

Self-adjoint operator

In mathematics, a **self-adjoint operator** on a finite-dimensional complex vector space V with inner product $\langle \cdot, \cdot \rangle$ is a linear map A (from V to itself) that is its own adjoint: $\langle Av, w \rangle = \langle v, Aw \rangle$. If V is finite-dimensional with a given orthonormal basis, this is equivalent to the condition that the matrix of A is Hermitian, i.e., equal to its conjugate transpose A^* . By the finite-dimensional spectral theorem, V has an orthonormal basis such that the matrix of A relative to this basis is a diagonal matrix with entries in the real numbers. In this article, we consider generalizations of this concept to operators on Hilbert spaces of arbitrary dimension.

Self-adjoint operators are used in functional analysis and quantum mechanics. In quantum mechanics their importance lies in the Dirac–von Neumann formulation of quantum mechanics, in which physical observables such as position, momentum, angular momentum and spin are represented by self-adjoint operators on a Hilbert space. Of particular significance is the Hamiltonian operator \hat{H} defined by

$$\hat{H}\psi = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi,$$

which as an observable corresponds to the total energy of a particle of mass m in a real potential field V . Differential operators are an important class of unbounded operators.

The structure of self-adjoint operators on infinite-dimensional Hilbert spaces essentially resembles the finite-dimensional case. That is to say, operators are self-adjoint if and only if they are unitarily equivalent to real-valued multiplication operators. With suitable modifications, this result can be extended to possibly unbounded operators on infinite-dimensional spaces. Since an everywhere-defined self-adjoint operator is necessarily bounded, one needs be more attentive to the domain issue in the unbounded case. This is explained below in more detail.

Contents

Bounded self-adjoint operators

Symmetric operators

- Subtleties of the unbounded case
- Definition of a symmetric operator
- A simple example

Self-adjoint operators

- Definition of a self-adjoint operator
- Essential self-adjointness
- Geometric interpretation
- An example

The distinction between symmetric and self-adjoint operators

- Boundary conditions
- Schrödinger operators with singular potentials

Spectral theorem

- Statement of the spectral theorem
- Functional calculus
- Resolution of the identity
- Formulation in the physics literature

Extensions of symmetric operators

- Self-adjoint extensions in quantum mechanics

Von Neumann's formulas

Examples

- A symmetric operator that is not essentially self-adjoint
- Constant-coefficient operators

Spectral multiplicity theory

- Uniform multiplicity
- Direct integrals

Example: structure of the Laplacian

Pure point spectrum

See also

Citations

References

Bounded self-adjoint operators

Suppose A is a bounded linear operator from a Hilbert space H to itself. Then there is a unique bounded operator A^* , called the **adjoint** of A such that (in bracket notation)

$$\langle Ax|y\rangle = \langle x|A^*y\rangle$$

for all x, y in H .^[1] We say that A is **self-adjoint** (physicists use the term "Hermitian") if $A^* = A$. Equivalently, a bounded operator A is self-adjoint if

$$\langle Ax|y\rangle = \langle x|Ay\rangle$$

for all x and y in H .

Symmetric operators

Subtleties of the unbounded case

In many applications, we are led to consider operators that are unbounded; examples include the position, momentum, and Hamiltonian operators in quantum mechanics, as well as many differential operators. In the unbounded case, there are a number of subtle technical issues that have to be dealt with. In particular, there is a crucial distinction between operators that are merely "symmetric" (defined in this section) and those that are "self-adjoint" (defined in the next section). In the case of differential operators defined on bounded domains, these technical issues have to do with making an appropriate choice of boundary conditions.

Definition of a symmetric operator

We now consider an unbounded operator A on a Hilbert space H . This means A is a linear map from a subspace of H —the "domain" of A , denoted **Dom**(A)—to H itself. We typically assume that **Dom**(A) is a dense subspace of H . Such an operator is called **symmetric** if, in bracket notation,

$$\langle Ax|y\rangle = \langle x|Ay\rangle$$

for all elements x and y in the domain of A .

If A is symmetric and **Dom**(A) = H , then A is necessarily bounded.^[2] That is to say, an unbounded symmetric operator cannot be defined on the whole Hilbert space. Since the operators considered in quantum mechanics are unbounded, it is impossible to define them as symmetric operators on the whole Hilbert space.

In the physics literature, the term **Hermitian** is used in place of the term symmetric. It should be noted, however, that the physics literature generally glosses over the distinction between operators that are merely symmetric and operators that are actually self-adjoint (as defined in the next section).

Although the notion of a symmetric operator is easy to understand, it is not the "right" notion in the unbounded case. Specifically, the spectral theorem applies only to operators that are self-adjoint (defined in the next section) and not to operators that are merely symmetric. In particular, although the eigenvalues of a symmetric operator are necessarily real, a symmetric operator need not have any eigenvectors, let alone an orthonormal basis of them.

