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# HILBERT SPACES

Hilbert spaces are an essential tool for formulating and proving theories in many fields of science and engineering. For example, in quantum mechanics corresponding to each observable (a quantity that can be measured, such as position, momentum, or energy) is a self-adjoint operator in an appropriate Hilbert space. In wave scattering theory the convergence of various computational (finite difference or finite element) methods can be validated in suitable Hilbert spaces, which can guide one to choose the most suitable (efficient, accurate, robust) computational methods for a particular simulation.

A Hilbert space is a vector space equipped with an inner product, also called a scalar product, together with the requirement that a sequence  $\{u_n\}$  of vectors has a limit within the space whenever it has the property that the distance between two members of the sequence  $u_n$  and  $u_m$  can be made arbitrarily small when the indices n and m are large. One familiar example is the Euclidean plane, where the vectors can be represented by ordered pairs (x, y) of real numbers. In this case the inner product between  $(x_1, y_1)$  and  $(x_2, y_2)$  is just  $x_1x_2 + y_1y_2$ . The plane is an example of a finite dimensional Hilbert space. In applications of Hilbert space theory to differential equations, one uses infinite dimensional Hilbert spaces in which the "vectors" are functions defined on some fixed set. The inner product in a Hilbert space enables one to define the distance and angle between vectors, which, in turn, leads to the expansion of vectors in terms of special sets of vectors called orthonormal bases. When applied to Hilbert spaces of functions, this includes expansions of functions in terms of Fourier series and other well-known orthogonal sets of functions, such as wavelets.

In a Hilbert space setting an operator is a mapping that takes an input from a Hilbert space and maps it to an output in the same or another Hilbert space. Operators are generalizations of functions that map complex numbers to complex numbers. In finite dimensions each matrix defines an operator by multiplication. In Hilbert spaces of functions one is interested in differential and integral operators, such as the Laplace operator and Fourier transform. Many of the boundary value problems in classical field theory can be formulated as operator equations in a Hilbert space. For example, Poisson's equation [see Eq. (11)] can be considered as an operator equation in a Hilbert space of functions. Similarly, partial differential equations such as the wave equation [Eq. (18)] can be viewed as an ordinary differential equation in which the value of the unknown at each time is an element of a Hilbert space of functions.

An important class of operators are linear operators, which preserve vector addition and multiplication by complex numbers. They can be measured in magnitude via their norms, which are analogous to the absolute value of a complex number. Furthermore, certain problems involving linear operators can be solved via their spectra, which are a generalization of the set of eigenvalues of a matrix. In particular, this enables one to form functions of an operator. When applied to quantum mechanics, this allows one to find the operator corresponding to a function of an observable and to prove that an observable can assume values only in the spectrum of its corresponding operator.

### The Geometry of Hilbert Space

The following is an overview of some important concepts and results in Hilbert space theory; for more details the reader can consult standard references in this area such as Blank, Exner, and Havlicek (1), Dunford and Schwartz (2), Kato (3), Naylor and Sell (4), Riesz and Sz.-Nagy (5), Schechter (6), von Neumann (7), and Yosida (8).

A Hilbert space H is a vector space equipped with an inner product such that H is complete in the sense defined in this section. An *inner product* is a function that assigns a complex number  $(\boldsymbol{u}, \boldsymbol{v})$  to each pair of elements  $\boldsymbol{u}, \boldsymbol{v}$  in H so that the following algebraic laws are satisfied:

 $(\boldsymbol{u}, \boldsymbol{u}) \ge 0$  for all  $\boldsymbol{u}$ , and  $(\boldsymbol{u}, \boldsymbol{u}) = 0$  if and only if  $\boldsymbol{u} = 0$  $(\boldsymbol{u} + \boldsymbol{v}, \boldsymbol{w}) = (\boldsymbol{u}, \boldsymbol{w}) + (\boldsymbol{v}, \boldsymbol{w})$  for all  $\boldsymbol{u}, \boldsymbol{v}$ , and  $\boldsymbol{w}$  $(\alpha \boldsymbol{u}, \boldsymbol{v}) = \alpha (\boldsymbol{u}, \boldsymbol{v})$  for all  $\boldsymbol{u}$  and  $\boldsymbol{v}$  in H and all complex numbers  $\alpha$  $(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{v}, \boldsymbol{u})^*$  for all  $\boldsymbol{u}$  and  $\boldsymbol{v}$  where \* denotes complex conjugate

H is called a *real* Hilbert space if "complex numbers" in the definition is replaced by "real numbers." A well-known example of a Hilbert space is the set of all *n*-tuples  $\mathbf{x} = (x_1, \ldots, x_n)$  of complex numbers  $x_i$  with the inner product  $(x, y) = x_1 y_1^* + \dots + x_n y_n^*$ . This space is often denoted by  $C^n$ , and by  $R^n$  if the  $x_i$  are restricted to be real numbers. An infinite dimensional analog of this is  $l^2$ , which denotes the Hilbert space of all infinite sequences  $\boldsymbol{x} = \{x_n\}$  of complex numbers such that  $\Sigma_n |x_n|^2 < \infty$ . The inner product is given by  $(\boldsymbol{x}, \boldsymbol{y}) = \Sigma_n x_n y^*_n$ . The  $L^2$  spaces are continuous analogs of  $l^2$  and are useful in problems where the independent variable is continuous instead of discrete, such as in differential equations and quantum mechanics. If T is a positive number, then the Hilbert space  $L^2(0, T)$  consists of all square integrable functions f(t) defined on the interval 0 < t < T; that is, the f(t) that satisfy  $\int_{0}^{T} |f(t)|^{2} dt < \infty$ . The inner product, defined by  $(f, g) = \int_{0}^{T} f(t)g(t) dt$ , is often associated with energy in many physical situations. For example, let v(t) be the voltage dropped between the two ports of a circuit element and let i(t) be the current through the element. Then  $\int_0^T v(t)i(t) dt = (v, i)$ is the energy lost in the element during the time interval 0 < t < T. The space  $L^2(a, b)$  is defined in a similar manner for any interval a < t < b in the real line. More generally, if E is a set in  $\mathbb{R}^n$ , then  $L^2(E)$  is the space of all functions  $\boldsymbol{u}(\boldsymbol{x})$  defined for  $\boldsymbol{x} = (x_1, \dots, x_n)$  in E such that  $\int_E |\boldsymbol{u}(\boldsymbol{x})|^2 d\boldsymbol{x} < \infty$ , where  $d\boldsymbol{x} = dx_1, \dots, dx_n$ , and the integral is a multiple integral over E. Throughout the following E will denote an open set in  $\mathbb{R}^n$  and B is the boundary of E. (E being open means that B is not included in E.) We shall just write  $L^2$  for  $L^2(E)$  when the set *E* is clear from the context.

A real Hilbert space H can naturally be extended to a complex Hilbert space consisting of all objects of the form u + iv, where u and v are in H. On the other hand, a complex Hilbert space can also be regarded as a real Hilbert space by introducing the real-valued inner product defined by  $\operatorname{Re}(u, v)$ , where Re denotes the operation of taking the real part of a complex number. In the following H can be either a real or complex Hilbert space except where noted otherwise. In the case of a real Hilbert space one may omit the complex operations such as \* and Re in the formulas.

An inner product provides a vector space with all the geometric structure of two- and three-dimensional Euclidean space. The *length* or *norm*  $\|\boldsymbol{u}\|$  of a vector  $\boldsymbol{u}$  in H is defined by  $\|\boldsymbol{u}\| = \sqrt{(u,u)}$ , while  $\|\boldsymbol{u} - \boldsymbol{v}\|$  is the *distance* between two vectors  $\boldsymbol{u}$  and  $\boldsymbol{v}$ . (Note, that the length  $|\boldsymbol{x}| = (|x_1|^2 + \dots + |x_n|^2)^{1/2}$  of a vector in  $C^n$  will be denoted by  $|\boldsymbol{x}|$  instead of  $\|\boldsymbol{x}\|$ .) This length satisfies a number of the familiar properties of the length of two- and three-dimensional vectors, including the triangle inequality and parallelogram law. The *triangle inequality*,  $\|\boldsymbol{u} + \boldsymbol{v}\| \leq \|\boldsymbol{u}\| + \|\boldsymbol{v}\|$ , says that the length of any side of a triangle is less than the sum of the lengths of the

other two sides. The parallelogram law,

$$\|\boldsymbol{u} + \boldsymbol{v}\|^{2} + \|\boldsymbol{u} - \boldsymbol{v}\|^{2} = 2\|\boldsymbol{u}\|^{2} + 2\|\boldsymbol{v}\|^{2}$$
(1)

expresses the fact that the sum of the squares of the lengths of the diagonals of a parallelogram is equal to the sum of the squares of the lengths of the sides. The parallelogram law is an easy consequence of the definition of length in terms of the inner product and the properties of the inner product. The triangle inequality follows from the easy-to-verify identity  $\|\boldsymbol{u} + \boldsymbol{v}\|^2 = \|\boldsymbol{u}\|^2 + \|\boldsymbol{v}\|^2 + 2 \operatorname{Re}(\boldsymbol{u}, \boldsymbol{v})$  and the Schwarz inequality

$$|(\boldsymbol{u}, \boldsymbol{v})| \le ||\boldsymbol{u}|| \, ||\boldsymbol{v}|| \tag{2}$$

which says that the absolute value of the inner product of two elements is no bigger than the product of the lengths of the elements. See Ref. 8 (p. 40) for a proof of the Schwarz inequality.

