Elements of Mathematical Quantum Mechanics

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Lecture 7 [June 5th 2024]

Dynamics on a canonical pair

So far we described the kinematics, that is the structure of the space of observables which holds at a specific time, because we imagine to perform a measurement described by \mathscr{A} on a state ω .

Example. Let us start from an example. Note that if $(W(z))_{z \in \mathbb{C}}$ is an irreducible Weyl system on some Hilbert space *H* then also

$$(\tilde{W}_t(z) := W(e^{it}z))_{z \in \mathbb{C}}$$

is a Weyl system for any $t \in \mathbb{R}$. Then it must be that there exists a unitary operator U_t such that

$$U_t W_t(z) U_t^* = W(z), \qquad t \in \mathbb{R}, z \in \mathbb{C}.$$

Moreover we can define an automorphism of the Weyl algebra by letting

$$\alpha_t(W(z)) = W(e^{it}z)$$

(i.e. a map of the Weyl algebra in itself which respects the *-operation and the algebraic relations in the *C**-algebra, and as a consequence is an isometry). This is an example of *dynamics*, i.e. the introduction of a time evolution in our description of a physical system.

Let us obseve that $\alpha_{2\pi}(W(z)) = W(z)$ so $\alpha_{2\pi} = id$. So the dynamics is periodic of period 2π , we will see that it corresponds to the quantum motion of an harmonic oscillator.

The time and dynamics enters into the model via a group $(\alpha_t)_t$ of (*-)automorphisms of \mathscr{A} , which have the following meaning $\omega(\alpha_t(a))$ is the measurement of the observable a at the time t. $\alpha_0 = id$. $\alpha_{t+s} = \alpha_t \circ \alpha_s$, i.e. is a representation of the additive group of \mathbb{R} onto automorphisms of the *C**-algebra \mathscr{A} .

We can let α act on the linear functional by duality: $(\alpha_t^*\omega)(a) := \omega(\alpha_t(a))$ and then this gives a group of linear transformations on linear functionals on \mathscr{A} and is easy to see that it preserves the states of \mathscr{A} .

Remark 1. Suppose that $\alpha_t^* \omega$ is not pure, then it can be decomposed into two states $\alpha_t^* \omega = \lambda \omega_1 + (1 - \lambda) \omega_2$ but then $\omega = \alpha_{-t}^* \alpha_t^* \omega = \lambda \alpha_{-t}^* \omega_1 + (1 - \lambda) \alpha_{-t}^* \omega_2$ so ω is not pure either. Therefore the dynamics preseves pure states.

Fix a specific setting $(\mathcal{H}, \tilde{\mathcal{A}}, \tilde{Q}_0)$ where $\tilde{\mathcal{A}}$ is a general C^* -algebra and \tilde{Q}_0 is a representation in \mathcal{H} .

Definition 2. Let $(\alpha_t)_{t \in \mathbb{R}}$ a set of C^* -automorphisms of $\tilde{\mathscr{A}}$. We call α a regular dynamics, *if*

- *i.* $(\alpha_t)_{t \in \mathbb{R}}$ *is a group wrt. t, i.e.* $\alpha_0 = \text{id } and \alpha_t \circ \alpha_s = \alpha_{t+s}$ for any $t, s \in \mathbb{R}$
- ii. the map $t \mapsto \alpha_t$ is weakly continuous, i.e. for any state ω and for any $a \in \tilde{A}$ the map $t \mapsto \omega(\alpha_t(a))$ is continuous.

Define $\tilde{Q}_t(a) := \tilde{Q}(\alpha_t(a))$ for $a \in \tilde{\mathcal{A}}$. In general this is understood as a *quantum stochastic process*.

Definition 3. The set $\{U(t)\}_{t\in\mathbb{R}} \subset \mathscr{B}(\mathscr{H})$ is a unitary group of strongly continuous operators, if U(t)U(s) = U(t+s) and $U(t)^* = U(-t)$ and if the map $t \mapsto U(t)$ is weakly (and thus strongly) continuous.

