TQ2 TEORIA SPETTRALE

CHAPTER 3

LINEAR FUNCTIONALS AND LINEAR OPERATORS

Simplicio: "*Concerning natural things we need not always seek the necessity of mathematical demonstrations.*"

Sagredo: "*Of course, when you cannot reach it. But if you can, why not?*"

GALILEO GALILEI, Dialogue on the Two Major Systems of the World

The two notions of linear functionals and linear operators are closely related and are treated in this chapter side by side. Sections 3-1 and 3-3 correspond to each other in this sense, and Section 3-2 on sesquilinear functionals is the link between the two. The central theorem here is the theorem of Riesz, which shows that linear functionals are scalar products. In Section 3-4 we collect a number of useful properties on projections, and introduce the notion of spectral measure. In Section 3-5 we expose enough of the difficulties which one encounters with unbounded operators to warn the unwary of the pitfalls. Our tactics will be to avoid if possible the unbounded operators, and, if that cannot be done, to subject them to such severe conditions of propriety that they cannot cause trouble. In the applications we shall be dealing mostly with symmetrical (Hermitian) operators; and here the reader should retain the important distinction between "symmetrical" and "self-adjoint."

3-1. BOUNDED LINEAR FUNCTIONALS

A bounded linear functional $\phi(f)$ on a Hilbert space is a function with domain $\mathscr{H}$, which has for its range the complex numbers C, and which satisfies the following conditions:

$$\phi(f+g) = \phi(f) + \phi(g) \qquad \text{for all } f, g \in \mathscr{H}$$

$$\phi(\lambda f) = \lambda\phi(f); \qquad \text{and all } \lambda \in C;$$

$$|\phi(f)| < M\,\|f\| \qquad (M < \infty).$$

The greatest lower bound of the numbers M which satisfy the last inequality is called the norm $\|\phi\|$ of the functional $\phi(f)$.

The simplest example of a functional is the scalar product of f with a fixed vector g,

$$\phi(f) = (g, f). \tag{3-1}$$

One verifies without difficulty that the norm of this functional is $\|\phi\| = \|g\|$ (Problem 1).

The bounded linear functionals form a linear vector space if one defines addition of $\phi_1(f)$ and $\phi_2(f)$ by $(\phi_1(f) + \phi_2(f))$, and multiplication of $\phi(f)$ with a scalar λ by $\lambda\phi(f)$. They are also a normed vector space with the norm defined by $\|\phi\|$.

We shall now show that the linear functionals also constitute a Hilbert space; that is, there exists a scalar product in this space. First we verify that $\phi(f)$ is a continuous function with respect to the strong topology in $\mathscr{H}$. To see this, let $f_n \to f$, so that $\|f_n - f\| \to 0$ as $n \to \infty$. Then

$$|\phi(f_n) - \phi(f)| = |\phi(f_n - f)| \le \|\phi\|\,\|f_n - f\|,$$

and the left side tends to zero with the right.

We can now prove the following theorem.

Theorem (Riesz): *Every bounded linear functional ϕ in a Hilbert space $\mathscr{H}$ is of the form $\phi(f) = (g, f)$ with g some fixed vector in $\mathscr{H}$.*

Proof: Let $\{\varphi_n\}$ be a complete orthonormal system in $\mathscr{H}$, and let $f = \sum_n x_n\varphi_n$. Since $\phi(f)$ is continuous we have

$$\phi(f) = \sum_{n=1}^{\infty} x_n\phi(\varphi_n).$$

We then define

$$g \equiv \sum_{n=1}^{\infty} \phi^*(\varphi_n)\varphi_n,$$

and find

$$(g, f) = \sum_{n=1}^{\infty} \phi(\varphi_n)x_n = \phi(f). \qquad \text{Q.E.D.}$$

With the theorem of Riesz we have no difficulty defining a scalar product for linear functionals as follows, by setting

$$(\phi_1, \phi_2) = (g_2, g_1)$$

where $\phi_1(f) = (g_1, f)$ and $\phi_2(f) = (g_2, f)$.

The linear functionals are thus a linear manifold with a scalar product (also called a pre-Hilbert space). Its closure in the norm is a Hilbert space called the *dual space* $\hat{\mathscr{H}}$ of $\mathscr{H}$. There exists a natural mapping of the linear functionals $\phi \in \hat{\mathscr{H}}$ onto the vectors of $\mathscr{H}$ by assigning to the linear functional $\phi(f) = (g, f)$ the vector $g \in \mathscr{H}$. If $\phi \to g$ in this mapping, then $\lambda\phi \to \lambda^* g$; and if $\phi_1 \to g_1$ and $\phi_2 \to g_2$, then $(\phi_1 + \phi_2) \to (g_1 + g_2)$. Such a mapping is called antilinear.

If in the linear functional $\phi(f) = (g, f)$ we keep the vector f fixed and let g vary over the space $\mathscr{H}$, then we obtain a *conjugate linear functional* $\Psi(g) = (g, f)$. If $\Psi(g)$ is conjugate linear, then $\Psi^*(g)$ (the complex conjugate of Ψ) is a linear functional.

It follows from the foregoing that the bounded linear functionals of $\mathscr{H}$ are again a Hilbert space $\hat{\mathscr{H}}$, and that there exists a natural norm preserving linear mapping of $\hat{\mathscr{H}}$ onto $\mathscr{H}$. We can thus identify $\hat{\mathscr{H}}$ with $\mathscr{H}$.

This duality property of Hilbert space is exploited by Dirac in his notation of the *bra* and *ket* vectors [1, p. 18]. In fact, a ket $|f\rangle$ is a vector $f \in \mathscr{H}$, and a bra $\langle g|$ is a linear functional over $\mathscr{H}$ which for f takes on the value $\langle g|f\rangle = (g, f)$.

PROBLEMS

1. The norm of the bounded linear functional $\phi(f) = (g, f)$ for some fixed vector g is equal to $\|g\|$.
2. The norm of a bounded linear functional satisfies the parallelogram law:

$$\|\phi_1 + \phi_2\|^2 + \|\phi_1 - \phi_2\|^2 = 2\,\|\phi_1\|^2 + 2\,\|\phi_2\|^2$$

(use the Riesz theorem).

3. A bounded linear functional is determined everywhere by its values on a subset $S \subset \mathscr{H}$ which spans $\mathscr{H}$.
4. A bounded linear functional is strongly and weakly continuous.

3-2. SESQUILINEAR FUNCTIONALS AND QUADRATIC FORMS

A sesquilinear functional is a complex-valued function $\phi(f, g)$ of two variable vectors f and $g \in \mathscr{H}$. Thus the domain of such a functional is the topological product $\mathscr{H} \times \mathscr{H}$ of the Hilbert space with itself consisting of all pairs of vectors, and the range is the complex numbers.

We shall restrict our discussion in this subsection to bounded sesquilinear functionals which we define by the requirements:

For fixed f the functional $\phi(f, g)$ is a bounded linear functional of g.

For fixed g the functional $\phi(f, g)$ is a bounded conjugate linear functional of f.

If, in addition to these properties, $\phi(f, g) = \phi^*(g, f)$, then the functional ϕ is called *symmetrical*.

Every sesquilinear functional defines a certain *quadratic form* $\hat{\phi}(f) \equiv \phi(f, f)$. Conversely, every such quadratic form defines uniquely a sesquilinear functional by the formula (Problem 1):

$$4\phi(f, g) \equiv \hat{\phi}(f + g) - \hat{\phi}(f - g) + i\hat{\phi}(f - ig) - i\hat{\phi}(f + ig).$$

The process expressed in this equation is known as *polarization*.

This last result shows that a sesquilinear functional $\phi(f, g)$ is in fact completely determined by its values on the diagonal $\phi(f, f)$, that is, by its associated quadratic form $\hat{\phi}(f)$. It follows from this remark that a sesquilinear functional is *symmetrical* if and only if its associated quadratic form is real.

A sesquilinear functional $\phi(f, g)$ is called *positive* if its associated quadratic form takes only positive values: $\hat{\phi}(f) \geq 0$. It is called *strictly positive* if $\hat{\phi}(f) = 0$ implies $f = \boldsymbol{\theta}$.

An example of a strictly positive sesquilinear functional is the scalar product $\phi(f, g) = (f, g)$.

If $\phi(f, g)$ is a sesquilinear functional, then for every fixed f this is a linear functional of g. Thus by Riesz' theorem we can associate an f' with every f by the formula

$$\phi(f, g) = (f', g) \qquad \text{for all } g \in \mathscr{H}.$$

The correspondence $f \to f'$ has the following properties: $\lambda f \to \lambda f'$ and $(f_1 + f_2)' = f_1' + f_2'$ (Problem 3). Such a correspondence is called a linear operator. We shall devote the next section to the study of such operators.

PROBLEMS

1. If $\hat{\phi}(f) \equiv \phi(f, f)$ for some sesquilinear functional ϕ, then

$$4\phi(f, g) = \hat{\phi}(f + g) - \hat{\phi}(f - g) + i\hat{\phi}(f - ig) - i\hat{\phi}(f + ig).$$

2. A sesquilinear functional is symmetrical if and only if its associated quadratic form is real.
3. The correspondence $f \to f'$ established by the equation

$$\phi(f, g) = (f', g) \qquad \text{for all } g \in \mathscr{H}$$

has the properties

$$(\lambda f)' = \lambda f', \qquad (f_1 + f_2)' = f_1' + f_2'.$$

3-3. BOUNDED LINEAR OPERATORS

A bounded linear operator T is a function with a linear manifold D_T as domain and a subset Δ_T in $\mathscr{H}$ as range, and such that

$$T(f + g) = Tf + Tg \qquad \text{for all } f, g \in D_T;$$

$$T(\lambda f) = \lambda Tf \qquad \text{for all } f \in D_T \text{ and all complex } \lambda;$$

$$\|Tf\| \leq M\,\|f\| \qquad \text{for } 0 \leq M < \infty.$$

It follows immediately from this definition that the range is also a linear manifold. The greatest lower bound of the numbers M which satisfy the last inequality is called the *norm* of the operator T and is denoted by $\|T\|$. If there does not exist such an $M < \infty$, then the operator is said to be *unbounded*. In this section we shall discuss only bounded operators.

If $f_1 \neq f_2$ implies $Tf_1 \neq Tf_2$, then there exists another linear operator T^{-1}, called the *inverse* of T, with domain $D_{T^{-1}} = \Delta_T$ and range $\Delta_{T^{-1}} = D_T$. It has the property

$$T^{-1}Tf = f \qquad \text{for all } f \in D_T,$$

$$TT^{-1}g = g \qquad \text{for all } g \in \Delta_T.$$

An operator is said to be *continuous* at $f \in D_T$ if $f_n \in D_T$ and $f_n \to f$ implies $Tf_n \to Tf$. Every bounded operator is continuous everywhere. Conversely, every linear operator which is continuous at one point is continuous everywhere and bounded. Continuity and boundedness are thus interchangeable concepts for linear operators. (See Problems 2 and 3.)

