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Topics from 20^{th} century physics.
An introductory course for students in mathematics

APPENDIX B: HILBERT SPACE

1. INTRODUCTION

Soon after quantum mechanics was introduced, in two different forms, as 'matrix mechanics' by Heisenberg and as 'wave mechanics' by Schrödinger, it was realized that a unified formulation could be given in terms of Hilbert space theory. Such a framework was developed in the early thirties by the mathematician John von Neumann in a series of papers and in his book 'Grundlagen der Quantenmechanik', later translated into English as 'The Mathematical Foundations of Quantum Mechanics'. The mathematics needed for this will be reviewed in this appendix. After the basic definitions of Hilbert space in Chapter 2 a general discussion of Hilbert space operators, bounded and unbounded, follows in Chapter 3. Projection operators, as a necessary tool for the further developments, are introduced in Chapter 4. Chapter 5 contains a discussion of the notions of hermitian symmetry and selfadjointness for unbounded operators. The centre piece of von Neumann's Hilbert space formalism for quantum mechanics is the spectral theorem for general unbounded selfadjoint operators and – with a slight generalization – for commuting systems of such operators. Related to this and only second in importance is his and Stone's theorem about continuous 1-parameter groups of unitary operators. Both theorems will be carefully and rigororously formulated, as natural but far-reaching generalizations to infinite dimensional spaces of well-known properties of finite dimensional linear algebra and matrix theory, the spectral theorem in Chapter 6 and the theorem about 1-parameter groups of unitary operators in Chapter 7. These theorems will not be proved, but will only be made plausible.

2. HILBERT SPACE: DEFINITION AND SOME PROPERTIES

2.1. *The definition of Hilbert space*

Analysis in an infinite dimensional vector space requires a *topology* to give notions of limit and convergence. A means to obtain this is a norm based on an inner product. This leads to a Hilbert space, the simplest and most useful example of an infinite dimensional topological vector space. The Hilbert spaces in quantum theory are always complex, so in this note only complex Hilbert spaces are discussed.

DEFINITION: A *Hilbert space* is a vector space over the complex numbers, provided with an inner product, and complete with respect to the norm given by this inner product.

More in detail: An *inner product* on a (complex) vector space $\mathcal{H}$ is a sesquilinear linear map

$$(\cdot,\cdot) : \mathcal{H} \times \mathcal{H} \to C,$$

i.e. linear in the second variable and conjugate linear in the first variable, which is hermitian symmetric, i.e. has

$$\overline{(\psi_1, \psi_2)} = (\psi_2, \psi_1),$$

for all ψ_1 and ψ_2 in $\mathcal{H}$, with the bar meaning complex conjugation of numbers, and which is positive definite, meaning

$$(\psi, \psi) \geq 0,$$

for all ψ in $\mathcal{H}$, with $(\psi, \psi) = 0$ implying $\psi = 0$. (Note that conjugate linearity of the inner product in the *second* variable is the standard convention in physics).

An inner product defines a *norm* according to $||\psi|| = (\psi, \psi)^{1/2}$; completeness in this norm means that every Cauchy sequence in $\mathcal{H}$ has a limit in $\mathcal{H}$.

DEFINITION: A Hilbert space is called *separable* iff the topology associated with the norm is separable, i.e. has a countable basis of open neighbourhoods.

A separable Hilbert space has a countable orthonormal basis. This is a sequence of vectors $\phi_1, \phi_2, \ldots$, with

$$(\phi_j, \phi_k) = \delta_{jk},$$

for $j, k = 1, 2, \ldots$, and such that an arbitrary vector ψ can written as

$$\psi = \sum_{j=1}^{\infty} a_j \phi_j,$$

with uniquely determined complex coefficients a_j, and the infinite sum absolutely convergent in the sense of the inner product norm.

The Hilbert spaces used in quantum theory are separable, and usually but not always infinite dimensional. In these notes separability – but not infinite dimensionality – will therefore be added to the definition of Hilbert space. All (separable) infinite dimemsional Hilbert spaces are isomorphic, so abstractly speaking there is only one such Hilbert space. There are of course many different concrete realizations of the same 'abstract' Hilbert space. The Hilbert spaces in quantum theory are usually but not always *function spaces*.

2.2. *Two basic examples of Hilbert spaces*

1. l^2: the space of all infinite sequences $a = (a_1, a_2, \ldots)$, such that the series $\sum_{j=1}^{\infty} |a_j|^2$ is absolutely convergent, with inner product

$$(a, b) = \sum_{j=1}^{\infty} a_j^* b_j.$$

One shows fairly easily that this space is indeed complete with respect to the norm $||a|| = (a, a)^{1/2} = (\sum_{j=1}^{\infty} |a_j|^2)^{1/2}$.

2. $L^2(R, dx)$: the space of all measurable functions $\psi(x)$ of the real variable x, square integrable in the sense of Lebèsgue, and with inner product

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

The proof that this space is complete with respect to the norm $||\psi|| = (\psi, \psi)^{1/2}$ is not completely elementary.

2.3. *Direct sum and tensor products of Hilbert spaces*

One can construct new Hilbert spaces from given ones. There are two main procedures for doing this.

a. Direct sums of Hilbert spaces

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be two given Hilbert spaces, with inner product $(\cdot,\cdot)_1$ and $(\cdot,\cdot)_2$. The direct sum $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ is in the first place the direct sum of $\mathcal{H}_1$ and $\mathcal{H}_2$ in the usual vector space sense, i.e. it is the cartesian product $\mathcal{H}_1 \times \mathcal{H}_2$, with the vector space structure given by

$$\{\psi_1, \psi_2\} + \{\phi_1, \phi_2\} = \{\psi_1 + \phi_1, \psi_2 + \phi_2\},$$

and

$$\lambda\{\psi_1, \psi_2\} = \{\lambda\psi_1, \lambda\psi_2\},$$

for all pairs $\{\psi_1, \psi_2\}$ and $\{\phi_1, \phi_2\}$ in $\mathcal{H}_1 \times \mathcal{H}_2$ and all complex numbers λ. This vector space direct sum is a Hilbert space with respect to the inner product

$$(\{\psi_1, \psi_2\}, \{\phi_1, \phi_2\}) = (\psi_1, \phi_1)_1 + (\psi_2, \phi_2)_2.$$

There is also a useful notion of *direct integral* of Hilbert spaces. This will not be discussed here.

b. Tensor product of Hilbert spaces

Let again $\mathcal{H}_1$ and $\mathcal{H}_2$ be two given Hilbert spaces. Let $\mathcal{H}_1 \otimes \mathcal{H}_2$ be the tensor product of $\mathcal{H}_1$ and $\mathcal{H}_2$ in the sense of vector spaces, such as one defines this in linear algebra. It consists of finite sums of elements denoted as $\psi_1 \otimes \psi_2$, $\phi_1 \otimes \phi_2$, etc., with ψ_1, ϕ_1 in $\mathcal{H}_1$ and ψ_2, ϕ_2 in $\mathcal{H}_2$. It has an inner product defined by linear extension of

$$(\psi_1 \otimes \psi_2, \phi_2 \otimes \phi_2) = (\psi_1, \phi_1)_1\,(\psi_2, \phi_2)_2.$$

In the case of infinite dimensional spaces, the usual case, this 'algebraic' tensor product space is not yet complete with respect to the inner product; it can be completed to give a Hilbert space tensor product, denoted as $\mathcal{H}_1 \widehat{\otimes} \mathcal{H}_2$.

2.4. *The inequality of Schwarz*

We have the following very useful inequality:

THEOREM (Schwarz's inequality): Let ψ_1 and ψ_2 be two arbitrary nonzero vectors in a complex Hilbert space $\mathcal{H}$. Then

$$|(\psi_1, \psi_2)| \leq ||\psi_1||\,||\psi_2||.$$

The equality holds if and only if one vector is a scalar multiple of the other.

