Elements of Mathematical Quantum Mechanics

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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 $\mathcal A$ 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

$$
(\,\tilde W_t(z)\,\!:=W(\mathit{e\,}^{it}z)\,)_{{z}\in\mathbb{C}}
$$

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

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

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 \mathcal{A} , which have the following meaning $ω(α_t(a))$ is the measurement of the observable *a* at the time *t*. α_0 =id. α_{t+s} = α_t ° α_s , i.e. is a representation of the additive group of \R onto automorphisms of the C^\ast -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 \mathcal{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 $(\mathscr{H},\tilde{\mathscr{A}},\tilde{\mathcal{Q}}_0)$ where $\tilde{\mathscr{A}}$ is a general C *-algebra and $\tilde{\mathcal{Q}}_0$ is a representation in ℋ.

Definition 2. *Let* (*αt*)*t*∈ℝ *a set of C* [∗]*-automorphisms of* ˜ *.We call α a regular dynamics, if*

- *i.* $(\alpha_t)_{t \in \mathbb{R}}$ *is a group wrt. t, i.e.* $\alpha_0 = id$ *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* $a \in \mathcal{A}$ *the map* $t \mapsto \omega(\alpha_t(a))$ *is continuous.*

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

Definition 3. *The set* {*U*(*t*)}*t*∈ℝ ⊂ℬ(ℋ) *is a unitary group of strongly continuous oper* ators, 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 repre*sentation space associated with ω ^h*⁰ *and h*0∈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 ${\{\tilde{Q}_0(a)h_0\}}_{a \in \tilde{A}}$ and prove that it is an isometry, here is where we use [\(1\)](#page-1-0).

Remark 5. Without the hypothesis that the state is invariant, then this construction is not true in general anymore. Take for example *⊘* commutative, i..e $C_{\infty}^{0}(\mathbb{R}^{2})$ 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 μ_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* ℋ*, then there exists a unique C* [∗]*-representation X of C^b* ⁰(ℝ,ℂ) *on* ℋ *such that*

- *i.* $X(e^{it}) = U(t)$
- *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. ${K(t)}_{t \in \mathbb{R}_+}$ ⊆ $\mathcal{B}(\mathcal{H})$ *. 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-adjointcontractions* t *hen there exists a unique representation* X *of* $C_b^0(\mathbb{R}_+)$ *on* $\mathscr H$ *such that*

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

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

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

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

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

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

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

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* $C \geq 0$ *such that*

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

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*

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

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 *₩* 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

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

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*

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

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 $C^0_b(\mathbb{R},\mathbb{C})$ on $\mathscr{B}(\mathscr{H})$ and if $(K(t))_{t\geqslant 0}$ 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.

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

 ${\bf Remark~17.}$ Assume that $f_1, f_2{\in}C_b^0({\mathbb R},{\mathbb C})$ such that $f_1{\sf = }f_2$ 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 $h \in \mathcal{H}$ μ_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 $U(t)$ = *XK*(*e it*⋅)*, then* (*U*(*t*))*t*∈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

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

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

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

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

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*∈ \mathcal{D}_H *iff*

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

If h_1 ∈ \mathcal{D}_H *and* h_2 ∈ \mathcal{H} *then*

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

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

Theorem 21. \mathscr{D}_H is dense in \mathscr{H} and $h_1, h_2 \in \mathscr{D}(H)$ 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∈ \mathcal{D}_H we define

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

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

Recall that $(\mathscr{H},\mathscr{A},Q_0)$ is our quantum space and if $h\!\in\!\mathscr{H}$ 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* $\mathcal{E}(h, h) \geq 0$ *for all* $h \in \mathcal{D}_H$.

Recall the definitions

$$
F_U(t, h) = \langle U(t)h, h \rangle = \int_{\mathbb{R}} e^{itx} \mu^{h,U}(\mathrm{d}x),
$$

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

Theorem 24. *The function* F_K *is holomorphic when* $t \in \mathbb{C}$ *and* $\text{Re}(t) > 0$ *and it is continuous when* $Re(t) \ge 0$ *. 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. $(K(t))_{t\geq0}$ is a strongy continuous, self-adjoint contraction semigroup.

Take f ∈ C^{∞} ∩ L^p for any p ≥ 1. Then in $L^2(\mathbb{R}^n)$ we have

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

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

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

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

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

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

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

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

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.

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