Algebraic Formulation of Quantum Theory

Seminar on Mathematical Aspects of Theoretical Physics

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We begin our study in the algebraic formulation of quantum theory, by defining some fundamental mathematical objects and notions.

Definition 1. *A C^*-algebra $A, \|\cdot\|, *$ is a complex, associative algebra A, together with a norm $\|\cdot\| : A \to \mathbb{R}_{\geq 0}$ and a $\mathbb{C}$ anti-linear map*

$$\begin{aligned} * : \quad & A \to A \\ & a \mapsto a^* \end{aligned}$$

(anti-linear meaning $(\lambda a + \mu b)^* = \bar{\lambda} a^* + \bar{\mu} b^*$)
such that the following hold:

1. *$(A, \|\cdot\|)$ is a complete topological vector space*
2. *$\|a \cdot b\| \leq \|a\| \cdot \|b\| \quad \forall a, b \epsilon A$*
3. *The map * is an involution, $a^{**} = a \quad \forall a \epsilon A$*
4. *The map * is an algebra anti-homomorphism, $(ab)^* = b^* a^*, \quad \forall a, b \epsilon A$*
5. *The C^* property holds, namely $\|a^* a\| = \|a\|^2, \quad \forall a \epsilon A$*

For morphisms of such unital C^* algebras, $\pi : A \to B$ holds the property:

$$\pi(a^*) = \pi(a)^*, \quad \forall a \epsilon A$$

Remark 1.
1. *An algebra for which only the first two axioms apply is called a Banach algebra*
2. *A consequence of the C^* property is that the adjoint preserves the norms. Using properties of the C^*-algebra we have:*

$$\|a\|^2 = \|a^* a\| \leq \|a^*\| \|a\|$$

*So, $\|a\| \leq \|a^*\|$. Exchanging roles for a, a^* and using the fact that * is an involution (property 3) we get*

$$\|a^*\|^2 = \|a^{**} a^*\| = \|a a^*\| \leq \|a\| \|a^*\|$$

So, $\|a^*\| \leq \|a\|$ as well, hence

$$\|a^*\| = \|a\| \tag{1}$$

In particular, since $1^* = 1$ we have $\|1\|^2 = \|1\| = 1$.

Elements $a \epsilon A$ such that $a^* = a$ are called $self-adjoint$ and form a real subspace, while elements for which $a^* a = a a^* = 1$ are called $unitary$.

Before we continue by defining the notion of bounded operators, we give the definition of a general *-representation.

Definition 2. *A representation of an involutive unital algebra A is a unital *-homomorphism π into the algebra of linear operators on a dense subspace D of a Hilbert space. A homomorphism is called *-homomorphism if*

$$\langle \Phi, \pi(A)\Psi \rangle = \langle \pi(A^*)\Phi, \Psi \rangle \quad \forall \Phi, \Psi \epsilon D \tag{2}$$

Definition 3. *Let $\mathcal{H}$ be a separable Hilbert space, namely a complete unitary vector space with a countable topological basis, with scalar product <-,-> that is linear in the first and anti-linear in the second argument.*
A $\mathbb{C}$-linear map $A : \mathcal{H} \to \mathcal{H}$ is called bounded, if the operator norm $\|A\| := sup_{\|x\|=1}\|Ax\|, \quad x\epsilon\mathcal{H}$ is finite. The space of bounded operators on a Hilbert space is a Banach algebra $B(\mathcal{H})$.

Remark 2. 1. *Such $\mathbb{C}$-linear maps are continuous due to the property:*

$$\|Ax - Ay\| = \|A(x-y)\| \leq \|A\| \cdot \|x-y\|$$

2. *$B(\mathcal{H})$ is also involutive through Riesz representation theorem, according to which, for $A\epsilon B(\mathcal{H})$ and $v\epsilon\mathcal{H}$ the continuous $\mathbb{C}$-linear function $\langle A\cdot, v\rangle : \mathcal{H} \to \mathbb{C}$ can be represented by the scalar product $\langle A\cdot, v\rangle = \langle \cdot, A^*v\rangle$, where $A^*v\epsilon\mathcal{H}$ and is unique. This defines an involution * on $B(\mathcal{H})$.*