If T_1 is a bounded linear operator defined on $D_{T_1} \supset D_T$ and agreeing with T on D_T, then we say T_1 is an *extension* of T, and we write $T_1 \supset T$ (or $T \subset T_1$).

If $f_n \in D_T$ is a Cauchy sequence and $f_n \to f$, then if $f \notin D_T$ we define

$$Tf = \lim_{n\to\infty} Tf_n.$$

This limit always exists, because with f_n, Tf_n is also a Cauchy sequence:

$$\|Tf_n - Tf_m\| \leq \|T\| \, \|f_n - f_m\|.$$

With this assignment we obtain an extension of the linear operator from D_T to the closure $\bar{D}_T$ (Problem 4). For this reason we can always assume that a bounded linear operator is defined on a subspace; in particular, if D_T is dense in $\mathscr{H}$, this is the entire space. The domain can even be extended to all of $\mathscr{H}$ if D_T is not dense in $\mathscr{H}$. We first extend T to $\bar{D}_T$ by continuity. Then we *define* T on $D_T^\perp$ as an arbitrary bounded linear operator; for instance, $Tf = 0$ for $f \in D_T^\perp$. On a general $f \in \mathscr{H}$, the extended operator is then defined by linearity; it has the same norm as the original operator. When nothing specific is said about the domain of a bounded operator T, we shall always assume that we are dealing with this maximal extension.

This remark is especially useful if we want to define the sum and the product of linear operators. For instance, let T_1 and T_2 be two operators; then the *sum* of these two operators is defined by the formula:

$$(T_1 + T_2)(f) = T_1 f + T_2 f.$$

Similarly we define the *product* T_1T_2 by setting

$$T_1T_2(f) = T_1(T_2 f).$$

We can also define a *multiplication with scalars* by

$$(\lambda T)(f) = \lambda(Tf),$$

and it is easily seen that if T_1, T_2, and T are bounded operators, their sum, product, and scalar multiples are also (Problem 5).

Every bounded linear operator defines a sesquilinear functional ϕ as follows:

$$\phi(f, g) \equiv (f, Tg).$$

At the end of the preceding section we have shown that the converse of this is also true. Actually, every such functional defines not one but two bounded linear operators T and T^* by the formula

$$\phi(f, g) = (T^*f, g) = (f, Tg).$$

The two operators T and T^* are said to be *adjoint* to one another. One easily verifies the following properties:

$$(T_1T_2)^* = T_2^*T_1^*;$$

$$(\lambda T)^* = \lambda^* T^* \qquad (\lambda^* = \text{complex conjugate } \lambda);$$

$$(T_1 + T_2)^* = T_1^* + T_2^*;$$

$$(T^*)^* = T.$$

An operator T for which $T^* = T$ is called *self-adjoint* or symmetrical. From the definition of the adjoint operator one easily verifies that $\|T^*\| = \|T\|$ (Problem 6).

We describe a few examples of bounded linear operators.

1) The *identity operator* I: This is the operator which does nothing to the vectors so that $If = f$, for all $f \in \mathscr{H}$.

2) The *projection operators* E, defined everywhere, are characterized by the property $E^*E = E$.

   Every projection operator determines a subspace which is its range; and conversely, every subspace M determines a unique projection E with range M (Problem 7).

   If $f = f_1 + f_2$ with $f_1 \in M$ and $f_2 \in M^\perp$, then the projection E with range M is defined by the equation

$$Ef = f_1.$$

3) The *partial isometries* Ω are linear operators with the property: $\Omega^*\Omega = E$ is a projection. It is easy to verify that $F = \Omega\Omega^*$ is then also a projection (Problem 8). E and F are called *right-* and *left*-projections respectively.

4) The *unitary operators* are a special class of isometries, namely those for which both E and F are unit operators. Thus U is unitary if

$$U^*U = UU^* = I.$$

The prototype of an isometry which is not unitary is the *shift-operator* defined as follows: Let $\{\varphi_n\}$ $(n = 1, 2, \ldots)$ be a complete orthonormal system, and define the operator Ω on all φ_n by

$$\Omega\varphi_n = \varphi_{n+1}.$$

One easily finds then that Ω^* satisfies

$$\Omega^*\varphi_{n+1} = \varphi_n \qquad \text{and} \qquad \Omega^*\varphi_1 = \mathbf{0}.$$

For all other f we define

$$\Omega f = \sum_{n=1}^{\infty} x_n \Omega\varphi_n \qquad \text{if} \quad f = \sum_{n=1}^{\infty} x_n\varphi_n.$$

From these definitions it follows that

$$\Omega^*\Omega\varphi_n = \varphi_n \qquad (n = 1, 2, \ldots).$$

Thus $\Omega^*\Omega = I$. Furthermore,

$$\Omega\Omega^*\varphi_n = \varphi_n \quad \text{with } n = 2, 3, \ldots, \qquad \text{and} \qquad \Omega\Omega^*\varphi_1 = \mathbf{0}.$$

Thus we have verified that $\Omega\Omega^*$ is a projection on the orthogonal complement of φ_1.

Another example of an isometry is the continuous shift operator defined as follows: Let $\mathscr{H} = L^2(0, \infty)$, so that $f = \{f(x)\}$ when $0 \le x < \infty$. If we set $f(x) = 0$ for $x < 0$, we can define an operator Ω by setting

$$(\Omega f)(x) = f(x - a), \qquad (\Omega^* f)(x) = f(x + a).$$

With this definition we find

$$(\Omega^*\Omega f)(x) = f(x),$$

$$(\Omega\Omega^* f)(x) = \begin{cases} f(x) & \text{for } x \ge a, \\ 0 & \text{for } x < a. \end{cases}$$

Thus we have verified that Ω is an isometry.

Examples of bounded self-adjoint linear operators are obtained easily as follows: Let $\{\varphi_n\}$ be a complete orthonormal system; define $A\varphi_n = \lambda_n\varphi_n$ (λ_n real) and extend by linearity to the entire space.

The sesquilinear functional associated with a self-adjoint operator is symmetrical (cf. Section 3-2), and every such functional defines a self-adjoint operator (Problem 10). We shall call a self-adjoint operator a *positive* operator if its associated quadratic form is positive.

PROBLEMS

1. The correspondence $f \to (\varphi, f)\varphi$ for some fixed normalized φ is a bounded linear operator with bound 1.
2. If a linear operator is continuous at one point, it is continuous everywhere.
3. A linear operator is continuous if and only if it is bounded.
4. Every bounded linear operator T with domain D_T admits a unique extension T_1 to the closure $\overline{D}_T$ without changing the norm, so that
$$D_{T_1} = \overline{D}_T \qquad \text{and} \qquad \|T_1\| = \|T\|.$$
5. If T_1 and T_2 are bounded linear operators, then $(T_1 + T_2)$ and T_1T_2 are, too. Furthermore, the bounds satisfy the inequalities
$$\|T_1 + T_2\| \le \|T_1\| + \|T_2\|, \qquad \text{and} \qquad \|T_1T_2\| \le \|T_1\|\,\|T_2\|.$$
6. $\|T^*\| = \|T\|$.
7. Every projection operator defines a unique subspace which is its range, and vice versa.
8. If Ω is a linear operator such that $\Omega^*\Omega = E$ is a projection, then $\Omega\Omega^* = F$ is also a projection.
9. In a finite-dimensional space, every isometry with right projection $E = I$ is unitary (that is, its left projection is also I).
10. A bounded self-adjoint operator defines a symmetrical sesquilinear functional, and vice versa.

3-4. PROJECTIONS

A linear operator E defined on all of $\mathscr{H}$ and satisfying the relation $EE^* = E$ is called a *projection*. It follows immediately from this relation that $E = E^*$ and consequently $E^2 = E$. Projections are thus self-adjoint and *idempotent*. The range Δ_E of a projection is a subspace, and to every subspace there corresponds a unique projection. We have therefore a one-to-one correspondence of projections to subspaces which permits us to replace one by the other.

It follows from this remark that the entire lattice structure of subspaces can be transferred to projections. They are, as are the subspaces, a partially ordered system. For instance, we say that $E_1 \le E_2$ if for the corresponding subspaces M_1 and M_2 we have $M_1 \subseteq M_2$. It is easy to show that $E_1 \le E_2$ if and only if $E_1E_2 = E_1$ (Problem 1).

If E is a projection with range M, then $(I - E)$ is the projection with range $M^\perp$. These remarks show that certain relations in the lattice of subspaces can be easily expressed in terms of *algebraic* operations on corresponding projections.

It is natural to ask the question how the operations of union and intersection of subspaces are expressed algebraically in terms of the corresponding projections: Let M_1 and M_2 be two subspaces, and E_1 and E_2 the projections with ranges M_1 and M_2 respectively. We have defined the intersection $M_1 \cap M_2$ as the subspace consisting of all the vectors common to M_1 and M_2. The projection F with range $N = M_1 \cap M_2$ must be a function of the projections E_1 and E_2. We shall denote it by $F = E_1 \cap E_2$, and it is by definition the largest projection contained in E_1 and in E_2. What is this function?

Our first impulse might be to suggest the answer $F = E_1E_2$. But this cannot be generally right, since F is a projection only if E_1 and E_2 commute (Problem 2). In that case the answer is correct, and $F \equiv E_1 \cap E_2 = E_1E_2$ (Problem 3).

If E_1 and E_2 do not commute, then the problem of finding $E_1 \cap E_2$ as a function of E_1 and E_2 is more difficult. We give here the result and shall be content with an illustration of the result in a special case.

Let us consider the situation of Fig. 3-1. The two projections E_1 and E_2 are represented by two (nonorthogonal) one-dimensional subspaces. The vectors $f_n = (E_1E_2)^n f$ are seen to converge to zero, illustrating that for this special case

$$E_1 \cap E_2 = \lim_{n\to\infty} (E_1E_2)^n = 0.$$

The general formula valid for any two projections is

$$E_1 \cap E_2 = \lim_{n\to\infty} (E_1E_2)^n. \tag{3-2}$$

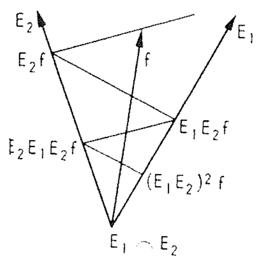

Fig. 3-1 Illustration of the formula

$$E_1 \cap E_2 = \lim_{n\to\infty} (E_1E_2)^n.$$

If E_1 and E_2 commute, then $(E_1E_2)^n = E_1E_2$, and we find, as before, that $E_1 \cap E_2 = E_1E_2$. It follows then that $E_1 \cup E_2 = E_1 + E_2 - E_1E_2$ (Problem 3).

