C*-dynamical systems from number theory

Part 1: C*- dynamical systems and KMS states: definitions, background and examples

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Dynamical systems and states

A C*-dynamical system is a pair (A, σ) with

- A a C*-algebra (whose self adjoint elements are the *observables*)
- $\sigma : \mathbb{R} \to \mathrm{Aut}(A)$ (the *dynamics* or time evolution on A)

(here $\sigma_0 = \mathrm{id}$, $\sigma_s \circ \sigma_t = \sigma_{s+t}$ and $t \mapsto \sigma_t(a)$ is norm continuous)

A *state* of A is a positive linear functional φ normalized so that $\|\varphi\| = 1$ and $\varphi(\sigma_t(a))$ is the *expectation value* of the observable $a \in A^{sa}$ corresponding to the state φ at time $t \in \mathbb{R}$.

Basic facts

1. The states of a commutative C*-algebra $A = C_0(\Omega)$ are in bijection with the probability measures on its spectrum Ω.

$$\varphi_\mu(f) = \int_\Omega f \, d\mu.$$

2. If A is a C*-subalgebra of $B(\mathcal{H})$ for a Hilbert space $\mathcal{H}$, each unit vector $\xi \in \mathcal{H}$ gives rise to a state

$$\omega_\xi(a) := \langle a\xi, \xi \rangle.$$

These *vector states* are not all there is, but...

3. **GNS construction:** for each state φ of A there is a Hilbert space $\mathcal{H}_\varphi$, a representation $\pi_\varphi : A \to B(\mathcal{H}_\varphi)$, and a cyclic unit vector $\xi_\varphi \in \mathcal{H}_\varphi$ such that

$$\varphi(a) = \langle \pi_\varphi(a)\xi_\varphi, \xi_\varphi \rangle.$$

Analytic elements

Let (A, σ) be a C*-dynamical system; an element $a \in A$ is called *σ-analytic if the map $t \mapsto \sigma_t(a) \in A$ extends to an A-valued entire function $z \mapsto \sigma_z(a)$. Equivalently, a is σ-analytic if $t \mapsto f(\sigma_t(a))$ extends to a complex-valued entire function for every bounded linear functional f on A.*

Fact: The σ-analytic elements form a dense *-subalgebra of A.

Key idea: For $a \in A$ the element

$$a_n := \sqrt{\frac{n}{\pi}} \int_{\mathbb{R}} \sigma_t(a) \exp(-nt^2)\, dt$$

is analytic for σ because the function

$$z \mapsto \sigma_z(a_n) := \sqrt{\frac{n}{\pi}} \int_{\mathbb{R}} \sigma_t(a) \exp(-n(t-z)^2)\, dt$$

is entire and $\|a_n - a\| \to 0$.

The KMS condition

Definition (Haag-Hugenholtz-Winnink, 1967)

A state φ on A satisfies the Kubo-Martin-Schwinger (KMS) condition with respect to σ at inverse temperature $\beta \in [0, \infty)$ (φ is a σ- KMS$_\beta$ state), if

$$\varphi(ab) = \varphi(b\sigma_{i\beta}(a))$$

for all σ-analytic elements $a, b \in A$.

Remark: This is a tracelike condition, twisted by σ along 'imaginary time'.

General reference for KMS condition [Bratteli-Robinson, *Operator algebras and quantum statistical mechanics. 2. Equilibrium states. 2nd ed. 1997. Springer Verlag; pdf downloadable*]

KMS condition (equivalent formulations)

1. Since $\|\varphi(\sigma_t(a))\| \leq \|a\|$ the state φ is KMS$_\beta$ for σ iff

$$\varphi(ab) = \varphi(b\sigma_{i\beta}(a))$$

   for a and b in a set of analytic elements with dense linear span. This formulation has the advantage of reducing the verification to a minimum. (hw: prove the equivalence)

   Also equivalent, and closer to the original boundary condition for Green functions used by Kubo, is the condition:

2. (For $\beta > 0$.) A state φ is a KMS$_\beta$-state if for any $a, b \in A$ there exists a continuous function

$$f : \{z \in \mathbb{C} \mid 0 \leq \Im z \leq \beta\} \to \mathbb{C}$$

   that is analytic in the open strip $0 < \Im z < \beta$ and satisfies

$$f(t) = \varphi(b\sigma_t(a)), \quad f(t + i\beta) = \varphi(\sigma_t(a)b) \quad \text{for all} \quad t \in \mathbb{R}.$$

   This has the advantage of not requiring analytic elements.

