CHAPTER XI

APPLICATIONS OF SPECTRAL THEORY

Let H be a separable, infinite-dimensional, complex Hilbert space. We exploit properties of the Spectral Theorem to investigate and classify operators on H. As usual, all Hilbert spaces considered will be assumed to be complex and separable, even if it is not explicitly stated.

If T is an element of the C^*-algebra $B(H)$, recall that the *resolvent* of T is the set $\mathrm{res}(T)$ of all complex numbers λ for which $\lambda I - T$ has a two-sided inverse in $B(H)$. The *spectrum* $\mathrm{sp}(T)$ of T is the complement of the resolvent of T. That is, λ belongs to $\mathrm{sp}(T)$ if $\lambda I - T$ does not have a bounded two-sided inverse.

THEOREM 11.1. (Existence of Positive Square Roots of Positive Operators) *Let H be a Hilbert space, and let T be a positive operator in $B(H)$; i.e., $(T(x), x) \geq 0$ for all $x \in H$. Then:*

1. *There exists an element R in $B(H)$ such that $T = R^*R$.*
2. *There exists a unique positive square root of T, i.e., a unique positive operator S such that $T = S^2$. Moreover, S belongs to the smallest sub-C^*-algebra of $B(H)$ that contains T and I.*
3. *If T is invertible, then its positive square root S is also invertible.*

PROOF. We know that a positive operator T is necessarily selfadjoint. Hence, writing $T = \int_{\mathbb{R}} \lambda \, dp(\lambda)$, let us show that $p_{(-\infty,0)} = 0$. That is, the spectrum of T is contained in the set of nonnegative real numbers. If not, there must exist a $\delta > 0$ such that $p_{(-\infty,-\delta]} \neq 0$. If x is a nonzero vector in the range of $p_{(-\infty,-\delta]}$, then

$$\begin{aligned}(T(x),x) &= (T(p_{(-\infty,-\delta]}(x)),x)\\ &= \int_{-\infty}^{-\delta} \lambda\,d\mu_x(\lambda)\\ &\leq -\delta\|x\|^2\\ &< 0.\end{aligned}$$

But this would imply that T is not a positive operator. Hence, p is supported on $[0,\infty)$. Clearly then $T = S^2 = S^*S$, where

$$S = \int \sqrt{\lambda}\,dp(\lambda).$$

Setting $R = S$ gives part 1.

Since S is the integral of a nonnegative function with respect to a projection-valued measure, it follows that S is a positive operator, so that S is a positive square root of T. We know from the Weierstrass Theorem that the continuous function $\sqrt{\lambda}$ is the uniform limit on the compact set $\mathrm{sp}(T)$ of a sequence of polynomials in λ. It follows that S is an element of the smallest sub-C^*-algebra A of $B(H)$ containing T and I.

Now, if S' is any positive square root of T, then S' certainly commutes with $T = {S'}^2$. Hence, S' commutes with every element of the algebra A and hence in particular with S. Let A' be the smallest sub-C^*-algebra of $B(H)$ that contains I, T and S'. Then A' is a separable commutative C^*-algebra with identity, and S and S' are two positive elements of A' whose square is T. But the Gelfand transform on A' is 1-1 and, by part 1 of this theorem and part b of Exercise 10.10, sends both S and S' to the function $\sqrt{\hat{T}}$. Hence, $S = S'$, completing the proof of part 2.

Finally, if T is invertible, say $TU = I$, then $S(SU) = I$, showing that S has a right inverse. Also, $(US)S = I$, showing that S also has a left inverse so is invertible.

EXERCISE 11.1. (a) Let T be a selfadjoint element of $B(H)$. Prove that there exist unique positive elements T_+ and T_- such that $T = T_+ - T_-$, T_+ and T_- commute with T and with each other, and $T_+T_- = 0$. HINT: Use the Gelfand transform. T_+ and T_- are called the *positive* and *negative* parts of the selfadjoint operator T.

(b) Let $T,\ T_+$, and T_- be as in part a. Verify that, for any $x \in H$, we have

$$\|T(x)\|^2 = \|T_+(x)\|^2 + \|T_-(x)\|^2.$$

Show further that $\sqrt{T^2} = T_+ + T_-$. How are T_+ and T_- represented in terms of the spectral measure for T? Conclude that every element $T \in B(H)$ is a complex linear combination of four positive operators.

(c) Suppose T is a positive operator, and let p denote its spectral measure. Suppose $0 \leq a < b < \infty$ and that x is an element of the range of $p_{[a,b]}$. Show that $a\|x\| \leq \|T(x)\| \leq b\|x\|$.

(d) If U is a unitary operator, prove that there exists a selfadjoint operator $T \in B(H)$ for which $U = e^{iT}$. HINT: Show that the function $\hat{U} = e^{ir}$ for some bounded real-valued Borel function r.

(e) If T is a positive operator, show that $I + T$ is invertible.

(f) Suppose T and S are invertible positive operators that commute. Assume that $S - T$ is a positive operator, i.e., that $S \geq T$. Prove that $T^{-1} - S^{-1}$ is a positive operator, i.e., that $T^{-1} \geq S^{-1}$.

(g) Suppose T is a positive operator and that S is a positive invertible operator not necessarily commuting with T. Prove that $S+T$ is positive and invertible.

DEFINITION. Let M be a subspace of a Hilbert space H. By a *partial isometry* of M into H we mean an element V of $B(H)$ that is an isometry on M and is 0 on the orthogonal complement $M^\perp$ of M.

EXERCISE 11.2. Let V be a partial isometry of M into H.

(a) Show that $(V(x), V(y)) = (x, y)$ for all $x, y \in \bar{M}$.

(b) Show that V^*V is the projection $p_{\bar{M}}$ of H onto $\bar{M}$ and that VV^* is the projection $p_{\overline{V(M)}}$ of H onto $\overline{V(M)}$.

(c) Show that V^* is a partial isometry of $V(M)$ into H.

(d) Let H be the set of square-summable sequences $\{a_1, a_2, \dots\}$, and let M be the subspace determined by the condition $a_1 = 0$. Define $V : M \to H$ by $[V(\{a_n\})]_n = a_{n+1}$. Show that V is a partial isometry of M into H. Compute V^*. (This V is often called the *unilateral shift*.)

THEOREM 11.2. (Polar Decomposition Theorem) *Let H be a Hilbert space, and let T be an element of $B(H)$. Then there exist unique operators P and V satisfying:*

(1) *P is a positive operator, and V is a partial isometry from the range of P into H.*
(2) *$T = VP$ and $P = V^*T$.*

Moreover, if T is invertible, then P is invertible and V is a unitary operator.

PROOF. Let $P = \sqrt{T^*T}$. Then P is positive. Observe that $\|P(x)\| = \|T(x)\|$ for all x, whence, if $P(x) = 0$ then $T(x) = 0$. Indeed,

$$(P(x), P(x)) = (P^2(x), x) = (T^*T(x), x) = (T(x), T(x)).$$

Therefore, the map V, that sends $P(x)$ to $T(x)$, is an isometry from the range M of P onto the range of T. Defining V to be its unique isometric extension to $\bar{M}$ on all of $\bar{M}$ and to be 0 on the orthogonal complement $M^\perp$ of M, we have that V is a partial isometry of M into H. Further, $T(x) = V(P(x))$, and $T = VP$, as desired. Further, from the preceding exercise, V^*V is the projection onto the closure $\bar{M}$ of the range M of P, so that $V^*T = V^*VP = P$.

If Q is a positive operator and W is a partial isometry of the range of Q into H for which $T = WQ$ and $Q = W^*T$, then W^*W is the projection onto the closure of the range of Q. Hence,

$$T^*T = QW^*WQ = Q^2,$$

whence $Q = P$ since positive square roots are unique. But then $V = W$, since they are both partial isometries of the range of P into H, and they agree on the range of P. Therefore, the uniqueness assertion of the theorem is proved.

Finally, if T is invertible, then P is invertible, and the partial isometry $V = TP^{-1}$ is invertible. An isometry that is invertible is of course a unitary operator.

DEFINITION. The operator $P = \sqrt{T^*T}$ of the preceding theorem is called the *absolute value* of T and is often denoted by $|T|$.

REMARK. We have defined the absolute value of an operator T to be the square root of the positive operator T^*T. We might well have chosen to define the absolute value of T to be the square root of the (probably different) positive operator TT^*. Though different, either of these choices would have sufficed for our eventual purposes. See part c of the following exercise.