Proof:

a. Consider for arbitrary real λ and α the obviously nonnegative expression $||\psi_1 + i\lambda e^{i\alpha}\psi_2||^2$. It can be written as

$$\begin{aligned}
&(\psi_1 + i\lambda e^{i\alpha}\psi_2, \psi_1 + i\lambda e^{i\alpha}\psi_2) = \\
&= (\psi_1, \psi_1) + i\lambda e^{i\alpha}(\psi_1, \psi_2) - i\lambda e^{-i\alpha}(\psi_2, \psi_1) + \lambda^2(\psi_2, \psi_2) = \\
&= ||\psi_1|| + i\lambda e^{i\alpha}(\psi_1, \psi_2) - i\lambda e^{-i\alpha}(\psi_1, \psi_2)^* + \lambda^2||\psi_2||.
\end{aligned}$$

The inner product (ψ_1, ψ_2) can be written as $e^{i\beta}|(\psi_1, \psi_2)|$ for some real number β. The above expression can then be written as

$$\begin{aligned}
&||\psi_1||^2 + i\lambda e^{i\alpha}e^{i\beta}|(\psi_1, \psi_2)| - i\lambda e^{-i\alpha}e^{-i\beta}|(\psi_1, \psi_2)| + \lambda^2||\psi_2|| = \\
&= ||\psi_1||^2 - 2\lambda\left(\frac{e^{i(\alpha+\beta)} - e^{-i(\alpha+\beta)}}{2i}\right)|(\psi_1, \psi_2)| + \lambda^2||\psi_2||^2 = \\
&= ||\psi_1||^2 - 2\lambda\sin(\alpha+\beta)\,|(\psi_1, \psi_2)| + \lambda^2||\psi_2||^2.
\end{aligned}$$

It is nonnegative for all real λ and β. We can choose α in such a way that $\sin(\alpha + \beta) = -1$. This gives us that

$$||\psi_1||^2 + 2\lambda|(\psi_1, \psi_2)| + \lambda^2||\psi_2||^2$$

is nonnegative for all real λ. We know from elementary algebra that the nonnegativity of the real quadratic expression $ax^2 + bx + c$ for all x, implies $b^2 - 4ac \leq 0$. We have here such an expression in λ and can therefore conclude that $4|(\psi_1, \psi_2)|^2 - 4||\psi_1||^2\,||\psi_2||^2 \leq 0$, which inequality is rewritten immediately as

$$|(\psi_1, \psi_2)| \leq ||\psi_1||\,||\psi_2||.$$

This was to be proved.

b. Verifying that $\psi_1 = \mu\psi_2$, for a complex number μ, implies $|(\psi_1, \psi_2)| = ||\psi_1||\,||\psi_2||$ is trivial. To prove the implication in the other direction we observe that ψ_2 can be written as $\psi_2 = P_1\psi_2 + (1 - P_1)\psi_2$, with

$$P_1\psi_2 = \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)}\psi_1,$$

In this P_1 is the orthogonal projection of ψ_2 on the 1-dimensional subspace of $\mathcal{H}$ spanned by ψ_1. We calculate

$$\begin{aligned}
&||(1 - P_1)\psi_2||^2 = ((1 - P_1)\psi_2, (1 - P_1)\psi_2) = \\
&= \left(\psi_2 - \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)}\psi_1, \psi_2 - \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)}\psi_1\right) = \\
&= (\psi_2, \psi_2) - \frac{|(\psi_1, \psi_2)|^2}{(\psi_1, \psi_1)} = \\
&= ||\psi_2||^2 - \frac{|(\psi_1, \psi_2)|^2}{||\psi_1||^2}.
\end{aligned}$$

This means that if $|(\psi_1, \psi_2)|$ is equal to $||\psi_1||\,||\psi_2||$ then $||(1-P_1)\psi_2|| = 0$, or $(1-P_1)\psi_2 = 0$, and consequently

$$\psi_2 = P_1\psi_2 = \frac{(\psi_1, \psi_2)}{(\psi_1, \psi_1)}\psi_1,$$

i.e. ψ_1 is a scalar multiple of ψ_1. This was to be proved.

2.5. *More general topological vector spaces*

If a vector space does not have an inner product it still may have a norm. Normed vector spaces that are complete in the topology defined by the norm are called *Banach spaces*. An example of a Banach space which is not a Hilbert space, is the space of all continuous linear transformations of a Hilbert space into it self. Such linear transformations will be discussed in the next chapter. A more general topological vector space which has a metric topology and is complete in this topology is called a Fréchet space. Spaces of this and related type are important in the theory of distributions or 'generalized functions'. In this course we need only Hilbert spaces.

3. OPERATORS IN HILBERT SPACE

3.1. *Operators and their domains*

Linear maps from a Hilbert space $\mathcal{H}$ into itself are called *linear operators* or just *operators*. It turns out that most of the operators that come up naturally in quantum mechanics cannot be defined on all vectors in $\mathcal{H}$, but only on a dense linear subspace of $\mathcal{H}$. This makes working with Hilbert space operators complicated, with many subtle technical points that have to be taken care of.

We consider therefore in general operators that are defined only on dense linear linear subspaces of $\mathcal{H}$. This means that – strictly speaking – an operator has to be specified as a *pair* $(A, \mathcal{D})$, with $\mathcal{D}$ a dense linear subspace, and A a linear map from $\mathcal{D}$ into $\mathcal{H}$. $\mathcal{D}$ is called the *domain* of the operator. Two operators will be considered equal if their domains coincide and if they are the same as maps on this common domain. Simple algebraic manipulations with operators may be complicated and nontrivial. The product AB of two operators A and B, for instance, makes sense only if $Im\,B$, the range of B is a subset of $\mathcal{D}_A$; the sum $A+B$ of two operators is defined if the two domains $\mathcal{D}_A$ and $\mathcal{D}_B$ coincide, or have at least a sufficiently large intersection $\mathcal{D}_A \cap \mathcal{D}_B$.

3.2. *Bounded operators*

We start with operators, for which such problems do not occur, or are inessential and can be removed in a unique way.

DEFINITION: An operator A, on a domain $\mathcal{D}_A$, is called *bounded* iff there exists a (positive) constant C such that $||A\psi|| \leq C||\psi||$, for all ψ in $\mathcal{D}$.

DEFINITION: An operator A' with domain $\mathcal{D}_{A'}$ is called an *extension* of an operator A with domain $\mathcal{D}_A$ if $\mathcal{D}_A$ is a subset of $\mathcal{D}_{A'}$ and $A'\psi = A\psi$, for all ψ in $\mathcal{D}_A$. This is denoted as $A \subseteq A'$.

THEOREM: A bounded operator has a unique extension to all of $\mathcal{H}$.

Proof: Let $(A, \mathcal{D})$ be a bounded operator, and let ψ be a vector in $\mathcal{H}$ not necessarily in $\mathcal{D}$. Because $\mathcal{D}$ is dense in $\mathcal{H}$, there exists a sequense of vectors $\psi_1, \psi_2, \ldots$ that converge to ψ, i.e. have the property that $\lim_{j\to\infty} ||\psi - \psi_j|| = 0$. Because of the boundedness property the sequence $A\psi_1, A\psi_2, \ldots$ is a Cauchy sequence and has therefore a limit ψ' in $\mathcal{H}$. Define $A\psi = \psi'$. This definition is in every way consistent, it is independent of the choice of the sequence $\psi_1, \psi_2, \ldots$, coincides with the given definition of $A\psi$ if ψ is already in $\mathcal{D}$, preserves linearity. etc. The boundednes condition is also preserved, with the same constant C.

Remark: For a bounded operator A the domain $\mathcal{D}$ is irrelevant, because A can be extended to all of $\mathcal{H}$. Speaking of a bounded operator we shall always assume that it has indeed been extended to all of $\mathcal{H}$.

3.3. *Some properties of bounded operators*

As a map from $\mathcal{D}$ or $\mathcal{H}$ into $\mathcal{H}$ a bounded operator is continuous in each point, as one verifies easily. In fact continuity and boundedness are equivalent. Note that a *linear* map is continuous in each point if and and only if it is continuous in 0. For a bounded operator A the set of constants C has an infinimum, in fact a minimum value, which is denoted as $||A||$ and is called the *norm* of A. It can be defined as

$$||A|| = \inf_{\psi \neq 0} \frac{||A\psi||}{||\psi||} = \inf_{||\psi||=1} ||A\psi||.$$

The number $||A||$ has indeed all the properties of a norm: $||A||$ is positive unless A is the operator which is identically 0, it satisfies $||\lambda A|| = |\lambda|\,||A||$ for every complex number λ and the sum $A + B$ of two bounded operators A and B is again bounded with $||A + B|| \leq ||A|| + ||B||$. One also has for products $||AB|| \leq ||A||\,||B||$, as is easily checked. The vector space of bounded operators in $\mathcal{H}$ will be denoted as $\mathcal{B}(\mathcal{H})$; with respect to the operator norm it is a *complete normed space*, i.e. it is a *Banach space*, and in fact a *Banach algebra*. This will not be used.

