Elements of Mathematical Quantum Mechanics

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Note 1 [v.1 April 23rd 2024]

Quantum phenomenology and the mathematical model

Table of contents

Basic bibliography: [Seg47] [Str08] [Haa96]

Additional biblio: [BSZ92] [BR87, BR97] [RS80]

Historical references: [Dir88] [Hei49]

1 The Stern–Gerlach experiment

We start this course by describing one of the experiments which led to some of the early discoveries in quantum mechanics, that of the quantisation of the intrinsic magnetic moment of the electron, the spin.

Otto Stern and Walther Gerlach conducted in Frankfurt in 1922 the experience described in Figure 1 (left). A beam of atoms experience an intense magnetic field and as a consequence is deflected. Upon detection by means of a screen the arrival positions of the atoms reveals a quantized patterns, in contrast with classical theory of the magnetic moment of atoms which would require a continuous distribution of arrival positions due to the uniform distributions

of the magnetic moment within the atom's population escaping from the oven. Figure 1 (right) shows the actual images obtained in the original experiment.
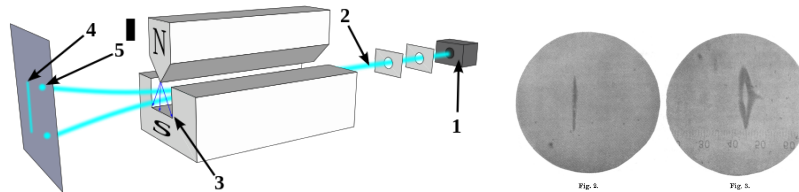

Figure 1. Left: Stern–Gerlach experiment: silver atoms travel through an inhomogeneous magnetic field and are deflected up or down depending on their spin. 1: furnace. 2: beam of silver atoms. 3: inhomogeneous magnetic field. 4: expected result. 5: what was actually observed. [from Wikipedia https://en.wikipedia.org/wiki/Stern–Gerlach_experiment]. Right: the experimental result of the Stern-Gerlach experiment. The beam has split into two components. From [Gerlach, Walther, and Otto Stern. "Der experimentelle Nachweis der Richtungsquantelung im Magnetfeld." *Zeitschrift für Physik* 9, no. 1 (December 1, 1922): 349–52. https://doi.org/10.1007/BF01326983.]

The Stern–Gerlach experiment shows the quantisation of the magnetic moment for the electron. Indeed the silver atoms have atomic number 47. In its fundamental state, 46 of these electrons do not contributed to the magnetic moment since they come in pairs of opposite intrinstic magnetic moment (*spin*) and in a spatially symmetric state which do not generate any angular momentum. Only the last electron, whose spatial distributions is also symmetric, has an uncompensated intrinsic magnetic moment which consitute the only relevant contribution to the total magnetic moment of the atom. This magnetic moment interacts with the non–uniform magnetic field deflecting the trajectory of the atom.

*Classically:* only one of the 47 electron matters. Intrinsic magnetic moment $m \in \mathbb{R}^3$ $|m| = M$. It interacts with the magnetic field $B(x) \in \mathbb{R}^3$. Atoms are reflected differently according to the value of $\langle B, m \rangle_{\mathbb{R}^3} = B_z m_z$ with $B = B_z \hat{z}$ and $m_z = \langle m, \hat{z} \rangle$. We expect that every atom has a magnetic moment $m \in \mathbb{R}^3$ with $|m| = M$ and oriented randomly in space so the quantity m_z is distributed like a continuous random variable.

Quantumly:

Fig. 2.   Fig. 3.
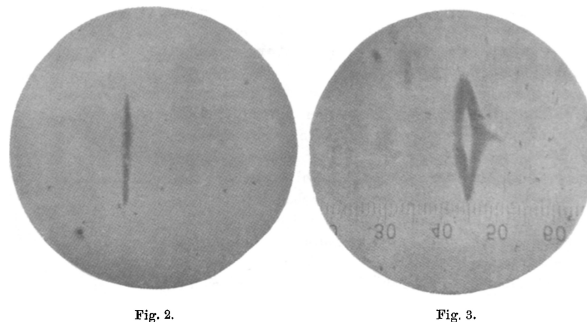
The presence of two well separated tracks means that this spin comes only in two varieties, oriented in the direction of the magnetic field or in the opposite direction. Conclusion: the electron intrinsic momentum (*spin*) is a quantum mechanical observable $m_z = \pm M$ (is *quantized*).

Indeed the spin of the electron seems to behave like a Bernoulli random variable. In order to explore other properties of this random variable we imagine a sequence of Stern–Gerlach experiments performed in series.
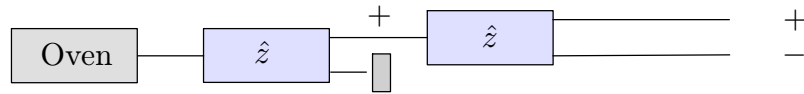
In this first case we first measure the $\hat{z}$ orientation, select those atoms which emerge from the + path after the first instrument and then again the $\hat{z}$ orientation and we obtain that all the atoms emerge from the + path.
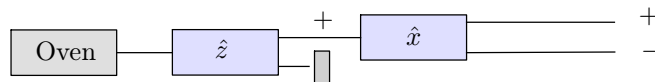

In this second situation we measure a different, orthogonal direction in the second instrument and we obtain that half of the atoms emerge from the + path and half from the − path. This is expected due to the symmetry of the problem.
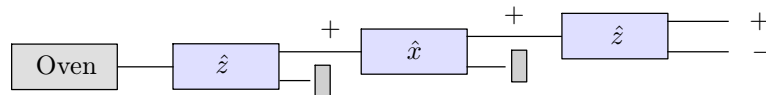
In this third installment we select the atoms which emerge from the + path after the $\hat{x}$ instrument and perform another selection with a $\hat{z}$ instrument. The result is that again half of the atoms emerge from the + path and half from the − path. The interpretation is that the measurement of $\hat{x}$ has completely destroyed the previous measurement of $\hat{z}$.

We now introduce another apparatus which undo the effect of a Stern–Gerlach instrument, this is not difficult to imagine, we just need to produce the opposite magnetic field to undo the effect of the first and arrange appropriately the geometry to recombine the atom beam. We label this instrument $\check{z}$ if it operates in the z direction.
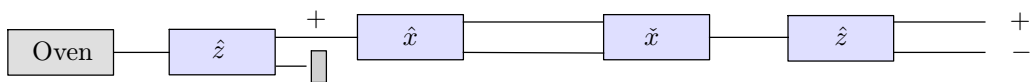
In this first case we use the new instrument to recombine the beams after a $\hat{x}$ beam splitter. If we have selected only atoms with spin in the $\hat{z} = +1$ direction right after the oven, then we will end up with all the atoms in the + beam after the last $\hat{z}$ instrument.
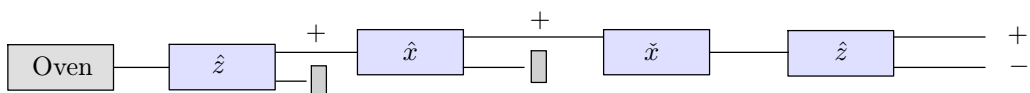
We now block the $\hat{x} = -1$ beam and we observe that atoms exit the instrument with probability $1/2$ in each of the two final beams.

Summarizing:

	+	−
	100%	0%
	50%	50%
	50%!	50%!
	100%	0%
	50%	50%
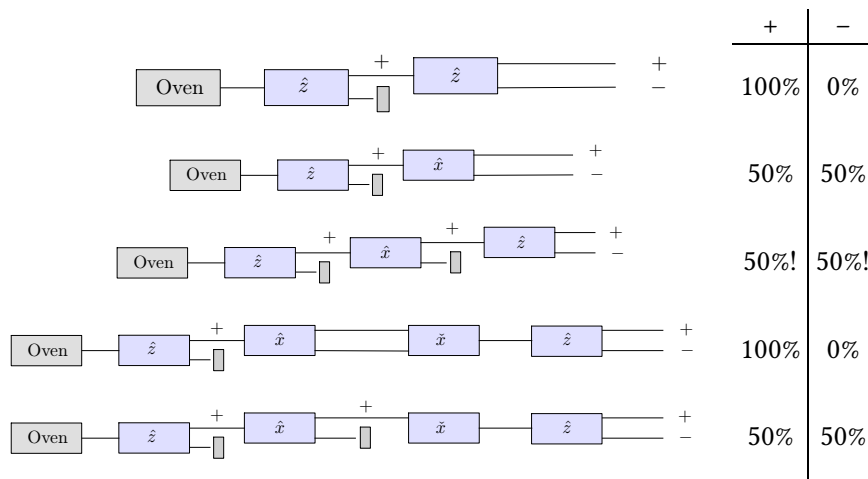
This is quite surprising. Allowing *more* atoms to go through the experiment depletes one of the exit beams! This property is not in agreement with a probabilistic description of the state of the atoms. Removing a conditioning cannot renders impossible events which were possible under the conditioning. This is a manifestation of quantum mechanical *interference* effects.

2 The mathematical model of a physical system

We describe now the basic mathematical model for a physical system from which we will later deduce the basic structure of quantum mechanics. For a more systematic discussion of various aspects of this modelling step refer to the following literature: [Str08, Seg47, SM63, Haa96].

We have two basic players in this game: observables and states.

- *Observables.* An observable is a physical quantity which we can measure (e.g. components of magnetic moment, position, speed/momentum, energy). Connected with some measuring apparatus which has a scale where you read a real number. We write $\mathcal{O}$ for the set of all observables. Given an observable $A \in \mathcal{O}$ more observables can be constructed from A by elementary procedures (i.e. relabeling the scale of the apparatus) E.g. $\lambda A, A^n \in \mathcal{O}$ $\lambda \in \mathbb{R}$. $A^n A^m = A^{n+m}$. In general we could imagine to define in a similar way $f(A)$ for any $f : \mathbb{R} \to \mathbb{R}$. An observable is *positive* if gives only positive results, in symbols we can reformulate this property as $A \geq 0 \Longleftrightarrow \exists B \in \mathcal{O} : A \equiv B^2$ (there with $\equiv$ we just mean that operationally the two observables A and B^2 gives the same values).