EXERCISE 11.3. Let T be an operator in $B(H)$.

(a) Prove that $\||T|(x)\| = \|T(x)\|$ for every $x \in H$.

(b) If T is a selfadjoint operator, and we write $T = T_+ - T_-$ (as in Exercise 11.1), show that $|T| = T_+ + T_-$.

(c) Show that there exists a unique positive operator P' and a unique partial isometry V' of the range of T^* into H such that $T = P'V'$ and $P' = TV'^*$. Is either P' or V' identical with the P and V of the preceding theorem?

We introduce next a number of definitions concerning the spectrum of an operator.

DEFINITION. Let T be a normal operator, and let p be its spectral measure.

(1) A complex number λ is said to belong to the *point spectrum* $\mathrm{sp}_p(T)$ of T if $p_{\{\lambda\}} \neq 0$. In this case we say that the *multiplicity* of λ is the dimension $m(\lambda)$ of the range of $p_{\{\lambda\}}$.

(2) An element λ of the spectrum of T, which is not in the point spectrum, is said to belong to the *continuous spectrum* $\mathrm{sp}_c(T)$ of T. The *multiplicity* $m(\lambda)$ of an element λ of the continuous spectrum is defined to be 0.

(3) A complex number λ is said to belong to the *discrete spectrum* $\mathrm{sp}_d(T)$ of T if $\{\lambda\}$ is an isolated point in the compact set $\mathrm{sp}(T)$. Note that if $\lambda \in \mathrm{sp}_d(T)$, then $\{\lambda\}$ is a relatively open subset of $\mathrm{sp}(T)$. It follows then from part a of Exercise 10.13 that $\mathrm{sp}_d(T) \subseteq \mathrm{sp}_p(T)$.

(4) A complex number λ is said to belong to the *essential spectrum* $\mathrm{sp}_e(T)$ if it is not an element of the discrete spectrum with finite multiplicity.

(5) T is said to have *purely atomic spectrum* if p is supported on a countable subset of $\mathbb{C}$.

EXERCISE 11.4. (Characterization of the Point Spectrum) Suppose T is a normal operator, that p is its spectral measure, and that v is a unit vector for which $T(v) = 0$. Write μ_v for the measure on $\mathrm{sp}(T)$ given by $\mu_v(E) = (p_E(v), v)$.

(a) Prove that $0 \in \mathrm{sp}(T)$.

(b) Show that $\int \lambda^n \, d\mu_v(\lambda) = 0$ for all positive integers n.

(c) Prove that $\int f(\lambda) \, d\mu_v(\lambda) = f(0)$ for all $f \in C(\mathrm{sp}(T))$.

(d) Show that $\mu_v = \delta_0$, whence $p_{\{0\}} \neq 0$.

(e) Let T be an arbitrary normal operator. Prove that $\lambda_0 \in \mathrm{sp}_p(T)$ if and only if λ_0 is an eigenvalue for T. HINT: Write $S = T - \lambda_0 I$, and use Exercise 10.14.

EXERCISE 11.5. Let H be the Hilbert space l^2 consisting of the square summable sequences $\{a_1, a_2, \dots\}$. Let $r_1, r_2, \dots$ be a sequence of (not necessarily distinct) numbers in the interval [0,1], and define an operator T on l^2 by

$$T(\{a_n\}) = \{r_n a_n\}.$$

(a) Prove that T is a selfadjoint operator–even a positive operator.

(b) Show that the point spectrum of T is the set of r_n's.

(c) Find the spectrum of T.

(d) Find the discrete spectrum of T.

(e) Find the essential spectrum of T.

(f) Choose the sequence $\{r_n\}$ so that $\mathrm{sp}_d(T) \subset \mathrm{sp}_p(T)$ and $\mathrm{sp}_e(T) \subset \mathrm{sp}(T)$.

(g) Construct a sequence $\{T_j\}$ of positive operators that converges in norm to a positive operator T, but for which the sequence $\{\mathrm{sp}_d(T_j)\}$ of subsets of $\mathbb{R}$ in no way converges to $\mathrm{sp}_d(T)$. Test a few other conjectures concerning the continuity of the map $T \to \mathrm{sp}(T)$.

THEOREM 11.3. *Let H be a separable Hilbert space, and let T be a normal operator in $B(H)$. Then the following are equivalent:*

(1) *T has purely atomic spectrum.*
(2) *There exists an orthonormal basis for H consisting of eigenvectors for T.*
(3) *There exists a sequence $\{p_i\}$ of pairwise orthogonal projections and a sequence $\{\lambda_i\}$ of complex numbers such that*

$$I = \sum_{i=1}^{\infty} p_i$$

and

$$T = \sum_{i=1}^{\infty} \lambda_i p_i.$$

PROOF. If T has purely atomic spectrum, and if $\lambda_1, \lambda_2, \ldots$ denotes a countable set on which the spectral measure p is concentrated, let $p_i = p_{\{\lambda_i\}}$. Then the p_i's are pairwise orthogonal, and

$$I = \sum_{i=1}^{\infty} p_i,$$

and

$$T = \int \lambda\, dp(\lambda)$$
$$= \sum_{i=1}^{\infty} \lambda_i p_{\{\lambda_i\}}$$
$$= \sum_{i=1}^{\infty} \lambda_i p_i,$$

showing that 1 implies 3.

Next, suppose $T = \sum_{i=1}^{\infty} \lambda_i p_i$, where $\{p_i\}$ is a sequence of pairwise orthogonal projections for which $I = \sum p_i$. We may make an orthonormal basis for H by taking the union of orthonormal bases for the ranges M_{p_i} of the p_i's. Clearly, each vector in this basis is an eigenvector for T, whence, 3 implies 2.

Finally, suppose there exists an orthonormal basis for H consisting of eigenvectors for T, and let $\{\lambda_1, \lambda_2, \dots\}$ be the set of distinct eigenvalues for T. Because T is a bounded operator, this set of λ_i's is a bounded subset of $\mathbb{C}$. For each $i = 1, 2, \dots$, let M_i be the eigenspace corresponding to the eigenvalue λ_i, and write p_i for the projection onto M_i. Then the p_i's are pairwise orthogonal, and $I = \sum p_i$.

Now, for each subset $E \subseteq \mathbb{C}$, define

$$p_E = \sum_{\lambda_i \in E} p_i.$$

Then $E \to p_E$ is a projection-valued measure supported on the compact set $\overline{\{\lambda_i\}}$, and we let S be the normal operator given by $S = \int \lambda\, dp(\lambda)$. If $v \in M_i$, then v belongs to the range of $p_{\{\lambda_i\}}$, whence $v = p_{\{\lambda_i\}}(v)$. It follows then that

$$\begin{aligned}
T(v) &= \lambda_i v \\
&= \lambda_i p_{\{\lambda_i\}}(v) \\
&= [\int \lambda \chi_{\{\lambda_i\}}(\lambda)\, dp(\lambda)](v) \\
&= [\int \lambda\, dp(\lambda)]([\int \chi_{\{\lambda_i\}}(\lambda)\, dp(\lambda)](v)) \\
&= S(p_{\{\lambda_i\}}(v)) \\
&= S(v).
\end{aligned}$$

Since this holds for each i, we have that $T = S$, showing that 2 implies 1.

The next theorem describes a subtle but important distinction between the spectrum and the essential spectrum. However, the true essence of the essential spectrum is only evident in Theorem 11.9.

THEOREM 11.4. *Let T be a normal operator on a separable Hilbert space H. Then*

(1) *$\lambda_0 \in sp(T)$ if and only if there exists a sequence $\{v_n\}$ of unit vectors in H such that*

$$\lim \|T(v_n) - \lambda_0 v_n\| = 0.$$

(2) *$\lambda_0 \in sp_e(T)$ if and only if there exists an infinite sequence $\{v_n\}$ of orthonormal vectors for which*

$$\lim \|T(v_n) - \lambda_0 v_n\| = 0.$$

PROOF. (1) If λ_0 belongs to the point spectrum of T, then there exists a unit vector v (any unit vector in the range of $p_{\{\lambda_0\}}$) such that $T(v) - \lambda_0 v = 0$. Therefore, the constant sequence $v_n \equiv v$ satisfies

$$\lim \|T(v_n) - \lambda_0 v_n\| = 0.$$

(2) If λ_0 belongs to the point spectrum of T, and the multiplicity $m(\lambda_0)$ is infinity, then there exists an infinite orthonormal sequence $\{v_n\}$ in the range of $p_{\{\lambda_0\}}$ such that $T(v_n) - \lambda_0 v_n \equiv 0$.

