Hilbert Space for Quantum Mechanics The Finite-Dimensional Spectral Theorem and The Functional Calculus for Self-Adjoint Operators

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November 6, 2014

I accept the division.

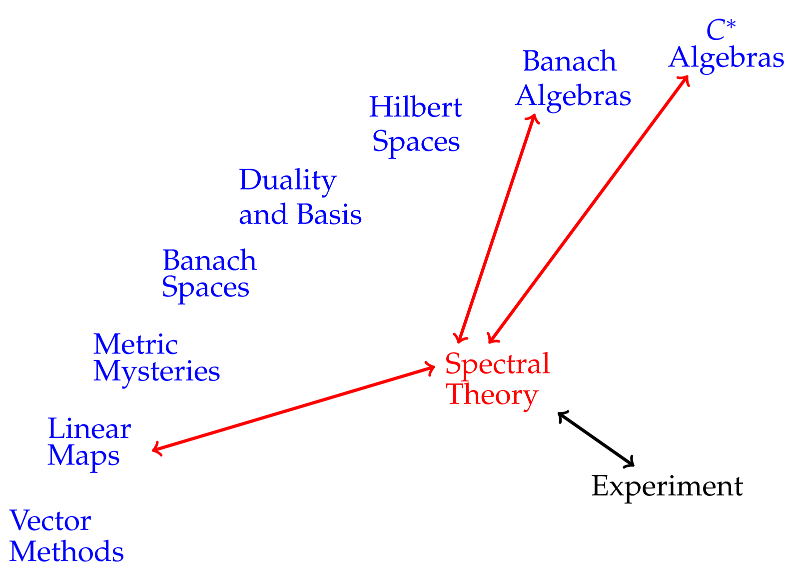
I even accept the question.

But I have trouble remembering which side of the glass I'm on.

Larry Susanka, Fall 2014

"Yes, they're all fools, gentlemen . . . But the question remains, 'What KIND of fools are they?'"

THE ARC OF QUANTUM WISDOM



$\mathbb{C}^n$

$\mathbb{C}^n$ can be conceived of as the set of ordered n-tuples $v = (v^1, v^2, \ldots, v^n)$ of complex numbers made into a vector space with the familiar properties of addition and scalar multiplication.

For typographical convenience we represent these as rows, but for compatibility with matrix operations and standard function notation they are, actually, columns.

$\mathbb{C}^n$ AND $\langle\, v\,, w\,\rangle_c$

Let the vector $\mathbf{e_i}$ denote the member of $\mathbb{C}^n$ that has a 1 in the ith row and zeroes elsewhere.

Then we have

$$v = (v^1, v^2, \ldots, v^n) = v^1\mathbf{e_1} + v^2\mathbf{e_2} + \cdots + v^n\mathbf{e_n}.$$

$\mathbb{C}^n$ is a Hilbert space with inner product

$$\langle\, v\,, w\,\rangle_c = v^1\,\overline{w^1} + v^2\,\overline{w^2} + \cdots + v^n\,\overline{w^n}.$$

$\mathbb{C}^n$ AND "REALITY" (PART I)

We identify $\mathbb{C}^n$ with some fragment of "reality" by identifying each $\mathbf{e_i}$ with a specific displacement of something measurable and "vector-like" in the "reality" fragment displacements.

The "reality" displacements we consider will be called **Reality**.

In the structure we build we will use a concept of "angle" so in **Reality** there should be some concept analogous to "orthogonal."

From the outset, we should have good reason to believe that **Reality** looks like an n-dimensional inner product (i.e. Hilbert) space.

$\mathbb{C}^n$ AND "REALITY" (PART II)

We will also be interested in operators $T\colon$ **Reality** $\to$ **Reality** and when we write $T(v) = w$ for certain $v, w \in \mathbb{C}^n$ what we really mean is that there are items A and B in **Reality** for which $T(A) = B$ and w is the member of $\mathbb{C}^n$ which we have associated with B and v is the member of $\mathbb{C}^n$ which we have associated with A.

