Elements of Mathematical Quantum Mechanics

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Complementary observables in finite quantum system

We want now to devise observables a, b for which the matrix $p_{\ell,k}^{b|a}$ is as uniform as possible, meaning that if we have measured a then there is no particular knowledge on b. We call these observables "complementary". We require also that either a or b provides an as complete as possible description of the physical system, i.e. that $C^*(a)$ and $C^*(b)$ are maximally abelian. Without loss of generality we can assume that $\sigma(a) = \sigma(b) = \{0, \ldots, n-1\}$ for some integer $n \geqslant 2$.

Actually, we assume that they have all the same spectrum with n points and to be given by

$$\Gamma = \{\gamma_k = e^{2\pi i k/n}\}_{k=0,\ldots,n-1}.$$

I call the observables u, v. I want that $\sigma(u) = \sigma(v) = \Gamma$. I consider them $\mathscr{L}(\mathbb{C}^n)$. Let $(\varphi_k)_k$ be the eigenvectors of u, i.e.

$$u\varphi_k = \gamma_k \varphi_k$$

and then take

$$v\varphi_k := \varphi_{k+1}$$

with $k+1$ understood modulus n. Now observe that $uv\varphi_k = u\varphi_{k+1} = \gamma_{k+1}\varphi_{k+1} = \gamma_{k+1} v\varphi_k = (\gamma_{k+1}/\gamma_k) vu\varphi_k$ for any $k = 0, \ldots, n-1$ so

$$uv = e^{2\pi i/n} vu. \tag{1}$$

If we assume that u, v generate the algebra of observables then this fixes the full algebraic structure. Observe also that $u^n = v^n = 1$.

Remark 1. Observe also that (1) implies that $u^n v = v u^n$ and also $v^n u = u v^n$ so the elements u^n, v^n belongs to the center (i.e. the elements which commutes with all the others) of the algebra generated by u, v. If we assume that u, v generate each of them a maximally abelian subalgebra then we can conclude from the commutation relation only that $u^n, v^n \in \mathbb{C}$. From this one can see that any irreducible representation of the commutation relation is n dimensional.

In particular

$$0=(\gamma_k^{-1}u)^n-1=(\gamma_k^{-1}u-1)\sum_{\ell=0}^{n-1}(\gamma_k^{-1}u)^\ell$$

and from this we deduce that

$$\pi_k^u:=n^{-1}\sum_{\ell=0}^{n-1}(\gamma_k^{-1}u)^\ell$$

satisfies

$$u\pi_k^u=\gamma_k\pi_k^u$$

so π_k^u is the orthogonal projection on the span of φ_k, indeed one can check that $(\pi_k^u)^*=\pi_k^u$ and $\pi_k^u\pi_\ell^u=\delta_{k,\ell}\pi_k^u$. So we have also $u=\sum_{k=0}^{n-1}\gamma_k\pi_k^u$. For v we can proceed in the same way and define π_k^v. Now let's compute $\sum_k\pi_k^u\pi_\ell^v\pi_k^u$ using (1) and get

$$\sum_k p_{\ell,k}^{v|u}\pi_k^u=\sum_k\pi_k^u\pi_\ell^v\pi_k^u=\frac{1}{n},\qquad \ell=1,\ldots,n-1$$

so as required we have $p_{\ell,k}^{v|u}=1/n$.

So we confirm that our choice of algebraic structure give indeed a maximally complementary pair of observables.

We want now to argue that u,v are sufficient to generate all $\mathscr{L}(\mathbb{C}^n)$ (i.e. all the $n\times n$ complex matrices).

Let $X\in\mathscr{L}(\mathbb{C}^n)$ and observe that the operator

$$Y=\frac{1}{n^2}\sum_{k,\ell}u^{-k}v^{-\ell}Xv^\ell u^k,$$

satisfy $uY=Yu$ and $vY=Yv$ so Y commutes with all the algebra generated by u,v (this actually depends only on the commutation relation (1)).

Then this means that Y is a multiple of the identity, because since it commutes with u we must have $Y=\sum_k y_k\pi_k^u$ but then $Y=vYv^*=\sum_k y_k v\pi_k^u v^*=\sum_k y_k\pi_{k+1}^u$ and this implies that $y_k=y_{k+1}$ that is $Y=\lambda\mathbb{1}$ for some $\lambda\in\mathbb{C}$.