(3) Suppose $\lambda_0 \in \mathrm{sp}(T)$ but $\lambda_0 \notin \mathrm{sp}_d(T)$. For each positive integer k, let $U_k = \mathrm{sp}(T) \cap B_{1/k}(\lambda_0)$. Then each U_k is a nonempty open subset of $\mathrm{sp}(T)$, whence $p_{U_k} \neq 0$ for all k. In fact, since λ_0 is not a discrete point in the spectrum of T, there exists an increasing sequence $\{k_n\}$ of positive integers such that $p_{F_n} \neq 0$ for every n, where $F_n = U_{k_n} - U_{k_{n+1}}$. (Why?) Choosing v_n to be a unit vector in the range of the projection p_{F_n}, we see that the sequence $\{v_n\}$ is infinite and orthonormal. Further,

we have

$$\begin{aligned}\|T(v_n) - \lambda_0 v_n\| &= \|T(p_{F_n}(v_n)) - \lambda_0 p_{F_n}(v_n)\| \\ &= \|[\int \lambda \chi_{F_n}(\lambda)\, dp(\lambda)](v_n) - [\int \lambda_0 \chi_{F_n}(\lambda)\, dp(\lambda)](v_n)\| \\ &= \|[\int (\lambda - \lambda_0)\chi_{F_n}(\lambda)\, dp(\lambda)](v_n)\| \\ &\leq \sup_{\lambda \in F_n} |\lambda - \lambda_0| \\ &\leq \sup_{\lambda \in U_{k_n}} |\lambda - \lambda_0| \\ &\leq 1/k_n.\end{aligned}$$

This shows that $\lim_n \|T(v_n) - \lambda_0 v_n\| = 0$.

(4) If $\lambda_0 \notin \mathrm{sp}(T)$, then $T - \lambda_0 I$ is invertible in $B(H)$. So, if $\{v_n\}$ were a sequence of unit vectors, for which $\lim_n (T(v_n) - \lambda_0 v_n) = 0$, then $\lim v_n = \lim (T - \lambda_0 I)^{-1}((T - \lambda_0 I)(v_n)) = 0$, which would be a contradiction.

The completion of this proof is left to the exercise that follows.

EXERCISE 11.6. Use results 1-4 above to complete the proof of Theorem 11.4.

We next introduce some important classes of operators on an infinite dimensional Hilbert space. Most of these classes are defined in terms of the spectral measures of their elements.

DEFINITION. Let H be an infinite-dimensional separable Hilbert space.

(1) An element $T \in B(H)$ is a *finite rank operator* if its range is finite dimensional.

(2) A positive operator T is a *compact operator* if it has purely atomic spectrum, and this spectrum consists of a (possibly finite) strictly decreasing sequence $\{\lambda_i\}$ of nonnegative numbers, such that $0 = \lim \lambda_i$, and such that the multiplicity $m(\lambda_i)$ is finite for every $\lambda_i > 0 \in \mathrm{sp}(T)$. (If the sequence $\lambda_1, \lambda_2, \ldots$ is finite, then the statement $0 = \lim \lambda_i$ means that $\lambda_N = 0$ for some (the last) N. Evidently each positive element λ_i of this spectrum is a discrete point, whence each positive λ_i of the spectrum is an eigenvalue for T.) A selfadjoint element $T = T_+ - T_- \in B(H)$ is a *compact operator* if its positive and negative parts T_+ and T_- are compact operators, and a general element $T = T_1 + iT_2 \in B(H)$ is a

compact operator if its real and imaginary parts T_1 and T_2 are compact operators.

(3) A positive operator T is a *trace class operator* if it is a compact operator, with positive eigenvalues $\lambda_1, \lambda_2, \ldots$, for which

$$\sum \lambda_i m(\lambda_i) < \infty.$$

A selfadjoint element $T = T_+ - T_- \in B(H)$ is a *trace class operator* if its positive and negative parts T_+ and T_- are trace class operators, and a general $T = T_1 + iT_2 \in B(H)$ is a *trace class operator* if its real and imaginary parts T_1 and T_2 are trace class operators.

(4) A positive operator T is a *Hilbert-Schmidt operator* if it is a compact operator, with positive eigenvalues $\lambda_1, \lambda_2, \ldots$, for which

$$\sum \lambda_i^2 m(\lambda_i) < \infty.$$

A selfadjoint element $T = T_+ - T_- \in B(H)$ is a *Hilbert-Schmidt operator* if its positive and negative parts T_+ and T_- are Hilbert-Schmidt operators, and a general $T = T_1 + iT_2 \in B(H)$ is a *Hilbert-Schmidt operator* if its real and imaginary parts T_1 and T_2 are Hilbert-Schmidt operators.

EXERCISE 11.7. Let H be a Hilbert space.

(a) Let T be in $B(H)$. Prove that the closure of the range of T is the orthogonal complement of the kernel of T^*. Conclude that T is a finite rank operator if and only if T^* is a finite rank operator.

(b) Show that the set of finite rank operators forms a two-sided selfadjoint ideal in $B(H)$.

(c) Show that T is a finite rank operator if and only if $|T|$ is a finite rank operator.

(d) Show that every finite rank operator is a trace class operator, and that every trace class operator is a Hilbert-Schmidt operator.

(e) Using multiplication operators on l^2 (see Exercise 11.5), show that the inclusions in part d are proper. Show also that the set of Hilbert-Schmidt operators is a proper subset of the set of compact operators on l^2 and that the set of compact operators is a proper subset of $B(l^2)$.

(f) Prove that every normal compact operator T has purely atomic spectrum. Conclude that, if T is a compact normal operator, then there exists an orthonormal basis of H consisting of eigenvectors for T.

THEOREM 11.5. (Characterization of Compact Operators) *Suppose T is a bounded operator on a separable infinite-dimensional Hilbert space H. Then the following properties are equivalent:*

(1) *T is a compact operator.*
(2) *If $\{x_n\}$ is any bounded sequence of vectors in H, then $\{T(x_n)\}$ has a convergent subsequence.*
(3) *$T(B_1)$ has a compact closure in H.*
(4) *If $\{x_n\}$ is a sequence of vectors in H that converges weakly to 0, then the sequence $\{T(x_n)\}$ converges in norm to 0.*
(5) *T is the limit in $B(H)$ of a sequence of finite rank operators.*

PROOF. Let us first show that 1 implies 5. It will suffice to show this for T a positive compact operator. Thus, let $\{\lambda_1, \lambda_2, \dots\}$ be the strictly decreasing (finite or infinite) sequence of positive elements of $\mathrm{sp}(T)$. Using the Spectral Theorem and the fact that T has purely atomic spectrum, write

$$T = \int \lambda \, dp(\lambda) = \sum_i \lambda_i p_{\{\lambda_i\}}.$$

Evidently, if there are only a finite number of λ_i's, then T is itself a finite rank operator, since the dimension of the range of each $p_{\{\lambda_i\}}$, for $\lambda_i > 0$, is finite, and 5 follows. Hence, we may assume that the sequence $\{\lambda_i\}$ is infinite. Define a sequence $\{T_k\}$ of operators by

$$\begin{aligned} T_k &= \sum_{i=1}^{k} \lambda_i p_{\{\lambda_i\}} \\ &= \int \chi_{[\lambda_k,\infty)}(\lambda)\lambda \, dp(\lambda). \end{aligned}$$

Then each T_k is a finite rank operator. Further,

$$\|T - T_k\| = \| \int \chi_{[0,\lambda_k)}(\lambda)\lambda \, dp(\lambda)\| \leq \lambda_k.$$

Hence, $T = \lim T_k$ in norm, giving 5.

We show next that 5 implies 4. Suppose then that $T = \lim T_k$ in norm, where each T_k is a finite rank operator. Let $\{x_n\}$ be a sequence in H that converges weakly to 0, and let $\epsilon > 0$ be given. Then, by the Uniform Boundedness Theorem, the sequence $\{x_n\}$ is uniformly bounded, and

$$\|T(x_n)\| \leq \|(T - T_k)x_n\| + \|T_k(x_n)\|.$$

Choose k so that $\|(T-T_k)(x_n)\| < \epsilon/2$ for all n. For this k, the sequence $\{T_k(x_n)\}$ is contained in the finite dimensional subspace M that is the range of T_k, and converges weakly to 0 there. Since all vector space topologies are identical on a finite dimensional space, we have that, for this fixed k, the sequence $\{T_k(x_n)\}$ also converges to 0 in norm. Choose N so that $\|T_k(x_n)\| < \epsilon/2$ for all $n \geq N$. Then $\|T(x_n)\| < \epsilon$ if $n \geq N$, and the sequence $\{T(x_n)\}$ converges to 0 in norm, as desired.