It is important that we make this clear: *without an explicit, up-front "legend" associating specific, measurable "reality" displacements with the* $\mathbf{e_i}$ *the equation* $T(v) = w$ *is meaningless.*

$\mathbb{C}^n$ and Matrix Representations of T

If $T\colon \mathbb{C}^n \to \mathbb{C}^n$ is any linear operator it can be represented using left multiplication by matrix $M = (T^i_j)$ where T^i_j is the coefficient on $\mathbf{e_i}$ in $T(\mathbf{e_j})$. So matrix M is the $n \times n$ matrix

$$M = (T(\mathbf{e_1})\, T(\mathbf{e_2}) \cdots T(\mathbf{e_n}))$$

and it follows by linearity and direct calculation that

$$T(v) = M\,v = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} T^i_j v^j \right) \mathbf{e_i}.$$

Adjoint in $\mathbb{C}^n$

The adjoint of an operator T is an operator $T^\dagger$ defined by

$$\langle\, T\,v\,, w\,\rangle_c = \langle\, v\,, T^\dagger w\,\rangle_c.$$

The matrix of $T^\dagger$ can be determined by applying this formula to the $\mathbf{e_i}$. Then

$$\langle\, T\,\mathbf{e_i}\,, \mathbf{e_j}\,\rangle_c = \langle\, \mathbf{e_i}\,, T^\dagger \mathbf{e_j}\,\rangle_c$$

producing the equality $\left(T^\dagger\right)^i_j = \overline{T^j_i}$.

In other words the matrix of $T^\dagger$ is $\overline{M^{\text{transpose}}}$.

Defining the conjugate transpose of any square matrix M to be $M^\dagger$ we have (by this definition) that

$$M \leftrightarrow T \quad \text{if and only if} \quad M^\dagger \leftrightarrow T^\dagger.$$

Normal Operators on $\mathbb{C}^n$ (Part I)

If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are complex numbers we define

$$diag(\lambda_1, \lambda_2, \ldots, \lambda_n)$$

to be the $n \times n$ matrix with $\lambda_1, \lambda_2, \ldots, \lambda_n$, in order, along the diagonal and zeroes elsewhere. Such matrices are called **diagonal matrices.**

A square matrix M is said to be **diagonalizable** if there is an invertible matrix P and diagonal matrix D for which

$$P^{-1}MP = D \quad \text{or, equivalently,} \quad MP = PD.$$

If M is diagonalizable and $D = diag(\lambda_1, \lambda_2, \ldots, \lambda_n)$ the numbers $\lambda_1, \lambda_2, \ldots, \lambda_n$ are unique except for order.

P is said to **diagonalize** M.

Normal Operators on $\mathbb{C}^n$ (Part II)

Operators that commute with their adjoint are called **normal** and those that are their own adjoint are called **self-adjoint**.

An invertible isometry on $\mathbb{C}^n$ is called **unitary**.

The vocabulary is also applied to the matrices that represent these operators.

If P is a unitary matrix, then $P^{-1} = P^\dagger$, and this property characterizes this type of matrix. Unitary matrices are normal.

It is a standard theorem of Linear Algebra that normal matrices are exactly those which are **diagonalizable** by a unitary **matrix of transition.**

Normal Operators on $\mathbb{C}^n$ (Part III)

Suppose M is normal $MP = PD$ for diagonal D and unitary P as above. Let P_i denote the ith column of P. We have

$$MP = (MP_1\ MP_2 \cdots MP_n) = (\lambda_1 P_1\ \lambda_2 P_2 \cdots \lambda_n P_n) = PD.$$

So the columns of P form a linearly independent set of eigenvectors for M and, of course, the operator T corresponding to M.

By virtue of the equation $P^{-1}M\,P = P^{\dagger}M\,P = D$ we say that any normal matrix (or operator) is **unitarily equivalent** to a diagonal matrix (or operator.)

Self-adjoint Operators on $\mathbb{C}^n$ (Part I)

Normal M is self-adjoint exactly when all the λ_i are real.

When M is self-adjoint, we will insist (by permuting the columns of P if necessary) that the λ_i are listed along the diagonal in decreasing order. Of course some of these numbers may coincide.

For each λ_i the eigenspace for λ_i, which is the span of the columns of P corresponding to this eigenvalue, will be denoted E_{λ_i}.

The sum of the dimensions of the eigenspaces for distinct eigenvalues is n.

Self-adjoint Operators on $\mathbb{C}^n$ (Part II)

Let's see how this looks working directly with the operator T.

Suppose we have self-adjoint T and diagonalizing unitary P so $M\,P = P\,D$ for diagonal D. Then $T(P_i) = \lambda_i P_i$ for $i = 1, \ldots, n$.

