

Elements of Mathematical Quantum Mechanics

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Pure states and irreducible representations

Definition 1. A representation φ on the Hilbert space H is **irreducible** if the only invariant subspaces of the family $(\varphi(a))_{a \in \mathcal{A}}$ are $\{0\}$ and H .

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

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

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

Lemma 2. The representation $\varphi: \mathcal{A} \rightarrow \mathcal{L}(H)$ is irreducible iff $\varphi(\mathcal{A})' = \mathbb{C} = \{\lambda \mathbb{1} : \lambda \in \mathbb{C}\}$.

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

$$\begin{aligned} \langle w, \varphi(a)Qv \rangle &= \langle \varphi(a)^*w, Qv \rangle = \langle \varphi(a)^*(P+Q)w, Qv \rangle \\ &= \langle P\varphi(a)^*w, Qv \rangle + \langle \varphi(a)^*Qw, Qv \rangle = \langle Qw, \varphi(a)v \rangle = \langle w, Q\varphi(a)v \rangle \end{aligned}$$

so $[\varphi(a), Q] = 0$. Then is clear that $Q \in \varphi(\mathcal{A})'$ so finished.

Reciprocally if $R \in \varphi(\mathcal{A})'$ is a nontrivial self-adjoint element of $\mathcal{L}(H)$, by spectral calculus we can produce a projection $P \in \varphi(\mathcal{A})'$ by setting $P = \chi(R)$ with $\chi: \mathbb{R} \rightarrow \mathbb{R}$ 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 $\varphi(\mathcal{A})$ since P commute with any $\varphi(a)$. \square

Proposition 3. The GNS representation φ_ω is irreducible iff ω is extremal in the set of states, i.e. a pure state for \mathcal{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 cyclicity 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

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

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

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

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 $X: H_\omega \rightarrow H_\omega$ such that

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

(exercise) Now observe that

$$B(a, cb) = \omega_1(a^*cb) = \omega_1((c^*a)^*b) = B(c^*a, b),$$

as a consequence

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

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

Example 4. $\omega = \lambda\omega_1 + (1 - \lambda)\omega_2$ 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 5. *A state ω on a commutative C^* algebra \mathcal{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 $\varphi_\omega(\mathcal{A}) \subseteq \varphi(\mathcal{A})' = \mathbb{C}$, 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. \square

In the commutative case, the pure state are the elements of the Gelfand spectrum $\Sigma(\mathcal{A})$ and any element of \mathcal{A} can be seen as a continuous complex function on $\Sigma(\mathcal{A})$. 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 combinations of such “delta measures”. So in particular any state ω can be written as an *average*

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

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

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.

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.

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 $\varphi_\omega(\mathcal{A})'$ and therefore there exists also an orthogonal projection $P \in \varphi_\omega(\mathcal{A})'$ 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 \mathcal{A} , so we have

$$\varphi_\omega = \begin{pmatrix} \varphi^{(1)} & \\ & \varphi^{(2)} \end{pmatrix}.$$

Given a representation φ on H we can construct a whole family of states associated to it, called its *folium*.

For example of a *state vector*

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

where ψ is a unit vector in H .

Or mixtures of state vectors ψ_1, \dots, ψ_n with weights $\lambda_1, \dots, \lambda_n$ such that $\lambda_1 + \dots + \lambda_n = 1$ and

$$\omega(a) = \sum_i \lambda_i \langle \psi_i, \varphi(a) \psi_i \rangle = \text{Tr} \left(\left(\sum_i \lambda_i |\psi_i\rangle \langle \psi_i| \right) \varphi(a) \right)$$

So a general element of the *folium* of φ is given by a density matrix ρ

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

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 6. *Any vector state of an irreducible representation is pure.*

I will not prove the following two interesting results.

Theorem 7. *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 8. (Fell) *The folium of a faithful representation is weakly-* dense in the set of all states.*

Remark 9. 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

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

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.

The quantum world

Somehow commutative setting does not fit the 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 \mathbb{S}^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. $\sim 0\text{K} \approx 273\text{C}$) 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:

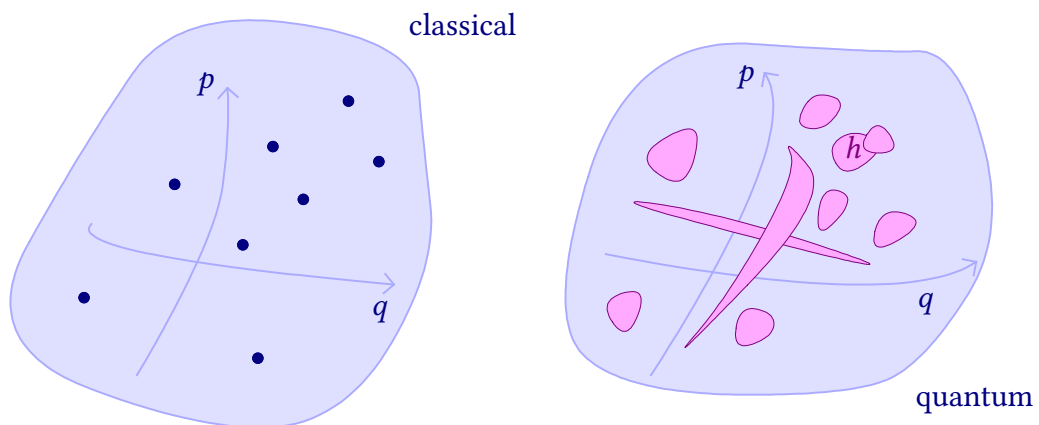
$$h = 6.62607004 \times 10^{-34} \text{ m}^2 \text{ kg} / \text{ s}.$$

- 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 $p = m v$ (i.e. mass times velocity) cannot be determined in any conceivable state ω with arbitrary precision, i.e.

$$\Delta_{\omega}(q)\Delta_{\omega}(p) \geq \frac{\hbar}{2} \quad (1)$$

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 $\delta_{\alpha, \beta}(dq, dp)$ 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.



This was the conclusion of Heisenberg [2] 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 [1] later showed that the two are equivalent descriptions. Von Neumann gave the standard mathematical axiomatization [3].

The quantum particle

We want now to construct a physical system (observables+states) that encodes Heisenberg's indetermination principle

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

for the position q and momentum p of a particle and other experimental observations.

The C^* -algebra of observables \mathcal{A} should contain the C^* -algebra \mathcal{Q} of all the bounded functions $f(q)$ of q and the C^* -algebra \mathcal{P} of all the bounded functions $g(p)$ of p but I need to rule out that q, p commutes otherwise I violate Heisenberg principle unless I restrict the set of states. But restricting the set of states is more difficult than dealing with a non-commutative algebra because we have more structure on \mathcal{A} than on \mathcal{S} .

$$f(q) = (q \wedge L) \vee (-L).$$

$$Q, P: C(\mathbb{R}; \mathbb{C}) \rightarrow \mathcal{A}.$$

$$f(q) = \mathbf{Q}(f), \quad g(p) = \mathbf{P}(g)$$

We want to explore how non-commutativity is related to the indetermination principle (2) and also to the notion of “complementarity”. Complementary observables are somehow observables which do not allow simultaneous measurement, that is if we are able to have states in which one of the is completely determined, then the other has to be completely “undetermined”. Think about the Stern-Gerlach experiment and the measurement of the magnetic moment in two orthogonal directions.

Anyway let us see what we can get from (2).

Observe that if $a, b \in \mathcal{A}$ and self-adjoint then $(a + i\lambda b)^*(a + i\lambda b) \geq 0$ for any $\lambda \in \mathbb{R}$ and if ω is a state we have

$$0 \leq \omega((a + i\lambda b)^*(a + i\lambda b)) = \omega(a^2) + \lambda^2 \omega(b^2) + i\lambda \omega(ab - ba),$$

therefore we need to have, letting $[a, b] = ab - ba$,

$$|\omega(i[a, b])| \leq 2(\omega(a^2))^{1/2}(\omega(b^2))^{1/2}.$$

So in any C^* algebra we have the (Schrödinger–Robertson) relation

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

So if we want to implement Heisenberg's principle for a pair of complementary observables q, p a way is to require that $i[p, q]$ is constant element of \mathcal{A} and therefore

$$[q, p] = i\hbar, \quad (3)$$

Unfortunately this is not possible in a C^* context.

First problem: these cannot be finite dimensional matrices, indeed if they were we could take the trace over the vector space \mathbb{C}^n they acts on and get

$$\text{Tr}([q, p]) = \sum_n \langle e_n, [q, p] e_n \rangle = 0, \quad \text{Tr}(i\hbar) = i\hbar n \dots$$

not very nice.

Moreover they cannot be implemented even in an abstract C^* algebra, indeed if $q, p \in \mathcal{A}_{sa}$ then

$$[q^n, p] = i\hbar n q^{n-1}$$

and therefore by the C^* condition

$$n\hbar \|q\|^{n-1} = n\hbar \|q^{n-1}\| = \|i\hbar n q^{n-1}\| = \|[q^n, p]\| \leq 2\|p\| \|q\|^n$$

which implies

$$\|p\| \|q\| \geq n\hbar / 2$$

if $\|q\| \neq 0$. This is true for any n and so either $\|p\|$ or $\|q\|$ has to be infinite.

This somehow is to be expected because “the position” is not really a bounded observable.