- *States.* We imagine that a certain physical object under study can be *prepared* in such a way that it is meaningful to speak about repeated experiments on the *same* entity. This entity is the *state* $\omega \in \mathcal{S}$ of the system under consideration. E.g. the state of the atoms in the Stern–Gerlach experiment beam, the state of a particle in motion in a particle accellerator. (And what about "the state of world"?) There is a relation between measurements on states and values of observables and it is "statistical" in the sense that $\omega(A) = \langle \omega, A \rangle \in \mathbb{R}$ represent the measuring of A on the state ω, has to be considered as an average over "experiences". Operationally we measure an observable A in a given state ω by perfoming a sequence of repeated experiments and taking the average

$$\omega(A) = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} m_{\omega}^{(i)}(A),$$

where each $m_{\omega}^{(i)}(A)$ is the i-th measurament of A in the state ω. A state is a map $\omega : \mathcal{O} \to \mathbb{R}$ understood as all the values it takes on every possible observable $\omega \equiv \{\omega(A) : A \in \mathcal{O}\}$.

We have the following relations between states and observables. You know that different states exists because when we measure an observable we get different numbers:

$$\omega(A) = \omega^{'}(A), \forall A \in \mathcal{O} \Longleftrightarrow \omega = \omega^{'}.$$

You know that two observables are different because there is a state where they give different values:

$$\omega(A) = \omega(B), \forall \omega \in \mathcal{S} \Longleftrightarrow A = B.$$

With respect to the operations we defined on observable we obtain the followin relations:

$$\omega(\lambda A) = \lambda \omega(A), \qquad \omega(A^n + A^m) = \omega(A^n) + \omega(A^m).$$

$$\omega(A^0) = 1 \Longrightarrow A^0 = 1, \omega(1) = 1.$$

An observable is positive iff its value on any state is positive:

$$A \geqslant 0 \Longleftrightarrow A = B^2 \Longleftrightarrow \forall \omega: \omega(A) = \omega(B^2) \geqslant 0.$$

Therefore states are positive and normalized linear functionals on $\mathcal{O}$. We introduce a norm on $\mathcal{O}$ which measure the size of an observable $A \in \mathcal{O}$ via the largest possible value of a state on it:

$$\|A\| = \sup_{\omega \in \mathcal{S}} |\omega(A)|$$

Then

$$\|\lambda A\| = |\lambda| \|A\|, \quad \|A\| = 0 \Longrightarrow A = 0.$$

We have also

$$\|A^2\| = \|A\|^2.$$

Indeed

$$\omega(\|A\| \pm A) = \|A\| \pm \omega(A) \geqslant 0 \text{``}\Longrightarrow\text{''} \|A\| \pm A \geqslant 0.$$

$$\|A\|^2 - A^2 = (\|A\| + A)(\|A\| - A) \geqslant 0 \Longrightarrow \omega(\|A\|^2 - A^2) \geqslant 0 \Longrightarrow \|A\|^2 - \omega(A^2) \geqslant 0.$$

On the other hand

$$0 \leqslant (\|A\| \pm A)^2 = \|A\|^2 + A^2 \pm 2\|A\|A \Longrightarrow 2\|A\||\omega(A)| \leqslant \|A\|^2 + \omega(A^2) \leqslant \|A\|^2 + \|A^2\|$$

taking sup over ω in $2\|A\||\omega(A)| \leqslant \|A\|^2 + \|A^2\|$ we get $\|A\|^2 \leqslant \|A^2\|$.

The states induce a linear structure over $\mathcal{O}$: we can define a new observable C by doing

$$\omega(C) = \omega(A) + \omega(B),$$

for given $A, B \in \mathcal{O}$. We can extend $\mathcal{O}$ to a linear space and

$$\|A + B\| \leqslant \|A\| + \|B\|.$$

So at this point if we assume completeness we will have a Banach space, but we are still not accounting for sequentials measurements. What about AB? Is not possible to define this using the previous arguments (i.e. via duality with states) if the observables are not simultaneously measurable (think about position and speed of a ball or frequency and duration of a musical note). If you cannot measure them simultaneously, then you cannot recover $\omega(AB)$ from $\omega(A)$ and $\omega(B)$.

It is reasonable to postulate that a **physical system** is defined by the set of its observable endowed with the operation of multiplication with scalars, addition and squaring (as we discussed above). That is to say that two physical systems are to be considered equivalent if their set of observables can be mapped one onto the other while preserving these structures. On such a structure one can define a notion of product (not associative in genera) via

$$A \circ B = \frac{1}{2}[(A+B)^2 - A^2 - B^2].$$

See in the book of Strocchi the discussion on this point at page 19, working with *Jordan algebras*. In order to obtain a well behaved mathematical theory we will introduce now an assumption which, while compatible with the previous discussion, cannot be justifyied on empirical ground.

Crucial techinical assumption. $\mathcal{O} \subseteq \mathcal{A}$ where $\mathcal{A}$ is a (non-commutative) algebra over $\mathbb{C}$ with involution $A \mapsto A^*$ and such that the following properties are true

$$(\lambda A + \beta B)^* = \bar{\lambda} A^* + \bar{\beta} B^*, \qquad (AB)^* = B^* A^*$$

$$\forall A \in \mathcal{A}, \quad A^* A \geq 0, \qquad \omega(A^* A) \geq 0 \qquad \omega \in \mathcal{S}$$

$$\|AB\| := \sup_{\omega \in \mathcal{S}} |\omega(AB)| \leq \|A\| \|B\|. \qquad \|A^* A\| = \|A\| \|A^*\|.$$

One simple consequence: take $\lambda \in \mathbb{R}$

$$0 \leq \omega((\lambda A + 1)^*(\lambda A + 1)) = \lambda^2 \omega(A^* A) + \lambda \omega(A^*) + \lambda \omega(A) + 1$$

then $\omega(A^*) = \overline{\omega(A)}$ and from this we have $\|A^*\| = \|A\|$.

These technical assumptions can be implemented by assuming the following more coincise setting:

Mathematical model for a physical system.

A physical system is the given of observables and states,

- Observables form a *C^*-algebra $\mathcal{A}$ with unity.*

- States $\mathcal{S}$ are normalized positive linear functionals on $\mathcal{A}$. We assume the set of states to be *full* (i.e. it separates the observables). Moreover observables should separate states (but this is by definition). Usually $\mathcal{S}$ is only a subset of all the positive linear functionals.

Example. Classical mechanical system $(q, p) \in \Gamma \subseteq T^* \mathbb{R}^n \approx \mathbb{R}^n \times \mathbb{R}^n$ where q is position and p momentum. The set of observables are the (continuous) functions $\mathcal{A} = C(\Gamma, \mathbb{C})$ $f^*(q, p) = \overline{f(q, p)}$. The states are (a subset of) the probability measures on Γ:

$$\omega(f) = \int_\Gamma f(q, p) \omega(\mathrm{d}q \times \mathrm{d}p).$$

$$\|f\| = \sup_{\omega \in \mathcal{S}} |\omega(f)|.$$

In classical physics one assume that states of the form $\omega = \delta_{(q_0, p_0)}$ are possible, these states are characterised by the fact that the *dispersion*

$$\Delta_\omega(f) = [\omega(f^2 - \omega(f)^2)]^{1/2} \geq 0,$$

is zero for all observables.

3 C^*-algebras

We discuss now the implication of the basic assumption on a physical system. Below a, b, c, are arbitrary elements of $\mathcal{A}$ and $\lambda, \mu \in \mathbb{C}$ with $\bar{\lambda}$ the complex conjugate of λ.

References: [Str08], [Nai11].

Definition 1. *A C^*-algebra $\mathcal{A}$ is an associative algebra over $\mathbb{C}$ which is endowed with the following additional structures: a norm $\|\cdot\|$ for which $\mathcal{A}$ is complete and which satisfy $\|ab\| \leq \|a\| \|b\|$ for all $a, b \in \mathcal{A}$ and an antilinear involution $*: \mathcal{A} \longrightarrow \mathcal{A}$ for which $(ab)^* = b^* a^*$. These structures satisfy the following compatibility condition (C^* condition)*

$$\|a^* a\| = \|a\|^2, \qquad a \in \mathcal{A}.$$

We will usually denote by $1 = 1_{\mathcal{A}}$ the unity of $\mathcal{A}$. An element $a \in \mathcal{A}$ is *self-adjoint* if $a = a^*$, is *normal* if $a^* a = a a^*$, is unitary if $a^* a = a a^* = 1_{\mathcal{A}}$.

Note that $\|a\|^2 = \|a^* a\| \leq \|a^*\| \|a\|$, therefore $\|a^*\| = \|a\|$, i.e. the involution is isometric. Moreover $1^* a = (a^* 1)^* = (a^*)^* = a$ and therefore $1^* = 1^* 1 = 1$, from which follows $\|1\| = 1$.

Example 2. The algebra of all continuous complex-valued functions $C(X)$ on a compact space topological Hausdorff space X wrt. the pointwise product and endowed with the supremum norm

$$\|f\| = \sup_{x \in X} |f(x)|, \qquad f \in C(X)$$

is a C^*-algebra.

Example 3. Let $\mathcal{H}$ be an Hilbert space. The set of all bounded linear operators $\mathcal{L}(\mathcal{H})$ on $\mathcal{H}$ together with the operator norm

$$\|A\| = \sup_{\varphi \neq 0} \frac{\|A\varphi\|}{\|\varphi\|}, \qquad A \in \mathcal{L}(\mathcal{H}),$$

and the involution given by the adjuction wrt. the scalar product of $\mathcal{H}$, is a C^* algebra, indeed by the property of the Hilbert space norm we have

$$\|A^* A\| = \sup_{\|\varphi\|=1} \|A^* A\varphi\| = \sup_{\|\varphi\|=\|\psi\|=1} \langle \psi, A^* A\varphi \rangle = \sup_{\|\varphi\|=\|\psi\|=1} \langle A\psi, A\varphi \rangle \leq \|A\|^2$$

and

$$\|A\|^2 = \sup_{\|\varphi\|=1} \|A\varphi\|^2 = \sup_{\|\varphi\|=1} \langle A\varphi, A\varphi \rangle = \sup_{\|\varphi\|=1} \langle \varphi, A^* A\varphi \rangle \leq \|A^* A\|.$$

Any norm-closed subalgebra $\mathcal{B}$ of $\mathcal{L}(\mathcal{H})$ which is self-adjoint, i.e. $\mathcal{B} = \mathcal{B}^*$ is a *concrete C^*-algebra*. For example, the compact operators form such a subalgebra or the C^*-algebra $C(T)$ generated by a single bounded self-adjoint operator T, i.e. the closure of all the polynomials in T, T^*, I.