Any vector v in $\mathbb{C}^n$ has a unique representation as

$$v = a^1 P_1 + a^2 P_2 + \cdots + a^n P_n \quad \text{where} \quad a = P^{-1}v \quad \text{because} \quad Pa = v.$$

Note that

$$\|\, v \,\|^2 = \sum_{i=1}^{n} v^i \overline{v^i} = \sum_{i=1}^{n} a^i \overline{a^i}.$$

The unitary operator given by matrix multiplication $P \colon \mathbb{C}^n \to \mathbb{C}^n$ is an isometry: that is, for every $v, w \in \mathbb{C}^n$

$$\langle\, v \,, w \,\rangle_c = \langle\, Pv \,, Pw \,\rangle_c.$$

Self-adjoint Operators on $\mathbb{C}^n$ (Part III)

$$T(v) = \lambda_1 a^1 P_1 + \lambda_2 a^2 P_2 + \cdots + \lambda_n a^n P_n$$

so representing vectors in terms of this basis makes T trivial to calculate.

Should you have mild regret concerning your initial choice of $\mathbf{e_1}, \mathbf{e_2}, \ldots, \mathbf{e_n}$, you can use P to tell you how to "change your mind" consistently.

Had you chosen $\mathbf{e_1}$ to be the "reality fragment" displacement represented by P_i for each i, as you very well could have, the matrix of T would have been diagonal from the outset.

P is your "new choice to original choice" translator!

Counting Measures

$\mu\colon \mathbb{P}(\mathbb{R}) \to [0,\infty]$ is called a **counting measure** on $\mathbb{R}$ if there is a countable subset S of $\mathbb{R}$, called the **support of μ**, so that $\mu(A)$ is the cardinality of $A \cap S$ for every $A \in \mathbb{P}(\mathbb{R})$.

For instance, if $S = \{1,2,5\}$ then $\mu(\mathbb{Q}) = 3$ and $\mu([0,3]) = 2$ and $\mu([10,20]) = 0$.

Or if $S = \mathbb{Q}$ then $\mu([0,3]) = \infty$ and $\mu(\{\sqrt{2}, 7/3, e\}) = 1$.

For each $\lambda \in \mathbb{R}$ we define δ_λ to be counting measure on the one-point set $\{\lambda\}$.

This is called (by mathematicians) a **point mass at λ**. Sometimes these measures are called **Dirac delta functions.**

Note that $\mu = \sum_{s\in S} \delta_s$ where we apply a sum of point masses to a set in the obvious way.

Counting Measures (Part II)

We define here a couple of relations between measures that are more pertinent, perhaps, for more general measures. But remember, our goal here is to run through the vocabulary involved in infinite dimensional spectral theory for unbounded operators but applied in a finite dimensional setting.

Suppose μ is a counting measure with support S and ν is a counting measure with support R.

μ called **absolutely continuous with respect to counting measure ν** if $\nu(A) = 0$ implies $\mu(A) = 0$.

This condition holds when and only when $S \subset R$.

μ and ν are called **mutually singular** if $S \cap R = \varnothing$.

$L^1(\mu)$ (Part I)

If $f\colon \mathbb{R} \to \mathbb{C}$ and if $\sum_{s\in S} |f(s)| < \infty$ we define

$$\int_{\mathbb{R}} f\, d\mu = \sum_{s\in S} f(s)\mu(\{s\}) = \sum_{s\in S} f(s).$$

The functions for which we have defined $\int_{\mathbb{R}} f\, d\mu$ are called **integrable** or **summable**.

$L^1(\mu)$ (Part II)

If $\sum_{s\in S} |f(s)| = 0$ we call f a **null function**, or, specifically, a **μ-null function**.

The set of equivalence classes of integrable functions, where f is equivalent to g when $f - g$ is a null function, is denoted $\boldsymbol{L^1(\mu)}$.

When $f - g$ is a null function we write

$$f = g \text{ almost everywhere,}$$

or $f = g$ a.e. as an abbreviation. If there is more than one measure around we may need to use the more specific

$$f = g \quad \mu\text{-a.e.}$$

$L^2(\mu)$ (Part I)

If $f: \mathbb{R} \to \mathbb{C}$ and if $\sum_{s \in S} |f(s)|^2 < \infty$ we call f **square integrable** or **square summable**.

$L^2(\mu)$ consists of equivalence classes of square integrable functions, where equivalent functions are those which are equal almost everywhere.

For reasons of custom and convenience, we conflate a function with its equivalence class.

This is harmless in our definitions and calculations because μ (and the inner product defined by μ) has no way to distinguish among functions in the same class.

$L^2(\mu)$ (Part II)

Products of square integrable functions are integrable (BCS inequality) and $L^2(\mu)$ with inner product given by

$$\langle f, g \rangle_\mu = \int_{\mathbb{R}} f \, \overline{g} \, d\mu = \sum_{s \in S} f(s) \, \overline{g(s)}$$

is a Hilbert space.