KMS states are stationary

Proposition

If $\beta \neq 0$ and φ is a KMS_β state, then φ is σ-invariant.

Proof: (assuming $1 \in A$ to simplify things).

Let b be analytic for σ. The entire function $z \mapsto \varphi(\sigma_z(b))$ has period $(i\beta)$ because the KMS condition implies

$$\varphi(\sigma_z(b)1) = \varphi(1\sigma_{z+i\beta}(b)).$$

Since $\|\phi(\sigma_t(b))\| \leq \|b\|$ for $t \in \mathbb{R}$ the function is bounded on the boundary of the strip $0 < \Im z < \beta$ and has period $i\beta$ so it is bounded on $\mathbb{C}$, hence it is constant. □

We will soon see that the converse is not true.

For $\beta = 0$ the KMS condition is simply a tracial condition that does not involve σ, but it is standard for this case to *require σ-invariance explicitly,* so the definition is (KMS_0 state) $\equiv$ (σ-invariant trace).

ground states

The state φ of A is a ground state for σ if

$$z \mapsto \varphi(b\sigma_z(a))$$

is bounded on the upper half plane for every $a, b \in A$ with a analytic for σ.

When the function is bounded it is bounded by $\|a\|\|b\|$ and it suffices to check the condition for a set of analytic elements with dense linear span. (hw: verify this) The proof involves a Phragmen-Lindelöf type result in complex variable:

Proposition

Let H denote the upper half plane and suppose f is continuous on $\overline{H}$ and holomorphic on H. If f is bounded on $\overline{H}$ then it is bounded by $\sup\{|f(x)| : x \in \mathbb{R}\}$.

KMS as an equilibrium condition

In 1967 H-H-W proposed the KMS condition as a definition of equilibrium for quantum systems. This was postulated from an insightful analogy with a property of boundary values of Green functions in statistical mechanics, motivated by work of Kubo, and of Martin and Schwinger.

Soon afterwards it was proved that KMS states have several of the properties characteristic of equilibrium, e.g.

- Stability
- Passivity
- Minimality

and that they also play a major role in the Tomita-Takesaki theory in von Neumann algebras.

The KMS condition is an essentially *noncommutative* phenomenon:

Proposition (see e.g Bratteli-Robinson vol.II ch 5)

If (A, σ) has a faithful KMS and A is commutative, then σ is trivial.

For us, KMS is simply a condition that generalizes the trace property in the presence of a dynamics.

Example (finite quantum systems)

'borrowed' from [Hugenholtz, *C*-algebras and statistical mechanics* Proc. Symp. Pure Math. **38** (1981)]

- $A = \mathrm{Mat}_n(\mathbb{C})$, so the observables are the selfadjoint $n \times n$ matrices.
- Every time evolution σ on $\mathrm{Mat}_n(\mathbb{C})$ arises as $\sigma_t(a) = e^{itH} a e^{-itH}$ with H a selfadjoint matrix (a *Hamiltonian*) which is determined up to an additive constant, and is usually normalized so that its smallest eigenvalue is 0. *Exercise: which matrices are analytic for σ?*
- There is a 1 to 1 correspondence between states φ of $\mathrm{Mat}_n(\mathbb{C})$ and *density matrices* Q_φ such that $\varphi(a) = \mathrm{Tr}(aQ_\varphi)$.
  ($Q \in \mathrm{Mat}_n(\mathbb{C})$ is a density matrix iff $Q \geq 0$ and $\mathrm{Tr}\, Q = 1$)
- φ is pure (i.e. extremal in the state space) iff Q_φ is a rank-one projection.