Example 4. The subalgebra $C^*(a) \subseteq \mathcal{A}$ generated by $a \in \mathcal{A}$ and the unity is a C^*-algebra with the restiction of the norm and the involutions of $\mathcal{A}$. The Banach algebra generated by a set of elements $a_1, \ldots, a_n$ is just the closure of all the polynomials in $a_1, \ldots, a_n$ and in their adjoints.

We call a self-adjoint iff $a = a^*$, a is *normal* if $a a^* = a^* a$. Any a can be decomposed into $a = b + ic$ with b, c self-adjoint. If a is normal then $C^*(a)$ is Abelian (i.e. commutative).

Keep in mind that, for us, the observables of a physical system will be self-adjoints elements of an (abstract) C^* algebra.

3.1 Spectral theory

Definition 5. *A Banach algebra $\mathcal{B}$ is a Banach space with a product such that $\|ab\| \leq \|a\| \|b\|$.*

Example 6. Take $L^1(\mathbb{R})$ or $L^1(\mathbb{R}_{\geq 0})$ with the convolution product and their natural norm. Then they are Banach algebras ($\|ab\| \leq \|a\| \|b\|$). (I think they are not C^*-algebras for the complex conjugation). For the convolution product on $L^1(\mathbb{R}_{\geq 0})$ take

$$(f * g)(t) = \int_0^t f(t - s) g(s) \mathrm{d}s, \qquad t \geq 0.$$

In the following we will work with Banach algebras (denoted $\mathcal{B}$) and I will tell explicitly when the algebra is supposed to satisfy the C^*-condition.

In any (unital) Banach algebra $\mathcal{B}$ we can define the *spectrum* $\sigma(a) = \sigma_{\mathcal{B}}(a)$ of an element $a \in \mathcal{B}$ to be the set of $\lambda \in \mathbb{C}$ for which $(\lambda - a)$ is not invertible in $\mathcal{B}$. The complement of the spectrum is called the *resolvent set* and $R_a(\lambda) = (\lambda - a)^{-1}$ is the resolvent function.

Theorem 7. *For any $a \in \mathcal{B}$, the spectrum $\sigma(a)$ is a non-empty compact set and the resolvent function is analytic in $\mathbb{C} \setminus \sigma(a)$.*

Proof. For $|\lambda|$ large enough (i.e. $|\lambda| > \|a\|$) we have

$$R_a(\lambda) = (\lambda - a)^{-1} = \sum_{n \geq 0} \lambda^{-1-n} a^n \tag{1}$$

where the series is convergent in $\mathcal{B}$. This shows that $R_a(\lambda)$ is analytic with Laurent expansion at infinity and there $R_a(\lambda) \to 0$. On the other hand, if $\mu - a$ is invertible, we have the convergent series expansion

$$R_a(\lambda) = (\lambda - a)^{-1} = \sum_{n \geq 0} (\mu - a)^{-n-1} (\lambda - \mu)^n$$

valid in a neighborhood of $\mu \in \mathbb{C}$. So the resolvent is analytic in the complement of $\sigma(a)$ and $(\sigma(a))^c$ is an open set containing all $\lambda \in \mathbb{C}$ such that $|\lambda| > \|a\|$, therefore $\sigma(a)$ is compact. Assume that $\sigma(a)$ is empty. Then $R_a(\lambda)$ would be an entire function of λ which go to zero at infinity. As a consequence $R_a(\lambda)$ should be constant. Indeed this is true for $f(R_a(\lambda))$ for any continuous linear functional f and by Hanh-Banach this implies that $R_a(\lambda) = 0$. Therefore the spectrum must be non-empty. $\square$

Proposition 8. *(Spectral radius formula) For any $a \in \mathscr{B}$ we have*

$$\rho(a) := \sup_{\lambda \in \sigma(a)} |\lambda| = \lim_{n \to \infty} \|a^n\|^{1/n} \leq \|a\|$$

with equality in case of a normal element of a C^*-algebra.

Remark 9. This shows that C^* are quite rigid, in the sense that the algebraic data defines the norm. The quantity $\varrho(a)$ is called the spectral radius of a.

Proof. Let $r = \inf_{n \to \infty} \|a^n\|^{1/n}$, then $r \leq \|a\|$. Take m such that $\|a^m\|^{1/m} \leq r + \varepsilon$, then

$$r \leq \liminf_{n \to \infty} \|a^n\|^{1/n} \leq \limsup_{n \to \infty} \|a^n\|^{1/n} = \limsup_{n \to \infty} \|a^{mk(n,m)+\ell(n,m)}\|^{1/n} \leq \limsup_{n \to \infty} \|a^m\|^{k(n,m)/n} \|a^{\ell(n,m)}\|^{1/n}$$

$$\leq \limsup_{n \to \infty} (r + \varepsilon)^{mk(n,m)/n} = r + \varepsilon.$$

Therefore the limit indeed exists and equality is true for normal elements since

$$\|a^2\|^2 = \|a^* a^* a a\| = \|a a^* a^* a\| = \|a^* a\|^2 = \|a\|^4$$

and therefore $\left\|a^{2^k}\right\| = \|a\|^{2^k}$ and $\|a\| = \lim_{k \to \infty} \left\|a^{2^k}\right\|^{2^{-k}} = \lim_{n \to \infty} \|a^n\|^{1/n}$. By the convergence of the resolvent series (1) we have that $r = \sup_{\lambda \in \sigma(a)} |\lambda|$. $\square$

A linear functional $\varphi: \mathscr{B} \to \mathbb{C}$ is multiplicative if $\varphi(ab) = \varphi(a) \varphi(b)$. The space $\mathscr{B}^*$ of linear functionals on $\mathscr{B}$ is a Banach space with the norm $\|\varphi\| = \sup_{a \in \mathscr{B}, \|a\| \leq 1} |\varphi(a)|$. The weak-$*$ topology on $\mathscr{B}^*$ is the topology generated by the system of neighborhoods of the form

$$N_{\psi, a_1, \ldots, a_n, \varepsilon} = \{\varphi \in \mathscr{B}' : |\psi(a_i) - \varphi(a_i)| \leq \varepsilon, \quad i = 1, \ldots, n\}$$

for $\psi \in \mathscr{B}'$, $a_1, \ldots, a_n \in \mathscr{B}$, $\varepsilon > 0$. It is the coarsest topology for which the maps $\varphi \in \mathscr{B}' \mapsto \hat{a}(\varphi) = \varphi(a) \in \mathbb{C}$ are continuous for all $a \in \mathscr{B}$. The Banach-Alaoglu theorem ensure that the closed unit ball of $\mathscr{B}^*$ is compact for the weak-$*$ topology.

Lemma 10. *The space $\Sigma(\mathscr{B})$ of all the multiplicative linear functionals on $\mathscr{B}$ is a compact Hausdorff space when endowed with the weak-$*$ topology.*

Proof. Let $\varphi \in \Sigma(\mathscr{B})$. Assume that $1 = \varphi(a) > \|a\|$, let b be the solution to $b = 1 + ab$ which exists since $\|a\| < 1$, then $\varphi(b) = \varphi(1) + \varphi(a)\varphi(b)$ which implies $\varphi(1) = 0$ and therefore $\varphi(a) = \varphi(a1) = \varphi(a)\varphi(1) = 0$ giving a contradiction. Therefore we have $|\varphi(a)| \leq \|a\|$, that is φ is continuous. On the space of all linear functionals we can consider the norm $\|\varphi\| = \sup_{\|a\|=1} |\varphi(a)|$ and obtain that $\|\varphi\| = 1$. Therefore by Banach-Alaoglu the unit ball is weakly-$*$ compact. Limits of multiplicative functionals are multiplicative, so $\Sigma(\mathscr{B})$ is also compact. $\square$

For any $a \in \mathscr{B}$ we can define a continuous function $\hat{a}: \Sigma(\mathscr{B}) \to \mathbb{C}$ as $\hat{a}(\varphi) = \varphi(a)$, it is called the Gelfand transform of a. The function is continuous by the definition of the weak-$*$ topology on linear functionals.

Theorem 11. *The Gelfand transform is a contractive algebra homomorphism from $\mathscr{B}$ to $C(\Sigma(\mathscr{B}))$. The image algebra separates the points of $\Sigma(\mathscr{B})$.*

Proof. We have $\widehat{ab}(\varphi) = \varphi(ab) = \varphi(a)\varphi(b) = \hat{a}(\varphi)\,\hat{b}(\varphi)$ and $\|\hat{a}\| = \sup_{\varphi\in\Sigma(\mathscr{B})}|\hat{a}(\varphi)| \le \|a\|$. For any two points $\varphi \ne \psi$ in $\Sigma(\mathscr{B})$ there exists $a\in\mathscr{B}$ such that $\varphi(a) \ne \psi(a)$, therefore $\hat{a}(\varphi) \ne \hat{a}(\psi)$. $\qquad\square$

For commutative Banach algebra $\mathscr{B}$ any proper maximal ideal is closed and any proper ideal is contained in a proper maximal ideal. Moreover let $\mathscr{J}$ a proper maximal ideal, then the quotient $\mathscr{B}\backslash\mathscr{J}$ is a Banach algebra and any $a\in\mathscr{B}\backslash\mathscr{J}$ is invertible, since otherwise $(a+\mathscr{J})\mathscr{B}$ would be a proper ideal containing $\mathscr{J}$. But a Banach algebra where any element is invertible must be $\mathbb{C}$ (Gelfand–Mazur theorem) so $\mathscr{B}\backslash\mathscr{J} = \mathbb{C}$ and $\mathscr{J}$ is of codimension 1.