An important technique in Hilbert space theory is the construction of solutions of various equations as the limit of a sequence or series. In a general Hilbert space there are two ways in which a vector  $\boldsymbol{u}$  can be the limit of a sequence of vectors  $\{\boldsymbol{u}_n\}$ . One says  $\{\boldsymbol{u}_n\}$  converges to  $\boldsymbol{u}$  (or converges strongly to  $\boldsymbol{u}$ ) if the distance from  $\boldsymbol{u}_n$  to  $\boldsymbol{u}$  approaches 0 as  $n \to \infty$  (i.e.,  $\|\boldsymbol{u}_n - \boldsymbol{u}\| \to 0$  as  $n \to \infty$ ; one often writes  $\boldsymbol{u}_n \to \boldsymbol{u}$  when this holds). One says  $\{\boldsymbol{u}_n\}$  converges weakly to  $\boldsymbol{u}$  if for each  $\boldsymbol{v}$  in H the sequence of complex numbers  $(\boldsymbol{u}_n, \boldsymbol{v})$  converges to  $(\boldsymbol{u}, \boldsymbol{v})$ . One writes  $u_n \to u$  in this case. For a sequence of vectors in  $C^m$  both methods of convergence are the same; that is,  $\{\boldsymbol{x}_n\} = \{(x_{n1}, \ldots, x_{nm})\}$  converges both strongly and weakly to  $\boldsymbol{x} = (x_1, \ldots, x_m)$  if for each j the sequence of complex numbers  $\{x_{nj}\}$  converges to  $x_j$ . However, in infinite dimensions these two methods of convergence differ. It follows from the Schwarz inequality that if  $\{\boldsymbol{u}_n\}$  converges strongly to  $\boldsymbol{u}$ , then it converges weakly to  $\boldsymbol{u}$ . However, a sequence can converge weakly but not strongly. Consider, for example,  $H = L^2(0, T)$ . Here a sequence of functions  $\{f_n(t)\}$  converges strongly to a function f(t) if  $\int^T_0 |f_n(t) - f(t)|^2 dt \to 0$  as  $n \to \infty$ . This is also called convergence in the  $L^2$  sense. On the other hand,  $\{f_n(t)\}$  converges weakly to f(t) if for each g(t) in  $L^2(0, T)$  one has  $\int^T_0 f_n(t)g(t) dt \to \int^T_0 f(t)g(t) dt$  as  $n \to \infty$ . For example, let  $f_n(t) = 1$  for n < t < n + 1 and  $f_n(t) = 0$  for all other t. Then, using Lebesque's convergence theorem (Ref. 9, p. 88), one can show that  $\{f_n(t)\}$  converges weakly to 0 in  $L^2(0, \infty)$  but not strongly to 0. A series  $\Sigma^{\infty}{_{n=1}} \boldsymbol{u}_n$  converges to  $\boldsymbol{u}$  if the sequence of partial sums  $\{\Sigma^N_{n=1} \boldsymbol{u}_n\}$  converges to  $\boldsymbol{u}$  as  $N \to \infty$ .

A sequence  $\{u_n\}$  is said to be a *Cauchy sequence* if the distance between different elements of the sequence approaches 0 as the indices get large (i.e.,  $||u_n - u_m|| \to 0$  as  $n, m \to \infty$ ). A sequence that converges is a Cauchy sequence since  $||u_n - u_m|| \leq ||u_n - u|| + ||u_m - u||$  by the triangle inequality. However, the opposite is not necessarily true (i.e., there are vector spaces equipped with inner products in which a vector space with some Cauchy sequences do not converge). The case in which a vector space with an inner product has the property that every Cauchy sequence converges is important for establishing the existence of solutions to various types of equations. A vector space *H* is said to be *complete* if every Cauchy sequence converges. It turns out that every vector space equipped with an inner product can be extended to a Hilbert space, which is called the *completion* of the original vector space; see Ref. 5, p. 331. In what follows many of the definitions and concepts are valid in any vector space with an inner product, while the theorems that show the existence of a solution to certain types of equations are usually valid only for a Hilbert space. The proof of the completeness of the  $L^2$  spaces involves the theory of Lebesgue integration; see Ref. 9, p. 117.

In the  $L^2$  spaces two functions f(t) and g(t) are considered to be the same if they are equal for almost all t (i.e., if they are equal except on a set of measure zero). A set S of real numbers has measure zero if for each positive number  $\epsilon$  there is a sequence of intervals such that the total length of the intervals is less than  $\epsilon$  and each point of S is contained in one of the intervals; see Ref. 9, p. 54. For example, the set S consisting of all the integers has measure zero.

A subset S of H is closed if, whenever a sequence  $\{u_n\}$  of elements of S converges to an element u of H, u is in S. In other words, S is closed if it contains the limit of any convergent sequence in S. For example, let S be the set of functions u(t) in  $L^2(-\infty, \infty)$  such that u(-t) = u(t) for almost all t (i.e. the set of even functions). Then S is closed. On the other hand, let  $S_1$  be the set of functions that are equal almost everywhere to a function that is continuous.  $S_1$  is not closed since there are sequences of continuous functions that converge in  $L^2$  to functions that are not continuous.

The closure of a subset S of H is the set of elements u in H such that there exists a sequence  $\{u_n\}$  in S which converges to u. A subset S of H is called *dense* if its closure is all of H. For example, let  $C^{\infty}_{0}(E)$  be the set of all functions u(x) that have continuous partial derivatives of all orders and for which there is a closed, bounded subset K of E such that u(x) = 0 outside K. Then  $C^{\infty}_{0}(E)$  is a dense subset of  $L^{2}(E)$ ; see Ref. 1, p. 1641. This fact can be used to show that most differential operators are defined on dense subsets of  $L^{2}(E)$ .

If a linear subspace M of a Hilbert space is closed, then it is a Hilbert space in its own right. If M is not closed, then it is not complete with the inner product of H, so it is an example of a vector space with an inner product that is not a Hilbert space. For example, the set  $S_1$  mentioned previously is an example of a vector space with an inner product that is not complete.

The Schwarz inequality allows one to define the *angle*  $\theta$  between two vectors via the formula  $\operatorname{Re}(\boldsymbol{u}, v) = \|\boldsymbol{u}\|$  $\|\boldsymbol{v}\| \cos \theta$ , which is familiar in two and three dimensions. Two elements  $\boldsymbol{u}$  and  $\boldsymbol{v}$  are said to be *orthogonal* if  $(\boldsymbol{u}, \boldsymbol{v}) = 0$ . In the case that H is a real Hilbert space, this says that the angle between  $\boldsymbol{u}$  and  $\boldsymbol{v}$  is  $\pi/2$ . We say that  $\boldsymbol{u}$  is orthogonal to a subset M of H if  $\boldsymbol{u}$  is orthogonal to every  $\boldsymbol{v}$  in M. The *orthogonal complement* of a set M is the set of all elements in H that are orthogonal to M.

Many interesting least squares problems can be viewed as finding the shortest distance from a vector to a subspace. More precisely, suppose M is a linear subspace of H and u is a vector in H and one wants to find vin M such that the distance from v to u is less than the distance from w to u for all other w in M. It is not hard to see (see Ref. 8, p. 82) that this occurs precisely if v - u is orthogonal to M. This v is called the *orthogonal projection* of u onto M, and the function P that maps u to v is called the *projection operator* of H onto M. The following *projection theorem* establishes that there is precisely one such v if M is closed:

**Theorem 1.** (projection theorem) Let M be a closed linear subspace of a Hilbert space H. For any u in H there is a unique v in H such that  $||u - v|| \le ||u - w||$  for all w in M. This v is characterized by (v - u, w) = 0 for all w in M. Thus u can be uniquely written as u = v + z, where v is in M and z is in the orthogonal complement of M.

The basic idea of the proof is quite simple. Let d be the greatest lower bound of the distances of elements of M to u. Take a sequence  $\{v_n\}$  of vectors in M such that the distance from  $v_n$  to u approaches d. Then one can use the parallelogram law to show that this is a Cauchy sequence and hence converges to an element v of M. It is then quite easy to show that the distance from v to u is d, and hence v is the desired element; see Ref. 8, p. 82 for details.

It is well known that in finite dimensions an orthogonal coordinate system can be defined by a finite orthonormal set of vectors. This is still useful in an arbitrary Hilbert space, but one has to allow infinite orthonormal sets. For simplicity we restrict our attention to countably infinite sets. A finite or infinite sequence  $\{u_n\}$  of elements is called an *orthonormal* set if each  $u_n$  has length one and  $u_n$  is orthogonal to  $u_m$  for different n and m. The set is called *complete* if there is no other vector in H orthogonal to all the  $u_n$ . A complete orthonormal set is also called an *orthonormal basis*. A classic example of a complete orthonormal set is the sequence of trigonometric functions

$$\frac{1}{\sqrt{2\pi}}, \frac{\cos t}{\sqrt{\pi}}, \frac{\sin t}{\sqrt{\pi}}, \dots, \frac{\cos(nt)}{\sqrt{\pi}}, \frac{\sin(nt)}{\sqrt{\pi}}, \dots$$
(3)

considered as elements of  $L^2(-\pi, \pi)$ . Showing that these are orthonormal is simply a matter of integration, but showing that they are complete requires more advanced tools; see Courant and Hilbert (10), p. 65. There are many more examples of complete orthonormal sets, including the well-known orthogonal polynomials such as the Legendre polynomials in  $L^2(-1, 1)$  and the spherical harmonics in  $L^2(S)$ , where S is the unit sphere in three dimensions; see Ref. 10, chap. II. Orthonormal bases are important because one can expand an arbitrary vector as a superposition of the basis elements, as in the next theorem. This, in turn, leads to formulas for the solution of differential equations for which the basis elements are particularly suited.

**Theorem 2.** Let  $\{u_n\}$  be an orthonormal set and  $\{a_n\}$  be a sequence of complex numbers. Then  $\sum_{n=1}^{\infty} a_n u_n$  converges if and only if  $\sum_{n=1}^{\infty} |a_n|^2 < \infty$ . In this case one has  $\|\sum_{n=1}^{\infty} a_n u_n\|^2 = \sum_{n=1}^{\infty} |a_n|^2$ , a generalization of the Pythagorean theorem. If u is in H, then  $\sum_{n=1}^{\infty} (u, u_n)u_n$  is the orthogonal projection of u on the subspace M, which is the closure of the set of all superpositions of the  $u_n$ , and *Bessel's inequality*  $\sum_{n=1}^{\infty} |(u, u_n)|^2 \le \|u\|^2$  holds. If the set is complete, then Bessel's inequality becomes an equality, called *Parseval's formula*, and  $u = \sum_{n=1}^{\infty} (u, u_n)u_n$ .