$L^2(\mu)$ (Part III)

For any subset A of $\mathbb{R}$ let

$$\chi_A : \mathbb{R} \to \{ 0, 1 \}$$

denote the function that evaluates to 1 on members of A and 0 otherwise. χ_A is called the **characteristic function for A**.

So if $f \in L^2(\mu)$ then $f = \sum_{s \in S} f(s) \, \chi_{\{s\}}$.

In fact, the set of characteristic functions $\{ \chi_{\{s\}} \mid s \in S \}$ forms an orthonormal basis for $L^2(\mu)$.

$L^2(\mu)$ (Part IV)

Select a member $g: \mathbb{R} \to \mathbb{C}$ and, for $f \in L^2(\mu)$, consider the a.e.-defined function $K_g(f) = gf$.

If g is in $L^2(\mu)$ then $K_g(f) \in L^1(\mu)$ by the BCS inequality.

If g is bounded on the support of μ then $K_g(f) \in L^2(\mu) \cap L^1(\mu)$.

K_g is called a **multiplication operator.**

An important example is when g is the constant function 1.

$K_1(f) = f$ for all f.

$L^2(\mu)$ (Part V)

Another multiplication operator, which will be key for us, is that corresponding to the identity function

$$Id\colon \mathbb{R} \to \mathbb{R} \quad \text{given by} \quad Id(x) = x.$$

If S is a bounded set, then the multiplication operator K_{Id} is bounded, and

$$K_{Id}(f) = \sum_{s \in S} s f(s) \chi_{\{s\}}.$$

For obvious reasons, it is customary to use $K_{Id}(f) = x f(x)$ to denote the output function, which is fine as long as you don't forget what it means.

$L^2(\mu)$ and the operator T (Part I)

We will suppose self-adjoint $T\colon \mathbb{C}^3 \to \mathbb{C}^3$ has real eigenvalues 7, 5 and 3.

Let P be the unitary matrix that diagonalizes T (or, actually, M_T). The columns of P are unit eigenvectors for 7, 5 and 3, respectively.

Let μ be the counting measure on $S = \{7, 5, 3\}$.

So $\mathbb{C}^3 = \mathbb{C}P_1 \oplus \mathbb{C}P_2 \oplus \mathbb{C}P_3$ where the summands are orthogonal subspaces of $\mathbb{C}^3$.

$L^2(\mu)$ and the operator T (Part II)

Define $U\colon L^2(\mu) \to \mathbb{C}^3$ by

$$U(f) = f(7)P_1 + f(5)P_2 + f(3)P_3.$$

U is an invertible isometry between these two Hilbert spaces, and satisfies (and could have been defined by)

$$U\left(\chi_{\{7\}}\right) = P_1, \quad U\left(\chi_{\{5\}}\right) = P_2, \quad U\left(\chi_{\{3\}}\right) = P_3$$

and extending to all of $L^2(\mu)$ by linearity.

$L^2(\mu)$ and the operator T (Part III)

$$\begin{tikzcd}
\mathbb{C}^3 \arrow[r, "T"] & \mathbb{C}^3 \arrow[d, "U^{-1}"] \\
L^2(\mu) \arrow[u, "U"] \arrow[r, "K_{Id}"] & L^2(\mu)
\end{tikzcd}$$

The isometry U lets us associate x (or rather multiplication by x) down in $L^2(\mu)$ with operator T. All operations involving $\mathbb{C}^3$ or T can be carried out in $L^2(\mu)$ using K_{Id}.

$L^2(\mu) \leftrightarrow T$ (Part IV)

$$\begin{tikzcd}
\mathbb{C}^3 \arrow[r, "f(T)"] & \mathbb{C}^3 \arrow[d, "U^{-1}"] \\
L^2(\mu) \arrow[u, "U"] \arrow[r, "K_f"] & L^2(\mu)
\end{tikzcd}$$

Then by continuity of U we can define $f(T)$ for any $f \in L^2(\mu)$.

Multiplicity (Part I)

The previous considerations are a complete rephrasing of the Spectral Theorem and the Functional Calculus for self-adjoint operators on a three dimensional space when the eigenspaces have dimension 1.

The theory of spectral multiplicity for these operators has an easy translation here to deal with possible eigenspace of dimension greater than one.

Multiplicity (Part II)

If μ is a counting measure on $\mathbb{R}$ with support S and $n \geq 1$ define $L^1(\mu, \mathbb{C}^n)$ to be the set of those functions $f \colon \mathbb{R} \to \mathbb{C}^n$ for which

$$\int_{\mathbb{R}} \|f\| \, d\mu = \sum_{s \in S} \|f(s)\| < \infty.$$

For these functions we define $\int_{\mathbb{R}} f \, d\mu$ to be $\sum_{s \in S} f(s)$.