Theorem 4. Assume that there exists a state

$$\omega^{h_0}(\alpha_t(a)) = \omega^{h_0}(a) \tag{1}$$

for all $t \in \mathbb{R}$ and $a \in \tilde{\mathcal{A}}$ and $(\alpha_t)_t$ is a regular dynamics of $\tilde{\mathcal{A}}$, then if \mathcal{H} is the GNS representation space associated with ω^{h_0} and $h_0 \in \mathcal{H}$ is the corresponding cyclic vector, then there exists a unitary strongly continuous group $(U(t))_{t \in \mathbb{R}}$ on \mathcal{H} such that

$$\tilde{Q}_t(\cdot) = U(t)\tilde{Q}_0(\cdot)U(-t)$$

and also $U(t)h_0 = h_0$.

The proof is in the notes. It is just GNS as soon as one realises that we can construct U(t) as

$$U(t)\tilde{Q}_0(a)h_0:=\tilde{Q}_0(\alpha_t(a))h_0$$

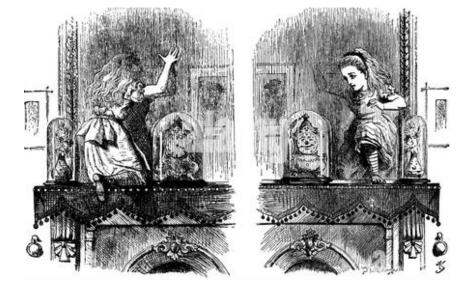
on the dense set $\{\tilde{Q}_0(a)h_0\}_{a\in\tilde{\mathcal{A}}}$ and prove that it is an isometry, here is where we use (1).

Remark 5. Without the hypothesis that the state is invariant, then this construction is not true in general anymore. Take for example \mathscr{A} commutative, i... $C^0_{\infty}(\mathbb{R}^2)$ and consider an Hilbert space $L^2(\mathbb{R}^2, \mu)$ where

$$\mu(\mathrm{d}x) = e^{-x^2/2}\mathrm{d}x + \delta_0(\mathrm{d}x)$$

and the usual moltiplication and take $\alpha_t(f(x)) = f(x - t)$. But here there is no unitary group associated to α . Indeed take the state $\omega^{\mu}(a) = \int a(x)\mu(dx)$. Consider the translated state $\omega^{\mu}(\alpha_t(\cdot))$, then GNS representation of it lives on $L^2(\mathbb{R}^n, \mu_t)$ where $\mu_t = T_t^* \mu$ the pull forward of μ by the translation operator. In order to have a unitary transformation we need that μ_t has to be absolutely continuous wrt. μ , but this is not the case.

Through the looking-glass



In this lectures we will require always to have a unitary implementation of the dynamics $(\alpha_t)_{t \in \mathbb{R}}$ for $(\mathcal{H}, \mathcal{A}, Q_0)$, i.e. to have a strongly continuous group of unitary operators $(U(t))_{t \in \mathbb{R}}$ so that $Q_t(\cdot) = Q_0(\alpha_t(\cdot)) = U(t)Q_0(\cdot)U(-t)$.

Recall that we have proven the following link between unitary groups and representations of $C(\mathbb{R})$:

Theorem 6. Consider an Hilbert space \mathcal{H} , a strongly continuous unitary group $(U(t))_{t \in \mathbb{R}}$ on \mathcal{H} , then there exists a unique C^* -representation X of $C_b^0(\mathbb{R}, \mathbb{C})$ on \mathcal{H} such that

- *i.* $X(e^{it \cdot}) = U(t)$
- *ii.* If $f_n \to f$ pointwise and $\sup_n ||f_n|| < \infty$ then $X(f_n) \to X(f)$ weakly.

Which could be considered a C^* version of the Fourier transform. We want now to do the same for certain semigroups. This essentially is the C^* analogon of the Laplace transform.

Definition 7. $\{K(t)\}_{t \in \mathbb{R}_+} \subseteq \mathscr{B}(\mathscr{H})$. We say that K(t) is a strongly continuous semigroup of self-adjoint contractions if

i.
$$K(0) = 1$$
, $K(t)K(s) = K(t+s)$, for $t, s \ge 0$.