The scalars  $(\boldsymbol{u}, \boldsymbol{u}_n)$  are called the *(generalized) Fourier coefficients* of  $\boldsymbol{u}$  with respect to  $\boldsymbol{u}_n$ . When this theorem is applied to the trigonometric sequence of Eq. (3), one obtains the classical Fourier series expansion

$$f(t) = a_0 + \sum_{n=1}^{\infty} [a_n \cos(nt) + b_n \sin(nt)]$$
  
$$a_0 = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(t) dt, \quad a_n = \frac{1}{\pi} \int_{-\pi}^{\pi} f(t) \cos(nt) dt$$
  
$$b_n = \frac{1}{\pi} f(t) \sin(nt) dt$$

Other examples include the expansions of functions in terms of other well-known orthogonal sets of functions, such as the Legendre polynomials and spherical harmonics; see Ref. 10, chap. II.

## Linear Operators

A linear operator A is a function that maps vectors  $\boldsymbol{u}$  in one vector space, called the domain of A and denoted by  $D_A$ , to vectors  $A\boldsymbol{u}$  in another vector space, which satisfies  $A(\alpha \boldsymbol{u} + \beta \boldsymbol{v}) = \alpha A \boldsymbol{u} + \beta A \boldsymbol{v}$  for all  $\boldsymbol{u}$  and  $\boldsymbol{v}$  in  $D_A$  and complex numbers  $\alpha$  and  $\beta$ . Here we shall be interested in the case where  $D_A$  is a subset of a Hilbert space H and A maps  $D_A$  into H, or possibly a different Hilbert space. In the case where H is  $R^n$  or  $C^n$ , a linear operator can be defined by an  $n \times n$  matrix  $\{a_{ik}\}$  by letting  $A\boldsymbol{x} = \boldsymbol{y}$ , where  $y_i = \sum_{k=1}^n a_{ik} x_k$ . The identity operator I defined by  $I\boldsymbol{u} = \boldsymbol{u}$  is a linear operator in any Hilbert space. Multiplication by a fixed function  $a(\boldsymbol{x})$  is a linear operator in  $L^2(E)$ . More precisely, let  $H = L^2(E)$  with  $a(\boldsymbol{x})$  a fixed scalar valued function defined for  $\boldsymbol{x}$  in E.  $D_A$  is the set of all functions  $\boldsymbol{u}(\boldsymbol{x})$  in H such that the function  $a(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x})$  is also in H, and one sets

$$(A\boldsymbol{u})(\boldsymbol{x}) = a(\boldsymbol{x})\boldsymbol{u}(\boldsymbol{x}) \tag{4}$$

for  $\boldsymbol{u}(\boldsymbol{x})$  in  $D_A$ . If  $a(\boldsymbol{x})$  is bounded, then  $D_A = H$ .

Perhaps the most important class of operators are *differential operators*, such as the ordinary differential operator

$$L\boldsymbol{u} = p(t)\frac{d^2\boldsymbol{u}}{dt^2} + q(t)\frac{d\boldsymbol{u}}{dt} + r(t)\boldsymbol{u}$$
(5)

where p(t), q(t), and r(t) are given functions defined for t in an interval a < t < b. When working with differential operators, another group of Hilbert spaces called the *Sobolev spaces* are very useful; see Ref. 8, p. 55. The Sobolev space  $H^1(a, b)$  consists of all functions f(t) in  $L^2(a, b)$  whose derivatives f'(t) = df/dt are also in  $L^2$ . The inner product and norm are given by  $(f, g)_1 = \int_a^b [f(t)g(t)* + f'(t)g'(t)*] dt$  and  $||f||^2_1 = \int_a^b (|f(t)|^2 + |f'(t)|^2) dt$ .  $H^2(a, b)$  is defined in an analogous manner by requiring that the second derivative of f(t) lie in  $L^2$  as well. If p(t), q(t), and r(t) are all bounded and u(t) is in  $H^2(a, b)$ , then Lu in  $L^2(a, b)$ . If one is solving an initial or boundary value problem associated with L, then one can incorporate the initial or boundary conditions into the domain of L. For example, if the problem requires the solution to be zero at t = a and t = b, then one can restrict the domain of L to functions u in  $H^2(a, b)$  such that u(a) = u(b) = 0. See Ref. 3, p. 146 for a more detailed discussion of these operators.

An important partial differential operator is the Laplacian  $\Delta \boldsymbol{u} = \partial^2 \boldsymbol{u}/\partial x_1^2 + \dots + \partial^2 \boldsymbol{u}/\partial x_n^2$ . As with ordinary differential operators, the Sobolev spaces are an invaluable tool when working with partial differential operators. If E is an open set in  $\mathbb{R}^n$ , then  $H^1(E)$  is the set of all functions  $\boldsymbol{u}(\boldsymbol{x})$  in  $L^2(E)$  with the property that all of its first partial derivatives also lie in  $L^2(E)$ . The inner product  $(.)_1$  in this space is given by  $(\boldsymbol{u}, \boldsymbol{v})_1 = (\boldsymbol{u}, \boldsymbol{v}) + \sum_{i=1}^n (\partial \boldsymbol{u}/\partial x_i, \partial \boldsymbol{v}/\partial x_i)$ , where (.) is the inner product in  $L^2(E)$ .  $H^2(E)$  is defined in a similar manner. In this context one can use the following generalization of the classical notion of partial derivatives: One says that  $\partial \boldsymbol{u}/\partial x_i = \boldsymbol{v}$  in E if there is a sequence of functions  $\{\boldsymbol{u}_m(\boldsymbol{x})\}$  in  $L^2(E)$  such that each  $\boldsymbol{u}_m$  has continuous first partial derivatives that lie in  $L^2(E)$  and such that  $\boldsymbol{u}_m \to \boldsymbol{u}$  and  $\partial \boldsymbol{u}_m/\partial x_i \to \boldsymbol{v}$  in  $L^2(E)$  as  $m \to \infty$ ; see Ref. 8, pp. 46–59 for more discussion of generalized derivatives or weak derivatives. Just as with ordinary differential operators, one often includes boundary conditions in the domain of the operator. Suppose one has a boundary value problem involving the Laplace operator on a subset E of  $\mathbb{R}^n$  with zero Dirichlet boundary conditions. Then the corresponding operator,  $\Delta_d$ , would have a domain,  $D\Delta_d$ , consisting of all functions in  $H^2(E)$  that are 0 on B and

$$\Delta_d \boldsymbol{u} = \frac{\partial^2 \boldsymbol{u}}{\partial x_1^2} + \dots + \frac{\partial^2 \boldsymbol{u}}{\partial x_n^2} \quad \text{for} \boldsymbol{u} \text{ in } D_{\Delta_d} \tag{6}$$

See Ref. 3, pp. 297–305 for more details and examples.

The solution of many differential equations can be expressed in terms of integral operators of the form

$$K\boldsymbol{u}(\boldsymbol{x}) = \int_{E} k(\boldsymbol{x}, \boldsymbol{y}) \boldsymbol{u}(\boldsymbol{y}) \, d\boldsymbol{y}$$
(7)

where the *kernel* k(x, y) is a given function of x and y in an open set E of  $\mathbb{R}^n$ . (For a boundary value problem, the kernel is often called the *Green's function*.) For example, the solution of  $d^2u/dt^2 = f(t)$  for 0 < t < 1 with boundary conditions u(0) = u(1) = 0 is  $u(t) = \int_0^1 k(t, s)f(s) ds$  with k(t, s) = (t-1)s for s < t and k(t, s) = (s-1)t for t < s; see Ref. 10, pp. 351, 371.

One possible domain for the integral operator of Eq. (7) is the set of all functions  $\boldsymbol{u}$  in  $H = L^2(E)$  such that the integral of Eq. (7) exists for almost all  $\boldsymbol{x}$  and the resulting function  $K\boldsymbol{u}$  is also in H. However, it often turns out that K has a natural extension to a larger domain; this is discussed further later in this article.

Convolution operators are integral operators of the form  $G\boldsymbol{u} = \boldsymbol{g} \ast \boldsymbol{u}$ , where

$$(\boldsymbol{g}^*\boldsymbol{u})(\boldsymbol{x}) = \int_{\mathbb{R}^n} \boldsymbol{g}(\boldsymbol{x} - \boldsymbol{y})\boldsymbol{u}(\boldsymbol{y}) \, d\boldsymbol{y}$$
(8)

with g(x) a function of x in  $\mathbb{R}^n$ . These operators arise in the solution of constant coefficient differential equations, in filtering problems, and in other translation invariant problems. For example, a solution of Poisson's equation,

 $\Delta \boldsymbol{u} = \boldsymbol{f}(\boldsymbol{x})$ , in three dimensions is  $\boldsymbol{u} = \boldsymbol{g} * \boldsymbol{f}$ , where  $\boldsymbol{g}(\boldsymbol{x}) = 1/(4\pi |\boldsymbol{x}|)$ ; see Ref. 10, p. 368. The *Hilbert transform*  $H\boldsymbol{u}(\boldsymbol{x}) = \int_{-\infty}^{\infty} u(\boldsymbol{y})/(\boldsymbol{x} - \boldsymbol{y}) d\boldsymbol{y}$  is a convolution operator with kernel 1/x.

An important integral operator is the *Fourier transform*  $\mathscr{F}$ , which maps the function f(t) to the function  $F(\omega) = 1/\sqrt{2\pi}$   $\int_{-\infty}^{\infty} e^{-j\omega t} f(t) dt$ , where  $j = \sqrt{-1}$ . Thus  $F = \mathscr{F} f$ . This integral exists for all  $\omega$  if  $\int_{-\infty}^{\infty} |f(t)| dt < \infty$ . Even though not every function f(t) in  $L^2(-\infty, \infty)$  meets this requirement, it turns out that the operator  $\mathscr{F}$  has a natural extension to all f(t) in  $L^2(-\infty, \infty)$  so that  $F = \mathscr{F} f$  also lies in  $L^2(-\infty, \infty)$ . In fact,  $\mathscr{F}$ , as well as differentiation and convolution, can be extended to the class of tempered distributions, which includes not only functions in  $L^2(-\infty, \infty)$  but also distributions like the Dirac delta function; see Ref. 8, p. 146. A function f(t) can be recovered from its Fourier transform  $F(\omega)$  via the *inverse Fourier transform*  $\mathscr{F}^{-1}$ , which is given by  $f(t) = 1/\sqrt{2\pi} \int_{-\infty}^{\infty} e^{j\omega t} F(\omega) d\omega$ ; see Ref. 8, p. 147. This can be written as  $\mathscr{F}^{-1}\mathscr{F} f = f$ . Thus  $\mathscr{F}^{-1}\mathscr{F} = I$ .

