KMS states and Tomita-Takesaki Theory

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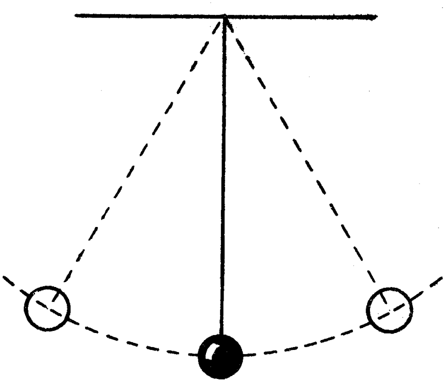
Motivation



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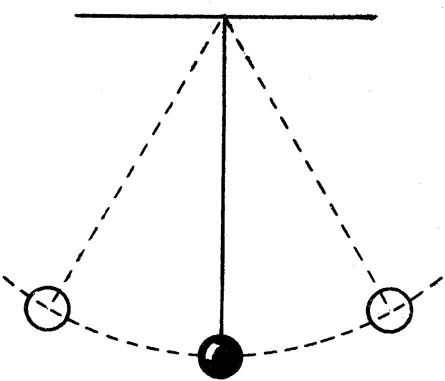

Can we obtain the equations of motion from the equilibrium state?

Maybe in quantum thermal systems.

$$e^{-\beta H} \circlearrowright e^{-iHt}$$

$$\text{temperature} \iff i \times \text{time}$$

Outline

Elements of Classical and Quantum Theories

Classical theories

- Auxiliary space: locally compact Hausdorff space X;

Quantum theories

- Auxiliary space: separable Hilbert space $\mathcal{H}$

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- States: probability measures P on X;

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- Auxiliary space: separable Hilbert space $\mathcal{H}$
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- States: positive, self-adjoint, normalized and trace-class operators ρ on $\mathcal{H}$;

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- States: probability measures P on X;
- Expectation values: $\int f dP$.

Quantum theories

- Auxiliary space: separable Hilbert space $\mathcal{H}$
- Observables: self-adjoint operators on $\mathcal{H}$
- States: positive, self-adjoint, normalized and trace-class operators ρ on $\mathcal{H}$;
- Expectation values: $\mathrm{tr}(A\rho)$.

Difference between Classical and Quantum theories

EPR paradox [Einstein et al., 1935]

Difference between Classical and Quantum theories

$$
\begin{tikzcd}
\text{EPR paradox [Einstein et al., 1935]} \arrow[rr] \arrow[d] & & \text{QM is incomplete} \arrow[d] \\
\text{QM is complete} \arrow[d] & & {} \arrow[d] \\
{} \arrow[uurr] & & {} \arrow[d] \\
& {} & {} \arrow[l]
\end{tikzcd}
$$

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\text{Entangled states } \lightning \arrow[uur] & {} \arrow[d] \\
{} & {} \arrow[l]
\end{tikzcd}
$$

Difference between Classical and Quantum theories

EPR paradox [Einstein et al., 1935] ⟶ QM is incomplete

QM is complete

Entangled states ↯

Search for complete theory:
Boolean propositions

Bell's inequalities [Bell, 1964]
[Reyes-Lega, 2013]

Difference between Classical and Quantum theories

$$
\begin{tikzcd}
\text{EPR paradox [Einstein et al., 1935]} \arrow[r] \arrow[d] & \text{QM is incomplete} \arrow[d] \\
\text{QM is complete} \arrow[d] & \begin{array}{c}\text{Search for complete theory:} \\ \text{Boolean propositions}\end{array} \arrow[d] \\
\text{Entangled states } \lightning \arrow[uur] & \begin{array}{c}\text{Bell's inequalities [Bell, 1964]} \\ \text{[Reyes-Lega, 2013]}\end{array} \arrow[d] \\
\text{Lattice of projections [Wilce, 2012]} & \text{Against experiment!} \arrow[l]
\end{tikzcd}
$$

Algebraic Quantum Mechanics

- Observables: A C^*-algebra $\mathcal{A}$:
  - Complete normed vector space with product and involution;
  - C^* property: $\|A^*A\| = \|A\|^2$;
  - We will assume that all the algebras we discuss are unital.
- States: Linear functionals $\omega : \mathcal{A} \to \mathbb{C}$ which are non-negative ($\omega(A^*A) \geq 0$) and normalized ($\omega(1) = 1$).