- *ii.* $K(t) = K(t)^*$,
- *iii.* $t \mapsto K(t)$ *is strongly continuous*
- *iv.* $||K(t)h|| \le ||h||, t \ge 0.$

Theorem 8. Assume that K is a strongly continuous semigroup of self-adjoint contractions then there exists a unique representation X of $C_b^0(\mathbb{R}_+)$ on \mathcal{H} such that

i.
$$X(e^{-t}) = K(t)$$

ii. If $f_n \rightarrow f$ pointwise and $\sup_n ||f_n|| < \infty$ then $X(f_n) \rightarrow X(f)$ weakly.

Remember that for proving the theorem on unitary operators we needed Bochner's theorem

Definition 9. If $G: \mathbb{R} \to \mathbb{C}$ we call G positive definite if for any $\lambda_1, ..., \lambda_k \in \mathbb{C}$ and $t_1, ..., t_k \in \mathbb{R}$ we have

$$\sum_{i,j=1}^k \lambda_i \bar{\lambda}_j G(t_i - t_j) \ge 0$$

Theorem 10. (Bochner) G is a continuous positive definite function iff there exists a bounded positive measure μ on \mathbb{R} such that

$$G(t) = \int_{\mathbb{R}} e^{itx} \mu(\mathrm{d}x).$$

In this case we will need Bernstein's theorem

Theorem 11. (Bernstein) F is a bounded totally monotone function iff there exists a bounded positive measure μ on \mathbb{R}_+ and a constant $C \ge 0$ such that

$$F(t) = C \int_{\mathbb{R}_+} e^{-tx} \mu(\mathrm{d}x).$$

where

Definition 12. We say that $F: \mathbb{R}_+ \to \mathbb{C}$ is totally monotone if for any $\lambda_1, \ldots, \lambda_k \in \mathbb{C}$ and $t_1, \ldots, t_k \in \mathbb{R}_+$ we have

$$\sum_{i,j=1}^k \lambda_i \bar{\lambda}_j F(t_i + t_j) \ge 0.$$

Lemma 13. Assume that *F* is a bounded, totally monotone function, then

a) For any a > 0, $-\Delta_a F$ is bounded totally monotone with $\Delta_a F(t) = F(t+a) - F(t)$.

Corollary 14. If *F* is bounded and totally monotone, for any $a_1, \ldots, a_n \in \mathbb{R}_+$

$$(-1)^n \Delta_{a_1} \cdots \Delta_{a_n} F$$

is totally monotone and therefore $(-1)^n \Delta_{a_1} \cdots \Delta_{a_n} F \ge 0$.

The idea to construct X is to consider

$$F_K(t,h) := \langle h, K(t)h \rangle$$

for h unit vector in $\mathcal H$ and check that it is totally monotone. So by Bernstein it exists a measure μ^h such that

$$\langle h, K(t)h \rangle = \int_{\mathbb{R}_+} e^{-tx} \mu^h(\mathrm{d}x).$$

From that one can construct *X* as

$$\langle h, X(f)h \rangle := \int_{\mathbb{R}_+} f(x)\mu^h(\mathrm{d}x) \, dx$$

The following lemma guarantees uniqueness

Lemma 15. There is only one C^* representation X_0 of $C_b^0(\mathbb{R}_+, \mathbb{C})$ such that

$$X_0(e^{-t\cdot}) = K(t).$$

See the notes for more details.

Now we have seen that if $(U(t))_{t\in\mathbb{R}}$ is a strongly continuous unitary group this is equivalent to have an representation X_U of $C_b^0(\mathbb{R}, \mathbb{C})$ on $\mathscr{B}(\mathscr{H})$ and if $(K(t))_{t\geq 0}$ is a selfadjoint, strongly continuous contraction semigroup, then we have a representation X_K of $C_b^0(\mathbb{R}_+, \mathbb{C})$ on $\mathscr{B}(\mathscr{H})$. We want to look into the relation between these two objects.

Definition 16. We say that $(U(t))_{t \in \mathbb{R}}$ (as before) has **positive energy** for each $f \in C_b^0(\mathbb{R}, \mathbb{C})$ such that $\sup p(f) \subseteq (-\infty, 0)$ we have that $X_U(f) = 0$.

Remark 17. Assume that $f_1, f_2 \in C_b^0(\mathbb{R}, \mathbb{C})$ such that $f_1 = f_2$ on $[0, \infty)$ then if *U* has positive energy then $X_U(f_1) = X_U(f_2)$.