We will now show that the algebra of bounded operators also satisfies to C^*-identity, hence it can be used a prototype structure for the following definitions that are governed by the notion of a C^*-algebra. For $A\epsilon B(\mathcal{H})$ we have

$$\begin{aligned}\|A\|^2 = sup_{\|x\|=1}\|Ax\|^2 = sup_{\|x\|=1}\langle Ax, Ax\rangle = sup_{\|x\|=1}\langle x, A^*Ax\rangle \\ \leq sup_{\|x\|=1}\|x\| \cdot \|A^*Ax\| = \|A^*A\| \leq \|A\| \cdot \|A^*\| = \|A\|^2\end{aligned}$$

So $\|A\|^2 \leq \|A^*A\| \leq \|A\|^2 \Rightarrow \|A^*A\| = \|A\|^2$ □

The main idea is that a C^*-algebra serves as an algebra of observables for a quantum mechanical system, providing thus a kinematical setting. As compared to classical Hamiltonian systems (N, ω, h) whose dynamics is specified by an element h in the Poisson algebra, the dynamics of quantum mechanical systems will be specified by an element of the C^*-algebra, as we will see later on. However, quantum mechanics is, as we know, a probabilistic theory. Hence, we must associate to every observable at least one expectation value.

Definition 4. *Let A be a unital C^*-algebra. A state ω on A is a normed positive linear functional*

$$\omega : A \to \mathbb{C}$$

In fact, the states belong to the dual vector space of A ($\omega\epsilon A^*$) with $\omega(a^*a) \geq 0, \quad \forall a\epsilon A$, and with normalization condition $\|\omega\| := sup_{\|a\|=1}|\omega(a)| = 1$.

Remark 3. *Particularly, on C^*-algebras continuity of a state follows from the positivity, so an ω that is linear, normed and positive is automatically an element of the topological dual space.*

We give some basic properties for the states of quantum systems.
Properties:

1. The set of all states is convex. Namely for ω_1, ω_2 two states, we have $\forall t \epsilon [0,1], \quad \omega_t = t\omega_1 + (1-t)\omega_2$ is also a state

2. A point x of a convex subset X of a real vector space V is called extremal if, for every segment $\bar{yz} \subset X$ containing x, we have $y = x$ or $z = x$. Extremal states on a C^*-algebra are called pure states. Non-pure states are called mixed states

Example: Density matrix

Consider the C^*-algebra B($\mathcal{H}$) of bounded operators on a Hilbert space $\mathcal{H}$. $\rho \epsilon End(\mathcal{H})$ is positive if $< \rho x, x > \geq 0, \quad \forall x \epsilon \mathcal{H}$. A positive endomorphism ρ of $\mathcal{H}$ is called density matrix if the endomorphism $\rho \cdot a$ is trace class $\forall a \epsilon A$. Namely a compact operator, for which a trace may be defined, so as to be finite and independent of the choice of basis. For $a = id_{\mathcal{H}}$, ρ itself is trace class, hence continuous. Then

$$\omega_\rho(a) := \frac{Tr(\rho a)}{Tr(\rho)} \tag{3}$$

is a state on C^*-algebra B($\mathcal{H}$).
Now let $\psi \epsilon \mathcal{H}$ be a unit vector, and

$$\begin{aligned} \rho :& \mathcal{H} \to \mathcal{H} \\ & x \mapsto \langle x, \psi \rangle \psi \end{aligned} \tag{4}$$

the orthogonal projection to the 1-dim subspace spanned by ψ. Then

$$\omega_\rho(a) = \langle a\psi, \psi \rangle \tag{5}$$

is a pure state.

In general, for every density matrix ρ on $\mathcal{H}$, the function

$$\omega_\rho(a) = \frac{Tr[\rho\pi(a)]}{Tr\rho}, \quad a \epsilon A \tag{6}$$

where $\pi : A \to B(\mathcal{H})$ a *-representation,(a *-preserving ring homomorphism of a C^*-algebra A on $\mathcal{H}$) is a state on A, called normal state.

Remark 4. *All states on a $C^* - algebra$ can be obtained this way.*

We continue, by giving the algebraic definition of two of the most important quantities in the quantum theory.

