

Why we do quantum mechanics on Hilbert spaces

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1 Why Hilbert space?

You will go through great pains to learn the profound mathematics of Hilbert spaces and operators on them.

What in experiment suggests the specific form of quantum mechanics with its “postulates”? Why should measurable quantities be represented by operators on a Hilbert space? Why should the complete information about a system be represented by a vector from a Hilbert space?

It looks like we make a lot of assumptions for setting up quantum mechanics. The arguments below will show, that we make one *less* than we make for classical mechanics, and that this entails all the strangeness. It is a bit like in general relativity: by omitting one postulate from geometry, we enter a whole new space of possibilities.

The short overview presented below is a severely diluted representation of the discussion in:

F. Strocchi, *Mathematical Structure of Quantum Mechanics*

W. Thirring, *Mathematical Physics III: Quantum Mechanics*

J.v. Neumann: Mathematische Grundlagen der Quantenmechanik

1.1 Overview

- Associate “physical quantity” \mathcal{Q} with a mathematical object \mathbf{Q}
- Key step: \mathbf{Q} should be part of an “algebra”
- Define the “state” of a system, that leads to an expectation value for any measurement on the system.
- Given a “state” and the algebra of observables, a Hilbert space can be constructed and the observables will be represented on it as linear operators in the Hilbert space (GNS representation).
- In turn, any Hilbert space that allows representing the algebra of observables as linear operators on it is equivalent to a direct sum of GNS representations.

1.2 Physical quantities and observables

Assume we have “physical quantities” \mathcal{Q} . The concept is deliberately vague to leave it as general as possible. It should be a number or set of numbers that are associated with something we can measure directly or determine indirectly by a set of manipulations on an something we call a physical system.

Our attitude: “Il libro della natura e scritto in lingua matematica” (this is an abbreviated and slightly dis-

torted quotation from Galileo’s writing ¹). For being able to establish logically consistent relations between physical quantities, we want to map them into mathematical objects.

1.3 An algebra for the observables!

Let \mathbf{Q} be the mathematical objects corresponding to the physical quantities. We want to be able to perform basic algebraic operations with them: add them, multiply them, scale them, in brief: they should be members of an “algebra” \mathcal{A} :

1. \mathcal{A} is a vector space
2. there is a multiplication: $(\mathbf{P}, \mathbf{Q}) \rightarrow \mathbf{O} =: \mathbf{PQ} \in \mathcal{A}$
3. $\mathbf{P}(\mathbf{Q}_1 + \mathbf{Q}_2) = \mathbf{PQ}_1 + \mathbf{PQ}_2$ for $\mathbf{P}, \mathbf{Q}_1, \mathbf{Q}_2 \in \mathcal{A}$
4. $\mathbf{P}(\alpha\mathbf{Q}) = \alpha(\mathbf{PQ})$ for $\alpha \in \mathbb{C}$
5. $\exists 1 \in \mathcal{A} : 1\mathbf{Q} = \mathbf{Q}1 = \mathbf{Q}$

Watch out: “Die Mathematiker sind eine Art Franzosen: redet man zu ihnen, so übersetzen sie es in ihre Sprache, und dann ist es alsobald ganz etwas anderes.” (Goethe). Here it has happened, we have given up control. We would need to come back later and see what “physical quantity” may correspond to $\mathbf{Q} + \mathbf{Q}'$ or \mathbf{QQ}' . How can we map this back into $\mathcal{Q} + \mathcal{Q}'$ etc.?

