Pontifícia Universidade Católica
do Rio de Janeiro

Edhin Franklin Mamani Castillo

Tomita-Takesaki theorem and KMS states

Dissertação de Mestrado

Dissertation presented to the Programa de Pós–graduação em Matemática da PUC-Rio in partial fulfillment of the requirements for the degree of Mestre em Matemática.

Advisor : Prof. Carlos Tomei
Co-advisor: Prof. George Svetlichny

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Abstract

Mamani Castillo, Edhin Franklin; Tomei, Carlos (Advisor); Svetlichny, George (Co-Advisor). **Tomita-Takesaki theorem and KMS states**. Rio de Janeiro, 2018. 80p. Dissertação de mestrado – Departamento de Matemática, Pontifícia Universidade Católica do Rio de Janeiro.

In this work we present the Tomita-Takesaki theory for a Von Neumann algebra $\mathcal{M}$ with cyclic separating vector u. We use the finite-dimensional case to motivate the theory, and then proceed to the analytical arguments usually employed to prove the infinite dimensional case. Also, we calculate the modular operators from the theory for three standard examples. In quantum statistical mechanics, the thermodynamic equilibrium states of a physical system with finitely many particles and finite volume are modeled by Gibbs states, while in the infinite case they are modeled by the so called KMS states through the operator-algebraic approach. We show how Tomita-Takesaki theory provides natural KMS states and the uniqueness of the time evolution of the physical system for those states.

Keywords

Tomita-Takesaki theorem; KMS states; Gibbs states; KMS condition; Cyclic and separating vector; Tomita Operator; Modular Operator; Modular group.

Resumo

Mamani Castillo, Edhin Franklin; Tomei, Carlos; Svetlichny, George. **O teorema de Tomita-Takesaki e os estados KMS**. Rio de Janeiro, 2018. 80p. Dissertação de Mestrado – Departamento de Matemática, Pontifícia Universidade Católica do Rio de Janeiro.

Neste trabalho apresentamos a teoria de Tomita-Takesaki para uma álgebra de Von Neumann $\mathcal{M}$ com vetor cíclico separante u. Usamos o caso finito dimensional para motivar a teoria, depois prosseguimos para os argumentos analíticos geralmente empregados para provar o caso infinito dimensional. Também calculamos os operadores modulares da teoria para três exemplos padrão. Na mecânica estatística quântica, os estados de equilíbrio termodinâmico de um sistema físico com um número de partículas e volume finito são modelados pelos estados de Gibbs, enquanto no caso infinito eles são modelados pelos chamados estados KMS através da abordagem de álgebra de operadores. Mostramos como a teoria de Tomita-Takesaki fornece estados KMS naturais e a unicidade da evolução temporal do sistema físico para esses estados.

Palavras-chave

Teorema de Tomita-Takesaki; Estados KMS; Estados de Gibbs; Condição KMS; Vetor cíclico e separador; Operador de Tomita; Operador Modular; Grupo Modular.

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1
Introduction

Thermodynamics is the study of the macroscopic properties of matter — pressure, temperature, heat capacity. The main goal of statistical mechanics is the ultimate explanation of thermodynamics in terms of the microscopic behavior of the system constituents. The original formalism, in which the constituents are supposed to obey classical physics, is called classical statistical mechanics. With the advent of quantum theory, it was soon noticed that in many systems the behavior of microscopic constituents was modeled more accurately by quantum mechanics, so quantum statistical mechanics was born with the same goal.

A pioneer in the modern approach of classical statistical mechanics was Josiah Willard Gibbs which in 1878 formalized the foundations of the subject [1]. He introduced statistical ensembles, a very useful concept to handle systems of large number of particles through probabilistic considerations. Later, the probabilistic approach was adapted to fit quantum mechanics. In both cases, the framework suggested by Gibbs defined heuristically the thermodynamic equilibrium states of the physical system, the Gibbs states. The subject found applications in a variety of branches of physics: the theory of metals, semiconductors, solid state, atomic and molecular physics. It also gave indications about new physical phenomena: superfluidity and superconductivity.

Meanwhile, in 1929 John Von Neumann suggested that the fundamental object in the mathematical setting of quantum mechanics was not the Hilbert space H of physical states, but families of quantum observables modeled by operators acting on H. He defined and studied rings of bounded operators on H which are closed in the weak operator topology, known today as Von Neumann algebras [2]. In a attempt to synthesize the essence of the quantum observables, other families of bounded operators were considered, among them C^* and Jordan algebras.

In 1943, Israel Gelfand and Mark Naimark characterized abstractly C^*-algebras without any reference to the underlying Hilbert space [3]. This remarkable achievement led Irving Segal in 1947 to state a set of axioms that any physical theory should satisfy [4]. These axioms were abstracted from the mathematical model of quantum mechanics and implied a complete reformulation of any physical theory in algebraic terms: physical observables are modeled by elements in a C^*-algebra $\mathcal{M}$ and physical states by normalized positive linear functionals on $\mathcal{M}$. This was the starting point of the operator algebraic approach of quantum mechanics, quantum statistical mechanics and quantum field theory.

The algebraic approach was a meaningful conceptual breakthrough, but was not particularly useful to connect theory with experimental data. The subject was largely ignored by the physics community until in 1957, when Rudolf Haag pointed out its importance in quantum field-theoretic models [5]. In the 1960's, it was applied to quantum statistical mechanics mostly to study the (Gibbs) equilibrium states of quantum systems.

In 1957 Ryogo Kubo [6] and in 1959 Paul Martin and Julian Schwinger [7] highlighted an algebraic property satisfied by the Gibbs states, the so called KMS (Kubo-Martin-Schwinger) condition. The states that satisfied this property were called KMS states. Physicists realized that this property characterized completely the Gibbs states for quantum systems in a finite dimensional state space: KMS states were exactly the Gibbs states. In 1967, Haag, Hugenholtz and Winnink proposed the KMS states as the thermodynamic equilibrium states for a general quantum system [8]. Despite the existence of other alternative proposals, KMS states were the most studied theoretical models of quantum statistical mechanics and quantum field theory.

In 1967, out of purely mathematical motivations, Minoru Tomita introduced an elaborate theory of Von Neumann algebras with a cyclic separating vector. His main achievement was the construction of a strongly continuous one-parameter unitary group of automorphisms of the Von Neumann algebra, the modular automorphism group. In 1970, Masamichi Takesaki improved the presentation of the theory and related it to KMS states: the cyclic separating vector induces a KMS state. This connection between pure mathematics and theoretical physics is now known as the Tomita-Takesaki theory [9].

In this dissertation we describe the Tomita-Takesaki theory and its connection with KMS states. Chapter 2 gives a basic account of some topics of operator theory which are needed for the development of the subsequent chapters. In particular, we consider Banach, C^* and Von Neumann algebras, with emphasis on the functional calculus that arises from the representation theorems of the correspondent commutative algebras. Specifically, we present the Gelfand transform, Von Neumann's bicommutant theorem, Kaplansky's density theorem and the functional calculus in three levels: for holomorphic, continuous and bounded functions of normal operators.

The Tomita-Takesaki theory is the subject of Chapter 3. The finite dimensional case is treated first to motivate some constructions, and then additional technical aspects are discussed in the infinite dimensional context. Three mathematical examples of the theory are presented.

Chapter 4 introduces the KMS states. First, we provide an introduction to the GNS (Gelfand-Naimark-Segal) construction. The Gibbs states and the elements of the operator algebraic approach to quantum statistical mechanics are motivated. We then present the KMS condition in a special case and show the equivalence between KMS and Gibbs states for finite quantum systems. The general definition follows, with some consequences. We finish with Takesaki's theorem, which relates the Tomita-Takesaki theory to KMS states. Our presentation of the algebraic operator approach of quantum statistical mechanics mainly follows the spirit of [10, 11].

Appendix A.1 and A.4 are tool boxes of standard topics in functional analysis while Appendix A.2 considers briefly anti-linear operators on a Hilbert space. Appendix A.3 gives miscellaneous applications of the holomorphic functional calculus.

2
Basic Operator Theory

This chapter is devoted to some basic topics in operator theory and is based mainly on [10, 12, 13]. The first two sections provide a brief introduction to Banach algebras and the holomorphic functional calculus. The next two sections handle C^*-algebras, the Gelfand-Naimark theorem and the continuous functional calculus for normal elements. Finally, the last two consider Von Neumann algebras, the density theorems of Von Neumann and Kaplansky, the representation theorem for commutative Von Neumann algebras and the bounded Borel functional calculus for normal elements.

2.1
Banach algebras

An *algebra* is a complex vector space $\mathcal{A}$ with a *product*, $(a,b) \in \mathcal{A} \times \mathcal{A} \mapsto ab \in \mathcal{A}$, which is distributive with respect to vector addition and associative.

The algebra $\mathcal{A}$ is a *normed algebra* if $\mathcal{A}$ admits a *multiplicative* norm, i.e., $|ab| \leq |a||b|$ for $a, b \in \mathcal{A}$. If the product has an unit element $e \in \mathcal{A}$ and $|e| = 1$ then $\mathcal{A}$ is *unital.* If it is commutative, $\mathcal{A}$ is *commutative.*

Definition 2.1. A *Banach algebra* $\mathcal{B}$ is a complete normed algebra.

The Banach space $\mathcal{B}$ has a dual $\mathcal{B}^*$, which in turn also has a dual $\mathcal{B}^{**} \supset \mathcal{B}$.

Example 2.1. z Let H be a complex Hilbert space and $B(H)$ be the set of linear bounded operators from H to itself, endowed with the operator norm. With the usual product given by composition of maps, $B(H)$ is a non-commutative unital Banach algebra. If $H = \mathbb{C}^n$ then $B(H) = M_n(\mathbb{C})$ is the set of $n \times n$ complex matrices.

Example 2.2. Let K be a compact Hausdorff space. The space $C(K)$ of continuous complex valued functions on K, endowed with the function sum and multiplication and the sup norm, is an unital commutative Banach algebra.

Example 2.3. Let $U \subset \mathbb{C}$ be a bounded open set with closure $\overline{U}$. The set $\mathcal{H}(U)$ of all functions of $C(\overline{U})$ admitting holomorphic restrictions to U. With the obvious induced structures, $\mathcal{H}(U)$ is a commutative unital Banach algebra.

Here, Banach algebras $\mathcal{B}$ are always unital, with identity denoted by e.

Spectral concepts on $B(H)$, which are of algebraic nature, extend to $\mathcal{B}$.

Definition 2.2. For $a \in \mathcal{B}$, the *spectrum* $\sigma(a)$ is

$$\sigma(a) \; = \; \{\lambda \in \mathbb{C} \mid \lambda e - a \;\text{ is not invertible}\},$$

its complement is the *resolvent* $\rho(a)$ and $r(a) \; = \; \sup|\sigma(a)|$ is the *spectral radius*. The *resolvent function* is the map $z \in \rho(a) \mapsto R_a(z) = (ze - a)^{-1} \in \mathcal{B}$.

Example 2.4. Let K be a compact Hausdorff space and $f \in C(K)$. The spectrum $\sigma(f)$ is the range of f, $\sigma(f) = f(K)$ and hence $r(f) = |f|$.

Example 2.5. Let $A \in M_n(\mathbb{C})$. The spectrum $\sigma(A)$ is the set of eigenvalues of A and $r(A)$ is the largest absolute value among the eigenvalues of A.

Clearly, polynomials induce functions $p : \mathcal{B} \to \mathcal{B}$. Convergent series, and hence analyticity, also make sense in $\mathcal{B}$. Since the usual estimates yielding absolute convergence of series on the complex numbers only require the properties of a multiplicative norm, standard results extend trivially. Among the examples are the uniqueness of the series at a point, analytic continuation and the fact that entire functions from $\mathbb{C}$ to itself give rise to entire functions from $\mathcal{B}$ to itself.

Another form of analyticity is very convenient. Let $U \subset \mathbb{C}$ be an open set. A function $f : U \mapsto \mathcal{B}$ is *analytic* if every point in U is a center of an open ball in which f admits an absolutely convergent power series. Again, from the properties of multiplicative norms, the Cauchy-Hadamard formula for the radius of convergence of a function $f : U \to \mathcal{B}$ at a point still holds. Explicitly, for $f(z) = \sum c_n z^n$, $c_n \in \mathcal{B}$, the radius of convergence R at 0 is given by

$$R \; = \; \frac{1}{\limsup |c_n|^{1/n}} \; .$$

Some results of complex theory from analytic functions $f : U \to \mathbb{C}$ transfer to analytic functions $f : U \to \mathcal{B}$ by use of Dunford's theorem [14].

Theorem 2.1. *A function $f : U \to \mathcal{B}$ is analytic if and only if it is weakly analytic, i.e., all compositions $f_\ell = \ell \circ f : U \to \mathbb{C}$ for $\ell \in \mathcal{B}^*$ are analytic*

Thus, for example, a bounded isolated singularity of an analytic function $f : U \to \mathcal{B}$ is removable. Cauchy's theorem — integration along a contractible smooth curve in U of an analytic $f : U \to \mathcal{B}$ is zero — also holds.

Proposition 2.1. *Let $\mathcal{B}$ be a Banach algebra and $a \in \mathcal{B}$.*

1. *(Neumann series) If $|a| < 1$, $(e - a)^{-1} = \sum_{n=0}^{\infty} a^n$.*

2. *The function R_a is analytic on $\rho(a) = \sigma(a)^c$ and $\lim_{z \to \infty} R_a(z) = 0$.*

3. *The spectrum $\sigma(a)$ is compact and non-empty.*

4. *(Gelfand's formula for the spectral radius) $r(a) = \lim_{n\to\infty} |a^n|^{1/n}$.*

Proof. The proof of (1) is standard, from which, as usual, three facts are immediate: the openness of the set of invertible elements, the openness of $\rho(a) \subset \mathbb{C}$ and the analyticity of R_a in $\rho(a)$. For $|z| > |a|$, write $w = 1/z$ so that $w \in B = \{w \in \mathbb{C}\ , |wa| < 1\}$. From the Neumann series, $R_a(z) = F(w) = w(e - wa)^{-1}$ is an analytic function in $B \setminus \{0\}$. On the other hand, F is analytic at a point $w_* \neq 0$ if and only if R_a is analytic at $z_* = 1/w_*$. Since $\lim_{z\to\infty} R_a(z) = \lim_{w\to 0} F(w) = 0$, the proof of (2) is complete. Also from $F(w) = R_a(z)$, we have that $z \in \rho(a)$ if $|z| > |a|$, so that $\sup|\sigma(a)| \leq |a|$ and thus $\sigma(a)$ is a compact set of $\mathbb{C}$. If $\sigma(a) = \emptyset$, from the behavior at ∞ of $R - a$ in (2), we learn that R_a is a bounded, entire — hence constant — function and (3) follows.

To obtain (4), we consider the radius of convergence R of F. Let $w_* \in \mathbb{C}$ with $|w_*| = R$. If $(e - w_* a) \in \mathcal{B}$ is invertible, F is analytic at w_*. Thus a point w_* in which F is not analytic (and then $R = |w_*|$) gives rise to $z_* = 1/w_* \in \sigma(a)$. Gelfand's formula now follows from the Cauchy-Hadamard formula for the radius of convergence $R = |w_*|$ of F at 0. ∎

A linear map $\phi : \mathcal{B}_1 \mapsto \mathcal{B}_2$ between Banach algebras is an *algebra homomorphism* if ϕ preserves product, i.e., $\phi(ab) = \phi(a)\phi(b)$ for $a, b \in \mathcal{B}_1$ and takes one identity to the other, $\phi(e_1) = e_2$. If ϕ is also bijective, it is an *algebra isomorphism* and $\mathcal{B}_1$ and $\mathcal{B}_2$ are *isomorphic.*

An algebra with every non-zero element invertible is a *division algebra.*

Proposition 2.2 (Gelfand-Mazur)**.** *A division Banach algebra $\mathcal{B}$ is isometrically isomorphic to $\mathbb{C}$.*

Proof. Let $a \in \mathcal{B}$. By (3) of proposition 2.1, there exists $\lambda_a \in \mathbb{C}$ such that $\lambda_a e - a$ is not invertible and hence equal to zero, so that $a = \lambda_a e$. The map $a \mapsto \lambda_a$ is the required isomorphism. ∎

Proposition 2.3. *Let $\phi : \mathcal{B}_1 \mapsto \mathcal{B}_2$ be an algebra homomorphism. Then, for $a \in \mathcal{B}_1$, $\sigma(\phi(a)) \subset \sigma(a)$ hence $r(\phi(a)) \leq r(a)$.*

Proof. We show that $\rho(a) \subset \rho(\phi(a))$ and taking complements gives the result. For $\mu \in \rho(a)$, $(\mu e - a)b = e$ for some $b \in \mathcal{B}_1$. Applying ϕ we have $(\mu\phi(e) - \phi(a))\phi(b) = \phi(e)$ and hence $\mu \in \rho(\phi(a))$. ∎

2.2 Holomorphic Functional Calculus

Let $U \subset \mathbb{C}$ be an open set, $\gamma \subset U$ be a smooth, simple, closed curve with positive orientation, bounding an open disk $D \subset U$. For a analytic function $f : U \mapsto \mathbb{C}$ and $z_0 \in D$, recall Cauchy's formula

$$f(z_0) = \frac{1}{2\pi i} \oint_\gamma f(z)(z - z_0)^{-1} dz.$$

Let $\mathcal{B}$ be a Banach algebra, $a \in \mathcal{B}$ and $U \subset \mathbb{C}$ be a bounded neighborhood of $\sigma(a)$. Let $\gamma \subset U$ be a finite set of smooth, simple, closed curves $\gamma_i, i = 1, \ldots, n$ surrounding open disks $D_i \subset U$ counterclockwise such that $\sigma(a) \subset \cup_i D_i$. For $f \in \mathcal{H}(U)$ (defined in example 2.3), set

$$f(a) = \frac{1}{2\pi i} \oint_\gamma f(z)(ze - a)^{-1} dz = \frac{1}{2\pi i} \oint_\gamma f(z) R_a(z) dz. \tag{2.1}$$

Lemma 2.2. *Any γ with the properties above obtains the same $f(a) \in \mathcal{B}$.*

Proof. Since f and R_a are holomorphic on $U \setminus \sigma(a)$, so is fR_a and in particular fR_a is continuous on γ. Thus, $f(a)$ is defined by the usual integration process on Banach spaces — one may approximate by Riemann sums uniformly, and conclude that $f(a) \in \mathcal{B}$. Two sets of curves γ and $\tilde{\gamma}$ satisfying the hypotheses above are homologically equivalent in $U \setminus \sigma(a)$ and the equality of the integrals follow from Cauchy's theorem on integration of analytic functions. ■

As we shall see, this definition coincides with the natural definition of $p(a)$ for a polynomial p, and extends for functions $f \in \mathcal{H}(U)$.

Theorem 2.3 (Holomorphic functional calculus)**.** *Let $\mathcal{B}$ be a Banach algebra, $a \in \mathcal{B}$ and $U \subset \mathbb{C}$ be a bounded neighborhood of $\sigma(a)$. There exists a unique continuous algebra homomorphism*

$$\phi = \phi_a : \mathcal{H}(U) \to \mathcal{B}$$

for which $\phi(1) = e, \phi(z) = a$. It is given by

$$f \in \mathcal{H}(U) \mapsto f(a) = \frac{1}{2\pi i} \oint_\gamma f(z) R_a(z) dz \in \mathcal{B}.$$

Proof. The linearity is clear. For the product, let γ as above and $f, g \in \mathcal{H}(U)$:

$$\begin{aligned} f(a)g(a) &= \frac{1}{2\pi i} \oint_\gamma f(z_1) R_a(z_1) dz_1 \, \frac{1}{2\pi i} \oint_\gamma g(z_2) R_a(z_2) dz_2 \\ &= (\frac{1}{2\pi i})^2 \oint_\gamma dz_1 \oint_\gamma dz_2 \Big(\, f(z_1) \, g(z_2) \, R_a(z_1) \, R_a(z_2) \Big) \, . \end{aligned}$$

We now use the familiar *resolvent identity*,

$$R_a(z_1)R_a(z_2) \;=\; \frac{R_a(z_1)-R_a(z_2)}{z_1-z_2}\ , \tag{2.2}$$

which in turn is a direct consequence of

$$(z_1e-a)[(z_1e-a)^{-1}-(z_2e-a)^{-1}](z_2e-a)=(z_2-z_1)e, \quad \text{for} \;\; z_1,z_2\in\rho(a)\ .$$

The integrand of the double integral above becomes

$$(\frac{1}{2\pi i})^2 f(z_1)R_a(z_1)\ \frac{g(z_2)}{z_1-z_2} - (\frac{1}{2\pi i})^2 g(z_2)R_a(z_2)\ \frac{f(z_1)}{z_1-z_2}.$$

The term z_1-z_2 becomes zero if both variables run through the same curve γ_i of the set γ. We dilate the curves in γ slightly, obtaining curves $\tilde\gamma$ surrounding those of γ: for the associated bounded disks, $D_i\subset\tilde D_i$. Clearly, the original integrals do not change their values. We are ready to continue: $f(a)g(a)$ is

$$(\frac{1}{2\pi i})^2\oint_\gamma f(z_1)R_a(z_1)dz_1\oint_{\tilde\gamma}\frac{g(z_2)dz_2}{z_1-z_2} - (\frac{1}{2\pi i})^2\oint_{\tilde\gamma} g(z_2)R_a(z_2)dz_2\oint_\gamma\frac{f(z_1)dz_1}{z_1-z_2}.$$

Use Cauchy's formula for the scalar integrals, taking into account that z_1 is surrounded by the curve $\tilde\gamma_i$ containing z_2, but z_2 is outside of the curve γ_i containing z_1: the second term vanishes and

$$f(a)g(a)=\frac{1}{2\pi i}\oint_\gamma f(z_1)g(z_1)R_a(z_1)dz_1=(fg)(a).$$

We now check that $\phi(1)=e$. Integrate the resolvent-like identity

$$(ze-a)^{-1}-e/z \;=\; (ze-a)^{-1}(a/z) \;=\; (1/z)(e-a/z)^{-1}(a/z), \quad \text{for } z\in\mathbb{C}$$

on a circle centered at the origin surrounding $\sigma(a)$ (any circle will obtain the same answer, by Cauchy's theorem). Up to a multiplicative scalar, the first integral gives $\phi(1)$, the second gives e and the third equals zero, by taking absolute values of the integrand on circles with large radius.

Similarly, to obtain $\phi(z)=a$, integrate on a large circle as above

$$(z-a)(z-a)^{-1}=z(z-a)^{-1}-a(z-a)^{-1}$$

to obtain $0=\phi(a)-a\phi(1)$.

Therefore the map ϕ is an algebra homomorphism. Moreover, the map is continuous: if $f_n \to f$ in $\mathcal{H}(U)$, we estimate norms on γ,

$$|f(a) - f_n(a)| = |\frac{1}{2\pi i}\oint_\gamma (f - f_n)(z)R_a(z)dz| \leq \frac{1}{2\pi}|f - f_n|_\infty |R_a|_\infty L(\gamma).$$

By compactness the norm of the resolvent function R_a is bounded. ■

Since ϕ is an algebra homomorphism and $\phi(z) = a$, we must have $\phi(p) = p(a)$ for polynomials. The map extends by continuity in a unique way. It is a nontrivial fact that polynomials are dense in $\mathcal{H}(U)$ [14].

Corollary 2.3.1 (Spectral mapping theorem for holomorphic functions)**.** *Let $\mathcal{B}$ be a Banach algebra, $a \in \mathcal{B}$ and $U \subset \mathbb{C}$ be a bounded neighborhood of $\sigma(a)$. Then, for $f \in \mathcal{H}(U)$,*

$$\sigma(f(a)) = f(\sigma(a)).$$

Proof. We prove first the direct inclusion. Suppose by contradiction that there exists $\lambda \in \sigma(f(a))$ such that $\lambda \notin f(\sigma(a))$. Thus, $\lambda \neq f(z)$ for $z \in \sigma(a)$. Now take an open set $\tilde{U} \subset U$ containing $\sigma(a)$ on which the function $g(z) = (\lambda - f(z))^{-1}$ is holomorphic. By theorem 2.3, $g(a) = (\lambda e - f(a))^{-1}$ exists, and from the fact that ϕ is an algebra homomorphism, it is indeed the inverse of $(\lambda e - f(a))$, contradicting $\lambda \in \sigma(f(a))$.

For the reverse inclusion, let $\lambda \in f(\sigma(a))$, for which $\lambda = f(\mu)$ for some $\mu \in \sigma(a)$. Since f is holomorphic on U, so is the function g defined through the formula $(\mu - z)g(z) = f(\mu) - f(z)$ (i.e., $z = \mu$ is a removable singularity). Applying theorem 2.3, we have $(\mu e - a)g(a) = \lambda e - f(a)$. If $\lambda e - f(a)$ is invertible then $(\mu e - a)\Big(g(a)(\lambda e - f(a))^{-1}\Big) = e$ and we conclude that $\mu e - a$ is invertible, contradicting $\mu \in \sigma(a)$. Thus $\lambda e - f(a)$ is not invertible: $\lambda \in \sigma(f(a))$. ■

To conclude this section, we remark that the main atraction of the holomorphic functional calculus and its spectral mapping theorem relies on the fact that they work for any element of the Banach algebra, while the continuous and bounded Borel functional calculus only work on a special class: the normal elements, as we shall see in later sections. Therefore, the holomorphic functional calculus has many interesting applications, few ones are showed in appendix A.3.

2.3 C*-algebras

The spectral theorem from self-adjoint and normal operators in $B(H)$ follows almost immediately from the fact that, for such operators, the norm is given by its spectral radius. This property, or better, a request that readily implies this property, characterizes C^*-algebras.

Let $\mathcal{A}$ be an algebra. An *involution* on $\mathcal{A}$ is a map $a \in \mathcal{A} \mapsto a^* \in \mathcal{A}$ such that for $\lambda \in \mathbb{C}$ and $a, b \in \mathcal{A}$,

$$(\lambda a + b)^* = \overline{\lambda} a^* + b^*, \qquad (a^*)^* = a, \qquad (ab)^* = b^* a^*.$$

Involutions extend the adjoint operation on $B(H)$.