Of special importance in quantum mechanics are families of commuting projections which are closed with respect to countable unions and intersections. If $\mathscr{L}$ is such a family and $E_n \in \mathscr{L}$ a sequence of projections in $\mathscr{L}$, then $\bigcup_n E_n$ and $\bigcap_n E_n$ are again in $\mathscr{L}$. Furthermore, with $E \in \mathscr{L}$, also $(I - E) \in \mathscr{L}$. If $\mathscr{L}$ contains also 0 and I, we obtain a Boolean algebra.

A canonical way of constructing such Boolean algebras of projections is the following:

Let $\mathscr{H} = L^2(S, M, \mu)$ and $\Delta \in M$ an arbitrary measurable set. To any such set one can associate a projection $E(\Delta)$ by defining, for any $f(x) \in L^2(S, M, \mu)$, $(x \in S)$, the operator $E(\Delta)$:

$$(E(\Delta)f)(x) = \chi_\Delta(x) f(x), \tag{3-3}$$

where $\chi_\Delta(x)$ is the characteristic function of the set Δ; that is, the function defined by

$$\chi_\Delta(x) = \begin{cases} 1 & \text{for } x \in \Delta, \\ 0 & \text{for } x \notin \Delta. \end{cases}$$

Because the class M of measurable sets is σ-additive, the projections $E(\Delta)$ are σ-additive, too. That is, if Δ_n is any sequence of disjoint sets, then

$$\text{(a)} \qquad \sum_{n=1}^{\infty} E(\Delta_n) = E\left(\bigcup_{n=1}^{\infty} \Delta_n\right).$$

Furthermore, for any two sets Δ_1, Δ_2, we have

$$\text{(b)} \qquad \begin{aligned} E(\Delta_1) \cap E(\Delta_2) &= E(\Delta_1 \cap \Delta_2), \\ E(\Delta_1) \cup E(\Delta_2) &= E(\Delta_1 \cup \Delta_2); \end{aligned}$$

and finally,

$$\text{(c)} \qquad \begin{aligned} E(\emptyset) &= 0, \\ E(S) &= I. \end{aligned}$$

Such a map from the class of sets M to a Boolean algebra of projections which satisfies the relations (a), (b), and (c) is called a *spectral measure* over the measure space (S, M, μ). This fundamental notion will be used constantly in the following discussion.

The canonical spectral measure defined by the special property (3-3) is, of course, especially simple to realize. The spectral measure is obviously a generalization of a numerical measure. Instead of assigning a number to the sets, the spectral measure assigns projections in a Hilbert space. From any spectral measure, one can easily obtain a large number of numerical measures. It suffices to define for an arbitrary vector f

$$\mu_f(\Delta) = (f, E(\Delta)f).$$

This definition of measures depending on vectors f will be of great importance later on.

PROBLEMS

1. If E_1 and E_2 are two projections, and Δ_{E_1} and Δ_{E_2} their corresponding ranges, then $\Delta_{E_1} \subseteq \Delta_{E_2}$ if and only if $E_1E_2 = E_1$.
2. If E_1 and E_2 are projections, then $F = E_1E_2$ is one if and only if $E_1E_2 = E_2E_1$.
3. If $E_1E_2 = E_2E_1$, then $E_1 \cap E_2 = E_1E_2$ and $E_1 \cup E_2 = E_1 + E_2 - E_1E_2$.
4. Three commuting projections E_1, E_2, and E_3 satisfy the distributive law,

$$E_1 \cap (E_2 \cup E_3) = (E_1 \cap E_2) \cup (E_1 \cap E_3),$$
$$E_1 \cup (E_2 \cap E_3) = (E_1 \cup E_2) \cap (E_1 \cup E_3).$$

3-5. UNBOUNDED OPERATORS

We cannot avoid discussing the unbounded operators since they are constantly used in quantum mechanics. We do it here primarily to acquaint the reader with the mathematical complications which one encounters with unbounded operators. (For a more complete discussion, see reference 2.)

An unbounded linear operator is such that $\|Tf\|/\|f\|$ exceeds all finite bounds. For such operators one can always find an f such that for any finite M we have

$$\|Tf\| > M\,\|f\|.$$

Such operators exist only in the infinite-dimensional Hilbert space. In the finite-dimensional case every linear operator is bounded (Problem 1).

An example of an unbounded operator is easily constructed, for instance as follows: Let $\{\varphi_n\}$ be a complete orthonormal system and define $A\varphi_n = n\varphi_n$. The domain D_A of this operator consists of all linear combinations

$$f = \sum_{n=1}^{\infty} x_n\varphi_n \qquad \text{such that} \qquad \sum_{n=1}^{\infty} n^2\,|x_n|^2 < \infty.$$

This is a dense linear manifold $\subset \mathscr{H}$. The operator is unbounded because $\|A\varphi_n\| = n$; thus for n sufficiently large this norm exceeds any finite quantity. It is easy to verify that this operator cannot be continuous. Consider, for instance, the sequence of vectors $f_n = (1/n)\varphi_n$. We obtain $Af_n = \varphi_n$, and this does not tend to zero, although f_n does. Thus A is not continuous. We also observe that A is not defined everywhere in $\mathscr{H}$ since the vector f with components $x_n = 1/n$ is not contained in D_A.

These properties are, in a certain sense, to be made precise now, also characteristic, for the unbounded operators. In order to explain this in more detail we need a new concept which replaces that of continuity in the unbounded case.

A linear operator T is called *closed* if, for every sequence of vectors f_n in the domain D_T of T, the relations

$$f_n \to f \qquad \text{and} \qquad Tf_n \to g$$

imply that $f \in D_T$ and that $Tf = g$. Superficially this definition seems to be like the definition of continuity. But there is an important difference: For the definition of continuity, f is assumed to be in D_T and $Tf_n \to Tf$ is asserted, while for a closed operator, f is *asserted* to be in D_T under the assumption that Tf_n converges.

Since the domain of a continuous operator is always closed (cf. Section 3-3), a continuous operator is always closed, but there are closed operators which are not continuous.

An operator which is not closed may be extended to a closed one. We shall not examine under what conditions such an extension is possible. Suffice it to remark here that all the unbounded operators which we need to consider do admit closures. If the closure is possible it is unique.

For closed unbounded operators one can prove that they cannot be defined in the entire space. We have the following theorem:

Theorem: *Every closed linear transformation on $\mathscr{H}$ is necessarily bounded* [3].

Let us now examine the definition of the adjoint transformation. This is a little more delicate, since D_T is not the entire space. We can and will, however, assume in the following discussion that D_T is dense in $\mathscr{H}$. This is not a severe restriction. Let us consider the expression $\Phi(g) = (f, Tg)$ for a fixed f. If there exists a vector f^* with the property

$$(f, Tg) = (f^*, g) \qquad \text{for all } g \in D_T,$$

then we say $f \in D_{T^*}$ and we *define* the operator T^* by setting $T^*f = f^*$. The operator T is called *symmetrical* (or Hermitian) if $T^* \supseteq T$; we have called an operator *self-adjoint* if $T^* = T$. Such an operator is thus always symmetrical.

In general we have the following situation for symmetrical operators T:

$$T \subseteq T^{**} \subseteq T^*,$$

and we may distinguish the following cases:

1) $T = T^{**}$ but $T^{**} \subset T^*$. The operator T is closed but not self-adjoint.
2) $T \subset T^{**} = T^*$. The operator T is not closed but its smallest closed extension T^{**} is self-adjoint (Problem 7). It is then called *essentially self-adjoint.*
3) $T \subset T^{**} \subset T^*$. The operator T is neither closed nor essentially self-adjoint.
4) $T = T^{**} = T^*$. The operator T is self-adjoint and hence closed.

A closed symmetrical operator, if it is not self-adjoint, may admit further symmetrical extensions. If there are no further extensions possible, then the symmetrical operator is called *maximal.* If there exists a maximal and self-adjoint extension, then the extended operator is called hypermaximal (see von Neumann [4]).

Von Neumann has given a complete characterization of symmetrical operators and their various extensions. In quantum mechanics the only symmetrical operators which have any useful physical interpretation are the essentially self-adjoint operators, in which we shall therefore be particularly interested.

The restriction in the domain of unbounded operators poses a great difficulty in the formation of sums and products of operators. Consider, for instance, the operators T_1 and T_2 with their respective domains D_1 and D_2.

The operator $T_1 + T_2$ is then definable only in the intersection $D_1 \cap D_2$, and there it is given by

$$(T_1 + T_2)f = T_1 f + T_2 f.$$

Similarly, for the definition of a product operator $T_1 T_2$, we need the conditions $f \in D_2$ and $T_2 f \in D_1$. Then we can define

$$(T_1 T_2)f = T_1(T_2 f).$$

The intersection of two domains is of course again a linear manifold, but it need not be dense. In fact it can be $\boldsymbol{\theta}$, even if both D_1 and D_2 are dense. It is seen from these remarks that the definition of sums and products of unbounded operators is already quite complicated for merely two operators.

There are two situations when a simplification is possible. The first occurs when there exists a common dense domain for two operators which is also invariant under the operations. The restriction of the operators to this dense domain permits the definition of unrestricted sums and products, and hence the formation of any algebraic expression.

The other simplification occurs when one of the two operators is bounded. Let T be an unbounded, and B any bounded operator; then $(T + B)$ and BT are defined in D_T. On the other hand, TB is defined only on the elements f for which $Bf \in D_T$.

This leads us to the definition: A bounded operator B commutes with the (unbounded) operator T if TB is an extension of BT,

$$BT \subseteq TB.$$

In particular, if B is a projection E, then $ET \subseteq TE$ implies $ETE = TE = ET$. A projection E which stands with an operator T in this relation is said to *reduce* T.

If the projection E reduces T, then $F = (I - E)$ also reduces T. We can then decompose the operator into two: $T = T^E + T^F$, where $T^E = TE$, $T^F = TF$ are called the reductions of T to the subspaces $M = E\mathscr{H}$ and $N = F\mathscr{H}$ respectively. T^E operates only in M and T^F only in N.