More generally, a partially defined linear operator A from a topological vector space E into its continuous dual space E^* is said to be **symmetric** if

$$\langle Ax|y\rangle = \langle x|Ay\rangle$$

for all elements x and y in the domain of A . This usage is fairly standard in the functional analysis literature.

A simple example

As noted above, the [spectral theorem](#) applies only to self-adjoint operators, and not in general to symmetric operators. Nevertheless, we can at this point give a simple example of a symmetric operator that has an orthonormal basis of eigenvectors. (This operator is actually "essentially self-adjoint.") The operator A below can be seen to have a [compact](#) inverse, meaning that the corresponding differential equation $Af = g$ is solved by some integral, therefore compact, operator G . The compact symmetric operator G then has a countable family of eigenvectors which are complete in L^2 . The same can then be said for A .

Consider the complex Hilbert space $L^2[0,1]$ and the [differential operator](#)

$$A = -\frac{d^2}{dx^2}$$

with $\text{Dom}(A)$ consisting of all complex-valued infinitely [differentiable](#) functions f on $[0, 1]$ satisfying the boundary conditions

$$f(0) = f(1) = 0.$$

Then [integration by parts](#) of the inner product shows that A is symmetric. The reader is invited to perform integration by parts twice and verify that the given boundary conditions for $\text{Dom}(A)$ ensure that the boundary terms in the integration by parts vanish.

The eigenfunctions of A are the sinusoids

$$f_n(x) = \sin(n\pi x) \quad n = 1, 2, \dots$$

with the real eigenvalues $n^2\pi^2$; the well-known orthogonality of the sine functions follows as a consequence of the property of being symmetric.

We consider generalizations of this operator below.

Self-adjoint operators

Definition of a self-adjoint operator

Briefly, a densely defined linear operator A on a Hilbert space is **self-adjoint** if it equals its adjoint. That is to say, A is self-adjoint if (1) the domain of A coincides with the domain of the adjoint, and (2) the operator A agrees with its adjoint on this common domain.

We now elaborate on the above definition. Given a densely defined linear operator A on H , its adjoint A^* is defined as follows:

- The domain of A^* consists of vectors x in H such that

$$y \mapsto \langle x | Ay \rangle$$

(which is a densely defined [linear map](#)) is a continuous linear functional. By continuity and density of the domain of A , it extends to a unique continuous linear functional on all of H .

- By the [Riesz representation theorem](#) for linear functionals, if x is in the domain of A^* , there is a unique vector z in H such that

$$\langle x | Ay \rangle = \langle z | y \rangle \quad \forall y \in \text{dom } A$$

This vector z is defined to be $A^* x$. It can be shown that the dependence of z on x is linear.

Notice that it is the denseness of the domain of the operator, along with the uniqueness part of Riesz representation, that ensures the adjoint operator is well defined.

A result of Hellinger-Toeplitz type says that an operator having an everywhere-defined bounded adjoint is bounded.

The condition for a linear operator on a Hilbert space to be *self-adjoint* is stronger than to be *symmetric*. Although this distinction is technical, it is very important; the spectral theorem applies only to operators that are self-adjoint and not to operators that are merely symmetric. For an extensive discussion of the distinction, see Chapter 9 of Hall (2013).

For any densely defined operator A on Hilbert space one can define its adjoint operator A^* . For a symmetric operator A , the domain of the operator A^* contains the domain of the operator A , and the restriction of the operator A^* on the domain of A coincides with the operator A , i.e. $A \subseteq A^*$, in other words A^* is extension of A . For a self-adjoint operator A the domain of A^* is the same as the domain of A , and $A = A^*$. See also [Extensions of symmetric operators](#) and [unbounded operator](#).

Essential self-adjointness

A symmetric operator A is always closable; that is, the closure of the graph of A is the graph of an operator. A symmetric operator is said to be **essentially self-adjoint** if the closure of A is self-adjoint. Equivalently, A is essentially self-adjoint if it has a *unique* self-adjoint extension. In practical terms, having an essentially self-adjoint operator is almost as good as having a self-adjoint operator, since we merely need to take the closure to obtain self-adjoint operator.

Geometric interpretation

There is a useful [geometric](#) way of looking at the adjoint of an operator A on H as follows: we consider the graph $G(A)$ of A defined by

$$G(A) = \{(\xi, A\xi) : \xi \in \text{dom}(A)\} \subseteq H \oplus H.$$

Theorem. Let J be the [symplectic mapping](#)

$$\begin{cases} H \oplus H \rightarrow H \oplus H \\ J : (\xi, \eta) \mapsto (-\eta, \xi) \end{cases}$$

Then the graph of A^* is the [orthogonal complement](#) of $JG(A)$:

$$G(A^*) = (JG(A))^\perp = \{(x, y) \in H \oplus H : \langle (x, y) | (-A\xi, \xi) \rangle = 0 \quad \forall \xi \in \text{dom}(A)\}$$

A densely defined operator A is symmetric [if and only if](#) $A \subseteq A^*$, where the subset notation $A \subseteq A^*$ is understood to mean $G(A) \subseteq G(A^*)$. An operator A is **self-adjoint** if and only if $A = A^*$; that is, if and only if $JG(A) = G(A^*)$.