Definition 2.3. A *C^*-algebra* $\mathcal{M}$ is a Banach algebra with an involution satisfying the *C^* condition*: $|a^* a| = |a|^2$ for $a \in \mathcal{M}$.

Since $|a|^2 = |a^* a| \leq |a^*||a|$, we have $|a^*| \leq |a|$. Interchanging a and a^*, we see that the involution is an isometry.

A subset $\mathcal{T} \subset \mathcal{M}$ that is itself a C^*-algebra with the induced operations is a *C^*-subalgebra* of $\mathcal{M}$.

Example 2.6. The set $B(H)$ is a non-commutative C^*-algebra with the adjoint operation for involution. The C^* condition plays the role of a fundamental property in $B(H)$: the usual operator norm is related to the quadratic form for self-adjoint operators. For a compact Hausdorff space K and a bounded open subset $U \subset \mathbb{C}$, $C(K)$ and $\mathcal{H}(U)$ are commutative C^*-algebras with the involution given by pointwise conjugation.

Definition 2.4. Let $\mathcal{M}$ be a C^*-algebra and $a \in \mathcal{M}$,

1. a is *self-adjoint* if $a^* = a$.
2. a is *unitary* if $a^* a = a a^* = e$ (and thus $a^* = a^{-1}$).
3. a is *normal* if $a^* a = a a^*$.

Every $a \in \mathcal{M}$ splits in real and imaginary parts,

$$a = Re(a) + i Im(a) \ , \quad \text{with} \ \ Re(a) = \frac{a + a^*}{2}, \quad Im(a) = \frac{a - a^*}{2i}. \tag{2.3}$$

Clearly, both real and imaginary parts are self-adjoint. An element a is normal if and only if real and imaginary parts commute. The relationship between normal and self-adjoint operators is analogous to the one between the complex and the real numbers.

Theorem 2.4. *Let $\mathcal{M}$ be a C^*-algebra. If $a \in \mathcal{M}$ is normal, then $r(a) = |a|$. Thus, for $a \in \mathcal{M}$, $|a|^2 = r(a^*a)$.*

Proof. First, if $a \in \mathcal{M}$ is self-adjoint then $|a^2| = |a^*a| = |a|^2$ hence $|a^{2^n}| = |a|^{2^n}$. Therefore $r(a) = \lim_{n\to\infty} |a^{2^n}|^{1/2^n} = |a|$. Thus, if $a \in \mathcal{M}$ is normal then

$$r^2(a) \leq |a|^2 = |a^*a| = \lim_{n\to\infty} |(a^*a)^n|^{1/n} = \lim_{n\to\infty} |a^{*n}a^n|^{1/n} \leq r(a^*)r(a) = r^2(a).$$

The second statement follows easily. ■

Thus, the norm in a C^*-algebra (which induces the metric and topological properties) is determined by the spectral radius (an algebraic property of elements of the C^*-algebra).

Definition 2.5. Let $\mathcal{M}_1$ and $\mathcal{M}_2$ be C^*-algebras. An algebra homomorphism $\phi : \mathcal{M}_1 \mapsto \mathcal{M}_2$ is a **-homomorphism* if ϕ preserves involution, i.e., $\phi(a^*) = \phi(a)^*$, for $a \in \mathcal{M}_1$. If additionally, ϕ is bijective, it is a **-isomorphism.* In this case, $\mathcal{M}_1$ and $\mathcal{M}_2$ are **-isomorphic.*

Corollary 2.4.1. *Every *-homomorphism is contractive, hence continuous, and every *-isomorphism is an isometry.*

Proof. The result follows from proposition 2.3 and theorem 2.4. ■

Proposition 2.4. *Let $\mathcal{M}$ be a C^*-algebra and $a \in \mathcal{M}$.*

1. *If a is unitary then $\sigma(a) \subset S^1$ (the unit circle).*

2. *If a is self-adjoint then $\sigma(a) \subset \mathbb{R}$.*

Proof. Let $a \in \mathcal{M}$ be unitary and $\lambda \in \sigma(a)$. Since $|a| = 1$, $|\lambda| \leq 1$. By corollary 2.3.1, $\sigma(a^{-1}) = \sigma(a)^{-1}$. But a^{-1} is also unitary: $|\lambda^{-1}| \leq 1$ and $\lambda \in S^1$.

Take now $a \in \mathcal{M}$ self-adjoint and consider $\exp(ia) = \sum_{n=0}^{\infty}(ia)^n/n!$. Since $(\exp(ia))^* = \exp(-ia)$ and $\exp(ia)\exp(-ia) = \exp(0) = e$, $\exp(ia)$ is unitary. By corollary 2.3.1, $\sigma(e^{ia}) = e^{i\sigma(a)} \subset S^1$, so that $\sigma(a) \subset \mathbb{R}$. ■

2.4
The Continuous Functional Calculus

A rather naive fact underlies the main constructions in this section. For $a \in \mathcal{B}$, if $\lambda \in \sigma(a)$, then $f(\lambda) \in \sigma(f(a))$ for $f \in \mathcal{H}(U)$ for which the holomorphic spectral mapping theorem holds (corollary 2.3.1). Said differently, the map $f \in \mathcal{H}(U) \mapsto f(\lambda) \in \mathbb{C}$ is an algebra homomorphism for each $\lambda \in \sigma(a)$. The Gelfand transform below relies on the identification between $\sigma(a)$ and a class of algebraic objects, which are interpreted as algebra homomorphisms or as maximal proper ideals (the kernels of such homomorphisms).

Definition 2.6. Let $\mathcal{B}$ be a commutative Banach algebra. A nonzero linear functional $\ell : \mathcal{B} \mapsto \mathbb{C}$ is a *character* on $\mathcal{B}$ if ℓ preserves product. The set $\Omega(\mathcal{B})$ of all characters is the *character space.*

Thus, the character ℓ is also an algebra homomorphism from $\mathcal{B}$ into $\mathbb{C}$ and takes invertible elements of $\mathcal{B}$ into invertible complex numbers.

Lemma 2.5. *Let $\mathcal{B}$ be a commutative Banach algebra, $a \in \mathcal{B}$ and $\ell \in \Omega(\mathcal{B})$. Then $\ell(a) \in \sigma(a)$ and $|\ell| = 1$.*

Proof. Since $\ell(\ell(a)e - a) = 0$, we have $\ell(a) \in \sigma(a)$. Also $|\ell(a)| \leq |a|$, so that $|\ell| \leq 1$. The result follows from $\ell(e) = 1$. ■

Thus, the character space $\Omega(\mathcal{B})$ is included in B_1^*, the closed unit ball of $\mathcal{B}^*$. We endow $\Omega(\mathcal{B})$ with the relative weak* topology. By the Banach-Alaoglu theorem, B_1^* is compact in the weak* topology.

Lemma 2.6. *For a commutative Banach algebra $\mathcal{B}$, the character space $\Omega(\mathcal{B})$ is a compact Hausdorff space.*

Proof. Clearly, $\Omega(\mathcal{B})$ is Hausdorff. Since B_1^* is weak* compact, it is enough to show that $\Omega(\mathcal{B})$ is weak* closed. Take $\ell \in \mathcal{B}^*$ in the weak* closure of $\Omega(\mathcal{B})$, and a net (ℓ_j) in $\Omega(\mathcal{B})$ such that $\ell_j \to \ell$ in the weak* topology. For $a, b \in \mathcal{B}$,

$$(ab)(\ell_j) = \ell_j(ab) = \ell_j(a)\ell_j(b) = a(\ell_j)b(\ell_j) \ .$$

Since the evaluation functionals are weak* continuous, $\ell \in \Omega(\mathcal{B})$. ■

Definition 2.7. Let $\mathcal{B}$ be a Banach algebra. The *Gelfand transform* is the map $\Gamma : \mathcal{B} \mapsto C(\Omega(\mathcal{B}))$ defined by $\Gamma(a)\ell = \ell(a)$ for $a \in \mathcal{B}$ and $\ell \in \Omega(\mathcal{B})$.

Lemma 2.7. *Let $\mathcal{B}$ be a commutative Banach algebra. Then, the Gelfand transform Γ is an algebra homomorphism with $\sigma(a) = \sigma(\Gamma(a))$ for $a \in \mathcal{B}$.*

Proof. Clearly Γ is an algebra homomorphism. From proposition 2.3 we know that $\sigma(\Gamma(a)) \subset \sigma(a)$.

To prove $\sigma(a) \subset \sigma(\Gamma(a))$, let $\lambda \in \sigma(a)$, so that $\lambda e - a$ is not invertible in $\mathcal{B}$. By Zorn's lemma there exists a maximal proper ideal I containing $\lambda e - a$. An ideal containing an invertible element coincides with $\mathcal{B}$, and thus the properness of I implies that it has no invertible elements, as well as its closure $\overline{I}$, since the set of invertible elements is open in $\mathcal{B}$. Thus, $\overline{I}$ is a closed proper ideal containing $\lambda e - a$. By maximality, $I = \overline{I}$.

Since I is closed and maximal, the quotient $\mathcal{B}/I$ is a division Banach algebra, and by proposition 2.2, $\mathcal{B}/I \cong \mathbb{C}$. Thus, the quotient map is a character $\ell \in \Omega(\mathcal{B})$ such that $\ell(\lambda e - a) = 0$, or equivalently, $\ell(a) = \lambda$. Therefore $\Gamma(a)\ell = \ell(a) = \lambda$ and $\lambda \in \sigma(\Gamma(a))$. ■

The result above extends to C^* algebras. In a nutshell, every commutative C^*-algebra $\mathcal{M}$ is the algebra of continuous functions of some compact space.

Theorem 2.8 (Gelfand-Naimark theorem)**.** *For a commutative C^*-algebra $\mathcal{M}$, the Gelfand transform $\Gamma : \mathcal{M} \mapsto C(\Omega(\mathcal{M}))$ is a *-isomorphism.*

Proof. We first show that Γ preserves involution. Split $a = Re(a) + iIm(a)$ as in eq. (2.3). Since $Re(a)$ and $Im(a)$ are self-adjoint, their spectrum is real and, for $\ell \in \Omega(\mathcal{M})$, by lemma 2.5, $\ell(Re(a))$ and $\ell(Im(a))$ are real numbers. Thus

$$\Gamma(a^*)\ell = \ell(Re(a)) - i\ell(Im(a)) = \overline{\ell(Re(a)) + i\ell(Im(a))} = \overline{\Gamma(a)}\ell.$$

We now show that Γ is a bijective isometry. For $a \in \mathcal{M}$, by theorem 2.4 and lemma 2.7,

$$|\Gamma(a)|^2 = r(\Gamma(a^*a)) = r(a^*a) = |a|^2$$

so that Γ is an isometry, hence injective, and the image $\Gamma(\mathcal{M})$, being a closed set, is a C^*-algebra. We apply the Stone-Weierstrass theorem: since $\Gamma(\mathcal{M})$ is a C^*-subalgebra of $C(\Omega(\mathcal{M}))$ that contains the constant functions and separates points of $\Omega(\mathcal{M})$ (recall that $\Omega(\mathcal{M})$ is Hausdorff in the weak* topology), it must be $C(\Omega(\mathcal{M}))$ itself. ■

An intersection of C^*-subalgebras is a C^*-subalgebra.

Definition 2.8. Let $\mathcal{M}$ be a C^*-algebra and $S \subset \mathcal{M}$. The C^*-subalgebra $C^*(S)$ *generated by* S is the smallest C^*-subalgebra of $\mathcal{M}$ containing S.

The subalgebra $C^*(S)$ can be viewed as the closure of the set of finite sums of products of elements in $S \cup S^*$. Therefore, for a normal element $a \in \mathcal{M}$, $C^*(a)$ is commutative C^*-algebra and consists of polynomials in a

and a^* together with their uniform limits. Every $\ell \in \Omega(C^*(a))$ is determined by the values $\ell(a)$ and $\overline{\ell(a)}$.

Theorem 2.9 (Continuous functional calculus)**.** *Let $\mathcal{M}$ be a C^*-algebra and $a \in \mathcal{M}$ be normal. Then, there is a *-isomorphism*

$$\phi : C(\sigma(a)) \to C^*(a), \quad f \mapsto f(a)$$

for which $\phi(1) = e$ and $\phi(z) = a$.

Proof. We first show that $\Gamma(a) : \Omega(C^*(a)) \mapsto \sigma(a)$ is a homeomorphism. By lemma 2.7, $\Gamma(a)$ is surjective. If $\Gamma(a)\ell = 0$ then $\ell(a)$ and $\overline{\ell(a)}$ vanish hence $\ell = 0$, implying injectivity. Since $\Gamma(a)$ is a weak* continuous bijection between compact Hausdorff spaces, it is a homeomorphism.

Identify $\Omega(C^*(a))$ with $\sigma(a)$. By theorem 2.8, $\Gamma : C^*(a) \mapsto C(\sigma(a))$ is a *-isomorphism and Γ^{-1} is the desired *-isomorphism. The facts $\phi(1) = e$ and $\phi(z) = a$ are easy. ■

Corollary 2.9.1 (Spectral mapping theorem for continuous functions)**.** *Let $\mathcal{M}$ be a C^*-algebra and $a \in \mathcal{M}$ be normal. If $f \in C(\sigma(a))$ then $\sigma(f(a)) = f(\sigma(a))$.*

Proof. By theorem 2.9, $f(\sigma(a)) = \sigma(f) = \sigma(f(a))$. ■

Let U be a bounded neighborhood of $\sigma(a)$. In a sense, we extend the functional calculus for $f \in \mathcal{H}(U)$(section 2.2) to $f \in C(\sigma)$ at a price of only consider normal elements. For a functional calculus on a 'intermediate' function class, see appendix A.3.3.

2.5
A clarifying example: group algebras

For a finite group G of order n, identify $\mathbb{C}^n$ with the formal linear combinations of the orthonormal basis elements $\{e_g : g \in G\}$. For $g, h \in G$, define the unitary operator $L_g : \mathbb{C}^n \mapsto \mathbb{C}^n$ by $L_g(e_h) = e_{gh}$ on basis elements. The linear span of the set $\{L_g : g \in G\}$ is a C^*-algebra, the *group algebra* of G. Note that the group algebra is commutative if and only if G is commutative.

Consider the group algebra $\mathcal{M}$ for $G = S_3$, and we interpret the group as the symmetries of an equilateral triangle centered at the origin of $\mathbb{R}^2$. Its elements are $\{I, r_1, r_2, x_1, x_2, x_3\}$: I is the identity, r_1 and r_2 represent rotations by $\pi/3$ and $2\pi/3$ while x_1, x_2, x_3 represent reflections on different axes of the triangle. Its multiplication table is

	I	r_1	r_2	x_1	x_2	x_3
I	I	r_1	r_2	x_1	x_2	x_3
r_1	r_1	r_2	I	x_3	x_1	x_2
r_2	r_2	I	r_1	x_2	x_3	x_1
x_1	x_1	x_2	x_3	I	r_1	r_2
x_2	x_2	x_3	x_1	r_2	I	r_1
x_3	x_3	x_1	x_2	r_1	r_2	I

and we then consider the representation of G by 6×6 permutation matrices, which can be read in each row of the multiplication table. The C^*-algebra $\mathcal{M}$ consists of the linear combinations of such matrices,

$$\mathcal{M} = \left\{ \begin{pmatrix} a & b & c & d & e & f \\ c & a & b & f & d & e \\ b & c & a & e & f & d \\ d & f & e & a & c & b \\ e & d & f & b & a & c \\ f & e & d & c & b & a \end{pmatrix}, \ a, b, c, d, e, f \in \mathbb{C} \right\}$$

The underlying Hilbert space is $\mathbb{C}^6$ and $\mathcal{M}$ is a 6-dimensional vector subspace of $M_6(\mathbb{C})$. Since $\{I, r_1, r_2\}$ is a commutative subgroup of S_3 then the correspondent 3-dimensional subalgebra $\mathrm{span}\{L_I, L_{r_1}, L_{r_2}\}$ is commutative.

2.6 Von Neumann algebras

We refer to the weak and strong operator topologies as the weak and strong topologies on $B(H)$. For some basic results, see appendix A.1.

Definition 2.9. A C^*-algebra $\mathcal{M} \subset B(H)$ is a *Von Neumann algebra* if $\mathcal{M}$ is weakly closed and contains the identity.

Example 2.7. In finite dimensional spaces, the operator topologies on $M_n(\mathbb{C})$ are equivalent and C^*-algebras and Von Neumann algebras coincide.

Example 2.8. Not every C^*-algebra is a Von Neumann algebra. Let K be a infinite compact Hausdorff space and μ be a finite positive Borel measure on K. Consider the map $M : L^\infty(K, \mu) \mapsto B(L^2(K, \mu))$ defined by $f \mapsto M_f(\psi) = f\psi$ for $\psi \in L^2(K, \mu)$. Clearly M is an isometric isomorphism from $L^\infty(K, \mu)$ onto its image $M(L^\infty(K, \mu))$. In particular, we may identify $C(K)$ and $L^\infty(K, d\mu)$ with their images under M.

Endow $L^\infty(K,\mu) \cong (L^1(K,\mu))^*$ with the weak* topology and $M(L^\infty(K,\mu))$ with the weak topology induced by $B(L^2(K,\mu))$. We now show that $M : L^\infty(K,\mu) \to M(L^\infty(K,\mu))$ is a homeomorphism for this choice of topologies(appendix A.1). Let (f_j) be a net in $L^\infty(K,\mu)$, with $f_j \to f$ in the weak* topology and $\psi \in L^2(K,\mu)$, then

$$(M(f_j)\psi, \psi) = \int_K f_j \, \psi \, \overline{\psi} \, d\mu = |\psi|^2 \, f_j$$

shows that indeed M and M^{-1} are continuous.

The image $M(C(K)) \cong C(K)$ is a C^*-algebra, but $C(K)$ is weak* dense in $L^\infty(K, d\mu)$, so that the image $M(C(K))$ is weakly dense in $M(L^\infty(K,\mu))$. Therefore $C(K)$ is a C^*-algebra that it is not a Von Neumann algebra. Still, $L^\infty(K,\mu)$ is a commutative Von Neumann algebra.

As for C^*-algebras, the intersection of Von Neumann algebras is again a Von Neumann algebra. Let $\mathcal{F} \subset B(H)$. The Von Neumann algebra $W^*(\mathcal{F})$ *generated* by $\mathcal{F}$ is the smallest Von Neumann algebra in $B(H)$ containing $\mathcal{F}$. Clearly, $W^*(\mathcal{F})$ is the weak closure of $C^*(\mathcal{F})$.

Given a subset $F \subset H$ of a Hilbert space, the (closed) vector space V spanned by F is obtained by applying twice the orthogonal complement, $V = F^{\perp\perp}$. It was Von Neumann's idea to describe $W^*(\mathcal{F})$ in a similar fashion using commutants instead of the (nonexistent) inner products. Closures are taken with respect to strong or weak topologies — recall that weak and strong closures of convex sets are equal(see appendix A.1).

Definition 2.10. The *commutant* of $\mathcal{F}$ is

$$\mathcal{F}' = \{T \in B(H) : TF = FT, \text{ for all } F \in \mathcal{F}\}$$

and $(\mathcal{F}')' = \mathcal{F}''$ is the *bicommutant* of $\mathcal{F}$.

Example 2.9. If $\mathcal{M} \subset B(H)$ is a Von Neumann algebra then $\mathcal{M}'$, $\mathcal{M}''$ and the center of $\mathcal{M}$, $\mathcal{Z}(\mathcal{M}) = \mathcal{M} \cap \mathcal{M}'$, are Von Neumann algebras. Additionally we have $\mathcal{M} \subset \mathcal{M}''$.

Example 2.10. We compute the commutant $\mathcal{M}'$ of the finite group algebra introduced in Section 2.5. The underlying fact is trivial: multiplications on the left and on the right commute. Let $\mathcal{S} = \text{span}\{R_g : g \in G\}$ with $R_g(e_h) = e_{hg}$ for $h \in G$. Clearly $L_g R_h e_m = R_h L_g e_m$ for $g, h, m \in G$ hence $\mathcal{S} \subset \mathcal{M}'$. If $A \in \mathcal{M}'$ then $Ae_g = AL_g e_I = L_g A e_I = \sum_m A_{mI} e_{gm}$ so that $A \in \mathcal{S}$ and $\mathcal{M}' = \mathcal{S}$.

Theorem 2.10 (Von Neumann density theorem)**.** *Suppose $\mathcal{M} \subset B(H)$ is a C^*-algebra containing the identity. Then $\mathcal{M}$ is strongly dense in $\mathcal{M}''$.*

Notice that $\mathcal{M}$ is not necessarily weakly closed, whereas $\mathcal{M}''$ is.

Proof. Let $T \in \mathcal{M}''$ and V be a strong neighborhood of T(appendix A.1): take $x_1, \ldots, x_n \in H$ and $\epsilon > 0$ such that $V = \{S \in B(H) : |Tx_i - Sx_i| < \epsilon,\ i = 1, \ldots, n\} \subset \mathcal{M}''$. Set $\tilde{x} = (x_1, \ldots, x_n) \in H^n$: we are led to consider n-uples

$$\tilde{\mathcal{M}}\tilde{x} \;=\; \{\tilde{S}\tilde{x} \;=\; (Sx_1, \ldots, Sx_n) \subset H^n \text{ for } S \in \mathcal{M}\} \;.$$

We show that $\tilde{T}\tilde{x} = (Tx_1, \ldots, Tx_n)$ lies in the (weak, strong) closure $\overline{\tilde{\mathcal{M}}\tilde{x}}$.

Let P be the orthogonal projection from H^n onto $\overline{\tilde{\mathcal{M}}\tilde{x}}$. The set $\tilde{\mathcal{M}} = \{\tilde{A} \in B(H^n) : A \in \mathcal{M}\}$ endowed with componentwise operations is a C^*-algebra. Clearly $\operatorname{Ran} P = \overline{\tilde{\mathcal{M}}\tilde{x}}$ is invariant by $\tilde{\mathcal{M}}$ and, because $\tilde{\mathcal{M}}$ is closed under the involution, $\ker P$ also is, so that $P \in \tilde{\mathcal{M}}'$.

A simple computation shows that $T \in \mathcal{M}''$ which implies that $\tilde{T} \in \tilde{\mathcal{M}}''$. Therefore $\tilde{T}$ commutes with P, so that $\operatorname{Ran} P$ is invariant under $\tilde{T}$ and $\tilde{T}\tilde{x} \in \operatorname{Ran} P = \overline{\tilde{\mathcal{M}}\tilde{x}}$. ∎

Corollary 2.10.1. *Let $\mathcal{M} \subset B(H)$ be a C^*-algebra containing the identity. Then $\mathcal{M}$ is a Von Neumann algebra if and only if $\mathcal{M} = \mathcal{M}''$.*

Adding up, by theorem 2.10, the weak and strong closures of a C^*-algebra $\mathcal{M}$ are equal to $\mathcal{M}''$. We use $\mathcal{M}''$ to refer to the strong or weak closure of $\mathcal{M}$.

A function $f : \mathbb{R} \mapsto \mathbb{C}$ is *strongly continuous* if for every Hilbert space H and every strongly convergent net (T_j) of self-adjoint operators in $B(H)$ with $T_j \to T$, one has $f(T_j) \to f(T)$ strongly. We quote Theorem 4.3.2 of [13].

Lemma 2.11. *If $f : \mathbb{R} \mapsto \mathbb{C}$ is a bounded and continuous function then it is strongly continuous.*

Recall that $\mathcal{M}_{sa}$ is the set of self-adjoint elements of $\mathcal{M}$. The map taking $A \in \mathcal{M}$ to its real part $Re(A) \in \mathcal{M}_{sa}$ is weakly continuous(see appendix A.1).

Theorem 2.12 (Kaplansky density theorem)**.** *Let $\mathcal{M} \subset B(H)$ be a C^*-algebra with strong closure $\mathcal{M}''$.*

1. *Every self-adjoint operator $A \in \mathcal{M}''$ is the strong limit of a net of self-adjoint operators (A_j) in $\mathcal{M}$, with $|A_j| \leq |A|$.*

2. *Every $A \in \mathcal{M}''$ is the strong limit of a net (A_j) in $\mathcal{M}$, with $|A_j| \leq |A|$.*

Proof. For (1), take a net (A_j) in $\mathcal{M}$ with $A_j \to A$ strongly (hence weakly, see appendix A.1) to the self-adjoint operator $A \in \mathcal{M}''$. We may suppose A_j to be in the weak (strong) closure of $\mathcal{M}_{sa}$ by taking real parts.

We show that we may bound each self-adjoint operator A_j by $|A|$. Define $f : \mathbb{R} \to \mathbb{R}$ so that $f(x) = x$ for $|x| \leq |A|$ which is continuous and constant outside of this interval. By lemma 2.11, $f(A_j) \to f(A) = A$, because f is the identity function on $\sigma(A)$. Moreover, f is real and $|f|_\infty = |A|$, so that $f(A_j)$ is self-adjoint and $|f(A_j)| \leq |A|$, and (1) is proved.

For (2), take again for each $A_j \to A \in \mathcal{M}''$ strongly. Embed the net and the limit as matrices with entries in $\mathcal{M}''$,

$$\tilde{A} = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix} \in M_2(\mathcal{M}'') = M_2(\mathcal{M})''$$

apply (1) to obtain a convergent net of self-adjoint matrices. The $(1, 2)$ entries of such matrices are the required net A_j. ■

2.7 Cyclic and separating vectors

Definition 2.11. Let $\mathcal{M} \subset B(H)$ be a C^*-algebra and $u \in H$. The vector u is *cyclic* for $\mathcal{M}$ if the set $\mathcal{M}u$ is dense in H. The vector u is *separating* for $\mathcal{M}$ if the map $A \in \mathcal{M} \mapsto Au \in H$ is injective.