Definition 5. *Let A be a C^*-algebra and ω a state on A. For $a \epsilon A$,*

$$\langle a \rangle_\omega := \omega(a) \tag{7}$$

is the expectation value of the observable a in the state ω.

Definition 6.

$$\Delta\omega(a)^2 := \langle (a - \langle a \rangle)^2 \rangle_\omega = \langle a^2 \rangle_\omega - \langle a \rangle_\omega^2 = \omega(a^2) - \omega(a)^2 \tag{8}$$

is the variance of a in the state ω.

Remark 5. *In quantum physics, a state assigns to an observable not a single a probability distribution of measured values. It is convenient to characterize the probability distributions in terms of their momenta. But since the n-th momentum is the expectation value of the n-th power, it is sufficient to know the expectation values of all elements of the algebra of observables. Namely*

$$\omega(a^n) = \int a^n dP_{\omega,A}(a), \quad n\epsilon\mathbb{N}_0 \tag{9}$$

Stricter mathematical definitions for the probability measure dP will be given shortly.

At this point, with the help of the mathematical objects, that we have defined so far, we introduce some of the most fundamental relations in the quantum theory, namely Heisenberg's uncertainty relations.

Proposition: Heisenberg's uncertainty relations:

Let A be a C^*-algebra, ω a state of A and $a, b\epsilon A$ self-adjoint. The following relation holds:

$$\Delta_\omega(a)\Delta_\omega(b) \geq \frac{1}{2}|\omega([a,b])| \tag{10}$$

We give the proof of the above proposition in the Appendix. A special case of this are the observables $p, q\epsilon A$ with

$$[p,q] = i\hbar \cdot 1, \quad \hbar\epsilon\mathbb{R}_{>0} \Rightarrow$$
$$\Delta_\omega(q)\Delta_\omega(p) \geq \frac{\hbar}{2}$$

An essential notion in the quantum theory is that of the spectrum of an observable. Namely the values that we can potentially measure for it.

Definition 7. *Let a be an element of a unital C^*-algebra. We call*

$$r_A(a) := \{\lambda\epsilon\mathbb{C} | \lambda 1_A - a \quad \epsilon A^\times\}$$

the resolvent set of a and

$$Spec_A(a) = \mathbb{C} \backslash r_A(a) \tag{11}$$

the spectrum of a. Essentially it is the set of all complex numbers $\lambda\epsilon\mathbb{C}$ for which $\lambda - a$ possesses no inverse in A.

For example, let $a^2 = 1$. We have that

$$(a-\lambda)(a-\mu) = a^2 - (\lambda+\mu)a + \lambda\mu = (1+\lambda\mu) - (\lambda+\mu)a \tag{12}$$

So for $\lambda^2 \neq 1$, $(1-\lambda^2)^{-1}(a+\lambda)$ is an inverse of $a-\lambda$. Therefore, Spec(a) is contained in the set $\{\pm 1\}$.
Considering the spectrum of a linear operator on a Hilbert space, its definition is the same if the C^*-algebra considered is B($\mathcal{H}$). There are mainly 3 contributions to the spectrum, namely 3 ways we can divide it according to why $\lambda 1_A - a$ is not invertible.

- If $\lambda 1_A - a$ is not injective, we say that λ is in the point spectrum of a. Elements of the point spectrum are called eigenvalues of a and non-zero elements of the kernel of $\lambda 1_A - a$ are known as eigenvectors of a. Thus λ is an eigenvalue of a if and only if there is a non-zero vector $v\epsilon\mathcal{H}$ such that $av = \lambda v$.
- If $\lambda 1_A - a$ does not have closed range, but the range is dense in H, we say that λ is in the continuous spectrum of a. The union of the point spectrum and the continuous spectrum is known as the set of generalized eigenvalues. Thus λ is a generalized eigenvalue of a if and only if there is a sequence of vectors $\{v_n\}$, bounded away from zero, such that $av_n - \lambda v_n \to 0$.
- If $\lambda 1_A - a$ has neither closed range, nor its range is dense in H, we say that λ is in the residual spectrum of a.