We leave to the exercises the fact that properties 2,3, and 4 are equivalent (for any element of $B(H)$). Let us show finally that 4 implies 1. Thus, suppose T satisfies 4. Then T^* also satisfies 4. For, if the sequence $\{x_n\}$ converges to 0 weakly, then the sequence $\{T^*(x_n)\}$ also converges to 0 weakly. Hence, the sequence $\{T(T^*(x_n))\}$ converges to 0 in norm. Since

$$\|T^*(x_n)\|^2 = (T^*(x_n), T^*(x_n)) = (T(T^*(x_n)), x_n) \leq \|T(T^*(x_n))\|\|x_n\|,$$

it follows that the sequence $\{T^*(x_n)\}$ converges to 0 in norm. Consequently, the real and imaginary parts T_1 and T_2 of T satisfy 4, and we may assume that T is selfadjoint. Write $T = T_+ - T_-$ in terms of its positive and negative parts. By part b of Exercise 11.1, we see that both T_+ and T_- satisfy 4, so that we may assume that T is a positive operator. Let p be the spectral measure for T, and note that for each positive ϵ, we must have that the range of $p_{(\epsilon,\infty)}$ must be finite dimensional. Otherwise, there would exist an orthonormal sequence $\{x_n\}$ in this range. Such an orthonormal sequence converges to 0 weakly, but, by part b of Exercise 9.11, $\|T(x_n)\| \geq \epsilon$ for all n, contradicting 4. Hence, $\mathrm{sp}(T) \cap (\epsilon, \infty)$ is a finite set for every positive ϵ, whence the spectrum of T consists of a decreasing sequence of nonnegative numbers whose limit is 0. It also follows as in the above that each $p_{\{\lambda\}}$, for $\lambda > 0 \in \mathrm{sp}(T)$, must have a finite dimensional range, whence T is a compact operator, completing the proof that 4 implies 1.

EXERCISE 11.8. (Completing the Proof of the Preceding Theorem) Let T be an arbitrary element of $B(H)$.

(a) Assume 2. Show that $T(B_1)$ is totally bounded in H, and then conclude that 3 holds. (A subset E of a metric space X is called *totally bounded* if for every positive ϵ the set E is contained in a finite union of sets of diameter less than ϵ.)

(b) Prove that 3 implies 4.

(c) Prove that 4 implies 2.

EXERCISE 11.9. (Properties of the Set of Compact Operators)

(a) Prove that the set K of all compact operators forms a proper closed two-sided selfadjoint ideal in the C^*-algebra $B(H)$.

(b) Prove that an element $T \in B(H)$ is a compact operator if and only if $|T|$ is a compact operator.

(c) Show that no compact operator can be invertible.

(d) Show that the essential spectrum of a normal compact operator is singleton 0.

THEOREM 11.6. (Characterization of Hilbert-Schmidt Operators) *Let H be a separable infinite-dimensional Hilbert space.*

(1) *If T is any element of $B(H)$, then the extended real number*

$$\sum_i \|T(\phi_i)\|^2$$

is independent of which orthonormal basis $\{\phi_i\}$ is used. Further,

$$\sum_i \|T(\phi_i)\|^2 = \sum_i \|T^*(\phi_i)\|^2.$$

(2) *An operator T is a Hilbert-Schmidt operator if and only if*

$$\sum_i \|T(\phi_i)\|^2 < \infty$$

for some (hence every) orthonormal basis $\{\phi_i\}$ of H.

(3) *The set of all Hilbert-Schmidt operators is a two-sided selfadjoint ideal in the algebra $B(H)$.*

PROOF. Suppose $T \in B(H)$ and that there exists an orthonormal basis $\{\phi_i\}$ such that

$$\sum_i \|T(\phi_i)\|^2 = M < \infty.$$

Let $\{\psi_i\}$ be another orthonormal basis.

Then

$$\begin{aligned}\sum_i \|T(\psi_i)\|^2 &= \sum_i \sum_j |(T(\psi_i), \phi_j)|^2 \\ &= \sum_i \sum_j |(\psi_i, T^*(\phi_j))|^2 \\ &= \sum_j \|T^*(\phi_j)\|^2 \\ &= \sum_j \sum_i |(T^*(\phi_j), \phi_i)|^2 \\ &= \sum_j \sum_i |(\phi_j, T(\phi_i))|^2 \\ &= \sum_i \|T(\phi_i)\|^2,\end{aligned}$$

which completes the proof of part 1.

Next, suppose T is a Hilbert-Schmidt operator. We wish to show that

$$\sum_i \|T(\phi_i)\|^2 < \infty$$

for some orthonormal basis $\{\phi_i\}$ of H. Since T is a linear combination of 4 positive Hilbert-Schmidt operators, and since

$$\|\sum_{i=1}^4 T_i(\phi)\|^2 \leq 16 \sum_{i=1}^4 \|T_i(\phi)\|^2,$$

it will suffice to show the desired inequality under the assumption that T itself is a positive operator. Thus, let $\{\lambda_n\}$ be the spectrum of T, and recall that the nonzero λ_n's are the eigenvalues for T. Since T has a purely atomic spectrum, there exists an orthonormal basis $\{\phi_i\}$ for H consisting of eigenvectors for T. Then,

$$\sum_i \|T(\phi_i)\|^2 = \sum_n \lambda_n^2 m(\lambda_n) < \infty.$$

Conversely, let T be in $B(H)$ and suppose there exists an orthonormal basis $\{\phi_i\}$ such that the inequality in part 2 holds for $T = T_1 + iT_2$. It follows from part 1 that the same inequality holds as well for $T^* = T_1 - iT_2$. It then follows that the inequality holds for the real and imaginary parts $T_1 = (T+T^*)/2$ and $T_2 = (T-T^*)/2i$ of T. It will suffice then to assume that T is selfadjoint, and we write $T = T_+ - T_-$ in terms of its positive and negative parts. Now, from part b of Exercise 11.1, it follows that the inequality in part 2 must hold for T_+ and T_-, so that it will suffice in fact to assume that T is positive. We show first that T is a compact operator. Thus, let $\{v_k\}$ be a sequence of vectors in H that converges weakly to 0, and write

$$v_k = \sum_i a_{ki}\phi_i.$$

Note that for each i, we have $0 = \lim_k (v_k, \phi_i) = \lim_k a_{ki}$. Let M be an upper bound for the sequence $\{\|v_k\|\}$. Then, given $\epsilon > 0$, there exists an N such that $\sum_{i=N}^\infty \|T(\phi_i)\|^2 < (\epsilon/2M)^2$. Then, there exists a K such that $|a_{ki}| \le \epsilon/2N\|T\|$ for all $1 \le i \le N-1$ and all $k \ge K$. Then,

$$\begin{aligned}
\|T(v_k)\| &= \|T(\sum_i a_{ki}\phi_i)\| \\
&= \|\sum_i a_{ki}T(\phi_i)\| \\
&\le \sum_{i=1}^{N-1} |a_{ki}|\|T(\phi_i)\| + \sum_{i=N}^{\infty} |a_{ki}|\|T(\phi_i)\| \\
&< \epsilon/2 + \sqrt{\sum_{i=N}^{\infty} |a_{ki}|^2} \times \sqrt{\sum_{i=N}^{\infty} \|T(\phi_i)\|^2} \\
&< \epsilon/2 + \|v_k\| \times \epsilon/2M \\
&\le \epsilon,
\end{aligned}$$

showing that the sequence $\{T(v_k)\}$ converges to 0 in norm. Hence, T is a (positive) compact operator. Now, using part 1 and an orthonormal basis of eigenvectors for T, we have that

$$\sum_i \lambda_i^2 m(\lambda_i) < \infty,$$

whence T is a Hilbert-Schmidt operator. This completes the proof of part 2.

We leave the verification of part 3 to an exercise.