This last formula is stated in terms of the product (or composition) of operators. If *A* and *B* are linear operators, then the product *AB* denotes the linear operator defined by (AB)u = A(Bu); the domain of *AB* is the set of all u in the domain of *B* such that Bu is in the domain of *A*. If *A* and *B* are operators defined by  $n \times n$  matrices, then the matrix of *AB* is the usual matrix product of the matrices of *A* and *B*. The Fourier transform extends to functions u(x) of *n* variables  $x = (x_1, \ldots, x_n)$  by the formula

$$\mathscr{T}\boldsymbol{u}(\boldsymbol{\xi}) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-j(\boldsymbol{\xi}, \boldsymbol{x})} \boldsymbol{u}(\boldsymbol{x}) \, d\boldsymbol{x}$$
(9)

where  $(\xi, \mathbf{x}) = \xi_1 x_1 + \dots + \xi_n x_n$ . The Fourier transform converts differentiation and convolution to multiplication; that is,

$$\mathscr{F}(\partial \boldsymbol{u}/\partial \boldsymbol{x}_{\boldsymbol{k}}) = j\xi_{\boldsymbol{k}}\mathscr{F}(f), \qquad \mathscr{F}(\boldsymbol{u} * \boldsymbol{v}) = (2\pi)^{n/2}\mathscr{F}(\boldsymbol{u})\mathscr{F}(\boldsymbol{v}) \quad (10)$$

See Ref. 8, p. 160. Thus taking Fourier transforms converts any constant coefficient differential operator on  $\mathbb{R}^n$  into a multiplication operator. For example, applying Eq. (7) twice gives  $\mathscr{F}(\Delta \boldsymbol{u}) = -|\xi|^2 \mathscr{F}(\boldsymbol{u})$ .

A linear operator A is *bounded* if there exists a constant M such that  $||A\boldsymbol{u}|| \leq M||\boldsymbol{u}||$  for all  $\boldsymbol{u}$  in  $D_A$ , and the smallest constant M is defined to be the *norm* of operator A, denoted by ||A||. A being bounded is equivalent to A being *continuous* (i.e., if  $\{\boldsymbol{u}_n\}$  is a sequence in  $D_A$  that converges to  $\boldsymbol{u}$ , which is also in  $D_A$ , then  $A\boldsymbol{u}_n \to A\boldsymbol{u}$ ). For example, a multiplication operator (5) is bounded if and only if  $a(\boldsymbol{x})$  is a bounded function; that is, there is a constant C such that  $|a(\boldsymbol{x})| \leq C$  for almost all  $\boldsymbol{x}$ . In this case  $||A|| \leq C$ . Showing that a particular integral operator of the form of Eq. (7) is bounded can require some sophisticated work with inequalities. For example, suppose  $\int_E |k(\boldsymbol{x}, \boldsymbol{y})| d\boldsymbol{y} \leq M$  for all  $\boldsymbol{x}$ , and  $\int_E |k(\boldsymbol{x}, \boldsymbol{y})| d\boldsymbol{x} \leq M$  for all  $\boldsymbol{y}$ . Then it can be shown that K is defined on all of  $L^2(E)$  and is bounded from  $L^2(E)$  into  $L^2(E)$  with  $||K|| \leq M$ ; see Ref. 3, p. 144. In particular, a convolution operator is bounded if  $\int R^n |g(\boldsymbol{x})| d\boldsymbol{x} < \infty$ . The Hilbert transform does not meet this condition, but it can also be shown to be bounded in  $L^2(-\infty, \infty)$ ; see Ref. 1, pp. 1041–1073.

A linear operator T is an *isometry* if the domain of T is all of H and it preserves inner products; that is, (Tu, Tv) = (u, v) for all u and v in H. This implies T also preserves lengths and distances ||Tu|| = ||u|| for all u. In particular, an isometry is bounded and ||T|| = 1. If, in addition, the equation Tu = f has a solution u for each f in H, then T is said to be *unitary*. The Fourier transform and its inverse are examples of unitary operators; see Ref. 8, p. 154.

Most differential operators are not bounded when regarded as an operator from  $L^2$  to itself. For example, consider  $L\mathbf{u} = d^2\mathbf{u}/dt^2$  as an operator from  $L^2(0, 2\pi)$  to itself. Then  $L(\sin(nt)) = -n^2 \sin(nt)$  for any n. So  $||L(\sin(nt))||/||\sin(nt)|| = n^2$ , which can be arbitrarily large. On the other hand, many of these same operators are bounded when regarded as operators from a Sobolev space to  $L^2$ . For example, the operator L given by Eq. (5) is a bounded operator from  $H^2$  to  $L^2$  if p(t), q(t), and r(t) are bounded.

A linear operator A is *closed* if whenever  $\{u_n\}$  is a sequence in  $D_A$ , and both  $u_n \to u$  and  $Au_n \to f$ , then u is in  $D_A$  and Au = f; that is, the set of ordered pairs (u, Au), where u varies over  $D_A$ , is a closed set in the product space  $H \times H$  of all ordered pairs (u, v), where u and v are in H. A bounded operator is closed if and only if  $D_A$  is a closed subset of H. If an operator is not closed, it may be possible to extend it to a closed operator  $A^c$ , by defining  $A^c u = f$  if  $\{u_n\}$  is a sequence in  $D_A$ , and both  $u_n \to u$  and  $Au_n \to f$ . This gives a unique f for the value of  $A^c u$  if A satisfies the condition that if whenever  $\{u_n\}$  is a sequence in  $D_A$ , and  $u_n \to 0$  and  $Au_n \to f$ , then f = 0; such an operator is called *closable*. For example, any bounded operator is closable and the closure is also bounded with the same norm as is defined on the closure of  $D_A$ . In particular, it is possible to extend the Fourier transform and its inverse in this way to all of  $L^2(\mathbb{R}^n)$ . For simplicity, we will denote the extended operators by  $\mathscr{F}$  and  $\mathscr{F}^{-1}$ .

## The Equation Au = f

Many problems in the classical theory of fields can be thought of as operator equations of the form Au = fin  $H = L^2(E)$ , where E, a subset of  $\mathbb{R}^n$ , is the domain of the independent variables. In the operator equation Au = f, the problem is to find u given A and f. Consider, for example, the boundary value problem consisting of Poisson's equation in E with zero Dirichlet boundary conditions on B, the boundary of E. Given f(x) defined in E, one wants to find u(x) such that

$$\Delta \boldsymbol{u} = \boldsymbol{f}(\boldsymbol{x}) \quad \text{in } \boldsymbol{E}, \text{ and } \boldsymbol{u}(\boldsymbol{x}) = 0 \text{ on } \boldsymbol{B}$$
(11)

This can be written as  $\Delta_d \boldsymbol{u} = \boldsymbol{f}$ , where  $\Delta_d$  is the Laplace operator defined by Eq. (6).

The problem Au = f is well posed if there is one and only one solution u for any f and u depends continuously on f. Given an operator A, its range, denoted by  $R_A$ , is the set of elements f for which the equation  $A\mathbf{u} = \mathbf{f}$  has a solution  $\mathbf{u}$  in  $D_A$ . Thus the equation  $A\mathbf{u} = \mathbf{f}$  has a solution for each  $\mathbf{f}$  in H if and only if the range of A is H. The operator A is said to be *invertible* if there is only one solution to the equation Au = f for any f in the range of A. If A is linear, this is equivalent to Au = 0 only if u = 0. If A is invertible, then one can define the inverse operator of A, denoted by  $A^{-1}$ , by setting  $A^{-1}f = u$  if Au = f. Often the term  $A^{-1}$  is used as a synonym for A being invertible. The domain of  $A^{-1}$  is the range of A, and one has  $A^{-1}A = I$  and  $AA^{-1} = I$ , where the identity operator is restricted to  $D_A$  in the first case and  $D_A^{-1}$  in the second. If A is the operator corresponding to an  $n \times n$  matrix, then A is invertible if and only if the determinant of the matrix is not zero and the matrix of  $A^{-1}$  is the usual matrix inverse of A. A multiplication operator of the form of Eq. (4) is invertible if  $a(\mathbf{x}) \neq 0$  for almost all  $\mathbf{x}$ , in which case  $A^{-1}$  is the multiplication operator by  $1/a(\mathbf{x})$ . In this case  $A^{-1}$  will be bounded with domain  $L^2(E)$  if  $1/a(\mathbf{x})$  is bounded uniformly almost everywhere. Since the Fourier transform converts differentiation into multiplication [see Eq. (10)], it follows that the Laplace operator on all of  $\mathbb{R}^n$  is invertible and its inverse is the convolution operator with kernel equal to  $\mathscr{T}^{-1}(-(2\pi)^{-n/2}|\xi|^{-2})$ . To summarize, the problem Au = f is well posed if and only if A is invertible and  $\hat{A}^{-1}$  is a bounded operator with domain equal to H.

Showing that an operator A is invertible and that  $A^{-1}$  is bounded is equivalent to showing that  $||A\boldsymbol{u}|| \geq c||\boldsymbol{u}||$  for some positive constant c. To obtain this inequality, it suffices to show an inequality such as  $|(A\boldsymbol{u}, \boldsymbol{u})| \geq c||\boldsymbol{u}||^2$  for some positive constant c. Then one can use the Schwarz inequality of Eq. (2) to conclude that  $||A\boldsymbol{u}|| = ||\boldsymbol{u}|| \geq c||\boldsymbol{u}||^2$ , which gives  $||A\boldsymbol{u}|| \geq c||\boldsymbol{u}||$ . Consider, for example, the Laplace operator  $\Delta_d$  with Dirichlet boundary values defined by Eq. (6). For simplicity, suppose that E is a bounded domain with smooth boundary B. Then

by Green's integral formula (see Ref. 11, p. 441) one has

$$(\Delta \boldsymbol{u}, \boldsymbol{v}) = -\sum_{k=1}^{n} \left( \frac{\partial \boldsymbol{u}}{\partial x_{k}}, \frac{\partial \boldsymbol{v}}{\partial x_{k}} \right)$$
(12)

if  $\boldsymbol{v} = 0$  on *B*. Here (,) is the inner product in  $L^2(E)$ . Applying this formula, one obtains  $(\Delta_d \boldsymbol{u}, \boldsymbol{u}) = -\Sigma^n_{k=1} \|\partial \boldsymbol{u}/\partial x_k\|^2$  for  $\boldsymbol{u}$  in  $D\Delta_d$ , where  $\| \|$  is the norm in  $L^2(E)$ . An inequality of Poincaré (see Ref. 12, p. 169) says that for a bounded domain *E* there is a constant *C* such that  $\|\boldsymbol{u}\|^2 \leq C \Sigma^n_{k=1} \|\partial \boldsymbol{u}/\partial x_k\|^2$  for all  $\boldsymbol{u}$  in  $H^1(E)$  that are 0 on *B*. Thus

$$-(\Delta_d \boldsymbol{u}, \boldsymbol{u}) \ge c \|\boldsymbol{u}\|_1^2 \ge c \|\boldsymbol{u}\|^2$$
(13)

where  $\| \|_1$  is the norm in  $H^1(E)$  and c is a positive constant. Thus  $\Delta_d$  has a bounded inverse. Showing that the range of  $\Delta_d$  is all of  $L^2(E)$  requires some more work; see the Lax–Milgram theorem later in this article.