A few extra mathematical properties we want for our \mathcal{Q} :

¹ “La filosofia naturale e scritta in questo grandissimo libro che continuamente ci sta aperto innanzi agli occhi, io dico l’universo, ma non si puo intendere se prima non s’impara a intender la lingua e conoscer i caratteri nei quali e scritto. Egli e scritto in lingua matematica, e i caratteri son triangoli, cerchi ed altre figure geometriche, senza i quali mezzi e impossibile a intenderne umanamente parola; senza questi e un aggirarsi vanamente per un oscuro labirinto. Il Saggiatore, Galileo Galilei (1564-1642)”

1. There should be a norm: we should be able to tell how “large” at most the quantity is and it should be compatible with multiplicative structure of the algebra. This norm should have the properties $\|\mathbf{PQ}\| \leq \|\mathbf{P}\|\|\mathbf{Q}\|$, $\|1\| = 1$
2. There should be an adjoint element with all the properties of a hermitian conjugate and $\|\mathbf{P}^*\| = \|\mathbf{P}\|$, $\|\mathbf{P}^*\mathbf{P}\| = \|\mathbf{P}\|^2$
3. \mathcal{A} should be *complete*: if a sequence of \mathbf{Q}_n “converges” (Cauchy series), there should be an element in \mathcal{A} such that the series converges to this element.

It is not obvious, whether these further assumptions are innocent or already imply deep postulates on the physics we want to mirror in our mathematics. Note, however, that the “observables” of classical mechanics are simply functions on the phase space and have all those properties with the norm $\|F\| = \sup_{x,p} |F(x,p)|$, if we restrict ourselves to *bounded* functions: after all, there is no single apparatus to measure infinitely large values. Note, that in this sense momentum p would not fit into the algebra, as it is unbounded. However, momentum restricted to any finite range *does* fit.

An algebra with these properties is called C^* algebra.

1.4 Spectrum of \mathbf{Q}

Any physical quantity \mathcal{Q} can assume a set of values, which should be identical with the spectrum of \mathbf{Q} : \mathbf{Q} , so to speak, is a general container for the possible values of the measurable quantity.

Let us remark that the spectrum $\sigma(\mathbf{Q})$ of an element of the algebra can be defined just like for a linear operator by looking at $(\mathbf{Q} - z)^{-1}$ for $z \in \mathbb{C}$:

$$\sigma(\mathbf{Q}) = \mathbb{C} \setminus \{z \in \mathbb{C} \mid \exists (\mathbf{Q} - z)^{-1}\}$$

1.5 The state of a system

We call an element of the algebra *positive*, if its spectrum has strictly non-negative values. A more fundamental definition of positivity is $A > 0 : A = B^*B, B \in \mathcal{A}$.

Using the definition of “positive”, we can introduce a partial ordering in the algebra by

$$\mathbf{Q} - \mathbf{Q}' > 0 : \mathbf{Q} > \mathbf{Q}'$$

The “**state of a system**” is a positive linear functional f with $f(1) = 1$

- **Linear:** $f(\alpha\mathbf{A} + \beta\mathbf{B}) = \alpha f(\mathbf{A}) + \beta f(\mathbf{B})$, we want that... (we have it in classical mechanics).
- **Positive:** $f(Q) \geq 0$ for $Q > 0$. Note the \geq rather than $>$: the observable Q may well have spectral values $=0$ in certain places. If a state f_0 only tests these places, the result $f_0(Q) = 0$, although $Q > 0$.

A state f is a very general definition of what we expect of something that gives an “expectation value” $f(\mathbf{Q})$ for a physical quantity \mathbf{Q} : linear, not negative if there are only positive values available, and $=1$, if we only measure that the system exists at all, without referring to any physical property ($\mathbf{Q} = 1$).

1.6 Gelfand isomorphism

Can be paraphrased as follows: “Any commuting C^* algebra is equivalent to an algebra of *continuous* functions from the *character set* of the algebra into the complex numbers”.

A **character of an abelian C^* -algebra** is a $*$ -homomorphism of the algebra into the complex numbers. For a discussion of “character” I refer you to the exercises. If you are not familiar with the concept, for simplicity, think of subset of the linear operators on the Hilbert space and imagine a single character as a common eigenvector shared by all the operators (bypassing also the question of possibly degenerate eigenvalues). For the algebra formed by the polynomials of a single “normal” operator, a character can be associated with a given spectral value of the operator.