Construct a linear functional ρ such that $\rho(X)=\lambda$ and by thinking a bit is clear that ρ: $\mathscr{L}(\mathbb{C}^n)\longrightarrow\mathbb{C}$ is a actually a positive linear functional (think about it, is clear from the definition of Y) and $\rho(\mathbb{1})=1$.

The definition of Y implies easily that for any $X\in\mathscr{L}(\mathbb{C}^n)$

$$X=\sum_{k,\ell}u^kv^\ell\rho((u^kv^\ell)^*X)$$

that is $(u^k v^\ell)_{k,\ell}$ is an orthornomal basis of $\mathscr{L}(\mathbb{C}^n)$ with respect to the non-degenerate scalar product $\langle X, Y\rangle = \rho(X^* Y)$. So in particular the algebra generated by u, v span all the $n \times n$ complex matrices.

This proves that the representation we gave is irreducible and therefore the pure states of this algebra are exactly the vector states of this representation. So to describe all the possible states is enough to restrict to states of the form

$$\omega(X) = \mathrm{Tr}_{\mathbb{C}^n}[\rho\pi(X)],$$

where $\rho \in \mathscr{L}(\mathbb{C}^n)$ is a density matrix (i.e. $\rho \geqslant 0$, $\mathrm{Tr}_{\mathbb{C}^n}(\rho) = 1$) and π is the concrete representation of this algebra that we have analyzed.

We would like now to take some limit $n \longrightarrow \infty$ in order to produce in this way continuous analogs of these algebras. This would give us an example of non-commutative C^* algebra generated by two abelian subalgebras with continuous spectrum.

The intuition we want to carry on is how we go from discrete uniform r.v. to continuous ones. In particular imagine that X is a r.v. with continuous distribution described by a density $p(x)$ on $\mathbb{R}$. I can imagine to approximate it in law by taking a discrete r.v. X_L such that $X_L = [X]_L$ for $L \in \mathbb{N}$ where $[x]_L = \lfloor Lx \rfloor / L$. Then we have for any continuous and bounded function $f: \mathbb{R} \longrightarrow \mathbb{R}$

$$\mathbb{E}[f(X_L)] = \int_{\mathbb{R}} f([x]_L) p(x) \mathrm{d}x \longrightarrow \int_{\mathbb{R}} f(x) p(x) \mathrm{d}x = \mathbb{E}[f(X)].$$

Let's try to implement the same procedure for a C^*-algebra. The first observation is that if we denote (u_n, v_n) a discrete canonical pair of degree n we have the following. We can take $L^2(\mathbb{T})$ as Hilbert space where $\mathbb{T} = \mathbb{R} \backslash \mathbb{Z}$ and represent each u_n and v_n as

$$u_n f(x) = \exp(2\pi i\,[x]_n) f(x), \qquad v_n f(x) = f(x - 1/n), \qquad x \in \mathbb{T}.$$

One can check that u_n, v_n is a representation of the algebra we constructed above. In this way we can embed all the operators $(u_n, v_n)_{n \geqslant 0}$ into $\mathscr{L}(L^2(\mathbb{T}))$.

We have to understand what plays the role of “continuous functions” in this context. We just take monomials of the form $u_n^k v_n^\ell$ (they suffice to determine any other element of $C^*(u_n, v_n)$ due to their commutation relation). However is easy to see that $u_n^k v_n^\ell \longrightarrow 1$ in the weak topology of $L^2(\mathbb{T})$. Somehow we need to look at high powers of u_n, v_n to see something interesting. We take $\ell_n = n^{1/2}[s]_{n^{1/2}}$ and $k_n = n^{1/2}[t]_{n^{1/2}}$ and now consider

$$\langle f_n, u_n^{k_n} v_n^{\ell_n} g_n \rangle_{L^2(\mathbb{T})} = \int_{\mathbb{T}} \overline{f_n(x)} \exp(2\pi i k_n [x]_n) g_n(x - \ell_n / n) \mathrm{d}x.$$

$$u_n^{k_n} v_n^{\ell_n} = e^{2\pi i k_n \ell_n / n} v_n^{\ell_n} u_n^{k_n} = e^{2\pi i [s]_{n^{1/2}} [t]_{n^{1/2}}} v_n^{\ell_n} u_n^{k_n}$$

By rescaling we have, for functions f_n, g_n supported on $(-\pi,\pi)$ and letting $x = y/n^{1/2}$.