EXERCISE 11.10. (The Space of All Hilbert-Schmidt Operators)
(a) If T is a Hilbert-Schmidt operator and S is an arbitrary element of $B(H)$, show that TS and ST are Hilbert-Schmidt operators.
(b) Show that T is a Hilbert-Schmidt operator if and only if $|T|$ is a Hilbert-Schmidt operator.
(c) Prove part 3 of the preceding theorem.
(d) For T and S Hilbert-Schmidt operators, show that

$$\sum_i (T(\phi_i), S(\phi_i)) = \sum_i (S^*T(\phi_i), \phi_i)$$

exists and is independent of which orthonormal basis $\{\phi_i\}$ is used.
(e) Let $B_{\mathrm{hs}}(H)$ denote the complex vector space of all Hilbert-Schmidt operators on H, and on $B_{\mathrm{hs}}(H) \times B_{\mathrm{hs}}(H)$ define

$$(T, S) = \sum_i (S^*T(\phi_i), \phi_i),$$

where $\{\phi_i\}$ is an orthonormal basis. Verify that (T, S) is a well-defined inner product on $B_{\mathrm{hs}}(H)$, and that $B_{\mathrm{hs}}(H)$ is a Hilbert space with respect to this inner product. This inner product is called the *Hilbert-Schmidt inner product.*
(f) If T is a Hilbert-Schmidt operator, define the *Hilbert-Schmidt norm* $\|T\|_{\mathrm{hs}}$ of T by

$$\|T\|_{\mathrm{hs}} = \sqrt{(T, T)} = \sqrt{\sum \|T(\phi_i)\|^2}.$$

Prove that $\|T\| \leq \|T\|_{\mathrm{hs}}$. Show further that, if T is a Hilbert-Schmidt operator and S is an arbitrary element of $B(H)$, then

$$\|ST\|_{\mathrm{hs}} \leq \|S\|\|T\|_{\mathrm{hs}}.$$

(g) Show that $B_{\mathrm{hs}}(H)$ is a Banach $*$-algebra with respect to the Hilbert-Schmidt norm.

THEOREM 11.7. (The Space of Trace Class Operators)
(1) *An operator $T \in B(H)$ is a trace class operator if and only if*

$$\sum_i |(T(\psi_i), \phi_i)| < \infty$$

for every pair of orthonormal sets $\{\psi_i\}$ and $\{\phi_i\}$.

(2) *The set of all trace class operators is a two-sided selfadjoint ideal in the algebra $B(H)$.*

(3) *An operator T is a trace class operator if and only if there exist two Hilbert-Schmidt operators S_1 and S_2 such that $T = S_1 \circ S_2$.*

PROOF. Since every trace class operator is a linear combination of four positive trace class operators, it will suffice, for the "only if" part of 1, to assume that T is positive. Thus, let $\{\eta_n\}$ be an orthonormal basis of eigenvectors for T, and write

$$M = \sum_n (T(\eta_n), \eta_n) = \sum_i \lambda_i m(\lambda_i),$$

where the λ_i's are the eigenvalues for T. If $\{\psi_i\}$ and $\{\phi_i\}$ are any orthonormal sets, write

$$\psi_i = \sum_n a_{ni}\eta_n,$$

where $a_{ni} = (\psi_i, \eta_n)$, and

$$\phi_i = \sum_n b_{ni}\eta_n,$$

where $b_{ni} = (\phi_i, \eta_n)$. Then

$$\begin{aligned}
\sum_i |(T(\psi_i), \phi_i)| &= \sum_i |\sum_n \sum_m a_{ni}\overline{b_{mi}}(T(\eta_n), \eta_m)| \\
&= \sum_i |\sum_n a_{ni}\overline{b_{ni}}(T(\eta_n), \eta_n)| \\
&\leq \sum_n (T(\eta_n), \eta_n) \times \sqrt{\sum_i |a_{ni}|^2} \times \sqrt{\sum_i |b_{ni}|^2} \\
&= \sum_n (T(\eta_n), \eta_n) \times \sqrt{\sum_i |(\eta_n, \psi_i)|^2} \times \sqrt{\sum_i |(\eta_n, \phi_i)|^2} \\
&\leq \sum_n (T(\eta_n), \eta_n)\|\eta_n\|\|\eta_n\| \\
&= M,
\end{aligned}$$

showing that the condition in 1 holds. We leave the converse to the exercises.

It clearly follows from part 1 that the set of trace class operators forms a vector space, and it is equally clear that if T is a trace class operator, i.e., satisfies the inequality in 1, then T^* is also a trace class operator. To see that the trace class operators form a two-sided selfadjoint ideal, it will suffice then to show that ST is a trace class operator whenever $S \in B(H)$ and T is a positive trace class operator. Thus, let $\{\eta_n\}$ be an orthonormal basis of eigenvectors for T, and let $\{\psi_i\}$ and $\{\phi_i\}$ be arbitrary orthonormal sets. Write

$$\psi_i = \sum_n a_{ni}\eta_n$$

and

$$S^*(\phi_i) = \sum_n b_{mi}\eta_m.$$

Then

$$\begin{aligned}
\sum_i |(ST(\psi_i), \phi_i)| &= \sum_i |\sum_n \sum_m a_{ni}\overline{b_{mi}}(T(\eta_n), \eta_m)| \\
&= \sum_i |\sum_n a_{ni}\overline{b_{ni}}(T(\eta_n), \eta_n)| \\
&\leq \sum_i \sum_n |a_{ni}b_{ni}|(T(\eta_n), \eta_n) \\
&\leq \sum_n (T(\eta_n), \eta_n) \\
&\qquad \times \sqrt{\sum_i |a_{ni}|^2}\sqrt{\sum_k |b_{nk}|^2} \\
&= \sum_n (T(\eta_n), \eta_n) \\
&\qquad \times \sqrt{\sum_i |(\eta_n, \psi_i)|^2}\sqrt{\sum_k |(\eta_n, S^*(\phi_k))|^2} \\
&= \sum_n (T(\eta_n), \eta_n)\|\eta_n\|\|S(\eta_n)\| \\
&\leq \|S\| \sum_n (T(\eta_n), \eta_n) \\
&< \infty,
\end{aligned}$$

showing, by part 1, that ST is trace class. This completes the proof of part 2.

We leave the proof of part 3 to the following exercise.

EXERCISE 11.11. (Completing the Preceding Proof)

(a) Suppose T is a positive operator. Show that

$$\sum_j (T(\psi_j), \psi_j) = \sum_n (T(\phi_n), \phi_n)$$

for any pair of orthonormal bases $\{\psi_j\}$ and $\{\phi_n\}$. Suppose next that

$$\sum_n (T(\phi_n), \phi_n) < \infty.$$

Prove that $\sqrt{T}$ is a Hilbert-Schmidt operator, and deduce from this that T is a trace class operator.

(b) Suppose T is a selfadjoint operator, and write $T = T_+ - T_-$ in terms of its positive and negative parts. Assume that $\sum_n |(T(\phi_n), \phi_n)| < \infty$ for every orthonormal set $\{\phi_n\}$. Prove that T is a trace class operator. HINT: Choose the orthonormal set to be a basis for the closure of the range of T_+.

(c) Prove the rest of part 1 of the preceding theorem.

(d) Prove that T is a trace class operator if and only if $|T|$ is a trace class operator.

(e) Prove part 3 of the preceding theorem.

EXERCISE 11.12. (The Space of Trace Class Operators)

(a) If T is a trace class operator, define

$$\|T\|_{\mathrm{tr}} = \sup_{\{\psi_n\},\{\phi_n\}} \sum_n |(T(\psi_n), \phi_n)|,$$

where the supremum is taken over all pairs of orthonormal sets $\{\psi_n\}$ and $\{\phi_n\}$. Prove that the assignment $T \to \|T\|_{\mathrm{tr}}$ is a norm on the set $B_{\mathrm{tr}}(H)$ of all trace class operators. This norm is called the *trace class norm.*

(b) If T is a trace class operator and $\{\phi_n\}$ is an orthonormal basis, show that the infinite series $\sum (T(\phi_n), \phi_n)$ is absolutely summable. Show further that

$$\sum_n (T(\phi_n), \phi_n) = \sum_n (T(\psi_n), \psi_n),$$

where $\{\phi_n\}$ and $\{\psi_n\}$ are any two orthonormal bases. We define the *trace* $\mathrm{tr}(T)$ of a trace class operator T by

$$\mathrm{tr}(T) = \sum_n (T(\phi_n), \phi_n),$$

where $\{\phi_n\}$ is an orthonormal basis.