The operator norm can in an obvious way be used to define *convergence* for sequences of operators.

DEFINITION: A sequence of bounded operators A_j is said to *converge in norm* to a bounded operator A iff $\lim_{j\to\infty} ||A - A_j|| = 0$.

This norm convergence is too strong for many purposes. A weaker notion of convergence, called – strangely enough – strong operator convergence, is often more useful:

DEFINITION: A sequence of bounded operators A_j is said to *converge strongly* to a bounded operator A iff $\lim_{j\to\infty} ||(A - A_j)\psi|| = 0$, for all ψ in $\mathcal{H}$.

It should be remembered that in the applications of Hilbert space theory to quantum theory, most of the important operators are unbounded. This necessitates a more detailed discussion of some of the technical subtleties of unbounded operators.

3.4. *Closed operators*

Let A be a (not necessarily bounded) operator with dense domain $\mathcal{D}$. Consider a Cauchy sequence $\psi_1, \psi_2, \ldots$ in $\mathcal{D}$. Due to the lack of continuity it is not necessary that the corresponding sequence $A\psi_1, A\psi_2, \ldots$ is again a Cauchy sequence.

DEFINITION: An operator A is called *closed* if and only is for every Cauchy sequence $\psi_1, \psi_2, \ldots$ such that $A\psi_1, A\psi_2, \ldots$ is also a Cauchy sequence, the sequence $\psi_1, \psi_2 \ldots$ converges to an element ψ in $\mathcal{D}$ and the sequence $A\psi_1, A\psi_2, \ldots$ converges to $A\psi$.

For an operator A there are two possibilities: A is closed or is closable, i.e. can be uniquely extended to a closed operator, denoted as $\overline{A}$, the *closure* of A, or A has no closed extension. In the present context there is not much use for operators that are not closable.

The notion of closure can be nicely formulated in terms of the *graph* of an operator, the cartesian product $\mathcal{D} \times Im\,A$, with $Im\,A$ the image of A. An operator A is closed if this product is closed as a linear subspace of $\mathcal{H} \times \mathcal{H}$, in the obvious product topology. The closure $\overline{A}$ of A is obtained by taking the topological closure of this subspace. An operator is not closable if the closed subspace obtained in this way is not the graph of an operator.

3.5. *Hermitian adjoints of operators*

For a bounded operator A defined on all of $\mathcal{H}$, the hermitian adjoint operator or just adjoint is defined as an operator A^* for which the action on an arbitrary vector ψ is defined by the inner product relation $(A^*\psi, \phi) = (\psi, A\phi)$, for all ϕ in $\mathcal{H}$. One can show that each bounded operator A^* has a unique bounded hermitian adjoint A^*. One has moreover $(A^*)^* = A$ and $||A^*|| = ||A||$. One also verifies easily that $(AB)^* = B^*A^*$, for A and B bounded.

For an unbounded operator A with dense domain $\mathcal{D}$ the definition of A^* requires more care than in the bounded case. One first defines a domain $\mathcal{D}'$ as

$$\mathcal{D}' \, : \{\psi \in \mathcal{H} \,|\, \exists \psi' : (\psi', \phi) = (\psi, A\phi), \forall \phi \in \mathcal{D}\}.$$

Next A^* is defined on $\mathcal{D}'$ by $A^*\psi = \psi'$. One proves that the new domain $\mathcal{D}'$ is a linear subspace of $\mathcal{H}$, which is dense if and only if the original operator A is closed or closable. In that case A^* is a well defined operator on the dense domain $\mathcal{D}'$, which is in general different from $\mathcal{D}$. It is moreover a *closed* operator and one has $(A^*)^* = \overline{A}$.

4. PROJECTION OPERATORS

4.1. *Definition and simple properties*

There is a class of simple bounded operators, which are important as building blocks for general operator theory:

DEFINITION: A bounded linear operator P in $\mathcal{H}$ is called an *orthogonal projection operator*, or shorter a *projection*, if $P^* = P$ and $P^2 = P$.

There is an obvious geometric intuition behind this algebraic definition, which is made precise by the contents of the following three lemmas:

LEMMA: Denote $Im\, P$, the *image* or *range* of P, as $\mathcal{M}$. This linear subspace is closed and is equal to the set $\{x \in \mathcal{H} \,|\, Px = x\}$.

Proof: $Px = x$ trivially implies that x is in the image of P, so that proves the second statement in one direction. Suppose, for the other direction, that x is in the image of P. This means that there is a y in $\mathcal{H}$ such that $x = Py$. This implies $x = P^2y = P(Py) = Px$. Let $x_1, x_2, \ldots$ be a sequence of vectors in $\mathcal{M}$ which converges to a vector x. The continuity of the operator P gives $Px = \lim_{j\to\infty}(Px_j) = \lim_{j\to\infty} x_j = x$, so $x \in \mathcal{M}$. Because we have a metric topology, this proves that the linear subspace $\mathcal{M}$ is closed. QED.

LEMMA: Denote $Ker\, P$, the *kernel* or *null space* of P, as $\mathcal{M}'$. One has that $\mathcal{H}$ is the direct sum of the closed subspaces $\mathcal{M}$ and $\mathcal{M}'$. (Note that $KerP = Im(1-P)$ and $ImP = Ker(1-P)$)

Proof: Note first that $\mathcal{M}'$ is also a closed subspace because the operator P is continuous. An arbitrary element x in $\mathcal{H}$ can be written as $x = Px + (1-P)x$. The first term is in $\mathcal{M}$, the second in $\mathcal{M}'$. Because $\mathcal{M} \cap \mathcal{M}' = \{0\}$, this proves $\mathcal{H} = \mathcal{M} \oplus \mathcal{M}'$. QED.

LEMMA: The direct sum $\mathcal{H} = \mathcal{M} \oplus \mathcal{M}'$ is an orthogonal direct sum.

Proof: So far we have only used the idempotency relation $P^2 = P$. The operator P also has the property $P^* = P$. This is needed for the proof of this lemma. Take arbitrary x in $\mathcal{M}'$ and x' in $\mathcal{M}'$. Then $(x, x') = (Px, x') = (x, Px') = 0$. QED.

This together shows that $x \mapsto Px$ is indeed an orthogonal projection in the usual geometric sense. Start from an arbitrary closed subspace $\mathcal{M}$, and let $\mathcal{M}'$ be its orthogonal complement, the closed linear subspace of all elements that are orthogonal to $\mathcal{M}$. One can show that $(\mathcal{M}')' = \mathcal{M}$ and that $\mathcal{H}$ is the direct sum of $\mathcal{M}$ and $\mathcal{M}'$. The operator P defined as $Px = x$ on $\mathcal{M}$ and as $Px = 0$ on $\mathcal{M}'$ is clearly a projection, the projection on $\mathcal{M}$.

All this can be summarized as:

There is a one-to-one correspondence between projections and closed subspaces.

THEOREM: The norm $||P||$ of a (nonzero) projection P is equal to 1.

Proof: One can write, for all ψ in $\mathcal{H}$,

$$||\psi||^2 = (\psi, \psi) = (P\psi + (1-P)\psi, P\psi + (1-P)\psi) =$$
$$= (P\psi, P\psi) + ((1-P)\psi, (1-P)\psi) = ||P\psi||^2 + ||(1-P)\psi||^2.$$

This shows that $||P\psi|| \leq ||\psi||$, so $||P|| \leq 1$. There are nonzero vectors ψ in the image of P; for these one has $P\psi = \psi$. This implies that $||P||$ is equal to 1.

4.2. *Partial ordering of projections*

One defines a partial ordering in the set of all projections in $\mathcal{H}$:

DEFINITION: Let P_1 and P_2 be projections in $\mathcal{H}$. The relation $P_1 \leq P_2$ means that P_1 and P_2 commute and that $P_1 P_2 = P_1$.