Quantum mechanics is a probabilistic theory, hence we require some elements of probability measure theory, in order to formulate our theory self consistently. Given a state ω on a unital C^*-algebra A, the map

$$\mathcal{B}(\mathbb{R}) \to^P A \to^\omega \mathbb{R}$$
$$E \mapsto \omega(P(E))$$

defines a probability measure on $\mathbb{R}$. Where $\mathcal{B}(\mathbb{R})$ is a sigma algebra and $P : \mathcal{B}(\mathbb{R}) \to A$ is a projector-valued measure on $\mathbb{R}$. The corresponding definitions are given in the Appendix.
If A is the algebra B($\mathcal{H}$) of bounded operators on a separable Hilbert space $\mathcal{H}$, for any $v\epsilon\mathcal{H}\backslash\{0\}$ the distribution function

$$P_v(\lambda) = \langle P(\lambda)v, v\rangle \tag{13}$$

defines a bounded measure on $\mathbb{R}$. For $v = 1$ it is a probability measure. Using von-Neumann's spectral theorem for self-adjoint operators on a separable Hilbert space, we can connect the operator action with probability measures. The theorem's importance is significant, since it allows us to define functions of operators.

Theorem 1. *For every self-adjoint operator A on a separable Hilbert space $\mathcal{H}$, there exists a unique projector-valued measure $P_A(\lambda)$, with the property that, for every continuous function f on $\mathbb{R}$, $f(A)$ is a linear operator with dense domain*

$$D(f(A)) = \left\{ v\epsilon\mathcal{H} | \int_{-\infty}^{+\infty} |f(\lambda)|^2 d\langle P_A(\lambda)v, v\rangle < \infty \right\} \tag{14}$$

and $\forall v \epsilon D(f(A))$

$$f(A)v = \int_{-\infty}^{+\infty} f(\lambda) dP_A(\lambda) v \tag{15}$$

Now if A is an abstract C^*-algebra and f a continuous function on Spec(a) we get

$$f(a) = \int_{Spec(a)} f(\lambda) dP_a(\lambda) \tag{16}$$

and in particular for any state ω, we obtain

$$\omega(a) = \int_{Spec(a)} \lambda \omega(dP_a(\lambda)) \tag{17}$$

We are now ready to formulate some of the basic axioms of a quantum mechanical system.

Axioms:

1. The first fundamental object is a unital C^*-algebra A. The self-adjoint elements of A are the observables.

2. The state of the system is described by a state of its C^*-algebra A. A state describes in principle the way the measurement is being prepared. In this sense, given an observable (an element of A) and a preparation of the system (the state ω) we can perform a measurement and obtain a number. The value $\omega(a)$ is the expectation value for this number.

3. Given a quantum system A in a state ω, the result of a measurement of an observable $a \epsilon A$ cannot be predicted. The possible outcomes are given by the spectrum $Spec(a) \subset \mathbb{R}$ and we can predict the probability measure $\rho_a = \omega(dP_a(\lambda))$. The expectation value is

$$\langle a \rangle_\omega = \int_{Spec(a)} \lambda \omega(dP_a(\lambda)) = \omega(a) \tag{18}$$

and the variance is

$$\Delta_\omega(a) = \langle (a - \langle a \rangle)^2 \rangle_\omega = \langle a^2 \rangle_\omega - \langle a \rangle_\omega^2 = \omega(a^2) - \omega(a)^2 \tag{19}$$

It is important that in this statistical interpretation of quantum mechanics we assume that an experiment can be repeated. In other words we have a whole ensemble of systems and we can prepare each of them in the same state. Then, by making repeated measurement of the value of an observable in the given state we obtain the probability distribution.

4. The measurement influences the state. If the value $a_0 \epsilon Spec(a)$ has been measured for an observable a, the system is in a state where a has zero variance. This is also known as wave function collapse.

5. The dynamics of a quantum mechanical system A is given by a map $\alpha : I \rightarrow A$ where $I \subset \mathbb{R}$ an interval which is continuous and takes values in the unitary elements of A.