Remark: The auxiliary Hilbert space will now be an emergent concept.

GNS Construction

Start with a C^*-algebra $\mathcal{A}$ and a state ω.

- $\mathcal{N}_\omega := \{A \in \mathcal{A} | \omega(A^*A) = 0\}$
- Hilbert space $\mathcal{H}_\omega := \overline{\mathcal{A}/\mathcal{N}_\omega}$ with $\langle [A], [B] \rangle := \omega(A^*B)$
- Define the representation extending

$$\begin{aligned} \pi_\omega : \mathcal{A} \to & \quad \mathcal{B}(\mathcal{H}_\omega) \\ A \mapsto & \pi_\omega(A) : \mathcal{H}_\omega \to \mathcal{H}_\omega \\ & \qquad [B] \mapsto [AB] \end{aligned}$$

- Cyclic vector $\Omega_\omega := [1]$, that is, $\overline{\mathcal{A}\Omega_\omega} = \mathcal{H}_\omega$
- This is the unique $*$-representation of $\mathcal{A}$ with a cyclic vector Ω_ω such that $\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle = \mathrm{tr}(\pi_\omega(A)\rho_{\Omega_\omega})$.

Example: $M_{2\times 2}(\mathbb{C})$

Consider the most general state on this algebra

$$\omega_\lambda(A) = \lambda A_{11} + (1-\lambda)A_{22} = \mathrm{tr}(\rho_\lambda A), \quad \rho = \begin{bmatrix} \lambda & 0 \\ 0 & 1-\lambda \end{bmatrix} \tag{1}$$

for $\lambda \in [0,1]$. Let E_{ij} be the matrix units so that $A = A_{ij}E_{ij}$

$$\omega_\lambda(A^*A) = \omega_\lambda(A^*_{ki}A_{kj}E_{ij}) = \lambda(|A_{11}|^2 + |A_{21}|^2) + (1-\lambda)(|A_{12}|^2 + |A_{22}|^2).$$

Therefore

$$\mathcal{N}_\lambda = \begin{cases} \mathrm{span}\{E_{11}, E_{21}\} & \lambda = 0 \\ \mathrm{span}\{E_{12}, E_{22}\} & \lambda = 1 \\ \{0\} & \lambda \in (0,1) \end{cases} \qquad \mathcal{H}_\lambda = \begin{cases} \mathrm{span}\{E_{12}, E_{22}\} & \lambda = 0 \\ \mathrm{span}\{E_{11}, E_{21}\} & \lambda = 1 \\ M_{2\times 2}(\mathbb{C}) & \lambda \in (0,1). \end{cases}$$

Inner product

Consider $\lambda \in (0,1)$. We have for $e_{ij} = [E_{ij}]$, $\lambda_1 := \lambda$, and $\lambda_2 := 1 - \lambda$

$$\langle e_{ij}, e_{kl} \rangle = \omega(E_{ij}^* E_{kl}) = \omega(E_{ji} E_{kl}) = \omega(\delta_{ik} E_{jl}) = \delta_{ik}\delta_{jl}\lambda_l \tag{2}$$

Therefore the basis $\{e_i^{(\alpha)} := [E_{i\alpha}]/\sqrt{\lambda_\alpha} | i, \alpha \in \{1,2\}\}$ is an orthonormal basis for $\mathcal{H}_\lambda$. Moreover, the representation splits as

$$\mathcal{H}_\lambda = \mathcal{H}_\lambda^{(1)} \oplus \mathcal{H}_\lambda^{(2)} \tag{3}$$

where $\mathcal{H}_\lambda^{(\alpha)} := \operatorname{span}\{e_i^{(\alpha)} | i \in \{1,2\}\}$. We have the corresponding orthogonal projections $P^{(\alpha)}$ onto $\mathcal{H}_\lambda^{(\alpha)}$. Another useful inner product to compute is

$$\langle \Omega_\lambda, e_i^{(\alpha)} \rangle = \frac{1}{\sqrt{\lambda_\alpha}} \langle [I_2], [E_{i\alpha}] \rangle = \frac{1}{\sqrt{\lambda_\alpha}} \omega(E_{i\alpha}) = \frac{1}{\sqrt{\lambda_\alpha}} \delta_{i\alpha}\lambda_\alpha. \tag{4}$$

