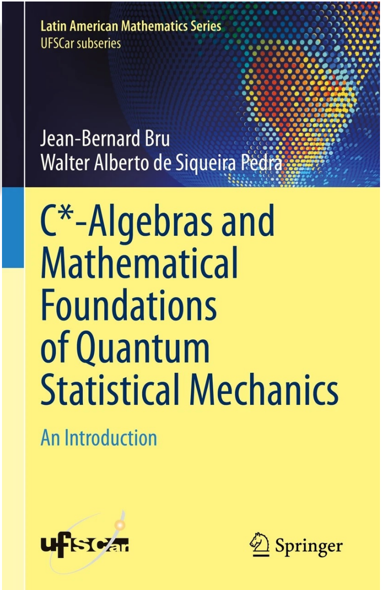
# $C^*$-Algebras and Mathematical Foundations of Quantum Statistical Mechanics

J.–B. Bru[1]

[1]BCAM - University of the Basque Country - Ikerbasque



# Outline

# $C^*$–Algebras

## Definition ($*$–Algebra)

The mapping $A \mapsto A^*$ from an algebra $\mathcal{X}$ to itself is an involution, when
*(i)* $\forall A \in \mathcal{X} : (A^*)^* = A$.
*(ii)* $\forall A, B \in \mathcal{X} : (AB)^* = B^* A^*$.
*(iii)* $\forall A, B \in \mathcal{X}$, $\forall \alpha, \beta \in \mathbb{C}$: $(\alpha A + \beta B)^* = \bar{\alpha} A^* + \bar{\beta} B^*$.
An algebra $\mathcal{X}$ with an involution is a $*$–algebra.

## Definition ($C^*$–Algebra)

*(i)* Let $\| \cdot \|_{\mathcal{X}}$ be a norm on a vector space $\mathcal{X}$. Then, $\mathcal{X} \equiv (\mathcal{X}, \| \cdot \|_{\mathcal{X}})$ is a normed algebra whenever $\mathcal{X}$ is an algebra and $\|AB\|_{\mathcal{X}} \leq \|A\|_{\mathcal{X}} \|B\|_{\mathcal{X}}$ for $A, B \in \mathcal{X}$.

*(ii)* A normed algebra $\mathcal{X}$ is a Banach algebra if $\mathcal{X}$ is complete w.r.t the norm $\| \cdot \|_{\mathcal{X}}$.

*(iii)* A Banach algebra $\mathcal{X}$ equipped with an involution such that $\|A\|_{\mathcal{X}} = \|A^*\|_{\mathcal{X}}$ for $A \in \mathcal{X}$ is a Banach $*$–algebra.

*(iv)* A Banach $*$–algebra $\mathcal{X}$ is a $C^*$–algebra whenever $\|A^* A\|_{\mathcal{X}} = \|A\|_{\mathcal{X}}^2$ for $A \in \mathcal{X}$.

# $C^*$–Algebras

## Definition ($C^*$–Algebra)

A $C^*$–algebra $\mathcal{X}$ is a complete, normed algebra equipped with an involution $*$ such that

$$\|A^*A\|_{\mathcal{X}} = \|A\|_{\mathcal{X}}^2 \ , \qquad A \in \mathcal{X} \ .$$

**Properties on $C^*$–algebras:**

- If the identity $1 \in \mathcal{X}$ exists then it is unique, self–adjoint, and $\|1\|_{\mathcal{X}} = 1$. In this case, $\mathcal{X}$ is a unital $C^*$–algebra. Any $C^*$–algebra can be extended to a unital $C^*$–algebra.
- If $\mathcal{X}$ is a Banach $*$–algebra, then there is a unique norm $\|\cdot\|_{\mathcal{X}}$ on $\mathcal{X}$ such that $(\mathcal{X}, \|\cdot\|_{\mathcal{X}})$ is a $C^*$–algebra.

**Notation**: From now, $\mathcal{X}$ is always a $C^*$–algebra with identity 1, i.e., a unital $C^*$–algebra.

# Examples of $C^*$–Algebras

**Example 1:** Let $\mathcal{H}$ be a Hilbert space. The space

$$(\mathcal{B}(\mathcal{H}), \|\cdot\|_{\mathrm{op}}, \cdot, ^*)$$

of bounded linear operators from $\mathcal{H}$ to $\mathcal{H}$ is a unital $C^*$–algebra. "$\cdot$" is the standard product of linear operators and, for all $A \in \mathcal{B}(\mathcal{H})$, $A^* \in \mathcal{B}(\mathcal{H})$ is its self–adjoint operator. Here, the norm is defined by

$$\|A\|_{\mathrm{op}} := \sup_{\varphi \in \mathcal{H}, \|\varphi\|=1} \|A\varphi\|_{\mathcal{H}} < \infty.$$