$$\langle f_n, u_n^{k_n} v_n^{\ell_n} g_n\rangle_{L^2(\mathbb{T})} = \int_{(-\pi,\pi)} \overline{f_n(x)} \exp(2\pi i [t]_{n^{1/2}} [x]_n n^{1/2}) g_n(x - [s]_{n^{1/2}}/n^{1/2}) \mathrm{d}x$$

$$= n^{-1} \int_{(-\pi n^{1/2}, \pi n^{1/2})} \overline{f_n(y/n^{1/2})} \exp(2\pi i [t]_{n^{1/2}} n^{1/2} [y/n^{1/2}]_n) g_n((y - [s]_{n^{1/2}})/n^{1/2}) \mathrm{d}y$$

so to have a well defined limit we can take $f_n(x) = n^{1/4} f(n^{1/2} x)$ and $g_n(x) = n^{1/4} g(n^{1/2} x)$ with $f, g \in C_0^\infty(\mathbb{R})$ so that for n large enough we have

$$\langle f_n, u_n^{k_n} v_n^{\ell_n} g_n\rangle_{L^2(\mathbb{T})} = \int_{\mathbb{R}} \overline{f(y)} \exp(2\pi i [t]_{n^{1/2}} n^{1/2} [y/n^{1/2}]_n) g(y - [s]_{n^{1/2}}) \mathrm{d}y$$

so here now we can take the limit and obtain that

$$\lim_n \langle f_n, u_n^{k_n} v_n^{\ell_n} g_n\rangle_{L^2(\mathbb{T})} = \langle f, U(t) V(s) g\rangle_{L^2(\mathbb{R})} \qquad (2)$$

where (U, V) are two **unitary groups** acting on $L^2(\mathbb{R})$ as

$$U(t) f(y) = \exp(2\pi i t y) f(y), \qquad V(s) f(y) = f(y - s).$$

$$U_n(t) = u_n^{k_n}, \qquad V_n(s) = v_n^{\ell_n}$$

$$u_n^{k_n} v_n^{\ell_n} = e^{2\pi i k_n \ell_n / n} v_n^{\ell_n} u_n^{k_n} = e^{2\pi i [s]_{n^{1/2}} [t]_{n^{1/2}}} v_n^{\ell_n} u_n^{k_n}$$

$$U_n(t) V_n(s) = e^{2\pi i [s]_{n^{1/2}} [t]_{n^{1/2}}} V_n(s) U_n(t)$$

$$\lim_{n \to \infty} \omega_n(U_n(t) V_n(s)) = C(t, s) = \omega(U(t) V(s))$$

which implies that for any non-commutative polynomial F we have

$$\omega_n(F(U_n, V_n)) \longrightarrow \omega(F(U, V))$$

since by the commutation relations we can rewrite $F(U, V)$ as a linear combination of monomials of the form $U(t) V(s)$ for various t, s.

Moreover they are weakly continuous, i.e. $t \mapsto \langle f, U(t) g\rangle$ is continuous for all $f, g \in L^2(\mathbb{R})$. Since they are unitary they are also strongly continuous.

They satisfying the commutation relations

$$U(t) V(s) = e^{2\pi i s t} V(s) U(t), \qquad t, s \in \mathbb{R}. \qquad (3)$$

These commutation relations are called the Weyl form of the canonical commutation relations and they are the implementation of the Heisenberg's commutation relations

$$[P, Q] = i\hbar,$$

within the C^*-framework (i.e. working only with bounded operators). The link between these formulas comes from interpreting the two unitary groups as being generated by the self-adjoint operators P, Q i.e. as

$$U(t) = \exp(iQt), \qquad V(s) = \exp(iPs),$$

Putting aside for the moment unbounded operators we obtained a pair of commutative C^* algebras $\mathscr{Q}, \mathscr{P}$ given by $\mathscr{Q} = C^*((U(t))_{t\in\mathbb{R}})$, $\mathscr{P} = C^*((V(s))_{s\in\mathbb{R}})$ which are concrete C^* algebras on $L^2(\mathbb{R})$. We denote $\mathscr{A} = C^*(\mathscr{Q}, \mathscr{P})$.

The C^*-algebra $\mathscr{A}$ is called the Weyl algebra. It is the fundamental example of two continuous observables which do not commute and in some sense they show complementarity.

Unitary representations of $\mathbb{R}$ and observables as homorphisms

Assume for the moment that we the family $(U(t))_{t\in\mathbb{R}}$ is a unitary family of bounded operators on an Hilbert space H (giving a representation of $\mathbb{R}$ on H).