Constructing a Density Operator from Decompositions

$$
\begin{aligned}
\omega(A) =&\langle\Omega_\omega, \pi_\omega(A)\Omega_\omega\rangle = \langle\Omega_\omega, \sum_{\alpha\in I} P^{(\alpha)}\pi_\omega(A)\Omega_\omega\rangle \\
=&\langle\Omega_\omega, \sum_{\alpha\in I} P^{(\alpha)}\pi_\omega(A)P^{(\alpha)}\Omega_\omega\rangle \\
=&\langle\Omega_\omega, \sum_{n\in J}\langle e_n, \sum_{\alpha\in I} P^{(\alpha)}\pi_\omega(A)P^{(\alpha)}\Omega_\omega\rangle e_n\rangle \\
=&\sum_{n\in J}\langle e_n, \sum_{\alpha\in I} P^{(\alpha)}\pi_\omega(A)P^{(\alpha)}\langle\Omega_\omega, e_n\rangle\Omega_\omega\rangle \\
=&\sum_{n\in J}\langle e_n, \sum_{\alpha\in I} P^{(\alpha)}\pi_\omega(A)P^{(\alpha)}\rho_{\Omega_\omega} e_n\rangle \\
=&\,\mathrm{tr}\left(\pi_\omega(A)\sum_{\alpha\in I} P^{(\alpha)}\rho_{\Omega_\omega}P^{(\alpha)}\right) = \mathrm{tr}(\pi_\omega(A)\rho_\omega)
\end{aligned}
\tag{5}
$$

The Density Operator of Our Decomposition

$$
\begin{aligned}
\rho_\lambda e_i^\alpha =& \sum_{\beta \in I} P^{(\beta)} \rho_{\Omega_\omega} P^{(\beta)} e_i^{(\alpha)} = \sum_{\beta \in I} P^{(\beta)} \rho_{\Omega_\omega} \delta_{\alpha\beta} e_i^{(\alpha)} = P^{(\alpha)} \rho_{\Omega_\omega} e_i^{(\alpha)} \\
=& P^{(\alpha)} \frac{1}{\sqrt{\lambda_\alpha}} \delta_{i\alpha} \lambda_\alpha \Omega_\omega = \frac{1}{\sqrt{\lambda_\alpha}} \delta_{i\alpha} \lambda_\alpha \sum_{j=1}^{2} \langle e_j^\alpha, \Omega_\omega \rangle e_j^{(\alpha)} \\
=& \frac{1}{\sqrt{\lambda_\alpha}} \delta_{i\alpha} \lambda_\alpha \sum_{j=1}^{2} \frac{1}{\sqrt{\lambda_\alpha}} \delta_{j\alpha} \lambda_\alpha e_j^{(\alpha)} = \frac{1}{\sqrt{\lambda_\alpha}} \delta_{i\alpha} \lambda_\alpha \frac{1}{\sqrt{\lambda_\alpha}} \lambda_\alpha e_\alpha^{(\alpha)} \\
=& \delta_{i\alpha} \lambda_\alpha e_\alpha^{(\alpha)}.
\end{aligned} \tag{6}
$$

Therefore, in the ordered basis $\mathcal{B} = \{e_1^{(1)}, e_2^{(1)}, e_1^{(2)}, e_2^{(2)}\}$ we have

$$
[\rho_\lambda]_{\mathcal{B}} = \begin{bmatrix} \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1-\lambda \end{bmatrix} \tag{7}
$$

The Representation

Finally we explicitly need the GNS representatives. Using the same approach

$$\pi_\lambda(A)e_i^{(\alpha)} = \frac{1}{\sqrt{\lambda_\alpha}}[AE_{i\alpha}] = \frac{1}{\sqrt{\lambda_\alpha}}[A_{jk}\delta_{ki}\delta_{\beta\alpha}E_{j\beta}] = \frac{1}{\sqrt{\lambda_\alpha}}A_{ji}[E_{j\alpha}] = A_{ji}e_j^{(\alpha)}.$$

Therefore

$$[\pi_\lambda(A)]_{\mathcal{B}} = \begin{bmatrix} A & 0 \\ 0 & A \end{bmatrix} (= A \otimes I_2) \tag{8}$$

and we explicitly check that neither ρ_{Ω_λ} or ρ_λ have an interpretation as observables.