A separating vector does not have to be cyclic.

Example 2.11. Let $\mathcal{M}$ be the group algebra of a finite group G, as in section 2.5. For $k \in G$, set $u = e_k$. Then, for $h \in G$, $L_{hk^{-1}} e_k = e_h$ hence u_k is cyclic for $\mathcal{M}$. Since $\dim \mathcal{M} = n$, the vector is also separating. Cyclic vectors are frequently abundant: we show that $u = e_I + i e_{r_1}$ also is cyclic separating for $\mathcal{M}$. For $k \in S_3$, the equation

$$e_k = (\sum_{g \in S_3} c_g L_g)(e_I + i e_{r_1})$$

must have solutions $\{c_g \in \mathbb{C} : g \in S_3\}$, with some $c_g \neq 0$ (exactly one, by the dimension count, so that u is also separating). The required system is

$$\begin{pmatrix} 1 & 0 & i & 0 & 0 & 0 \\ i & 1 & 0 & 0 & 0 & 0 \\ 0 & i & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & i \\ 0 & 0 & 0 & i & 1 & 0 \\ 0 & 0 & 0 & 0 & i & 1 \end{pmatrix} \begin{pmatrix} c_I \\ c_{r_1} \\ c_{r_2} \\ c_{x_1} \\ c_{x_2} \\ c_{x_3} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{2.4}$$

whose matrix has non-zero determinant and hence u is cyclic for $\mathcal{M}$.

Inverting eq. (2.4),

$$\begin{pmatrix} c_I \\ c_{r_1} \\ c_{r_2} \\ c_{x_1} \\ c_{x_2} \\ c_{x_3} \end{pmatrix} = -\frac{1}{2} \begin{pmatrix} 1 & -1 & -i & 0 & 0 & 0 \\ -i & 1 & -1 & 0 & 0 & 0 \\ -1 & -i & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -i & -1 \\ 0 & 0 & 0 & -1 & 1 & -i \\ 0 & 0 & 0 & -i & -1 & 1 \end{pmatrix},$$

where the k-th column gives the coefficients c_g to obtain $e_k = \sum_g c_g L_g u$. For example, $e_I = -L_I/2 + iL_{r_1}/2 + L_{r_2}/2$.

Lemma 2.13. *Let H be a separable Hilbert space. Every commutative C^*-algebra $\mathcal{M} \subset B(H)$ has a separating vector.*

Proof. Take $u_1 \in H_1$, the unit sphere of H. If $\mathcal{M}u_1$ is dense in H, stop, otherwise take $u_2 \in H_1$ with $u_2 \perp \mathcal{M}u_1$. Then necessarily $Tu_1 \perp Tu_2$ for $T \in \mathcal{M}$ (recall $\mathcal{M}$ is closed by taking adjoints). By Zorn's lemma and the separability of H, there is a sequence of unitary vectors (u_n) such that $\cup_{n=1}^{\infty}\mathcal{M}u_n$ is dense in H with an additional property: for all $T \in \mathcal{M}$, $Tu_n \perp Tu_m$ for $n \neq m$.

We will show that $u = \sum_{n=1}^{\infty} 2^{-n}u_n$ is separating for $\mathcal{M}$. The series converges because the u_n's are normal. If $T \in \mathcal{M}$ satisfies $Tu = 0$, then $Tu_n = 0$ for $n \in \mathbb{N}$, because $Tu_n \perp Tu_m$ for $n \neq m$. Using the commutativity of $\mathcal{M}$ in $T(\cup_{n=1}^{\infty}\mathcal{M}u_n)$ yields $T = 0$. ∎

Proposition 2.5. *Let $\mathcal{M} \subset B(H)$ be a C^*-algebra and $u \in H$. Then u is cyclic for $\mathcal{M}$ if and only if u is separating for $\mathcal{M}'$.*

Proof. If $A' \in \mathcal{M}'$ with $A'u = 0$, then $A'Au = 0$ for $A \in \mathcal{M}$. Since u is cyclic, $A' = 0$ and hence u is separating for $\mathcal{M}'$. Conversely, take a separating vector u of $\mathcal{M}'$ and let P be the orthogonal projection onto $\overline{\mathcal{M}u}$. As in theorem 2.10, this space is invariant under $\mathcal{M}$, so that $P \in \mathcal{M}'$. Now, $(I - P)u$ is also separating for $\mathcal{M}'$. Indeed, if $A', B' \in \mathcal{M}'$ satisfy $A'(I - P)u = B'(I - P)u$, then $(A' - B')u = (A' - B')Pu$. But $A' - B', (A' - B')P \in \mathcal{M}'$, contradicting the separability of u. Therefore $u \in \ker P$ and then $I, (I - P) \in \mathcal{M}'$ and from $Iu = (I - P)u$ either $I = I - P$ or $I = P$. But $P = 0$ implies $\overline{\mathcal{M}u} = \{0\}$, and it contains Iu. Thus $P = I$, so that $\overline{\mathcal{M}u} = H$ and thus u is cyclic. ∎

Corollary 2.13.1. *Let $\mathcal{M} \subset B(H)$ be a Von Neumann algebra. Then $u \in H$ is cyclic and separating for $\mathcal{M}$ if and only if u is cyclic and separating for $\mathcal{M}'$.*

Proof. Combine proposition 2.5 and corollary 2.10.1. ∎

2.8 The bounded Borel functional calculus

The main result in this section is the representation theorem for commutative Von Neumann algebras acting on separable Hilbert spaces.

Theorem 2.14. *Let H be a separable Hilbert space and $\mathcal{M} \subset B(H)$ be a commutative Von Neumann algebra. Then $\mathcal{M}$ is *-isomorphic to $L^\infty(K, \mu)$ for a compact Hausdorff space K and a finite positive Borel measure μ on K.*

The result follows immediately from lemma 2.15 and lemma 2.16 below.

Lemma 2.15. *Let H be a separable Hilbert space and $\mathcal{M} \subset B(H)$ be a commutative Von Neumann algebra. Then $\mathcal{M}$ is *-isomorphic and weak homeomorphic to a commutative Von Neumann algebra with a cyclic vector.*

Proof. By lemma 2.13, $\mathcal{M}$ has a separating vector $u_0 \in H$. For $H_0 = \overline{\mathcal{M}u_0}$, consider the orthogonal projection $P : H \to H_0$ and the restriction map $\phi : \mathcal{M} \subset B(H) \mapsto B(H_0)$ that carries $A \in \mathcal{M}$ to the restriction of A to H_0. Since H_0 is invariant by $\mathcal{M}$, ϕ is well-defined. We show that ϕ is injective: if $\phi A = 0$, then $A = 0$. Indeed, $u_0 = Iu_0 \in H_0$, so that $\phi A u_0 = A u_0 = 0$ and since u is separating, $A = 0$.

Clearly, $\phi : \mathcal{M} \mapsto \phi(\mathcal{M})$ is a weakly continuous *-isomorphism. Also, $u_0 \in H_0$ is a cyclic vector of the commutative C^*-algebra $\phi(\mathcal{M})$. From the Kaplansky density theorem, ϕ^{-1} is weakly continuous: ϕ is a homeomorphism and $\phi(\mathcal{M})$ is a Von Neumann algebra. ∎

Lemma 2.16. *Let $\mathcal{M} \subset B(H)$ be a commutative C^*-algebra with cyclic vector $u \in H$. Then, there exist a finite positive Borel measure μ on the character space $K = \Omega(\mathcal{M})$ such that $\mathcal{M}''$ and $L^\infty(K, \mu)$ are *-isomorphic.*

The new ingredient provides a proof of the self-adjoint spectral theorem. For $T \in B(H)$ and $v \in H$, the map $f \in C(\sigma(T)) \mapsto \langle f(T)v, v\rangle \in \mathbb{C}$ belongs to $C(\sigma(T))^*$. By the Riesz representation theorem, there is a measure μ_v such that the map is given by $f \mapsto \int_{\sigma(T)} f \, d\mu_v$. The use of the cyclic vector is also standard: for the multiplication operator $Tf = xf$, the constant function $1 \in L^2(\sigma(T), d\mu)$ gives rise to monomials $T^k 1 = x^k$, which by Gram-Schmidt obtain the orthogonal polynomials with respect to $d\mu$. The process converts the rather abstract vector space spanned by $v, Tv, T^2, \ldots$ into a bona fide subspace of polynomials. The two arguments above are implemented in the context of Von Neumann algebras in the first two paragraphs of the proof.

Proof. For $K = \Omega(\mathcal{M})$, let $\Gamma : \mathcal{M} \mapsto C(K)$ be the Gelfand transform. The Riesz representation theorem applied to $f \in C(K) \mapsto (\Gamma^{-1}(f)u, u) \in \mathbb{C}$ gives a unique finite regular Borel measure μ on K such that for $f \in C(K)$,

$$(\Gamma^{-1}(f)u, u) = \int_K f d\mu. \tag{2.5}$$

A calculation with positive functions $f \in C(K)$ implies that μ is positive.

Define $U_0 : \mathcal{M}u \subset H \mapsto C(K) \subset L^2(K,\mu)$ by $U_0(Au) = \Gamma(A)$. A calculation using eq. (2.5) shows that U_0 is an isometry, so that it extends to a unitary operator $U : H \mapsto L^2(K,\mu)$ since u is cyclic. The map

$$\phi : B(H) \ \mapsto \ B(L^2(K,\mu)) \ , \quad A \ \mapsto \ UAU^*$$

is a *-isomorphism (hence an isometry) and a weak homeomorphism and

$$\phi(A)\ \Gamma(B) \ = \ \Gamma(A)\ \Gamma(B) \ , \quad \text{for } A, B \in \mathcal{M}$$

so that $\phi(A) = \Gamma(A)$ because $C(K)$ is dense in $L^2(K,\mu)$. Thus,

$$\phi(\mathcal{M}) = C(K) \subset L^\infty(K,\mu) \ .$$

Since $\mathcal{M}$ is weakly dense in $\mathcal{M}''$, $\phi(\mathcal{M}'') \subset L^\infty(K,\mu)$. Therefore, the restriction $\phi : \mathcal{M}'' \mapsto L^\infty(K,\mu)$ is an isometric *-homomorphism.

We are left with showing that ϕ is surjective. The unit ball $(B(H))_1$ is weakly compact(see appendix A.1) so that $(\mathcal{M}'')_1$ also is and $(\phi(\mathcal{M}''))_1$ is weakly closed. An application of Kaplansky density theorem (theorem 2.12) shows that $\phi(\mathcal{M}'')$ is weakly closed, and hence is a Von Neumann algebra containing $C(K)$. Therefore $\phi(\mathcal{M}'') = L^\infty(K,\mu)$. ∎

We are ready for the last extension of the (normal) functional calculus.

Theorem 2.17 (Bounded Borel functional calculus)**.** *Let H be a separable Hilbert space and $T \in B(H)$ be a normal operator. Then there is a finite positive Borel measure μ on $\sigma(T)$ such that the Gelfand transform $\Gamma : C^*(T) \mapsto C(\sigma(T))$ extends to an *-isomorphism $\tilde{\Gamma} : W^*(T) \mapsto L^\infty(\sigma(T),\mu)$.*

Proof. By lemma 2.15, we may suppose that $W^*(T)$ possess a cyclic vector $u \in H$, so that u is also cyclic for $C^*(T)$. The result follows from lemma 2.16 applied to $C^*(T)$. ∎

The functional calculus does not exist only for holomorphic, continuous and bounded Borel functions. In appendix A.3.3, we show a functional calculus for C^k functions is the natural context in the presence of nilpotent parts.

3
The Tomita-Takesaki theory

We describe the Tomita-Takesaki theory for Von Neumann algebras with a cyclic separating vector. We first present the finite dimensional case, then the infinite dimensional case without giving proofs. After providing three examples of modular operators — two of which in finite dimensions — we indicate the proof of the main theorem. We follow [10, 15, 16].

We need some rather unusual concept of anti-linear operators between Hilbert spaces, stated in appendix A.1, associated to anti-isomorphisms between C^*-algebras. A linear bijection $\phi : \mathcal{M}_1 \mapsto \mathcal{M}_2$ between C^*-algebras is an *anti-isomorphism* if it preserves involution and for $A, B \in \mathcal{M}_1$, $\phi(AB) = \phi(B)\phi(A)$. In this case, $\mathcal{M}_1$ and $\mathcal{M}_2$ are *anti-isomorphic*.

We consider three examples of maps ϕ for which $\phi(AB) = \phi(B)\phi(A)$. The first is an involution $* : \mathcal{B} \mapsto \mathcal{B}$, a self-inverse anti-linear map for which $(AB)^* = B^*A^*$. For the inverse operation in $GL(\mathcal{B})$, the group of invertible elements of $\mathcal{B}$, we also have $(AB)^{-1} = B^{-1}A^{-1}$. Finally, from section 2.5, recall the group algebra of a finite group G and the right multiplication map $R : G \mapsto M_n(\mathbb{C})$, $g \mapsto R_g(e_k) = e_{kg}$, for $k \in G$: clearly $R_{gh} = R_h R_g$.

3.1
The Tomita-Takesaki theory for $H = \mathbb{C}^n$

In finite dimensions, the Tomita-Takesaki theory is easier. Von Neumann algebras $\mathcal{M} \subset M_n(\mathbb{C})$ are simply C^* algebras and all operators are bounded.

We show that for a C^* algebra $\mathcal{M} \subset M_n(\mathbb{C})$ and its commutant $\mathcal{M}' \subset M_n(\mathbb{C})$ with common cyclic separating vector $u \in \mathbb{C}^n$ (recall Corollary 2.13.1), there is an anti-isomorphism $\phi_u : \mathcal{M} \mapsto \mathcal{M}'$ induced by u.

The vector $u \in \mathbb{C}^n$, induces a natural linear map, the evaluation at u,

$$\theta_u : \mathcal{M} \mapsto \mathbb{C}^n \qquad A \mapsto Au.$$

From the separating property of u, θ_u is injective, while the fact that u is cyclic in a finite dimensional space yields surjectivity: θ_u is an isomorphism of vector spaces. Thus, the C^*-algebra structures of $\mathcal{M} \subset M_n(\mathbb{C})$, i.e., the involution and product algebra, are induced on $\mathbb{C}^n$. Similarly, the inner product of $\mathbb{C}^n$ induces one in $\mathcal{M} \subset M_n(\mathbb{C})$.

Now, u is also cyclic and separating for $\mathcal{M}'$ and

$$\psi_u : \mathcal{M}' \mapsto \mathbb{C}^n \;, \qquad A' \mapsto A'u$$

is also an isomorphism of vector spaces, as well as

$$\phi_u = \psi_u^{-1} \circ \theta_u : \mathcal{M} \mapsto \mathcal{M}'.$$

The explicit form of ϕ_u is hard do find. Instead, note that, for $A \in \mathcal{M}$,

$$Au = \phi_u(A)u,$$

since $A \in \mathcal{M}$ and $\phi_u(A) \in \mathcal{M}'$ are related through Au.

The diagram below should help the reader to get used with the new definitions. In the first row are the maps θ_u and ψ_u. The central (identity) map identifies $H = \mathbb{C}^n$ with its dual through a *linear* (and not antilinear) map. The composition of bijections on the top row is $\phi_u : \mathcal{M} \to \mathcal{M}'$.

$$\begin{array}{ccccccc}
\mathcal{M} & \xrightarrow{\theta_u} & \mathcal{M}u \simeq H & \xrightarrow{id} & H^* \simeq \mathcal{M}'u & \xleftarrow{\psi_u} & \mathcal{M}' \\
{\scriptstyle *}\big\downarrow & & {\scriptstyle S}\big\uparrow & & {\scriptstyle S^*}\big\downarrow & & {\scriptstyle *}\big\downarrow \\
\mathcal{M} & \xrightarrow{\theta_u} & \mathcal{M}u \simeq H & \xrightarrow{\Delta} & H^* \simeq \mathcal{M}'u & \xleftarrow{\psi_u} & \mathcal{M}'
\end{array}$$

The vertical arrows are anti-linear bijections. The arrows at each side are involutions in $\mathcal{M}$ and $\mathcal{M}'$. Define the *Tomita operator* associated to $(\mathcal{M}, u)$,

$$S : \mathcal{M}u \;\to\; \mathcal{M}u \qquad Au \mapsto A^*u, \tag{3.1}$$

which completes a commutative square on the left of the diagram. Clearly S is anti-linear (see appendix A.2 for basic facts about anti-linear maps and their duals) and $S = S^{-1}$. In the same fashion, one defines its dual $S^* : \mathcal{M}'u \to \mathcal{M}'u$. We compute $S^* : \mathcal{M}'u \;\to\; \mathcal{M}'u$: let $A \in \mathcal{M}$ and $A' \in \mathcal{M}'$,

$$(SAu, A'u) = (A^*u, A'u) = (A'^*u, Au), \tag{3.2}$$

hence $S^*A'u = A'^*u$ and again $(S^*)^{-1} = S^*$.

The map $\Delta = S^*S : H \to H$ ensures the commutativity of the central square of the diagram. Horizontal maps are linear bijections. For an example in which Δ is not a unitary map, see section 3.3.1.

The map ϕ_u is easily described in terms of S.

Proposition 3.1. *For $A \in \mathcal{M}$, $\phi_u(A) = SA^*S$ and $S\mathcal{M}S = \mathcal{M}'$, in the sense that $S\mathcal{M}Su = \mathcal{M}'u$ for the cyclic vector u. Also, $S^*\mathcal{M}'S^* = \mathcal{M}$.*

Proof. For $A \in \mathcal{M}$, $\phi_u(A)u = Au = S(A^*u) = SA^*S(Iu) = SA^*Su$. Thus, if $SA^*S \in \mathcal{M}'$, the separability of u implies $\phi_u(A) = SA^*S$. We must then show that for $A \in \mathcal{M}$, SAS commutes with $\mathcal{M}$. Thus, for $B, C \in \mathcal{M}$ and since every vector in $H = \mathbb{C}^n$ is of the form Cu by cyclicity of u,

$$SASB(Cu) = SAC^*B^*u = BCA^*u = BS(AC^*u) = BSAS(Cu). \tag{3.3}$$

so that $S\mathcal{M}S \subset \mathcal{M}'$. For the other inclusion, imitate eq. (3.3) to obtain $S^*\mathcal{M}'S^* \subset \mathcal{M}'' = \mathcal{M}$, where the last equality is corollary 2.10.1. Applying involutions on both sides yields $S\mathcal{M}'S \subset \mathcal{M}$. Now compose with $S = S^{-1}$ on both sides and get $\mathcal{M}' \subset S\mathcal{M}S$. Similarly, $S^*\mathcal{M}'S^* = \mathcal{M}$. ■

We consider additional structure. Thus, for example, ϕ_u *reverses* products. Indeed, from section 3.1, for $A, B \in \mathcal{M}$, we have $\phi_u(B) \in \mathcal{M}'$ and

$$\phi_u(AB)u = ABu = A\phi_u(B)u = \phi_u(B)Au = \phi_u(B)\phi_u(A)u\ .$$

However, usually ϕ_u does not preserve the involution.

Proposition 3.2. *The map ϕ_u preserves the involution if and only if*

$$(u, ABu) = (u, BAu), \quad \textit{for all } A, B \in \mathcal{M}\ .$$

Commutative C^*-algebras satisfy this condition. The Tomita-Takesaki theorem, presented in this section for finite dimensions, constructs a family of anti-isomorphisms between $\mathcal{M}$ and $\mathcal{M}'$ which preserve involution.

Proof. Suppose that ϕ_u preserves involution. Recall that H is a Hilbert space: in particular, an inner product is defined. We have

$$\begin{aligned}(u, ABu) &= (A^*u, Bu) = (\phi_u(A^*)u, Bu) = (\phi_u(A)^*u, Bu) = (u, \phi_u(A)Bu)\\ &= (u, B\phi_u(A)u) = (u, BAu).\end{aligned}$$

A similar calculation shows the converse. ■

Consider the polar decomposition of Tomita's operator (see appendix A.2),

$$S = J\ (S^*S)^{1/2} = J\ \Delta^{1/2} \tag{3.4}$$

where J is an anti-linear unitary operator, $J^* = J^{-1}$, and $\Delta = S^*S$ is a (self-adjoint) positive operator with positive square root $\Delta^{1/2}$ (a positive operator T is a self-adjoint operator for which $(Tu, u) \geq 0$). The operators Δ and J are the *modular* and *conjugation* operators associated to the pair $(\mathcal{M}, u)$.

Proposition 3.3. *Let S be the Tomita operator associated to $(\mathcal{M}, u)$. Then*

1. $J = J^* = J^{-1}$ *and* $\Delta^{-1} = SS^*$.

2. $S = J\Delta^{1/2} = \Delta^{-1/2}J$.

Proof. The first claim is immediate. Since $J = J^{-1}$, eq. (3.4) gives

$$S = S^{-1} = (SS^*)^{1/2}J = \Delta^{-1/2}J \ .$$

■

For $A \in \mathcal{M}$, we compare $\phi_u(A^*)$ and $\phi_u(A)^*$,

$$\phi_u(A^*) = SA^*S = J\Delta^{1/2}A\Delta^{-1/2}J, \quad \phi_u(A)^* = J\Delta^{-1/2}A\Delta^{1/2}J \ .$$

There is no reason why ϕ_u should preserve involutions. Tomita's wonderful idea is to replace the self-adjoint operator $\Delta^{1/2}$ by the skew adjoint $\Delta^{i/2}$ (a simple consequence of the functional calculus): we will show that the map

$$\tau(A) : \mathcal{M} \to \mathcal{M}' \ , \quad A \mapsto J\Delta^{i/2}A^*\Delta^{-i/2}J$$

is a linear bijection which preserves involutions and reverses products.

To see what should be proved, express τ in terms of the Tomita operator,

$$\tau(A) = J(\Delta^{1/2}\Delta^{-1/2})\Delta^{i/2}A^*\Delta^{-i/2}(\Delta^{1/2}\Delta^{-1/2})J$$

$$= S\Delta^{(-1+i)/2}A^*\Delta^{-(-1+i)/2}S.$$

If we could prove that $\Delta^{(-1+i)/2}\mathcal{M}\Delta^{-(-1+i)/2} \subset \mathcal{M}$, then $\tau(A) \in \mathcal{M}'$ since, by proposition 3.1, $S\mathcal{M}S = \mathcal{M}'$. Furthermore,

$$A = \Delta^{-(1+i)/2}S^*(\tau(A))^*S^*\Delta^{(1+i)/2} \tag{3.5}$$

which suggests that $\Delta^{-(1+i)/2}\mathcal{M}'\Delta^{(1+i)/2} \subset \mathcal{M}$ because $S^*\mathcal{M}'S^* = \mathcal{M}$, again by proposition 3.1.

We prove more: $\Delta^z\mathcal{M}\Delta^{-z} \subset \mathcal{M}$ for $z \in \mathbb{C}$, where the operators Δ^z and Δ^{-z} are well defined by the continuous functional calculus for a suitable definition of the map $w \in \mathbb{C} \mapsto w^z \in \mathbb{C}$.

We use a special case of Carlson's theorem (see page 186 of [17]).

Theorem 3.1. *Let $f : \mathbb{C} \mapsto \mathbb{C}$ be analytic. If f vanishes on $\mathbb{Z}$ and it is bounded on $\operatorname{Re} z \geq 0$, then f is identically zero.*

Theorem 3.2. *Let $\mathcal{M} \subset M_n(\mathbb{C})$ be a Von Neumann algebra with cyclic separating vector $u \in \mathbb{C}^n$. Then $\Delta^z\mathcal{M}\Delta^{-z} = \mathcal{M}$ for every $z \in \mathbb{C}$.*

Proof. We first prove the direct inclusion: we show that elements of $\Delta^z \mathcal{M} \Delta^{-z}$ commute with $\mathcal{M}'$, so that $\Delta^z \mathcal{M} \Delta^{-z} \subset \mathcal{M}'' = \mathcal{M}$. Let $A \in \mathcal{M}$, $A' \in \mathcal{M}'$, $e_j, e_k \in \mathbb{C}^n$ be basis elements, and define the function

$$f : \mathbb{C} \mapsto \mathbb{C}, \qquad z \mapsto |\Delta|^{-2z}([\Delta^z A \Delta^{-z}, A']e_j, e_k),$$

where $[A, B] = AB - BA$, for $A, B \in M_n(\mathbb{C})$, is the commutator of matrices. We show that f satisfies the hypotheses of theorem 3.1.

To see that f is zero at $n \in \mathbb{Z}$, we prove $\Delta^n \mathcal{M} \Delta^{-n} = \mathcal{M}$. We use proposition 3.3. Write $\Delta \mathcal{M} \Delta^{-1} = S^*(S\mathcal{M}S)S^* = S^*\mathcal{M}'S^* = \mathcal{M}$. Similarly,

$$\Delta^2 \mathcal{M} \Delta^{-2} = \Delta(\Delta \mathcal{M} \Delta^{-1})\Delta^{-1} = \mathcal{M}$$

and the result for $n \in \mathbb{N}$ follows by induction. For $-n \in \mathbb{N}$, $\Delta^{-n}\mathcal{M}\Delta^n = \Delta^{-n}(\Delta^n \mathcal{M} \Delta^{-n})\Delta^n = \mathcal{M}$.

Since Δ is an invertible positive operator, its eigenvalues λ_k are strictly positive. The maps $z \mapsto \lambda_k^z = e^{z \log \lambda_k}$ are entire maps for, say, the usual real valued logarithm. From the analytical functional calculus we obtain an entire function $z \mapsto \Delta^z$. The spectral theorem $\Delta^z = UD^zU^*$ gives the bounds

$$\|\Delta^{-z}\| = \min_k \ \lambda_k^{Rez} = m^{Rez} \ , \quad \|\Delta^z\| \ = \ \max_k \ \lambda_k^{Rez} = M^{Rez} \ .$$

Since J is anti-unitary, by proposition 3.3,

$$|\Delta^{-1}| = |SS^*| = |J\Delta^{1/2}\Delta^{1/2}J| = |J\Delta J| = |\Delta|,$$

which implies that $mM = 1$. Finally,

$$f(z) \leq 2\|\Delta\|^{-2z} \ \|\Delta^z\| \ \|\Delta^{-z}\| \ \|A\| \ \|A'\| \leq 2M^{-2Rez}M^{Rez}m^{-Rez}\|A\| \ \|A'\| \ ,$$

which is bounded for $Rez \geq 0$.