Example (finite quantum systems)

- The stationary (i.e. σ-invariant) states are those for which

$$\mathrm{Tr}(e^{itH} a e^{-itH} Q) = \mathrm{Tr}(aQ) \qquad \forall a \in \mathrm{Mat}_n(\mathbb{C});$$

  by the trace property this is equivalent to $\mathrm{Tr}(a e^{-itH} Q e^{itH}) = \mathrm{Tr}(aQ)$ hence φ is stationary iff Q_φ commutes with e^{itH}, and thus with H.

- Extremal stationary states are pure; their density matrices are the projections onto the eigenvectors of H.

- The *von Neumann entropy* of a state $\varphi = \mathrm{Tr}(\cdot\, Q_\varphi)$ is

$$S(\varphi) := -\mathrm{Tr}(Q_\varphi \log Q_\varphi).$$

  $S(\varphi) = 0$ (minimal) when φ is pure, and $S(\varphi) = \log n$ (maximal) when φ is the normalized trace. *"A pure state has maximal information, and the normalized trace has minimal information."*

Example (finite quantum systems)

Definition

The *free energy:* of the state φ of $\mathrm{Mat}_n(\mathbb{C})$ with Hamiltonian H at inverse temperature $\beta = 1/T$ is $\quad F(\varphi) := -S(\varphi) + \beta\varphi(H)$,

The free energy (for fixed β and H) is minimized at a unique state:

Proposition (thermodynamic inequality)

1) $\quad F(\varphi) := -S(\varphi) + \beta\varphi(H) \geq -\log \mathrm{Tr}(e^{-\beta H})$;

2) equality holds if and only if φ is the **Gibbs state** φ_G*, having density matrix* $Q_G = \frac{1}{\mathrm{Tr}(e^{-\beta H})} e^{-\beta H}$.

For a proof see e.g. the appendix in [Hugenholtz, *C*-algebras and statistical mechanics*]. (or try it as an exercise, for which you will need a few basic but nontrivial facts about matrices and convex functions)

Convex functions and matrices

- For self adjoint matrices A and B,

$$|\log \operatorname{Tr} e^{A} - \log \operatorname{Tr} e^{B}| \leq \|A - B\|$$

- If, in addition $f : \mathbb{R} \to \mathbb{R}$ is a convex function, then

$$\operatorname{Tr}\left(f(A) - f(B) - (A - B)f'(B)\right) \geq 0$$

  When f is strictly convex, then equality holds iff $A = B$.

- If A and B are positive, then setting $f(t) = t \log t$ gives

$$\operatorname{Tr}(A \log A) - \operatorname{Tr}(A \log B) \geq \operatorname{Tr}(A - B)$$

  and if A and B are density matrices (trace one and positive), this yields

$$\operatorname{Tr}(A \log A) - \operatorname{Tr}(A \log B) \geq 0$$

Convex functions and matrices

- (Peierls's inequality) For self adjoint $A \in \mathrm{Mat}_n(\mathbb{C})$ and $\{x_i\}$ an orthonormal set in H
$$\sum_i e^{\langle Ax_i, x_i\rangle} \leq \operatorname{Tr} e^A.$$
- The function $A \mapsto \log \operatorname{Tr} A$ is an increasing convex function of the selfadjoint matrices to $\mathbb{R}$.
- The function $\Omega \mapsto \operatorname{Tr}(\Omega \log \Omega)$ is convex on the set of density matrices $\{\Omega \in \mathrm{Mat}_n : \Omega \geq 0,\ \operatorname{Tr}\Omega = 1\}$

Example (finite quantum systems)

Proposition

The Gibbs state φ_G is the unique state on $\mathrm{Mat}_n(\mathbb{C})$ such that

$$\varphi(ab) = \varphi(b\sigma_{i\beta}(a))$$

for all $a, b \in \mathrm{Mat}_n(\mathbb{C})$, where $\sigma_{i\beta}(a) = e^{-\beta H} a e^{\beta H}$.

HW project: Prove the proposition. You will need to show that the Gibbs density is the only density that satisfies

$$\mathrm{Tr}(abQ) = \mathrm{Tr}(be^{-\beta H} a e^{\beta H} Q)$$

for every pair of matrices a, b in $\mathrm{Mat}_n(\mathbb{C})$ (an interesting exercise in linear algebra).

Thus the KMS condition characterizes equilibrium for finite systems. For some infinite systems, equilibrium states are defined as thermodynamical limits of local Gibbs states, and are also characterized by KMS.