(c) Let T be a positive trace class operator. Show that $\|T\|_{\mathrm{tr}} = \mathrm{tr}(T)$. For an arbitrary trace class operator T, show that $\|T\|_{\mathrm{tr}} = \mathrm{tr}(|T|)$. HINT: Expand everything in terms of an orthonormal basis consisting of eigenvectors for $|T|$.

(d) Let T be a trace class operator and S be an element of $B(H)$. Prove that

$$\|ST\|_{\mathrm{tr}} \leq \|S\|\|T\|_{\mathrm{tr}}.$$

(e) Show that $B_{\mathrm{tr}}(H)$ is a Banach *-algebra with respect to the norm defined in part a.

EXERCISE 11.13. (a) Let (S, μ) be a σ-finite measure space. Show that if a nonzero multiplication operator m_f on $L^2(\mu)$ is a compact operator, then μ must have some nontrivial atomic part. That is, there must exist at least one point $x \in S$ such that $\mu(\{x\}) > 0$.

(b) Suppose μ is a purely atomic σ-finite measure on a set S. Describe the set of all functions f for which m_f is a compact operator, a Hilbert-Schmidt operator, a trace class operator, or a finite rank operator.

(c) Show that no nonzero convolution operator K_f on $L^2(\mathbb{R})$ is a compact operator. HINT: Examine the operator $U \circ K_f \circ U^{-1}$, for U the L^2 Fourier transform.

(d) Let (S, μ) be a σ-finite measure space. Suppose $k(x, y)$ is a kernel on $S \times S$, and assume that $k \in L^2(\mu \times \mu)$. Prove that the integral operator K, determined by the kernel k, is a Hilbert-Schmidt operator, whence is a compact operator.

(e) Let (S, μ) be a σ-finite measure space, and let T be a positive Hilbert-Schmidt operator on $L^2(\mu)$. Suppose $\{\phi_1, \phi_2, \dots\}$ is an orthonormal basis of $L^2(\mu)$ consisting of eigenfunctions for T, and let λ_i denote the eigenvalue corresponding to ϕ_i. Define a kernel $k(x, y)$ on $S \times S$ by

$$k(x, y) = \sum_{i=1}^{\infty} \lambda_i \phi_i(x) \overline{\phi_i(y)}.$$

Show that $k \in L^2(\mu \times \mu)$ and that T is the integral operator determined by the kernel k. Show in general that, if T is a Hilbert-Schmidt operator on $L^2(\mu)$, then there exists an element $k \in L^2(\mu \times \mu)$ such that

$$Tf(x) = \int k(x, y) f(y) \, d\mu(y)$$

for all $f \in L^2(\mu)$. Conclude that there is a linear isometry between the Hilbert space $L^2(\mu \times \mu)$ and the Hilbert space $B_{\mathrm{hs}}(L^2(\mu))$ of all Hilbert-Schmidt operators on $L^2(\mu)$.

(f) Let S be a compact topological space, let μ be a finite Borel measure on S, and let k be a continuous function on $S \times S$. Suppose $\phi \in L^2(\mu)$ is an eigenfunction, corresponding to a nonzero eigenvalue, for the integral operator T determined by the kernel k. Prove that ϕ may be assumed to be continuous, i.e., agrees with a continuous function μ almost everywhere. Give an example to show that this is not true if μ is only assumed to be σ-finite.

(g) (Mercer's Theorem) Let S, μ, k, and T be as in part f. Suppose T is a positive trace class operator. Prove that

$$\mathrm{tr}(T) = \int_S k(x,x)\, d\mu(x).$$

We turn next to an examination of "unbounded selfadjoint" operators. Our definition is derived from a generalization of the properties of bounded selfadjoint operators as described in Theorem 8.7.

DEFINITION. A linear transformation T from a subspace D of a Hilbert space H into H is called an *unbounded selfadjoint operator* on H if

(1) D is a proper dense subspace of H.
(2) T is not continuous on D.
(3) T is symmetric on D; i.e., $(T(x), y) = (x, T(y))$ for all $x, y \in D$.
(4) Both $I + iT$ and $I - iT$ map D onto H.

If, in addition, $(T(x), x) \geq 0$ for all $x \in D$, then T is called an *unbounded positive operator* on H.

The subspace D is called the *domain* of T.

REMARK. Observe, from Theorem 9.8, that if p is an H-projection-valued measure on a Borel space $(S, \mathcal{B})$, then $\int f\, dp$ is an unbounded selfadjoint operator on H for every real-valued Borel function f on S that is not in $L^\infty(p)$.

THEOREM 11.8. (Spectral Theorem for Unbounded Selfadjoint Operators) *Let H be a (separable and complex) Hilbert space.*

(1) *If T is an unbounded selfadjoint operator on H, then there exists a unique H-projection-valued measure p on $(\mathbb{R}, \mathcal{B})$ such that T is the integral with respect to p of the unbounded function*

$f(\lambda) = \lambda$; i.e., $T = \int \lambda\, dp(\lambda)$. See Theorem 9.8. Further, p is not supported on any compact interval in $\mathbb{R}$.

(2) *If p is an H-projection-valued measure on $(\mathbb{R}, \mathcal{B})$, that is not supported on any compact interval in $\mathbb{R}$, then $T = \int \lambda\, dp(\lambda)$ is an unbounded selfadjoint operator.*

(3) *The map $p \to \int \lambda\, dp(\lambda)$ of part 2 is a 1-1 correspondence between the set of all H-projection-valued measures p on $(\mathbb{R}, \mathcal{B})$ that are not supported on any compact interval in $\mathbb{R}$ and the set of all unbounded selfadjoint operators T on H.*

PROOF. Part 2 follows from Theorem 9.8. To see part 1, let $T : D \to H$ be an unbounded selfadjoint operator, and note that $I \pm iT$ is norm-increasing on D, whence is 1-1 and onto H. Define $U = (I - iT)(I + iT)^{-1}$. Then U maps Honto itself and is an isometry. For if $y = (I+iT)^{-1}(x)$, then $x = (I+iT)(y)$, whence $\|x\|^2 = \|y\|^2 + \|T(y)\|^2$. But then

$$\begin{aligned}\|U(x)\|^2 &= \|(I - iT)(y)\|^2 \\ &= \|y\|^2 + \|T(y)\|^2 \\ &= \|x\|^2.\end{aligned}$$

Moreover,

$$I + U = (I + iT)(I + iT)^{-1} + (I - iT)(I + iT)^{-1} = 2(I + iT)^{-1},$$

showing that $I + U$ maps H 1-1 and onto D. Similarly, we see that

$$I - U = 2iT(I + iT)^{-1},$$

whence

$$T = -i(I - U)(I + U)^{-1}.$$

This unitary operator U is called the *Cayley transform* of T.

By the Spectral Theorem for normal operators, we have that $U = \int \mu\, dq(\mu)$, where q is the spectral measure for U. Because U is unitary, we know that q is supported on the unit circle $\mathbb{T}$ in $\mathbb{C}$, and because $I + U = 2(I + iT)^{-1}$ is 1-1, we know that -1 is not an eigenvalue for U. Therefore, $q_{\{-1\}} = 0$, and the function h defined on $\mathbb{T} - \{-1\}$ by

$$h(\mu) = -i(1 - \mu)/(1 + \mu)$$

maps onto the real numbers $\mathbb{R}$. Defining $S = \int h(\mu)\, dq(\mu)$, we see from Theorem 9.8 that S is an unbounded selfadjoint operator on H. By part c of Exercise 9.15, we have that

$$\int (1/(1 + \mu))\, dq(\mu) = (I + U)^{-1},$$

and hence that

$$S = -i(I - U)(I + U)^{-1} = T.$$

Finally, let $p = h_*(q)$ be the projection-valued measure defined on $(\mathbb{R}, \mathcal{B})$ by

$$p_E = h_*(q)_E = q_{h^{-1}(E)}.$$

From part e of Exercise 9.15, we then have that

$$\int \lambda \, dp(\lambda) = \int h(\mu) \, dq(\mu) = S = T,$$

as desired.

We leave the uniqueness of p to the exercise that follows. Part 3 is then immediate from parts 1 and 2.

DEFINITION. Let $T : D \to H$ be an unbounded selfadjoint operator and let p be the unique projection-valued measure on $(\mathbb{R}, \mathcal{B})$ for which $T = \int \lambda \, dp(\lambda)$. The projection-valued measure p is called the *spectral measure* for T.