A functional on a vector space V is a mapping from V to the complex numbers; a linear functional is one that is linear. The conjugate (or dual) space of H, denoted by  $H_*$ , consists of all bounded linear functionals F on H such that  $D_F = H$ . A simple example is  $F(f) = 1/2\pi \int^{2\pi} f(t) dt$ , which is the functional that assigns to each function f in  $H = L^2(0, 2\pi)$  its average value. This is a special case of the following general way to obtain linear functionals. Let v be a fixed element of H and let  $F_v(\mathbf{u}) = (\mathbf{u}, \mathbf{v})$ . Then this linear functional that is bounded linear functional that is bounded by the Schwarz inequality. In fact,  $||F_v|| = ||\mathbf{v}||$ . The Riesz representation theorem says that any bounded linear functional on H can be obtained from an element  $\mathbf{v}$  of H in this way.

**Theorem 3.** (Riesz) Let *F* be a bounded linear functional defined everywhere on a Hilbert space *H*. Then there exists a unique element v in *H* such that ||v|| = ||F|| and F(u) = (u, v) for all u in *H*.

The proof is quite easy. Let M be the set of all u such that F(u) = 0. M is a closed linear subspace of H. By the projection theorem there is a v in H that is orthogonal to M and has length 1. By multiplying F by a constant, we may reduce to the case where F(v) = 1. Now let u be any element of H. Note that u - F(u)v is in M. Thus (u, v) = (u - F(u)v, v) + (F(u)v, v) = F(u).

The Riesz representation theorem can be used to prove the *Lax-Milgram theorem*, which, in turn, is useful for proving the existence of solutions to many elliptic boundary value problems. This theorem is often stated in terms of bilinear forms that are closely related to linear operators. A *sesquilinear form* B associates a scalar  $B(\boldsymbol{u}, \boldsymbol{v})$  to each pair of elements  $\boldsymbol{u}$  and  $\boldsymbol{v}$  in a vector space  $D_B$ , called the domain of B, such that  $B(\boldsymbol{u}, \boldsymbol{v})$  is linear in  $\boldsymbol{u}$  for each fixed  $\boldsymbol{v}$  and conjugate linear in  $\boldsymbol{v}$  for each fixed  $\boldsymbol{u}$ ; that is,  $B(\boldsymbol{u}, \alpha \boldsymbol{v}_1 + \beta \boldsymbol{v}_2) = \alpha * B(\boldsymbol{u}, \boldsymbol{v}_1) + \beta * B(\boldsymbol{u}, \boldsymbol{v}_2)$ . An example is the *Dirichlet form* 

$$D(\boldsymbol{u},\boldsymbol{v}) = \sum_{k=1}^{n} \int_{E} \frac{\partial \boldsymbol{u}}{\partial x_{k}} \frac{\partial \boldsymbol{v}^{*}}{\partial x_{k}} dx = \sum_{k=1}^{n} \left( \frac{\partial \boldsymbol{u}}{\partial x_{k}}, \frac{\partial \boldsymbol{v}^{*}}{\partial x_{k}} \right)$$
(14)

where (,) is the inner product in  $L^2(E)$ . The domain is the set of functions in  $H^1(E)$  that are 0 on *B*, the boundary of *E*. A bilinear form  $B(\boldsymbol{u}, \boldsymbol{v})$  is said to be *bounded* if there is a constant *C* such that  $|B(\boldsymbol{u}, \boldsymbol{v})| \leq C ||\boldsymbol{u}|| ||\boldsymbol{v}||$  for all  $\boldsymbol{u}$  and  $\boldsymbol{v}$  in  $D_B$ . For example, the Dirichlet form is bounded with respect to the norm in  $H^1(E)$  but not  $L^2(E)$ .

Given a sesquilinear form *B* with dense domain, there is a linear operator *A* associated with *B*. Its domain is the set of all  $\boldsymbol{u}$  such that there is an  $\boldsymbol{f}$  such that  $B(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{f}, \boldsymbol{v})$  for all  $\boldsymbol{v}$  in  $D_B$ . This  $\boldsymbol{f}$  is uniquely determined since  $D_B$  is assumed to be dense. Consider the Dirichlet form defined by Eq. (14). Since  $(-\Delta_d \boldsymbol{u}, \boldsymbol{v}) = D(\boldsymbol{u}, \boldsymbol{v})$  for  $\boldsymbol{u}$  and  $\boldsymbol{v}$  in  $D\Delta_d$ , it follows that the operator associated with the Dirichlet form is either equal to or an extension of  $-\Delta_d$ . In fact, the two operators are equal; this is an important theorem of Friedrichs; see Ref. 1, p. 1789.

The importance of sesquilinear forms is that they are a useful tool for proving the existence of solutions to the equation Au = f when A is the associated operator. This is the content of the following theorem.

**Theorem 4.** (Lax–Milgram) Let  $H_1$  be a Hilbert space with norm  $|| ||_1$  and  $B(\boldsymbol{u}, \boldsymbol{v})$  a bounded bilinear form on  $H_1$ . Assume that B is coercive on  $H_1$ —that is, there exists a constant c > 0 such that  $|B(\boldsymbol{u}, \boldsymbol{u})| \ge c ||\boldsymbol{u}||^2_1$  for all  $\boldsymbol{u}$  in  $H_1$ . Then for any bounded linear functional F on  $H_1$  there exists a unique element  $\boldsymbol{w}$  in  $H_1$  such that  $B(\boldsymbol{u}, \boldsymbol{u}) = F(\boldsymbol{u})$  for all  $\boldsymbol{u}$  in  $H_1$ . Suppose H is another Hilbert space with norm || || such that  $H_1$  is a dense subset of H and there exists a constant C such that  $||\boldsymbol{u}|| \le C ||\boldsymbol{u}||_1$  for all  $\boldsymbol{u}$  in  $H_1$ . Let A be the operator in H associated with B. Then A is invertible, the range of A is all of H, and  $A^{-1}$  is a bounded linear operator on H.

For a proof, see Ref. 8, p. 92. According to Eq. (13), the Dirichlet form defined by Eq. (14) satisfies the hypotheses of the Lax-Milgram theorem with  $H_1$  being the subspace of  $H^1(E)$  consisting of functions in  $H^1(E)$  that are 0 on *B*. If one takes  $H = L^2(E)$ , then we have noted that the operator in *H* associated with the Dirichlet form is  $\Delta_d$ . Thus the Lax-Milgram theorem establishes the existence of a solution to Poisson's equation [Eq. (11)].

A linear operator defined by a matrix mapping  $C^n$  to itself has the property that its range is all of  $C^n$  if and only if it is invertible. This is not true for a general operator in infinite dimensions, but there are some important special cases in which this is true. One of these involves compact operators. A linear operator on a Hilbert space is said to be *compact* if it maps any bounded sequence into a sequence with a convergent subsequence. In particular, a compact operator is bounded. It can also be shown that the identity mapping is a compact operator from  $H^1(E)$  to  $L^2(E)$  if E is a bounded set; see Ref. 1, p. 1691. This can be used to show that  $\Delta^{-1}_D$  is a compact operator in  $L^2(E)$  if E is bounded. The following theorem, called the Fredholm alternative theorem, extends the aforementioned result of matrices in finite dimensions; for a proof see Ref. 8, sec. X.5.

**Theorem 5.** (Fredholm) Let  $A = C - \lambda I$ , where *C* is compact and  $\lambda \neq 0$  is a complex number. Then *A* is invertible if and only if the range of *A* is all of *H*.

Let *H* be a Hilbert space and *A* an operator on it with  $D_A$  is dense in *H*. The function  $B(\boldsymbol{u}, \boldsymbol{v}) = (\boldsymbol{u}, A\boldsymbol{v})$ is a sesquilinear form. The associated operator A\* is called the adjoint of *A*; that is,  $(\boldsymbol{u}, A\boldsymbol{v}) = (A*\boldsymbol{u}, \boldsymbol{v})$  for  $\boldsymbol{u}$  in  $D_{A*}$  and  $\boldsymbol{v}$  in  $D_A$ . For example, if *A* is an  $n \times n$  matrix  $\{a_{ik}\}$ , then the matrix  $\{b_{ik}\}$  of A\* is just the conjugate of the transpose of *A* (i.e.,  $b_{ik} = a^*_{ki}$ ). If *A* is the multiplication operator of Eq. (4), then A\* is the multiplication operator by a(x)\*. If *K* is an integral operator of the form of Eq. (7), then K\* is equal to or an extension of the integral operator with kernel p(x, y) given by p(x, y) = k(y, x)\*. For a unitary operator *T* one has  $T*=T^{-1}$ .