3-6. EXAMPLES OF OPERATORS

1. The position operator Q. The position operator Q is defined in a subset D_Q of the space $L^2(-\infty, +\infty)$ consisting of all Lebesgue square-integrable functions $\psi(x)$ by setting

$$(Q\psi)(x) = x\psi(x).$$

The subset D_Q is defined by

$$D_Q = \left\{\psi(x) : \int_{-\infty}^{+\infty} x^2 \, |\psi(x)|^2 \, dx < \infty\right\}.$$

The operator Q is symmetrical, since for every $\varphi \in D_Q$ and every $\psi \in D_Q$, we have

$$(\psi, Q\varphi) = \int_{-\infty}^{+\infty} x\psi^*(x)\varphi(x)\, dx = (Q\psi, \varphi).$$

This equation shows that for all such ψ, $Q^*\psi$ is defined and, in fact, $Q^*\psi = Q\psi$. Thus $D_Q \subseteq D_{Q^*}$ and $Q \subseteq Q^*$.

We shall now show that, for this domain D_Q, the operator Q is also self-adjoint. To see this, we verify that in fact $D_{Q^*} \subseteq D_Q$ so that $Q = Q^*$. Thus let $\psi \in D_{Q^*}$ and define $\psi_1 = Q^*\psi$; then

$$(\psi, Q\varphi) = (\psi_1, \varphi) \qquad \text{for all } \varphi \in D_Q.$$

Thus

$$\int_{-\infty}^{+\infty} (x\psi^*(x) - \psi_1(x))\varphi(x)\, dx = 0 \qquad \text{for all } \{\varphi(x)\} \in D_Q.$$

Since D_Q is dense in $\mathscr{H}$ we must have, a.e.,

$$x\psi(x) = \psi_1(x).$$

Therefore $\psi \in D_Q$ and $\psi_1 = Q\psi$.

2. The momentum operator. The operator P is defined on the subset D_P which consists of all absolutely continuous functions $\psi(x)$ which are differentiable a.e., and for which $(d\psi/dx) \in L^2(-\infty, +\infty)$. On this the set operator P is defined by

$$(P\psi)(x) = -i\,\frac{d\psi(x)}{dx}.$$

One can show that this operator, too, is self-adjoint [2, Chapter IV].

There exists, furthermore, a common dense domain D which is invariant under the operations Q and P, and on which both operators are defined. For any $\varphi \in D$ one finds (Problem 8)

$$(QP - PQ)\varphi = i\varphi. \tag{3-4}$$

We see that the operator $QP - PQ$ is bounded on the dense domain D, and therefore admits a unique extension to the entire space; so we may write the operator equation

$$QP - PQ \subset iI. \tag{3-5}$$

We shall call this the *canonical commutation rule*. It plays a fundamental role in quantum mechanics.

It is usually (incorrectly) written $QP - PQ = iI$, which disregards the fact that the left-hand side is defined only on a dense domain.

3. The creation and annihilation operators A^* and A. Let φ_n $(n = 0, 1, \ldots)$ be a complete orthonormal system in an abstract Hilbert space $\mathscr{H}$. Define

$$A\varphi_n = \sqrt{n}\varphi_{n-1} \qquad (n = 1, 2, \ldots),$$
$$A^*\varphi_n = \sqrt{n+1}\varphi_{n+1} \qquad (n = 0, 1, 2, \ldots),$$
$$A\varphi_0 = 0.$$

By linearity we can extend the definition of A and A^* to all linear combinations

$$f = \sum_{n=0}^{\infty} x_n\varphi_n \qquad \text{for which} \qquad \sum_{n=0}^{\infty} |x_n|^2 n < \infty.$$

On such f we define

$$Af = \sum_{n=0}^{\infty} x_n A\varphi_n = \sum_{n=1}^{\infty} x_n\sqrt{n}\varphi_{n-1}$$

and

$$A^*f = \sum_{n=0}^{\infty} x_n A^*\varphi_n = \sum_{n=0}^{\infty} x_n\sqrt{n+1}\varphi_{n+1}.$$

The two operators A and A^* are then the adjoint of one another, and $D_A = D = D_{A^*}$, so that the * has the usual significance of the adjoint for unbounded operators. There is a simple relation between the operators A, A^* on the one hand and Q, P on the other (Problem 9).

PROBLEMS

1. In a finite-dimensional Hilbert space, every linear operator is bounded.
2. The set of elements f with the property that, for some unbounded operator T with dense domain, there exists a vector f^* such that

$$(f, Tg) = (f^*, g) \qquad \text{for all } g \in D_T,$$

is a linear manifold D_{T^*}.
3. If D_T is dense, then the vector f^* of Problem 2 is unique.
4. The operator T^* is always closed.
5. Every symmetrical operator T admits a closed symmetrical extension, namely T^{**}.
6. If E reduces the operator T, then $F = (I - E)$ also reduces T.
7. If the symmetrical operator A has the property $A^{**} = A^*$, then its smallest closed symmetrical extension $A = A^{**}$ is self-adjoint.

8. The functions

$$\varphi_n(x) = \frac{1}{\sqrt{\sqrt{\pi}\,2^n n!}} e^{-x^2/2} H_n(x) \qquad (n = 0, 1, \ldots),$$

where $H_n(x)$ are the polynomials of Hermite [5, p. 62], are a complete orthonormal system in $L^2(-\infty, +\infty)$; and the finite linear combinations of the $\varphi_n(x)$ are a dense linear manifold D which is invariant under P and Q, and on which both P and Q are defined. For every $\varphi \in D$ one verifies

$$(QP - PQ)\varphi = i\varphi.$$

9. The operators

$$A = \frac{1}{\sqrt{2}}(Q + iP) \qquad \text{and} \qquad A^* = \frac{1}{\sqrt{2}}(Q - iP)$$

are adjoints of each other on the domain

$$D = \left\{f : \sum_{n=0}^{\infty} |(f, \varphi_n)|^2 n < \infty\right\},$$

and they satisfy

$$A\varphi_n = \sqrt{n}\varphi_{n-1} \qquad (n = 1, 2, \ldots),$$
$$A\varphi_0 = 0,$$
$$A^*\varphi_n = \sqrt{n+1}\varphi_{n+1} \qquad (n = 0, 1, 2, \ldots).$$

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CHAPTER 4

SPECTRAL THEOREM AND SPECTRAL REPRESENTATION

Unless the vessel's pure, all you pour in turns sour.

HORACE

In this chapter we are concerned primarily with those aspects of self-adjoint linear operators which have to do with their realizations in a function space. Most of the practical calculations in the applications are done by means of such realizations. There is a canonical realization which we call the spectral representation. It uses for its Hilbert space a certain function space over the spectrum of the operator.

In order to formulate the spectral representation, we need several basic concepts and theorems which we introduce in an informal manner in Section 4-1, in the context of finite-dimensional spaces. There we present the notions of spectrum, spectral measure, simple spectrum, and spectral representation unencumbered by technical details of topology and measure theory.

In Section 4-2, we give the definition of the spectrum of a self-adjoint operator in terms of the domain of the resolvent operator. The central theorem of this chapter, the spectral theorem, is stated without proof in Section 4-3. It establishes a unique correspondence between spectral measures and self-adjoint operators, and it is an indispensable tool in the establishment of a functional calculus as explained in the following section (4-4). In Section 4-5, we prepare the ground for the spectral representation by studying some properties of the spectral density functions. This clarifies the role of the cyclic vector and leads to two equivalent definitions of the simple spectrum of an operator.

Section 4-6 gives a formulation of the spectral representation. The case of one operator is explained in sufficient detail to complete the existence proof without too much trouble, and to make the subsequent generalization to a countable family of operators at least plausible. In the final section (4-7), we sketch the method of eigenfunction expansion which, if available, gives a convenient method for calculating the spectral representation.

4-1. SELF-ADJOINT OPERATORS IN FINITE-DIMENSIONAL SPACES

In this section $\mathscr{H}$ will be a finite-dimensional Hilbert space, and we denote its dimension by $n < \infty$. We shall briefly recapitulate the principal properties of the self-adjoint linear operators A in $\mathscr{H}$. Since $n < \infty$,

$$D_A = \Delta_A = \mathscr{H}.$$

The equation $f' = Af$, which associates with every $f \in \mathscr{H}$ another $f' \in \mathscr{H}$, can always be realized as a finite linear system of equations by introducing a complete orthonormal system $\{\varphi_r\}$ with $r = 1, \ldots, n$, and $(\varphi_r, \varphi_s) = \delta_{rs}$. If

$$f = \sum_{r=1}^{n} x_r \varphi_r \qquad \text{and} \qquad f' = \sum_{r=1}^{n} x'_r \varphi_r,$$

then

$$x'_r = \sum_{s=1}^{n} A_{rs} x_s,$$

where

$$A_{rs} = (\varphi_r, A\varphi_s) = A^*_{sr} \qquad (r, s = 1, \ldots, n).$$

The structure of the operator is revealed by referring it to a particular coordinate system, consisting of *eigenvectors*. They are the nontrivial solutions of the equations

$$A\psi_r = \lambda_r \psi_r \qquad (r = 1, \ldots, n).$$

One can show that there always exist n nontrivial solutions of this equation where the numbers λ_r, *the eigenvalues*, are the solutions of the *secular equation*

$$|A_{rs} - \lambda \delta_{rs}| = 0.$$

The determinant of the left-hand side of this equation is a polynomial in λ and it has, according to the fundamental theorem of algebra, exactly n solutions; since A_{rs} is Hermitian, they are all real. These solutions are called the spectrum of the operator A. Some of these solutions may coincide; they must then be counted with their proper multiplicity. In the special case in which the roots are all simple (that is, of multiplicity 1), we shall call the eigenvalues *nondegenerate* and the spectrum *simple*.

The following facts are easily verified: If $\lambda_r \neq \lambda_s$, then the corresponding eigenvectors ψ_r and ψ_s are orthogonal: $(\psi_r, \psi_s) = 0$. Furthermore, if the eigenvalue λ_r has multiplicity $\alpha(r)$, then there exist $\alpha(r)$ linearly independent eigenvectors ψ_r with this eigenvalue (Problems 1 and 2). The eigenvectors which belong to λ_r are then an $\alpha(r)$-dimensional subspace of $\mathscr{H}$.

From the preceding remarks it follows that there always exists a coordinate system in $\mathscr{H}$ consisting of eigenvectors ψ_r $(r = 1, 2, \ldots, n)$. If the λ_r are all nondegenerate, the ψ_r are already orthogonal and complete. If they are degenerate we can choose them to be so in many different ways. In this coordinate system the operator A appears in a particularly simple form: If $f = \sum_{r=1}^{n} x_r \psi_r$, then $f' = Af = \sum_{r=1}^{n} x_r' \psi_r$ with $x_r' = \lambda_r x_r$. This is the *spectral representation* of A.

For the sake of later generalizations of this important result, we shall formulate it as follows.