The reverse inclusion is clear: $\mathcal{M} = \Delta^z(\Delta^{-z}\mathcal{M}\Delta^z)\Delta^{-z} \subset \Delta^z\mathcal{M}\Delta^{-z}$. ∎

We are ready for the Tomita-Takesaki theorem. There is nothing special in the computations above about the exponent $i/2$.

Theorem 3.3. *Let $\mathcal{M} \subset M_n(\mathbb{C})$ be a Von Neumann algebra with cyclic separating vector $u \in \mathbb{C}^n$. Then $J\mathcal{M}J = \mathcal{M}'$. For $t \in \mathbb{R}$, the map*

$$A \in \mathcal{M} \mapsto J\Delta^{it}A^*\Delta^{-it}J \in \mathcal{M}'$$

is as an anti-isomorphism which preserves involutions.

Proof. Indeed, $J\mathcal{M}J = J(\Delta^{1/2}\mathcal{M}\Delta^{-1/2})J = S\mathcal{M}S = \mathcal{M}'$, so that

$$\tau(\mathcal{M}) = J(\Delta^{i/2}\mathcal{M}\Delta^{-i/2})J = J\mathcal{M}J = \mathcal{M}' \ .$$

Furthermore, eq. (3.5) is an inverse of τ because of theorem 3.2: $\tau : \mathcal{M} \mapsto \mathcal{M}'$ is a bijection which preserves involutions and $\mathcal{M}$ and $\mathcal{M}'$ are anti-isomorphic. ■

3.2 The infinite dimensional case

Throughout this section, $\mathcal{M} \subset B(H)$ is a Von Neumann algebra with a cyclic separating vector $u \in H$. Tomita's ideas provide a whole family of anti-isomorphisms preserving involution between $\mathcal{M}$ and $\mathcal{M}'$ in the infinite dimensional case. We state results analogous to theorem 3.2 and theorem 3.3 and obtain some consequences.

Call S_0 to Tomita operator associated to $(\mathcal{M}, u)$ given by eq. (3.1). From the separability of u, S_0 is well defined. The cyclic property of u only implies that S_0 is densely defined, since S_0 may be unbounded (see section 4 of [15] for an example). Fortunately, S_0 is closable (see appendix A.4 for definitions).

Proposition 3.4. *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as above. Then*

1. *For $A' \in \mathcal{M}'$, $S_0^*(A'u) = A'^*u$ and hence $S_0^* = (S_0^*)^{-1}$ on $\mathcal{M}'u$.*

2. *S_0 is a well-defined closable operator.*

Proof. The first fact is proved as in finite dimensions: since S_0 is densely defined, S_0^* is well defined and one follows eq. (3.2). From corollary 2.13.1, $\mathcal{M}'u$ is dense in H and hence S_0^* is densely defined which implies that S_0 is closable (see appendix A.4). ■

For S, the closure of S_0, we have a polar decomposition (see appendix A.2): there exists a densely defined positive linear operator $\Delta = S^*S$ and a partial anti-isometry $J : \overline{\mathrm{Ran}(\Delta^{1/2})} \to \overline{\mathrm{Ran}(S)}$ such that

$$S = J\Delta^{1/2}. \tag{3.6}$$

The invertible positive operator Δ, the anti-unitary operator J and the closed operator S are the *modular operator*, the *modular conjugation* and the *Tomita operator* associated to the pair $(\mathcal{M}, u)$. For simplicity, from now on, we refer to (Δ, J) as the *modular pair* associated to $(\mathcal{M}, u)$.

Proposition 3.5. *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as above. Then*

$$S = J\Delta^{1/2} = (SS^*)^{1/2}J,$$

$$\Delta^{-1} = SS^*, \quad J = J^{-1} = J^*, \quad Ju = \Delta u = \Delta^{-1}u = u,$$

$$S = J\Delta^{1/2} = \Delta^{-1/2}J, \qquad S^* = \Delta^{1/2}J = J\Delta^{-1/2}.$$

Proof. First, observe that $S_0 = (S_0)^{-1}$ on $\mathrm{Dom}(S_0) = \mathrm{Ran}(S_0) \subset \mathcal{M}u$. Since S is closed, $S_0^2 = I$ implies $S^2 = I$ on $\mathrm{Dom}(S)$ and $\mathrm{Dom}(S) = \mathrm{Ran}(S)$. From properties of unbounded operators(appendix A.4), $S^* = S_0^*$ and $S^{**} = S$. As before, (1) of proposition 3.4 implies that, $(S^*)^2 = I$ on $\mathrm{Dom}(S^*)$ and $\mathrm{Dom}(S^*) = \mathrm{Ran}(S^*)$. From these, we conclude that $S^*SSS^* = I$ on $\mathrm{Dom}(\Delta)$, and hence that $\Delta^{-1} = SS^*$ and we also obtain the first equality above.

Since S and Δ (hence $\Delta^{1/2}$) have dense ranges, J is an anti-unitary operator, i.e., $J^* = J^{-1}$. From eq. (3.6), we get $S = J\Delta^{1/2} = \Delta^{-1/2}J$ and taking adjoints gives $S^* = \Delta^{1/2}J = J\Delta^{-1/2}$. Also, $I = S^2 = J\Delta^{1/2}\Delta^{-1/2}J = J^2$ on the dense subspace $\mathrm{Dom}(S)$, and hence $J^2 = I$. We thus get $J = J^* = J^{-1}$.

Finally, $Su = S_0(Iu) = u$ and using the previous results,

$$S^*u = \Delta u = \Delta^{-1}u = \Delta^{-1/2}u = u$$

together with $Ju = J\Delta^{1/2}u = Su = u$. ■

We present the infinite dimensional Tomita-Takesaki theorem.

Theorem 3.4 (Tomita-Takesaki)**.** *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as above. Then, for $t \in \mathbb{R}$,*

$$\Delta^{it}\mathcal{M}\Delta^{-it} = \mathcal{M} \qquad \textit{and} \qquad J\mathcal{M}J = \mathcal{M}'.$$

The proof is given in section 2.5. The first conclusion is no longer true for an arbitrary complex exponent as happened in finite dimension.

Corollary 3.4.1. *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as above. Then, for $t \in \mathbb{R}$, $A \in \mathcal{M} \mapsto J\Delta^{it}A^*\Delta^{-it}J \in \mathcal{M}'$ is an anti-isomorphism preserving involutions.*

Also, theorem 3.4 provide easier proofs for standard results. For example, for a commutative Von Neumann algebra $\mathcal{M} \subset B(H)$ the inclusion $\mathcal{M} \subset \mathcal{M}'$ is usually strict. The algebra $\mathcal{M}$ is *maximally Abelian* if $\mathcal{M} = \mathcal{M}'$.

Proposition 3.6. *Let $\mathcal{M} \subset B(H)$ be a commutative Von Neumann algebra. If $\mathcal{M}$ has a cyclic vector $u \in H$, then it is maximally Abelian.*

Proof. Clearly, $\mathcal{M}u \subset \mathcal{M}'u$. Thus $\mathcal{M}'u$ is dense in H, since u is cyclic for $\mathcal{M}$: u is also cyclic for $\mathcal{M}'$. By proposition 2.5, u is separating for $\mathcal{M}$. We use theorem 3.4 to show the reverse inclusion

$$\mathcal{R}' = J\mathcal{M}J \subset J\mathcal{M}'J = J(J\mathcal{M}J)J = \mathcal{M}.$$

■

From proposition 3.2 we obtain a characterization of algebras with trivial modular pair.

Proposition 3.7. *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as above, with modular pair (Δ, J) and Tomita operator S. Then $\Delta = I$ if and only if, for $A, B \in \mathcal{M}$, $(u, ABu) = (u, BAu)$.*

Proof. For the direct implication, observe that S is an anti-unitary operator, so that $(u, ABu) = (A^*u, Bu) = (S(Bu), S(A^*u)) = (u, BAu)$ for $A, B \in \mathcal{M}$.

Conversely, a calculation shows that $|S(Au)|^2 = |Au|^2$ and thus S is an anti-unitary operator. By uniqueness of the polar decomposition, $S = SI$ hence $S = J$ and $\Delta = I$. ■

For a C^*-algebra $\mathcal{M}$, a *-isomorphism from $\mathcal{M}$ onto itself is a *-*automorphism* of $\mathcal{M}$. The set $\mathrm{Aut}(\mathcal{M})$ of all *-automorphisms on $\mathcal{M}$ is a group: multiplication is given by composition.

Since Δ is an invertible positive operator, the functional calculus for (unbounded) self-adjoint operators implies that $H = \log \Delta$ is self-adjoint, the *modular Hamiltonian* associated to the pair $(\mathcal{M}, u)$. From Stone's theorem, $(e^{iHt})_{t\in\mathbb{R}} = (\Delta^{it})_{t\in\mathbb{R}}$ is a unitary, strongly continuous one-parameter group and hence $(\sigma_t)_{t\in\mathbb{R}}$ is a σ-weakly continuous one-parameter group of *-automorphisms (by theorem 3.4) of $\mathcal{M}$:

$$\sigma_t : \mathcal{M} \mapsto \mathcal{M} \ , \qquad A \mapsto \Delta^{it} A \Delta^{-it}. \tag{3.7}$$

The action σ_t the *modular automorphism group* associated to the pair $(\mathcal{M}, u)$, or, more briefly, the modular group of $\mathcal{M}$.

The modular group σ_t is important in mathematical physics because it can be interpreted as providing a temporal evolution for the self-adjoint elements of $\mathcal{M}$, which represent physical objects, the so called observables of the physical system. We shall see an application in chapter 4.

3.3 Modular Operators in different contexts

We compute the modular operators for three cases. To do this, we provide cyclic separating vectors for each Von Neumann algebra being considered.

3.3.1 Finite group algebras

Let $\mathcal{M}$ be the group algebra of section 2.5 and I be the identity of G. For each $k \in G$, $u = e_k$ is cyclic separating for $\mathcal{M}$, as seen in example 2.11.

We compute the action of the Tomita operator S. For $g \in G$,

$$S(e_g) = S(L_{gk^{-1}}e_k) = L^*_{gk^{-1}}e_k = L_{kg^{-1}}e_k = e_{kg^{-1}k},$$

while for the adjoint S^*, for $g, h \in G$, we see that $S = S^*$:

$$(Se_g, e_h) = \delta_{kg^{-1}k,h} = \delta_{kh^{-1}k,g} = (e_{kh^{-1}k}, e_g) = (Se_h, e_g).$$

Thus, for each $k \in G$ the pair $(\mathcal{M}, e_k)$ is trivial, i.e., $\Delta = S^*S = I$, $J = S$ and the modular group is also trivial. For some cyclic separating vectors, non-commutative Von Neumann algebras may have trivial modular operator Δ.

We next show the modular operator is not trivial for the group algebra $\mathcal{M}$ of $G = S_3$ for the cyclic separating vector $u = e_I + ie_{r_1}$ (see example 2.11). The formula obtained there give rise to the matrix representations of the Tomita and modular operators,

$$S = \begin{pmatrix} 0 & i & 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1+i & i \\ 0 & 0 & 0 & i & -i & 0 \\ 0 & 0 & 0 & 0 & -1+i & 0 \end{pmatrix}, \qquad \Delta = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & -1 & 4 & 1-i \\ 0 & 0 & 0 & 0 & 1+i & 1 \end{pmatrix}.$$

Since $\{I, r_1, r_2\}$ is a commutative subgroup of S_3, the correspondent 3-dimensional subalgebra $\mathrm{span}\{L_I, L_{r_1}, L_{r_2}\} \subset M_n(\mathbb{C})$ is commutative which gives $\Delta = I$ on the correspondent vector subspace $\mathrm{span}\{e_I, e_{r_1}, e_{r_2}\} \subset \mathbb{C}^n$.

Different cyclic separating vectors for the same Von Neumann algebra give in general different modular operators.

3.3.2
Tensor products

Let H and K be n-dimensional Hilbert spaces with bases $\{e_k\}$ and $\{f_k\}$. The set $\{e_i \otimes f_j\}$ is a basis for the tensor product $H \otimes K$. Let $I_K \in B(K)$ be the identity matrix. The tensor product of algebras $\mathcal{M} = B(H) \otimes \mathbb{C}I_K$ acts on $H \otimes K$ through $(A \otimes \lambda I_K)(e_i \otimes f_j) = A(e_i) \otimes \lambda I_K(f_j)$. The operations

$$(A_1 \otimes B_1) \circ (A_2 \otimes B_2) = (A_1 \circ A_2) \otimes (B_1 \circ B_2) \quad \text{and} \quad (A \otimes B)^* = A^* \otimes B^*,$$

are well defined, so that $\mathcal{M}$ is a finite dimensional C^*-algebra, and hence a Von Neumann algebra. Clearly $\mathcal{M}' = (B(H) \otimes \mathbb{C}I_K)' = \mathbb{C}I_H \otimes B(K)$.

We show that the vector $u = \sum_{i=1}^{n} a_i e_i \otimes f_i \in H \otimes K$ with $a_i > 0$ for every i is cyclic separating for $\mathcal{M}$.

To show that u is cyclic, let $A_{ij} \in B(H)$ be the operator that carries e_i into e_j and the other basis vectors to zero. Then

$$(a_j^{-1} A_{ji} \otimes I_K)(\sum_k a_k e_k \otimes f_k) = e_i \otimes f_j.$$

For the separability, let $B \otimes I_K \in \mathcal{M}$ with $(B \otimes I_K)(u) = 0$. Then

$$0 = (B \otimes I_K)(\sum_i a_i e_i \otimes f_i) = \sum_{i,j} a_i B_{ji} e_j \otimes f_i \ ,$$

shows that $B_{ji} = 0$ since $a_i > 0$ for every i.

We compute the action of the Tomita operator S and its adjoint S^*:

$$S(e_i \otimes f_j) = S\left(\left(\frac{A_{ji}}{a_j}\right) u\right) = \left(\frac{A_{ij}}{a_j}\right) u = \frac{a_i}{a_j} e_j \otimes f_i,$$

while $S^*(e_m \otimes f_n) = (a_n/a_m) e_n \otimes f_m$ because

$$(S(e_i \otimes f_j), e_m \otimes f_n) = \frac{a_i}{a_j} \delta_{jm} \delta_{in} = (\frac{a_n}{a_m} e_n \otimes f_m, e_i \otimes f_j).$$

Similar calculations using the action of S and S^*, yields

$$\Delta(e_i \otimes f_j) = \left(\frac{a_i}{a_j}\right)^2 e_i \otimes f_j, \quad J(e_i \otimes f_j) = e_j \otimes f_i.$$

Note that Δ is diagonal: this simplifies the calculation of J, Δ^{it} and the modular group σ_t. Thus, for example,

$$\Delta^{it}(A \otimes I_K)\Delta^{-it}(e_k \otimes f_j) = \sum_m \left(\frac{a_m}{a_k}\right)^{2it} A_{mk} e_m \otimes f_j = (\tilde{A} \otimes I)(e_k \otimes f_j),$$

where $\tilde{A} \in B(H)$ is a matrix with entries $\tilde{A}_{kj} = \left(\frac{a_k}{a_j}\right)^{2it} A_{kj}$. Again, for each $t \in \mathbb{R}$, this relationship is a bijection from $B(H)$ onto itself. From this we deduce that $\Delta^{it} \mathcal{M} \Delta^{-it} = \mathcal{M}$.

The freedom in the choice of $(a_i) > 0$ allows to enlarge the trivial part of Δ. For 4-dimensional vector spaces H and K, $\Delta = I$ on the 4-dimensional vector subspace $\mathrm{span}\{e_k \otimes f_k : k = 1, 2, 3, 4\}$. Furthermore, if

$$\begin{aligned}
a_1 = a_2 \neq a_3 \neq a_4 &\quad \text{then } \Delta = I \text{ in 6 dimensions,}\\
a_1 = a_2 = a_3 \neq a_4 &\quad \text{then } \Delta = I \text{ in 10 dimensions,}\\
a_1 = a_2 = a_3 = a_4 &\quad \text{then } \Delta = I \text{ in all the 16 dimensions.}
\end{aligned}$$

Observe that, while the modular operator changes with these choices of u, the modular conjugation remains the same.

3.3.3 Crossed products

The crossed product of a Von Neumann algebra $\mathcal{M}$ and a group G acting on $\mathcal{M}$ gives rise to a Von Neumann algebra containing copies of $\mathcal{M}$ and G.

We consider a special case. Let $(\Omega, \Sigma, \mathbb{P})$ be a separable measure space with a probability measure $\mathbb{P}$ defined on the Borel σ-algebra Σ. A bijective map $S : \Omega \mapsto \Omega$ is an *automorphism* of $(\Omega, \Sigma, \mathbb{P})$ if, for $W \in \Sigma$,

1. $S(W),\ S^{-1}(W) \in \Sigma$.
2. $\mathbb{P}(W) = 0$ if and only if $\mathbb{P}(S^{-1}(W)) = 0$.

The set $Aut(\Omega, \Sigma, \mathbb{P})$ of automorphisms of Ω is a group under composition. The space $\mathcal{M} = L^\infty(\Omega, \mathbb{P})$ is a commutative Von Neumann algebra with automorphism group $Aut(\mathcal{M})$ consisting of $*$-isomorphisms of $\mathcal{M}$ to itself. For $\alpha \in Aut(\Omega)$, the map $f \mapsto f \circ \alpha$ belongs to $Aut(\mathcal{M})$.

Let G be a group of order n and consider a group action $T : G \mapsto Aut(\Omega)$ which preserves probability, in the sense that $\mathbb{P}(T_g(W)) = \mathbb{P}(W)$ for $W \in \Sigma$ and $g \in G$. This action induces canonically a group action α on $\mathcal{M}$ by

$$\begin{aligned}
\alpha : G &\to Aut(\mathcal{M}), & \alpha_g(f) : \Omega &\to \mathbb{C}\\
g &\mapsto \alpha_g & w &\mapsto f(T_{g^{-1}}(w)).
\end{aligned}$$

We proceed to describe the cross product of G acting by α on $\mathcal{M}$.

Let $H = L^2(\Omega, \mathbb{P}) \oplus \ldots \oplus L^2(\Omega, \mathbb{P})$ (n copies) and $(x_g) \in H$ with components $x_g \in L^2(\Omega, \mathbb{P})$ for $g \in G$. For $f \in \mathcal{M}$ and $h \in G$, we define the operators (the *copies*) $\pi(f), U(h) \in B(H)$ by

$$(\pi(f)x)_g = \alpha_h^{-1}(f)x_g, \qquad (U(h)x)_g = x_{h^{-1}g}.$$

The Von Neumann algebra generated by these operators,

$$\mathcal{M} = W^* \left(\{\pi(f) : f \in L^\infty(\Omega, \mathbb{P})\} \cup \{U(h) : h \in G\}\right) \subset B(H)$$

is the *finite crossed product* of $L^\infty(\Omega, \mathbb{P})$ by G.

It is useful to consider the matrix representations of elements of $\mathcal{M}$. First, note that every operator $B \in B(H)$ can be represented by a matrix with entries $B_{ij} \in B(L^2(\Omega, \mathbb{P}))$. Thus, fix $g, h \in G$ and $(x_m) \in H$, then for any $f \in \mathcal{M}$ and $k \in G$, the matrix entries of $\pi(f)U(k) \in \mathcal{M}$ are

$$B_{gh}(x_m) = P_g \pi(f)U(k)((P_h(x))_m) = \alpha_g^{-1}(f)((P_h x)_{k^{-1}g}) = \alpha_g^{-1}(f)\delta_{k^{-1}g,h}(x_m),$$

where P_g is the projection operator onto the g-th summand $L^2(\Omega, \mathbb{P})$. Adding up, $\pi(f)U(k)$ has matrix entries $B_{gh} = \alpha_g^{-1}(\delta_{k^{-1}g,h}) \in B(L^2(\Omega, \mathbb{P}))$.

Similar calculations show that the matrix entries of $B \in \mathcal{M} \subset B(H)$ are of the form $B_{gh} = \alpha_h^{-1}(E_B(gh^{-1}))$ for some map $E_B : G \mapsto L^\infty(\Omega, \mathbb{P})$: we can generate elements of $\mathcal{M}$ by specifying E_B.

We now compute a cyclic separating vector. Let e be the identity of G and 1 be the constant map $x \in \Omega \mapsto 1$. Consider the vector $u = (u)_g \in H$ with components $u_g = \delta_{g,e} 1 \in L^2(\Omega, \mathbb{P})$.

To check the separability of u, let $B \in \mathcal{M}$ with $Bu = 0$. Thus, for $g \in G$,

$$0 = (Bu)_g = \sum_h B_{gh} u_h = \alpha_h^{-1}(E_B(gh^{-1}))\delta_{h,e} 1 = E_B(g),$$

which implies that $B_{gh} = 0$ and so $B = 0$.

To show that u is cyclic, we approximate $(y)_g \in H$ by an element of $\mathcal{M}u$. Fix $\epsilon > 0$. By the density of $L^\infty(\Omega, \mathbb{P})$ in $L^2(\Omega, \mathbb{P})$, for $g \in G$ we can choose $f_g \in L^\infty(\Omega, \mathbb{P})$ such that $|y_g - f_g|_{L^2} < \epsilon$. Define $B \in \mathcal{M}$ by its matrix entries B_{gh}: the choice $E_B(g) = f_g$ yields the cyclicity,

$$|(y)_g - Bu|_H^2 = \sum_g |y_g - E_B(g)|_{L^2}^2 = \sum_g |y_g - f_g|_{L^2}^2 < n\epsilon^2.$$

We calculate the matrix entries S_{gh} of the Tomita operator. For $B \in \mathcal{M}$,

$$\begin{aligned} (S(Bu))_g &= (B^* u)_g \\ \sum_h S_{gh} E_B(h) &= \sum_h B^*_{gh} u_h = \sum_h \overline{B}_{hg} u_h = \alpha_g^{-1}(\overline{E_B(g^{-1})}), \end{aligned}$$

which implies that $S_{gh} = \delta_{h,g^{-1}} \alpha_g(C(.))$, where C is the complex conjugation.

Thus S is an isometry:

$$\begin{aligned} |S(Bu)|_H^2 &= \sum_g |(S(Bu))_g|_{L^2}^2 = \sum_g |\alpha_g^{-1}(\overline{E_B(g^{-1})})|_{L^2}^2 \\ &= \sum_g |E_B(g^{-1})|_{L^2}^2 = |Bu|_H^2 \end{aligned}$$

and S extends to an anti-unitary operator. By the uniqueness of the polar decomposition $S = SI$, $J = S$ and $\Delta = I$.

3.4 Proof of the Tomita-Takesaki theorem

We have to be careful with operator domains (again, see appendix A.4 for the basic definitions). As usual, $\mathcal{M} \subset B(H)$ is a Von Neumann algebra with cyclic separating vector $u \in H$ and modular pair (Δ, J).

The proof of the following lemma is given at the end of this section.

Lemma 3.5. *Let $\mathcal{M}$ and $u \in H$ as above, and w be a weakly continuous functional on $B(H)$. If $w(J\mathcal{M}'J) = 0$ then $w(\Delta^{it}\mathcal{M}\Delta^{-it}) = 0$ for $t \in \mathbb{R}$.*

The proof of Tomita-Takesaki theorem follows below.

Proof. We first show that, for $t \in \mathbb{R}$,

$$\Delta^{it}\mathcal{M}\Delta^{-it} \subset J\mathcal{M}'J. \tag{3.8}$$

Suppose by contradiction that $\Delta^{it_0}B\Delta^{-it_0} \notin J\mathcal{M}'J$ for $t_0 \in \mathbb{R}$ and $B \in \mathcal{M}$. The linear functional

$$w_0 : J\mathcal{M}'J \oplus \mathbb{C}\ \Delta^{it_0}B\Delta^{-it_0} \to \mathbb{C}, \qquad A + \lambda\Delta^{it_0}B\Delta^{-it_0} \mapsto \lambda$$

is weakly continuous, because $\ker(w_0) = J\mathcal{M}'J$ is weakly closed. Extend w_0 to a weakly continuous functional w in all $B(H)$ by the Hahn-Banach theorem (see theorem 5.3 of [18]). Clearly $w(J\mathcal{M}'J) = 0$ and $w(\Delta^{it_0}B\Delta^{-it_0}) \neq 0$, contradicting lemma 3.5.

Thus eq. (3.8) holds and we take $t = 0$:

$$\mathcal{M} \subset J\mathcal{M}'J. \tag{3.9}$$

We prove the symmetric inclusion

$$\mathcal{M}' \subset J\mathcal{M}J. \tag{3.10}$$

By corollary 2.13.1, u is also cyclic separating for $\mathcal{M}'$ and we identify in $\mathcal{M}'$ facts which we already know about $\mathcal{M}$. Let $\tilde{S}$ and $(\tilde{\Delta}, \tilde{J})$ be the Tomita operator and the modular pair for $(\mathcal{M}', u)$. From proposition 3.4 (1), $\tilde{S} = S^*$ and $(\tilde{S})^* = S$ on $\mathcal{M}'u$ and $\mathcal{M}u$ respectively, and hence $\tilde{\Delta} = (\tilde{S})^*\tilde{S} = SS^* = \Delta^{-1}$ on a dense subset of H.

From proposition 3.5, $\tilde{J}\Delta^{-1/2} = \tilde{J}\tilde{\Delta}^{1/2} = \tilde{S} = S^* = J\Delta^{-1/2}$ on a dense subset of H and hence $\tilde{J} = J$. Therefore, eq. (3.9) applied to $(\mathcal{M}', u)$ implies that $\mathcal{M}' \subset \tilde{J}\mathcal{M}''\tilde{J} = J\mathcal{M}J$. From this it follows that, $\mathcal{M} = J\mathcal{M}'J$ and $\mathcal{M}' = J\mathcal{M}J$ because $J = J^{-1}$.