THEOREM: The relation $P_1 \leq P_2$ is a partial ordering. The following statements are equivalent.

a. $P_1 \leq P_2$.

b. For the closed linear subspaces $\mathcal{M}_1$ and $\mathcal{M}_2$ on which P_1 and E_2 project one has $\mathcal{M}_1 \subset \mathcal{M}_2$.

c. $||P_1\psi|| \leq ||P_2\psi||$, for all ψ in $\mathcal{H}$.

d. $(\psi, P_1\psi) \leq (\psi, P_2\psi)$, for all ψ in $\mathcal{H}$.

Proof: Because $||P_j\psi||^2 = (P_j\psi, P_j\psi) = (\psi, P_j^2\psi) = (\psi, P_j\psi)$, for all ψ in $\mathcal{H}$, there is equivalence between c. and d.

$a \Rightarrow b$: Suppose that $P_1P_2 = P_2P_1 = P_1$. Take ψ in $\mathcal{M}_1$. This means $P_1\psi = \psi$. From this $P_2P_1\psi = \psi \Rightarrow P_2\psi = \psi$, or ψ in $\mathcal{M}_2$. This proves $\mathcal{M}_1 \subset \mathcal{M}_2$.

$b \Rightarrow a$: Suppose that $\mathcal{M}_1 \subset \mathcal{M}_2$. For ψ in $\mathcal{H}$ one has $P_1\psi \in \mathcal{M}_1$ and therefore $P_1\psi \in \mathcal{M}_2$, which implies $P_2P_1\psi = P_1\psi$. This holds for all ψ in $\mathcal{H}$, so $P_2P_1 = P_1$. Taking hermitian adjoint gives $P_1P_2 = P_1$. Together one has $P_1P_2 = P_2P_1 = P_1$

$a \Rightarrow c$: Suppose that $P_1P_2 = P_2P_1 = P_1$. Because the operator norm $||P_1||$ of P_1 is equal to 1, one obtains $||P_1\psi|| = ||P_1P_2\psi|| \leq ||P_2\psi||$, for all ψ in $\mathcal{H}$.

$c \Rightarrow b$: Suppose $||P_1\psi|| \leq ||P_2\psi||$, for all ψ in $\mathcal{H}$. For a ψ in $\mathcal{M}_1$ this becomes $||\psi|| \leq ||P_2\psi||$. One has also $||P_2\psi|| \leq ||\psi||$. Together this gives $P_2\psi|| = ||\psi||$. A simple calculation gives then for the complementary projection

$$||(1-P_2)\psi||^2 = ((1-P_2)\psi, (1-P_2)\psi) = ||\psi||^2 - ||P_2\psi||^2 = 0,$$

which implies $(1-P_2)\psi = 0$ or $P_2\psi = \psi$, i.e. $\psi \in \mathcal{M}_2$.

All this together proves the proposition.

Remark: In the set of all projections there is a 'smallest' and a 'largest' projection: the two trivial projections, $P = 0$ and $P = 1$, corresponding with the trivial subspaces $\mathcal{M} = \{0\}$ and $\mathcal{M} = \mathcal{H}$.

Remark: There is a notion of 'complement' in the set of projections: if P is the projection on $\mathcal{M}$ then the complementary projection $1 - P$ is the projection on the orthogonal complement $\mathcal{M}'$.

5. SYMMETRIC AND SELFADJOINT OPERATORS

5.1. *Introductory remarks*

In standard text books on quantum mechanics a central role is played by what is called 'hermitian operators'. They represent physical observables and are assumed to have complete orthormal bases of eigenvectors, with real eigenvalues interpreted as the possible results of measurements. This is a generalization of what is known of finite dimensional hermitian matrices to the case of operators in Hilbert space. It is intuitively appealing but the actual mathematical situation is more complicated. This is due to the fact that most observables in quantum theory are represented by *unbounded operators*, and that even for bounded operators there is the possibility of *continuous spectrum* in addition to discrete eigenvalues. We therefore need a more refined notion: that of selfadjointness. Observables in quantum theory are described by *selfadjoint* operators. We first define a notion that is weaker in general, that of a symmetric operator.

5.2. *Symmetric operators*

DEFINITION: An operator A with dense domain of definition $\mathcal{D}_A$, is called symmetric iff $(\psi_1, A\psi_2) = (A\psi_1, \psi_2)$, for all ψ_1 and ψ_2 in $\mathcal{D}_A$.

An operator A has a hermitian adjoint A^*, with domain $\mathcal{D}_{A^*}$, as was discussed in 3.5. This definition says that A is symmetric if the domain $\mathcal{D}_A$ is a subset of the domain $\mathcal{D}_{A^*}$ and $A = A^*$ on $\mathcal{D}_A$, or, in the terminology introduced in 3.2, A^* is an extension of A. It is easy to verify whether a given operator, for instance a differential operator, is symmetric. This property is however too weak, not good enough for quantum theory; we want $A = A^*$ instead of $A \subseteq A^*$, i.e. with *equality of domains*.

5.3. *Selfadjoint operators*

DEFINITION: An operator A with dense domain $\mathcal{D}$ is called *selfadjoint* iff for a vector ψ_1 in $\mathcal{H}$ the existence of a ψ_1' with $(\psi_1, A\psi_2) = (\psi_1', \psi_2)$, for all ψ_2 in $\mathcal{D}_A$, implies that ψ_1 is in $\mathcal{D}_A$ and $A\psi_1 = \psi_1'$.

Note that selfadjointnessof A implies symmetry, as one sees by taking ψ_1 in $\mathcal{D}_A$. The definition can be simply stated as $A = A^*$, with the understanding that this equality implies equality of domains. For a bounded operator the definitions of symmetry and selfadjointness clearly coincide. In that case one may fall back on the notion of hermicity as it is used in the physics text books.

5.4. *From symmetry to selfadjointness*

An operator may be symmetric but not selfadjoint. This is sometimes a trivial problem that can be removed. For a densily defined operator A its hermitian adjoint is closed. Therefore a symmetric operator that is not closed cannot be selfadjoint. Closing A is extending it to an operator $\overline{A}$ with domain $\mathcal{D}_{\overline{A}} \supset \mathcal{D}_A$. One can check that the closure of a symmetric operator is again symmetric.

Note also that in general $A \subseteq B$ implies $A^* \subseteq A^*$, i.e. $\mathcal{D}_{B^*} \subset \mathcal{D}_{A^*}$. Extending the symmetric operator A to its closure may close the gap between the domain of the operator and of its hermitian adjoint, giving a selfadjoint operator. A symmetric operator A on a domain $\mathcal{D}_A$ for which this happens is called *essentially selfadjoint* on $\mathcal{D}_A$. Examples are the multplication and differentiation operators used in quantum mechanics, $X : \psi(x) \mapsto x\psi(x)$ and $D : \psi(x) \mapsto -i\frac{d}{dx}\psi(x)$ in $\mathcal{H} = L^2(R^1, dx)$. They are both essentially selfadjoint on the domain $\mathcal{D} = \mathcal{S}(R^1)$, the space of Schwartz functions.

It may happen that a symmetric operator is after closure still not selfadjoint. There is a standard method (by 'Cayley transforms') by which one can try to find selfadjoint extensions. Two outcomes are possible:

a. The operator may have a selfadjoint extension. In that case there is more than one. This happens sometime for certain quantum mechanical systems. The different extensions describe different physical situations. An example is discussed in the main text of this course.

b. There are no selfadjoint extensions; the procedure comes to a halt, with the result still symmetric but not selfadjoint. In that case the operator is useless for quantum mechanics. An example is the differentiation operator $D : \psi(x) \mapsto -i\frac{d}{dx}\psi(x)$, for $\mathcal{H}$ the square integrable functions on the interval $[0, +\infty)$. A second example is the operator $DX^3 + X^3D$ on $L^2(R^1, dx)$. Both operators are symmetric, and for both no domain of definiton exists on which they are selfadjoint.

For selfadjoint operators there exist in a generalized sense complete orthonormal bases of eigenvectors with real eigenvalues. This is stated by the *spectral theorem*, a theorem which is valid for selfadjoint but not for symmetric operators. It is of central importance for quantum theory and will be discussed in the next chapter.