The discussion below is inspired by the following papers:

- Accardi, Luigi. “Some Trends and Problems in Quantum Probability.” In *Quantum Probability and Applications to the Quantum Theory of Irreversible Processes*, edited by Luigi Accardi, Alberto Frigerio, and Vittorio Gorini, 1055:1–19. Lecture Notes in Mathematics. Berlin, Heidelberg: Springer Berlin Heidelberg, 1984. <https://doi.org/10.1007/BFb0071706>.
- Ohya, Masanori, and Dénes Petz. *Quantum Entropy and Its Use*. Texts and Monographs in Physics. Berlin; New York: Springer-Verlag, 1993.
- Schwinger, Julian. “Unitary Operator Bases.” *Proceedings of the National Academy of Sciences* 46, no. 4 (April 1, 1960): 570–79. <https://doi.org/10.1073/pnas.46.4.570>.

1 Non-commutativity and probability

To start simpler we consider first system which possess “finitely many” pure states. Think about the two states in the Stern–Gerlach experiment.

Let us assume we have two observables a, b which generates \mathcal{A} and such that $\sigma(a), \sigma(b)$ are finite.

We would like to inquire about the “most indeterminate” relative position of a and b inside the C^* -algebra $\mathcal{A} = C^*(a, b)$ they generate.

First of all it is clear that since $\sigma(a)$ is finite, let's say with n elements, we can find function $(\rho_k \in C(\mathbb{R}))_{k=1, \dots, n}$ such that $\rho_k(x) \in [0, 1]$ and $\sum_{k=1}^n \rho_k(x) = 1$ for all $x \in \mathbb{R}$ and $\rho_k(x)\rho_\ell(x) = \delta_{k,\ell}$ for all $x \in \sigma(a)$.

Let $\pi_k^a := \rho_k(a)$ and observe that by construction

$$\sum_{k=1}^n \pi_k^a = 1, \quad \pi_k^a \pi_\ell^a = \delta_{k,\ell}, \quad k, \ell = 1, \dots, n,$$

i.e. $(\pi_k^a)_k$ form a partition of unity in self-adjoint projections. We let $(\pi_k^b)_{k=1, \dots, m}$ the analogous objects associated to b where m is the size of $\sigma(b)$.

Clearly there exists constants $(a_k)_k$ such that $f(a) = \sum_k f(a_k) \pi_k^a$ for any $f \in C(\mathbb{R})$ and similarly for b so we need that $[\pi_k^a, \pi_\ell^b] \neq 0$ for some $k = \ell$ in order to have a non-commutative algebra.

Let us assume that $C^*(a)$ and $C^*(b)$ are maximally abelian subalgebras in \mathcal{A} .

Then observe that the observable

$$\sum_k \pi_k^a \pi_\ell^b \pi_k^a$$

commutes with any element in $C^*(a)$ and therefore it should belong to it. As a consequence there exist complex numbers $(p_{\ell,k}^{b|a})_{k,\ell}$ such that

$$\sum_k \pi_k^a \pi_\ell^b \pi_k^a = \sum_k p_{\ell,k}^{b|a} \pi_k^a.$$

Since the l.h.s. is positive on any state and there exist states (ω_k^a) such that $\omega_k^a(\pi_\ell^a) = \delta_{k,\ell}$ we have that $(\pi_k^a)_k$ is a basis of $C^*(a)$, that $(p_{\ell,k}^{b|a})_{k,\ell}$ are uniquely determined and that

$$p_{\ell,k}^{b|a} \geq 0, \quad \sum_k p_{\ell,k}^{b|a} = \sum_\ell p_{\ell,k}^{b|a} = 1.$$

Therefore we have a set of probabilities $(p_{\ell,k}^{b|a})_{k,\ell}$ which are generated intrinsically by the non-commutativity of the algebra, even before we consider the states on that algebra.

This shows that, as soon as we allow for non-commutativity, some “randomness” is already built into our algebra of observables.

For any state ω we can construct a new state

$$\omega^a(h) = \sum_k \omega(\pi_k^a h \pi_k^a)$$

and now observe that

$$\omega^a(f(a)) = \omega(f(a)), \quad \omega^a(f(b)) = \sum_{k,\ell} f(b_\ell) \omega(\pi_k^a \pi_\ell^b \pi_k^a) = \sum_{\ell,k} f(b_\ell) p_{\ell,k}^{b|a} \omega(\pi_k^a)$$

so $\omega^a(\pi_\ell^b) = \sum_k p_{\ell,k}^{b|a} \omega(\pi_k^a)$.

Bibliography

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- [3] Léon Van Hove. Von Neumann's contributions to quantum theory. *Bulletin of the American Mathematical Society*, 64(3):95–99, 1958.