Lemma 18. U has positive energy iff for any $h \in \mathcal{H} \mu_U^h$ is supported on $\mathbb{R}_+ = [0, \infty)$ where

 μ_U^h is the measure such that

$$\langle h, X_U(f)h \rangle = \int f(x)\mu^{h,U}(\mathrm{d}x).$$

Theorem 19. Assume $(U(t))_{t\in\mathbb{R}}$ is a strongly continuous unitary group with positive energy, then $K(t) = X_U(e^{-t})$ is a strongly continuous self-adjoint contraction semigroup and also $X_U = X_K$ on $C_b^0(\mathbb{R}_+, \mathbb{C})$. The converse is true, i.e. if we have K and we define $U(t) = X_K(e^{it})$, then $(U(t))_{t\in\mathbb{R}}$ is a strongly continuous unitary group with positive energy and $X_K = X_U$.

We want to justify now the name of "positive energy". This is not fundamental in the following but will give a better grasp of the connection with standard physical intuition.

By the way note that

$$U(t)X_U(f)U(-t) = X_U(e^{-it}fe^{+it}) = X_U(f)$$

so the homomorphism X_U is invariant under the time dynamics. It is a generalized observable called "energy".

Let \mathscr{D}_H be a subspace of \mathscr{H} such that $h \in \mathscr{D}_H$ iff $t \mapsto U(t)h$ is strongly differentiable in 0. For any $h \in \mathscr{D}_H$ we define

$$Hh = \frac{1}{i} \lim_{t \to 0} \frac{U(t)h - h}{t} \in \mathscr{H}.$$

Is simple to prove that *H* is a linear operator $H: \mathcal{D}_H \to \mathcal{H}$. For generic *U*, the operator *H* is not bounded, which implies that *H* cannot be extended as a continuous operator on all \mathcal{H} . *H* is an *unbounded operator* and \mathcal{D}_H is called the domain of *H*.

Lemma 20. $h \in \mathcal{D}_H$ iff

$$\int_{\mathbb{R}} x^2 \mu^{h,U}(\mathrm{d} x) < \infty, \quad and \ then \qquad \|Hh\|^2 = \int_{\mathbb{R}} x^2 \mu^{h,U}(\mathrm{d} x).$$

If $h_1 \in \mathcal{D}_H$ and $h_2 \in \mathcal{H}$ then

$$\int_{\mathbb{R}} |x| |\mu^{h_1, h_2, U}|(\mathrm{d}x) < \infty, \quad and \qquad \langle Hh_1, h_2 \rangle = \int_{\mathbb{R}} x \mu^{h_1, h_2, U}(\mathrm{d}x).$$

where $\mu^{h_1,h_2,U}$ is the polarization of the hermitian map $h \mapsto \mu^{h,U}$.

Theorem 21. \mathcal{D}_H is dense in \mathcal{H} and $h_1, h_2 \in \mathcal{D}(H)$ we have $\langle Hh_1, h_2 \rangle = \langle h_1, Hh_2 \rangle$, so H is symmetric.

Remark 22. Is possible to prove that (H, \mathcal{D}_H) is self-adjoint, i.e. $H^* = H$. (given the natural definition of the adjoint of a densely defined unbounded operator)

If $h_1, h_2 \in \mathcal{D}_H$ we define

$$\mathscr{E}(h_1,h_2) = \langle Hh_1,h_2 \rangle$$

If $h_1 \in \mathcal{D}_H$ and $||h||_{\mathcal{H}} = 1$ then we define $\mathcal{C}(h, h)$ to be the energy of the state $h \in \mathcal{H}$.

Recall that $(\mathcal{H}, \mathcal{A}, Q_0)$ is our quantum space and if $h \in \mathcal{H}$ gives the vector state $\omega^h(a) = \langle Q_0(a)h, h \rangle$. So the energy is an extension of this formula for the unbounded operator H which formally is the derivative of the time-evolution group U. We had $Q_t(a) = U(-t)Q_0(a)U(t)$. If it is possible to take the derivative wrt. to t then we obtain

$$\partial_t Q_t(a) = \frac{1}{i} [H, Q_t(a)]$$

Theorem 23. *U* has positive energy iff $\mathscr{C}(h,h) \ge 0$ for all $h \in \mathscr{D}_{H}$.