We have really two different spaces: $\mathscr{H}$ and ℓ_n^2. The latter consists of all sequences of n complex numbers $\{x_r\}$ with $r = 1, 2, \ldots, n$. By the formula $x_r = (\psi_r, f)$ we establish a one-to-one correspondence Ω between vectors f in the abstract space $\mathscr{H}$ and sequences $\{x_r\}$ in ℓ_n^2. This correspondence is isometric if the norm of sequences $\{x_r\}$ is defined by

$$\|\{x_r\}\|^2 = \sum_{r=1}^{n} |x_r|^2$$

(Problem 4). Isometric means that if $\{x_r\} = \Omega f$, then

$$\sum_{r=1}^{n} |x_r|^2 = \|f\|^2.$$

Two Hilbert spaces which are the linear isometric image of each other are identical in their abstract structure.

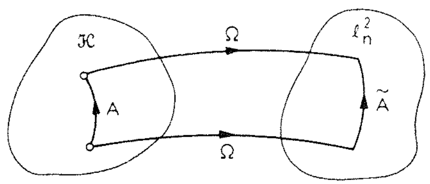

Fig. 4–1 Illustrating the equation $\tilde{A} = \Omega A \Omega^{-1}$.

The operator A defined in $\mathscr{H}$ may be considered an operator in ℓ_n^2 via the isometric image Ω of $\mathscr{H}$ onto ℓ_n^2. We shall denote it by $\tilde{A}$. Thus $\tilde{A} = \Omega A \Omega^{-1}$, and (cf. Fig. 4–1)

$$\tilde{A}\{x_r\} = \{\lambda_r x_r\}. \qquad (4\text{–}1)$$

Every self-adjoint operator permits a spectral representation in finite-dimensional spaces. We are interested in the generalization of this result to the infinite-dimensional Hilbert space. In order , formulate the spectral representation in Hilbert space, it is necessary to introduce some new concepts which will permit an alternative but equivalent formulation of the above result. The main difficulty which we must negotiate is connected with the use of the coordinate system $\{\psi_r\}$. In Hilbert space a complete system of eigenvectors does not necessarily exist. It is thus necessary to seek a formulation which does not use such a system.

Let us begin by an alternative definition of the spectrum Λ of the operator A. We have seen that Λ is the set of numbers λ for which the equation $(A - \lambda \cdot I)\psi = \mathbf{0}$ has nontrivial solutions. In other words, if $\lambda \notin \Lambda$, then

this equation has only the trivial solution $\psi = \mathbf{0}$. A linear operator which has this property admits an inverse, which is again a linear operator. This means the operator

$$R_\lambda = (A - \lambda \cdot I)^{-1} \qquad (4\text{–}2)$$

exists for $\lambda \notin \Lambda$. The operator R_λ is called the *resolvent operator*.

If (still in finite-dimensional spaces) $\lambda_r \in \Lambda$, then the set of ψ for which $(A - \lambda_r I)\psi = \mathbf{0}$ spans a finite-dimensional subspace M_r. Let P_r be the projection with range M_r. If λ_r is nondegenerate, then M_r is one-dimensional. Generally, the degree of degeneracy of λ_r equals dim M_r. The previous statements concerning the orthogonality and completeness of the ψ_r can now be expressed by the equations

$$P_r P_s = \delta_{rs} P_r, \qquad \text{and} \quad \sum_r P_r = I. \qquad (4\text{–}3)$$

A system of projections which satisfy such relations is sometimes called a decomposition of unity. In terms of the projections P_r, the operator A has the simple form $\Sigma \lambda_r P_r$ (Problem 7).

We have already stated what we mean by a simple spectrum. Now we shall take up this notion once more, and cast it into a different form, which at first sight may seem more complicated but which in the end will be the only useful form of expressing this notion for general operators.

Consider the set of all polynomials

$$u(A) = a_1 A^{n-1} + a_2 A^{n-2} + \cdots + a_n.$$

They form an algebra $\mathscr{A}$, that is a vector space with a multiplication law: If T_1 and $T_2 \in \mathscr{A}$, then $\lambda_1 T_1 + \lambda_2 T_2 \in \mathscr{A}$ for complex λ_1, λ_2 and $T_1 T_2 \in \mathscr{A}$.

The dimension of this vector space cannot exceed n since the operator A satisfies an algebraic equation of order n, that is, the Cayley equation:

$$\prod_{r=1}^{n} (\lambda_r - A) = 0.$$

If the dimension of $\mathscr{A}$ is exactly equal to n, then the spectrum of A is simple. If the dimension is less than n, it is degenerate.

Another equally useful way of characterizing the simple spectrum is the following: if g is a fixed vector in $\mathscr{H}$, we can consider the set of all the elements of the form $f = Tg$ with $T \in \mathscr{A}$. We denote this set by $\{\mathscr{A}g\}$. It is clearly a subspace of $\mathscr{H}$. The size of this subspace will depend on g as well as on $\mathscr{A}$. Concerning the dependence of g, it is convenient to select vectors for which dim $\{\mathscr{A}g\}$ is maximal. For such vectors the dimension of $\{\mathscr{A}g\}$ depends only on the structure of the algebra, and will therefore depend on its dimension. More precisely, we have the following theorem.

Theorem: *The spectrum of A is simple if and only if there exist vectors g such that $\{\mathscr{A}g\}$ is equal to the entire space.*

Instead of giving a proof of this theorem we merely make some heuristic remarks which can easily be expanded and sharpened to a complete proof (Problem 6).

The vectors g with the property that $\{\mathscr{A}g\} = \mathscr{H}$ are called *cyclic vectors* of the algebra $\mathscr{A}$. They are characterized by the property $P_r g \neq \mathbf{0}$ for all r. If the P_r are all one-dimensional, then $f = u(A)g = \sum_r u(\lambda_r)P_r g$.

By suitable choice of $u(\lambda_r)$ one can reach any arbitrary vector $f \in \mathscr{H}$. Thus we see that we may characterize the operators with simple spectrum by saying that they give the highest mobility of the vector Tg with $T \in \mathscr{A}$. The other extreme would be obtained if the spectrum of A is completely degenerate. Then the operator A is merely a multiple of the unit operator, and we have the least mobility: The degree of mobility of vectors Tg with $T \in \mathscr{A}$ thus measures the degree of degeneracy of the spectrum.

Both of the preceding definitions of the simple spectrum can, with suitable modifications, be transferred to the infinite-dimensional Hilbert space. Before we do this, we shall introduce the notion of the spectral measure (still for the finite-dimensional case).

Let Δ be a Borel set on the real line. To every set we can associate a projection $E(\Delta)$ defined by

$$E(\Delta) = \sum_{\lambda_r \in \Delta} P_r.$$

In this way we obtain a projection-valued set function, defined on all Borel sets and satisfying the relations

$$\begin{aligned} E(\Delta_1) \cup E(\Delta_2) &= E(\Delta_1 \cup \Delta_2), \\ E(\Delta_1) \cap E(\Delta_2) &= E(\Delta_1 \cap \Delta_2), \\ E(0) &= 0, \\ E(R^1) &= I. \end{aligned} \tag{4–4}$$

At the end of Chapter 3 we called a projection-valued set function with these properties a *spectral measure*. Thus we see that every self-adjoint operator A defines a unique spectral measure E. With every such measure we can also define, for any fixed vector f, a finite numerical-valued measure μ_f by the formula

$$\mu_f(\Delta) = (f, E(\Delta)f).$$

In our particular case (finite dimension of $\mathscr{H}$), every μ_f is a discrete Lebesgue-Stieltjes measure concentrated at the points λ_r. The weights ρ_r at the points λ_r depend on the choice of f, and they may be zero for certain vectors f. However, for cyclic vectors g we have

$$\mu_g(\lambda_r) - \mu_g(\lambda_r - 0) = (g, P_r g) \neq 0,$$

where we have used the notation $\mu_g(\lambda) \equiv \mu_g((-\infty, \lambda])$. From this remark we

see immediately that the measure μ_f for any f must be absolutely continuous with respect to any measure μ_g with g cyclic.

Thus, in the notation of Section 1-4,

$$\mu_f \prec \mu_g.$$

In particular if f is also a cyclic vector, we have

$$\mu_g \prec \mu_f;$$

the two measures are equivalent: $\mu_f \sim \mu_g$. One verifies easily with the Radon-Nikodym theorem that, conversely, if $\mu_f \sim \mu_g$, then f must be cyclic. We summarize this situation with the following theorem:

Theorem: *Two numerical spectral measures μ_{g_1} and μ_{g_2} are equivalent if both g_1 and g_2 are cyclic vectors. Every other numerical measure μ_f is inferior to them.*

All of the results in this section have analogues in the infinite-dimensional case, and the rest of this chapter is devoted to the explicit formulation of these analogues and their applications for establishing the spectral representation.

PROBLEMS

1. Let A be a self-adjoint operator in the finite-dimensional space $\mathscr{H}$. Then
$$A\psi_1 = \lambda_1\psi_1, \qquad A\psi_2 = \lambda_2\psi_2 \qquad \text{and} \qquad \lambda_1 \neq \lambda_2$$
imply that $(\psi_1, \psi_2) = 0$. Is this result also valid in infinite-dimensional spaces?
2. If λ is a root of multiplicity α of the secular equation $|A - \lambda \cdot I| = 0$, then there exist exactly α linearly independent solutions ψ of the equation $A\psi = \lambda\psi$.
3. If ψ_1 and ψ_2 are two linearly independent eigenvectors belonging to the same eigenvalue λ, then all vectors in the subspace spanned by ψ_1 and ψ_2 are eigenvectors with eigenvalue λ.
4. The correspondence $\Omega : f \to \{x_r\}$, where $x_r = (\psi_r, f)$ and ψ_r is a complete orthonormal system in $\mathscr{H}$, is one-to-one and isometric provided that the norm of the sequence $\{x_r\}$ is defined by
$$\|\{x_r\}\|^2 = \sum_{r=1}^{n} |x_r|^2.$$
5. A vector g is cyclic with respect to a self-adjoint operator A if and only if $P_r g \neq \mathbf{0}$ for all spectral projections P_r.
6. The spectrum of A is simple if and only if $\{\mathscr{A}g\} = \mathscr{H}$ for cyclic vectors g.
7. In a finite-dimensional space the self-adjoint operator A has the form $A = \sum \lambda_r P_r$, where P_r is the projection with range M_r and M_r is the linear subspace of vectors ψ_r which satisfy
$$(A - \lambda_r \cdot I)\psi_r = \mathbf{0}.$$

4-2. THE RESOLVENT AND THE SPECTRUM

In this section we consider a self-adjoint operator A in Hilbert space. A may be bounded or unbounded; in any case it is closed. For any complex $z = x + iy$, we consider the operator $A - z \cdot I$, and we denote by D its domain and by $\Delta(z)$ its range, so that $\Delta \equiv \Delta(0)$ is the range of A.