Remark 12. (Gelfand–Mazur) Assume that all the elements except 0 of a Banach algebra $\mathscr{B}$ are invertible, then take $a\in\mathscr{B}$ and $\lambda\in\sigma(a)$. Since $\lambda - a$ is assumed to be not invertible we must have $\lambda - a = 0$ and therefore $a = \lambda$. That is $\mathscr{B} = \mathbb{C}$.

A consequence is:

Corollary 13. *Assume $\mathscr{B}$ is commutative. If $a\in\mathscr{B}$ is invertible iff $\hat{a}\in\Sigma(\mathscr{B})$ is invertible, that is $\hat{a}(\varphi) \ne 0$ for all $\varphi\in\Sigma(\mathscr{B})$. Therefore $\sigma(a) = \sigma(\hat{a}) = \{\varphi(a): \varphi\in\Sigma(B)\}$ and $\sup\{|\lambda|: \lambda\in\sigma(a)\} = \|\hat{a}\|_\infty$.*

Proof. If a is invertible then $1 = \varphi(aa^{-1}) = \varphi(a)\varphi(a^{-1})$ so $(\hat{a})^{-1} = \widehat{(a^{-1})}$ and therefore $\hat{a}(\varphi) \ne 0$ for all φ. If a is not invertible, then $a\mathscr{B}$ is a proper ideal of $\mathscr{B}$ since $1\notin a\mathscr{B}$. Let $\mathscr{J}$ be a maximal proper ideal containing $a\mathscr{B}$ and let $\varphi = 0$ on $\mathscr{J}$ and $\varphi(1) = 1$. Then φ is multiplicative and $\hat{a}(\varphi) = 0$. To prove that $\sigma(\hat{a}) = \{\varphi(a): \varphi\in\Sigma(B)\}$ observe that if $\lambda\in\sigma(\hat{a})$ then $\lambda - a$ is not invertible and $\mathscr{J} = (\lambda - a)\mathscr{B}$ is an ideal contained in a maximal ideal. If φ is the corresponding linear functional then $\varphi(\lambda - a) = 0$ since obviously $\lambda - a\in\mathscr{J}$ and therefore $\varphi(a) = \lambda$. So for any $\lambda\in\sigma(a)$ there is a multiplicative φ for which $\lambda = \varphi(a)$. So $\sigma(\hat{a}) \subseteq \{\varphi(a): \varphi\in\Sigma(B)\}$. On the other hand if $\varphi(\lambda - a) = 0$ then $(\lambda - a)\mathscr{B} \subseteq \ker(\varphi)$ therefore $\lambda - a$ cannot be invertible because otherwise if $(\lambda - a)^{-1}$ exists then $1 = (\lambda - a)^{-1}(\lambda - a)\in(\lambda - a)\mathscr{B}\subseteq\ker(\varphi)$ so $\ker(\varphi)$ cannot be a proper ideal. $\qquad\square$

Example 14. For $L^1(\mathbb{R};\mathbb{C})$ with product given by convolution the Gelfand transform is the Fourier transform. For $L^1(\mathbb{R}_+;\mathbb{C})$ with half-line convolution the Gelfand transform is the Laplace transform.

In the case of C^* algebras we have an isomorphism $\mathscr{A} \approx C(\Sigma(\mathscr{A}))$ of C^* algebras.

Theorem 15. (Gelfand–Naimark) *Any abelian C^*-algebra $\mathscr{A}$ is isometrically isomorphic to $C(\Sigma(\mathscr{A}))$.*

Proof. We need to check the correct behaviour of the involution, that is $\varphi(a^*) = \overline{\varphi(a)}$. Assume a is self-adjoint, then we can form (by convergent series in the Banach algebra)

$$U(t) = \exp(iat) = \sum_{n\ge 0} \frac{(it)^n}{n!}a^n$$

and check that it is unitary in $\mathscr{A}$, i.e. $U(-t) = U(t)^*$ and $U(-t)U(t) = \exp(-iat)\exp(iat) = 1$.

$$\varphi(U(t)) = \sum_{n \geqslant 0} \frac{(it)^n}{n!} \varphi(a^n) = \sum_{n \geqslant 0} \frac{(it)^n}{n!} \varphi(a)^n = \exp(it\varphi(a))$$

but now

$$|\varphi(U(t))| \leqslant \|\varphi\| \, \|U(t)\| = \|U(t)\| = 1$$

since $\|U(t)\|^2 = \|U(t)^*U(t)\| = \|1\| = 1$. Therefore $|\exp(it\varphi(a))| \leqslant 1$ for all $t \in \mathbb{R}$ and this implies that $\varphi(a) \in \mathbb{R}$.

Decomposing any $a \in \mathscr{A}$ as $a = b + ic$, with b, c self-adjoint, we obtain that

$$\varphi(a^*) = \varphi(b - ic) = \varphi(b) - i\varphi(c) = \overline{\varphi(b) + i\varphi(c)} = \overline{\varphi(a)},$$

that is $\hat{a}^* = \bar{\hat{a}}$. Remember that for C^*-algebras we have that if a is normal then $\|a\|_{\mathscr{A}} = \varrho_{\mathscr{A}}(a)$ therefore we have

$$\|a\|_{\mathscr{A}} = \|\hat{a}\|_{C(\Sigma(\mathscr{B}))}.$$

Now use againg the C^*condition to get for any $a \in \mathscr{A}$ (observe that a^*a is self-adjoint)

$$\|a\|^2 \underset{C^*}{=\!=} \|a^*a\| = \|\widehat{a^*a}\| = \|\hat{a}^* \hat{a}\|_\infty = \|\bar{\hat{a}} \hat{a}\|_{C(\Sigma(\mathscr{A}))} \underset{C^*}{=\!=} \|\hat{a}\|^2_{C(\Sigma(\mathscr{A}))}$$

so we conclude that the transform is an isomorphism. It is one to one since if $\varphi(a) = \varphi(b)$ for all φ then $\varphi(a - b) = 0$ for all φ, this implies that $\|a - b\| = 0$. □

Remark 16. Multiplicative linear functionals in $\mathscr{B}$ corresponds to maximal proper ideals. See Strocchi for the details.

> **Exercise 1.** Take the commutative C^* algebra $\mathscr{A}$ of diagonal $n \times n$ matrices. Prove that it is a C^*-algebra with the structure inherited from the space of all matrices, i.e. norm is the operator norm, involution is the adjoint, product is product of matrices. Try to work out the space $\Sigma(\mathscr{A})$.

The Gelfand–Naimark theorem allows a functional calculus on the normal elements of a C^* algebra.

If $a \in \mathscr{A}$ is normal, then the C^* algebra $C^*(a)$ (generated by $1, a, a^*$) is Abelian and therefore isomorphic to $C(\Sigma(C^*(a)))$ but $\varphi \in \Sigma(C^*(a))$ is uniquely determined by the value of $\varphi(a) \in \mathbb{C}$ since for any polynomial $p(a, a^*)$ we have $\varphi(p(a, a^*)) = p(\varphi(a), \overline{\varphi(a)})$. Then $\sigma(a) = \sigma(\hat{a}) = \{\varphi(a): \varphi \in \Sigma(C^*(a))\}$ and $\Sigma(C^*(a)) = \sigma(a)$. This means that for any $f \in C(\sigma(a))$ there exists a unique $h \in C^*(a)$ such that $\hat{h} = f$ under the Gelfand transform map. In this case we write $h = f(a)$.

Is easy to see that $f(g(a)) = (f \circ g)(a)$, that $f(a)$ is self-adjoint if f is real, etc...

Observe that, since $C^*(f(a)) \subseteq C^*(a)$ for any continuous $f: \sigma(a) \to \mathbb{R}$ and normal a we have

$$\sigma(f(a)) = \{\varphi(f(a)): \varphi \in \Sigma(C^*(a))\} = \{f(\varphi(a)): \varphi \in \Sigma(C^*(a))\} = f(\sigma(a)).$$

With non-normal elements one has a similar relations, however not is such great generality. Let $a \in \mathscr{A}$ and $f(z) = \sum_{n \geqslant 0} c_n z^n$ be holomorphic in a neighborhood of $\sigma(a)$, then $f(a) = \sum c_n a^n$ is well defined and $\sigma(f(a)) = f(\sigma(a))$ (spectral mapping principle). This is easy to see for polynomials. An interesting case is $\sigma(a^{-1}) = (\sigma(a))^{-1}$.

Moreover $\sigma(ab)$ and $\sigma(ba)$ differ at most by $\{0\}$. Indeed let $\lambda \notin \sigma(ba)$ and let $c = (\lambda - ba)^{-1}$ then

$$(\lambda - ab)(1 + acb) = (\lambda + \lambda acb - ab - abacb) = (\lambda - ab + a(\lambda - ba)cb) = (\lambda - ab + ab) = \lambda$$

so $\lambda - ab$ is also inverible unless $\lambda = 0$.

If a is unitary (i.e $aa^* = 1 = a^* a$) then $\sigma(a) \subseteq \{z : |z| = 1\}$.

If a is self-adjoint then $\sigma(a)$ contains either $\pm\|a\|$: indeed recall that $\sigma(a)$ is compact. For selfadjoint a we have $\sigma(a) \subseteq \mathbb{R}$ and by compactness and the fact that $\varrho(a) = \|a\|$ we conclude that there exists $\lambda \in \mathbb{R}$ such that $|\lambda| = \|a\|$.

The continuous functional calculus for a self-adjoint element a can be developed also as follows. Consider the map $T : p \mapsto p(a)$ where p runs over complex polynomials. Then by the spectral mapping principle we have $\sigma(p(a)) = p(\sigma(a))$ and $\|p(a)\| = \varrho(p(a)) = \sup_{\lambda \in \sigma(a)} |p(\lambda)|$ so $\|p(a)\| = \|p\|_{C(\sigma(a))}$. By Stone-Weierstrass, polynomials are dense in $C(\sigma(a))$ (since $\sigma(a)$ is compact) and we have that T extends by continuity to a map on $T : C(\sigma(a)) \to C^*(a)$ moreover $T(f)T(g) = T(fg)$, $T(f)^* = T(\bar{f})$ and $\|T(f)\| = \|f\|$ so it is an isomorphism of C^* algebras.