Ambiguity in functions of states

Consider the von Neumann entropy

$$S(\rho) = -\operatorname{tr}(\rho \log(\rho)) \tag{9}$$

of a density matrix ρ. In our example the entropy of our initial density matrix describing the state is

$$-\lambda \log(\lambda) - (1-\lambda)\log(1-\lambda) = S(\rho) = \omega(\log(\rho)). \tag{10}$$

This is in particular the expected value of an observable! However, in the GNS representation we have encountered two density operators ρ_{Ω_λ} and ρ_λ which also do the job but are not observables. However their entropies differ!

$$S(\rho_{\Omega_\lambda}) = 0 \neq S(\rho) = S(\rho_\lambda). \tag{11}$$

The ambiguity is worse

What is going on here? In reality, the ambiguity is much more dramatic. Redefining the orthonormal basis by $e_i^{\alpha}(U) = \sum_{\beta=1}^{2} e_i^{(\beta)} U_{\beta\alpha}$ for U unitary yields a new decomposition and thus a new density operator

$$\rho_\lambda(U) = \sum_{\alpha \in I} P^{(\alpha)}(U) \rho_{\Omega_\omega} P^{(\alpha)}(U). \tag{12}$$

The spectrum of the density operator will depend on U and therefore the entropy as well. As it turns out, such a shift in the decomposition of the representation can be understood as the action of the gauge group through Tomita-Takesaki theory. More about this will be discussed in Souad's lecture right after this!

W^*-algebras

What is Tomita-Takesaki theory? To understand this we must specialize our algebras. A C^*-algebra can always be realized as a uniformly closed subset of the bounded operators on a Hilbert space[Bratteli and Robinson, 1987].

Definition

A C^*-algebra $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is called a von Neumann algebra or W^*-algebra if $\mathcal{A}'' = \mathcal{A}$ where

$$\mathcal{A}' = \{B \in \mathcal{B}(\mathcal{H}) | AB = BA \text{ for all } A \in \mathcal{A}\}. \tag{13}$$

Cyclic representations of W^*-algebras

Theorem (★)

If $\mathfrak{M}$ is a W^*-algebra and ω is a faithful ($\omega(A^*A) = 0 \to A = 0$) normal ($\omega(A) = \mathrm{tr}(\rho A)$) state then its cyclic representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ satisfies

- *π_ω is faithful (injective);*
- *$\pi_\omega(\mathfrak{M})$ is a von Neumann algebra;*
- *Ω_ω is separating for $\pi_\omega(\mathfrak{M})$ ($\pi_\omega(A)\Omega_\omega = 0 \to \pi_\omega(A) = 0$).*

Dynamical Systems

Time evolution is represented by a one-parameter group of automorphisms

$$\tau : \mathbb{R} \to \mathrm{Aut}(\mathcal{A})$$
$$t \mapsto \tau_t.$$

Dynamical systems consist of an $C(W)^*$-algebra with a time evolution which satisfies certain continuity properties.

Example

Given a Hamiltonian H on a Hilbert space $\mathcal{H}$ the Schrödinger time evolution s is given by

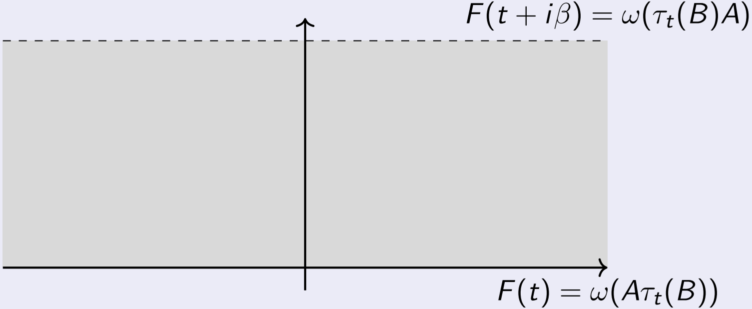
$$s_t(O) = e^{iHt} O e^{-iHt} \tag{14}$$

and $(\mathcal{B}(\mathcal{H}), s)$ is a dynamical system.