The equation $Af - zf = g$ establishes a correspondence between the elements of D and the elements of $\Delta(z)$. If this correspondence is one-to-one, then there exists the resolvent operator $R_z = (A - z \cdot I)^{-1}$ with domain $\Delta(z)$ and range D.

We adopt the following definition of the spectrum of the operator A: The values of z for which $\Delta(z) = \mathscr{H}$ are called *regular* values for A; all other values are called the *spectrum* of A. All the values $z = x + iy$, with $y \neq 0$, are regular values for A (Problems 1 and 2). Thus the spectrum of a self-adjoint operator A is always real; in particular the proper values are real.

For real values $z = \lambda$, $\Delta(\lambda)$ may or may not be equal to $\mathscr{H}$. There are four cases possible, depending on whether $\Delta(\lambda)$ is closed or not, and whether we have $\overline{\Delta(\lambda)} \subset \mathscr{H}$ or $\overline{\Delta(\lambda)} = \mathscr{H}$. We can thus divide the spectrum Λ into two parts, $\Lambda = \Lambda_c + \Lambda_d$, called the *continuous* and the *discrete* part. If $\Delta(\lambda) \subset \overline{\Delta(\lambda)}$, then $\lambda \in \Lambda_c$ and if $\overline{\Delta(\lambda)} \subset \mathscr{H}$, then $\lambda \in \Lambda_d$. The four cases which arise is this way are given in Table 4-1.

Table 4-1

THE SPECTRUM OF A SELF-ADJOINT OPERATOR

Property of $\Delta(\lambda)$	Spectrum
$\Delta(\lambda) = \overline{\Delta(\lambda)} = \mathscr{H}$	$\lambda \notin \Lambda_c, \quad \lambda \notin \Lambda_d$
$\Delta(\lambda) \subset \overline{\Delta(\lambda)} = \mathscr{H}$	$\lambda \in \Lambda_c, \quad \lambda \notin \Lambda_d$
$\Delta(\lambda) = \overline{\Delta(\lambda)} \subset \mathscr{H}$	$\lambda \notin \Lambda_c, \quad \lambda \in \Lambda_d$
$\Delta(\lambda) \subset \overline{\Delta(\lambda)} \subset \mathscr{H}$	$\lambda \in \Lambda_c, \quad \lambda \in \Lambda_d$

We see from this table that the range $\Delta(\lambda)$ of the operator $A - \lambda \cdot I$ furnishes a convenient means to identify the structure of the spectrum of a self-adjoint operator.

This characterization does not say anything about the multiplicity of the spectrum. In the discrete spectrum, it is easy to verify that the dimension of $\Delta(\lambda)^{\perp}$ is exactly equal to the multiplicity of the eigenvalue λ (Problem 6). To characterize the multiplicity in the continuous part of Λ is more difficult. In order to do this, we need the functional calculus to which we devote much of the remaining part of this chapter.

We conclude this section with some remarks on the resolvent operator $R_z = (A - z \cdot I)^{-1}$. If z is a regular value for A (for instance, for all z with $\operatorname{Im} z \neq 0$), then R_z is a bounded operator defined for all elements $g \in \mathscr{H} = \Delta(z)$.

From the two equivalent relations $(A - \lambda \cdot I)f = g$ and $R_\lambda g = f$, we easily obtain, for all $g \in \mathscr{H}$,

$$R_{z_1} g = R_{z_2}(A - z_2 \cdot I) R_{z_1} g,$$

$$R_{z_2} g = R_{z_2}(A - z_1 \cdot I) R_{z_1} g.$$

By taking the difference of the two equations we obtain

$$R_{z_1} - R_{z_2} = (z_1 - z_2) R_{z_2} R_{z_1}. \tag{4–5}$$

This is called the Hilbert relation. It follows immediately that two bounded resolvents commute:

$$R_{z_1} R_{z_2} = R_{z_2} R_{z_1}.$$

Finally one can prove the relation (Problem 7)

$$R_z^* = R_{z^*}.$$

PROBLEMS

1. The operator $(A - zI)^{-1}$, with A self-adjoint and $z = x + iy\ (y \neq 0)$, exists and is bounded.
2. If $z = x + iy\ (y \neq 0)$, then $\Delta(z) = \mathscr{H}$.
3. The solutions of the eigenvalue problem $A\psi = \lambda\psi$ are the orthogonal complement of $\Delta(\lambda)$.
4. The spectrum of the operator Q (Section 3-5) is the entire real line.
5. The point λ is in the continuous spectrum of the self-adjoint operator if and only if there exists a sequence of normalized vectors φ_n ($\|\varphi_n\| = 1$) such that
$$\|(A - \lambda)\varphi_n\| \to 0 \quad \text{for} \quad n \to \infty.$$
6. The multiplicity of an eigenvalue $\lambda \in \Lambda_d$ of a self-adjoint operator is equal to the dimension of $\Delta(\lambda)^{\perp}$.
7. The resolvent R_z of a self-adjoint operator satisfies the relation $R_z^* = R_{z^*}$ for all $z \notin \Lambda$.

4-3. THE SPECTRAL THEOREM

At the end of Section 4-1 we introduced the notion of the spectral measure for the finite-dimensional case. We shall now generalize this notion to the operators in the infinite-dimensional Hilbert space. The fundamental spectral theorem may then be stated in the following way.

To every self-adjoint operator A there corresponds a unique spectral measure $\Delta \to E(\Delta)$ defined on the Borel sets of the real line R^1 such that

$$A = \int_{-\infty}^{+\infty} \lambda \, dE_\lambda, \tag{4-6}$$

where $E_\lambda \equiv E((-\infty, \lambda])$ and the integral is to be interpreted as the Lebesgue-Stieltjes integral valid for any $f \in D_A$

$$(f, Af) = \int_{-\infty}^{+\infty} \lambda \, d(f, E_\lambda f). \tag{4-7}$$

The proof of this important theorem is found in reference 1.

It suffices here to see that it is an obvious generalization of the corresponding theorem for the discrete case (Section 4-1).

The one-to-one correspondence of the spectral measures on the real line to the self-adjoint operators permits us to replace one by the other.

To every spectral measure on the real line belongs a *spectral family* of projections E_λ with $-\infty < \lambda < +\infty$.

The general projection of such a spectral family is defined $E_\lambda \equiv E((-\infty, \lambda])$. The spectral family satisfies the relations

$$\begin{aligned} E_\lambda &\le E_\mu \qquad \text{for } \lambda < \mu, \\ E_{\lambda+0} &= E_\lambda, \\ E_{-\infty} &= 0, \\ E_{+\infty} &= I. \end{aligned} \tag{4-8}$$

If the spectral family is known, the spectral measure can be reconstructed by the formula

$$E(\Delta) = \int_\Delta dE_\lambda$$

for any Borel set Δ. This formula is an abbreviated notation for the numerical integral, valid for any $f \in \mathscr{H}$:

$$(f, E(\Delta)f) = \int_{-\infty}^{+\infty} \chi_\Delta(\lambda) \, d(f, E_\lambda f) \equiv \int_\Delta d(f, E_\lambda f)$$

PROBLEMS

1. If the spectrum Λ of a self-adjoint operator is continuous (that is Λ_d is the null set), then $(f, E_\lambda f)$ is a continuous function of λ for all vectors f.
2. The spectral measure $E(\Delta)$ of a self-adjoint operator A reduces the resolvent operator $R_z = (A - z \cdot I)^{-1}$: $R_z E(\Delta) = E(\Delta) R_z$.

4-4. THE FUNCTIONAL CALCULUS

The last formula of the preceding section is a special case of a much more general relation between certain functions $u(\lambda)$ of a real variable λ and linear operators in Hilbert space.

If T is a bounded operator defined in $D_T = \mathscr{H}$, then it is clear what we mean by the operator T^2. It is the operator which assigns to every vector f the vector $T^2 f = T(Tf)$. It is not difficult to extend this to any finite positive power of T, by a recursive definition: $T^n f = T(T^{n-1} f)$. If $u(\lambda) \equiv \lambda^n + a_1 \lambda^{n-1} + \cdots + a_n$ is a polynomial of λ, then we define the operator $u(T) = T^n + a_1 T^{n-1} + \cdots + a_n$ by setting

$$u(T)f = T^n f + a_1 T^{n-1} f + \cdots + a_n f.$$

This assignment of polynomials to operators satisfies the relations

$$\begin{aligned} (u_1 + u_2)(T) &= u_1(T) + u_2(T), \\ (u_1 u_2)(T) &= u_1(T) u_2(T), \\ (cu)(T) &= cu(T) \end{aligned} \tag{4-9}$$

for all complex c. Furthermore, all the operators $u(T)$ commute with each other.

The correspondence of functions $u(\lambda)$, with operators $u(T)$, which satisfies relations (4-9) is called a *functional calculus*. It is desirable to extend this calculus to the largest possible class of functions for self-adjoint operators. A convenient way to do this is the following.

We define $u(\lambda)$ as *measurable* with respect to the spectral family E_λ if for every $f \in \mathscr{H}$ the function $u(\lambda)$ is measurable with respect to the Lebesgue-Stieltjes measure defined by the spectral density functions $\rho_f = (f, E_\lambda f)$.

Similarly, we say $u(\lambda)$ is *integrable* with respect to the spectral family E_λ if for every $f \in \mathscr{H}$ the function $u(\lambda)$ is integrable with respect to the measure defined by $\rho_f(\lambda)$.

Let A be a self-adjoint linear operator and E_λ its spectral family. If $u(\lambda)$ is measurable and integrable with respect to E_λ, then we can define, for any pair of vectors $f, g \in \mathscr{H}$, the expression

$$L_g^*(f) \equiv \int_{-\infty}^{+\infty} u(\lambda) \, d(f, E_\lambda g),$$

and one verifies easily that $L_g(f)$ is a bounded linear functional of f. By Riesz' theorem there thus exists a unique vector g^* with the property $L_g(f) = (g^*, f)$.

The correspondence $g \to g^*$ defines a bounded linear operator $u(A)$ so that we have the formula

$$(f, u(A)g) = \int_{-\infty}^{+\infty} u(\lambda) \, d(f, E_\lambda g).$$

This will be written in an abbreviated notation as

$$u(A) = \int_{-\infty}^{+\infty} u(\lambda)\, dE_\lambda.$$

One can verify that the correspondence $u(\lambda) \to u(A)$ of functions with operators has the properties (4–9), (Problem 6).

The operator $u(A)$ is bounded if the function $u(\lambda)$ is essentially bounded with respect to E_λ; that is, if there exists a real number $M < \infty$ such that the set $\{\lambda : u(\lambda) < M\}$ has measure zero for all measures ρ_f. The greatest lower bound of the numbers M with this property is the bound of the operator $u(A)$ (Problem 1).