3.2 Positive elements

Definition 17. *We call $a \in \mathscr{A}$ positive if a is self-adjoint and $\sigma(a) \subseteq \mathbb{R}_+$ and we denote with $\mathscr{A}_+$ the set of positive elements of $\mathscr{A}$ and also write $a \geqslant 0$.*

Some properties of positive elements have simple and clever proofs.

- If $a, b \in \mathscr{A}_+$ and $a + b = 0$ then $a = b = 0$. Indeed $\sigma(-b) = -\sigma(b) \in \mathbb{R}_+ \Longrightarrow \sigma(b) = \{0\} \Longrightarrow b = 0$. (use the spectral mapping principle and that $\|b\| = \varrho(b) = 0$). Now take $a + b + c = 0$ with $a, b, c \in \mathscr{A}_+$

- If a is self-adjoint and $\|a\| \leqslant 1$ then $a \in \mathscr{A}_+$ iff $\|1 - a\| \leqslant 1$. Indeed if $a \geqslant 0$ then $\sigma(1 - a) \subseteq [0, 1]$ and $\varrho(1 - a) = \|1 - a\| \leqslant 1$. Conversely $\|1 - a\| \leqslant 1, \|a\| \leqslant 1$ imply that $\sigma(a)$ is contained in the intersection of two balls of radius 1 centred in 1 and 0, that is $\sigma(a) \subseteq [0, 1] \subseteq \mathbb{R}_+$.

- $\mathscr{A}_+$ is a cone, i.e. $\lambda a \geqslant 0$ if $a \geqslant 0$ for all $\lambda > 0$. Moreover if $a, b \geqslant 0$ and $\|a\|, \|b\| \leqslant 1$ then let $c = (a + b)/2$ and observe that $\|c\| \leqslant 1$ and

$$\|1 - c\| \leqslant \frac{1}{2}\|1 - a\| + \frac{1}{2}\|1 - b\| \leqslant 1$$

so $c \geqslant 0$. Therefore $\mathscr{A}_+$ is closed convex cone. It is closed since if $a_n \to a$ and $a_n \geqslant 0$ then we can rescale the sequence in such a way to get $\sup_n \|a_n\| \leqslant 1$ and therefore $\|1 - a\| = \lim \|1 - a_n\| \leqslant 1$ and $\|a\| \leqslant 1$ so $a \geqslant 0$.

- By functional calculus every positive element has a positive square root $a^{1/2}$. It can be constructed as limit of polynomials in a (without constant term). Therefore the product of two commuting positive elements is positive. The positive square root is unique, indeed if $b, c \geqslant 0$ are such that $b^2 = c^2 = a$ we have that a, b, c commute among themselves and

$$0 = (b^2 - c^2)(b - c) = b^3 + b^2 c + c^2 b - c^3 = (b - c)^2(b + c) \geqslant 0$$

so we need to have $(b - c)^2 b = (b - c)^2 c = 0$ so $0 = (b - c)^2 b - (b - c)^2 c = (b - c)^3$ and therefore $b = c$.

- By functional calculus one can decompose any self-adjoint element into the difference of two positive elements $a = a_+ - a_-$.

- Any element $a \in \mathscr{A}$ is the sum of four unitaries. Indeed write $a = p + iq$ with self-adjoint elements p, q and then assuming $\|p\|, \|q\| \leq 1$ consider the unitaties $p \pm i(1 - p^2)^{1/2}$ and $q \pm i(1 - q^2)^{1/2}$.

Note that in $\mathscr{L}(\mathscr{H})$ any operator in the form A^*A is positive (i.e. it has positive spectrum) .

This was conjectured to be true also in abstract C^* algebras but Gelfand and Naimark could not prove it. The result was proven later by Kelley and Vaught and surprisingly the proof is quite nontrivial (but not long). We skip it, just register the fact as

Theorem 18. *In a C^* algebra the following properties are equivalent:*

1) $a \in \mathscr{A}_+$,   *2) $a = b^2, b = b^*$,*   *3) $\|1 - a / \|a\|\| \leq 1$,*   *4) $a = c^*c$.*

As we have seen property 3) implies that $\mathscr{A}_+$ is a closed convex cone. We say that $a \geq b$ if $a - b \in \mathscr{A}_+$.

Remark 19. If $a, b \geq 0$ then $a + b \geq 0$ however positivity is tricky due to non-commutativity. For example even if $0 \leq a \leq b$ it does not follow in general that $a^2 \leq b^2$ unless a, b commute. If we try to define $|a| = (a^*a)^{1/2}$ then is not true that $|a + b| \leq |a| + |b|$.

Let us give some true inequalities.

- We have $a \leq \|a\|$ and $a^2 \leq \|a\| a$ as easily seen from spectral consideations.

- $a \geq 0$ implies $cac^* \geq 0$ and by difference $a \geq b \Longrightarrow cac^* \geq cbc^*$.

- $a \geq b \geq 0$ then $(\lambda - a)^{-1} \leq (\lambda - b)^{-1}$ for $\lambda \geq 0$. (see Meyer for a proof)

- $a \geq b \Longrightarrow f(a) \geq f(b)$ for functions of the form $f(x) = x^\alpha$ with $\alpha \in (0, 1)$.

Let us note the following.

Proposition 20. *Let ω is a continuous linear functional such that $\|\omega\| = \omega(1) = 1$ then $\omega(a^*) = \overline{\omega(a)}$.*

Proof. We can assume that a is s.a. since then is easy to conclude. Assume that $\omega(a) = f + ig$ with $f, g \in \mathbb{R}$ I need to prove that $g = 0$. Take $a + ic$ with $c \in \mathbb{R}$ and observe that $(a + ic)^*(a + ic) = a^2 + c^2$ then $\omega(a + ic) = f + i(g + c)$ so

$$f^2 + (g + c)^2 = |\omega(a + ic)|^2 \leq \|a + ic\|^2 \underset{C^*}{=} \|(a + ic)^*(a + ic)\| = \|a^2 + c^2\| \leq \|a^2\| + c^2 \leq \|a\|^2 + c^2.$$

Now c is arbitrary so we get that $g^2 + 2gc \leq \|a\|^2$ which is impossible unless $g = 0$.   □

3.3 States on C^* algebras

A linear functional on $\mathscr{A}$ is positive if $\omega(a) \geq 0$ for all $a \in \mathscr{A}_+$.

For positive linear functionals Cauchy-Schwarz inequality holds true:

$$|\omega(a^*b)|^2 \leqslant \omega(a^*a)\omega(b^*b).$$

Then we have

Proposition 21. *A linear functional $\omega \in \mathscr{A}^*$ is positive iff $\|\omega\| = \omega(1)$.*

Proof. Note that $\|a\| - a \geqslant 0$ then if ω is positive we have $\|a\|\omega(1) \geqslant \omega(a)$. On the other hand the Cauchy–Schwartz inequality holds for ω and

$$|\omega(a)|^2 \leqslant \omega(1)\omega(a^*a) \leqslant \omega(1)^2\|a^*a\| \leqslant \omega(1)^2\|a\|^2,$$

so ω is bounded and $\|\omega\| \leqslant |\omega(1)| = \omega(1)$. On the other hand if ω is bounded and $\|\omega\| = \omega(1)$ we can assume that $\omega(1) = 1$. Then for any $a \geqslant 0$ with $\|a\| = 1$ we have also $|\omega(1-a)| \leqslant \omega(1) = 1$ which implies $|1 - \omega(a)| \leqslant 1$ but since $\omega(a) = \omega(a^*) = \overline{\omega(a)}$ we have $\omega(a) \in \mathbb{R}$ and therefore $\omega(a) \geqslant 0$.   □

Proposition 22. *Positive linear functionals separate $\mathscr{A}$ and $a \in \mathscr{A}_+$ iff $\omega(a) \geqslant 0$ for all positive linear functionals ω.*

Proof. Assume that $\omega(a) = 0$ for all positive ω. Decompose $a = b + ic$ with self-adjoint b, c. Then $\omega(b) = \omega(c) = 0$. But this implies that $\hat{b} = \hat{c} = 0$ and by Gelfand's isomorphism that $b = c = 0$ (recall that multiplicative functionals are bounded and therefore positive). Let us now prove the second part. If $\omega(a) \geqslant 0$ we have that $\omega(a) = \omega(a^*)$ and $\omega(a - a^*) = 0$. Since positive functionals separate $\mathscr{A}$ we must have $a = a^*$. But then taking ω to be multiplicative we deduce that $\sigma(a) \subseteq \mathbb{R}_+$, that is $a \in \mathscr{A}_+$. Let us prove the first part.   □

Recall that a state is a normalized positive linear functional on $\mathscr{A}$. The set of positive linear functionals of norm $\leqslant 1$ is a compact convex closed set (in the weak-$*$ topology). By a theorem of Krein–Milman it is the closed convex hull of its extreme points which are called *pure states*. Recall that an extreme point of a convex set is a point which cannot be written as the convex combination of other points. Pure states separate points in $\mathscr{A}$.

Example 23. On $\mathscr{L}(H)$ the states given by $\omega(A) = \langle x, Ax \rangle$ for some normalized $x \in H$ are pure states.

3.4 The Gelfand–Naimark–Segal representation and the GN theorem

So far we conceptualized the basic structure of a physical system and the related observation and measurement theory (algebra of observables and the convex set of state of physical system). This applies both to classical and quantum (i.e. non-classical) systems. We also argued that a classical system is given by an algebra of observables given by continuous functions on a "state space". For the moment anything escaping this point of view will be *quantum* therefore we need to take a non-commutative algebra (by the Gelfand-Naimark theorem).

How do we do computations in a non-commutative C^* algebra? We need (concrete) representations of non-commutative C^*-algebras in order to use the theory to make prediction and compare to experiments.