An operator A is said to be *Hermitian* if (Au, v) = (u, Av) for all u and v in  $D_A$ . If A is Hermitian, then A\* is equal to or an extension of A. For example, it follows from Eq. (12) that  $\Delta_d$  is Hermitian. If A is invertible, then A is Hermitian if and only if  $A^{-1}$  is Hermitian. If A\*=A, then A is said to be *self-adjoint*. For example, if A is an  $n \times n$  matrix  $\{a_{ik}\}$ , then A is self-adjoint if  $a_{ik} = a^*_{ki}$  for all i and k. The multiplication operator of Eq. (4) is self-adjoint if a(x) is real for all x. If A is a Hermitian operator with domain equal to H, then A is self-adjoint. If A is self-adjoint. If A is normal for all x. If A is self-adjoint. If  $A = a^*_{ki}$  for all i and k. The multiplication operator of Eq. (4) is self-adjoint if a(x) is real for all x. If A is a Hermitian operator with domain equal to H, then A is self-adjoint. If A is normal for all x. If  $A = a^*_{ki}$  and only if  $A^{-1}$  is self-adjoint. If A is normal invertible and  $A^{-1}$  has domain equal to H, then A is self-adjoint. For example,  $\Delta_d$  is self-adjoint. An operator A is normal if AA\*=A\*A. Any self-adjoint or unitary operator is normal. If A is normal, then  $\alpha A$  is normal for any complex number  $\alpha$ . Any multiplication operator given by Eq. (4) is normal. Normal operators are important because of their spectral properties, which are considered next.

# **Spectral Theory and Evolution Equations**

A number of initial boundary value problems of classical field theory can be cast in the form of an ordinary differential equation of one of the following two forms:

$$\frac{d\boldsymbol{u}}{dt} = A\boldsymbol{u}(t), \quad \text{for } t > 0 \text{ together with } \boldsymbol{u}(0) = \boldsymbol{\phi} \qquad (15)$$

$$\frac{d^2 \boldsymbol{u}}{dt^2} = A \boldsymbol{u}(t), \quad \text{for } t > 0 \text{ together with } \boldsymbol{u}(0) = \boldsymbol{\phi} \text{ and } \frac{d \boldsymbol{u}}{dt}(0) = \boldsymbol{\psi}$$
(16)

In these equations *A* is a linear operator in a Hilbert space *H* and the unknown  $\boldsymbol{u}(t)$  is a function of  $t \ge 0$  whose value at each *t* is an element of *H*. The solution  $\boldsymbol{u}(t)$  should satisfy the differential equation for t > 0 and the initial conditions for t = 0. For example, the initial boundary value for the heat (or diffusion) equation

$$\begin{aligned} \frac{\partial \boldsymbol{u}}{\partial t} &= \Delta \boldsymbol{u}, \quad \text{for } t \ge 0, \boldsymbol{x} \text{ in } \boldsymbol{E} \\ \boldsymbol{u}(t, \boldsymbol{x}) &= 0, \quad \text{for } t \ge 0, \boldsymbol{x} \text{ on } \boldsymbol{B} \\ \boldsymbol{u}(0, \boldsymbol{x}) &= \boldsymbol{\phi}(\boldsymbol{x}), \quad \text{for } x \text{ in } \boldsymbol{E} \end{aligned}$$
(17)

can be viewed as an equation of the form of Eq. (15) with  $A = \Delta_d$  defined by Eq. (6). Similarly, the corresponding problem for the wave equation

$$\frac{\partial^2 \boldsymbol{u}}{\partial t^2} = \Delta \boldsymbol{u}, \quad \text{for } t \ge 0, \boldsymbol{x} \text{ in } E$$
$$\boldsymbol{u}(t, \boldsymbol{x}) = 0, \quad \text{for } t \ge 0, \boldsymbol{x} \text{ on } B \qquad (18)$$
$$\boldsymbol{u}(0, \boldsymbol{x}) = \boldsymbol{\phi}(\boldsymbol{x}), \quad \frac{\partial \boldsymbol{u}}{\partial t}(0, \boldsymbol{x}) = \boldsymbol{\psi}(\boldsymbol{x}) \quad \text{for } \boldsymbol{x} \text{ in } E$$

has the form of Eq. (16) with the same A. Equations (15) and (16) are examples of simple evolution equations; for more general evolution equations, see Ref. 8, chap. XIV. In many cases the solution of these equations can be obtained in terms of the eigenvalues  $\lambda_n$  and eigenvectors  $\boldsymbol{u}_n$  of the operator A (i.e.,  $A\boldsymbol{u}_n = \lambda_n \boldsymbol{u}_n$ ). Eigenvalues are part of the *spectrum*  $\sigma(A)$  of A, which consists of all complex numbers that are not in the resolvent set of A. The *resolvent set*,  $\rho(A)$ , of A consists of all complex numbers  $\lambda$  such that  $A - \lambda I$  is invertible and  $(A - \lambda I)^{-1}$ is bounded and with domain H; the operator valued function  $R(\lambda; A) = (A - \lambda I)^{-1}$  defined for  $\lambda$  in the resolvent set is called the *resolvent* of A. A number  $\lambda$  can be in the spectrum for one of three reasons:

- (1)  $A \lambda I$  does not have an inverse (i.e., there exists  $\boldsymbol{u} \neq 0$  satisfying  $A\boldsymbol{u} = \lambda \boldsymbol{u}$ ). We say  $\lambda$  is an eigenvalue of A (or  $\lambda$  belongs to the *point spectrum* of A) and that  $\boldsymbol{u}$  is an eigenvector corresponding to  $\lambda$ .
- (2)  $A \lambda I$  is invertible, but the domain of  $(A \lambda I)^{-1}$  is not dense in *H*. In this case one says that  $\lambda$  is in the *residual spectrum* of *A*.
- (3)  $A \lambda I$  is invertible, and  $(A \lambda I)^{-1}$  has a dense domain, but it is unbounded. In this case one says that  $\lambda$  is in the *continuous spectrum* of A.

Note that cases 2 and 3 are impossible if *H* is infinite dimensional. In the case where *A* is an operator in a Hilbert space of functions like  $L^2(E)$ , it is common to use the term *eigenfunction* for an eigenvector. For an operator *A* given by a matrix  $\{a_{ik}\}$ , a number  $\lambda$  is an eigenvalue if det $\{a_{ik} - \lambda \delta_{ik}\} = 0$ ; otherwise  $\lambda$  is in the resolvent. Here det is the determinant and  $\delta_{ik}$  is 1 if i = k and 0 otherwise.

For the multiplication operator of Eq. (4) a number  $\lambda$  is in the resolvent if  $a(\mathbf{x}) \neq \lambda$  for almost all  $\mathbf{x}$  and the function  $1/(a(\mathbf{x}) - \lambda)$  is bounded and  $R(\lambda, A)$  is the multiplication operator by  $1/(a(\mathbf{x}) - \lambda)$ . If  $a(\mathbf{x}) \neq \lambda$  for almost all  $\mathbf{x}$ , but the function  $1/(a(\mathbf{x}) - \lambda)$  is not bounded, then  $\lambda$  is in the continuous spectrum. A number  $\lambda$  is an eigenvalue for this operator if the set S of  $\mathbf{x}$  where  $a(\mathbf{x}) = \lambda$  has positive measure. In this case any function that is 0 outside S is a corresponding eigenfunction.

Suppose two operators A and B are related by  $A = T^{-1}BT$ , where T is an invertible operator, and both T and  $T^{-1}$  are bounded and defined on all of H. Then A and B have the same spectrum and points in the spectrum have the same type. For example, Consider the Laplacian  $\Delta$  as an operator in  $L^2(\mathbb{R}^n)$ . It follows from Eq. (10) that  $\Delta = \mathscr{F}^{-1}M\mathscr{F}$ , where M is the multiplication operator by  $-|\xi|^2$ ; that is,  $M\mathbf{v}(\xi) = -|\xi|^2\mathbf{v}(\xi)$ . Hence the spectrum of  $\Delta$  is the negative real axis together with the number 0 and the spectrum consists entirely of continuous spectra.

It can be shown that for an operator the spectrum is a closed set; see Ref. 3, p. 174. Furthermore, the spectrum of a self-adjoint operator lies on the real axis. The eigenvectors of a normal operator corresponding to distinct eigenvalues are orthogonal; see Ref. 3, pp. 271, 274. In the case where the eigenvectors of A form a complete orthonormal set  $\{u_n\}$  and there exists a constant C such that the real part of each eigenvalue does not exceed C, then the solution to Eq. (15) is

$$\boldsymbol{u}(t) = \sum_{n=1}^{\infty} (\boldsymbol{\phi}, \boldsymbol{u}_n) e^{\lambda_n t} \boldsymbol{u}_n$$
(19)

If, in addition, the eigenvalues are all real, then the solution to Eq. (16) is

$$\boldsymbol{u}(t) = \sum_{n=1}^{\infty} \left[ (\boldsymbol{\phi}, \boldsymbol{u}_n) \cos(\sqrt{-\lambda_n} t) + (\boldsymbol{\psi}, \boldsymbol{u}_n) \sin(\sqrt{-\lambda_n} t) / \sqrt{-\lambda_n} \right] \boldsymbol{u}_n$$
(20)

See Ref. 12, pp. 149–150. Thus it is important to know when a normal operator has the property that its eigenvectors form a complete orthonormal set. One case where this occurs is when the operator is compact.

**Theorem 6.** (Riesz–Schauder and Hilbert–Schmidt) If *C* is a compact operator, then the spectrum of *C* consists of a finite or infinite sequence  $\{\lambda_n\}$  of eigenvalues and possibly the number 0 (which can also be an eigenvalue, but need not be). Any nonzero eigenvalue  $\lambda$  has *finite multiplicity* (i.e., the collection of eigenvectors corresponding to  $\lambda$  is a subspace of finite dimension). If, in addition, *C* is normal, then there is a complete orthonormal set consisting of eigenvectors of *C*. If *A* is an operator such that  $(A - \lambda I)^{-1}$  is compact for some  $\lambda$ , then the spectrum of *A* consists of a finite or infinite sequence of eigenvalues. In the infinite case the eigenvalues have no finite accumulation point. Every eigenvalue is of finite multiplicity. If, in addition, *A* is normal, then there is a complete orthonormal set consisting of eigenvectors of *A*.

See Ref. 3, pp. 185–188, 280 for a proof of this theorem. According to this theorem, it follows that if *E* is a bounded set, then the eigenvalues of  $\Delta_d$  form a sequence having no finite limit point, every eigenvalue is of finite multiplicity, and any complex number that is not an eigenvalue is in the resolvent. Furthermore, there is a complete orthonormal set consisting of eigenvectors of  $\Delta_d$ . In the case of one dimension, where *E* is the interval  $0 < x < \pi$  and  $\Delta_d \mathbf{u} = d^2 \mathbf{u}/dx^2$  and functions  $\mathbf{u}$  in the domain  $\Delta_d$  are 0 at x = 0 and  $x = \pi$ , the eigenvalues are the positive integers and the eigenfunctions are the functions  $\sin(nx)$ .