Recall the definitions

$$F_{U}(t,h) = \langle U(t)h,h \rangle = \int_{\mathbb{R}} e^{itx} \mu^{h,U}(dx),$$
$$F_{K}(t,h) = \langle K(t)h,h \rangle = \int_{\mathbb{R}^{+}} e^{-tx} \mu^{h,K}(dx).$$

Theorem 24. The function F_K is holomorphic when $t \in \mathbb{C}$ and $\operatorname{Re}(t) > 0$ and it is continuous when $\operatorname{Re}(t) \ge 0$. Moreover, we have that

$$F_U(s,h) = F_K(is,h) = \lim_{y \downarrow 0} F_K(is+y,h).$$

Remark 25. We can define the generator H' of K similarly as we defined the generator H of U. Namely $\mathcal{D}_{H'}$ is defined as the set of vectors $h \in \mathcal{H}$ such that K(t)h is strongly differentiable in zero and define

$$H'h = -\lim_{t\downarrow 0} \frac{K(t)h - h}{t}.$$

But if *U* and *K* are related so that $X_U = X_K$ then H' = H and $\mathcal{D}_H = \mathcal{D}_{H'}$.

Consider now $\mathcal{H} = L^2(\mathbb{R}^n, dx)$. $\mathcal{A} = C_b^0(\mathbb{R}^n, \mathbb{C})$ and $(Q_0(a)h)(x) = a(x)h(x)$. Define

$$K(t)h = \rho_t * h = \frac{1}{(2\pi t)^{n/2}} \int e^{-|x-y|^2/(2t)} h(y) dy.$$

Theorem 26. $(K(t))_{t \ge 0}$ is a strongy continuous, self-adjoint contraction semigroup.

Take $f \in C^{\infty} \cap L^p$ for any $p \ge 1$. Then in $L^2(\mathbb{R}^n)$ we have

$$\lim_{t\downarrow 0} \mathscr{F}\left(\frac{K(t)f-f}{t}\right)(k) = \lim_{t\downarrow 0} \frac{e^{-tk^2/2}-1}{t} \mathscr{F}(f)(k) = -k^2 \mathscr{F}(f)(k) = \mathscr{F}(\Delta f)(k)$$

so $H = -\Delta$ and one can prove that $\mathcal{D}_H = H^2$. Moreover $\mathscr{C}(h, h) = \int_{\mathbb{R}^n} |\nabla h|^2 dx \ge 0$. So the semigroup has positive energy (it was already clear from the fact that it is a contraction). So now

$$F_K(t,h) = \int_{\mathbb{R}^{2n}} \frac{e^{-|x-y|^2/2t}}{(2\pi t)^{n/2}} h(x) \overline{h(y)} dx dy$$

and for $h \in L^2 \cap L^1$ we have the explicit representation

$$F_U(s,h) = F_K(is,h) = \int_{\mathbb{R}^{2n}} \frac{e^{-|x-y|^2/2(is)}}{(2\pi i s)^{n/2}} h(x)\overline{h(y)} dxdy$$

where $(i)^{n/2} = e^{\pi i n/4}$ given the kind of limit we had to perform.

We conclude therefore that for $h \in L^2 \cap L^1$

$$(U(s)h)(x) = \int_{\mathbb{R}^n} \frac{e^{-|x-y|^2/2(is)}}{(2\pi i s)^{n/2}} h(y) \mathrm{d}y.$$

This is the model of the free particle in \mathbb{R}^n , i.e. a particle not interacting with any external system. In this case $(U(t))_{t\in\mathbb{R}}$ is a unitary group on $L^2(\mathbb{R}^n)$ and the expectation of any observable $Q_t(a)$ on the state ω^h evolves according to the equation

$$\omega_t^h(a) = \langle Q_t(a)h, h \rangle = \langle U(-t)Q_0(a)U(t)h, h \rangle = \langle Q_0(a)U(t)h, U(t)h \rangle$$

To construct more complex dynamics we will look at the Euclidean strategy next time.

In two weeks: Wightman and Schwinger functions.