The character set is nothing newly introduced, no new condition on our algebra: given a commuting C^* algebra, we can give its character set. For defining “continuity” we need a topology. A weak topology is used: a sequence of characters χ_n converges, if the sequence of real numbers $\chi_n(\mathbf{Q})$ converges for each $\mathbf{Q} \in \mathcal{A}$.

1.6.1 Illustration on the example of bounded linear operators

Gelfand isomorphism is the correspondence of what you know as “any set of commuting operators can be diagonalized simultaneously”. The statement can be derived without any reference to a “Hilbert space” or “states on the Hilbert space”. It only uses the precise definition of “character”. However, to develop a feeling for its mean-

ing, it can be helpful to discuss a very simplified version for linear operators on a Hilbert space.

Assume a *commutative* C^* algebra \mathcal{A} of bounded linear operators on a Hilbert space. You have learnt that all operators of the algebra can be “diagonalized” simultaneously. Assume for simplicity that all these operators have a strictly discrete spectrum with eigenfunctions from the Hilbert space. Let $\{|i\rangle\}$ denote the set of simultaneous eigenvectors of all operators in the algebra. Assume for simplicity that we can choose the $|i\rangle$ orthonormal: $\langle i|j\rangle = \delta_{ij}$. Then any operator $\mathbf{A} \in \mathcal{A}$ can be written as

$$\mathbf{A} = \sum_{\chi_i} |\chi_i\rangle f_{\mathbf{A}}(i) \langle \chi_j| =: \sum_{\chi_i} |\chi_i\rangle \chi_i(\mathbf{A}) \langle \chi_j|$$

The set shared eigenvectors $\{|i\rangle\}$ defines the character set $X = \{\chi_i\}$ of this particular C^* algebra:

$$\chi_i(A) = \langle i|A|i\rangle$$

The $f_{\mathbf{A}}(i)$ can be understood as mapping one particular character χ_i into the complex numbers.

1.7 States, measures, and integrals

We can identify states with integration measures on the spectrum of an element \mathbf{Q} .

1.7.1 What is an integral?

It is a continuous (in the sense of some topology) linear map from a space of functions f into the complex numbers.

We write it as

$$\int_{\chi \in X} d\mu(\chi) f(\chi)$$

where $d\mu(\chi)$ is the integration “measure” on the set of χ 's

1.7.2 What is a state?

It is a (positive, continuous) linear map from the C^* -algebra into the complex numbers.

1.7.3 State \leftrightarrow measure on the character set

To the extent that we can associate the character set with the “spectrum” of the observable any measure on the character set is a measure on the spectrum.

1.7.4 Illustration

Using again the analogy with a C^* algebra of bounded linear operators: a state can be constructed using a “density matrix” ρ by:

$$f_\rho(\mathbf{A}) := \text{Tr} \rho \mathbf{A}$$

In the simplest case of a *pure state* $\rho = |\Psi\rangle\langle\Psi|$ ($\|\Psi\| = 1$)

$$f_\rho(\mathbf{A}) = \text{Tr} \rho \mathbf{A} = \sum_i |\langle\Psi|i\rangle|^2 \chi_i(\mathbf{A}) =: \sum_{\chi \in X} \mu(\chi) f_{\mathbf{A}}(\chi)$$

The integration measure induced by f_ρ with $\rho = |\Psi\rangle\langle\Psi|$ is just $\mu(\chi_i) = |\langle\Psi|i\rangle|^2$. We are back to the simplest quantum mechanical situation.

1.8 The structure of classical and quantum mechanics

Postulate: Observables of a physical system are described by hermitian $\mathbf{Q} = \mathbf{Q}^*$ elements of a C^* algebra \mathcal{A} and the state of a physical system is mapped into a state on \mathcal{A} . The possible measurement results for \mathbf{Q} are the spectrum of \mathbf{Q} and their probability distribution in a state f is given by the measure df , which is the probability measure induced by it on the spectrum of \mathbf{Q} .