6. THE SPECTRAL THEOREM

6.1. *The spectral theorem in finite dimensional Hilbert space*

A hermitian symmetric $n \times n$ matrix $\{A_{jk}\}$ can be brought in diagonal form by means of a transformation with a suitable unitary matrix $\{U_{jp}\}$ according to

$$\sum_{p,q=1}^{n} U_{jp} A_{pq} U^{-1}_{qk} = \delta_{jk}\alpha_j,$$

with the α_j real numbers, the *characeristic values* or *eigenvalues* of the matrix $\{A_{jk}\}$. This is a central result from standard linear algebra. A more intrinsic formulation says that a selfadjoint operator A in an n-dimensional Hilbert space $\mathcal{H}$, has an orthonormal basis of eigenvectors with real eigenvalues, i.e. a system of vectors $\phi_1, \ldots, \phi_n$, with $(\phi_j, \phi_k) = \delta_{jk}$, for $j, k = 1, \ldots, n$, and an unique expansion $\psi = \sum_{j=1}^{n} c_j\phi_j$ for each ψ in $\mathcal{H}$, together with real numbers $\alpha_1, \ldots, n$ such that $A\phi_j = \alpha_j\phi_j$, for $j = 1, \ldots, n$. If the eigenvalues α_j are degenerate this orthonormal basis is not uniquely determined; even in the nondegenerate case there is still the freedom of multiplying each ϕ_j by a phase factor. To eliminate this nonuniqeness from the formulation it is better to consider eigenvalues which are all different, $\alpha_1 < \alpha_2 < \ldots < \alpha_p$, with $p \leq n$, and instead of eigenvectors the eigenspaces $\mathcal{M}_j$, for each eigenvalue α_j. Let P_j be the orthogonal projections on the $\mathcal{M}_j$. One has $P_j P_k = P_k P_j = 0$ and $\sum_{j=1,\ldots,p} P_j = 1$. The statement about eigenvalues and eigenvectors, or rather eigenspaces, can then be formulated as a theorem:

THEOREM: A selfadjoint operator A in a finite dimensional Hilbert space $\mathcal{H}$ has a unique set of real numbers $\alpha_1 < \alpha_2 < \ldots < \alpha_p$, together with a unique system of mutually orthogonal projection operators $P_1, P_2, \ldots, P_p$ with $P_j P_k = P_k P_j = 0$ and $P_1 + \ldots + P_p = 1$, for $j, k = 1, \ldots, p$, such that

$$A = \sum_{j=1,\ldots,p} \alpha_j P_j.$$

The set of eigen values $\alpha_1, \ldots, \alpha_p$ is called the *spectrum* of the operator A; the theorem is therefore called the *spectral theorem* for a selfadjoint operator in a finite dimensional Hilbert space.

6.2. *The problem of formulating a spectral theorem in infinite dimension*

When $\mathcal{H}$ is infinite dimensional the spectral theorem retains in some cases the same form, apart from summing now from 1 to ∞. An example is the operator $D^2 + X^2 = -\frac{d^2}{dx^2} + x^2$ in $L^2(R^1, dx)$, up to constants a well-known operator from quantum mechanics . It has discrete nondegenerate eigenvalues $\lambda_j = 2j+1$ for $j = 0, 1, \ldots \infty$, and a corresponding complete orthogonal system of eigenvectors $\phi_0, \phi_1, \ldots$. This is however an exception. Consider as a typical example the operator $D = -i\frac{d}{dx}$ itself. It is clealy symmetric on the space $\mathcal{S}(R^1)$ and it is known that it can be uniquely extended to a selfadjoint operator, in the strict sense of the preceding chapter, on the larger domain of functions which are square integrable and differentiable with the derivative again square integrable. It has eigenfunctions $\phi_k(x) = e^{-ikx}$ with eigenvalues k, for each real number k. An arbitrary ψ in $\mathcal{H} = L^2(R^1, dx)$ can be uniquely expanded as $\psi(x) = \int_{-\infty}^{+\infty} c_k \phi_k dk$, with the 'expansion coefficients' c_k the Fourier transform of $\psi(x)$. The selfadjoint operator has eigenfunctions, real eigenvalues and a corresponding eigenfunction expansion. One is tempted to write a continuous version of the formula for the spectral theorem in finite dimensional space, something like

$$D = \int_{-\infty}^{+\infty} k \, dP_k.$$

It is however not clear what the precise meaning of this heuristic formula is. In any case, the eigenfunctions ϕ_k are *not* square integrable, i.e. *not* in $\mathcal{H}$, so what we have is *not* a Hilbert space property, in this form at least. To find a proper we first reformulate the spectral theorem for the finite dimensional case.

6.3. *Spectral resolutions in finite dimensional space*

Let A be again a selfadjoint operator in a finite dimensional Hilbert space $\mathcal{H}$, $\alpha_1 < \ldots < \alpha_p$ its eigenvalues, and $P_1, \ldots, P_p$ the corresponding projections on the eigenspaces $\mathcal{M}_1, \ldots, \mathcal{M}_p$. Define first new operators $E_1, \ldots, E_p$ by $E_j = P_1 + P_2 + \ldots + P_j$, clearly again a system of commuting projection operators, now on the direct sum spaces $\mathcal{N}_j = \mathcal{M}_1 \oplus \mathcal{M}_2 \oplus \ldots \oplus \mathcal{M}_j$, for $j = 1, \ldots, p$. The operators E_j form a finite sequence of projections which is monotone increasing, i.e $E_j < E_{j+1}$, in the sense discussed in section 4.2. The P_j can be recovered from the E_j as $P_j = E_j - E_{j-1}$, for $j = 1, \ldots p$, so the formula for the spectral theorem for the operator A becomes $A = \sum_{j=1}^{p} \alpha_j (E_j - E_{j-1})$. One next converts in a trivial way the finite sequence $E_1, \ldots, E_p$ into an infinite set $\{P_\alpha\}$, depending on a continuous parameter $\alpha \in R$, by defining for each α in the half open interval $[\alpha_j, \alpha_{j+1})$, $j = 1, \ldots, p-1$, the projection operator E_α as E_j and in addition to that $E_\alpha = 0$ for $\alpha < \alpha_1$ and $E_\alpha = 1$ for $\alpha \geq \alpha_p$. The result is an infinite set of commuting projections that is monotone nondecreasing in the parameter $\alpha \in R$, has $\lim_{\alpha \to -\infty} E_\alpha = 0$ and $\lim_{\alpha \to +\infty} E_\alpha = 1$ and is also (by definition) continuous from the right in α. The new 1-parameter system $\{E_\alpha\}$ is completely equivalent to the original sequence $P_1, \ldots P_p$. Note that in the formulation of the properties of the new set nothing remains that would not be meaningful in the infinite dimensional case.

For an arbitrary ψ in $\mathcal{H}$ the function $F_\psi(\alpha) = (\psi, E_\alpha \psi)$ is a step function with a finite number of increasing values, starting at 0 and ending at 1, and as such an elementary example of a right continuous, real, monotone nondecreasing function with $\lim_{\alpha \to -\infty} F_\psi(\alpha) = 0$ and $\lim_{\alpha \to +\infty} F_\psi(\alpha) = 1$. The spectral theorem gives

$$
\begin{aligned}
(\psi, A\psi) &= \sum_{j=1}^{p} \alpha_j \, (\psi, P_j \psi) = \\
&= \sum_{j=1}^{p} \alpha_j (\psi, (E_j - E_{j-1})\psi) = \\
&= \sum_{j=1}^{p} \alpha_j \, (F_\psi(\alpha_{j+1}) - F_\psi(\alpha_j))
\end{aligned}
$$

Monotone functions lead naturally to Stieltjes integrals; because the monotone function $F_\psi(\alpha)$ is a step function, we can trivially write

$$
(\psi, A\psi) = \sum_{j=1}^{p} \alpha_j (\psi, P_j \psi) = \int_{-\infty}^{+\infty} \alpha \, dF_\psi(\alpha) = \int_{-\infty}^{+\infty} \alpha \, d(\psi, E_\alpha \psi).
$$

This holds for every ψ in $\mathcal{H}$, so we can regard it as a definition of the operator-valued Stieltjes integral

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

With this we have obtained a formulation of the spectral theorem for a selfadjoint operator in a finite dimensional Hilbert space which is completely equivalent to the original one and which can be used for the infinite dimensional case.