EXERCISE 11.14. (a) Prove the uniqueness assertion in part 1 of the preceding theorem.

(b) Let $T : D \to H$ be an unbounded selfadjoint operator, let p be its spectral measure, and let $U = (I - iT)(I + iT)^{-1}$ be its Cayley transform. Prove that

$$U = \int [(1 - i\lambda)/(1 + i\lambda)] \, dp(\lambda).$$

(c) Show that there is a 1-1 correspondence between the set of all projection-valued measures on $(\mathbb{R}, \mathcal{B})$ and the set of all (bounded or unbounded) selfadjoint operators on a Hilbert space H.

DEFINITION. Let T be an unbounded selfadjoint operator with domain D. A complex number λ is said to belong to the *resolvent* of T if the linear transformation $\lambda I - T$ maps D 1-1 and onto H and $(\lambda I - T)^{-1}$ is a bounded operator on H. The *spectrum* $\mathrm{sp}(T)$ of T is the complement of the resolvent of T.

If f is a real-valued (bounded or unbounded) Borel function on $\mathbb{R}$, we write $f(T)$ for the operator $\int f(\lambda) dp(\lambda)$.

As in the case of a bounded normal operator, we make analogous definitions of *point spectrum, continuous spectrum, discrete spectrum,* and *essential spectrum.*

The following exercise is the natural generalization of Exercise 11.4 and Theorem 11.4 to unbounded selfadjoint operators.

EXERCISE 11.15. Let T be an unbounded selfadjoint operator. Verify the following:

(a) The spectral measure p for T is supported on the spectrum of T; the spectrum of T is contained in the set of real numbers; if E is a closed subset of $\mathbb{C}$ for which $p_E = I$, then E contains the spectrum of T.

(b) $\lambda \in \mathrm{sp}(T)$ if and only if there exists a sequence $\{v_n\}$ of unit vectors in H such that

$$\lim \|T(v_n) - \lambda v_n\| = 0.$$

(c) $\lambda \in \mathrm{sp}_p(T)$ if and only if λ is an eigenvalue for T, i.e., if and only if there exists a nonzero vector $v \in D$ such that $T(v) = \lambda v$.

(d) $\lambda \in \mathrm{sp}_e(T)$ if and only if there exists a sequence $\{v_n\}$ of orthonormal vectors for which

$$\lim \|T(v_n) - \lambda v_n\| = 0.$$

(e) T is an unbounded positive operator if and only if $\mathrm{sp}(T)$ is a subset of the set of nonnegative real numbers.

THEOREM 11.9. (Invariance of the Essential Spectrum under a Compact Perturbation) *Let $T : D \to H$ be an unbounded selfadjoint operator on a Hilbert space H, and let K be a compact selfadjoint operator on H. Define $T' : D \to H$ by $T' = T + K$. Then T' is an unbounded selfadjoint operator, and*

$$sp_e(T') = sp_e(T).$$

That is, the essential spectrum is invariant under "compact perturbations."

EXERCISE 11.16. Prove Theorem 11.9.

EXERCISE 11.17. (a) Let T be an unbounded selfadjoint operator with domain D on a Hilbert space H. Prove that the graph of T is a closed subset of $H \times H$.

(b) Let $H = L^2([0,1])$, let D be the subspace of H consisting of the absolutely continuous functions f, whose derivative f' belongs to H and for which $f(0) = f(1)$. Define $T : D \to H$ by $T(f) = if'$. Prove that T is an unbounded selfadjoint operator on H. HINT: To show that $I \pm iT$

is onto, you must find a solution to the first order linear differential equation:

$$y' \pm y = f.$$

(c) Let $H = L^2([0,1])$, let D be the subspace of H consisting of the absolutely continuous functions f, whose derivative f' belongs to H and for which $f(0) = f(1) = 0$. Define $T : D \to H$ by $T(f) = if'$. Prove that T is not an unbounded selfadjoint operator.

(d) Let $H = L^2([0,1])$, let D be the subspace of H consisting of the absolutely continuous functions f, whose derivative f' belongs to H and for which $f(0) = 0$. Define $T : D \to H$ by $T(f) = if'$. Prove that T is not an unbounded selfadjoint operator.

We give next a different characterization of unbounded selfadjoint operators. This characterization essentially deals with the size of the domain D of the operator and is frequently given as the basic definition of an unbounded selfadjoint operator. This characterization is also a useful means of determining whether or not a given $T : D \to H$ is an unbounded selfadjoint operator.

THEOREM 11.10. *Let D be a proper dense subspace of a separable Hilbert space H, and let $T : D \to H$ be a symmetric linear transformation of D into H. Then T is an unbounded selfadjoint operator if and only if the following condition on the domain D holds: If $x \in H$ is such that the function $y \to (T(y), x)$ is continuous on D, then x belongs to D.*

PROOF. Suppose $T : D \to H$ is an unbounded selfadjoint operator and that an $x \in H$ satisfies the given condition. Then the map sending $y \in D$ to $((I + iT)(y), x)$ is continuous on D, and so has a unique continuous extension to all of H. By the Riesz Representation Theorem for Hilbert spaces, there exists a $w \in H$ such that

$$((I + iT)(y), x) = (y, w)$$

for all $y \in D$. Since $I - iT$ maps D onto H, there exists a $v \in D$ such that $w = (I - iT)(v)$. Therefore,

$$\begin{aligned} ((I + iT)(y), x) &= (y, w) \\ &= (y, (I - iT)(v)) \\ &= ((I + iT)(y), v) \end{aligned}$$

for all $y \in D$, showing that $(z, x) = (z, v)$ for all $z \in H$, whence $x = v$, and $x \in D$.

Conversely, assume that the condition holds. We must show that T is an unbounded selfadjoint operator. We must verify that $I \pm iT$ maps D onto H. We show first that the range of $I + iT$ is dense. Thus, let x be a vector orthogonal to the range of $I + iT$. Then the map $y \rightarrow ((I+iT)(y), x)$ is identically 0 on D, showing that $(T(y), x) = i(y, x)$, and therefore the map $y \rightarrow (T(y), x)$ is continuous on D. By the condition, $x \in D$, and we have

$$0 = ((I + iT)(x), x) = (x, x) + i(T(x), x),$$

implying that $\|x\|^2 = -i(T(x), x)$, which implies that $x = 0$ since $(T(x), x)$ is real. Hence, the range of $I + iT$ is dense in H. Of course, a similar argument shows that the range of $I - iT$ is dense in H.

To see that the range of $I + iT$ is closed, let $y \in H$, and suppose $y = \lim y_n$, where each $y_n = (I + iT)(x_n)$ for some $x_n \in D$. Now the sequence $\{y_n\}$ is a Cauchy sequence, and, since $I + iT$ is norm-increasing, it follows that the sequence $\{x_n\}$ also is a Cauchy sequence. Let $x = \lim x_n$. Then, for any $z \in D$, we have

$$\begin{aligned}(T(z), x) &= \lim(T(z), x_n) \\ &= \lim(z, T(x_n)) \\ &= \lim(z, (1/i)(y_n - x_n)) \\ &= (z, (1/i)(y - x)),\end{aligned}$$

which shows that the map $z \rightarrow (T(z), x)$ is a continuous function of z. Therefore, $x \in D$, and

$$(z, T(x)) = (T(z), x) = (z, (1/i)(y - x)),$$

showing that $T(x) = (1/i)(y - x)$, or $(I + iT)(x) = y$, and y belongs to the range of $I + iT$. Again, a similar argument shows that the range of $I - iT$ is closed, and therefore T is an unbounded selfadjoint operator.

REMARK. We see from the preceding exercise and theorem that a symmetric operator $T : D \rightarrow H$ can fail to be an unbounded selfadjoint operator simply because its domain is not quite right. The following exercise sheds some light on this observation and leads us to the notion of "essentially selfadjoint" operators.

EXERCISE 11.18. Let H be a separable Hilbert space, and let $T : D \to H$ be a symmetric linear transformation from a dense subspace D of H into H.

(a) Suppose D' is a proper subspace of D. Show that $T : D' \to H$ can never be an unbounded selfadjoint operator. (No smaller domain will do.)

(b) Let G denote the graph of T, thought of as a subset of $H \times H$. Prove that the closure $\bar{G}$ of G is the graph of a linear transformation $S : D'' \to H$. Show further that $D \subseteq D''$, that S is an extension of T, and that S is symmetric on D''. This linear transformation S is called the *closure* of T and is denoted by $\bar{T}$. T is called *essentially selfadjoint* if $\bar{T}$ is selfadjoint.