An example

Consider the complex Hilbert space $L^2(\mathbf{R})$, and the operator which multiplies a given function by x :

$$Af(x) = xf(x)$$

The domain of A is the space of all L^2 functions $f(x)$ for which $xf(x)$ is also square-integrable. Then A is self-adjoint.^[3] On the other hand, A does not have any eigenfunctions. (More precisely, A does not have any *normalizable* eigenvectors, that is, eigenvectors that are actually in the Hilbert space on which A is defined.)

As we will see later, self-adjoint operators have very important spectral properties; they are in fact multiplication operators on general measure spaces.

The distinction between symmetric and self-adjoint operators

As has been discussed above, although the distinction between a symmetric operator and a self-adjoint (or essentially self-adjoint) operator is a subtle one, it is important since self-adjointness is the hypothesis in the spectral theorem. Here we discuss some concrete examples of the distinction; see the section below on extensions of symmetric operators for the general theory.

Boundary conditions

In the case where the Hilbert space is a space of functions on a bounded domain, these distinctions have to do with a familiar issue in quantum physics: One cannot define an operator—such as the momentum or Hamiltonian operator—on a bounded domain without specifying *boundary conditions*. In mathematical terms, choosing the boundary conditions amounts to choosing an appropriate domain for the operator. Consider, for example, the Hilbert space $L^2([0, 1])$ (the space of square-integrable functions on the interval $[0, 1]$). Let us define a "momentum" operator A on this space by the usual formula, setting Planck's constant equal to 1:

$$Af = -i \frac{df}{dx}.$$

We must now specify a domain for A , which amounts to choosing boundary conditions. If we choose

$$\mathbf{Dom}(A) = \{\text{smooth functions } f | f(0) = f(1) = 0\},$$

then using integration by parts, one can easily verify that A is symmetric. This operator is not essentially self-adjoint,^[4] however, basically because we have specified too many boundary conditions on the domain of A , which makes the domain of the adjoint too big. (This example is discussed also in the "Examples" section below.)

Specifically, with the above choice of domain for A , the domain of the closure \mathbf{A}^{cl} of A is

$$\mathbf{Dom}(A^{\text{cl}}) = \{\text{functions } f \text{ with two derivatives in } L^2 | f(0) = f(1) = 0\},$$

whereas the domain of the adjoint \mathbf{A}^* of A is

$$\mathbf{Dom}(A^*) = \{\text{functions } f \text{ with two derivatives in } L^2\}.$$

That is to say, the domain of the closure has the same boundary conditions as the domain of A itself, just a less stringent smoothness assumption. Meanwhile, since there are "too many" boundary conditions on A , there are "too few" (actually, none at all in this case) for \mathbf{A}^* . If we compute $\langle g, Af \rangle$ for $f \in \mathbf{Dom}(A)$ using integration by parts, then since f vanishes at both ends of the interval, no boundary conditions on g are needed to cancel out the boundary terms in the integration by parts. Thus, any sufficiently smooth function g is in the domain of \mathbf{A}^* , with $\mathbf{A}^* g = -i dg/dx$.^[5]

Since the domain of the closure and the domain of the adjoint do not agree, A is not essentially self-adjoint. After all, a general result says that the domain of the adjoint of \mathbf{A}^{cl} is the same as the domain of the adjoint of A . Thus, in this case, the domain of the adjoint of \mathbf{A}^{cl} is bigger than the domain of \mathbf{A}^{cl} itself, showing that \mathbf{A}^{cl} is not self-adjoint, which by definition means that A is not essentially self-adjoint.

The problem with the preceding example is that we imposed too many boundary conditions on the domain of A . A better choice of domain would be to use periodic boundary conditions:

$$\mathbf{Dom}(A) = \{\text{smooth functions } f | f(0) = f(1)\}.$$

With this domain, A is essentially self-adjoint.^[6]

In this case, we can understand the implications of the domain issues for the spectral theorem. If we use the second choice of domain (with periodic boundary conditions), we can find an orthonormal basis of eigenvectors for A , the functions $f_n(x) := e^{2\pi i n x}$. If we used the first domain, with "too many" boundary conditions, A would not have any eigenvectors at all.