Using eq. (3.8), $\Delta^{it}\mathcal{M}\Delta^{-it} \subset \mathcal{M}$. The reverse inclusion follows from a by now familiar trick: $\mathcal{M} = \Delta^{it}(\Delta^{i(-t)}\mathcal{M}\Delta^{it})\Delta^{-it} \subset \Delta^{it}\mathcal{M}\Delta^{-it}$. ∎

The rest of the section is devoted to prove the technical results needed to show lemma 3.5.

Let $\mathcal{M} \subset B(H)$ be a Von Neumann algebra and $T : D \subset H \mapsto H$ be an unbounded linear operator. We say that T is *affiliated to* $\mathcal{M}$, denoted by $T\ \eta\ \mathcal{M}$, if TA extends AT for $A \in \mathcal{M}'$, i.e., if T commutes with $A \in \mathcal{M}'$ on D. Said differently, T fails to belong to $\mathcal{M}$ just because it is unbounded.

Lemma 3.6. *Let $T : D \subset H \mapsto H$ be a densely-defined closed operator with polar decomposition $T = UP$. Then $T\ \eta\ \mathcal{M}$ if and only if $U \in \mathcal{M}$ and $P\ \eta\ \mathcal{M}$.*

Proof. Clearly if $U \in \mathcal{M}$ and $P\ \eta\ \mathcal{M}$, then $T\ \eta\ \mathcal{M}$. For the converse, let $V \in \mathcal{M}'$ be unitary and observe that, the assertion: T commutes with V on D, is equivalent to $V^*TV = T$ on D. Using the polar decomposition of T gives $V^*TV = (V^*UV)(V^*PV)$. Thus, $T\eta\mathcal{M}$ if and only if $T = (V^*UV)(V^*PV)$. By the uniqueness of polar decomposition, $V^*UV = U$ and $V^*PV = P$ on D. From this we deduce that $U \in \mathcal{M}$ and $P\eta\mathcal{M}$ because every element of $\mathcal{M}'$ is a linear combination of unitary elements of $\mathcal{M}'$. ∎

The spectral theorem applied to P asserts that if $A \in B(H)$ commutes with P(on D) then A commutes with each spectral projector E of P. Thus, if $P\eta\mathcal{M}$ then $A \in \mathcal{M}'$ commutes with E. Therefore, $E \in \mathcal{M}'' = \mathcal{M}$ and so $\mathcal{M}$ contains all the spectral projectors of P.

Lemma 3.7. *Let $\mathcal{M}$ and $u \in H$ as above. Then for $A \in \mathcal{M}$ and $r > 0$, there exists $A' \in \mathcal{M}'$ such that*

$$A'u = (\Delta^{-1} + rI)^{-1}Au. \tag{3.11}$$

Proof. Let $A \in \mathcal{M}$, $r > 0$ and set $y = (\Delta^{-1} + rI)^{-1}Au$. First, note that

$$y \in \mathrm{Dom}(\Delta^{-1} + rI) = \mathrm{Dom}(\Delta^{-1}) \subset \mathrm{Dom}(S^*)\ .$$

Set $z = S^*y$ and define the linear operators

$$\begin{aligned} Y_0 : \mathcal{M}u &\longrightarrow H \\ Bu &\longrightarrow By \end{aligned} \qquad\qquad \begin{aligned} Z_0 : \mathcal{M}u &\longrightarrow H \\ Bu &\longrightarrow Bz. \end{aligned}$$

A calculation gives $(Y_0(Bu), Cu) = (Bu, Z_0(Cu))$, for $B, C \in \mathcal{M}$, i.e., Y_0^* extends Z_0. This implies that Y_0^* is densely defined, and so Y_0 is closable (see appendix A.4). Let Y be the closure of Y_0.

For $B, C \in \mathcal{M}$, $Y_0 B(Cu) = BCy = BY_0(Cu)$, i.e., Y_0 commutes with the elements of $\mathcal{M}$ on $\mathrm{Dom}(Y_0)$. Since Y is closed, it commutes with elements of $\mathcal{M}$ on $\mathrm{Dom}(Y)$: $Y \;\eta\; \mathcal{M}'$. We claim that Y is bounded, and so $Y \in \mathcal{M}'$. This suffices to prove the lemma:

$$Yu = Y_0(Iu) = Iy = (\Delta^{-1} + rI)^{-1} Au.$$

We now prove the claim. Suppose by contradiction that Y is unbounded and let $Y = UP$ be its polar decomposition. Since the spectrum $\sigma(P)$ is unbounded (otherwise P and hence $Y = UP$ would be bounded), there are positive numbers a and b such that

$$\frac{|A|}{2r^{1/2}} < a < b \quad \text{and} \quad PE \neq 0, \tag{3.12}$$

where $E \in \mathcal{M}$ is the spectral projector of P corresponding to $[a, b]$. Since $Y \;\eta\; \mathcal{M}'$, lemma 3.6 gives $P \;\eta\; \mathcal{M}'$ and $U, E, EP \in \mathcal{M}'$. We now show

$$|A|^2 |Ez|^2 \geq 4ra^2 |Ez|^2. \tag{3.13}$$

Since $z = Z_0 u = Y_0^* u = PU^* u$ and $Au = (\Delta^{-1} + rI)y$, by inverting eq. (3.11),

$$\begin{aligned} |A|^2|Ez|^2 &\geq |AEz|^2 = |AEPU^*u|^2 = |PEU^*Au|^2 = |PEU^*(\Delta^{-1} + rI)y|^2 \\ &\geq |PEU^*\Delta^{-1}y + rPEU^*y|^2 \\ &\geq |PEU^*\Delta^{-1}y + rPEU^*y|^2 - |PEU^*\Delta^{-1}y - rPEU^*y|^2. \end{aligned} \tag{3.14}$$

Use $|x+y|^2 - |x-y|^2 = 4Re(x, y)$ in eq. (3.14) to obtain

$$\begin{aligned} |A|^2|Ez|^2 &\geq 4Re(PEU^*\Delta^{-1}y, rPEU^*y) = 4rRe(\Delta^{-1}y, UEP^2EU^*(Yu)) \\ &= 4rRe(SS^*y, UP^2EU^*(UPu)) = 4rRe(S^*(UP^2EU^*UPu), S^*y) \\ &= 4rRe(PU^*UEP^2U^*u, z) = 4rRe(P^2E(PU^*u), z) \\ &= 4rRe(P^2Ez, z). \end{aligned} \tag{3.15}$$

For the spectral projector E on $[a, b]$ we have $P^2 E \geq a^2 E$, and eq. (3.15) gives eq. (3.13).

Combining eqs. (3.12) and (3.13) yields $Ez = 0$. Thus, for $A \in \mathcal{M}$,

$$0 = AEz = E(Az) = EZ_0(Au) = E(PU^*)Au = PEU^*(Au)$$

and hence $PEU^* = 0$ on H. Finally, $PE = U^*UPE = U^*(PEU^*)^* = 0$ contradicting $PE \neq 0$ from eq. (3.12). ■

Fix $A \in \mathcal{M}$ and $r > 0$. In what follows, $A' = A'(A, r) \in \mathcal{M}$ is defined in the previous lemma, i.e., A, A' and r satisfy eq. (3.11).

Lemma 3.8. *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as usual, $A \in \mathcal{M}$ and $r > 0$. Then, for $x_1, x_2 \in D = Dom(\Delta^{1/2}) \cap \mathrm{Dom}(\Delta^{-1/2})$, $X = JA'^*J$ solves*

$$(Ax_1, x_2) = (X\Delta^{1/2}x_1, \Delta^{-1/2}x_2) + r(X\Delta^{-1/2}x_1, \Delta^{1/2}x_2). \tag{3.16}$$

Proof. We first show eq. (3.16) for $x_1 = B_1'u, x_2 = B_2'u \in \mathcal{M}'u \subset D$.

$$\begin{aligned}
(A(B_1'u), B_2'u) &= (Au, B_1'^*B_2'u) = ((\Delta^{-1} + rI)A'u, B_1'^*B_2'u) \\
&= (SS^*(A'u) + rA'u, B_1'^*B_2'u) \\
&= (SA'^*u, B_1'^*B_2'u) + r(A'u, B_1'^*B_2'u) \\
&= (S^*(B_1'^*B_2'u), A'^*u) + r(B_1'A'u, B_2'u) \\
&= (B_1'u, B_2'A'^*u) + r(S^*(A'^*B_1'^*u), B_2'u) \\
&= (B_1'u, S^*A'S^*B_2'u) + r(S^*A'^*S^*B_1'u, B_2'u).
\end{aligned}$$

Now use $S^* = \Delta^{1/2}J = J\Delta^{-1/2}$ to complete the computation:

$$\begin{aligned}
(A(B_1'u), B_2'u) &= (B_1'u, \Delta^{1/2}JA'J\Delta^{-1/2}B_2'u) + r(\Delta^{1/2}JA'^*J\Delta^{-1/2}B_1'u, B_2'u) \\
&= (JA'^*J\Delta^{1/2}B_1'u, \Delta^{-1/2}B_2'u) + r(JA'^*J\Delta^{-1/2}B_1'u, \Delta^{1/2}B_2'u).
\end{aligned} \tag{3.17}$$

We prove the general case, with $x_1, x_2 \in D$, with a limiting argument. We first show that, for $x \in D$, there exists a sequence (B_n') in $\mathcal{M}'$ such that

$$B_n'u \longrightarrow x, \qquad \Delta^{1/2}B_n'u \longrightarrow \Delta^{1/2}x, \qquad \Delta^{-1/2}B_n'u \longrightarrow \Delta^{-1/2}x. \tag{3.18}$$

Since u is cyclic, for $x \in D$, there exists a sequence (B_n) in $\mathcal{M}$ such that

$$B_n^*u \longrightarrow J\Delta^{-1/2}x + J\Delta^{1/2}x, \quad \text{hence} \quad J(B_n^*u) \longrightarrow \Delta^{-1/2}x + \Delta^{1/2}x.$$

Since $\Delta^{1/2}B_nu = J^2\Delta^{1/2}B_nu = JSB_nu = J(B_n^*u)$, we have

$$\Delta^{1/2}B_nu = J(B_n^*u) \longrightarrow \Delta^{-1/2}x + \Delta^{1/2}x = (\Delta^{-1} + I)\Delta^{1/2}x. \tag{3.19}$$

By lemma 3.7, for $B_n \in \mathcal{M}$, there exists $B_n' \in \mathcal{M}'$ such that

$$B_n'u = (\Delta^{-1} + I)^{-1}B_nu. \tag{3.20}$$

If $t \in [0, 1]$, then $f(z) = z^{-t}(z^{-1} + 1)^{-1}$ is a bounded Borel function for $z \in (0, \infty)$ hence $\Delta^{-t}(\Delta^{-1} + I)^{-1}$ is a bounded operator. Applying this operator to both sides of eq. (3.19) and using eq. (3.20) shows the claim:

$$\Delta^{1/2-t}B_n'u \to \Delta^{1/2-t}x, \qquad t = 0, 1/2, 1. \tag{3.21}$$

Finally approximate $x_1, x_2 \in D$ by sequences of the form above and take limits in eq. (3.17) using eq. (3.18). ■

Lemma 3.9. *Let $\mathcal{M} \subset B(H)$ and $u \in H$ as usual, $A \in \mathcal{M}$ and $r > 0$. Then, for $y_1, y_2 \in H$, $X = JA'^*J$ solves*

$$(Xy_1, y_2) = \int_{\mathbb{R}} \frac{r^{it-1/2}}{e^{\pi t} + e^{-\pi t}} (\Delta^{it} A \Delta^{-it} y_1, y_2)\, dt. \tag{3.22}$$

Roughly speaking, this equation is an inverse of eq. (3.16).

Proof. We first show the result for a bounded Δ, so that $D = H$. By lemma 3.8, for $y_1, y_2 \in H$, $B = JA'^*J$ satisfies eq. (3.16) for $\Delta^{-it}y_1, \Delta^{-it}y_2 \in H$:

$$\begin{aligned}(A\Delta^{-it}y_1, \Delta^{-it}y_2) = \\ (B\Delta^{1/2}\Delta^{-it}y_1, \Delta^{-1/2}\Delta^{-it}y_2) + r(B\Delta^{-1/2}\Delta^{-it}y_1, \Delta^{1/2}\Delta^{-it}y_2)\end{aligned}$$

$$(\Delta^{it}A\Delta^{-it}y_1, y_2) = (\Delta^{-1/2+it}B\Delta^{1/2-it}y_1, y_2) + r(\Delta^{1/2+it}B\Delta^{-1/2-it}y_1, y_2).$$

Using the projection valued measure for Δ, the right side turns into

$$\int\int x^{-1/2+it}y^{1/2-it}d(E_xBE_yy_1, y_2) + r\int\int x^{1/2+it}y^{-1/2-it}d(E_xBE_yy_1, y_2). \tag{3.23}$$

Setting $s = x/y$, from eq. (3.23) we obtain

$$(\Delta^{it}A\Delta^{-it}y_1, y_2) = \int\int s^{it}(s^{-1/2} + rs^{1/2})d(E_xBE_yy_1, y_2). \tag{3.24}$$

Since $(\Delta^{it})_{t\in\mathbb{R}}$ is an unitary strongly continuous one-parameter group, the left side is a bounded Borel function. Integrate eq. (3.24) to get

$$\begin{aligned}\int_{\mathbb{R}} \frac{r^{it-1/2}}{e^{\pi t} + e^{-\pi t}}(\Delta^{it}A\Delta^{-it}y_1, y_2)dt = \\ \int\int d(E_xBE_yy_1, y_2)(s^{-1/2} + rs^{1/2}) \int_{\mathbb{R}} \frac{s^{it}r^{it-1/2}}{e^{\pi t} + e^{-\pi t}}dt.\end{aligned} \tag{3.25}$$

From the residue theorem,

$$\int_{\mathbb{R}} \frac{s^{it}r^{it-1/2}}{e^{\pi t} + e^{-\pi t}}dt = \frac{1}{s^{-1/2} + rs^{1/2}}$$

yielding the result for a bounded Δ:

$$\int_{\mathbb{R}} \frac{r^{it-1/2}}{e^{\pi t} + e^{-\pi t}}(\Delta^{it}A\Delta^{-it}y_1, y_2)dt = \int\int d(E_xBE_yy_1, y_2) = (By_1, y_2). \tag{3.26}$$

We prove the general case. For $n \in \mathbb{N}$, let E_n be the spectral projector of Δ in $[n^{-1}, n]$ and consider the operators E_nBE_n, $E_nAE_n, \Delta_0 = \Delta E_n$, the last one being the restriction of Δ to the subspace $E_n(H)$. For $y_1, y_2 \in H$,

$$E_n y_1, E_n y_2 \;\in\; \mathrm{Dom}(\Delta_0^{1/2}) \cap \mathrm{Dom}(\Delta_0^{-1/2})$$

and hence the operators satisfy eq. (3.16). Since Δ_0 is bounded,

$$(BE_n y_1, E_n y_2) = \int_{\mathbb{R}} \frac{r^{it-1/2}}{e^{\pi t} + e^{-\pi t}} dt (\Delta^{it} A \Delta^{-it} E_n y_1, E_n y_2).$$

The general result follows by dominated convergence, since $E_n \to I$ strongly. $\blacksquare$

We finally prove lemma 3.5.

Proof. Let w be a weakly continuous functional on $B(H)$ with $w(J\mathcal{M}'J) = 0$. Then, there are $x_k, y_k \in H$ such that $w(A) = \sum_{k=1}^{n} (Ax_k, y_k)$ for $A \in \mathcal{M}$. Taking finite sums in eq. (3.22) with $X = JA'^*J$ by lemma 3.9, and setting $k = \log r$ gives

$$0 = w(JA'^*J) = \int_{\mathbb{R}} \frac{r^{it-1/2} w(\Delta^{it} A \Delta^{-it}) dt}{e^{\pi t} + e^{-\pi t}} = r^{-1/2} \int_{\mathbb{R}} e^{ikt} \left(\frac{w(\Delta^{it} A \Delta^{-it})}{e^{\pi t} + e^{-\pi t}} \right) dt.$$

Thus, the function

$$\frac{w(\Delta^{it} A \Delta^{-it})}{e^{\pi t} + e^{-\pi t}}$$

has zero Fourier transform and hence it is identically zero. From this, $w(\Delta^{it} A \Delta^{-it}) = 0$ and $w(\Delta^{it} \mathcal{M} \Delta^{-it}) = 0$. $\blacksquare$

4
KMS states

This chapter presents the main application of Tomita-Takesaki theorem to mathematical physics, the KMS states. We first review basic facts related to positivity in C^*-algebras and introduces the GNS construction. We then introduce the Gibbs states together with a brief introduction to quantum statistical mechanics and KMS states. In Section 3, we consider some properties of states in the the operator algebraic approach of quantum statistical mechanics. KMS states in a abstract setting come up in Section 4. The Takesaki theorem for KMS states is the subject of Section 5. The material is based on [10, 11, 16, 19].

4.1
The GNS construction

Standard examples of C^*-algebras are the C^*-subalgebras of $B(H)$ for a Hilbert space H and $C(K)$, the space of continuous functions on a compact Hausdorff space K, which is the standard model of a commutative C^*-algebra, as seen in theorem 2.8. In this section we describe a *-homomorphism from any C^*-algebra onto a C^*-subalgebra of $B(H)$ for some Hilbert space H, the *GNS construction* after Gelfand, Naimark and Segal.

In this section $\mathcal{M}$ denotes a C^*-algebra.

We first review some elementary facts regarding positivity on a C^*-algebra. The following commutation relation is very convenient.

Proposition 4.1. *Let $a, b \in \mathcal{M}$. Then $\sigma(ab) \setminus \{0\} = \sigma(ba) \setminus \{0\}$.*

Proof. If $\lambda \in \sigma(ab) \setminus \{0\}$, then $c(\lambda e - ab) = (\lambda e - ab)c = e$ for some $c \in \mathcal{M}$, so that $c(ab) = (ab)c$. Thus, $(e + bca)(\lambda e - ba) = \lambda e$ which means that $\lambda \in \sigma(ba) \setminus \{0\}$. Swapping roles, we get $\sigma(ab) \setminus \{0\} = \sigma(ba) \setminus \{0\}$. ■

A self-adjoint element $a \in \mathcal{M}$ is *positive* if $\sigma(a) \subset [0, \infty)$. We denote a positive element by $a \geq 0$ and the set of all positive elements of $\mathcal{M}$ by $\mathcal{M}_+$. A subset $P \subset \mathcal{M}$ is a *cone* if for $\lambda \geq 0$ and each $a, b \in P$, then $\lambda a, a + b \in P$. Recall that $\mathcal{M}_{sa}$ is the set of self-adjoint elements of $\mathcal{M}$.

Proposition 4.2. *Let $a \in \mathcal{M}$.*

1. *$a \geq 0$ if and only if $a \in \mathcal{M}_{sa}$ and $|te - a| \leq t$ for $t \geq |a|$.*

2. *If $a \in \mathcal{M}_{sa}$, then $a = a_+ - a_-$, $a_+a_- = 0$ with $a_+, a_- \in \mathcal{M}_+$.*

3. *$\mathcal{M}_+$ is a closed cone.*

4. *$\mathcal{M}_{sa}$ is partially ordered: $a \geq b$ if $a - b \geq 0$.*

5. *a is positive if and only if $a = b^*b$ for some $b \in \mathcal{M}$.*

Proof. Let $I \in C(\sigma(a))$ be the identity function on $\sigma(a)$.

For (1), note that $\sigma(a) \subset [0, \infty)$ if and only if $|t.1 - I|_\infty \leq t$ for $t \geq |a|$, which is equivalent to $|te - a| \leq t$ for $t \geq |a|$, by the functional calculus.

For (2), for $t \in \sigma(a)$, set $I_\pm(t) = 2^{-1}(|t| \pm t)$ then $I = I_+ - I_-$, $I_+I_- = 0$ with $I_+, I_- \geq 0$. By the continuous functional calculus on a, the result follows.

For (3), take limits of sequences on (1), to obtain the closedness of $\mathcal{M}_+$. Let $a, b \in \mathcal{M}_+$ and $t, s \in \mathbb{R}$ with $t \geq |a|$ and $s \geq |b|$, then $t + s \geq |a + b|$ and $|(t + s)e - (a + b)| \leq |te - a| + |se - b| \leq t + s$ hence $a + b \in \mathcal{M}_+$. The other cone condition is clear.

For (4), if $a \geq b$ and $b \geq a$, then $\sigma(a-b) \subset [0, \infty)$ and $\sigma(b-a) \subset [0, \infty)$. Thus, $\sigma(a - b) = -\sigma(b - a) \subset (-\infty, 0]$ hence $\sigma(a - b) = \{0\}$. Thus, $|a - b| = r(a - b) = 0$. If $a \geq b$ and $b \geq c$, then $a - b \geq 0$ and $b - c \geq 0$ hence $a - c = (a - b) + (b - c) \geq 0$ because $\mathcal{M}_+$ is a cone.

For the direct implication of (5), note that $I = I^{1/2}I^{1/2} = (I^{1/2})^*I^{1/2}$, then $a = (a^{1/2})^*a^{1/2}$ by the functional calculus.

Conversely, by (2), $a = b^*b = a_+ - a_-$. Setting $c = ba_-$, we see that $-c^*c = -a_-b^*ba_- = -a_-(a_+ - a_-)a_- = a_-^3 \geq 0$. Since $\mathcal{M}_+$ is a cone, we have $cc^* = 2(Re^2(c)+Im^2(c))+(-c^*c) \geq 0$ hence $\sigma(cc^*) \subset [0, \infty)$. Excluding $0 \in \mathbb{C}$, we also have $\sigma(cc^*) = \sigma(c^*c) = -\sigma(-c^*c) \subset (-\infty, 0]$ hence $\sigma(cc^*) = \{0\}$. Thus, $|c|^2 = |c^*|^2 = |cc^*| = r(cc^*) = 0$ hence $a_-^2 = (a_- - a_+)a_- = -b^*ba_- = -b^*c = 0$. This implies that $a_- = 0$ and hence $a = a_+ \geq 0$. ■

We also use $a \leq b$ for $b \geq a$. A linear functional $\ell : \mathcal{M} \mapsto \mathbb{C}$ is *positive* if $\ell(a) \geq 0$ for $a \geq 0$. From the definition, we see that ℓ preserves positivity: for $a \geq b$ we have $\ell(a) \geq \ell(b)$. Also, ℓ is *positive definite* if it is positive and $\ell(a) > 0$ for $a \geq 0, a \neq 0$.

Lemma 4.1. *Let ℓ be a positive linear functional on $\mathcal{M}$ and $a, b \in \mathcal{M}$. Then*

1. *ℓ is bounded.*

2. *The map $(a, b) \mapsto \ell(a^*b)$ is a positive semi-definite sesquilinear form.*

3. *$|\ell(a^*b)|^2 \leq \ell(a^*a)\ell(b^*b)$.*

4. *$\ell(e) = |\ell|$.*

5. *$|\ell(b^*ab)| \leq |a|\ell(b^*b)$.*

6. *The set $\mathcal{J}_\ell = \{a \in \mathcal{M} : \ell(a^*a) = 0\}$ is a left ideal.*

Proof. For (1), suppose by contradiction that ℓ is unbounded and take a sequence $(a_n) \in (\mathcal{M})_1$, the unit sphere of $\mathcal{M}$, with $\ell(a_n) > 2^n$ for $n \in \mathbb{N}$. By eq. (2.3) and (2) of proposition 4.2, we assume $a_n \geq 0$. Clearly $a = \sum_{n=1}^{\infty} 2^{-n} a_n \in \mathcal{M}$ and for $n \in \mathbb{N}$, $n \leq \sum_{k=1}^{n} 2^{-k}\ell(a_k) \leq \ell(a)$, a contradiction.

Item (2) is clear and implies (3). For (4), observe that $\ell(e) \leq |\ell|$ and for $a \in (\mathcal{M})_1$, by (3), we have $|\ell(a)|^2 = |\ell(e^*a)|^2 \leq \ell(e)\ell(a^*a) \leq \ell(e)|\ell|$. Taking sups we obtain $|\ell| \leq \ell(e)$.

Item (5) is clear if $\ell(b^*b) = 0$. Thus, suppose that $\ell(b^*b) \neq 0$. The map $a \mapsto v(a) = \ell(b^*b)^{-1}\ell(b^*ab)$ is a positive linear functional on $\mathcal{M}$. By (5), $|v| = 1$ hence $\ell(b^*b)^{-1}|\ell(b^*ab)| \leq |a|$. Item (6) follows from the previous items. ■

From the lemma, positive definite functionals induce inner products.

For a Hilbert space H and a *-homomorphism $\pi : \mathcal{M} \mapsto B(H)$ the pair (H, π) is a *representation* of $\mathcal{M}$. If $u \in H$ is a cyclic vector for the image $\pi(\mathcal{M}) \subset B(H)$, (H, π, u) is a *cyclic representation* of $\mathcal{M}$. We now describe the so-called GNS construction.

Theorem 4.2 (GNS representation)**.** *Given a positive linear functional ℓ on $\mathcal{M}$, there exists a cyclic representation $(H_\ell, \pi_\ell, u_\ell)$ of $\mathcal{M}$, for which $|u_\ell| = |\ell|$ and $\ell(a) = (u_\ell, \pi_\ell(a)u_\ell)$ for $a \in \mathcal{M}$.*

Proof. From lemma 4.1, the quotient space $H = \mathcal{M}/\mathcal{J}_\ell$ admits the inner product $(\tilde{a}, \tilde{b}) \in H \times H \mapsto \ell(a^*b)$, hence its completion H_ℓ is a Hilbert space.