**Example 2:** Let $K$ be a compact set and $C(K)$ be the complex vector space of continuous functions from $K$ to $\mathbb{C}$. For all $f \in C(K)$, let

$$\|f\|_\infty := \sup_{x \in K} |f(x)| < \infty.$$

Then, $(C(K), \|\cdot\|_{C(K)})$ is a Banach space and by defining the involution by

$$f^*(x) := \overline{f(x)}$$

and the pointwise product, $(C(K), \|\cdot\|_\infty, \cdot, ^*)$ is a commutative unital $C^*$–algebra and all **commutative unital** $C^*$–algebras are of this form.

# Representation of $C^*$–Algebras

## Definition (Representation of $C^*$–algebras)

*(i)* A representation of $\mathcal{X}$ is a pair $(\pi, \mathcal{H})$, $\mathcal{H}$ being a Hilbert space and $\pi : \mathcal{X} \to \mathcal{B}(\mathcal{H})$ a $*$–homomorphism.

*(ii)* A representation $(\pi, \mathcal{H})$ is faithful if $\pi$ is injective.

*(iii)* Let $(\pi, \mathcal{H})$ be a representation of $\mathcal{X}$. If

$$\overline{\pi(\mathcal{X})\Omega} = \mathcal{H}$$

for some $\Omega \in \mathcal{H}$ then $\Omega$ is called a cyclic vector and the triplet $(\pi, \mathcal{H}, \Omega)$ is called a cyclic representation of $\mathcal{X}$.

- Any $C^*$–algebra has a faithful representation, by Gelfand–Naimark's theorem.
- The notion of representation is pivotal to understand the difference between the algebraic and Hilbert space formulation of quantum mechanics.

# States on $C^*$–algebras

**Notation**: $\mathcal{X}$ is a unital $C^*$–algebra. The identity is always denoted by 1. The topological dual space is denoted by $\mathcal{X}^*$.

## Definition (States on $C^*$–algebras)

*(i)* $\rho : \mathcal{X} \to \mathbb{C}$ is positive ($\rho \geq 0$) if $\rho(A^*A) \geq 0$ for all $A \in \mathcal{X}$.

*(ii)* $\rho : \mathcal{X} \to \mathbb{C}$ is a state if $\rho \geq 0$ and $\rho(1) = 1$.

## Theorem (Equivalent definition of states)

*$\rho$ is a state iff $\rho : \mathcal{X} \to \mathbb{C}$ is a linear functional and*

$$\|\rho\|_{\mathcal{X}^*} := \sup_{A \in \mathcal{X}, \|A\|_{\mathcal{X}} = 1} |\rho(A)|^2 = \rho(1) = 1.$$

- In fact, a linear functional $\rho : \mathcal{X} \to \mathbb{C}$ is positive iff $\|\rho\|_{\mathcal{X}^*} = \rho(1)$.
- Positive functionals $\rho : \mathcal{X} \to \mathbb{C}$ are continuous, i.e., $\rho \in \mathcal{X}^*$.

# Examples of States

**Example 1:** Let $\mathcal{H}$ be a Hilbert space and $\mathcal{X} \subset \mathcal{B}(\mathcal{H})$ be a unital $C^*$–algebra.
*(i)* For $\psi \in \mathcal{H}$ with $\|\psi\|_{\mathcal{H}} = 1$, one defines a state $\rho_\psi : \mathcal{X} \to \mathbb{C}$ by

$$\rho_\psi(A) = \langle \psi, A\psi \rangle, \qquad A \in \mathcal{X},$$

*(ii)* Let $D \in L^1(\mathcal{H})$ (trace–class operators) with $D \geq 0$ and $\mathrm{Tr}\, D = 1$. Then the map $\rho_D : \mathcal{X} \to \mathbb{C}$ defined by

$$\rho_D(A) = \mathrm{Tr}\,(DA), \qquad A \in \mathcal{X},$$

is well–defined as $L^1(\mathcal{H})\mathcal{B}(\mathcal{H}) \in L^1(\mathcal{H})$ and is a state.

**Example 2:** Let $K$ be a compact set and $\mathcal{X} = C(K)$. Let $a \in K$ and $\rho_a : \mathcal{X} \to \mathbb{C}$ defined by $\rho_a(f) = f(a)$. Then $\rho_a(1) = 1$ and $\rho_a(f^* f) \geq 0$ for all $f \in \mathcal{X}$, i.e., $\rho_a$ is a state of $\mathcal{X}$.