6.4. *Spectral resolutions in the general case*

Let $\mathcal{H}$ now be a general, i.e. not necessarily finite dimensional Hilbert space.

DEFINITION: A 1-*parameter spectral resolution* or short *spectral resolution*, in $\mathcal{H}$ is a system of commuting projection operators $\{E_\alpha\}$, for $\alpha \in R$, which possesses the following properties:

a. the E_α are monotone nondecreasing, i.e. $E_{\alpha_1} \leq E_{\alpha_2}$, or equivalently, $E_{\alpha_1}E_{\alpha_2} = E_{\alpha_2}E_{\alpha_1} = E_{\alpha_1}$, for $\alpha_1 \leq \alpha_2$,

b. there is continuity from the right, i.e. $\lim_{\alpha\downarrow\alpha_0} E_\alpha = E_{\alpha_0}$, for all α_0 in R,

c. $\lim_{\alpha\to-\infty} E_\alpha = 0$ and $\lim_{\alpha\to+\infty} E_\alpha = 1$.

The continuity in c and the limits in d are in the sense of strong operator convergence. The choice of continuity from the right instead of from the left is a convention, which agrees with a similar convention in Appendix C.

A spectral resolution has a property which is very important for quantum theory:

THEOREM: For every ψ in $\mathcal{H}$ with $||\psi|| = 1$, the function F defined as $F(\alpha) = (\psi, E_\alpha\psi)$ is real, monotone nondecreasing, continuous from the right, and has $\lim_{\alpha\to-\infty} = 0$ and $\lim_{\alpha\to+\infty} = 1$. Note that these are precisely the properties that in probability theory characterize a *distribution function* of a stochastic variable. (See Appendix C).

Proof: Follows immediately from the definition of spectral resolution and from the general properties of projections as discussed in Chapter 4.

6.5. *The spectral theorem for a general selfadjoint operator*

Let $\{E_\alpha\}$ be a general spectral resolution as defined in the preceding section. It can be shown that the collection of vectors ψ for which the Stieltjes integral $\int_{-\infty}^{+\infty} \alpha\, d(\psi, E_\alpha\psi)$ converges is a dense linear subspace of $\mathcal{H}$ and that the integral defines the action of a selfadjoint operator on this domain. Conversely every selfadjoint operator A in $\mathcal{H}$ possesses a unique spectral resolution from which the action of the operator can be recovered in this way. This is the *spectral theorem for general selfadjoint operators*:

THEOREM: A selfadjoint operator A in a Hilbert space $\mathcal{H}$ possesses a unique spectral resolution $\{E_\alpha\}$ such that

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

meaning that for each ψ in the domain $\mathcal{D}_A$ one has the convergent Stieltjes integral

$$(\psi, A\psi) = \int_{-\infty}^{+\infty} \alpha\, d(\psi, E_\alpha\psi).$$

In fact, ψ is in the domain of A if and only if this integral converges.

The full proof of this theorem is nonelementary and cannot be given here. Note that in this situation the Riemann-Stieltjes and Lebèsgue-Stieltjes integrals coincide.

6.6. *Examples*

a. *The operator* X . It can be shown that this operator is essentially selfadjoint on $\mathcal{S}(R^1)$ and selfadjoint on the subspace of all square integrable functions $\psi(x)$ for which also $x\psi(x)$ is square integrable. The operator X has no eigenfunctions, not even eigenfunctions that are not square integrable like in the case of D. (In physics text books one uses sometimes the *Dirac δ-function* $\delta_{x_0}(x) = \delta(x - x_0)$, for an arbitrary real number x_0, as an eigenfunction of X with eigenvalue x_0. The Dirac δ-function is extremely usful as a heuristic tool for all sorts of formula manipulations. In this course the use of δ-functions and the like will be avoided, because we do not want to discuss its mathematical justification, the theory of 'generalized functions' or distributions in the sense of Laurent Schwartz.) The spectral projections of X are simply given as

$$(E_{x_0}\psi)(x) = \psi(x),$$

for $x < x_0$ and

$$(E_{x_0}\psi)(x) = 0,$$

for $x \geq x_0$. Note that $\leq$ and $>$ in this definition instead of $<$ and $\geq$ would not change E_α; this spectral resolution is continuous both from the left and the right. Note also that

$$(\psi, E_{x_0}\psi) = \int_{-\infty}^{x_0} ||\psi(x)||^2 dx.$$

This means that we can write

$$d(\psi, E_x\psi) = ||\psi(x)||^2 \, dx$$

and that we are therefore, in the context of probability theory, in the special case of absolute continuity, which means that the distribution function $F_\psi(x) = (\psi, E_x\psi)$ can be represented by a *probability density* $\rho(x) = ||\psi(x)||^2$. (See Appendix C, section 3.2.)

b. *The operator* D: The operator D can be obtained from X as $D = FXF^{-1}$, with F the Fourier transform, here seen as the bounded linear operator defined on $\mathcal{S}(R^1)$ by the integral formula

$$(F\psi)(k) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{+\infty} \psi(x) e^{-ikx} dx,$$

and then extended to an invertible operator on all of $\mathcal{H}$ by continuity. (F is in fact a *unitary* operator, an important notion that will be discussed later). The spectral resolution of D is the Fourier transform of the spectral resolution of X, so it is given in terms of Fourier transforms $F\psi$ as:

$$(E_{k_0} F\psi)(k) = (F\psi)(k),$$

for $k < k_0$ and

$$(E_{k_0} F\psi)(k) = 0,$$

for $k \geq k_0$. The operator D has as eigenfunctions the plane waves $\phi_k(x) = e^{ikx}$, which are not square integrable and are therefore not proper eigenvectors in the Hilbert space sense, as we already discussed. Note in this context that, formally at least, plane wave functions and Dirac δ-functions are each others Fourier transforms.

6.7. *The spectrum of a selfadjoint operator*

We have discussed the generalization of the eigenvalue and and eigenvector problem for hermitian matrices to selfadjoint operators in Hilbert space. Eigenvectors became first eigenspaces and then projections in spectral resolutions. The set of eigenvalues of a hermitean matrix becomes the *spectrum* of a selfadjoint operator. Such operators still may have eigenvalues in the usual sense, i.e. numbers α such that there exist a nonzero vector ψ with $A\psi = \alpha\psi$, but the notion of spectrum is more general:

DEFINITION: The *spectrum* of a densely defined closed operator A in the Hilbert space $\mathcal{H}$ is the set of complex numbers λ such that $A - \lambda I$, as a map from the domain of A onto its range, is not invertible.

For a finite dimensional $\mathcal{H}$ the operator $A - \lambda I$ is not invertible if and only if the nullspace of $A - \lambda I$ is non trivial, i.e. if there is a nonzero vector ψ such that $(A - \lambda I)\psi = 0$, or $A\psi = \lambda\psi$. This shows that in the finite dimensional case the spectrum is just the set of *eigenvalues* of A. In the infinite dimensional case the situation is more complicated. It is possible that an operator, even a bounded operator, has a trivial null space and is still not invertible. If that happens for $A - \lambda I$ the number λ belongs to the spectrum, but it is *not* an eigenvalue.

One can show that the spectrum is a closed subset of the complex plane; for a selfadjoint operator it consists of *real numbers*. There is an equivalent description of the spectrum of a selfadjoint operator A in terms of its spectral resolution $\{E_\alpha\}$. We state this without proof as a theorem:

THEOREM: The real number α belongs to the spectrum of A iff for every positive ε the difference $E_{\alpha+\varepsilon} - E_{\alpha-\varepsilon}$ is nonzero. If $\lim_{\varepsilon\downarrow 0}(E_{\alpha+\varepsilon} - E_{\alpha-\varepsilon})$, which in any case exists, is nonzero, then α is moreover an eigenvalue. The eigenvalues form a discrete set; the remainder of the spectrum is by definition the continuous spectrum.

The spectrum of A can also be described in terms of the distribution functions $F_\psi(\alpha) = (\psi, E_\alpha\psi)$, for all possible unit vectors ψ. This shows that there is a close relation between the spectrum of A and the support of the distributions

F_ψ, as defined in Section 3.2 of Appendix C, and through this with the support of the probability measures on the real line induced by the F_ψ. This is of central important for the application to quantum theory.