Schrödinger operators with singular potentials

A more subtle example of the distinction between symmetric and (essentially) self-adjoint operators comes from Schrödinger operators in quantum mechanics. If the potential energy is singular—particularly if the potential is unbounded below—the associated Schrödinger operator may fail to be essentially self-adjoint. In one dimension, for example, the operator

$$\hat{H} := \frac{P^2}{2m} - X^4$$

is not essentially self-adjoint on the space of smooth, rapidly decaying functions.^[7] In this case, the failure of essential self-adjointness reflects a pathology in the underlying classical system: A classical particle with a $-x^4$ potential escapes to infinity in finite time. This operator does not have a *unique* self-adjoint, but it does admit self-adjoint extensions obtained by specifying "boundary conditions at infinity". (Since \hat{H} is a real operator, it commutes with complex conjugation. Thus, the deficiency indices are automatically equal, which is the condition for having a self-adjoint extension. See the discussion of extensions of symmetric operators below.)

In this case, if we initially define \hat{H} on the space of smooth, rapidly decaying functions, the adjoint will be "the same" operator (i.e., given by the same formula) but on the largest possible domain, namely

$$\mathbf{Dom}(\hat{H}^*) = \left\{ \text{twice differentiable functions } f \in L^2(\mathbb{R}) \mid \left(-\frac{\hbar^2}{2m} \frac{d^2 f}{dx^2} - x^4 f(x) \right) \in L^2(\mathbb{R}) \right\}.$$

It is then possible to show that \hat{H}^* is not a symmetric operator, which certainly implies that \hat{H} is not essentially self adjoint. Indeed, \hat{H}^* has eigenvectors with pure imaginary eigenvalues,^{[8][9]} which is impossible for a symmetric operator. This strange occurrence is possible because of a cancellation between the two terms in \hat{H}^* : There are functions f in the domain of \hat{H}^* for which neither d^2f/dx^2 nor $x^4f(x)$ is separately in $L^2(\mathbb{R})$, but the combination of them occurring in \hat{H}^* is in $L^2(\mathbb{R})$. This allows for \hat{H}^* to be nonsymmetric, even though both d^2/dx^2 and x^4 are symmetric operators. This sort of cancellation does not occur if we replace the repelling potential $-x^4$ with the confining potential x^4 .

Conditions for Schrödinger operators to be self-adjoint or essentially self-adjoint can be found in various textbooks, such as those by Berezin and Schubin, Hall, and Reed and Simon listed in the references.

Spectral theorem

In the physics literature, the spectral theorem is often stated by saying that a self-adjoint operator has an orthonormal basis of eigenvectors. Physicists are well aware, however, of the phenomenon of "continuous spectrum"; thus, when they speak of an "orthonormal basis" they mean either an orthonormal basis in the classic sense *or* some continuous analog thereof. In the case of the momentum operator $P = -i d/dx$, for example, physicists would say that the eigenvectors are the functions $f_p(x) := e^{ipx}$, which are clearly not in the Hilbert space $L^2(\mathbb{R})$. (Physicists would say that the eigenvectors are "non-normalizable.") Physicists would then go on to say that these "eigenvectors" are orthonormal in a continuous sense, where the usual Kronecker delta δ_{ij} is replaced by a Dirac delta function $\delta(p - p')$.

Although these statements may seem disconcerting to mathematicians, they can be made rigorous by use of the Fourier transform, which allows a general L^2 function to be expressed as a "superposition" (i.e., integral) of the functions e^{ipx} , even though these functions are not in L^2 . The Fourier transform "diagonalizes" the momentum operator; that is, it converts it into the operator of multiplication by p , where p is the variable of the Fourier transform.

The spectral theorem in general can be expressed similarly as the possibility of "diagonalizing" an operator by showing it is unitarily equivalent to a multiplication operator. Other versions of the spectral theorem are similarly intended to capture the idea that a self-adjoint operator can have "eigenvectors" that are not actually in the Hilbert space in question.

Statement of the spectral theorem

Partially defined operators A, B on Hilbert spaces H, K are **unitarily equivalent** if and only if there is a unitary transformation $U : H \rightarrow K$ such that

- U maps $\text{dom } A$ bijectively onto $\text{dom } B$,
- $BU\xi = UA\xi, \quad \forall \xi \in \text{dom } A.$

A multiplication operator is defined as follows: Let (X, Σ, μ) be a countably additive measure space and f a real-valued measurable function on X . An operator T of the form

$$[T\psi](x) = f(x)\psi(x)$$

whose domain is the space of ψ for which the right-hand side above is in L^2 is called a multiplication operator.

One version of the spectral theorem can be stated as follows.

Theorem. Any multiplication operator is a (densely defined) self-adjoint operator. Any self-adjoint operator is unitarily equivalent to a multiplication operator.^[10]

Other version of the spectral theorem can be found in the spectral theorem article linked to above.

The spectral theorem for unbounded self-adjoint operators can be proved by reduction to the spectral theorem for unitary (hence bounded) operators.^[11] This reduction uses the Cayley transform for self-adjoint operators which is defined in the next section. We might note that if T is multiplication by f , then the spectrum of T is just the essential range of f .