**Example 3:** Let $K$ be a compact set and $\mathcal{X} = C(K)$. Let $\mu$ be a probability measure on $K$ and the map $\rho_\mu : \mathcal{X} \to \mathbb{C}$ be defined by

$$\rho_\mu(f) = \int_K f(x)\, \mathrm{d}\mu(x).$$

Then $\rho_\mu(1) = 1$ and $\rho_\mu(f^* f) \geq 0$ for all $f \in \mathcal{X}$, which means that $\rho_\mu$ is a state of $\mathcal{X}$.

# Examples of States

**Example 3:** Let $K$ be a compact set and $\mathcal{X} = C(K)$. Let $\mu$ be a probability measure on $K$ and the map $\rho_\mu : \mathcal{X} \to \mathbb{C}$ be defined by

$$\rho_\mu(f) = \int_K f(x)\,\mathrm{d}\mu(x).$$

Then $\rho_\mu(1) = 1$ and $\rho_\mu(f^* f) \geq 0$ for all $f \in \mathcal{X}$, which means that $\rho_\mu$ is a state of $\mathcal{X}$.

## Theorem (Riesz–Markov)

*Let $K$ be a compact metrizable set, $\mathcal{X} = C(K)$ and $\rho$ be a state. Then there is a unique probability measure $\mu_\rho$ on $K$ such that*

$$\rho(f) = \int_K f(x)\,\mathrm{d}\mu_\rho(x), \qquad f \in \mathcal{X}.$$

- Recall that all commutative unital $C^*$–algebras are of the form $C(K)$ for some compact set $K$. In particular, in this case, states can always be seen as probability measures.

# Properties of States

## Theorem (Properties of states)

*(i)* $\rho \geq 0$ *implies that* $\rho(A) = \overline{\rho(A^*)}$ *for all* $A \in \mathcal{X}$.

*(ii)* $\rho(A) = 0$ *for all states* $\rho \Rightarrow A = 0$.

*(iii)* $\rho(A) \in \mathbb{R}$ *for all states* $\rho \Rightarrow A^* = A$.

*(iv)* $\rho(A) \geq 0$ *for all states* $\rho \Rightarrow A = B^*B \geq 0$.

*(v)* $A \in \mathcal{X}$ *is normal (i.e.,* $AA^* = A^*A$*)* $\Rightarrow \exists$ *a state* $\rho$ *so that* $|\rho(A)| = \|A\|_{\mathcal{X}}$.

## Lemma (Cauchy–Schwarz inequality)

$\rho \in \mathcal{X}^*$ *and* $\rho \geq 0$ *imply that, for all* $A, B \in \mathcal{X}$,

$$|\langle A, B\rangle_\rho|^2 := |\rho(B^*A)|^2 \leq \rho(A^*A)\rho(B^*B) =: \langle A, A\rangle_\rho \langle A, B\rangle_\rho .$$

*and*

$$\rho(B^*AB) \leq \|A\|_{\mathcal{X}} \ \rho(B^*B).$$

# GNS (Gel'fand–Naimark–Segal) Representation

- Let $\mathcal{X}$ be a unital $C^*$–algebra and $\rho$ a state. Define

$$\mathcal{L}_\rho := \{A \in \mathcal{X} \ : \ \rho(A^* A) = 0\}$$

- A scalar product $\langle \cdot, \cdot \rangle_\rho$ in $\mathcal{X}/\mathcal{L}_\rho$ can be defined by

$$\langle A + \mathcal{L}_\rho, B + \mathcal{L}_\rho \rangle_\rho = \rho(B^* A)$$

- $\mathcal{L}_\rho$ is a closed left–ideal of $\mathcal{X}$, i.e., $\mathcal{L}_\rho$ is a closed subspace such that $\mathcal{X}\mathcal{L}_\rho \subset \mathcal{L}_\rho$. For all $A \in \mathcal{X}$,

$$\tilde{\pi}_\rho(A)(B + \mathcal{L}_\rho) = AB + \mathcal{L}_\rho$$

defines a linear operator $\tilde{\pi}_\rho(A) : \mathcal{X}/\mathcal{L}_\rho \to \mathcal{X}/\mathcal{L}_\rho$ with

$$\|\tilde{\pi}_\rho(A)\|_{\mathcal{X}/\mathcal{L}_\rho} := \sup_{B \in \mathcal{X}/\mathcal{L}_\rho, B \neq 0} \sqrt{\frac{\rho\left(B^* A^* A B\right)}{\rho\left(B^* B\right)}} \leq \|A\|_{\mathcal{X}}.$$

- $\mathcal{H}_\rho := \overline{\mathcal{X}/\mathcal{L}_\rho}^{\langle \cdot, \cdot \rangle_\rho}$ is an Hilbert space and $\tilde{\pi}_\rho$ has a continuous extension denoted by $\pi_\rho : \mathcal{X} \to \mathcal{B}(\mathcal{H}_\rho)$. It leads to the GNS–representation of $\rho$.