The Gelfand–Naimark–Segal theorem allows to construct representations of C^* algebras on an Hilbert space starting from any state ω (i.e. normalized positive linear functional).

Namely we want to construct a map $\varphi \colon \mathscr{A} \to \mathscr{L}(H)$ for some complex Hilbert space H such that φ is linear, $\varphi(1) = 1$, $\varphi(ab) = \varphi(a)\varphi(b)$ and $\varphi(a^*) = \varphi(a)^*$ where on the r.h.s. the involution is understood as the adjoint in the Hilbert space. This is also called a $*$-homomorphism.

Remark 24. Any multiplicative functional $\varphi \colon \mathscr{A} \to \mathbb{C}$ give a one-dimensional representation on the Hilbert space $H = \mathbb{C}$.

Let us observe that any such representation is necessarily a contraction. Indeed note that if $\lambda - a$ is invertible in $\mathscr{A}$ then exists $c \in \mathscr{A}$ s.t. $c(\lambda - a) = 1$ that implies $\varphi(c)(\lambda - \varphi(a)) = 1$ so $\lambda - \varphi(a)$ is also invertible, that is $\sigma_{\mathscr{L}(H)}(\varphi(a)) \subseteq \sigma_{\mathscr{A}}(a)$. So for C^*-algebras

$$\|\varphi(a)\|_{\mathscr{L}(H)} \underset{C}{=} \varrho_{\mathscr{L}(H)}(\varphi(a)) \leqslant \varrho_{\mathscr{A}}(a) \underset{C}{=} \|a\|.$$

If φ is an isomorphism (on his image), i.e. $\ker(\varphi) = \{0\}$ on has that φ is an isometry since φ^{-1} is another representation and $\|a\| = \|\varphi^{-1}(\varphi(a))\| \leqslant \|\varphi(a)\| \leqslant \|a\|$.

Each unit vector $x \in H$ give rise to a state $\omega \colon a \mapsto \omega(a) = \langle x, \varphi(a)x \rangle$ on $\mathscr{A}$ (generally not a pure one). We will see now that every state on $\mathscr{A}$ arises in this way.

Assume ω is a state and define the Hermitean form on $\mathscr{A}$:

$$\langle a, b \rangle_\omega = \omega(a^*b).$$

The linear space $\mathscr{A}$ with this scalar product is a pre-Hilbert space. Let

$$\mathscr{N} = \{a \in \mathscr{A} \colon \langle a, a \rangle = 0\}$$

the set of zero elements and define the Hilbert space $H_\omega = \overline{\mathscr{A} \backslash \mathscr{N}}$ where the bar denotes the completion wrt. the topology generated by the scalar product $\langle, \rangle_\omega$. Denotes $\|a\|_\omega = \langle a, a \rangle_\omega^{1/2}$ the corresponding norm. Observe that

$$\langle ba, ba \rangle_\omega = \omega(a^*b^*ba) \leqslant \|b^*b\|\omega(a^*a) = \|b\|^2\omega(a^*a) = \|b\|^2\langle a, a \rangle_\omega$$

so the operator $L_b \colon H_\omega \to H_\omega$ defined by $L_b a = ba$ on the dense subset $\mathscr{A}$ is bounded with norm $\|L_b\| \leqslant \|b\|$. Note that it is well defined, since $L_b a = 0$ if $a \in \mathscr{N}$. Moreover $L_b L_c = L_{bc}$ and $L_b^* = L_{b^*}$ as can be easily checked. Therefore $a \mapsto L_a$ is an homomorphism of C^* algebras (since $\{L_a \colon a \in \mathscr{A}\}$ is a C^* subalgebra of $\mathscr{L}(H_\omega)$), indeed recall that $\|L_b\|^2_{\mathscr{L}(H_\omega)} = \|L_b^* L_b\|_{\mathscr{L}(H_\omega)}$. So $\varphi_\omega(a) = L_a$ is a representation of $\mathscr{A}$ on H_ω and if we denote by $\Omega_\omega = [1] \in \mathscr{H}_\omega$ we have $\omega(a) = \langle \Omega_\omega, L_a \Omega_\omega \rangle$.

Note that the set $\{L_a \Omega_\omega \colon a \in \mathscr{A}\} \subseteq H_\omega$ is dense in H_ω. Then one says that Ω_ω is a cyclic vector for the representation φ_ω and that the representation is cyclic.

If K is another Hilbert space supporting a cyclic representation $\pi \colon \mathscr{A} \to \mathscr{L}(K)$ with cyclic vector $\psi \in K$ such that $\omega(a) = \langle \psi, \pi(a)\psi \rangle_K$ then the map $a \in \mathscr{A} \mapsto \pi(a)\psi \in K$ is an densely defined isometry from H_ω to K since

$$\langle a, a \rangle_{H_\omega} = \omega(a^*a) = \langle \pi(a)\psi, \pi(a)\psi \rangle_K.$$

Therefore the cyclic representations of $\mathscr{A}$ associated to a state ω are unique up to isomorphism. In general one call it the GNS representation associated to the state ω.

- A state ω is *faithful* is $\omega(a^*a) = 0 \Rightarrow a = 0$. Which implies that $\|L_a \Omega_\omega\|_\omega = 0 \Rightarrow a = 0$. The GNS representation is faithful if $L_a = 0 \Rightarrow a = 0$ which is a weaker property.

- Consider the commutative setting and let $H = L^2(\Omega, \mathscr{F}, \mu)$ for some probability space $(\Omega, \mathscr{F}, \mu)$ then on this space there are three different C^* algebras acting with pointwise multiplication on the elements of H: that of the continuous functions (taking $\mathscr{F}$ to be the Borel σ-algebra on some compact space K), that of the measurable functions and that of the $L^\infty(\mu)$ functions (i.e. equivalence classes modulo μ-null sets).

- A measure μ on a compact space K with the Borel σ-algebra $\mathscr{F}$ gives a faithful representation of $C(K)$ if the support of μ is K. μ is never faithful on measurable function and by construction is faithful on $L^\infty(\mu)$.

- The space H_ω of the GNS construction can be thought as a non-commutative version of the commutative $L^2(\Omega, \mathscr{F}, \mu)$. However here right multiplication $R_b a = ab$ is not in general given by a bounded operator.

- And one cannot obtain faithful representations by quotienting (like in $L^\infty(\mu)$ because $\mathscr{N}$ is only a left ideal). This is however possible if the state is tracial, i.e. $\omega(ab) = \omega(ba)$.

Since states separate elements of $\mathscr{A}$ there are enough GNS representations to build a faithful representation of any C^* algebra, as stated by the (non-commutative) Gelfand–Naimark theorem.

Theorem 25. *(Gelfand–Naimark) The exists a faithful representation of $\mathscr{A}$ in Hilbert space H*

The Gelfand–Naimark theorem construct faithful representation of $\mathscr{A}$ in Hilbert space by a direct sum of the GNS representations over *all* the states.

Let $\mathscr{S}$ be the set of all the positive normalized states of $\mathscr{A}$ and consider the Hilbert space $H = \oplus_{\omega \in \mathscr{S}} H_\omega$ where the elements are (finite) families $x = (x_\omega)_{\omega \in \mathscr{S}}$ with $x_\omega \in H_\omega$, where the scalar product is

$$\langle x, x \rangle_H = \sum_{\omega \in \mathscr{S}} \langle x_\omega, x_\omega \rangle_{H_\omega}$$

and where $\varphi(a)x = (\varphi_\omega(a)x_\omega)_{\omega \in \mathscr{S}}$. Then φ is a isometric representation of $\mathscr{A}$ in $\mathscr{L}(H)$. (Gelfand–Naimark theorem)

Assume that $\varphi(a) = 0$. Then $0 = \|\varphi_\omega(a)\|^2_{H_\omega} = \omega(a^*a)$ for all $\omega \in \mathscr{S}$. However we have already seen that positive linear functionals separate elements of $\mathscr{A}$ so $a^*a = 0$ and $a = 0$. Therefore φ is injective and this implies that it is an isomorphism.

If $\mathscr{A}$ is separable is possible to take a countable subset of $\mathscr{S}$ to perform the construction, in this case H will become separable.

Then GN theorem shows that there is no loss of generality to consider representations of physical systems in Hilbert space.

Remark 26. Consider a state ω and a self-adjoint a such that ω is dispersion-free wrt. a, i.e. $0 = \Delta_\omega(a) = [\omega((a - \omega(a))^2)]^{1/2}$ then in the corresponding GNS representation we have

$$\omega((a - \omega(a))^2) = \langle \Omega_\omega, (\varphi(a) - \omega(a))^2 \Omega_\omega \rangle = \|(\varphi(a) - \omega(a))\Omega_\omega\|^2$$

so $(\varphi(a) - \omega(a))\Omega_\omega = 0$ and $\omega(a)$ is an eigenvalue of $\varphi(a)$ with eigenvector Ω_ω. In particular $\omega(a)$ should be in $\sigma(\varphi(a)) \subseteq \sigma(a)$.

3.5 Pure states and irreducible representations

Indeed is clear that if you have two representations φ, ψ acting on two Hilbert spaces H_1, H_2 you can alway form another representation $\varphi \otimes \psi$ acting on the tensor product Hilbert space $H_1 \otimes H_2$ (revise the definition) as

$$(\varphi \otimes \psi)(a)(v \otimes w) = \varphi(a)v \otimes \psi(a)w \qquad v \in H_1, w \in H_2.$$

We want now to discuss briefly the "simplest" representations.

Definition 27. *A representation φ on the Hilbert space H is irreducible if the only invariant subspaces of the family $(\varphi(a))_{a \in \mathscr{A}}$ are $\{0\}$ and H.*

For any family $\mathscr{B} \subseteq \mathscr{L}(H)$ we denote by $\mathscr{B}'$ the commutant of $\mathscr{B}$, that is the set

$$\mathscr{B}' = \{C \in \mathscr{L}(H): [C, B] = 0, \forall B \in \mathscr{B}\},$$

where $[C, B] = CB - BC$. Note that $\mathscr{B} \subseteq \mathscr{B}''$ and that $\mathscr{B}' \supseteq \mathbb{C} = \{\lambda \mathbb{1} : \lambda \in \mathbb{C}\}$.