We define $\pi_\ell : \mathcal{M} \mapsto B(H_\ell)$: for $a \in \mathcal{M}$, set $\pi_\ell(a) : H \mapsto H$ by $\pi_\ell(a)(\tilde{b}) = \widetilde{ab}$, a well-defined linear operator on H. Since $|\pi_\ell(a)\tilde{b}|^2 \leq \ell(b^*a^*ab) \leq |\ell||a|^2|\tilde{b}|^2$, π_ℓ extends to a bounded linear operator denoted by same letter on H_ℓ. A direct calculation shows that π_ℓ is a *-homomorphism and hence (H_ℓ, π_ℓ) is a representation of $\mathcal{M}$.

For $u_\ell = \tilde{e} \in H$, we have $\pi_\ell(\mathcal{M})\tilde{e} = H$ so that $(H_\ell, \pi_\ell, u_\ell)$ is a cyclic representation of $\mathcal{M}$. The remaining properties are clear. ■

We refer to $(H_\ell, \pi_\ell, u_\ell)$ as the *GNS-representation* induced by ℓ.

A state $w \in \mathcal{M}$ is a positive functional of norm one. The GNS construction applied to a state w leads to a cyclic representation (H_w, π_w, u_w) with unit cyclic vector, since $|w| = |u| = 1$.

4.2 Gibbs states

An important question in quantum statistical mechanics is the following: given a physical system composed of large number of particles that obey the rules of quantum mechanics, what are the equilibrium states of the system? In this section we shall sketch the physical meaning of the question and introduce the costumary answer: the Gibbs states.

The bulk properties of matter — pressure, temperature, heat capacity, volume — are studied by thermodynamics, which provides laws determining the behavior of these properties when matter is in the so called equilibrium thermodynamic state. Thermodynamics works very well without information of the microscopic structure of matter. The classical and quantum statistical mechanics try to derive the thermodynamic properties from microscopic laws that governs the (classical, quantum) behavior of the particles composing the system. The statistical approach circumvents the difficulties arising from an analytic method having to model a large number of particles.

We sketch the basic procedure of quantum statistical mechanics. Denote by S a physical system enclosed in a finite volume $V \subset \mathbb{R}^3$, composed of n particles obeying the rules of quantum mechanics. To model S, we consider its *state space*, a separable Hilbert space H with the following specifications.

1. The pure physical states of S are represented by unit vectors of H.
2. The physical quantities of the system S that can be measured — the *physical observables* — are represented by self-adjoint operators belonging to $B(H)$, also called observables. The set of all observables is denoted by $\mathcal{O} \subset B(H)$.

An important observable is the *Hamiltonian operator* $\mathcal{H} \in \mathcal{O}$: it encodes the forces acting on the particles of S and generates the time evolution of S. More explicitly, the *time evolution* τ of S is given by

$$\tau : \mathbb{R} \times \mathcal{O} \to \mathcal{O} \qquad (t, A) \mapsto \tau_t(A) = e^{it\mathcal{H}} A e^{-it\mathcal{H}}. \tag{4.1}$$

It is natural to extend τ from $\mathcal{O}$ to $B(H)$.

Proposition 4.3. *The evolution τ of the Hamiltonian $\mathcal{H} \in \mathcal{O}$ is a strongly continuous one-parameter group of automorphisms of $B(H)$.*

Proof. This is a consequence of Stone's theorem: $\mathcal{H}$ is a self-adjoint operator, so that $(e^{it\mathcal{H}})_{t\in\mathbb{R}}$ is a strongly(operator) continuous unitary one-parameter group and clear calculations shows the strongly continuity of the time evolution. ∎

More general physical states, the *ensembles*, are identified with a special class of observables, the *density operators.* A *density operator* $\rho \in B(H)$ is a positive trace-class operator of trace one. An operator $T \in B(H)$ is *trace class* if, for an orthonormal basis $\{e_k\}$ of H , the *trace*

$$\|T\|_1 \;=\; \mathrm{Tr}\,|T| \;=\; \sum_k \Big(\,(T^*T)^{1/2}e_k, e_k\,\Big)$$

is finite. The trace is independent of basis. Trace class operators are compact.

Proposition 4.4. *Every density operator $\rho \in B(H)$ induces a state*

$$w_\rho : B(H) \to \mathbb{R} \qquad A \mapsto \mathrm{Tr}(\rho A). \tag{4.2}$$

Proof. Clearly, $w_\rho \in B(H)^*$ and $w_\rho(I) = 1$. For $A \in B(H)$,

$$w_\rho(A^*A) = \mathrm{Tr}(\rho A^*A) = \mathrm{Tr}(\rho^{1/2}\rho^{1/2}A^*A) = \mathrm{Tr}((A\rho^{1/2})^*(A\rho^{1/2})) \geq 0,$$

so that w_ρ is a positive functional, hence a state. ■

If $A \in \mathcal{O}$, then $w_\rho(A)$ gives the *expected value* of the observable A in the physical state ρ. Physically, if we measure n times the observable A, exactly in the same physical state ρ, we obtain n real numbers $a_1, \ldots, a_n$. The expected value of A in ρ is the usual limit,

$$\lim_{n\to\infty} \frac{a_1 + \ldots + a_n}{n}.$$

For the evolution $\tau_t(A)$, $w_\rho(\tau_t(A))$ describes the corresponding variation of the expected value.
Despite of the abundance of density operators (and hence of physical states), the thermodynamic properties of matter only make sense (and thus can be measured) in the *equilibrium states.* Rather than providing a definition, we list some properties that a physical system S in a equilibrium state ρ should have.

Time Invariance: The expected values of the physical observables should be constant in time in ρ.

Stability: If the system S is disturbed slightly, then S returns smoothly to ρ as the time passes.

Maximal Entropy: The system S should reach the maximal entropy when it is in the state ρ. Entropy should be understood as the number of all possible physical configurations of the particles of the system.

For the system S with Hamiltonian $\mathcal{H}$, we postulate a family of *Gibbs states*, which are equilibrium states ρ_β parameterized by the *inverse tempera-*

ture $\beta \in \mathbb{R}$. The β-Gibbs state is the state w_β induced by the density operator

$$\rho_\beta = \frac{e^{-\beta \mathcal{H}}}{Z} \qquad Z = \operatorname{Tr}(e^{-\beta\mathcal{H}}), \tag{4.3}$$

where Z is the *partition function.*

A way to motivate these states is to consider the principle of maximum entropy. For simplicity, assume that H is finite dimensional.

Definition 4.1. Let ρ_1, ρ_2 be density operators and $\beta \in \mathbb{R}$.

1. The *entropy* $\mathcal{S}$ of a state ρ is defined as $\mathcal{S}(\rho) = -\operatorname{Tr}(\rho \log(\rho))$.

2. The *free energy* F of a state ρ is $F(\rho) = \beta w_\rho(\mathcal{H}) - S(\rho)$.

3. The *entropy* of ρ_1 *relative* to ρ_2 is

$$\mathcal{S}(\rho_1|\rho_2) = -\operatorname{Tr}(\rho_1 \log \rho_1 - \rho_1 \log \rho_2) \tag{4.4}$$

Additionally, we shall need lemma 6.2.21 from [11].

Lemma 4.3. *Let A be a positive $n \times n$ matrix and B a strictly positive matrix. Then*

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

with equality if and only if $A = B$.

We shall see that Gibbs states are characterized by a variational principle: they maximize entropy and minimize free energy. Denote by $E_{\min}$ and $E_{\max}$ the minimum and maximum elements of the spectrum $\sigma(\mathcal{H})$.

Theorem 4.4. *Let H be finite dimensional. If $E \in \sigma(\mathcal{H})$ and $E \in (E_{min}, E_{max})$ then there exists a Gibbs state w_β maximizing entropy and minimizing free energy for which $w_\beta(\mathcal{H}) = E$.*

Proof. We first show that the energy $E = w(\mathcal{H}) \in (E_{\min}, E_{\max})$ for every state w. To see this, write $E_{\min} I < \mathcal{H} < E_{\max} I$. Applying w to this equation gives

$$E_{\min} w(I) < w(\mathcal{H}) < E_{\max} w(I)$$
$$E_{\min} < E < E_{\max}.$$

We now show that for any $E \in (E_{\min}, E_{\max})$ there exists a Gibbs state w_β for which $w_\beta(\mathcal{H}) = E$. We note that

$$
\begin{aligned}
\frac{dE}{d\beta} &= \frac{d}{d\beta} w(\mathcal{H}) = \frac{d}{d\beta}\left(\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H})}{\operatorname{Tr}(e^{-\beta\mathcal{H}})}\right) \\
&= -\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H}^2)\operatorname{Tr}(e^{-\beta\mathcal{H}}) + \operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H})\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H})}{\operatorname{Tr}(e^{-\beta\mathcal{H}})^2} \\
&= -\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H}^2)}{Z} + \left(\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H})}{Z}\right)^2 = -\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H}^2)}{Z} + 2E^2 - E^2 \\
&= -\left[-\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H}^2)}{Z} - 2E\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H})}{Z} + \frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}E^2 I)}{Z}\right] \\
&= -\frac{\operatorname{Tr}\left[e^{-\beta\mathcal{H}}(\mathcal{H}^2 - 2E\mathcal{H} + E^2)\right]}{Z} = -w_\beta\left[(\mathcal{H} - E)^2\right] \leq 0.
\end{aligned}
$$

Thus, E is decreasing with respect to β and strictly decreasing unless $\mathcal{H}$ is constant hence $E = w_\beta(\mathcal{H})$ is injective. Since E depends continuously of β, this relation is actually a bijective correspondence and so for every E there exists w_β such that $w_\beta(\mathcal{H}) = E$.

Also, from lemma 4.3 setting $A = \rho_1$ and $B = \rho_2$ in eq. (4.4) gives

$$\mathcal{S}(\rho_1|\rho_2) \leq \operatorname{Tr}(\rho_1 - \rho_2) = 0.$$

Therefore, the relative entropy is always decreasing. By similar calculations for $\rho_1 = \rho$ and $\rho_2 = \rho_\beta = e^{-\beta\mathcal{H}}/Z$ we obtain

$$
\begin{aligned}
\mathcal{S}(\rho|\rho_\beta) &= -\operatorname{Tr}\left(\rho\log\rho - \rho\log\frac{e^{-\beta\mathcal{H}}}{Z}\right) = -\operatorname{Tr}(\rho\log\rho) + \operatorname{Tr}\left(\rho\log\frac{e^{-\beta\mathcal{H}}}{Z}\right) \\
&= \mathcal{S}(\rho) + \operatorname{Tr}(\rho\log e^{-\beta\mathcal{H}}) + \log Z = S(\rho) - \beta\operatorname{Tr}(\rho\mathcal{H}) + \log\operatorname{Tr}(e^{-\beta\mathcal{H}}) \\
&= \mathcal{S}(\rho) - \beta w_\rho(\mathcal{H}) + \log\operatorname{Tr}(e^{-\beta\mathcal{H}}). \qquad (4.5)
\end{aligned}
$$

While the free energy of the Gibbs state w_β is

$$
\begin{aligned}
F(\rho_\beta) &= \beta w_\beta(\mathcal{H}) + \operatorname{Tr}(\rho_\beta\log\rho_\beta) = \beta w_\beta(\mathcal{H}) + \operatorname{Tr}\left(\frac{e^{-\beta\mathcal{H}}}{Z}\log\frac{e^{-\beta\mathcal{H}}}{Z}\right) \\
&= \beta w_\beta(\mathcal{H}) - \beta\frac{\operatorname{Tr}(e^{-\beta\mathcal{H}}\mathcal{H})}{Z} + \log(\operatorname{Tr}(e^{-\beta\mathcal{H}})) = \log(\operatorname{Tr}(e^{-\beta\mathcal{H}})).
\end{aligned}
$$

From this and eq. (4.5) we deduce that $\mathcal{S}(\rho|\rho_\beta) = -F(\rho) + F(\rho_\beta) \leq 0$ and hence w_β minimizes free energy: $F(\rho_\beta) \leq F(\rho)$. Moreover w_β maximizes entropy:

$$\mathcal{S}(\rho) = \beta w_\rho(\mathcal{H}) - F(\rho) \leq \beta w_\rho(\mathcal{H}) - F(\rho_\beta) = \mathcal{S}(\rho_\beta).$$

■

Frequently $e^{-\beta\mathcal{H}}$ is a trace-class operator, hence compact: for simplicity we suppose so as a hypothesis, so that H admits an orthonormal basis of eigenvectors. By the continuous functional calculus ρ_β is positive since $e^{-\beta t}, \beta \in \mathbb{R}$, is a positive function . Thus, ρ_β is a density operator and w_β is a state on $B(H)$ by proposition 4.4.

Let $\mathcal{M} \subset B(H)$ be a Von Neumann algebra. A state w on $\mathcal{M}$ is *faithful* if $A \in \mathcal{M}_+ \setminus \{0\}$ implies that $w(A) > 0$. Equivalently, w is faithful if $A \in \mathcal{M}_+$ with $w(A) = 0$ implies that $A = 0$.

Finally, a state w is a (τ, β)-*KMS state* if satisfies the *KMS condition*:

$$w_\beta(A\tau_{i\beta}B) = w_\beta(BA), \qquad \text{for } A, B \in B(H), \tag{4.6}$$

where $\tau_{i\beta}$ is obtained setting $t = i\beta$ in eq. (4.1) through the continuous functional calculus for the Hamiltonian $\mathcal{H}$.

Proposition 4.5. *Let w_β be a β-Gibbs state for the physical system S. Then*

1. *For $A \in \mathcal{O}, t \in \mathbb{R}$, $w_\beta(\tau_t(A)) = w_\beta(A)$: w_β is invariant under τ_t.*
2. *w_β is faithful.*
3. *w_β is a (τ, β)-KMS state.*

Proof. From the functional calculus, $e^{-\beta\mathcal{H}}$ and $e^{it\mathcal{H}}$ commute. We prove (1):

$$Zw_\beta(\tau_t(A)) = \mathrm{Tr}(e^{-\beta\mathcal{H}}e^{it\mathcal{H}}Ae^{-it\mathcal{H}}) = \mathrm{Tr}(e^{it\mathcal{H}}e^{-\beta\mathcal{H}}Ae^{-it\mathcal{H}}) = \mathrm{Tr}(e^{-\beta\mathcal{H}}A).$$

To show (2), let $A \geq 0$ with $w_\beta(A) = 0$ and (ψ_n) be the orthonormal basis of eigenvectors of $\mathcal{H}$ with eigenvalues (E_n). Then

$$\begin{aligned} 0 = w_\beta(A) &= \frac{1}{Z}\,\mathrm{Tr}(e^{-\beta\mathcal{H}}A) = \frac{1}{Z}\,\mathrm{Tr}(Ae^{-\beta\mathcal{H}}) \\ &= \sum_{n=1}^{\infty}(\psi_n, Ae^{-\beta\mathcal{H}}\psi_n) = \sum_{n=1}^{\infty}(\psi_n, Ae^{-\beta E_n}\psi_n) = \sum_{n=1}^{\infty} e^{-\beta E_n}(\psi_n, A\psi_n). \end{aligned}$$

Since $A \geq 0$, $|A^{1/2}\psi_n|^2 = (\psi_n, A\psi_n) = 0$ for $n \in \mathbb{N}$. Hence $A^{1/2}$ and A vanish: w_β is faithful.

To see (3), for $A, B \in B(H)$ we have

$$w_\beta(A\tau_{i\beta}B) = \frac{1}{Z}\,\mathrm{Tr}(e^{-\beta\mathcal{H}}Ae^{-\beta\mathcal{H}}Be^{\beta\mathcal{H}}) = \frac{1}{Z}\,\mathrm{Tr}(Ae^{-\beta\mathcal{H}}B) = w_\beta(BA).$$

■

Property (3) was proved by Kubo(1957) and Martin and Schwinger(1959). It is fundamental for the characterization of equilibrium states in general settings, as we shall see in section 3.4, because for a special family of quantum physical systems, the KMS states are equivalent to the Gibbs states. A *finite quantum system* is a system S with finite dimensional state space H.

Proposition 4.6. *Let $\beta \in \mathbb{R}$. Every (τ, β)-KMS state of a finite quantum system S is a β-Gibbs state.*

Proof. Let w be a (τ, β)-KMS state and (ψ_i) be the orthonormal basis of eigenvectors of $\mathcal{H}$ with eigenvalues (E_i). The rank one operators

$$\psi_i \otimes \psi_j : \mathbb{C}^n \to \mathbb{C}^n \qquad v \mapsto (\psi_j, v)\psi_i,$$

satisfy $(\psi_i \otimes \psi_k)(\psi_k \otimes \psi_j) = \psi_i \otimes \psi_j$. Using the KMS condition,

$$\begin{aligned} &w(\psi_i \otimes \psi_j)) = w((\psi_i \otimes \psi_k)(\psi_k \otimes \psi_j)) = w((\psi_k \otimes \psi_j)e^{-\beta\mathcal{H}}(\psi_i \otimes \psi_k)e^{\beta\mathcal{H}}) \\ &= w((\psi_k \otimes \psi_j)e^{-\beta E_i}(\psi_i \otimes \psi_k)e^{\beta E_k}) = e^{-\beta E_i}e^{\beta E_k}w((\psi_k \otimes \psi_j)(\psi_i \otimes \psi_k) \\ &= e^{\beta E_k}e^{-\beta E_i}\delta_{ij}w((\psi_k \otimes \psi_k)). \end{aligned}$$

Summing over k,

$$\sum_k e^{-\beta E_k} w(\psi_i \otimes \psi_j) = e^{-\beta E_i}\delta_{ij}\sum_k w(\psi_k \otimes \psi_k) = e^{-\beta E_i}\delta_{ij}w(I) = e^{-\beta E_i}\delta_{ij}.$$

Since $Z = \mathrm{Tr}(e^{-\beta\mathcal{H}}) = \sum_k e^{-\beta E_k}$, we obtain $w(\psi_i \otimes \psi_j) = e^{-\beta E_i}\delta_{ij}/Z$.

We now turn to the general case. Write $A \in B(H)$ as $A = \sum_{i,j} A_{ij}\psi_i \otimes \psi_j$ with $A_{ij} = (\psi_i, A\psi_j)$ and recall that ρ_β has the matrix representation $e^{-\beta E_i}\delta_{ij}$ on the basis $\{\psi_n\}$. Then

$$w(A) = \sum_{i,j} A_{ij}w(\psi_i \otimes \psi_j) = \frac{1}{Z}\sum_j\sum_i (e^{-\beta E_i}\delta_{ji})A_{ij} = \frac{1}{Z}\,\mathrm{Tr}(\rho_\beta A),$$

so that w is a β-Gibbs state. ■

Abstracting some of the facts above we are led to the algebraic approach of quantum statistical mechanics. For a physical system S and a separable Hilbert space H, we require the following axioms.

Axiom 1: The physical observables of S are represented by the self-adjoint elements of a Von Neumann algebra $\mathcal{M} \subset B(H)$.

Axiom 2: The physical states of S are represented by normal states on $\mathcal{M}$, to be defined in the next section.

Axiom 3: The expected value of an observable $A \in \mathcal{M}$ in the state w is given by $w(A)$.

Axiom 4: The time evolution of S is given by a σ-weakly continuous one-parameter group τ of automorphisms of $\mathcal{M}$.

Finally, there is an axiom concerning physical symmetries that we omit, since we do not use it in the sequel.

4.3 Normal states

In this section, we define normal states and show that they are equivalent to states induced by density operators. As a consequence, we obtain interesting properties about *-homomorphisms between Von Neumann algebras.

Let $\mathcal{T}(H)$ be the set of trace class operators of H. The norm given by the trace converts $\mathcal{T}(H)$ into a Banach space. We quote theorem 6.26 of [18].

Proposition 4.7. *The following facts are true.*

1. *$B(H)$ is the dual of $\mathcal{T}(H)$ under the map*

$$\phi : B(H) \to (\mathcal{T}(H))^* \qquad A \mapsto \phi(A)(\rho) = \mathrm{Tr}(\rho A),\ \ \rho \in \mathcal{T}(H).$$

2. *The weak* and σ-weak topology on $B(H)$ coincide.*

3. *For a σ-weakly continuous functional w on $B(H)$, there is $\rho \in \mathcal{T}(H)$ such that $w(A) = \mathrm{Tr}(\rho A)$, for $A \in B(H)$.*

We extend the well known fact that the commutative Von Neumann algebra $L^\infty(K, \mu)$ is the dual space of $L^1(K, \mu)$ for some compact Hausdorff space K with finite positive Borel measure μ.

Definition 4.2. The *predual* of a Von Neumann algebra $\mathcal{M}$ is the set $\mathcal{M}_*$ of linear functionals on $\mathcal{M}$, which are σ-weakly continuous on the unit ball $\mathcal{M}_1$.

In this section, $\mathcal{M} \subset B(H)$ is a Von Neumann algebra.

Proposition 4.8. *The predual $\mathcal{M}_*$ is a uniformly closed subspace of $\mathcal{M}^*$. The dual of $\mathcal{M}_*$ is $\mathcal{M}$.*

Proof. First, note that $\mathcal{M}_1 = \mathcal{M} \cap B(H)_1$ is weakly compact because $B(H)_1$ is and $\mathcal{M}_1$ is σ-weakly compact because it is bounded. Therefore, if $w \in \mathcal{M}_*$, then $w(\mathcal{M}_1) \subset \mathbb{C}$ is compact, hence bounded. This implies that $w \in \mathcal{M}^*$ and hence $\mathcal{M}_* \subset \mathcal{M}^*$.

We now show that $\mathcal{M}_*$ is uniformly closed. Let $w_n \in \mathcal{R}_* \to w$ uniformly and $A_m \in \mathcal{M}_1 \to A$ σ-weakly. We must show that $w(A_m) \to w(A)$ uniformly, so that $w \in \mathcal{M}_*$. Indeed, if $m, n \to \infty$

$$\begin{aligned}|w(A) - w(A_m)| &\leq |w(A) - w_n(A)| + |w_n(A) - w_n(A_m)| + |w_n(A_m) - w(A_m)| \\ &\leq 2|w - w_n| + |w_n(A) - w_n(A_m)| \to 0,\end{aligned}$$

since each w_n is σ-weakly continuous on $\mathcal{M}_1$.

To prove the duality, consider $J : \mathcal{M} \to (\mathcal{M}_*)^*$ defined for $A \in \mathcal{M}$ by

$$J(A) : \mathcal{M}_* \subset \mathcal{M}^* \to \mathbb{C} \qquad w \mapsto w(A).$$

We first show that J is an isometry, and hence injective. Denote by $|.|_1$ the norm on $(\mathcal{M}_*)^*$. Then $|J(A)|_1 = \sup_{w\in(\mathcal{R}_*)_1} |J(A)w| \le \sup_{w\in(\mathcal{R}_*)_1} |w||A| = |A|$, for $A \in \mathcal{M}$. To see the reverse inequality, take $x, y \in H$ and define

$$w_{x,y} : \mathcal{M} \to \mathbb{C} \qquad A \mapsto (y, Ax) \ .$$

Clearly $w_{x,y} \in \mathcal{M}_*$ and $w_{x,y} \in (\mathcal{R}_*)_1$ if $|x| = |y| = 1$, and thus

$$|A| = \sup_{|x|=|y|=1} |(x, Ay)| = \sup_{w_{x,y}\in(\mathcal{R}_*)_1} |w_{x,y}(A)| \le \sup_{w\in(\mathcal{R}_*)_1} |J(A)w| = |J(A)|_1.$$

It remains to prove that J is surjective. For $\phi \in (\mathcal{M}_*)^*$,

$$\phi(w_{(\cdot,\cdot)}) : H \times H \to \mathbb{C} \qquad (x, y) \mapsto \phi(w_{x,y})$$

is a sesquilinear form on H, hence $\phi(w_{x,y}) = (y, Ax)$ for some $A \in B(H)$. Actually, $A \in \mathcal{M}$. Indeed, for $A' \in \mathcal{M}'$ self-adjoint, $w_{A'x,y} = w_{x,A'y}$ and

$$(y, AA'x) = \phi(w_{A'x,y}) = \phi(w_{x,A'y}) = (A'y, Ax) = (y, A'Ax).$$

Hence A commutes with $\mathcal{M}'$ and $A \in \mathcal{M}'' = \mathcal{M}$, since each element in $\mathcal{M}'$ is a complex linear combination of self-adjoint elements(eq. (2.3)). Thus $\phi(w_{x,y}) = (y, Ax) = J(A)(w_{x,y})$, i.e., $\phi = J(A)$ on the subspace $F = \{w_{x,y} \in \mathcal{M}_* : x, y \in H\}$. Recall(appendix A.1) that $w \in \mathcal{M}_*$ has the form $w = \sum_{n=1}^{\infty} w_{x_n,y_n}$ for sequences $(x_n), (y_n) \in H$ with $\sum_n |x_n|^2$ and $\sum_n |y_n|^2$ finite. Therefore F is dense in $\mathcal{M}_*$ and $\phi = J(A)$: J is surjective. ■

A net $(A_j)_{j\in J} \in \mathcal{M}_+$ is *increasing* if for $j, k \in J$ with $j \le k$, then $A_j \le A_k$. It is *bounded* in $\mathcal{M}_+$ if there is $B \in \mathcal{M}_+$ such that $A_j \le B$ for every j: in this case, B is an *upper bound* for (A_j). An upper bound $C \in \mathcal{M}_+$ for (A_j), is the *supremum* $\sup_j A_j$ of (A_j), if for every upper bound B for (A_j), we have $C \le B$.