We define $L^2(\mu, \mathbb{C}^n)$ to be the set of those functions $f \colon \mathbb{R} \to \mathbb{C}^n$ for which

$$\int_{\mathbb{R}} \|f\|^2 \, d\mu = \sum_{s \in S} \|f(s)\|^2 < \infty.$$

Multiplicity (Part III)

Note that $L^2(\mu, \mathbb{C}^1)$ was the space we previously called $L^2(\mu)$.

For each Dirac delta measure, or "function," the space $L^2(\delta_\lambda, \mathbb{C}^n)$ has dimension n.

A specific basis consists of the n functions $b_{\lambda,k} \colon \mathbb{R} \to \mathbb{C}^n$ which are 0 except at λ and for which $b_{\lambda,k}(\lambda) = \mathbf{e_k}$, for $1 \leq k \leq n$.

Any function $f \colon \mathbb{R} \to \mathbb{C}^n$ is defined as a member of $L^2(\delta_\lambda, \mathbb{C}^n)$ by the single vector

$$f(\lambda) = v^1 \mathbf{e_1} + \cdots + v^n \mathbf{e_n}.$$

Then, again as members of $L^2(\delta_\lambda, \mathbb{C}^n)$, we have

$$f = v^1 b_{\lambda,1} + \cdots + v^n b_{\lambda,n}.$$

Multiplicity (Part III)

$L^2(\mu, \mathbb{C}^n)$ is a Hilbert space with inner product

$$\begin{aligned}\langle f, h\rangle &= \int_{\mathbb{R}} \langle f(s), h(s)\rangle \, d\mu = \sum_{s\in S} \langle f(s), h(s)\rangle \\ &= \sum_{s\in S} \sum_{j=1}^{n} f^{j}(s)\, \overline{h^{j}(s)}.\end{aligned}$$

Finite-Dimensional Spectral Theorems The Arc TOC $\mathbb{C}^n$ Adjoint Measures $L^2(\mu)$ and T Multiplicity

Multiplicity (Part IV)

Now suppose $T\colon \mathbb{C}^3 \to \mathbb{C}^3$ is a self-adjoint operator, as before, but which only has two distinct eigenvalues 5 and 3.

Suppose the eigenspace for 5 has dimension 1, so the eigenspace for 3 has dimension 2.

Let P be the unitary change of basis matrix with columns P_1, P_2 and P_3 where P_1 is an eigenvector for eigenvalue 5 and the remaining columns two span the eigenspace for eigenvalue 3.

$$\mathbb{C}^3 = \mathbb{C}P_1 \oplus (\mathbb{C}P_2 \oplus \mathbb{C}P_3)\,.$$

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Multiplicity (Part V)

Let $L = L^2(\delta_5, \mathbb{C}^1) \times L^2(\delta_3, \mathbb{C}^2)$.

L consists of ordered pairs of functions (f, g) where f is complex valued and g has values in $\mathbb{C}^2$.

It has a basis consisting of the three function-pairs

$$(\chi_5, 0) \quad \text{and} \quad (0, b_{3,1}) \quad \text{and} \quad (0, b_{3,2})$$

L is a Hilbert space of dimension 3 with inner product:

$$\begin{aligned}\langle (f,g), (h,k)\rangle &= \langle f, h\rangle + \langle g, k\rangle \\ &= f(5)\overline{h(5)} + g^1(3)\overline{k^1(3)} + g^2(3)\overline{k^2(3)}.\end{aligned}$$

Finite-Dimensional Spectral Theorems The Arc TOC $\mathbb{C}^n$ Adjoint Measures $L^2(\mu)$ and T Multiplicity

Multiplicity (Part VI)

Define $U\colon L \to \mathbb{C}^3$ by

$$U(\chi_5, 0) = P_1 \quad \text{and} \quad U(0, b_{3,1}) = P_2 \quad \text{and} \quad U(0, b_{3,2}) = P_3$$

extending to all of L by linearity.

U is an isometry onto $\mathbb{C}^3$, just as before.

If $h\colon \mathbb{R} \to \mathbb{C}$ define, for each $(f, g) \in L$ the pair

$$K_h(f, g) = (hf, hg).$$

K_h is called a multiplication operator on L, and once again the multiplication operator K_{Id} of the identity map $Id(x) = x$ corresponds to the operator T, and this allows us to define $h(T)$, for a wide class of functions h, as the operator $h(T)$ that corresponds to the multiplication operator K_h.