Functional calculus

One important application of the spectral theorem is to define a "functional calculus." That is to say, if h is a function on the real line and T is a self-adjoint operator, we wish to define the operator $h(T)$. If T has a true orthonormal basis of eigenvectors e_j with eigenvalues λ_j , then $h(T)$ is the operator with eigenvectors e_j and eigenvalues $h(\lambda_j)$. The goal of functional calculus is to extend this idea to the case where T has continuous spectrum.

Of particular importance in quantum physics is the case in which T is the Hamiltonian operator \hat{H} and $h(x) := e^{-itx/\hbar}$ is an exponential. In this case, the functional calculus should allow us to define the operator

$$U(t) := h(\hat{H}) = e^{-it\hat{H}/\hbar},$$

which is the operator defining the time-evolution in quantum mechanics.

Given the representation of T as the operator of multiplication by f —as guaranteed by the spectral theorem—it is easy to characterize the functional calculus: If h is a bounded real-valued Borel function on \mathbf{R} , then $h(T)$ is the operator of multiplication by the composition $h \circ f$.

Resolution of the identity

It has been customary to introduce the following notation

$$E_T(\lambda) = \mathbf{1}_{(-\infty, \lambda]}(T)$$

where $\mathbf{1}_{(-\infty, \lambda]}$ is the characteristic function of the interval $(-\infty, \lambda]$. The family of projection operators $E_T(\lambda)$ is called **resolution of the identity** for T . Moreover, the following Stieltjes integral representation for T can be proved:

$$T = \int_{-\infty}^{+\infty} \lambda dE_T(\lambda).$$

The definition of the operator integral above can be reduced to that of a scalar valued Stieltjes integral using the weak operator topology. In more modern treatments however, this representation is usually avoided, since most technical problems can be dealt with by the functional calculus.

Formulation in the physics literature

In physics, particularly in quantum mechanics, the spectral theorem is expressed in a way which combines the spectral theorem as stated above and the Borel functional calculus using Dirac notation as follows:

If H is self-adjoint and f is a Borel function,

$$f(H) = \int dE |\Psi_E\rangle f(E) \langle \Psi_E|$$

with

$$H|\Psi_E\rangle = E|\Psi_E\rangle$$

where the integral runs over the whole spectrum of H . The notation suggests that H is diagonalized by the eigenvectors Ψ_E . Such a notation is purely formal. One can see the similarity between Dirac's notation and the previous section. The resolution of the identity (sometimes called projection valued measures) formally resembles the rank-1 projections $|\Psi_E\rangle\langle \Psi_E|$. In the Dirac notation, (projective) measurements are described via eigenvalues and eigenstates, both purely formal objects. As one would expect, this does not survive passage to the resolution of the identity. In the latter formulation, measurements are described using the spectral measure of $|\Psi\rangle$, if the system is prepared in $|\Psi\rangle$ prior to the measurement. Alternatively, if one would like to preserve the notion of eigenstates and make it rigorous, rather than merely formal, one can replace the state space by a suitable rigged Hilbert space.

If $f = 1$, the theorem is referred to as resolution of unity:

$$I = \int dE |\Psi_E\rangle\langle \Psi_E|$$

In the case $H_{\text{eff}} = H - i\Gamma$ is the sum of an Hermitian H and a skew-Hermitian (see skew-Hermitian matrix) operator $-i\Gamma$, one defines the biorthogonal basis set

$$H_{\text{eff}}^* |\Psi_E^*\rangle = E^* |\Psi_E^*\rangle$$

and write the spectral theorem as:

$$f(H_{\text{eff}}) = \int dE |\Psi_E\rangle f(E) \langle \Psi_E^*|$$

(See Feshbach–Fano partitioning method for the context where such operators appear in scattering theory).

Extensions of symmetric operators

The following question arises in several contexts: if an operator A on the Hilbert space H is symmetric, when does it have self-adjoint extensions? An operator that has a unique self-adjoint extension is said to be **essentially self-adjoint**; equivalently, an operator is essentially self-adjoint if its closure (the operator whose graph is the closure of the graph of A) is self-adjoint. In general, a symmetric operator could have many self-adjoint extensions or none at all. Thus, we would like a classification of its self-adjoint extensions.

The first basic criterion for essential self-adjointness is the following:^[12]

Theorem: If A is a symmetric operator on H , then A is essentially self-adjoint if and only if the range of the operators $A - i$ and $A + i$ are dense in H .

Equivalently, A is essentially self-adjoint if and only if the operators $A^* - i$ and $A^* + i$ have trivial kernels.^[13] That is to say, A fails to be self-adjoint if and only if A^* has an eigenvector with eigenvalue i or $-i$.

Another way of looking at the issue is provided by the Cayley transform of a self-adjoint operator and the deficiency indices. (We should note here that it is often of technical convenience to deal with closed operators. In the symmetric case, the closedness requirement poses no obstacles, since it is known that all symmetric operators are closable.)