Lemma 4.5. *Let $(A_j) \in \mathcal{M}_+$ be an increasing net with an upper bound in $\mathcal{M}_+$. Then (A_j) has a supremum $A \in \mathcal{M}_+$ and $A_j \to A$ σ-weakly.*

Proof. For each $i \in J$, let S_i be the weak closure of $\{A_j : j > i\}$. Since (A_i) has an upper bound, we see that S_i is bounded. The balls of $\mathcal{M}$ are weakly compact and each S_i is weakly closed, hence S_i is weakly compact. Thus, there exists $A \in \cap_{i\in J} S_i$ such that for $i \in J$, $A_i \leq A$, $A \in S_i$ and $A = w - \lim A_i$. Moreover it is easy to see that $A = \sup_i(A_i)$. Finally, $A_i \to A$ strongly hence weakly (and hence σ-weakly since the weak and σ-weak topologies coincide in bounded sets), because

$$|(A - A_i)x|^2 = |(A - A_i)^{1/2}(A - A_i)^{1/2}x|^2 \leq 2|A|((A - A_i)x, x) \to 0 \ .$$

∎

A positive linear functional $w \in \mathcal{M}$ is *normal* if for every bounded increasing net $(A_j) \in \mathcal{M}_+$, $w(\sup_j A_j) = \sup_j w(A_j)$.

Theorem 4.6. *Let $w \in \mathcal{M}$. The following conditions are equivalent.*

1. *w is normal.*

2. *w is σ-weakly continuous.*

3. *There is a density operator ρ such that $w(A) = \mathrm{Tr}(\rho A)$ for $A \in \mathcal{M}$.*

Proof. For (1)⇒(2), see theorem 2.4.21 of [10]. For the converse, let (A_j) be a bounded increasing net in $\mathcal{M}_+$. Then $A_j \to A = \sup_j A_j$ σ-weakly hence $w(A_j) \to w(A)$ uniformly. Thus $w(A) = \sup_j w(A_j)$ and w is normal.

For (3)⇒(2), extend w to $B(H)$, and by (2) of proposition 4.7, w is σ-weakly continuous. Similarly, for (2)⇒(3), the extended state w satisfies (3) by item (3) of proposition 4.7. ∎

We present some applications. The first is yet another context in which order relates to topology.

Lemma 4.7. *Let $\phi : \mathcal{M}_1 \mapsto \mathcal{M}_2$ be a *-homomorphism between Von Neumann algebras. If for a normal state w on $\mathcal{M}_2$, $w \circ \phi$ is a normal state on $\mathcal{M}_1$, then ϕ is σ-weakly continuous.*

Proof. A σ-weakly continuous functional $w \in \mathcal{M}_2^*$ is a linear combination of σ-weakly continuous states, hence a linear combination of normal states. From the hypothesis, $w \circ \phi$ is a linear combination of normal states on $\mathcal{M}_1$, i.e., $w \circ \phi \in \mathcal{M}_1^*$ is a σ-weakly continuous functional. ∎

By proposition 2.3, a *-homomorphism ϕ between Von Neumann algebras preserves positivity and hence order. Thus, if (A_j) is a bounded increasing net in $(\mathcal{M}_1)_+$, so is $(\phi(A_j))$ in $(\mathcal{M}_2)_+$. Also, from corollary 2.4.1, *-homomorphisms between C^*-algebras are uniformly continuous.

Theorem 4.8. *Let $\phi : \mathcal{M}_1 \subset B(H_1) \mapsto \mathcal{M}_2 \subset B(H_2)$ be a surjective *-homomorphism between Von Neumann algebras. Then ϕ is σ-weakly and strongly continuous. In particular, *-isomorphisms are homeomorphisms in the σ-weak and strong topologies.*

Proof. We first show σ-weak continuity. Let w be a normal state on $\mathcal{M}_2$ and (A_j) be a bounded increasing net in $(\mathcal{M}_1)_+$. Since ϕ is surjective, a computation with the order relations gives $\phi(\sup_j A_j) = \sup_j \phi(A_j)$. By the normality of w, $w(\phi(\sup_j A_j)) = \sup_j w(\phi(A_j))$, i.e., $w \circ \phi$ is a normal state of $\mathcal{M}_1$. Thus ϕ is σ-weakly continuous by lemma 4.7.

Strong continuity will follow from σ-weak continuity. First notice that, for each net $(A_j) \in \mathcal{M}_1$, $|A_j x|^2 = (A_j^* A_j x, x)$, for $x \in H_1$: $A_j \to 0$ strongly if and only if $A_j^* A_j \to 0$ weakly. From the previous paragraph, $\phi(A_j)^*\phi(A_j) \to 0$ weakly, and hence $\phi(A_j) \to 0$ strongly. Therefore, ϕ is strongly continuous. ■

Let $\mathcal{J}$ be a right ideal of a C^*-algebra $\mathcal{M}$. An increasing net (E_j) in $\mathcal{J}_+ \cap \mathcal{J}_1$ is an *approximate identity* of $\mathcal{J}$ if $E_j A \to A$ uniformly, for $A \in \mathcal{J}$. From proposition 2.2.18 of [10], every right ideal $\mathcal{J}$ has an approximate identity.

Lemma 4.9. *Let $\mathcal{M} \subset B(H_1)$ be a Von Neumann algebra and $\phi : \mathcal{M} \mapsto B(H_2)$ be a σ-weakly continuous *-homomorphism. Then there exists a projection $E \in \mathcal{Z}(\mathcal{M})$ (the center of $\mathcal{M}$) such that the restriction map $\phi : \mathcal{M}E \mapsto \phi(\mathcal{M})$ is a *-isomorphism and $\phi(\mathcal{M}(I-E)) = 0$.*

Proof. Suppose for the moment the following claim: $\ker\phi$ is closed by taking adjoints. Let (F_j) be an approximate identity of (the right ideal) $\ker\phi$, and set $F = \sup_j F_j \in (\ker\phi)_+$. For $A \in \ker\phi$, $F_j A^* \to FA^* = A^*$ uniformly because multiplication is weakly continuous. Thus $AF_j \to AF = A$, since taking adjoints is an isometry. Similarly $FA = A$ and $F^2 = F$: said differently, F is a projection onto $\ker\phi$. Moreover, for $A \in \mathcal{M}$,

$$AF = (AF)F = F(AF) = (FA)F = FA,$$

so that $F \in \mathcal{Z}(\mathcal{M})$. Clearly $\ker\phi = (\ker\phi)F \subset \mathcal{M}F \subset \ker\phi$ and $\ker\phi = \mathcal{M}F$. Also $E = I - F \in \mathcal{Z}(\mathcal{M})$ is a projection and $\mathcal{M} = \ker\phi \oplus \mathcal{M}E$, and thus the restriction $\phi : \mathcal{M}E \mapsto \phi(\mathcal{M})$ is a *-isomorphism together with $\phi(\mathcal{M}(I-E)) = 0$.

We now prove the claim. First, observe that $\ker\phi$ is a σ-weakly closed two-sided ideal since ϕ is σ-weakly continuous. Let $A \in \ker\phi$ with polar decomposition $U(A^*A)^{1/2}$ then $A^*A, (A^*A)^{1/2} \in \ker\phi$ and so does $A^* = (A^*A)^{1/2}U^*$. Therefore, $\ker\phi$ is closed under adjoints. ■

From section 3.1, a positive linear functional w on a Von Neumann algebra (hence a C^*-algebra) $\mathcal{M}$ induces a cyclic representation (H, π, w) for which the image $\pi(\mathcal{M})$ is a C^*-algebra (hence uniformly closed), however it is not necessarily a Von Neumann algebra. The normality of w does it.

Theorem 4.10. *Let w be a normal state on the Von Neumann algebra $\mathcal{M} \subset B(H)$ and (H_w, π, w) be the GNS-representation of w. Then, the image $\pi(\mathcal{M})$ is a Von Neumann algebra.*

Proof. We first show that π is σ-weakly continuous. For a bounded increasing net $(A_j) \in \mathcal{M}_+$ with $A = \sup_j A_j$, $(B^* A_i B)$ is also a bounded increasing net with $\sup_j B^* A_j B = B^* A B$, for $B \in \mathcal{M}$. Since w is normal,

$$(\pi(B)u, \pi(A)\pi(B)u) = w(B^* A B)$$

$$= \sup_j w(B^* A_j B) = (\pi(B)u, \sup_j \pi(A_j)\pi(B)u).$$

Thus $\pi(A) = \sup_j \pi(A_j)$ since $\pi(\mathcal{M})u$ is dense in H_w. Since w is a normal state on $B(H_w)$, $w \circ \pi$ is a normal state on $\mathcal{M}_1$ and $\pi : \mathcal{M}_1 \mapsto B(H_w)$ is σ-weakly continuous by lemma 4.7.

By lemma 4.9, there is a projection $E \in \mathcal{Z}(\mathcal{M})$ such that $\pi : \mathcal{M}E \mapsto \pi(\mathcal{M})$ is a *-isomorphism, hence an isometry. Since $\mathcal{M}_1$ is weakly compact and π is weakly continuous, $(\pi(\mathcal{M}))_1$ is weakly closed. Now use theorem 2.12 to see that $\pi(\mathcal{M})$ is weakly closed and thus $\pi(\mathcal{M})$ is a Von Neumann algebra. ■

4.4
KMS states

In section 3.2 Gibbs states were defined as the equilibrium states for a physical system of n particles in a finite volume $V \subset \mathbb{R}^3$. A real system has something like 10^{23} particles and a large volume: going to infinity is a reasonable approximation of it. An *infinite system* is a limiting situation in which the number of particles and volume increase but keep a finite particle density n/V. What are the equilibrium states of an infinite system? Here we introduce the operator algebraic answer: the KMS states.

In order to be of any use, the limiting process has to apply to observables, in particular equilibrium states. The resulting system, consisting of states and observables, is the *thermodynamic limit* of the (finite) system.

The algebraic approach, instead, describes its axioms for the infinite system directly. For the infinite system S, we model the physical observables by the self-adjoint elements of a Von Neumann algebra $\mathcal{M} \subset B(H)$, the physical states by normal states w on $\mathcal{M}$, the time evolution by a σ-weakly continuous one-parameter group τ of *-automorphisms of $\mathcal{M}$ and the expected value of the observable $A \in \mathcal{M}$ in the state w by $w(A)$.

By proposition 4.6, the equilibrium states of finite quantum systems are exactly the KMS states on $B(H)$. By analogy, we later define the KMS states on $\mathcal{M}$ as the equilibrium states of the infinite system.

Let $\mathcal{M}$ be a Von Neumann algebra and τ be a σ-weakly continuous one-parameter group of *-automorphisms of $\mathcal{M}$. The pair $(\mathcal{M}, \tau)$ is called a *W^*-dynamical system.* We refer to τ as the *time evolution* of $\mathcal{M}$.

In section 3.2, the time evolution $\tau_t = e^{it\mathcal{H}}(\cdot)e^{-it\mathcal{H}}$ extended analytically from $t \in \mathbb{R}$ to $z \in \mathbb{C}$. For an arbitrary time evolution τ on $\mathcal{M}$, this is not necessarily true. This is a problem: $\tau_{i\beta}$ for $\beta \in \mathbb{R}$ appears in the KMS condition(eq. (4.6)). We are interested in elements $A \in \mathcal{M}$ for which this analytic extension is possible.

Let $(\mathcal{M}, \tau)$ be a W^*-dynamical system. An element $A \in \mathcal{M}$ is *τ-analytic* if there are $s > 0$ and $f : \mathbb{R} \times (-s, s)i \subset \mathbb{C} \mapsto \mathcal{M}$ such that

1. $f(z) = \tau_z(A) \in \mathcal{M}$ is well defined in the strip $z \in \mathbb{R} \times (-s, s)i$.

2. (Weak analyticity) $\ell \circ f$ is analytic for $\ell \in \mathcal{M}_*$.

Thus, the map $t \in \mathbb{R} \mapsto \tau_t(A) \in \mathcal{M}$ is extended from $\mathbb{R}$ to $\mathbb{R} \times (-s, s)$ for τ-analytic elements. Condition 2 is actually equivalent to strong analyticity. We will frequently prove weak analiticity and then use properties of strong analyticity. Thus, by analytic continuation, $\tau_{z+w} = \tau_z\tau_w$. When f is defined in $\mathbb{C}$, A is a *τ-entire* element. The set of all τ-entire elements of $\mathcal{M}$ is $\mathcal{M}_\tau$.
We now approximate $A \in \mathcal{M}$ by τ-entire elements in the σ-weak topology.

Lemma 4.11. *Let $(\mathcal{M}, \tau)$ be a W^*-dynamical system and μ be a Borel measure of bounded variation on $\mathbb{R}$. Then for $A \in \mathcal{M}$ there exists $B \in \mathcal{M}$ such that*

$$\ell(B) = \int \ell(\tau_t A)d\mu(t) \quad \text{for } \ell \in \mathcal{M}_*.$$

Proof. For $\ell \in \mathcal{M}_*$, the function $\ell \mapsto \int \ell(\tau_t A)d\mu(t)$ is a bounded linear functional on $\mathcal{M}_*$: $|\int \ell(\tau_t A)d\mu(t)| \leq |\ell||A||\mu|$. Hence

$$\ell(B) = \int \ell(\tau_t A)d\mu(t)$$

for some $B \in (\mathcal{M}_*)^* = \mathcal{M}$. ■

We express the relationship between A and B by

$$B = \int \tau_t(A)d\mu(t).$$

Proposition 4.9. *The set of τ-entire elements $\mathcal{M}_\tau$ is σ-weakly dense in $\mathcal{M}$.*

Proof. For $A \in \mathcal{M}$ we obtain a sequence of elements $(A_n) \in \mathcal{M}_\tau$ which we then show to converge σ-weakly to A. By lemma 4.11, the map

$$z \in \mathbb{C} \mapsto f_n(z) = \sqrt{\frac{n}{\pi}} \int \tau_t(A) e^{-n(t-z)^2} dt \in \mathcal{M}$$

is well defined, since $t \mapsto e^{-n(t-z)^2} \in L^1(\mathbb{R})$. Moreover, for $\ell \in \mathcal{M}_*$, $|\ell(\tau_t(A))| \leq |\ell||A|$. By dominated convergence, the integral differentiation commute,

$$\frac{d}{dz}\ell(f_n(z)) = \sqrt{\frac{n}{\pi}} \int \ell(\tau_t(A)) \frac{d}{dz}(e^{-n(t-z)^2}) dt,$$

so that $\ell \circ f_n$ is entire. Define

$$A_n = \sqrt{\frac{n}{\pi}} \int \tau_t(A) e^{-nt^2} dt.$$

For $z = s \in \mathbb{R}$,

$$f_n(s) = \sqrt{\frac{n}{\pi}} \int \tau_{s+u}(A) e^{-nu^2} du = \tau_s \left(\sqrt{\frac{n}{\pi}} \int \tau_u(A) e^{-nu^2} du \right) = \tau_s(A_n),$$

i.e., A_n is a τ-entire element. Moreover,

$$|A_n| \leq \sup_{t \in \mathbb{R}} |\tau_t(A)| \sqrt{\frac{n}{\pi}} \int e^{-nt^2} dt \leq |A|.$$

We show that $A_n \to A$ σ-weakly. For a σ-weakly continuous functional $\ell \in \mathcal{M}_*$,

$$\ell(A_n - A) = \sqrt{\frac{n}{\pi}} \int [\ell(\tau_t A) - \ell(A)] e^{-nt^2} dt. \tag{4.7}$$

For $|t| \leq \delta$ we have $|\ell(\tau_t(A)) - \ell(\tau_0(A))| \leq 2^{-1}\epsilon$ since τ is σ-weakly continuous and if additionally N is large enough,

$$\sqrt{\frac{N}{\pi}} \int_{|t|>\delta} e^{-Nt^2} dt \leq \frac{\epsilon}{4|\ell||A|}.$$

Thus, by eq. (4.7), for $n > N$,

$$|\ell(A_n - A)| \leq \frac{\epsilon}{2} \sqrt{\frac{n}{\pi}} \int_{|t|\leq\delta} e^{-nt^2} dt + 2|\ell||A| \sqrt{\frac{n}{\pi}} \int_{|t|>\delta} e^{-nt^2} dt \leq \epsilon\ ,$$

i.e., $A_n \to A$ σ-weakly and $\mathcal{M}_\tau$ is σ-weakly dense in $\mathcal{M}$. ■

Let $(\mathcal{M}, \tau)$ be a W^*-dynamical system and $\beta \in \mathbb{R}$. A normal state w on $\mathcal{M}$ is a (τ, β)-*KMS state* if for $A, B \in \mathcal{M}_\tau$,

$$w(AB) = w(B\tau_{i\beta}(A)). \tag{4.8}$$

A $(\tau, -1)$-KMS state is a *τ-KMS state*. This special choice relates to the Tomita-Takesaki theory in the next section.

As in section 3.2, an equilibrium state w is labeled by β, the inverse temperature. But now we do not have a given family of equilibrium states. An important and difficult problem is to find all the equilibrium states of a W^*-dynamical system $(\mathcal{M}, \tau)$.

Just for mention, the most interesting and important problem in statistical mechanics are the *phase transitions*. For example, if we reduce the pressure of a confined liquid at fixed temperature then at certain critical pressure the liquid vaporizes and slight variations around this critical value produces different equilibrium states or *phases*, i.e., mixtures of vapor and liquid can coexist and large changes in thermodynamic properties such as: density, specific heat, entropy, etc. occur. From theoretical viewpoint, thermodynamic properties vary sharply with pressure at those critical points. Thus, in the finite volume physical system, these quantities vary rapidly which in the thermodynamic limit appear as sharp discontinuities of the thermodynamic properties. These discontinuities are sometimes cited as justification of the thermodynamic limit.

We may assume that w is a τ-KMS state by rescaling the time evolution τ: set $\tilde{\tau}_t = \tau_{-\beta t}$ and w is a (τ, β)-KMS state if and only if it is a $\tilde{\tau}$-KMS state.

We now show that (τ, β)-KMS states exhibit the time invariance property.

Proposition 4.10. *Let $(\mathcal{M}, \tau)$ be a W^*-dynamical system and w be a (τ, β)-KMS state with $\beta \neq 0$. Then $w(\tau_t A) = w(A)$ for $A \in \mathcal{M}$ and $t \in \mathbb{R}$.*

Proof. By rescaling we assume $\beta = -1$. We first show time invariance for τ-entire elements. For $A \in \mathcal{M}_\tau$, recall the entire function $f : \mathbb{C} \mapsto \mathcal{M}, f(z) = \tau_z(A)$. Then $w \circ f$ is entire, since $w \in \mathcal{M}^*$. For the identity operator $I \in \mathcal{M}$ and $z \in \mathbb{C}$, by the KMS condition (eq. (4.8)), $w \circ f$ is periodic with period i:

$$w(f(z - i)) = w(I\tau_{-i}(\tau_z A)) = w((\tau_z A)I) = w(f(z)) \ .$$

Moreover, $w \circ f$ is bounded on the strip $\mathbb{R} \times [-1, 0]$:

$$|w(f(z))| \leq |\tau_{\mathrm{Re}\, z}\tau_{i\,\mathrm{Im}\, z}A| \leq |\tau_{i\,\mathrm{Im}\, z}A| \leq M.$$

From the periodicity, $w \circ f$ is bounded on $\mathbb{C}$, hence a constant, by Liouville's theorem. Time invariance then follows: $w(\tau_t(A)) = w(f(t)) = w(f(0)) = w(A)$.

Time invariance for arbitrary elements of $\mathcal{M}$ follows from an approximation argument. For $A \in \mathcal{M}$, by proposition 4.9, there is a sequence (A_n) in

$\mathcal{M}_\tau$ with $A_n \to A$ σ-weakly. Since τ and w are σ-weakly continuous,

$$w(\tau_t(A)) = w(\tau_t(\lim_n A_n)) = \lim_n w(\tau_t(A_n)) = \lim_n w(A_n) = w(A)$$

and the proof is complete. ■

The definition of KMS states in terms σ-weakly density on $\mathcal{M}$ is harder to handle when unbounded operators are involved. We provide an alternative characterization of KMS states which emphasizes their analytic aspects.

Recall two basic properties of analytic functions (theorems 3.7 (chapter 4) and 3.9 (chapter 6) of [14]).

Theorem 4.12. *Let $\Omega \subset \mathbb{C}$ be an open connected subset and $f : \Omega \mapsto \mathbb{C}$ be analytic. If the set $\{z \in \Omega : f(z) = 0\}$ has an accumulation point in Ω, then f is identically zero.*

Theorem 4.13. *Let $f : \mathbb{R}\times[a,b]i \subset \mathbb{C} \mapsto \mathbb{C}$ be a bounded continuous function, analytic on $\mathbb{R}\times(a,b)$. Then*

$$\sup_{z\in\mathbb{R}\times[a,b]} |f(z)| \leq \max\left(\sup_{t\in\mathbb{R}} |f(t+ia)|, \sup_{t\in\mathbb{R}} |f(t+ib)|\right).$$

Proposition 4.11. *Let w be a state on a W^*-dynamical system $(\mathcal{M},\tau)$, $\beta \in \mathbb{R}$. Then w is a (τ,β)-KMS state if and only if for each $A, B \in \mathcal{M}$ there is a bounded continuous function $F_{A,B} : \mathbb{R}\times[0,\beta] \mapsto \mathbb{C}$, analytic on $\mathbb{R}\times(0,\beta)$, such that*

$$F_{A,B}(t) = w(B\tau_t A), \qquad F_{A,B}(t+i\beta) = w(\tau_t(A)B)\ ,\ \text{for } t \in \mathbb{R}. \tag{4.9}$$

Proof. We prove the case $\beta > 0$: the proof for $\beta < 0$ is the same.

For the reverse implication, let $A, B \in \mathcal{M}_\tau$ and define the entire function $G(z) = w(B\tau_z A)$. For $t \in \mathbb{R}$, $G(t) = w(B\tau_t A) = F_{A,B}(t)$, i.e., $G = F_{A,B}$ on $\mathcal{M}$. By theorem 4.12, $F_{A,B} = G$ on $\mathbb{R}\times[0,\beta]$ and w is a (τ,β)-KMS state:

$$w(B\tau_{i\beta}A) = G(i\beta) = F_{A,B}(i\beta) = w(AB).$$

We first prove the direct implication for τ-entire elements $A, B \in \mathcal{M}_\tau$. Define the entire function $F_{A,B}(z) = w(B\tau_z A)$. For $t \in \mathbb{R}$, $F_{A,B}$ satisfies $F_{A,B}(t) = w(B\tau_t A)$ and $F_{A,B}(t+i\beta) = w(B\tau_{i\beta}\tau_t A) = w(\tau_t(A)B)$ by the KMS condition (eq. (4.8)). Moreover, $F_{A,B}$ is bounded on $\mathbb{R}\times[0,\beta]$ since $|F_{A,B}(z)| \leq |B||\tau_{\mathrm{Im}\, z}A|$. Thus, the restriction of $F_{A,B}$ to the strip $\mathbb{R}\times[0,\beta]$ is the desired function.

We now extend the result for arbitrary elements. Approximate $A, B \in \mathcal{M}$ by bounded nets (A_j) and (B_j) in $\mathcal{M}_\tau$, using Kaplansky's theorem 2.12. Thus

$|A_j| \leq |A|$, $|B_j| \leq |B|$, with $A_j \to A$ and $B_j \to B$ strongly. Define for each j, $F_j = F_{A_j,B_j}$ as above and suppose for the moment that (F_j) is a Cauchy net, uniformly on $\mathbb{R} \times [0,\beta]$. Then F_j converges uniformly to a bounded continuous function $F : \mathbb{R} \times [0,\beta] \mapsto \mathbb{C}$ which is analytic on $\mathbb{R} \times (0,\beta)$, from the analogous properties for the F_{A_j,B_j}'s. For $t \in \mathbb{R}$, $F(t) = \lim_j w(B_j \tau_t A_j) = w(B\tau_t A)$ and $F(t+i\beta) = w(\tau_t(A)B)$. We now prove the claim.

Let (H, π, u) be the GNS-representation of w. By theorem 4.13, $|F_j - F_k|_\infty$ occurs on the boundary of the strip $\mathbb{R} \times [0,\beta]$. So, for $t \in \mathbb{R}$ and $\mathbb{R} + i\beta$,

$$\begin{aligned} \sup_{t\in\mathbb{R}} |(F_j - F_k)(t)| &= \sup_{t\in\mathbb{R}} |w((B_j - B_k)\tau_t A_j) + w(B_k \tau_t (A_j - A_k))| \\ &\leq |A||\pi(B_j^* - B_k^*)u| + |B||\pi(A_j - A_k)u|, \end{aligned}$$

$$\sup_{t\in\mathbb{R}} |(F_j - F_k)(t+i\beta)| \leq |A||\pi(B_j - B_k)u| + |B||\pi(A_j^* - A_k^*)u|.$$

Combine the estimates to obtain

$$\begin{aligned} |F_j - F_k|_\infty \leq |A| &\left\{ |\pi(B_j^* - B_k^*)u| + |\pi(B_j - B_k)u| \right\} \\ &+ |B| \left\{ |\pi(A_j - A_k)u| + |\pi(A_j^* - A_k^*)u| \right\}. \end{aligned} \tag{4.10}$$

Finally, by theorem 4.8 and lemma 3.7, π is strongly continuous, yielding the following uniform convergences:

$$\pi(A_j)u \to \pi(A)u, \quad \pi(B_j)u \to \pi(B)u,$$

$$\pi(A_j^*)u \to \pi(A^*)u, \quad \pi(B_j^*)u \to \pi(B^*)u.$$

Thus, eq. (4.10) implies that (F_j) is a uniform Cauchy net on $\mathbb{R} \times [0,\beta]$. ■

4.5 The Takesaki theorem for KMS states

We finish this text with Takesaki's theorem, a profound link between Tomita-Takesaki theory and KMS states, considered a deep connection between pure mathematics and theoretical physics. We interpret physically a special case of this result.

We begin with two properties of a faithful state on its GNS representation. Throughout this section, $\mathcal{M}$ is a Von Neumann algebra.