KMS States

Definition

Let $(\mathcal{A}, \tau)$ be a dynamical system. ω is said to be a (τ, β)-KMS state if for all $A, B \in \mathcal{A}$ there exists a bounded continuous F on the strip analytic on its interior such that for all for all $t \in \mathbb{R}$



KMS states as Equilibrium states

KMS states are a candidate for a general definition of thermodynamic equilibrium in quantum systems[Haag et al., 1967]:

- KMS states are invariant under the dynamics $\omega(\tau_t(A)) = \omega(A)$;
- In finite dimensional Hilbert spaces with Schrödinger's time evolution τ, the only possible (τ, β)-KMS states are the β-Gibbs states

$$\begin{aligned}\mathcal{B}(\mathcal{H}) &\to \mathbb{C} \\ A &\mapsto \frac{\operatorname{tr}\left(Ae^{-\beta H}\right)}{\operatorname{tr}\left(e^{-\beta H}\right)}.\end{aligned}$$

- It is clear that the Gibbs prescription cannot be the characterization of equilibrium in the thermodynamic limit since coexistence of different phases demands that there cannot be a general unique correspondence between the Hamiltonian (evolution group) and states[Connes, 1994].

Tomita-Takesaki Theory

For a W^*-algebra $\mathfrak{M}$ equipped with a cyclic and separating vector Ω the polar decomposition of the closure of

$$\begin{aligned} S_0 : \mathfrak{M}\Omega &\to \mathcal{H} \\ A\Omega &\mapsto A^*\Omega \end{aligned} \tag{15}$$

yields:

- a one-parameter unitary group $t \mapsto \Delta^{it}$;
- a modular conjugation J.

Theorem (Tomita-Takesaki)

- $J\mathfrak{M}J = \mathfrak{M}'$;
- $\Delta^{it}\mathfrak{M}\Delta^{-it} = \mathfrak{M}$ *for all* $t \in \mathbb{R}$.

Modular Automorphism Group

Definition

Let $\mathfrak{M}$ be a von Neumann algebra and ω be a faithful normal state. Due to ★ we can perform the modular constructions on the cyclic representation $(\pi_\omega(\mathfrak{M}), \pi_\omega, \Omega_\omega)$. We define the modular automorphism group of $(\mathfrak{M}, \omega)$ by

$$\alpha_t = \pi_\omega^{-1}(\Delta^{it}\pi_\omega(A)\Delta^{-it}). \tag{16}$$

Theorem (★★)

$(\mathfrak{M}, \alpha)$ *is a* W^**-dynamical system*

Proof.

[Duvenhage, 1999] □

The Canonical Time Evolution

Theorem (★★★)

Let $\mathfrak{M}$ be a von Neumann algebra and ω be a faithful normal state. Then $(\mathfrak{M}, \tau)$ with $\tau_t(A) = \alpha_{-t/\beta}(A)$ and α the modular group of $(\mathfrak{M}, \omega)$ is the unique W^*-dynamical system such that ω is a (τ, β)-KMS state.

Proof.

[Duvenhage, 1999] □

On von Neumann Algebras as Dynamical Objects

- Through the modular group, states induce dynamics on the algebra of operators.
- The physical relevance of such prescription for evolution is guaranteed by the fact that it is the unique dynamical law which makes the state an equilibrium state.
- One can use an analog of the Radon-Nikodym theorem to connect the modular groups induced by different states. Such a connection brings forward a canonical homomorphism from $\mathbb{R}$ into the automorphism group of $\mathfrak{M}$ modulus inner automorphisms. This suggests that the emergence of the dynamical law might have a deeper origin.

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