shows that any $\psi \in AC[0,1]$ is in the domain of $T^\star$ and $T^\star\psi = \mathrm{i}\dfrac{\mathrm{d}\psi}{\mathrm{d}x}$. Therefore $T^\star = \mathrm{i}\dfrac{\mathrm{d}}{\mathrm{d}x}$ on $D(T^\star) = AC[0,1]$. It is easy to see that T is not essentially self-adjoint since

$$e^{\pm x} \in D(T^\star) \quad \text{and} \quad \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}e^{\pm x} = \pm\mathrm{i}e^{\pm x}\ . \tag{65}$$

In fact, T is closed (Problem 6) so T is a closed, symmetric but not self-adjoint operator. Does T have any self-adjoint extensions? Yes, uncountably many different ones! Let $\alpha \in \mathbb{C}$, $|\alpha| = 1$, and define

$$T_\alpha = \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x} \quad \text{on} \quad D(T_\alpha) = \{\phi|\phi \in AC[0,1],\ \phi(0) = \alpha\phi(1)\}\ . \tag{66}$$

Each of these operators T_α is a different self-adjoint extension of T (Problem 7), Of course, each T_α is in turn extended by $T^\star$. These extensions are depicted in Figure VIII.1. The reason why there is exactly a circle of different possible extensions will be made clear in Section X.1.
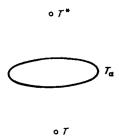

Figure 1: The self-adjoint extensions of T.

4 SPECTRAL THEOREM

4.1 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 $\mathcal{H}$, we can always find a measure pu on a measure space M and a unitary operator $U : \mathcal{H} \to L^2(M, d\mu)$ so that

$$(UAU^{-1}f)(x) = F(x)f(x) \tag{67}$$

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 $\lambda_1, \cdots, \lambda_n$ so that

$$(UAU^{-1}f)_i = \lambda_i f_i \quad \text{for each} \quad f = (f_1, \cdots, f_n) \in \mathbb{C}^n. \tag{68}$$

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 $f \mapsto [\psi, f(A)\psi]$ for fixed $\psi \in \mathcal{H}$.

Given a fixed operator A, for which f can 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 $\|A\| \leq R$, then $\sum_{n=0}^{\infty} c_n A^n$ converges in $\mathcal{L}(\mathcal{H})$ 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 fis 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 6 (Continuous functional calculus). *Let* A *be a self-adjoint operator on a Hilbert space* $\mathcal{H}$. *Then there is a unique map* $\phi : C(\sigma(A)) \to \mathcal{L}(\mathcal{H})$ *with the following properties:*

1. *ϕ is an algebraic $\star$-homomorphism, that is,*

$$\phi(fg) = \phi(f)\phi(g), \quad \phi(\lambda f) = \lambda \phi(f), \tag{69}$$

$$\phi(1) = I, \quad \phi(\overline{f}) = \phi(f)^\star. \tag{70}$$

2. *ϕ is continuous, that is, $\|\phi(f)\|_{\mathcal{L}(\mathcal{H})} \leq C \|f\|_\infty$.*

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

   Moreover, ϕ has the additional properties:

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

5. *$\sigma[\phi(f)] = \{f(\lambda)|\lambda \in \sigma(A)\}$ (spectral mapping theorem).*

6. *If $f \leq 0$, then $\phi(f) \leq 0$.*

7. *$\|\phi(f)\| = \|f\|_\infty$ (this strengthens (2)).*

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. (1) and (3) 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

$$\|P(A)\|_{\mathcal{L}(\mathcal{H})} = \|P(x)\|_{C(\sigma(A))} = \sup_{\lambda \in \sigma(A)} |P(\lambda)|. \tag{71}$$

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 (5) (which holds for arbitrary bounded operators):

Lemma 3. *Let $P(x) = \sum_{n=0}^{N} a_n x^n$. Let $P(A) = \sum_{n=0}^{N} a_n A^n$. Then*

$$\sigma(P(A)) = \{P(\lambda)|\lambda \in \sigma(A)\} . \tag{72}$$

Proof. Let $\lambda \in \sigma(A)$. Since $x = \lambda$ is a root of $P(x) - P(\lambda)$, we have $P(x) - P(\lambda)$, we have $P(x) - P(\lambda) = (x - \lambda)Q(x)$, so $P(A) - P(\lambda) = (A - \lambda)Q(A)$. $\square$