It is possible to extend the functional calculus to unbounded operators by restricting the vectors f and g to suitably defined dense linear manifolds. Some slight modifications of the relations (4–9) are then needed because of the restrictions of the domains of definition.

Some important applications of the functional calculus are the following examples:

1) The integral representation of the self-adjoint operator A with the spectral family λ is given by

$$A = \int_{-\infty}^{+\infty} \lambda\, dE_\lambda.$$

It is bounded if and only if

$$\int_{-\infty}^{+\infty} \lambda^2\, d(f, E_\lambda f)$$

exists for all $f \in \mathscr{H}$. If it is unbounded, then the domain of definition D_A is given by the set of vectors f for which

$$\int_{-\infty}^{+\infty} \lambda^2\, d(f, E_\lambda f) < \infty.$$

2) Let $\chi_\Delta(\lambda)$ be the characteristic function of the Borel set Δ. It is measurable and integrable with respect to E_λ. The operator

$$\chi_\Delta(A) \equiv \int_{-\infty}^{+\infty} \chi_\Delta(\lambda)\, dE_\lambda = \int_\Delta dE_\lambda \equiv E(\Delta)$$

defines the projection of the spectral measure associated with Δ.

3) For every real t and every self-adjoint operator A one can define

$$U_t = e^{iAt} = \int_{-\infty}^{+\infty} e^{i\lambda t}\, dE_\lambda. \tag{4–10}$$

One verifies that this is a family of unitary operators which satisfies

$$U_{t_1} U_{t_2} = U_{t_1 + t_2}.$$

This relation between self-adjoint operators and unitary one-parameter groups has a converse in the form of

Stone's theorem: *Every unitary one-parameter group U_t for which $(f, U_t g)$ is a continuous function in t for all $f, g \in \mathscr{H}$ defines a unique spectral measure such that*

$$U_t = \int_{-\infty}^{+\infty} e^{i\lambda t}\, dE_\lambda.$$

The self-adjoint operator A which corresponds to this spectral measure is called the *generating operator* of the group. We may then write the preceding relation equivalently $U_t = e^{iAt}$.

The set of all bounded operators of the form $u(A)$, with A some self-adjoint operator, forms an algebra $\mathscr{A}$. We shall denote it the algebra *generated* by A.

If $T_1, T_2 \in \mathscr{A}$, then $T_1 + T_2 \in \mathscr{A}$ and $T_1 T_2 \in \mathscr{A}$. Furthermore if $T \in \mathscr{A}$, then $\lambda T \in \mathscr{A}$ for all complex λ. The algebra is *abelian*; this means that for every pair of operators T_1 and T_2 one has $T_1 T_2 = T_2 T_1$. The algebra can also be characterized in the following equivalent way:

Let $\mathscr{S}$ be any set of self-adjoint operators; then we denote by $\mathscr{S}'$ the set of all bounded operators which commute with $\mathscr{S}$. The algebra generated by $\mathscr{S}$ is then the set $\mathscr{S}'' \equiv (\mathscr{S}')'$. The algebra $\mathscr{A}$ defined above is then also the algebra defined by $\mathscr{A} = \{A\}''$ (Problem 4). The fact that $\mathscr{A}$ is abelian is expressed by the relation $\mathscr{A} \subseteq \mathscr{A}'$. If $\mathscr{A} = \mathscr{A}'$, then the algebra is called *maximal abelian*. It then does not admit any abelian extension.

In Section 4-1 we stated that the self-adjoint operator A has simple spectrum if and only if the algebra generated by the operator A has maximal dimension. We can now transfer this property to the infinite dimensional case by defining: The operator A has simple spectrum if the algebra $\mathscr{A} = \{A\}''$ is a maximal abelian algebra: $\mathscr{A} = \mathscr{A}'$.

At this point we have succeeded in transferring the notion of simple spectrum to the infinite-dimensional case without making use of the notion of eigenvector.

PROBLEMS

1. The operator $u(A) = \int u(\lambda)\, dE_\lambda$ is bounded if and only if the function $u(\lambda)$ is essentially bounded.
2. The domain of definition of the unbounded operator $u(A)$ is the set of vectors f for which

$$\int_{-\infty}^{+\infty} |u(\lambda)|^2\, d(f, E_\lambda f) < \infty.$$

3. The operator $u(A)$ for A self-adjoint is unitary if and only if $|u(\lambda)| = 1$ a.e. with respect to the spectral family E_λ.

*4. The algebra $\mathscr{A} = \{A\}''$ consists of all the operators of the form $u(A)$ where $u(\lambda)$ is an essentially bounded measurable and integrable function with respect to the spectral family E_λ of A [2, Section 129].

5. If the spectrum of the self-adjoint operator A is discrete and $\{A\}'' = \mathscr{A} \subset \mathscr{A}'$, then there exists at least one degenerate eigenvalue λ of A.

6. The correspondence

$$u(\lambda) \to u(A) \equiv \int_{-\infty}^{+\infty} u(\lambda)\, dE_\lambda$$

is a functional calculus; that is, it satisfies relations (4–9).

4-5. SPECTRAL DENSITIES AND GENERATING VECTORS

In this section we shall study in more detail the spectral density function introduced in the preceding section. Let E_λ be a spectral family, and f a vector in $\mathscr{H}$; then we define the spectral density function $\sigma_f(\lambda) = (f, E_\lambda f)$. This function will depend on the spectral family E_λ on the one hand, and on the vector f on the other. We shall study the dependence on f for a fixed spectral family E_λ.

First we list a few simple properties of any function $\sigma(\lambda) = (f, E_\lambda f)$ which follow directly from the basic properties (4–8) of a spectral family.

$$\begin{aligned} \sigma(\lambda_1) &\le \sigma(\lambda_2) \qquad \text{for } \lambda_1 < \lambda_2, \\ \sigma(\lambda + 0) &= \sigma(\lambda), \\ \sigma(-\infty) &= 0, \\ \sigma(+\infty) &= 1 \qquad \text{for } \|f\| = 1. \end{aligned} \tag{4–11}$$

Furthermore the function $\sigma(\lambda)$ is discontinuous for certain values $\lambda \in \Lambda_d$. For all other values of λ it is continuous. In particular for all values $\lambda \notin \Lambda$ the function $\sigma(\lambda)$ is constant.

Any function $\sigma(\lambda)$ with these properties defines a measure $\mu(\Delta)$ for all Borel subsets Δ of the real line through the formula:

$$\mu(\Delta) = \int \chi_\Delta(\lambda)\, d\sigma(\lambda).$$

Thus for each f we have defined a measure.

We shall now examine the dependence of this measure on the vector f. We recall from Section 1-2 that measures are a partially ordered set. A measure μ_1 is inferior with respect to μ_2 ($\mu_1 \prec \mu_2$) if μ_1 is absolutely continuous with respect to μ_2.

For the measures which we are studying there is another partial ordering possible by using the dependence of σ on the vector f. Let

$$\sigma_1(\lambda) = (f_1, E_\lambda f_1) \qquad \text{and} \qquad \sigma_2(\lambda) = (f_2, E_\lambda f_2).$$

To any vector f we can associate a subspace

$$M(f) = \overline{\{\mathscr{A}'f\}}$$

where the right-hand side denotes the subspace generated by all vectors of the form Sf with $S \in \mathscr{A}'$. If we denote by

$$M_1 \equiv M(f_1), \qquad M_2 \equiv M(f_2),$$

then we may define a partial ordering of the measure by denoting σ_1 inferior to σ_2 if $M_1 \subseteq M_2$. We have adopted a terminology which is justified in anticipation of the following.

Theorem: *Let E_λ be a spectral family and $f_1, f_2 \in \mathscr{H}$ two arbitrary vectors in $\mathscr{H}$; then the spectral density function σ_1 is absolutely continuous with respect to σ_2 if and only if $M_1 \subseteq M_2$* [3].

This theorem shows that the notions of partial ordering derived from absolute continuity and from the partial ordering of associated subspaces are equivalent. It follows from this that the measure associated with a cyclic vector of $\mathscr{A}'$ has a maximal property:

If g is a vector such that $\overline{\{\mathscr{A}'g\}} = \mathscr{H}$, then the measure defined by $\rho(\lambda) = (g, E_\lambda g)$ is maximal in the partially ordered set of measures. That is for any $f \in \mathscr{H}$, we have

$$\sigma_f \prec \rho.$$

It follows immediately from this remark that if g' is any other cyclic vector and ρ' the associated measure, then $\rho \sim \rho'$ (Problem 4). The spectral density functions for two different cyclic vectors define the same (maximal) measure class.

In conclusion of this subsection we can now give an alternate definition of the operator with simple spectrum which generalizes the one given in Section 4-1. We have defined an operator A to have simple spectrum if $\{A\}'' = \mathscr{A} = \mathscr{A}'$. An equivalent definition is possible with the cyclic vectors by using the following.

Theorem: *An operator A has simple spectrum if and only if there exists a cyclic vector for the algebra $\mathscr{A} = \{A\}''$* (Problem 5).

This theorem generalizes the corresponding elementary theorem for the finite-dimensional case.

PROBLEMS

1. If $\mathscr{A}$ is abelian and $M = \overline{\{\mathscr{A}'g\}}$, then the projection P with range M is contained in $\mathscr{A}$.
2. If $M \equiv \overline{\{\mathscr{A}'g\}} \subset \mathscr{H}$, then there exists a vector g_1, such that
$$M \subset \overline{\{\mathscr{A}'g_1\}}.$$
*3. There exists a cyclic vector g for $\mathscr{A}'$, such that
$$\overline{\{\mathscr{A}'g\}} = \mathscr{H}.$$
(Use Zorn's lemma.)
4. If g and g' are two cyclic vectors for $\mathscr{A}'$, then the associated measures ρ and ρ' are equivalent ($\rho \sim \rho'$).
5. $\mathscr{A} \equiv \{A\}'' = \mathscr{A}'$ if and only if there exists a vector g such that $\overline{\{\mathscr{A}g\}} = \mathscr{H}$. In that case the spectrum of A is simple.

4-6. THE SPECTRAL REPRESENTATION

This chapter started out with a discussion of the spectral representation in the finite-dimensional case. We have now all the tools on hand to demonstrate the existence of a spectral representation in the infinite-dimensional case. Let us recall the finite situation.

We have seen in Section 4-1 that any self-adjoint operator in an abstract space $\mathscr{H}$ defines an ℓ_n^2-space consisting of finite sequences $\{x_\nu\}$ ($\nu = 1, 2, \ldots, n$) together with an isometric mapping Ω of $\mathscr{H}$ onto ℓ_n^2 such that the transformed operator $\tilde{A} = \Omega A \Omega^{-1}$ is a multiplication operator.