Not every self-adjoint operator has a complete orthonormal set of eigenvectors. The spectral theorem (Theorem 7) is the generalization of the Hilbert–Schmidt theorem to arbitrary self-adjoint operators. It requires a generalization of the notion of a complete orthonormal set called a spectral family. A *projection* P is a self-adjoint operator satisfying  $P^2 = P$  and ||P|| = 1 if  $P \neq 0$ . It can be shown that every projection is given by the orthogonal projection of H on some closed linear subspace, as in Theorem 1. A family of projections  $\{E(r)\}, -\infty < r < \infty$  is called a *spectral family* if (1) E(r)E(s) = E(s)E(r) = E(r) for r < s,  $(2) E(r) \rightarrow E(s)u$  as  $r \rightarrow s-$ , (3) E(r) has a limit as  $r \rightarrow s$ ,  $(4) E(r)u \rightarrow 0$  as  $r \rightarrow -\infty$ , and  $(5) E(r)u \rightarrow u$  as  $r \rightarrow \infty$ . Given a complete orthonormal set that is the eigenvectors of an operator A, the associated spectral family is defined by  $E(r)u = \Sigma \lambda_n \leq r (u, u_n)u_n$ . Using a spectral family a series of the form  $\Sigma^{\infty}{}_{n=1} f(\lambda_n)(u, u_n)u_n$  like the ones in Eqs. (19) and (20) can be generalized to an integral. If f(r) is a complex-valued function defined for real r, then the operator  $\int_{-\infty}^{\infty} f(r) dE(r)u = \int_{-\infty}^{\infty} f(r) d(E(r)u, v)$ ; see Ref. 3, p. 357.

**Theorem 7.** (Spectral Theorem) To every self-adjoint operator A in a Hilbert space H there corresponds a unique spectral family, called the spectral family of A, such that any bounded linear operator that commutes with A commutes with each E(r) and  $A = \int_{-\infty}^{\infty} r \, dE(r)$ .

See Ref. 3, p. 360 for a proof. For any complex-valued function f(r) defined for real r, let  $f(A) = \int_{-\infty}^{\infty} f(r) dE(r)$ . Using the spectral theorem, the formulas of Eq. (19) for the solution to Eq. (15) can be generalized to  $\boldsymbol{u}(t) = e^{tA}\phi$  provided that A is a self-adjoint operator whose spectrum lies entirely to the right of some number C. The formula of Eq. (20) for the solution of Eq. (25) can be generalized to  $\boldsymbol{u}(t) = \cos(\sqrt{-A} t)\phi + (-A)^{-1/2} \sin(\sqrt{-A} t)\psi$  for the same type of operator A.

## **Applications to Quantum Mechanics**

To formulate the quantum mechanical description of a physical system, it is first necessary to have a description of the system in terms of classical Hamiltonian mechanics, so we begin with a brief review of this; for more details see Ref. 13. A physical system is described by position coordinates  $\mathbf{q} = (q_1, \ldots, q_n)$  and their time derivatives  $\dot{\mathbf{q}} = (\dot{q}_1, \ldots, \dot{q}_n) = d\mathbf{q}/dt$ , and the time evolution of the system is described by a system of differential equations. For example, the Cartesian coordinates  $\mathbf{q} = (q_1, q_2, q_3)$  of a single particle of mass m in three dimensions acted on by a force F satisfy *Newton's equations:*  $m d\dot{\mathbf{q}}/dt = F$ . For conservative systems the equations of motion can be put in the form of *Lagrange's equations:* 

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_i} \right) - \frac{\partial L}{\partial q_i} = 0, \qquad i = 1, 2, \dots, n$$
(21)

where the Lagrangian L = T - U is the difference between the kinetic energy T and potential energy U. In the preceding example of a particle in three dimensions, suppose  $F = -\nabla U$ , where U = U(q) depends only on q. Then  $L(q, \dot{q}) = (m|\dot{q}|^2/2) - U(q)$  and Eq. (21) is equivalent to  $m d\dot{q}/dt = F$ . Quantities that are constant in time are called *integrals of motion*. For example, the *energy function*  $h(q, \dot{q}) = \sum_i \dot{q}_i \partial L/\partial \dot{q}_i - L$  is an integral of motion since Eq. (21) implies that dh/dt = 0. If enough integrals of motion can be found so that the relation between q and t can be expressed in terms of known functions, then the system is said to be *completely integrable* or to be a *classical integrable system*.

To obtain Hamilton's equations of motion, one introduces the *conjugate momenta*  $\boldsymbol{p} = (p_1, ..., p_n)$  by  $p_i = \partial L/\partial \dot{q}_i$ . The *Hamiltonian*  $H(\boldsymbol{q}, \boldsymbol{p})$  is the result of replacing  $\dot{\boldsymbol{q}}$  by  $\boldsymbol{p}$  in  $h(\boldsymbol{q}, \dot{\boldsymbol{q}})$ . One can show that Eq. (21) is

equivalent to Hamilton's equations:

$$\frac{dq_i}{dt} = \frac{\partial H(\boldsymbol{q}, \boldsymbol{p})}{\partial p_i}, \quad \frac{dp_i}{dt} = -\frac{\partial H(\boldsymbol{q}, \boldsymbol{p})}{\partial q_i}$$
(22)

For details see Ref. 13, pp. 340–342, and Ref. 14, p. 174. In the preceding example of a single particle, one has  $H(\boldsymbol{q}, \boldsymbol{p}) = (|\boldsymbol{p}|^2/2m) + U(\boldsymbol{q})$ . If  $F = F(\boldsymbol{q}, \boldsymbol{p})$  is some physical quantity, then it follows from Eq. (22) that

$$\frac{dF}{dt} = \{F, H\} \tag{23}$$

where

$$\{F,H\} = \sum_{i} \left( \frac{\partial F}{\partial q_{i}} \frac{\partial H}{\partial p_{i}} - \frac{\partial F}{\partial p_{i}} \frac{\partial H}{\partial q_{i}} \right)$$

is the *Poisson bracket* of *F* and *H*. Thus *F* is conserved if  $\{F, H\} = 0$ . For simplicity, we assume that *L* and *H* are independent of *t*; the preceding equations can be generalized to the case where *L* and *H* depend on *t*. See Ref. 13, pp. 397, 405, and Ref. 14, p. 174 for details.

Quantization is the process of transforming a classical mechanical description of a system into a quantum mechanical one. In quantum mechanics observables such as coordinates, momenta, and energy are represented by self-adjoint operators acting on a Hilbert space H, and the state of the system is described by a vector  $\boldsymbol{u}$  in H having length 1. Observables are usually not subject to precise measurement. Rather there is a probability of measuring a certain value for an observable if the system is in a particular state. The following fundamental principle of quantum mechanics makes this more precise.

**Principle 1 (P1).** If u is the state of the system and A is the operator corresponding to an observable, then the inner product (u, Au) represents the average of a series of measurements of the observable over an ensemble of systems that are all described by the state u.

As we shall see, the only case when a measurement can be precise is when the state is an eigenvector of A, in which case the value of the observable is the corresponding eigenvalue. This is of particular importance for the energy operator  $\mathscr{X}$  whose eigenvalues  $E_n$  and eigenvectors  $\boldsymbol{u}_n$  satisfy

$$\mathcal{H}\boldsymbol{u}_n = \boldsymbol{E}_n \boldsymbol{u}_n \tag{24}$$

The  $u_n$  are called *stationary states* because, as we shall see, they are time invariant. When the system is in a stationary state  $u_n$ , a measurement of the energy results in the corresponding eigenvalue  $E_n$ . The correspondence between the classical mechanical variables and corresponding quantum mechanical operators should satisfy the next two fundamental principles.

**Principle 2** (**P2**). If F(q, p) and G(q, p) are two functions of coordinates and momentum, with corresponding operators *A* and *B*, then the operator corresponding to the Poisson bracket  $\{F, G\}$  of *F* and *G* should be [A, B]/j.

**Principle 3 (P3).** If  $v_1, \ldots, v_n$  are classical variables with corresponding operators  $A_1, \ldots, A_n$  that commute and  $f(v_1, \ldots, v_n)$  is any function of  $v_1, \ldots, v_n$ , then  $f(A_1, \ldots, A_n)$  should be the operator corresponding to  $f(v_1, \ldots, v_n)$ .

Here  $=h/(2\pi)$  and *h* is Planck's constant and [A, B] = AB - BA is the commutator of the operators *A* and *B*. The observables are said to commute if [A, B] = 0. Also, a function of commuting self-adjoint operators can

be defined in a manner similar to the case of one operator, as in the spectral theorem; see Ref. 15, p. 270. One implication of this is the following. Suppose  $\boldsymbol{v}$  is an observable with operator A and let  $f(\boldsymbol{v})$  be the function that is 1 in an interval I and 0 outside the interval. Then  $(\boldsymbol{u}, f(A)\boldsymbol{u})$  coincides with the probability of the value of  $\boldsymbol{v}$  being in the interval I if the state is  $\boldsymbol{u}$ . However, by the spectral theorem this is equal to  $\int_{-\infty}^{\infty} f(\lambda) d(\boldsymbol{u}, E(\lambda)\boldsymbol{u}) = \int_{I} d(\boldsymbol{u}, E(\lambda)\boldsymbol{u})$ , where  $\{E(\lambda)\}$  is the spectral family associated with A. Thus  $d(\boldsymbol{u}, E(\lambda)\boldsymbol{u})$  corresponds to the probability distribution of observing a particular value of the observable when the state is  $\boldsymbol{u}$ ; see Ref. 7, p. 201. Furthermore,  $E(A) = E(A, \boldsymbol{u}) = \int_{-\infty}^{\infty} \lambda d(\boldsymbol{u}, E(\lambda)\boldsymbol{u}) = (\boldsymbol{u}, A\boldsymbol{u})$  is the mean of this distribution. The usual measure of the uncertainty in observations of the values of A is the standard deviation  $\sigma(A)$  given by  $\sigma(A) = \sigma(A, \boldsymbol{u}) = [\int_{-\infty}^{\infty} (\lambda - E(A))^2 d(\boldsymbol{u}, E(\lambda)\boldsymbol{u})]^{1/2} = |(A - E(A)I)\boldsymbol{u}|$ . If  $I = [\lambda, \lambda] = \{\lambda\}$  consists of a single number, then the probability of measuring the value  $\lambda$  is  $(E(\lambda) - E(\lambda^{-}))\boldsymbol{u}$ . This will be 0 unless  $\lambda$  is an eigenvalue. If  $\lambda$  is an eigenvalue, then this becomes  $|P(\lambda)\boldsymbol{u}|^2$ , where  $P(\lambda) = E(\lambda) - E(\lambda^{-})$  is the projection on the eigenspace corresponding to  $\lambda$ . In particular, if  $\boldsymbol{u}$  is an eigenvector corresponding to  $\lambda$ , then the probability of observing the value  $\lambda$  of  $\boldsymbol{v}$  and  $\boldsymbol{v}$  and  $\boldsymbol{v}$  and  $\boldsymbol{v}$  and the probability of an observable earlier, the only possible result of a precise measurement of an observable is one of the eigenvalues of the corresponding operator.