Theorem. Suppose A is a symmetric operator. Then there is a unique partially defined linear operator

$$W(A) : \text{ran}(A + i) \rightarrow \text{ran}(A - i)$$

such that

$$W(A)(Ax + ix) = Ax - ix, \quad x \in \text{dom}(A).$$

Here, ran and dom denote the image (in other words, range) and the domain, respectively. $W(A)$ is isometric on its domain. Moreover, the range of $1 - W(A)$ is dense in H .

Conversely, given any partially defined operator U which is isometric on its domain (which is not necessarily closed) and such that $1 - U$ is dense, there is a (unique) operator $S(U)$

$$S(U) : \text{ran}(1 - U) \rightarrow \text{ran}(1 + U)$$

such that

$$S(U)(x - Ux) = i(x + Ux) \quad x \in \text{dom}(U).$$

The operator $S(U)$ is densely defined and symmetric.

The mappings W and S are inverses of each other.

The mapping W is called the **Cayley transform**. It associates a partially defined isometry to any symmetric densely defined operator. Note that the mappings W and S are monotone: This means that if B is a symmetric operator that extends the densely defined symmetric operator A , then $W(B)$ extends $W(A)$, and similarly for S .

Theorem. A necessary and sufficient condition for A to be self-adjoint is that its Cayley transform $W(A)$ be unitary.

This immediately gives us a necessary and sufficient condition for A to have a self-adjoint extension, as follows:

Theorem. A necessary and sufficient condition for A to have a self-adjoint extension is that $W(A)$ have a unitary extension.

A partially defined isometric operator V on a Hilbert space H has a unique isometric extension to the norm closure of $\text{dom}(V)$. A partially defined isometric operator with closed domain is called a partial isometry.

Given a partial isometry V , the **deficiency indices** of V are defined as the dimension of the orthogonal complements of the domain and range:

$$\begin{aligned} n_+(V) &= \dim \text{dom}(V)^\perp \\ n_-(V) &= \dim \text{ran}(V)^\perp \end{aligned}$$

Theorem. A partial isometry V has a unitary extension if and only if the deficiency indices are identical. Moreover, V has a *unique* unitary extension if and only if the deficiency indices are both zero.

We see that there is a bijection between symmetric extensions of an operator and isometric extensions of its Cayley transform. The symmetric extension is self-adjoint if and only if the corresponding isometric extension is unitary.

A symmetric operator has a unique self-adjoint extension if and only if both its deficiency indices are zero. Such an operator is said to be **essentially self-adjoint**. Symmetric operators which are not essentially self-adjoint may still have a canonical self-adjoint extension. Such is the case for *non-negative* symmetric operators (or more generally, operators which are bounded below). These operators always have a canonically defined Friedrichs extension and for these operators we can define a canonical functional calculus. Many operators that occur in analysis are bounded below (such as the negative of the Laplacian operator), so the issue of essential adjointness for these operators is less critical.

Self-adjoint extensions in quantum mechanics

In quantum mechanics, observables correspond to self-adjoint operators. By Stone's theorem on one-parameter unitary groups, self-adjoint operators are precisely the infinitesimal generators of unitary groups of time evolution operators. However, many physical problems are formulated as a time-evolution equation involving differential operators for which the Hamiltonian is only symmetric. In such cases, either the Hamiltonian is essentially self-adjoint, in which case the physical problem has unique solutions or one attempts to find self-adjoint extensions of the Hamiltonian corresponding to different types of boundary conditions or conditions at infinity.

Example. The one-dimensional Schrödinger operator with the potential $V(x) = -(1 + |x|)^\alpha$, defined initially on smooth compactly supported functions, is essentially self-adjoint (that is, has a self-adjoint closure) for $0 < \alpha \leq 2$ but not for $\alpha > 2$. See Berezin and Schubin, pages 55 and 86, or Section 9.10 in Hall.

The failure of essential self-adjointness for $\alpha > 2$ has a counterpart in the classical dynamics of a particle with potential $V(x)$: The classical particle escapes to infinity in finite time.^[14]

Example. There is no self-adjoint momentum operator p for a particle moving on a half-line. Nevertheless, the Hamiltonian p^2 of a "free" particle on a half-line has several self-adjoint extensions corresponding to different types of boundary conditions. Physically, these boundary conditions are related to reflections of the particle at the origin (see Reed and Simon, vol.2).

Von Neumann's formulas

Suppose A is symmetric densely defined. Then any symmetric extension of A is a restriction of A^* . Indeed, $A \subseteq B$ and B symmetric yields $B \subseteq A^*$ by applying the definition of $\text{dom}(A^*)$.

Theorem. Suppose A is a densely defined symmetric operator. Let

$$N_\pm = \text{ran}(A \pm i)^\perp,$$

Then

$$N_\pm = \ker(A^* \mp i),$$

and

$$\text{dom}(A^*) = \text{dom}(\bar{A}) \oplus N_+ \oplus N_-,$$

where the decomposition is orthogonal relative to the graph inner product of $\text{dom}(A^*)$:

$$\langle \xi | \eta \rangle_{\text{graph}} = \langle \xi | \eta \rangle + \langle A^* \xi | A^* \eta \rangle.$$

These are referred to as von Neumann's formulas in the Akhiezer and Glazman reference.