For any unit vector $v \in H$ we can form the function $\varphi^v(t) = \langle v, U(t)v\rangle$, it is easy to show that $\varphi^v(0) = 1$, and φ^v is positive definite, i.e.

$$\sum_{i,j} \bar{\lambda}_i \lambda_j \varphi^v(t_j - t_i) \geq 0 \qquad (\lambda_i)_i \subseteq \mathbb{C}, (t_i)_i \subseteq \mathbb{R}.$$

This are the same properties of the characteristic function of a measure, so we want to show that there exist a measure μ^v on $\mathbb{R}$ so that

$$\varphi^v(t) = \int_{\mathbb{R}} e^{itx} \mu^v(\mathrm{d}x), \qquad t \in \mathbb{R}.$$

This is essentially Bochner's theorem (given some continuity of φ^v), but are going to sketch a proof because will give us a simple example of more involved reconstruction we encouter later on.

Let $f \in \mathcal{S}(\mathbb{R})$ a Schwartz function and define

$$T_f := \int_{\mathbb{R}} U(t) \hat{f}(t) \mathrm{d}t$$

where $\hat{f}$ is the Fourier transform of f. In order for this definition to make sense I need some condition on the family $(U(t))_{t\in\mathbb{R}}$ to be able to integrate it. Is easy to check in simple cases that $(U(t))_{t\in\mathbb{R}}$ is essentially never continuous in the operator norm.

Note that it is a bounded operator because

$$|\langle v, T_f v\rangle| \leqslant \int_{\mathbb{R}} |\varphi^v(t)||\hat{f}(t)|\mathrm{d}t \leqslant \|v\|^2 \int_{\mathbb{R}} |\hat{f}(t)|\mathrm{d}t \leqslant C_f \|v\|^2$$

for all $f \in \mathcal{S}(\mathbb{R})$ and for all $f \in \mathcal{F}L^1 = \{f \in C(\mathbb{R}) : \|\hat{f}\|_{L^1} < \infty\}$. This define a linear functional ℓ^v on $\mathcal{S}(\mathbb{R})$ such that

$$|\ell^v(f)| \leqslant C_v \|\hat{f}\|_{L^1}.$$

In order to extend this functional to all $C_0(\mathbb{R})$ I need to show that $|\ell^v(f)| \lesssim \|f\|_\infty$ for $f \in \mathcal{S}(\mathbb{R})$.

In order to do this one has to use that ℓ^v is positive, that is if $f = g^2 \geqslant 0$ then provided $g \in \mathcal{S}(\mathbb{R})$ we have

$$\ell^v(f) = \ell^v(g^2) \geqslant 0$$

because we use that

$$\int_{\mathbb{R}} \varphi^v(t)\hat{f}(t)\mathrm{d}t = \int_{\mathbb{R}}\int_{\mathbb{R}} \varphi^v(t+s)\hat{g}(t)\hat{g}(s)\mathrm{d}t\mathrm{d}s \geqslant 0$$

by positive definiteness of φ^v.

Then one argue by approximation that for any $f \in \mathcal{S}(\mathbb{R})$ one has $\|f\|_\infty - f = h \geqslant 0$ and this can be approximated by h_ε in $\mathcal{S}(\mathbb{R})$ to get that $\ell^v(h) \geqslant 0$ and this will imply that

$$\ell^v(f) \leqslant \|f\|_\infty$$

and the the functional can be extended to all $C_0(\mathbb{R})$ by approximation.

To make rigorous this argument one need that φ^v is continuous in t.

As soon as we have extended ℓ^v continously we can define a $*$-representation Q of $C_0(\mathbb{R})$ on $\mathcal{L}(H)$. For any $f \in C_0(\mathbb{R})$ define the operator $Q(f)$ by the relation $\langle v, Q(f)v\rangle = \ell^v(f)$ and its polarization. This define a bounded operator such that $\|Q(f)\|_{\mathcal{L}(H)} \leqslant \|f\|_\infty$ and $Q(f)^* = Q(\bar{f})$ and Q is linear in f and $Q(f)Q(g) = Q(fg)$ (by continuity is enough to check there relations of $f \in \mathcal{S}(\mathbb{R})$ and this case we have the more precise relation

$$Q(f) = \int_{\mathbb{R}} U(t)\hat{f}(t)\mathrm{d}t$$

(remember that the r.h.s is defined as a weak integral). I would like to use $f(x) = e^{isx}$, in order to do this observe that for any $v \in H$