One of the fundamental principles of quantum mechanics, Heisenberg's uncertainty principle, is closely related to this. It says that for two observables *A* and *B* that do not commute it is not possible to find a state where the uncertainty of measuring each of these observables is arbitrarily small. More precisely, for any state  $\boldsymbol{u}$  one has  $2\sigma(A)\sigma(B) \ge |E(AB - BA)|$ ; for a proof see Ref. 7, pp. 230–247.

One implication of property (P2) is the following: Let  $Q_1, ..., Q_n$  and  $P_1, ..., P_n$  denote the operators corresponding to coordinates and momenta. Since  $\{q_i, q_k\} = \{p_i, p_k\} = 0$  and  $\{q_i, p_k\} = \delta_{ik}$ , then

$$[Q_i, Q_k] = [P_i, P_k] = 0, \quad [Q_i, P_k] = j\hbar\delta_{ik}I$$
(25)

where  $\delta_{ik} = 1$  if i = k and  $\delta_{ik} = 0$  if  $i \neq k$ . It follows from the uncertainty principle that for any state  $\boldsymbol{u}$  one has  $\sigma(\boldsymbol{Q}_i)\sigma(\boldsymbol{P}_i) \geq 2$  (i.e., the product of the uncertainties in the measurements of any position and corresponding momentum is at least  $\hbar/2$ ).

There are two formulations of quantum mechanics. One of these, developed by Schrödinger, is called wave mechanics and is the most widely used, and a discussion of it is given first. The other, developed by Heisenberg, is called matrix mechanics and a discussion of it follows. In wave mechanics the operators are time independent and the state variable describing the system varies with time. For a system described by Hamiltonian H(q, p) the state propagates according to *Schrödinger's equation*:

$$j\hbar \frac{d\boldsymbol{u}}{dt} = \mathscr{H}\boldsymbol{u} \tag{26}$$

where  $\mathcal{H} = H(Q, P)$  is the energy operator corresponding to H(q, p). This is an equation of the form of Eq. (15) with  $A = -j\mathcal{H}/$ . Using the spectral theorem, one can construct the solution to this differential equation as

$$\boldsymbol{u}(t) = e^{-j\mathcal{H}t/\hbar}\boldsymbol{u}(0) = \int_{-\infty}^{\infty} e^{-j\lambda t/\hbar} d\boldsymbol{E}(\lambda)\boldsymbol{u}(0)$$
(27)

where u(0) is the state when t = 0 and  $\{E(\lambda)\}$  is the spectral family for  $\mathscr{H}$ . If the eigenvectors of  $\mathscr{H}$  form a complete orthonormal set, then Eq. (27) takes the form similar to Eq. (18); that is,

$$\boldsymbol{u}(t) = \sum_{n} (\boldsymbol{u}(0), \boldsymbol{u}_{n}) e^{-j\lambda_{n}t/\hbar} \boldsymbol{u}_{n}$$
(28)

In the Schrödinger formulation the standard choice of the Hilbert space is  $H = L^2(\mathbb{R}^n)$  with

$$(Q_i \boldsymbol{u})(\boldsymbol{x}) = x_i \boldsymbol{u}(\boldsymbol{x}) \qquad P_i \boldsymbol{u} = -j\hbar \frac{\partial \boldsymbol{u}}{\partial x_i}$$
(29)

which satisfy Eq. (25). In this case one can show that  $E(\lambda, Q_i)$  is given by  $E(\lambda, Q_i)u(x) = u(x)$  for  $x_i \leq \lambda$  and  $E(\lambda, Q_i)u(x) = 0$  for  $x_i > \lambda$ ; see Ref. 7, p. 131. From this it follows that  $|u(x)|^2$  is the probability density function of finding the particle at position x if the state is u. In fact, many authors take this result as one of the basic assumptions of quantum mechanics; see Ref. 7, p. 198, and Ref. 14, p. 25. To get the spectral family for  $P_i$  one can use the fact that the Fourier transform transforms constant coefficient differential operators into multiplication [see Eq. (10)] so that  $P_i = \mathcal{F}^{-1}Q_i \mathcal{F}$ . Since  $\mathcal{F}$  is a unitary operator,  $E(\lambda, P_i/) = \mathcal{F}^{-1}E(\lambda, Q_i)\mathcal{F}$ . Consequently, if u is the state of the system, then  $|\mathcal{F}u(\xi)|^2$  is the probability density of observing a value of  $\xi$  for p/.

When the  $Q_i$  and  $P_i$  are given by Eq. (29), Schrödinger's equation becomes

$$j\hbar \frac{d\boldsymbol{u}}{dt} = \mathbf{H}\left(q, -j\hbar \frac{\partial}{\partial x_i}\right)\boldsymbol{u}$$
(30)

In the case of a single particle in Cartesian coordinates acted on by a potential U(q), this becomes

$$j\hbar \frac{\partial \boldsymbol{u}}{\partial t} = -\frac{\hbar^2}{2m} \Delta \boldsymbol{u} + U(\boldsymbol{q})\boldsymbol{u}$$
(31)

To make the formula of Eq. (27) for the solution more explicit, it is necessary to determine  $E(\lambda, \mathscr{H})$  more precisely. For example, in the case of a free particle where  $U(\mathbf{q}) \equiv 0$ , one has  $\mathscr{H} = \mathscr{F}^{-1}M\mathscr{F}$ , where M is the multiplication operator by  ${}^{2}|\xi|^{2}/2m$ . It follows that  $e^{-j\mathscr{H}/2} = \mathscr{F}^{-1}N\mathscr{F}$ , where N is the multiplication operator by  $\exp(-j|\xi|^{2}t/2m)$ .

For nonzero potentials  $U(\mathbf{q})$  it is sometimes possible to find the eigenvalues and eigenfunctions of  $\mathscr{H}$  in terms of familiar functions. If this is possible, one says that the system is a *quantum integrable system*. One important system that falls into this category is the one-dimensional harmonic oscillator where  $U(\mathbf{q}) = K\mathbf{q}^2/2$ . In this case it can be shown (see Ref. 14, p. 66) that the eigenvalues are  $E_n = (n + 1/2)\hbar\omega$  for n = 0, 1, 2, ... and  $\omega = (K/m)^{1/2}$  and the eigenfunctions are given as  $\mathbf{u}_n(x) = N_n H_n(\alpha x) \exp(-\alpha^2 x^2)$ , where  $N_n = (\alpha/\pi^{1/2} 2^n n!)^{1/2}$ ,  $\alpha = (mK/\hbar^2)^{1/4}$ , and  $H_n(x)$  is the *n*th Hermite polynomial. These eigenfunctions are a complete orthonormal set. It is not always possible to find a complete orthonormal set consisting of eigenvectors of a given self-adjoint operator. However, often when this is not the case it is still possible to find generalized eigenfunctions and an integral representation that plays a similar role.

In Heisenberg's formulation of quantum mechanics the state vector  $\boldsymbol{u}$  describing a system is time independent, and the operators associated with observables vary with time according to the equation

$$\frac{dA}{dt} = \frac{1}{j\hbar} [A, \mathcal{H}]$$

which is just the quantum mechanical analog of Eq. (23) under the correspondence (P2). It can be shown that this is equivalent to Schrodinger's equation; see Ref. 14, pp. 170–171.

# **Other Methods**

In the preceding discussion the solution to the differential equation  $d\boldsymbol{u}/dt = A\boldsymbol{u}$  for a self-adjoint operator A in a Hilbert space was given as  $\boldsymbol{u}(t) = e^{tA}\boldsymbol{u}(0) = \int_{-\infty}^{\infty} e^{tr} dE(r)\boldsymbol{u}(0)$ . This construction involving a spectral integral requires A to be self-adjoint. In 1948 E. Hille and K. Yosida constructed the solution to this equation under weaker assumptions, which allow application to a broader class of differential equations. They assumed Re( $A\boldsymbol{u}, \boldsymbol{u} ) \leq M \|\boldsymbol{u}\|^2$  for some constant M independent of  $\boldsymbol{u}$ , and the equation  $A\boldsymbol{u} - \lambda \boldsymbol{u} = \boldsymbol{f}$  has a solution  $\boldsymbol{u}$  for all  $\boldsymbol{f}$  in H if  $\lambda > M$ . (See Ref. 3, chap. 9; Ref. 8, chap. IX; and Ref. 16, chap. XII for details.) Their work has been extended to more general equations of evolution of the form  $d\boldsymbol{u}/dt = A(t)\boldsymbol{u}(t) + \boldsymbol{f}(t)$ , where the operators A(t) may vary with t; see Ref. 8, chap. XIV.

The length of a vector  $\|\boldsymbol{u}\| = (\boldsymbol{u}, \boldsymbol{u})^{1/2}$  expressed in terms of an inner product is only one example of a norm that gives a measure of the length or size of a vector. There are other useful norms in vector spaces that, when applied to linear operators, yield interesting results concerning the solution of differential equations. This forms the basis of the theory of Banach spaces and locally convex linear topological spaces that generalizes the theory of Hilbert spaces (2,3,4,8).

The preceding discussion has been concerned with the theory of linear operators and applies to linear partial differential equations. There is a corresponding theory of nonlinear operators in Hilbert and Banach spaces that applies to nonlinear partial differential equations. See Ref. 8, chap. XIV, and Ref. 16 for information on this.

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