6. The Heisenberg picture is defined as follows. The observables evolve in time according to

$$a(t) = \alpha_t^{-1} a \alpha_t \tag{20}$$

Time evolution is described by automorphisms of A. The states do not depend on time. Furthermore, in the Heisenberg picture we get a time-dependent family of probability measures for any pair $(a, \omega) \rightsquigarrow (observable, state)$. Using the GNS theorem (described below) we can find a Hilbert space $\mathcal{H}_w$ and a vector $\Omega \epsilon \mathcal{H}_w$ such that

$$\omega(a(t)) = \langle a(t)\Omega, \Omega \rangle \tag{21}$$

is the expectation value.

7. For a quantum system (A, α_t) with time-independent dynamics, if we consider the C^*-algebra A to be a subalgebra of B($\mathcal{H}$), there is a description of the unitary one-parameter subgroup

$$\begin{aligned} \mathbb{R} &\rightarrow B(\mathcal{H}) \\ t &\mapsto \alpha_t \end{aligned}$$

in terms of an unbounded self-adjoint operator H on $\mathcal{H}$:

$$\alpha_t = e^{\frac{i}{\hbar} H t} \tag{22}$$

Where H is the Hamiltonian and $\forall a \epsilon A$ holds the law:

$$\frac{d}{dt} a(t) = \frac{i}{\hbar} [H, a] \tag{23}$$

which can be roughly regarded as a quantized analogue of the classical Poisson bracket.

GNS Theorem (Gelfand-Naimark-Segal)

The content of this important theorem is strongly related to the algebraic formulation of quantum theory.

Theorem 2. *Let ω be a state on a unital C^*-algebra A. Then there exists a representation π of the algebra by linear operators on a dense subspace D of some Hilbert space $\mathcal{L}$ and a unit vector $\Omega \epsilon D$ such that:*

$$\omega(a) = \langle \Omega, \pi(a)\Omega \rangle_\omega \tag{24a}$$

$$D = \{\pi(a) | a \epsilon A\} \tag{24b}$$

Proof: We introduce the scalar product on the algebra:

$$\langle A, B \rangle_\omega := \omega(A^* B)$$

having the properties of linearity for the right and anti-linearity for the left factor, while hermiticity ($\langle A^*, B \rangle_\omega = \overline{\langle B^*, A \rangle_\omega}$) follows from positivity of ω, as well as the fact that the scalar product is positive semi-definite: $\langle A, A \rangle_\omega = \omega(A^* A) \geq 0$.
Consider the set $R = \{a \epsilon A | \omega(a^* a) = 0\}$. R is a closed left ideal of A,
$\lceil$since for $a \epsilon R, b \epsilon A$ we have from Cauchy-Schwartz inequality:

$$\omega\left((ba)^*(ba)\right) = \omega(a^* b^* ba) = \langle b^* ba, a \rangle \leq \sqrt{(b^* ba, b^* ba)}\sqrt{(a, a)} = 0 \Rightarrow ba \epsilon R \rfloor$$

We define D as the quotient space $D := A/R$, where the scalar product is positive definite by construction. Hence D can be completed giving a Hilbert space $\mathcal{H}$. Now the representation π is induced by left multiplication of the algebra: $\pi(a)(b + R) := ab + R$, which is well-defined since R is a left ideal of A. Finally set $\Omega = 1 + R$ and the conditions of the theorem are satisfied. □

Remark 6. *It is easy to see that the construction is unique up to a unitary equivalence. Consider $(\pi', D', \mathcal{H}', \Omega')$ satisfying the theorem's conditions and we define an operator $U : D \to D'$ by*

$$U\pi(A)\Omega = \pi'(A)\Omega' \tag{25}$$

U is well-defined, since $\pi(a)\Omega = 0$ if and only if $\omega(a^* a) = 0$, but then we will also have $\pi'(a)\Omega' = 0$. U preserves the scalar product and is invertible, hence it has a unique extension to a unitary operator from $\mathcal{H}$ to $\mathcal{H}'$. As a result, the representations π, π' are unitarily equivalent:

$$\pi'(a) = U\pi(a)U^*, \quad a \epsilon A \tag{26}$$

Remark 7. *It is trivial to see that any unit vector $\Phi \epsilon D$ induces a state of the algebra by $\omega(A) = (\Phi, \pi(A)\Phi)$. The GNS construction proves us that the converse is also true.*

The importance of the GNS theorem is that it allows us to consider the Hilbert space as a derived concept in the quantum theory and the C^*-algebra of observables as the fundamental object.