The spectrum of the operators D and X are purely continuous and consist of the real line. The spectrum of the operator $D^2 + X^2$ is purely discrete and consists of the numbers $2n+1$, for $n = 0, 1, \ldots$.

6.8. *A functional calculus for selfadjoint operators*

Because of domain problems simple algebraic manipulations with unbounded operators may cause problems. The domain of the polynomial $\sum_{p=0}^{n} c_p A^p$ in a densely defined operator A is in general smaller than the domain of A itself; in fact it may be no longer dense. In the case of an unbounded selfadjoint operator there is however a general *functional calculus*, which avoids such problems. It is based on the spectral theorem and allows us to give a precise meaning not just to arbitrary polynomials, but to a wide class of more general functions of a selfadjoint operator. One can prove the following statement:

THEOREM: Let A be a selfadjoint operator in the Hilbert space $\mathcal{H}$ and f a real-valued function defined on the real line, which is continuous or a pointwise limit of continuous functions. Let $\{E_\alpha\}$ be the spectral resolution of A. The operator $f(A)$ defined by

$$f(A) = \int_{-\infty}^{+\infty} f(\alpha)\, dE_\alpha$$

is selfsadjoint, or more precisely:

a. The vectors ψ in $\mathcal{H}$, for which the Stieltjes integral

$$\int_{-\infty}^{+\infty} f(\alpha)\, d(\psi, E_\alpha \psi),$$

is convergent, form a dense subspace $\mathcal{D}_{f(A)}$.

b. The operator $f(A)$, defined on all vectors ψ in $\mathcal{D}_{f(A)}$ by

$$(\psi, f(A)\psi) = \int_{-\infty}^{+\infty} f(\alpha)\, d(\psi, E_\alpha \psi),$$

is selfadjoint.

6.9. *Systems of commuting selfadjoint operators*

It is well-known that two commuting selfadjoint operators A and B in a finite dimensional Hilbert space $\mathcal{H}$ have an orthonormal base consisting of common eigenvectors, in general not unique, or in a more intrinsic formulation, a unique system of common eigenspaces. Let the operator A have eigenvalues $\alpha_1 < \ldots < \alpha_p$, eigenspaces $\mathcal{M}_1^A, \ldots, \mathcal{M}_p^A$ with projection operators $P_1^A, \ldots, P_p^A$ and similarly B eigenvalues $\beta_1 < \ldots < \beta_q$, eigenspaces $\mathcal{M}_1^B, \ldots, \mathcal{M}_q^B$ and projections

$P_1^B, \dots, P_q^B$. The common eigenspaces of A and B are then $\mathcal{M}_{jk}^{AB} = \mathcal{M}_j^A \cap \mathcal{M}_k^B$, with projections $P_{jk}^{AB} = P_j^A P_k^B$, for $j = 1, \dots, p$ and $K = 1, \dots, q$. To prepare for the infinite dimensional situation one may introduce first a set of projection operators $E_{jk}^{AB} = \sum_{s \leq j; t \leq k} P_{st}^{AB}$ on the subspaces $\mathcal{N}_{jk}^{AB} = \oplus_{s \leq j; t \leq k} \mathcal{M}_{st}^{AB}$, and then convert this in a set $\{E_{\alpha\beta}^{AB}\}$ depending on two continuous real variables α and β, in the same way as this was done for the case of a single operator A. All this can be extended immediately to the case of a finite number of commuting selfadjoint operators. With this the stage is set for the discussion of systems of commuting selfadjoint operators in an *infinite dimensional* Hilbert space. We start with a general definition of the notion of spectral resolution.

DEFINITION: A n-parameter spectral resolution is a system $\{E_{\alpha_1 \dots \alpha_n}\}$ of commuting projection operators, for α_j in R, $j = 1, \dots, n$, with the properties:

a. the system is monotone nondecreasing in each variable α_j separately,

b. there is continuity from the right in each α_j separately,

c. $\lim_{\alpha_1 \to -\infty, \dots, \alpha_n \to -\infty} E_{\alpha_1 \dots \alpha_n} = 0$ and $\lim_{\alpha_1 \to +\infty, \dots, \alpha_n \to +\infty} E_{\alpha_1 \dots \alpha_n} = 1$.

One easily shows that taking the limit α_j to 1 for all variables α_j except one gives a 1-variable spectral resolution in the remaining parameter.

The notion of n-parameter spectral resolution forms the basis for a generalization of the spectral theorem from one operator to a finite system of commuting selfadjoint operators. Let $A_1, \dots, A_n$ be a system of commuting selfadjoint operators. Note that 'A_j commutes with A_k' means that all spectral projections of A_j commute with all spectral projections of A_k; the definition $[A_j, A_k] = A_j A_k - A_k A_j = 0$ would be unsatisfactory because of obvious domain problems.

THEOREM: A system of commuting selfadjoint operators $A_1, \dots, A_n$ possesses a unique n-parameter spectral resolution $\{E_{\alpha_1 \dots \alpha_n}\}$ such that, for $j = 1, \dots n$,

$$A_j = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} \alpha_j \, dE_{\alpha_1 \dots \alpha_n},$$

meaning that for each ψ in the domain of A_j one has the covergent Stieltjes integral

$$(\psi, A_j \psi) = \int_{-\infty}^{+\infty} \dots \int_{-\infty}^{+\infty} \alpha_j \, d(\psi, E_{\alpha_1 \dots \alpha_n} \psi).$$

The n-fold integral in this theorem reduces immediately to a one dimensional integral over the 1-parameter spectral resolution E_{α_1}, so in this sense this theorem is not much of a generalization of the spectral theorem for a single operator. The value of the theorem lies however in the possibility of applying it to general expressions in the n operators. There is an obvious extension of the functional calculus discussed in Section 6.8 to *systems* of selfadjoint operators. One has the following theorem:

THEOREM: Let $A_1, \ldots, A_n$ be a system of commuting selfadjoint operators, and f a real-valued function on R^n, which is continuous or a pointwise limit of continuous functions. Let $\{E_{\alpha_1 \ldots \alpha_n}\}$ be the n-parameter spectral resolution of this system. The vectors ψ in $\mathcal{H}$, for which the Stieltjes integral

$$\int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} f(\alpha_1, \ldots, \alpha_n)\, d(\psi, E_{\alpha_1 \ldots \alpha_n} \psi).$$

converges, form the domain of a selfadjoint operator, denoted as $f(A_1, \ldots, A_n)$, and given on this domain by the integral

$$(\psi, f(A_1 \ldots A_n)\psi) = \int_{-\infty}^{+\infty} \cdots \int_{-\infty}^{+\infty} f(\alpha_1, \ldots, \alpha_n)\, (\psi, E_{\alpha_1 \ldots \alpha_n} \psi).$$

Important for its application to quantum theory is the following theorem:

THEOREM: Let $\{E_{\alpha_1 \ldots \alpha_n}\}$ be an n-parameter spectral resolution and ψ a unit vector in $\mathcal{H}$. The function

$$F_\psi(\alpha_1, \ldots, \alpha_n) = (\psi, E_{\alpha_1 \ldots \alpha_n} \psi)$$

is an *n-variable distribution function* in the sense of probability theory, and determines as such a probability measure on R^n. (See for this Appendix C, Section 3.3.)

7. GROUPS OF UNITARY OPERATORS

7.1. *Unitary operators*

The automorphisms of a Hilbert space $\mathcal{H}$ are the unitary operators, the invertible linear maps that leave the inner product $(\cdot, \cdot)$ invariant. Various slightly different but equivalent definitions can be given:

DEFINITION: A linear operator U in $\mathcal{H}$ is called *unitary* if one of the following equivalent conditions hold:

a. U is invertible and $(U\psi_1, U\psi_2) = (\psi_1, \psi_2)$, for all ψ_1 and ψ_2 in $\mathcal{H}$,

b. U is invertible and $||U\psi|| = ||\psi||$, for all ψ in $\mathcal{H}$,

c. U is invertible and $U^*U = 1$,

d. U is invertible and $UU^* = 1$,

e. $U^*U = UU^* = 1$.