In classical mechanics, all \mathbf{Q} commute. In quantum mechanics, they do not commute. Here is the fundamental mathematical difference between the two theories.

1.9 Where is the Hilbert space?

C^* algebras can always be represented as bounded operators on a Hilbert space. “Represented”: what matters about the algebra is its addition and multiplication laws, and, as it is C^* , also the conjugation operation. Let $\pi : \mathcal{A} \rightarrow \mathcal{B}(\mathcal{H})$ be a mapping that assigns a bounded operator on the Hilbert space to each element of $\mathcal{A} : \mathbf{Q} \rightarrow \pi(\mathbf{Q})$. We call π a $*$ -homomorphism, if it preserves the C^* algebraic properties.

If we have a state f , we can use it to define a scalar product

$$\langle \mathbf{Q} | \mathbf{Q}' \rangle := f(\mathbf{Q}^* \mathbf{Q}').$$

and with it turn the algebra into a Hilbert space. We can then use this Hilbert space to represent the algebra on it. Let us call this Hilbert space $\mathcal{H}(\mathcal{A}, f)$.

Note: $f(\mathbf{Q}^* \mathbf{Q}')$ will not be a legitimate scalar product on the complete algebra as in general there will be $0 \neq$

$\mathbf{A} \in \mathcal{A}$ such that $w(\mathbf{A}^*\mathbf{A}) = 0$.

This can be fixed, loosely speaking, by removing those \mathbf{A} from the space used for representing \mathcal{A} . Using the concepts of quotient algebra and left sided ideal this can be done as follows: first observe that the $\mathbf{A} \in \mathcal{N}$ with $f(\mathbf{A}^*\mathbf{A}) = 0$ are a left-sided ideal of the algebra:

$$f(\mathbf{A}^*\mathbf{A}) = 0 \Rightarrow f(\mathbf{A}^*\mathbf{B}^*\mathbf{B}\mathbf{A}) = 0 \quad \forall \mathbf{B} \in \mathcal{A}$$

The go into the quotient algebra

$$\mathcal{A}/\mathcal{N} = \{[\mathbf{B}] | \mathbf{B} \in \mathcal{A}\}, \quad [\mathbf{B}] = \{\mathbf{B} + \mathbf{A} | \mathbf{A} \in \mathcal{N}\}$$

The scalar product of quotient algebra is defined by

$$\langle [\mathbf{B}] | [\mathbf{B}] \rangle := \inf_{\mathbf{A} \in \mathcal{N}} f(\mathbf{B} + \mathbf{A})^*(\mathbf{B} + \mathbf{A}) > 0 \quad \text{for } [\mathbf{B}] \neq [0]$$

Note that $[0] = \{\mathbf{A} | \mathbf{A} \in \mathcal{N}\}$.

1.9.1 GNS representation

(Gelfand, Naimark, Segal) Having constructed $\mathcal{H}(\mathcal{A}, f)$. We get a representation of the algebra on that Hilbert space as follows. Let $|q\rangle \in \mathcal{H}(\mathcal{A}, f)$ be the vector in the Hilbert space that corresponds to an element $\mathbf{Q} \in \mathcal{A}$. Let \mathbf{P} be any element in \mathcal{A} . Then $\mathbf{P}\mathbf{Q} \in \mathcal{A}$ with a corresponding $|pq\rangle \in \mathcal{H}(\mathcal{A}, f)$. We define the linear operator on $\mathcal{H}(\mathcal{A}, f)$ $\pi_f(\mathbf{P}) : |q\rangle \rightarrow \pi_f(\mathbf{P})|q\rangle := |pq\rangle$.

1.9.2 Cyclic vector

A vector $|c\rangle$ from the a Hilbert space is called ‘‘cyclic’’ w.r.t. a representation π , if the vectors $\{\pi(\mathbf{Q})|c\rangle | \pi(\mathbf{Q}) \in \pi(\mathcal{A})\}$ are dense in the Hilbert space.