Lemma 28. *The representation $\varphi: \mathscr{A} \to \mathscr{L}(H)$ is irreducible iff $\varphi(\mathscr{A})' = \mathbb{C} = \{\lambda \mathbb{1} : \lambda \in \mathbb{C}\}$.*

Proof. If φ is reducible then let P the orthogonal projection on a non-trivial invariant subspace. Let $v \in PH$ then we have $\varphi(a)v \in PH$ and $\varphi(a)Pv = \varphi(a)v = P\varphi(a)v$. If $v \notin PH$ then $v \in QH$ with $Q = 1 - P$ and then for any w

$$\langle w, \varphi(a)Qv \rangle = \langle \varphi(a)^* w, Qv \rangle = \langle \varphi(a)^*(P + Q)w, Qv \rangle$$

$$= \langle P\varphi(a^*)w, Qv \rangle + \langle \varphi(a)^* Qw, Qv \rangle = \langle Qw, \varphi(a)v \rangle = \langle w, Q\varphi(a)v \rangle$$

so $[\varphi(a), Q] = 0$. Then is clear that $P \in \varphi(\mathscr{A})'$. Reciprocally if $H \in \varphi(\mathscr{A})'$ is a nontrivial self-adjoint element of $\mathscr{L}(H)$, by spectral calculus we can produce a projection $P \in \varphi(\mathscr{A})'$ by setting $P = \chi(H)$ with $\chi: \mathbb{R} \to \mathbb{R}$ some characteristic function of a subset of $\mathbb{R}$, then $P^2 = P$ so P is indeed a projection and the associated subspace is invariant under $\varphi(\mathscr{A})$ since P commute with any $\varphi(a)$. □

Remark 29. Remember that a representation φ is cyclic if there exists a vector $v \in H$ such that $\{\varphi(a)v : a \in \mathscr{A}\}$ is dense in H. Note that any irreducible representation is cyclic for any vector (otherwise there would be nontrivial invariant subspaces). However not all the cyclic representations are irreducible (see below).

Recall that the set of all states $\mathscr{S}$ (positive normalized linear functionals on $\mathscr{A}$) is a convex set, closed for the weak-∗ topology. A *pure state* is (by definition) an extremal point in this convex set, i.e. cannot be written as linear combination of other states. By Krein–Milman theorem the set of all states is the closure (in the weak-∗ topology) of the convex combitations of pure states.

Proposition 30. *The GNS representation φ_ω is irreducible iff ω is extremal in the set of states, i.e. a pure state for $\mathscr{A}$.*

Proof. Let's assume that φ_ω is reducible, that is there exists a non-trivial orthogonal projection P in $\varphi_\omega(\mathcal{A})'$, then observe that, with $\Omega_\omega \in H_\omega$ the vacuum vector for φ_ω and with $Q = 1 - P$

$$\omega(a) = \langle \Omega_\omega, \varphi_\omega(a)\Omega_\omega \rangle_{H_\omega} = \langle P\Omega_\omega, \varphi_\omega(a)P\Omega_\omega \rangle_{H_\omega} + \langle Q\Omega_\omega, \varphi_\omega(a)Q\Omega_\omega \rangle_{H_\omega},$$

where the cross terms disappear since P commutes with $\varphi_\omega(a)$. Observe that

$$\lambda = \langle P\Omega_\omega, P\Omega_\omega \rangle_{H_\omega} \in (0,1)$$

indeed if for example $\lambda = 0$ we would have $P\Omega_\omega = 0$ but then $P\varphi_\omega(a)\Omega_\omega = 0$ and by ciclicity of Ω_ω and continuity of P we would deduce that $Pw = 0$ for any $w \in H_\omega$ which is ruled out by non-triviality of P. Similarly $\lambda = 1$ is also ruled out by an analogous argument. Now let

$$\omega_1(a) := \frac{\langle P\Omega_\omega, \varphi_\omega(a)P\Omega_\omega \rangle_{H_\omega}}{\langle P\Omega_\omega, P\Omega_\omega \rangle_{H_\omega}}, \qquad \omega_2(a) := \frac{\langle Q\Omega_\omega, \varphi_\omega(a)Q\Omega_\omega \rangle_{H_\omega}}{\langle Q\Omega_\omega, Q\Omega_\omega \rangle_{H_\omega}},$$

and observe that ω_1, ω_2 are states on $\mathcal{A}$ and that $\omega = \lambda \omega_1 + (1 - \lambda)\omega_2$. If $\omega_1 = \omega_2$ then $\omega = \omega_1 = \omega_2$ and this cannot happen since then

$$\langle \Omega_\omega, \varphi_\omega(a)\Omega_\omega \rangle_{H_\omega} = \frac{\langle P\Omega_\omega, \varphi_\omega(a)\Omega_\omega \rangle_{H_\omega}}{\langle P\Omega_\omega, P\Omega_\omega \rangle_{H_\omega}}, \qquad a \in \mathcal{A}$$

but then $\varphi_\omega(a)\Omega_\omega$ approximate any vector $\psi \in QH_\omega$ but then this implies

$$\langle \Omega_\omega, \psi \rangle_{H_\omega} = \frac{\langle P\Omega_\omega, \psi \rangle_{H_\omega}}{\langle P\Omega_\omega, P\Omega_\omega \rangle_{H_\omega}} = 0,$$

which in turn implies that $Q\Omega_\omega = 0$ but this is a contradiction with $\langle P\Omega_\omega, P\Omega_\omega \rangle_{H_\omega} < 1$. This implies that the state is not extremal, i.e. no pure.

Let's prove the converse, assume that the state ω is not pure, i.e. there exists $\lambda \in (0,1)$ and states $\omega_1 \neq \omega_2$ such that $\omega = \lambda \omega_1 + (1 - \lambda)\omega_2$. This implies that ω_1 is dominated by ω in the sense that if $a \geq 0$ we have

$$\omega(a) = \lambda \omega_1(a) + \underbrace{(1 - \lambda)\omega_2(a)}_{\geq 0} \geq \lambda \omega_1(a).$$

So the Hermitian form $B(a,b) \mapsto \omega_1(a^*b)$ on $\mathcal{A}$ satisfies $(\overline{B(a,b)} = \overline{\omega_1(a^*b)} = \omega_1(b^*a) = B(b,a))$

$$B(a,a) \leq \frac{1}{\lambda}\omega(a^*a) = \frac{1}{\lambda}\langle a,a \rangle_{H_\omega}.$$

In particular $B(a,b)$ is well defined on $\mathcal{A} \setminus \mathcal{N}_\omega$ with $\mathcal{N}_\omega = \{a \in \mathcal{A} : \langle a,a \rangle_{H_\omega} = 0\}$ as a consequence it defines a bounded self-adjoint operator $X : H_\omega \to H_\omega$ such that

$$B(a,b) = \langle a, Xb \rangle_{H_\omega}, \qquad a,b \in \mathcal{A}.$$

(exercise) Now observe that $B(a,cb) = \omega_1(a^*cb) = \omega_1((c^*a)^*b) = B(c^*a,b)$, as a consequence

$$\langle a, X\varphi_\omega(c)b \rangle_{H_\omega} = B(a,cb) = B(c^*a,b) = \langle \varphi_\omega(c^*)a, Xb \rangle_{H_\omega} = \langle a, \varphi_\omega(c)Xb \rangle_{H_\omega}, \qquad a,b \in \mathcal{A}$$

from which we conclude that $X\varphi_\omega(c) = \varphi_\omega(c)X$ using the density of $\mathscr{A}$ in H_ω. This holds for any $c \in \mathscr{A}$ therefore we conclude that $X \in \varphi(\mathscr{A})'$. Now X is a non-trivial self-adjoint operator so the representation is not irreducible. □

A pure state represent a situation which cannot be reduced to "simpler ones". If a state is not pure then one can imagine that is obtained probabilistically by sampling one among is pure components with certain probabilities.

Example 31. $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$ represents the situation where with probability λ_1 the system is in the state ω_1 and with probability $1-\lambda$ it is in the state ω_2.

Corollary 32. *A state ω on a commutative C^* algebra $\mathscr{A}$ is pure iff it is multiplicative.*

Proof. Let ω be a pure state, then the representation φ_ω is irreducible but it is also Abelian $\varphi_\omega(\mathscr{A}) \subseteq \varphi(\mathscr{A})' = \mathbb{C}$, so it is a one-dimensional representation and $H_\omega = \mathbb{C}$ is also a one-dimensional Hilbert space. Therefore

$$\omega(ab) = \langle \Omega_\omega, \varphi_\omega(a)\varphi_\omega(b)\Omega_\omega\rangle_{H_\omega} = \langle \Omega_\omega, \varphi_\omega(a)\Omega_\omega\rangle_{H_\omega}\langle \Omega_\omega, \varphi_\omega(b)\Omega_\omega\rangle_{H_\omega} = \omega(a)\omega(b)$$

so ω is multiplicative. On the hand if ω is multiplicative the $\omega(a^*b) = \omega(a^*)\omega(b) = \overline{\omega(a)}\omega(b)$ so $\varphi_\omega(a) = \omega(a)$ is the GNS representation resulting from it and is one dimensional, therefore irreducible. □

Therefore irreducible representations of commutative C^* algebras corresponds to multiplicative functionals (think why). And constitute the Gelfand spectrum of the algebra which, as we have seen, can be thought of as a space where the algebra is represented as continuous functions. Any irreducible representation is therefore a point in this space and the element of the algebra act via point-wise multiplication.

In the non-commutative case and in concordance with the GN theorem, one think to the space of all irreducible representations as the equivalent "non-commutative space". Indeed it is clear that pure states separate points and that they are labelled by the corresponding irreducible representation (because of cyclicity and of uniqueness of the GNS representation). However here the elements of the algebra acts in a more complex way on each "point" ω, namely as linear operators $\varphi_\omega(a)$ on the corresponding Hilbert space H_ω.