Examples

A symmetric operator that is not essentially self-adjoint

We first consider the Hilbert space $L^2[0, 1]$ and the differential operator

$$D : \phi \mapsto \frac{1}{i}\phi'$$

defined on the space of continuously differentiable complex-valued functions on $[0, 1]$, satisfying the boundary conditions

$$\phi(0) = \phi(1) = 0.$$

Then D is a symmetric operator as can be shown by integration by parts. The spaces N_+ , N_- are given respectively by the distributional solutions to the equation

$$\begin{aligned} -iu' &= iu \\ -iu' &= -iu \end{aligned}$$

which are in $L^2[0, 1]$. One can show that each one of these solution spaces is 1-dimensional, generated by the functions $x \rightarrow e^{-x}$ and $x \rightarrow e^x$ respectively. This shows that D is not essentially self-adjoint,^[15] but does have self-adjoint extensions. These self-adjoint extensions are parametrized by the space of unitary mappings $N_+ \rightarrow N_-$, which in this case happens to be the unit circle \mathbf{T} .

In this case, the failure of essential self-adjointness is due to an "incorrect" choice of boundary conditions in the definition of the domain of D . Since D is a first-order operator, only one boundary condition is needed to ensure that D is symmetric. If we replaced the boundary conditions given above by the single boundary condition

$$\phi(0) = \phi(1),$$

then D would still be symmetric and would now, in fact, be essentially self-adjoint. This change of boundary conditions gives one particular essentially self-adjoint extension of D . Other essentially self-adjoint extensions come from imposing boundary conditions of the form $\phi(1) = e^{i\theta}\phi(0)$.

This simple example illustrates a general fact about self-adjoint extensions of symmetric differential operators P on an open set M . They are determined by the unitary maps between the eigenvalue spaces

$$N_{\pm} = \{u \in L^2(M) : P_{\text{dist}} u = \pm iu\}$$

where P_{dist} is the distributional extension of P .

Constant-coefficient operators

We next give the example of differential operators with constant coefficients. Let

$$P(\vec{x}) = \sum_{\alpha} c_{\alpha} x^{\alpha}$$

be a polynomial on \mathbf{R}^n with *real* coefficients, where α ranges over a (finite) set of multi-indices. Thus

$$\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$$

and

$$x^{\alpha} = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}.$$

We also use the notation

$$D^{\alpha} = \frac{1}{i^{|\alpha|}} \partial_{x_1}^{\alpha_1} \partial_{x_2}^{\alpha_2} \cdots \partial_{x_n}^{\alpha_n}.$$

Then the operator $P(D)$ defined on the space of infinitely differentiable functions of compact support on \mathbf{R}^n by

$$P(D)\phi = \sum_{\alpha} c_{\alpha} D^{\alpha} \phi$$

is essentially self-adjoint on $L^2(\mathbf{R}^n)$.

Theorem. Let P a polynomial function on \mathbf{R}^n with real coefficients, \mathbf{F} the Fourier transform considered as a unitary map $L^2(\mathbf{R}^n) \rightarrow L^2(\mathbf{R}^n)$. Then $\mathbf{F}^* P(D) \mathbf{F}$ is essentially self-adjoint and its unique self-adjoint extension is the operator of multiplication by the function P .

More generally, consider linear differential operators acting on infinitely differentiable complex-valued functions of compact support. If M is an open subset of \mathbf{R}^n

$$P\phi(x) = \sum_{\alpha} a_{\alpha}(x) [D^{\alpha} \phi](x)$$

where a_{α} are (not necessarily constant) infinitely differentiable functions. P is a linear operator

$$C_0^\infty(M) \rightarrow C_0^\infty(M).$$

Corresponding to P there is another differential operator, the formal adjoint of P

$$P^{*\text{form}}\phi = \sum_{\alpha} D^{\alpha} (\overline{a_{\alpha}} \phi)$$

Theorem. The adjoint P^* of P is a restriction of the distributional extension of the formal adjoint to an appropriate subspace of L^2 . Specifically:

$$\text{dom } P^* = \{u \in L^2(M) : P^{*\text{form}} u \in L^2(M)\}.$$

Spectral multiplicity theory

The multiplication representation of a self-adjoint operator, though extremely useful, is not a canonical representation. This suggests that it is not easy to extract from this representation a criterion to determine when self-adjoint operators A and B are unitarily equivalent. The finest grained representation which we now discuss involves spectral multiplicity. This circle of results is called the Hahn-Hellinger theory of spectral multiplicity.