The set of KMS-states

Let Σ_β be the set of σ-KMS$_\beta$-states. Then

- if $\varphi_i \in \Sigma_{\beta_i}$ and $\beta_i \to \beta$ then any weak* limit point of $\{\varphi_i\}_i$ is a KMS$_\beta$-state;
- if $\varphi \in \Sigma_\beta$ then the normal extension $\bar{\varphi}$ of φ to $\pi_\varphi(A)''$ is faithful and $\sigma_t^{\bar{\varphi}} \circ \pi_\varphi = \pi_\varphi \circ \sigma_{-\beta t}$; in particular, for $\beta \neq 0$ a state φ with faithful GNS-representation can be a σ-KMS$_\beta$-state for at most one dynamics σ, and then if such a nontrivial dynamics σ is fixed, β is also uniquely determined;
- a point $\varphi \in \Sigma_\beta$ is extremal if and only if $\pi_\varphi(A)''$ is a factor (i.e. has trivial center)
- extremal KMS$_\beta$ states are also called pure phases.
- if A is unital then Σ_β is a Choquet simplex in A^*, that is, it is a convex weakly*-closed subset of A^* and (assuming A is separable) every point in Σ_β is the barycenter of a unique probability measure concentrated on the extremal points of Σ_β;

Partition function

Some C*-dynamical systems have no Hamiltonian (that is, σ_t is not of the form $e^{itH} \cdot e^{-itH}$ for any H associated to the C*-algebra A). To get around this, we consider A represented on a Hilbert space $\mathcal{H}$.
However, the following situation often arises

- Let $\pi \colon A \to B(\mathcal{H})$ be an irreducible representation. Assume there exists an (unbounded) self-adjoint operator H on $\mathcal{K}$ such that

$$\pi(\sigma_t(a)) = e^{itH}\pi(a)e^{-itH} \quad \text{for all} \quad a \in A.$$

- The operator H is uniquely determined if we require that zero is the smallest point in its spectrum. The function $\beta \mapsto \mathrm{Tr}(e^{-\beta H})$ is then called the **partition function** associated to π.
- When $\mathrm{Tr}(e^{-\beta H}) < \infty$, then $\varphi(\cdot) = \mathrm{Tr}(\cdot\, e^{-\beta H})/\mathrm{Tr}(e^{-\beta H})$ is a σ-KMS$_\beta$-state. This is similar to the Gibbs state of the finite system over $A = \mathrm{Mat}_n(\mathbb{C})$.

- Equivalently, if φ is an extremal σ-KMS$_\beta$-state such that the von Neumann algebra $M = \pi_\varphi(A)''$ has type I, then $\varphi(a) = \mathrm{Tr}(ae^{-\beta H})/\,\mathrm{Tr}(e^{-\beta H})$ for a unique positive operator H affiliated with M, having zero in the spectrum.
- For each $\beta' > \beta$, we have $e^{-\beta' H} \leq e^{-\beta H}$, and hence

$$\varphi'(\cdot) = \mathrm{Tr}(\cdot\, e^{-\beta' H})/\,\mathrm{Tr}(e^{-\beta' H})$$

  is a KMS$_{\beta'}$ state.
  (So 'cooling down' to a larger inverse temperature has the effect of improving equilibrium.)

cf. [Powers-Sakai, '75], [Jorgensen, '77] and others.

Phase transition and symmetry breaking

A **phase transition** is an abrupt change in physical properties of a system.

Example: transition between the solid, liquid, and gaseous phases as temperature increases.

Phase transitions often (but not always) take place between phases with different symmetry. Some intuitive examples are:

- A snowflake is less symmetric than a (spherical) drop of water.
- Ferromagnets are capable of spontaneous magnetization (dipoles "align" each other) at low temperatures.

In C*-algebraic terms, the group of automorphisms of A commuting with σ and preserving every KMS$_\beta$-state changes as β varies.
Typically the symmetry group gets smaller as temperature decreases. This is known as **spontaneous symmetry breaking:** only symmetric configurations can be at equilibrium at high temperature while the system admits asymmetric equilibrium configurations upon cooling down.