In the commutative case, the pure state are the elements of the Gelfand spectrum $\Sigma(\mathscr{A})$ and any element of $\mathscr{A}$ can be seen as a continuous complex function on $\Sigma(\mathscr{A})$. A pure state is just evaluation in a point for these functions $\omega(f) = f(\omega)$, i.e. a Dirac measure and a impure state is the limit of convex combintations of such "delta measures". So in particular any state ω can be written as an *average*

$$\omega(f) = \int_{\sigma(\mathscr{A})} \hat{f}(\rho)\mu(\mathrm{d}\rho)$$

for some measure $\mu \in \Pi(\Sigma(\mathscr{A}))$.

So the commutative situation corresponds to standard probability theory and measuraments are "incertain" just because we do not know the pure state that represent the system but maybe only a probability distribution over them.

Note that on pure states ω we have $\Delta_\omega(f) = \omega(f^2) - \omega(f)^2 = 0$. So they represent the more precise determination of the state of a system. This of course if the algebra is Abelian.

Our setting (i.e. algebras of observables + states) contains standard probability theory, at least in the case where the algebra is commutative.

Let's agree that an observable is a self-adjoint element of the algebra.

However in general any observable $a \in \mathscr{A}$ define a commutative $(C^*\text{-})$algebra $C^*(a)$ and therefore any state define a probability measure on $\Sigma(C^*(a)) = \sigma(a) \subseteq \mathbb{R}$.

This can be generalised to a set of commuting observables $(a_1, \ldots, a_n)$ which give the Abelian algebra $C^*(a_1, \ldots, a_n)$ and a measure on $\Sigma(C^*(a_1, \ldots, a_n))$, the set of the pure states (i.e. the multiplicative states) are uniquely labeled by n reals numbers $\{(\omega(a_1), \ldots, \omega(a_n)) : \omega \in \Sigma(C^*(a_1, \ldots, a_n))\} \subseteq \mathbb{R}^n$ So we can identify $\Sigma(C^*(a_1, \ldots, a_n)) = \sigma(a_1) \times \cdots \times \sigma(a_n) \subseteq \mathbb{R}^n$ and any state on this algebra as a probability measure on $\mathbb{R}^n$ with a support on that set.

However in general irreducible representations are not one dimensional if the algebra is non-commutative and they do not corresponds to multiplicative functionals, nor to a probabilistic situation.

Purification. We also saw last time that if a state ω dominates another, e.g. ω_1 (that is if $\omega_1(a) \leq C\omega(a)$ for any $a \geq 0$) then there exists a non-trivial self-adjoint operator in $\varphi_\omega(\mathscr{A})'$ and therefore there exists also an orthogonal projection $P \in \varphi_\omega(\mathscr{A})'$ and using it is not-difficult to see that H_ω splits into a direct sum $H_\omega = V \oplus W$ and that φ_ω restricts leaves these subspaces invariant and restricts to a sub-representation of $\mathscr{A}$, so we have $\varphi_\omega = \varphi^{(1)} \otimes \varphi^{(2)}$.

Given a representation φ on H we can construct a whole family of states associated to it, called its *folium* they are of the form, for example of a *state vector*

$$\omega^\psi(a) = \langle \psi, \varphi(a)\psi \rangle$$

where ψ is a unit vector in H. Or mixures of state vectors $\psi_1, \ldots, \psi_n$ with weights $\lambda_1, \ldots, \lambda_n$ such that $\lambda_1 + \cdots + \lambda_n = 1$ and

$$\omega(a) = \sum_i \lambda_i \langle \psi_i, \varphi(a)\psi_i \rangle = \mathrm{Tr}\Big(\sum_i \lambda_i |\psi_i\rangle\langle\psi_i|\varphi(a)\Big)$$

where $|\psi_i\rangle\langle\psi_i|$ denotes the rank-1 operator on H given by $|\psi_i\rangle\langle\psi_i|\varphi = \psi_i\langle\psi_i, \varphi\rangle$ for any $\varphi \in H$. More generally we can replace $\sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$ by any trace class, positive operator $\rho \in \mathscr{L}(H)$. This operator is usually called a density matrix. Recall that Tr is defined on $\mathscr{L}_1(H)$ by

$$\mathrm{Tr}(A) = \sum_n \langle e_n, A e_n \rangle, \qquad A \in \mathscr{L}_1(H) = \Big\{ A \in \mathscr{L}(H) : \sum_n |\langle e_n, A e_n \rangle| < \infty \Big\}$$

(the definition does not depend on the basis). So a general element of the folium of φ is given by a density matrix ρ

$$\omega^\rho(a) = \mathrm{Tr}(\rho\varphi(a)).$$

Note that ω^ρ is a vector state for its own GNS representation φ_{ω^ρ}, i.e.

$$\omega^\rho(a) = \langle \Omega_{\omega^\rho}, \varphi_{\omega^\rho}(a)\Omega_{\omega^\rho} \rangle_{H_{\omega^\rho}}.$$

Corollary 33. *Any vector state of an irreducible representation is pure.*

I will not prove the following two interesting results.

Theorem 34. *The folium of a representation and the set of vector states of a representation are norm closed subsets in the space of all states $\mathcal{S}$.*

Theorem 35. (Fell) *The folium of a faithful representation is weakly-$*$ dense in the set of all states.*

Remark 36. From a physical point of view we can only do a finite amount of experiments (and with finite precision), which means that we can only identify a weak-$*$ neighborhood of set of all possible states of the system, i.e. a subset of the form

$$\{\omega \in \mathcal{S} : |\omega(a_i) - v_i| \leq \varepsilon_i \text{ for all } i = 1, \ldots, n\}$$

where $(a_i)_i$ are observables and $\varepsilon_i > 0$ and $v_i \in \mathbb{R}$. So any faithful representation is as good to be used to approximate a realistic situation. However for mathematical purposes sometimes is useful to single out specific representations which have additional properties.

3.6 The quantum world

As we saw, it the commutative setting we are able to have states (the pure states) which assign precise values to all observables and where the only source of variance is then described by a probabilistic model. That's something not possible anymore when dealing with microscopic phenomena. This has been discovered at the beginning of the 1900 in various situations and experiments:

- Stern–Gerlach experiment show that the magnetic moment of the electron $M = (M_x, M_y, M_z)$ is quantized (so does not corresponds to the state space which we expect from a vector in $\$^2$) and moreover it seems not to agree with probabilistic reasoning.

- Black-body radiation. The thermodynamical analysis of a particular situation (Plack) at very low temperatures (i.e. $\sim 0^\circ K \approx 273^\circ C$) pointed out (Einstein) that the degrees of freedom (i.e. different possible states) in the electromagnetic radiation field (light) has to be discrete and not continuous. I.e. light is composed by discrete entities, i.e. photons. That is somehow the set of different possible (pure) states is discrete and not continuous. Planck's constant:

$$h = 6.62607004 \times 10^{-34} \, m^2 \, \text{kg} \, / \, s.$$

- Heisenberg's analysis of a quantum particle shows that when you try to measure the position and the speed of a particle you get in trouble. In the sense that measurements of position will disturb the velocity of the particle and vice-versa and one should make the hypothesis that both position q and momentum $p = mv$ (i.e. mass times velocity) cannot be determined in any conceivable state ω with arbitrary precision, i.e.

$$\Delta_\omega(q)\Delta_\omega(p) \geq \frac{\hbar}{2} \tag{2}$$

This is Heisenberg's indetermination principle. It somehow implies that the states of a particle cannot be labelled by position and momentum variables, i.e. we need to forbid states which have precise values of position *and* momentum. Note that if (q, p) were forming a commutative algebra then you will have such states like $\delta_{\alpha,\beta}(\mathrm{d}q, \mathrm{d}p)$ which give precise value to $p = \alpha$ and $q = \beta$.

The set of all (elementary) states of a quantum system cannot be put in direct correspondence with the possible values of all the observables. And in particular it is suggested that the set of elementary states is discrete and not continuous.

In classical mechanics the state of a particle is described by a point in the phase space (q, p) of positions and momenta. Any point is possible and any two very nearby points are conceptually distinct. But the existence of the *elementary quantum h* suggests that in every small volume element of size $\delta q \, \delta p \approx h$ there is only one possible quantum state for a particle.
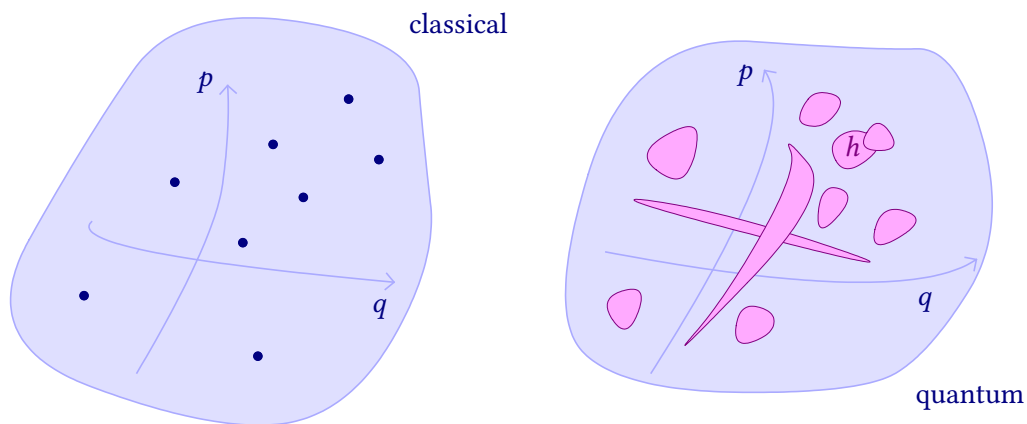
One could put in question the mathematical framework (i.e. restricting states or observables), but actually our setting contains a way out because allows us to introduce *non-commutative* algebras.

This was the conclusion of Heisenberg [Hei49] and he created matrix mechanics, while somehow Schrödinger constructed a different model for the states (i.e. wave-functions constrained by PDEs) and he created wave mechanics. Dirac [Dir88] later showed that the two are equivalent descriptions. Von Neumann gave the standard mathematical axiomatization [Van58].

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