(c) Suppose $D \subseteq E$ and that $V : E \to H$ is an unbounded selfadjoint operator. We say that V is a *selfadjoint extension* of T if V is an extension of T. Prove that any selfadjoint extension of T is an extension of $\bar{T}$. That is, $\bar{T}$ is the minimal possible selfadjoint extension of T.

(d) Determine whether or not the operators in parts c and d of Exercise 11.17 have selfadjoint extensions and/or are essentially selfadjoint.

EXERCISE 11.19. Let H be a separable Hilbert space.

(a) (Stone's Theorem) Let $t \to U_t$ be a homomorphism of the additive group $\mathbb{R}$ into the group of unitary operators on H. Assume that for each pair of vectors $x, y \in H$ the function $t \to (U_t(x), y)$ is continuous. Prove that there exists a unique unbounded selfadjoint operator A on H, having spectral measure p, such that

$$U_t = e^{itA} = \int e^{it\lambda}\, dp(\lambda)$$

for all $t \in \mathbb{R}$. The operator A is called the *generator* of the one-parameter group U_t.

(b) Let A be an unbounded positive operator on H, having spectral measure p, with domain D. For each nonnegative t define

$$P_t = e^{-tA} = \int e^{-t\lambda}\, dp(\lambda).$$

Prove that the P_t's form a continuous semigroup of contraction operators. That is, show that each P_t is a bounded operator of norm ≤ 1 and that $P_{t+s} = P_t \circ P_s$ for all $t, s \geq 0$. Further, show that

$$A(x) = \lim_{t \to 0+} \frac{P_t(x) - x}{-t}$$

for every $x \in D$.

We conclude this chapter by summarizing our progress toward finding a mathematical model for experimental science. No proofs will be supplied for the theorems we quote here, and we emphasize that this is only a brief outline.

We have seen in Chapter VIII that the set $\mathcal{P}$ of all projections on an infinite-dimensional complex Hilbert space H could serve as a model for the set Q of all questions. Of course, many other sets also could serve as a model for Q, but we use this set $\mathcal{P}$.

Each observable A is identified with a question-valued measure, so in our model the observables are represented by projection-valued measures on $\mathbb{R}$, and we have just seen that these projection-valued measures are in 1-1 correspondence with all (bounded and unbounded) selfadjoint operators. So, in our model, the observables are represented by selfadjoint operators.

What about the states? How are they represented in this model? In Chapter VII we have seen that each state α determines a character μ_α of the set Q of questions. To see how states are represented in our model, we must then determine what the characters of the set $\mathcal{P}$ are.

THEOREM 11.11. (Gleason's Theorem) *Let H be a separable infinite dimensional complex Hilbert space, and let $\mathcal{P}$ denote the set of all projections on H. Suppose μ is a mapping of $\mathcal{P}$ into [0,1] that satisfies:*

(1) *If $p \leq q$, then $\mu(p) \leq \mu(q)$.*
(2) *$\mu(I - p) = 1 - \mu(p)$ for every $p \in \mathcal{P}$.*
(3) *If $\{p_i\}$ is a pairwise orthogonal (summable) sequence of projections, then $\mu(\sum p_i) = \sum \mu(p_i)$.*

Then there exists a positive trace class operator S on H, for which $\|S\|_{\mathrm{tr}} = tr(S) = 1$, such that $\mu(p) = tr(Sp)$ for every $p \in \mathcal{P}$.

Hence, the states are represented by certain positive trace class operators. Another assumption we could make is that every positive trace class operator of trace 1 corresponds, in the manner above, to a state. Since each such positive trace class operator S with $\mathrm{tr}(S) = 1$ is representable in the form

$$S = \sum \lambda_i p_i,$$

where $\sum \lambda_i m(\lambda_i) = 1$, we see that the pure states correspond to operators that are in fact projections onto 1-dimensional subspaces. Let α be a pure state, and suppose it corresponds to the projection q_v onto the

1-dimensional subspace spanned by the unit vector v. Let A be an observable (unbounded selfadjoint operator), and suppose A corresponds to the projection-valued measure $E \to p_E$. That is, $A = \int \lambda\, dp(\lambda)$. Then we have

$$\begin{aligned}\mu_{\alpha,A}(E) &= \mu_{\alpha,\chi_E(A)}(\{1\})\\ &= \mu_\alpha(\chi_E(A))\\ &= \mu_\alpha(q_E^A)\\ &= \mu_\alpha(p_E)\\ &= \mathrm{tr}(q_v p_E)\\ &= (q_v p_E(v), v)\\ &= (p_E(v), v)\\ &= \mu_v(E).\end{aligned}$$

If we regard the probability measure μ_v as being the probability distribution corresponding to a random variable X, then

$$(A(v), v) = ([\int \lambda\, dp(\lambda)](v), v) = \int \lambda\, d\mu_v(\lambda) = E[X],$$

where $E[X]$ denotes the expected value of the random variable X. We may say then that in our model $(A(v), v)$ represents the expected value of the observable A when the system is in the pure state corresponding to the projection onto the 1-dimensional subspace spanned by v.

How are time evolution and symmetries represented in our model? We have seen that these correspond to automorphisms ϕ_t' and π_g' of the set Q. So, we must determine the automorphisms of the set $\mathcal{P}$ of projections.

THEOREM 11.12. (Wigner's Theorem) *Let H be a separable infinite dimensional complex Hilbert space, and let $\mathcal{P}$ denote the set of all projections on H. Suppose η is a $1-1$ mapping of $\mathcal{P}$ onto itself that satisfies:*

(1) *If $p \leq q$, then $\eta(p) \leq \eta(q)$.*
(2) *$\eta(I - p) = I - \eta(p)$ for every $p \in \mathcal{P}$.*
(3) *If $\{p_i\}$ is a pairwise orthogonal (summable) sequence of projections, then $\{\eta(p_i)\}$ is a pairwise orthogonal sequence of projections, and*

$$\eta(\sum p_i) = \sum \eta(p_i).$$

Then there exists a real-linear isometry U of H onto itself such that $\eta(p) = UpU^{-1}$ for all $p \in \mathcal{P}$. Further, U either is complex linear or it is conjugate linear.

Applying Wigner's Theorem to the automorphisms ϕ'_t, it follows that there exists a map $t \to U_t$ from the set of nonnegative reals into the set of real-linear isometries on H such that $\phi'_t(p) = U_t p U_t^{-1}$ for every $p \in \mathcal{P}$. Also, if G denotes a group of symmetries, then there exists a map $g \to V_g$ of G into the set of real-linear isometries of H such that $\pi'_g(p) = V_g p V_g^{-1}$ for every $p \in \mathcal{P}$.

THEOREM 11.13.

(1) *The transformations U_t can be chosen to be (complex linear) unitary operators that satisfy*

$$U_{t+s} = U_t \circ U_s$$

for all $t, s \geq 0$.

(2) *The transformations V_g can be chosen to satisfy*

$$V_{g_1 g_2} = \sigma(g_1, g_2) V_{g_1} \circ V_{g_2}$$

for all $g_1, g_2 \in G$, where $\sigma(g_1, g_2)$ is a complex number of absolute value 1. Such a map $g \to V_g$ is called a representation of G.

(3) *The operators U_t commute with the operators V_g; i.e.,*

$$U_t \circ V_g = V_g \circ U_t$$

for all $g \in G$ and all $t \geq 0$.

We have thus identified what mathematical objects will represent the elements of our experimental science, but much remains to specify. Depending on the system and its symmetries, more precise descriptions of these objects are possible. One approach is the following:

(1) Determine what the group G of all symmetries is.
(2) Study what kinds of mappings $g \to V_g$, satisfying the conditions in the preceding theorem, there are. Perhaps there are only a few possibilities.
(3) Fix a particular representation $g \to V_g$ of G and examine what operators commute with all the V_g's. Perhaps this is a small set.
(4) Try to determine, from part 3, what the transformations U_t should be.

Once the evolution transformations ϕ'_t are specifically represented by unitary operators U_t, we will be in a good position to make predictions, which is the desired use of our model. Indeed, if α is a state of the system, and if α is represented in our model by a trace class operator S, then the state of the system t units of time later will be the one that is represented by the operator $U_t^{-1}SU_t$.