$$\langle v, Q(f)v\rangle = \int_{\mathbb{R}} \varphi^v(t)\hat{f}(t)\mathrm{d}t,$$

looking at this formula is clear that if $f_n \longrightarrow f$ in such a way that the r.h.s. converges, so we can take $f_n(x) = e^{isx}e^{-x^2/(2n)}$ so that

$$\langle v, Q(f_n)v\rangle = \int_{\mathbb{R}} \varphi^v(t)\hat{f}_n(t)\mathrm{d}t = (2\pi n^{-1})^{-1/2} \int_{\mathbb{R}} \varphi^v(t) e^{-n(t-s)^2/2}\mathrm{d}t \longrightarrow \varphi^v(s)$$

by continuity of φ^v. So this suggest that we can define $Q(e^{is\cdot}) = U(s)$. In order for this to make full sense we need to extend Q to all continuous bounded functions. Short way to do this is to realise that ℓ^v corresponds to a measure μ^v By Riesz-Markov and then just extend it using measure theory. In this case actually you can extend it to all bounded measurable functions on $\mathbb{R}$.

Note also that if $f_n \uparrow f$ then the sequence $(\langle v, Q(f_n)v\rangle)_n$ is monotone increasing since if $f \geq 0$ then $\langle v, Q(f)v\rangle \geq 0$ so we can extend Q to all $C_b(\mathbb{R})$. To check that the extension is unique the following argument works.

Take now the family $(h_n(x) = \exp(-nx^2))_n$ then by continuity of φ^v it is easy to prove that

$$Q(h_n) \longrightarrow 1_{\mathscr{L}(H)}.$$

Observe that if $f \in C_b(\mathbb{R})$ then $h_n f \in C_0(\mathbb{R})$ and it follows that for any extension Q' of Q to $C_b(\mathbb{R})$ we have

$$Q'(h_n)Q'(f) = Q'(h_n f) = Q(h_n f) = Q(h_n)Q(f)$$

and taking limits we have $Q'(f) = Q(f)$.

So today we proved that for any weakly-continuous one-parameter unitary group in $\mathscr{L}(H)$ we can construct a representation Q of the C^*-algebra $C_b(\mathbb{R})$ on $\mathscr{L}(H)$. It is suggestive to write $f(Q) = Q(f)$ and think to $f(Q)$ as a function computed on an operator Q in such a way that the formula

$$U(t) = \exp(itQ)$$

has now a sense. We could of course associate to Q an unbounded linear operator $\hat{Q}$ on a dense domain within H in such a way that by Stone theorem $\hat{Q}$ is the generator of the group $(U(t))_{t\in\mathbb{R}}$.

From the operational point of view such an homomorphism Q represent an observable in the sense that we can measure its expectation value on any state ω and also we can see it as a random variable with a law given by the linear functional

$$f \mapsto \omega(f(Q)).$$

If we go back to the Weyl relation we now understand that they describe two observables P, Q which satisfy the commutation relations

$$\exp(itQ)\exp(isP) = \exp(2\pi ist)\exp(isP)\exp(itQ).$$

Combining unbouded operators is a task of the same difficulty of combining two homomorphism or two unitary representations of $\mathbb{R}$.

There is no simple way to understand, for example, the sum $P+Q$.

Tentantively in this course we take the attitude that an observable is really a *-homomorphism of $C_b(\mathbb{R})$ into either some abstract C^*-algebra or into a C^*-algebra of operators. This extends to the non-commutative/quantum context the probabilistic notion of real random variable.

This is coherent with our modelisation which sees observables as self-adoint elements of a C^*-algebra in that if $f:\mathbb{R}\longrightarrow\mathbb{R}$ then $f(Q)$ is a self-adjoint operator.

The reason to use this different notion is that it can accomodate the case where we have dealing with "unbounded" obserables. Think for example to a Gaussian random variable X. A Gaussian random variable is not an element of a C^*-algebra since X can take arbitrarily large values. However if we look at X has a $*$-homomorphism by letting $X(f):=f(X)$ for any $f\in C(\mathbb{R})$ then X is a well defined observable. In this case it has a concrete realisation on $L^2(\mathbb{P})$ and if we take $v(\omega)=1$ we have that

$$\langle v, X(f)v\rangle = \mathbb{E}[f(X)].$$