The proof that these conditions are equivalent is elementary and is left to the reader. Note that in the finite dimensional case invertibility follows from the invariance of the inner product or the norm, or separably from $U^*U = 1$ or $UU^* = 1$. In an infinite dimensional Hilbert space an operator U can be *isometric*, i.e. have $||U\psi|| = ||\psi||$, for all ψ, without being unitary.

Example: Shift operators. Choose an orthonormal basis $\phi_1, \phi_2, \ldots$ in $\mathcal{H}$. Define the operator U by $U\phi_j = \phi_{j+1}$, for $j = 1, 2 \ldots$. This operator is clearly isometric but not invertible; its range is the subspace of codimension 1 spanned by the vectors $\phi_2, \phi_3, \ldots$.

Unitary operators are obviously bounded with operator norm equal to 1. They form a group, which may be denoted as $\mathcal{U}(\mathcal{H})$.

7.2. 1-*parameter groups of unitary operators*

Consider a continuous complex-valued function $f : R \to C$ with the property that $f(t_1 + t_2) = f(t_1)f(t_2)$, for all t_1 and t_2 in R. One can show, using elementary analysis, that in this case continuity implies differentiability, and that moreover f has the form $f(t) = e^{ita}$, for some complex number a. If the image of the function f is contained in the unit circle this number a is real. Conversely, each complex number a gives an exponential function $f(t) = e^{ita}$, defined, for instance, as the sum of the absolutely convergent power series $f(ta) = \sum_{n=0}^{\infty} \frac{1}{n!}(ita)^n$.

This idea can be generalized from complex-valued functions to operator-valued functions in Hilbert space. One has the following theorem: a function $F : R \to \mathcal{B}(\mathcal{H})$, continuous in the *operator norm* topology, and with the property $F(t_1 + t_2) = F(t_1)F(t_2)$, for all t_1 and t_2 in R, is an exponential function $F(t) = e^{itA}$, for some *bounded* operator A, with e^{itA} defined as the the sum of the power series $\sum_{n=0}^{\infty} \frac{1}{n!}(itA)^n$, now absolutely convergent in the operator norm. If the operators $F(t)$ are unitary then A is selfadjoint. Conversely, a bounded operator A gives a function $F(t) = e^{itA} \equiv \sum_{n=0}^{\infty} \frac{1}{n!}(itA)^n$, with the power series absolutely convergent in the operator norm. The proof is an easy generalization in which arguments using absolute values of complex numbers are replaced by similar arguments using operator norms.

For applications in quantum theory this theorem is too crude; the operators that are exponentiated there, like the Hamiltonian operator H, are usually *unbounded*. For an unbounded operator A, with dense domain of definition $\mathcal{D}_A$, the simple definition of e^{itA} as the sum of the series $1 + itA + \frac{1}{2}(itA)^2 + \ldots$ runs into obvious domain problems and therefore does not make sense in general. However, for the particular case in which A is selfadjoint there is again a one-to-one correspondence between 'generators' A and *unitary* 'exponential functions' $F(t)$. This is a nontrivial result. To formulate it properly, we first give in a more formal fashion the definition of the notion of a strongly continous 1-parameter groups of unitary operators.

DEFINITION: A collection $\{U(t)\}_{t \in R^1}$ of unitary groups is called a a *strongly continuous* 1-*parameter group of unitary operators*, or just 1-*parameter group of unitary operators*, if

a. $U(t_1)U(t_2) = U(t_1 + t_2)$, for all real numbers t_1 and t_2,

b. the vector-valued function $U(t)\psi$ is continuous for all ψ in $\mathcal{H}$, in the strong operator topology, as defined in 3.3, i.e. in terms of the vector-valued functions $U(t)\psi$, for all ψ in $\mathcal{H}$.

A direct consequence of the definition is that all the $U(t)$ commute, that $U(0)$ is the unit operator and that $U(-t)$ is the inverse of $U(t)$. Note that one can show that it is in fact sufficient to assume that $U(t)\psi$ is continuous for $t = 0$, for all ψ in $\mathcal{H}$.

THEOREM (Stone - von Neumann): Let $\{U(t)\}_{t \in R^1}$ be a strongly continuous 1-parameter group of unitary operators. The vectors ψ in $\mathcal{H}$, for which the limit

$$\lim_{t \to 0} -i \, \frac{U(t) - 1}{t} \psi$$

exists, form a dense linear subspace $\mathcal{D}$ of $\mathcal{H}$. This limit defines an operator A, which is selfadjoint on $\mathcal{D}$. The operator A is called the *infinitesimal generator* of the 1-parameter group.

The proof of this theorem, a nontrivial exercise in standard Hilbert space theory, will not be given here.

This theorem is complemented by the statement that the operator-valued function $t \mapsto U(t)$ can in an appropriate sense be written as the exponential function $U(t) = e^{itA}$, a statement which is based on the spectral theorem for selfadjoint operators, in particular on the functional calculus discussed in 6.8. For this we have the following theorem:

THEOREM: Let A be a selfadjoint operator, with spectral resolution $\{E_\alpha\}_{\alpha \in R^1}$. Then the operators defined by

$$U(t) = \int_{-\infty}^{+\infty} e^{it\alpha} \, dE_\alpha,$$

or, more explicitly,

$$(\psi, U(t)\psi) = \int_{-\infty}^{+\infty} e^{it\alpha} \, d(\psi, E_\alpha \psi),$$

for all ψ in $\mathcal{H}$, form a 1-parameter group of unitary operators with A as infinitesimal generator.

These two theorems together give the one-to-one correspondence between selfadjoint operators and strongly continuous 1-parameter groups of unitary operators, with the second theorem providing a precise meaning for the notion of exponential of a selfadjoint operator.

For an arbitrary *bounded* operator B the exponential e^B can be defined as the sum of the exponential series $\sum_{n=1}^{\infty} \frac{1}{n!} B^n$, just as in the case of complex numbers. This is meaningless for general unbounded operators. For the special case of unbounded selfadjoint operators a good definition of exponential is provided by the spectral theorem. How tricky it would be to rely on the exponential series in this case is shown by the following example.

Example: Consider in $\mathcal{H} = L^2(R^1, dx)$ the translation operators $U(a)$, defined as $(U(a)\psi)(x) = \psi(x - a)$. These operators form a strongly continuous

1-parameter group of unitary operators, with as infinitesimal generator the differential operator $D' = -D = i\frac{d}{dx}$, in agreement with the Taylor expansion of a function $\psi(x)$, so we can write $U(a)\psi = e^{iaD'}\psi$. The operator D' and all its powers $(D')^n$ are well-defined on the dense linear subspace of infinitely differentiable functions with compact support in R^1, so all the partial sums $S_n = 1 + iaD' + \frac{1}{2}(iaD')^2 + \ldots + \frac{1}{n!}(iaD')^n$ are well defined on this domain. Nevertheless, the action of the successive S_n will in the limit of $n \to \infty$ clearly not result in a translation of such functions, because the support of each $S_n\psi$ will remain contained in the support of ψ.

7.3. *General groups of unitary operators*

A *group* of unitary operators in $\mathcal{H}$ is a collection of unitary operators that includes the unit operator, contains with every operator its inverse and with each pair of operators its product. As such it is a subgroup of $\mathcal{U}(\mathcal{H})$. In quantum theory groups of unitary operators play an important role, usually as *representations* of externally given *symmetry groups*, i.e. as the images under homomorphisms of these symmetry groups into $\mathcal{U}(\mathcal{H})$. In this respect *Lie groups* with their continuous unitary representations are of particular importance. Such representations are in a certain sense generated by 1-parameter subgroups. These have infinitesimal generators representing the *Lie algebra* of the group.

Example: The 3-dimensional rotation group, usually denoted as $O(3)$, is a Lie group. It consists of all 3×3 orthogonal matrices $\{O_{jk}\}$. It can be represented in the Hilbert space $\mathcal{H} = L^2(R^3, d\vec{x})$ by the unitary operators $U(O)$ acting as $(U(O)\psi)(\vec{x}) = \psi(O^{-1}\vec{x})$, with $(O^{-1}\vec{x})_j = \sum_{k=1}^{3} O^{-1}_{jk} x_k$. See Appendix D for further information on groups and group representations.