Lemma 4.14. *Let w be a state on $\mathcal{M}$ with GNS-representation (H, π, u). Then w faithful on $\mathcal{M}$ if and only if π is injective and u is separating for $\pi(\mathcal{M})$.*

Proof. For the direct inclusion, let $A \in \mathcal{M}$ with $\pi(A) = 0$, so that

$$w(A^*A) = (u, \pi(A^*A)u) = |\pi(A)u|^2 = 0, \tag{4.11}$$

which implies that $A^*A = 0$, since w is faithful on $\mathcal{M}$. Thus, $A = 0$ and π is injective. For the separability, let $A \in \mathcal{M}$ with $\pi(A)u = 0$. By eq. (4.11), $w(A^*A) = 0$ and hence $A^*A = 0$. Again, since w is faithful on $\mathcal{M}$, $A = 0$. Therefore, $\pi(A) = 0$ and u is separating for $\pi(\mathcal{M})$.

Conversely, let $A \in \mathcal{M}$ such that $w(A^*A) = 0$. By the same calculation of eq. (4.11), $\pi(A)u = 0$. Since u is separating and π is injective, we obtain $A = 0$: w is faithful on $\mathcal{M}$. ■

Gibbs states are faithful (proposition 4.5), KMS states are too.

Proposition 4.12. *Let $(\mathcal{M}, \tau)$ be a W^*-dynamical system and w be a (τ, β)-KMS state with GNS-representation (H, π, u). Then u is cyclic separating for $\pi(\mathcal{M})$ and w is faithful for $\pi(\mathcal{M})$.*

Proof. From the GNS construction, u is cyclic, we now prove separability. Let $A \in \mathcal{M}$ such that $\pi(A) = 0$. By proposition 4.11, for $B, C \in \mathcal{M}$, there exists $F = F_{C,A^*B} : \mathbb{R} \times [0, \beta] \mapsto \mathbb{C}$ satisfying eq. (4.9). Since $F(t) = w(A^*B\tau_t C) = (\pi(A)u, \pi(B\tau_t C)u) = 0$, F vanishes on $\mathcal{M}$ and therefore vanishes identically, by theorem 4.12. Thus, $0 = F(i\beta) = (\pi(C)^*u, \pi(A)^*\pi(B)u)$ which implies $\pi(A)^* = 0$ since u is cyclic. We then have $\pi(A) = 0$: u is separating for $\pi(\mathcal{M})$.

To prove faithfulness, let $A = \pi(B)^*\pi(B) \in \pi(\mathcal{M})_+$ with $w(\pi(B)^*\pi(B)) = 0$. Then $\pi(B) = 0$: indeed,

$$|\pi(B)u|^2 = (u, \pi(B)^*\pi(B)u) = w(\pi(B)^*\pi(B)) = 0,$$

since u is separating for $\pi(\mathcal{M})$. Therefore $A = 0$ and w is faithful for $\pi(\mathcal{M})$. ■

We now apply the Tomita-Takesaki theorem and create a time evolution τ for which the state w is a τ-KMS state.

Theorem 4.15 (Takesaki)**.** *Let w be a normal state on the Von Neumann algebra $\mathcal{M} \subset B(H)$. The following are equivalent.*

1. *There is a σ-weakly continuous one-parameter group τ of *-automorphisms of $\mathcal{M}$ such that w is a τ-KMS state.*

2. *There exists a projection $E \in \mathcal{Z}(\mathcal{M})$ with $\mathcal{M} = \mathcal{M}E \oplus \mathcal{M}(I - E)$, such that w faithful on $\mathcal{M}E$ and $w(\mathcal{M}(I - E)) = 0$.*

If these conditions are satisfied, the restriction of τ to $\mathcal{M}E$ is uniquely determined by w. This restriction is then the modular group of $\mathcal{M}E$.

Proof. To see that (1) implies (2), let (H_w, π, u) be the GNS-representation of w. By lemma 4.9, $\pi : \mathcal{M}E \mapsto \pi(\mathcal{M})$ is a *-isomorphism and $\pi(\mathcal{M}(I-E)) = 0$, for some projection $E \in \mathcal{Z}(\mathcal{M})$. By proposition 4.12, w is faithful on $\pi(\mathcal{M})$ and hence it is faithful on $\mathcal{M}E$. Finally, $w(\mathcal{M}(I-E)) = (u, \pi(\mathcal{M}(I-E))u) = 0$.

Conversely, first notice that as $w(\mathcal{M}(I-E)) = 0$, every definition of τ on $\mathcal{M}(I-E)$ satisfies the KMS condition(eq. (4.8)) trivially. Thus, we can assume that $E = I$, so that w is faithful on $\mathcal{M}$. We now verify that the modular group given by Tomita-Takesaki theory is the time evolution with the desired properties. Let (H_w, π, u) be the GNS-representation of w. By lemma 4.14, the faithfulness of w implies that u is cyclic separating for $\pi(\mathcal{M})$. Then eq. (3.7) in the Tomita-Takesaki theorem (theorem 3.4) specifies the modular group τ associated to $(\pi(\mathcal{M}), u)$. Clearly $(\pi(\mathcal{M}), \tau)$ is a W^*-dynamical system. By lemma 4.14, π is injective and hence a *-isomorphism from $\mathcal{M}$ onto its image. From theorem 4.8, π is a σ-weakly homeomorphism. Thus we may identify $\mathcal{M}$ with $\pi(\mathcal{M})$ and conclude that $(\mathcal{M}, \tau)$ is a W^*-dynamical system. We now check that w is a τ-KMS state: for $A, B \in \mathcal{M}_\tau$,

$$w(B\tau_{-i}A) = (u, B\Delta A\Delta^{-1}u) = (B^*u, S^*SAu) = (u, ABu) = w(AB).$$

To prove the uniqueness claim, suppose that there exist another σ-weakly continuous one-parameter group κ of *-automorphisms of $\mathcal{M}$ for which w is a κ-KMS state. By proposition 4.11, for $A, B \in \mathcal{M}$ there are bounded continuous functions $F, G : \mathbb{R} \times [-1, 0] \mapsto \mathbb{C}$, analytic on $\mathbb{R} \times (-1, 0)$ such that

$$\begin{aligned} F(t) &= w(B\tau_t A), & F(t-i) &= w(\tau_t(A)B), \\ G(t) &= w(B\kappa_t A), & G(t-i) &= w(\kappa_t(A)B). \end{aligned}$$

For $s \in [-1, 0]$, $F(si) = w(BA) = G(si)$, i.e., $F = G$ on $\{0\} \times [-1, 0]$ and thus on $\mathbb{R} \times [-1, 0]$ by theorem 4.12. Since u is cyclic, for $t \in \mathbb{R}$,

$$(B^*u, \tau_t(A)u) = F(t) = G(t) = (B^*u, \kappa_t(A)u),$$

implies $\tau_t(A)u = \kappa_t(A)u$. The separability of u gives $\tau = \kappa$. ∎

Choosing $E = I$ yields the following interesting consequence.

Corollary 4.15.1. *Let w be a normal state on the Von Neumann algebra $\mathcal{M}$. Then w is faithful if and only if there exists an unique σ-weakly continuous one-parameter group τ of *-automorphisms of $\mathcal{M}$ for w is a τ-KMS state.*

As before, suppose that for the infinite system S, we model the physical observables by self-adjoint elements of a Von Neumann algebra $\mathcal{M} \subset B(H)$, the physical states by normal states w on $\mathcal{M}$ and the time evolution by a σ-weakly continuous one-parameter group κ of *-automorphisms of $\mathcal{M}$. By corollary 4.15.1, a faithful physical state w corresponds to a unique time evolution τ (the modular group associated to w) for which w is an equilibrium state (with respect to τ) at $\beta = -1$.

Thus, the notion of a (τ, β)-KMS state, hence of an equilibrium state, depends on the time evolution τ proposed for the physical system.

If w is also a (κ, β)-KMS state then κ must be a rescaling of τ. Equivalently, if τ and κ are not related by rescaling then w cannot be a equilibrium state for the time evolution κ: a faithful physical state w induces an intrinsically related time evolution τ for which it is an equilibrium state.

5
Conclusions

Um sistema de microscopia digital com reconhecimento e classificação automática dos cristais de hematita em minérios de ferro foi desenvolvido.

O método utiliza operações tradicionais de processamento digital de imagens e propõe uma segmentação automática de cristais baseada no cálculo da distância espectral, a fim de controlar ...

É fundamental também comentar que ...

Assim, como uma proposta para trabalho futuro, pode-se buscar combinar os dois enfoques...

A
Some Functional Analysis

A.1
Topologies on $B(H)$

We define the weak, strong and σ-weak topologies on $B(H)$ and then enumerate some of their properties. For a treatments of locally convex topologies and nets, see [18, 20]. For more about topologies on $B(H)$, see [10, 21, 12].

Let H be a complex Hilbert space and $l^2(H)$ be the space of sequences (x_n) in H such that $\sum_n |x_n|^2 < \infty$. The *strong, weak and σ-weak operator topologies* on $B(H)$ are the locally convex topologies induced respectively by the following seminorms

$$p_x(A) = |Ax|,\ p_{x,y}(A) = (Ax, y),\ p_{x_n,y_n}(A) = \sum_n |(Ax_n, y_n)|^2,\ \text{for}\ \ A \in B(H)\ .$$

Thus, neighborhoods of $A \in B(H)$ in the strong and weak topologies are given by a choice of $x_i \in H, i = 1, \ldots, n$ and $\epsilon > 0$: they consist of $B \in B(H)$ for which, respectively $|(A - B)x_i| < \epsilon$ or $|((A - B)x_i, x_i)| < \epsilon$.

By the polarization identity in Hilbert spaces, the weak and σ-weak topologies are actually induced by $(p_{x,x})_{x\in H}$ and $\{p_{x_n,x_n} : (x_n) \in l^2(H)\}$. In what follows, we refer to the weak operator topology and strong operator topology as the weak and strong topologies on $B(H)$.

The weak topology is included in the strong and σ-weak topologies (think of a topology as a collection of open sets satisfying certain axioms). The strong and σ-weak topologies in turn are included in the norm topology. These inclusions are strict if H is infinite dimensional. Moreover, the weak and σ-weak topologies coincide in bounded sets of $B(H)$.

These topologies do not satisfy in general the first axiom of countability: some properties must be characterized by nets instead of sequences. The convergence of a net $(A_j) \subset B(H)$ to $A \in B(H)$ is *strong* if $|A_jx| \to |Ax|$, *weak* if $(A_jx, x) \to (Ax, x)$ for every $x \in H$, or *σ-weak* if $\sum_n (A_jx_n, x_n) \to \sum_n (Ax_n, x_n)$ for $(x_n) \in l^2(H)$.

Let H_1 and H_2 be Hilbert spaces. The map $f : B(H_1) \mapsto B(H_2)$ is *weakly continuous* if for every weakly convergent net $(A_j) \to A$ in $B(H_1)$, one has $f(A_j) \to f(A)$ weakly (in $B(H_2)$).

Additional well known properties of these topologies are the following.

1. The unit closed ball of $B(H)$ is weakly compact.

2. The weak and strong closures of a convex subset $V \subset B(H)$ coincide.

3. The operator product in $B(H)$, $(A, B) \mapsto A \circ B$ is weakly and strongly separately continuous.

4. The adjoint operation in $B(H)$, $A \mapsto A^*$ is weakly continuous.

5. The map $Re : B(H) \mapsto B(H), Re(A) = (A+A^*)/2$, is weakly continuous.

6. For w be a weakly continuous linear functional on $B(H)$, there exist $x_1, \ldots, x_n, y_1, \ldots, y_n \in H$ such that for $A \in B(H)$,
$$w(A) = \sum_{k=1}^{n} (x_n, Ay_n).$$

7. For w be a σ-weakly continuous functional on $B(H)$, there exist sequences $(x_n), (y_n) \in l^2(H)$ such that for $A \in B(H)$,
$$w(A) = \sum_{n=1}^{\infty} (x_n, Ay_n).$$

A.2 Anti-linear operators

We give some basic facts about anti-linear operators. We follow [21, 16].

Let H be a complex Hilbert space with scalar multiplication $(\lambda, x) \mapsto \lambda x$ and inner product (x, y) for $\lambda \in \mathbb{C}$ and $x, y \in H$. The conjugate Hilbert space of H, denoted by $\tilde{H}$, is the set H with the same vector addition of H but scalar multiplication and inner product defined by
$$(\lambda, x) \mapsto \lambda.x = \overline{\lambda}x, \qquad (x, y)_c = \overline{(x, y)}\ .$$

For $x \in H$, $|x|^2 = (x, x) = (x, x)_c = |x|_c^2$ hence the norm topologies on H and $\tilde{H}$ are the same. Thus, topological properties do not depend on the Hilbert space being used.

Let A be an anti-linear operator acting on H. We can consider $A : \tilde{H} \mapsto H$ as a map. We see that, for $\lambda \in \mathbb{C}$ and $x \in \tilde{H}$, $A(\lambda.x) = A(\overline{\lambda}x) = \lambda Ax$ hence $A : \tilde{H} \mapsto H$ is a linear operator. Similarly, $A : H \mapsto \tilde{H}$. An analogous calculation shows that $A : H \mapsto \tilde{H}$ is also a linear operator.

Conversely, if $A : H \mapsto H$ is a linear operator then $A : \tilde{H} \mapsto H$ and $A : H \mapsto \tilde{H}$ are anti-linear. Changing both domain and range of A preserves linearity and anti-linearity.

Let $A : D \subset H \mapsto H$ be an anti-linear operator defined on a densely defined subspace $D \subset H$. Then $A : D \subset \tilde{H} \mapsto H$ is linear with an adjoint $A^* : Dom(A^*) \subset H \mapsto \tilde{H}$ for which $A^* y = z$ for y in

$$\mathrm{Dom}(A^*) = \{y \in H : \text{ there is } z \in H, (Ax, y) = (x, z)_c = (z, x) \text{ for all } x \in H\}.$$

For $x \in D$ and $y \in \mathrm{Dom}(A^*)$, $(Ax, y) = (x, A^* y)_c = (A^* y, x)$.

Thus, we can consider the adjoint A^* without reference to $\tilde{H}$: the anti-linear operator $A^* : Dom(A^*) \subset H \mapsto H$ is the *adjoint of the anti-linear* operator $A : D \subset H \mapsto H$, with domain

$$\mathrm{Dom}(A^*) = \{y \in H : \text{ there is } z \in H, (Ax, y) = (z, x) \text{ for } x \in D\},$$

satisfying $(Ax, y) = (A^* y, x)$ for $x \in D$ and $y \in \mathrm{Dom}(A^*)$.

Let $A : D \subset H \mapsto H$ be a closed densely defined anti-linear operator. Then $A : D \subset \tilde{H} \mapsto H$ is a closed, densely defined linear operator and hence admits a polar decomposition, i.e., $A = V(A^*A)^{1/2} = (AA^*)^{1/2} V$ for some partial isometry $V : \overline{Ran(A^*A)^{1/2}} \to \overline{Ran(A)}$.

The map $AA^* : Dom(A^*) \subset H \mapsto H$ is linear, and so are $A^*A : D \subset \tilde{H} \mapsto \tilde{H}$ and $A^*A : D \subset H \mapsto H$. The maps $V : \tilde{H} \mapsto H$ and $V : H \mapsto \tilde{H}$ are linear and $V : H \mapsto H$ is anti-linear: it is a *partial anti-isometry*. The closures do not change if H is replaced by $\tilde{H}$.

Thus every closed densely defined anti-linear operator $A : D \subset H \mapsto H$ admits a polar decomposition $A = V(A^*A)^{1/2} = (AA^*)^{1/2} V$ for some partial anti-isometry $V : \overline{Ran(A^*A)^{1/2}} \to \overline{Ran(A)}$.

A.3
Some applications of the functional calculus

A.3.1
Riesz projections

For a Banach space X and $A \in \mathcal{B}(X)$, an important problem is to find the notrivial invariant subspaces of A — actually, it is an open problem if such an operator admits such a subspace. When X is a Hilbert space and A is a normal operator, the spectral theorem solves the problem positively. Here, we show that the holomorphic functional calculus gives a positive answer if $\sigma(A) \subset \mathbb{C}$ has two or more connected components. Indeed, there are *Riesz projections* P_i

for each connected component σ_i of $\sigma(A)$ such that the P_i's commute, their ranges provide a direct sum decomposition of X in invariant subspaces and the restriction AP_i has spectrum σ_i.

In particular, if A is a square complex matrix, the Jordan decomposition of A follows from the existence of Riesz projections once a structure theorem for nilpotent matrices is known.

Split $\sigma(A)$ in n disjoint sets σ_k, $k = 1, \ldots, n$ consisting of unions of connected components of $\sigma(A)$: $\sigma(A)$ and hence each σ_k are compact. Fix an open bounded neighborhood $U \subset \mathbb{C}$ of $\sigma(A)$ and draw smooth simple positively oriented curves γ_k enclosing each σ_k respectively. Let D_k be the connected region bounded by γ_k and χ_k be the characteristic function of D_k: clearly $\chi_k \in \mathcal{H}(U)$. Moreover,

$$\sum_{k=1}^{n} \chi_k = 1 \quad \text{and} \quad \chi_i \chi_j = 0, i \neq j.$$

The holomorphic functional calculus provides the Riesz projections $P_k = \chi_k(A)$. Their ranges $X_k = P_k(X)$ are closed, invariant subspaces, since

$$\sum_{k=1}^{n} P_k = I \quad \text{and} \quad P_i P_j = 0, i \neq j.$$

Let A_k be the restriction of A to X_k, $A_k = AP_k$. Then

$$X = X_1 \oplus \ldots \oplus X_n \quad \text{and} \quad A = A_1 \oplus \ldots \oplus A_n.$$

Thus, the topological separation of $\sigma(A)$ in components provides an algebraic decomposition of X and A in terms of direct sums. Said differently, a topological property of $\sigma(A)$ induces an algebraic property of A. Note that A does not need to satisfy an algebraic condition of symmetry.

If $A \in M_n(\mathbb{C})$ and its eigenvalues λ_k are all distinct, then $\sigma(A) = \cup_{k=1}^{n} \{\lambda_k\}$: the invariant closed subspaces X_k are the one-dimensional eigenspaces associated to each λ_k. Thus, choosing a basis of eigenvectors, A is diagonalized:

$$A = A_1 \oplus \ldots \oplus A_n = \begin{pmatrix} A_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & A_n \end{pmatrix} = \begin{pmatrix} \lambda_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \lambda_n \end{pmatrix}.$$

If the eigenvalues have algebraic multiplicity, we have $\sigma(A) = \cup_{k=1}^{m} \{\lambda_k\}$ with $m < n$. The invariant closed subspaces X_k associated to each λ_k are not necessarily one-dimensional. Choosing an arbitrary basis for each X_k,

$$A = A_1 \oplus \ldots \oplus A_m = \begin{pmatrix} A_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & A_m \end{pmatrix},$$

i.e., a diagonalization by blocks, almost a Jordan decomposition of A. The topology of $\sigma(A)$ does not distinguish the algebraic multiplicity of the eigenvalues λ_k, and the Jordan decomposition does not follow from $\sigma(A)$ and the functional calculus. It takes a special basis of (generalized) eigenvectors in each X_k to obtain the Jordan decomposition of A.

A.3.2
Large powers of an operator

Let $\mathcal{B}$ be a Banach algebra and $A \in \mathcal{B}$ with spectral radius $r(A) < 1$, i.e., the spectrum $\sigma(A)$ is contained in D_1, the unit open disk of $\mathbb{C}$. We prove, using the holomorphic functional calculus that $A^n \to 0$ uniformly.

Since $\sigma(A) \subset D_1$ is compact, there is a circle of radius $r < 1$ centered at the origin (positively oriented) $\gamma \subset D_1$ enclosing $\sigma(A)$. Thus,

$$|A^n| \;=\; |\frac{1}{2\pi i}\int_\gamma z^n R_A(z)dz| \;\leq\; \frac{|R_A|_\infty L(\gamma)}{2\pi} r^n \to 0,$$

where the resolvent function $R_A(z)$ has bounded norm by compactness.

This nice consequence of the holomorphic functional calculus is striking, when one considers for example, for $s < 1$, the matrix

$$A = \begin{pmatrix} s & 100 & 0 \\ 0 & s & 100 \\ 0 & 0 & s \end{pmatrix}, \text{ with } A^n = \begin{pmatrix} s^n & 100ns^{n-1} & 500n(n-1)s^{n-2} \\ 0 & s^n & 100ns^{n-1} \\ 0 & 0 & s^n \end{pmatrix},$$

then $r(A) < 1$ and $|A|_\infty = 100 + s$. The decay to zero of A takes a while.

A.3.3
Functional calculus for C^k differentiable functions

Let $\mathcal{B}$ be a Banach algebra, $A \in \mathcal{B}$ and U be a bounded neighborhood of $\sigma(A)$. The holomorphic functional calculus computes $f(A)$ for $f \in \mathcal{H}(U)$. However, depending of the properties of A, the functional calculus for classes extend to smooth functions. We consider complex matrices with real spectrum.

Let $A \in M_n(\mathbb{C})$ have Jordan decomposition $A = BJB^{-1}$ and p be a real polynomial of a single variable. Clearly, for $\lambda_j \in \sigma(A)$,

$$p(A) = Bp(J)B^{-1} = B \begin{pmatrix} p(J_{\lambda_1}) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & p(J_{\lambda_m}) \end{pmatrix} B^{-1}.$$

Thus, to define $f(A)$, we first define $p(J_{\lambda_j})$ and then take a limit.

A Jordan block of dimension k splits in $J_{\lambda_j} = \lambda_j I + N_j$, where $N_j^k = 0$. For a polynomial p expanded at the point λ_j, we obtain the finite expansion

$$\begin{aligned} p(J_{\lambda_j}) = p(\lambda_j I + N_j) &= p(\lambda_j I) + p^{(1)}(\lambda_j I)N_j + \ldots + \frac{p^{(k)}(\lambda_j I)N_j^k}{k!} \\ &= p(\lambda_j)I + p^{(1)}(\lambda_j)N_j + \ldots + \frac{p^{(k)}(\lambda_j)N_j^k}{k!}. \end{aligned}$$

Taking the supremum norm of p and its derivatives on $[a, b]$ (the C^k norm),

$$|p(J_{\lambda_j})| \leq |p|_\infty + |p^{(1)}|_\infty |N_j| + \ldots + \frac{|p^{(k)}|_\infty |N_j|^k}{k!} \leq C|p|_{C^k}.$$

From this bound, the functional calculus extends to functions $f \in C^k[a, b]$, better still, for C^k functions defined in real neighborhood U of $\sigma(A)$. By continuity, the algebra homomorphism properties — which hold for polynomials — are preserved.

We present a convenient tool to exponentiate or invert matrices of small dimension with known spectrum.

Proposition A.1. *Let M be an $n \times n$ matrix, with minimal polynomial $m(\lambda) = \Pi_i(\lambda_i)$, where the eigenvalue λ_i has multiplicity μ_i. For two C^k functions f and g in the neighborhood of $\sigma(M)$, $f(M) = g(M)$ if and only if the functions agree on each λ_i up to the derivative of order $\mu_i - 1$.*

Thus, every entire function of a 3×3 matrix is computed by a polynomial of degree 2. The computation of the eigenvectors of M is not needed.

A.4
Unbounded operators

We revise some definitions and elementary results about unbounded operators. The material is based on [18]. There is no way out: some of the most important operators in quantum theory and mathematical physics are unbounded. In one dimension, for example, consider the position, momentum, Laplacian operators on appropriate dense subspaces $D \subset L^2(\mathbb{R})$,

$$q : D \to L^2(\mathbb{R}) \qquad p : D \to L^2[0,1] \qquad \Delta : D \to L^2[0,1]$$
$$f \mapsto xf \qquad f \mapsto \frac{df}{dx} \qquad f \mapsto \frac{d^2 f}{dx^2}$$

The Hellinger-Toeplitz theorem asserts that an everywhere defined symmetric operator $A : H \to H$ ($(Ax, y) = (x, Ay)$ for $x, y \in H$) is necessarily bounded. Thus unbounded operators are naturally associated to subspaces of H.

Let D be a dense subspace of H. The linear map $A : D \subset H \to H$ is a *densely defined* linear operator. The *graph* of A is the subspace

$$\Gamma(A) = \{(x, Ax) : x \in D\} \subset H \oplus H.$$

Let $A : D_1 \subset H \to H$ and $B : D_2 \subset H \to H$. If $D_1 \subset D_2$ and B restricted to D_1 coincides with A, B is an *extension* of A. Equivalently, B is an extension of A if $\Gamma(A) \subset \Gamma(B)$.

Consider the Hilbert space $H \oplus H$ with the inner product

$$\langle (x_1, y_1), (x_2, y_2) \rangle = (x_1, x_2) + (y_1, y_2).$$

A densely defined operator $A : D \subset H \to H$ is *closed* if its graph $\Gamma(A)$ is closed in $H \oplus H$.

Equivalently, A is closed if the convergences $x_n \to x \in H$ with (x_n) in D and $Ax_n \to y \in H$ imply $x \in D$ and $Ax = y$. Thus, closed operators are rather similar to bounded (continuous) operators.

An operator A which admits a closed extension is *closable*. Since the intersection of all graphs of closed extensions of A is again a closed graph, every closable operator A has a smallest closed extension $\overline{A}$, the *closure* of A. For a closable operator A, $\Gamma(\overline{A}) = \overline{\Gamma(A)}$.

Densely defined unbounded operators are still amenable to taking adjoints. For such an $A : D \subset H \to H$, let

$$D^* = \{y \in H : \exists w \in H, (Ax, y) = (x, w) \text{ for } x \in D\}.$$

The *adjoint* of A is the linear operator

$$A^* : D^* \subset H \to H \qquad y \mapsto w.$$

The familiar adjoint formula states $(Ax, y) = (x, A^* y)$ for $x \in D$ and $y \in D^*$. Also note that A^* can only be defined if A is densely defined, and then we write $A^{**} = (A^*)^*$. For the reader's convenience, we recall some basic properties.

Proposition A.2. *Let $A : D \subset H \to H$ be a densely defined operator. Then*

1. *A^* is closed.*
2. *A is closable if and only if A^* is densely defined. In this case $\overline{A} = A^{**}$.*
3. *If A is closable then $(\overline{A})^* = A^*$.*

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