Irreducibility of a representation can be also phrased as: all vectors of the Hilbert space are cyclic.

By construction, the vector corresponding to $|1\rangle_f$ in the GNS representation π_f for state f representation is cyclic.

1.9.3 Pure-state \Leftrightarrow GNS construction is irreducible

States form a convex space, i.e. if f_1 and f_2 are states, then also $f = \alpha f_1 + (1 - \alpha)f_2$, $\alpha \in [0, 1]$ is a state. States that cannot be decomposed in this way are called “pure”. Without discussing this further, we mention

- The density matrix corresponding to pure states has the form $\rho_{pure} = |\Psi\rangle\langle\Psi|$
- The GNS representation π_p for a pure state p is irreducible.

1.10 Direct sum of representations

Suppose there are two representations π_1 and π_2 of an algebra on two Hilbertspaces, \mathcal{H}_1 and \mathcal{H}_2 , respectively. With the direct sum of the Hilbert spaces

$$\Psi \in \mathcal{H}_1 \oplus \mathcal{H}_2 : \Psi = \psi_1 \oplus \psi_2; \quad \langle\Psi|\Psi'\rangle = \langle\psi_1|\psi'_1\rangle + \langle\psi_2|\psi'_2\rangle$$

the direct sum of the two representations is constructed by

$$\pi(\mathbf{A})\Psi = \pi_1(\mathbf{A})\psi_1 \oplus \pi_2(\mathbf{A})\psi_2$$

1.11 Equivalence of any cyclic representation to GNS

Clearly, two representations that are related by a unitary transformation (“change of basis”) will be consid-

ered equivalent. If the transformation is between two different Hilbert spaces, we must replace “unitary transformation” with “isomorphism”, i.e. a linear, bijective, norm-conserving transformation:

$$\mathcal{H}_1 \xrightarrow{U} \mathcal{H}_2 : \|U\Psi_1\|_2 = \|\Psi_1\|_1.$$

Two representations related by an isomorphism

$$\pi_2(\mathbf{A}) = U\pi_1(\mathbf{A})U^{-1}$$

are called *equivalent*.

Theorem:

Any representation of the C^* algebra on a Hilbert space with a cyclic vector is equivalent to a GNS representation.

Sketch of the proof: Assume a specific representation π which has a cyclic vector $|c\rangle$. Then we can define a state on the algebra by

$$f_c(\mathbf{A}) := \langle c|\pi(\mathbf{A})|c\rangle.$$

The GNS representation π_{f_c} is then equivalent to π . The map U between the two representations

$$|a\rangle := \pi(\mathbf{A})|c\rangle \xrightarrow{U} |[\mathbf{A}]\rangle_{f_c},$$

is obviously isometric and invertible as $\langle [A]|[A]\rangle_{f_c} = 0 \Leftrightarrow \langle a|a\rangle = 0$.

1.11.1 Equivalence any representation to a sum of GNS

From representation theory: “Any representation π of a C^* algebra (with unity) on a Hilbert space is the direct sum of representations of with a cyclic vector.”

Therefore: any representation of a C^* algebra is equivalent to a direct sum of GNS representations.

1.12 Conclusion

Let the mathematical dust settle and try to see what we have done. Using only the algebra of observables and one or several states, we have constructed one or several Hilbert spaces. We can map the algebraic structure onto linear operators on each of these Hilbert spaces. These are the GNS representations.

If, in turn, we more or less arbitrarily pick a Hilbert space and represent our algebra on it, this Hilbert space can be put into a one-to-one relation to a sum of the GNS representations. It is equivalent to it.

It is all in the C^* algebra and the states. These states we introduced in the closest analogy to probability measures on phase space. The Hilbert space representation pops out automatically.

What is new in quantum mechanics is non-commutativity. For handling this, the Hilbert space representation turned out to be a convenient — by many considered the best — mathematical environment. For classical mechanics, working in the Hilbert space would be an overkill: we just need functions on the phase space.