When we try to transfer this theorem to the infinite-dimensional case, the first question that comes up is: what is the measure in the continuous part of the spectrum of A? From the remarks in Section 4-1 it seems fairly natural to suspect that only the class of equivalent measures will be uniquely determined, and that the measure which is thus defined is the measure associated with the cyclic vector.

We consider thus an operator A with simple spectrum, and define a measure over the spectrum with the spectral density function $\rho(\lambda) = (g, E_\lambda g)$. The space $L_\rho^2(\Lambda)$ consists of functions $u(\lambda)$ where $\lambda \in \Lambda$, over the spectrum Λ of the operator A. The norm is defined by $\|\{u(\lambda)\}\|^2 = \int |u(\lambda)|^2\, d\rho(\lambda)$, with $\rho(\lambda) \equiv (g, E_\lambda g)$. In this expression E_λ is the uniquely determined spectral family of A, and g is a cyclic vector. To every $f \in \{\mathscr{A}g\}$, that is, to every f of the form $f = Tg$ with $T \in \mathscr{A}$, we can associate a function $u(\lambda)$ by the rule $T = u(A)$. Furthermore, because

$$\|f\|^2 = \|Tg\|^2 = \|u(A)g\|^2 = \int_{-\infty}^{+\infty} |u(\lambda)|^2\, d\rho(\lambda),$$

we see that the correspondence $f \leftrightarrow \{u(\lambda)\} \in L_\rho^2(\Lambda)$ is an isometry from $\{\mathscr{A}g\}$ onto a dense linear subset of $L_\rho^2(\Lambda)$. Since $\{\mathscr{A}g\}$ is dense in $\mathscr{H}$, we can extend this correspondence by continuity to an isometric mapping of $\mathscr{H}$ onto $L_\rho^2(\Lambda)$. We denote this mapping by Ω.

What becomes of the operator A when it is transformed into an operator $\tilde{A}$ in $L_\rho^2(\Lambda)$? Since the functional calculus is multiplicative, the operator $Au(A)$ corresponds to the function $\lambda u(\lambda)$. This is true without qualification if $\lambda u(\lambda)$ is essentially bounded. If it is unbounded, certain precautions are required in order to take account of the restricted domain of definition. Let us therefore concentrate on the bounded case.

It follows then, from the definition of Ω, that

$$\Omega A \Omega^{-1}\{u(\lambda)\} = \Omega A f = \Omega A u(A) g = \{\lambda u(\lambda)\},$$

so that

$$\tilde{A}\{u(\lambda)\} = \{\lambda u(\lambda)\} \qquad \text{and} \qquad \tilde{A} = \Omega A \Omega^{-1}.$$

This is the spectral representation of the operator A.

The spectral representation is unique in the sense of equivalence. If $f \leftrightarrow \{u_1(\lambda)\}$ is another such representation, then there exists an equivalent density function $\rho_1 \sim \rho$, and the two representations are connected by a transformation

$$u_1(\lambda)\sqrt{\frac{d\rho_1}{d\rho}}\, e^{i\alpha(\lambda)} = u(\lambda),$$

where $d\rho_1/d\rho$ is the Radon-Nikodym derivative of the two equivalent measures.

The spectral representation has a generalization to a finite or countably infinite set of commuting self-adjoint operators. Let A_r ($r = 1, 2, \ldots$) be such a set, and let Λ_r be the spectrum of A_r; then there exists a uniquely defined measure class $\{\rho\}$ on the Borel sets of the Cartesian product space $S = \Lambda_1 \times \Lambda_2 \times \cdots$ and an isometric mapping of $\mathscr{H}$ onto $L_\rho^2(S)$ such that if $f \leftrightarrow \{u(\lambda)\}$, where $\lambda = \{\lambda_1, \lambda_2, \ldots\} \in S$, then

$$\|f\|^2 = \int_S |u(\lambda)|^2\, d\rho.$$

If we write as before $\{u(\lambda)\} = \Omega f$, then the transformed operators $\tilde{A}_r$ are defined by

$$\tilde{A}_r = \Omega A_r \Omega^{-1}.$$

One can prove that if $P_r(\Delta_r)$ is a spectral projection of the operator A_r, then $\tilde{P}_r(\Delta_r) \equiv \Omega P_r(\Delta_r)\Omega^{-1}$ is given explicitly by

$$\tilde{P}_r(\Delta_r)\{u(\lambda)\} = \chi_{\Delta_r}(\lambda_r)u(\lambda),$$

where $\chi_{\Delta_r}(\lambda_r)$ is the characteristic function of the set Δ_r. However, this does not mean that the operator $\tilde{A}_r$ is a multiplication operator in L^2. In order to prove this property, a further assumption is needed which expresses something which we might describe as independence of the operators and which we shall not give in detail [3]. Under this additional assumption, one finds that

$$\tilde{A}_r\{u(\lambda_r)\} = \{\lambda_r u(\lambda)\}, \qquad (r = 1, 2, \ldots). \tag{4–12}$$

PROBLEMS

1. If $f = \{f(\lambda)\} \in L^2(-\infty, +\infty)$ and A is the operator $Af = \{-i(df/d\lambda)\}$ defined on a certain dense linear subset D_A of L^2 such that A is self-adjoint, then the transformation

$$\Omega f = \tilde{f}, \qquad \tilde{f}(\mu) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(\lambda) e^{i\lambda\mu}\, d\lambda$$

is isometric and transforms A into the spectral representation

$$\tilde{A} = \Omega A \Omega^{-1}, \qquad (\tilde{A}\tilde{f})(\mu) = \mu \tilde{f}(\mu).$$

*2. If two self-adjoint operators A and B commute, and if A has simple spectrum, then B is a function of A : $B = u(A)$. B has simple spectrum, too, if and only if the function $u(\lambda)$ has an inverse.

4-7. EIGENFUNCTION EXPANSIONS

Let us consider a self-adjoint operator A with spectrum Λ. From the preceding sections we know that such an operator defines a unique spectral measure $E(\Delta)$, $(\Delta \subseteq \Lambda)$ and that this spectral measure determines the operator. All the properties of the operator A are known if an explicit method is known for calculating the projections $E(\Delta)$ of the spectral measure. One such explicit method, which often works in practice, is obtained by utilizing the *eigenfunction expansion.* This method resembles in some respects the expansion in eigenvectors used for illustrative purposes in Section 4-1. The difference here is that we use solutions of the eigenvalue equation which fall outside the Hilbert space. We illustrate this in a special case.

Let $\mathscr{H} = L^2(-\infty, +\infty)$ be the space of square-integrable functions on the real line and A some self-adjoint operator in $\mathscr{H}$. The solutions $\varphi_n(x)$ of the equation $A\varphi_n = \lambda_n \varphi_n$ which are square-integrable are called eigenvectors of A, and they may be chosen so as to form an orthonormal system in $\mathscr{H}$. If this system is complete, then the spectrum of A is discrete, and we have essentially the case discussed in Section 4-1. If the system is not complete, then there may exist other solutions of the operator equation

$$A\varphi = \lambda\varphi \tag{4–13}$$

for which $\varphi \notin \mathscr{H}$. In order for this equation to make sense, it is evidently necessary to extend the domain of definition of the operator A to such func-

tions; this can often be done. For instance, if A is the differential operator P discussed in Section 3-6, then we may define it on functions $\varphi(x)$ which are not in L^2. The only property of $\varphi(x)$ which we need to define the operator $P = -i(d/dx)$ is that $\varphi(x)$ be differentiable. Such a function is, for instance, the exponential $\varphi(x) = e^{ikx}$ (k real), and one verifies that in this case one has an equation

$$P\varphi = k\varphi \qquad \text{for all } -\infty < k < +\infty.$$

It may be that there exists a complete set of eigenfunctions, that is, solutions of Eq. (4–12) which are not contained in $\mathscr{H}$. By "complete" we mean that the solutions depend on some (or several) parameters $k : \varphi(k, x)$, such that every vector $f(x)$ of $\mathscr{H}$ which is orthogonal to the eigenvectors $\varphi_n(x)$ is a linear superposition of the eigenfunctions $\varphi(k, x)$:

$$f(x) = \int_K \hat{f}(k) \varphi(k, x)\, d\mu(k),$$

where the integral extends to the entire range K of the parameter k. If such a complete set of eigenfunctions exists, then we can also normalize them suitably so that the norm of f satisfies Parseval's equation

$$\int_{-\infty}^{+\infty} |f(x)|^2\, dx = \int_K |\hat{f}(k)|^2\, d\mu(k).$$

For instance, in the above example with $A = P$, the system

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx} \qquad (-\infty < k < +\infty)$$

is such a complete system, and the transformation

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_K \hat{f}(k) e^{ikx}\, dk$$

is simply the Fourier transformation of the function $f(x)$.

If such a complete system exists for all f orthogonal to the eigenvectors φ_n, then we say the operator A admits an *eigenfunction expansion*. It is then possible to prove that

$$(Af)(x) = \int_K \hat{f}(k)\lambda(k)\varphi(k, x)\, d\mu(k),$$

where $\lambda(k)$ is the eigenvalue belonging to $\varphi(k, x)$. When A is considered as an operator in the system of functions $\hat{f}(k)$, it is a multiplication operator. The eigenfunction expansion, if it exists, can thus serve the same purpose as the spectral representation.

Just as in the case of the Fourier transforms, there exists an inversion of the transformation (4–13) given by an equation such as

$$\hat{f}(k) = \int_{-\infty}^{+\infty} f(x)\varphi^*(k, x)\, dx.$$

The correspondence $f(x) \leftrightarrow \hat{f}(k)$ is thus an isometric mapping of the space $L^2(-\infty, +\infty)$ onto the space $L^2(K, \mu)$ such that A appears in the latter space as a multiplication operator.

The usefulness of this method of obtaining a spectral representation for self-adjoint operators is evident if the operator A is a differential operator. The solution of Eq. (4–13) is then obtained as the solution of an ordinary partial differential equation.

However, the expansion theorem is not generally true; and even if it is true, as, for instance, for certain partial differential operators, Eq. (4–13) does not suffice to determine the eigenfunctions uniquely. It is then necessary to add further conditions, which determine the eigenfunctions. For further detail on these questions the reader should refer to references 4 and 5.

The mathematical theory of eigenfunction expansions is not yet sufficiently developed to guarantee its availability in every case of practical interest. In general situations we must fall back on the spectral representation, which always exists. For certain special cases, however, especially for some elementary problems in one-particle quantum mechanics, the expansion theorem is available; and then it is a most convenient tool to calculate the spectrum and the spectral representation.

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PART 2

Physical Foundations