Appendix

Definition 8. *A topological vector space X is a vector space over some field k ($\mathbb{R}$ or $\mathbb{C}$) which is endowed with a topology such that the vector addition: $X \times X \to X$ and scalar multiplication: $k \times X \to X$ are continuous functions.*

Definition 9. *A topology is a collection τ of subsets of $X \neq \emptyset$ (X being the topological space), satisfying:*

1. *$X, \emptyset \quad \epsilon \tau$*
2. *τ is closed under arbitrary union*
3. *τ is closed under finite intersection*

e.g.: $X = \{1, 2, 3, 4\}$, then $\tau = P(X)$ the power set of X forms a topology. (discrete topology)

Definition 10. *Supremum. Given a subset S of an ordered set T, supS is the least element of T that is greater or equal to every element of S. If supS exists, then it is unique.*

Proof of Heisenberg relations:
We will use the following property: Let ω be a state on a unital C^*-algebra A. Then $\omega(a^*) = \overline{\omega(a)} \quad \forall a \epsilon A$.
We decompose:

$$ab = \frac{1}{2}(ab + ba) + \frac{1}{2}(ab - ba) = \frac{1}{2}\{a, b\} + \frac{1}{2}[a, b]$$

a,b are self-adjoint, hence

$$\{a, b\} = ab + ba = a^*b^* + b^*a^* = (ba)^* + (ab)^* = \{a, b\}^*$$

and

$$[a, b] = -[b, a]^*$$

By use of the above property ω yields a real value on the anticommutator and an imaginary on the commutator. Namely

$$|\omega(ab)|^2 = \frac{1}{4}|\omega(\{a, b\}) + \omega([a, b])|^2$$

By Cauchy-Schwartz inequality we also have that

$$|\omega(ab)|^2 \leq \omega(b^2)\omega(a^2)$$

Altogether:

$$\omega(a^2)\omega(b^2) \geq \frac{1}{4}\omega(\{a, b\})^2 + \frac{1}{4}|\omega([a, b])|^2 \Rightarrow$$

$$\omega(a^2)\omega(b^2) \geq \frac{1}{4}|\omega([a, b])^2$$

We now set $\tilde{a} := a - \omega(a) \cdot 1$, $\tilde{b} := b - \omega(b) \cdot 1$ where $[\tilde{a}, \tilde{b}] = [a, b]$. Applying the inequality we arrive at

$$\Delta_\omega(a)^2 \Delta_\omega(b)^2 \geq \frac{1}{4}|\omega([a, b])|^2$$

Definition 11. *For a set X, a* <u>*sigma algebra*</u> *is a collection χ of subsets of X such that:*

1. *χ is not empty*
2. *χ is closed under complements, i.e. if $U \subset X$ is in χ, then also $X \backslash U \epsilon \chi$*
3. *χ is closed under countable unions, i.e. if each element of the family $(U_i)_{i \epsilon \mathbb{N}}$ is in χ, then $\bigcup_{i \epsilon \mathbb{N}} U_i \quad \epsilon \chi$.*

Definition 12. *A* <u>*Borel set*</u> *is a subset of X that can be obtained from open sets in X through the operations of countable unions, intersections and relative complements.*

Definition 13. *For A a unital C^*-algebra, denote $\mathcal{B}(\mathbb{R})$ the sigma-algebra of Borel subsets in $\mathbb{R}$. A normalized* <u>*projector-valued measure*</u> *on $\mathbb{R}$ with values in A is a map*

$$P : \mathcal{B}(\mathbb{R}) \to A$$

such that

1. *$\forall E \subset \mathbb{R}$ Borel subset, $P(E) = P(E)^2$ and $P(E) = P(E)^*$ (projector-valued)*
2. *$P(\emptyset) = 0$ and $P(\mathbb{R}) = 1_A$ (normalized)*
3. *$\forall E = \bigsqcup_{n=1}^{\infty} E_n$ and $P(E) = \lim_{n \to \infty} \sum_{i=1}^{n} P(E_i)$*