Uniform multiplicity

We first define *uniform multiplicity*:

Definition. A self-adjoint operator A has uniform multiplicity n where n is such that $1 \leq n \leq \omega$ if and only if A is unitarily equivalent to the operator M_f of multiplication by the function $f(\lambda) = \lambda$ on

$$L^2_{\mu}(\mathbf{R}, \mathbf{H}_n) = \{\psi : \mathbf{R} \rightarrow \mathbf{H}_n : \psi \text{ measurable and } \int_{\mathbf{R}} \|\psi(t)\|^2 d\mu(t) < \infty\}$$

where \mathbf{H}_n is a Hilbert space of dimension n . The domain of M_f consists of vector-valued functions ψ on \mathbf{R} such that

$$\int_{\mathbf{R}} |\lambda|^2 \|\psi(\lambda)\|^2 d\mu(\lambda) < \infty.$$

Non-negative countably additive measures μ, ν are **mutually singular** if and only if they are supported on disjoint Borel sets.

Theorem. Let A be a self-adjoint operator on a *separable* Hilbert space H . Then there is an ω sequence of countably additive finite measures on \mathbf{R} (some of which may be identically 0)

$$\{\mu_{\ell}\}_{1 \leq \ell \leq \omega}$$

such that the measures are pairwise singular and A is unitarily equivalent to the operator of multiplication by the function $f(\lambda) = \lambda$ on

$$\bigoplus_{1 \leq \ell \leq \omega} L^2_{\mu_\ell}(\mathbf{R}, \mathbf{H}_\ell).$$

This representation is unique in the following sense: For any two such representations of the same A , the corresponding measures are equivalent in the sense that they have the same sets of measure zero.

Direct integrals

The spectral multiplicity theorem can be reformulated using the language of direct integrals of Hilbert spaces:

Theorem.^[16] Any self-adjoint operator on a separable Hilbert space is unitarily equivalent to multiplication by the function $\lambda \mapsto \lambda$ on

$$\int_{\mathbf{R}}^\oplus H_\lambda d\mu(\lambda).$$

Unlike the multiplication-operator version of the spectral theorem, the direct-integral version is unique in the sense that the measure equivalence class of μ (or equivalently its sets of measure zero) is uniquely determined and the measurable function $\lambda \mapsto \dim(H_\lambda)$ is determined almost everywhere with respect to μ .^[17] The function $\lambda \mapsto \dim(H_\lambda)$ is the **spectral multiplicity function** of the operator.

We may now state the classification result for self-adjoint operators: Two self-adjoint operators are unitarily equivalent if and only if (1) their spectra agree as sets, (2) the measures appearing in their direct-integral representations have the same sets of measure zero, and (3) their spectral multiplicity functions agree almost everywhere with respect to the measure in the direct integral.^[18]

Example: structure of the Laplacian

The Laplacian on \mathbf{R}^n is the operator

$$\Delta = \sum_{i=1}^n \partial_{x_i}^2.$$

As remarked above, the Laplacian is diagonalized by the Fourier transform. Actually it is more natural to consider the *negative* of the Laplacian $-\Delta$ since as an operator it is non-negative; (see elliptic operator).

Theorem. If $n=1$, then $-\Delta$ has uniform multiplicity $\text{mult} = 2$, otherwise $-\Delta$ has uniform multiplicity $\text{mult} = \omega$. Moreover, the measure μ_{mult} may be taken to be Lebesgue measure on $[0, \infty)$.

Pure point spectrum

A self-adjoint operator A on H has pure point spectrum if and only if H has an orthonormal basis $\{e_i\}_{i \in I}$ consisting of eigenvectors for A .

Example. The Hamiltonian for the harmonic oscillator has a quadratic potential V , that is

$$-\Delta + |x|^2.$$

This Hamiltonian has pure point spectrum; this is typical for bound state Hamiltonians in quantum mechanics. As was pointed out in a previous example, a sufficient condition that an unbounded symmetric operator has eigenvectors which form a Hilbert space basis is that it has a compact inverse.

See also

- Compact operator on Hilbert space
- Theoretical and experimental justification for the Schrödinger equation
- Unbounded operator

Citations

1. Hall 2013 Proposition A.53
2. Hall 2013 Corollary 9.9
3. Hall 2013 Proposition 9.30
4. Hall 2013 Proposition 9.27
5. Hall 2013 Proposition 9.28
6. Hall 2013 Example 9.25
7. Hall 2013 Theorem 9.41
8. Berezin 1991 p. 85
9. Hall 2013 Section 9.10
10. Hall 2013 Theorems 7.20 and 10.10
11. Hall 2013 Section 10.4
12. Hall 2013 Theorem 9.21
13. Hall 2013 Corollary 9.22
14. Hall 2013 Chapter 2, Exercise 4
15. Hall 2013 Section 9.6
16. Hall 2013 Theorems 7.19 and 10.9
17. Hall 2013 Proposition 7.22
18. Hall 2013 Proposition 7.24

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