# GNS (Gel'fand–Naimark–Segal) Representation

- A representation of $\mathcal{X}$ is a pair $(\pi, \mathcal{H})$, $\mathcal{H}$ being Hilbert space and $\pi : \mathcal{X} \to \mathcal{B}(\mathcal{H})$ a $*$–homomorphism. If $\overline{\pi(\mathcal{X})\Omega} = \mathcal{H}$ for some $\Omega \in \mathcal{H}$ then $\Omega$ is a cyclic vector and the triplet $(\pi, \mathcal{H}, \Omega)$ is a cyclic representation of $\mathcal{X}$.
- Let $\mathcal{L}_\rho := \{A \in \mathcal{X} \ : \ \rho(A^* A) = 0\}$.

## Definition (GNS-representation $(\mathcal{H}_\rho \Omega_\rho, \pi_\rho)$ of a state $\rho$)

(a) $\mathcal{H}_\rho :=$ completion of $\mathcal{X}/\mathcal{L}_\rho$ with respect to the scalar product;
(b) $\Omega_\rho := (1 + \mathcal{L}_\rho) \in \mathcal{H}_\rho$;
(c) $\pi_\rho :=$ representation on $\mathcal{H}_\rho$ of $\mathcal{X}$ defined by $\pi_\rho(A)(B + \mathcal{L}_\rho) = AB + \mathcal{L}_\rho$, $A, B \in \mathcal{X}$.

## Theorem

*Let $\rho$ be a state on a unital $C^*$–algebra $\mathcal{X}$. There is a unique (up to a unitary transformation) cyclic representation $(\pi_\rho, \mathcal{H}_\rho, \Omega_\rho)$ such that*

$$\rho(A) = \langle \Omega_\rho, \pi_\rho(A)\Omega_\rho \rangle_{\mathcal{H}_\rho}, \qquad A \in \mathcal{X}.$$

# Observations

- The GNS representation has led to very important applications of the Tomita–Takesaki theory, developed in seventies, to Quantum Field Theory and Statistical Mechanics.
- These developments mark the beginning of the algebraic approach to Quantum Mechanics and Quantum Field Theory.
- The algebraic formulation turned out to be extremely important and fruitful for the mathematical foundations of Quantum Statistical Mechanics (mainly until the nineties).
- Formalism constructed to study thermodynamic limits of quantum systems at any **fixed particle density and temperature** (notion of KMS states).
- Last but not least, no reasonable microscopic theory of first order phase transitions is possible within the Hilbert space based approach, and **the use of the algebraic setting is imperative**.

# Outline

# Schrödinger / Heisenberg Pictures of Quantum Mechanics

(S1) **Schrödinger picture:** Let $H = H^* \in \mathcal{B}(\mathcal{H})$ acting on some Hilbert space $\mathcal{H}$. For any $t \in \mathbb{R}$ and initial state $\psi(0) \in \mathcal{H}$ at $t = 0$, the Schrödinger equation is

$$i\partial_t \psi(t) = H\psi(t), \qquad \text{i.e.,} \qquad \psi(t) = \mathrm{e}^{-itH}\psi(0).$$

Expectation value at time $t \in \mathbb{R}$ of an observable $B = B^* \in \mathcal{B}(\mathcal{H})$:

$$\langle \psi(t), B\psi(t)\rangle = \langle \psi(0), \mathrm{e}^{itH} B \mathrm{e}^{-itH}\psi(0)\rangle, \qquad t \in \mathbb{R}.$$

(H2) **Heisenberg picture:** The map $B \mapsto \tau_t(B) := \mathrm{e}^{itH} B \mathrm{e}^{-itH}$ defines a (automorphism) group which satisfies

$$\forall t \in \mathbb{R}: \quad \partial_t \tau_t(B) = \tau_t \circ \delta(B), \qquad \text{with } \delta(B) := i[H, B].$$

If $H_t = H_t^*$ is time–dependent, we obtain a two–parameter family $\{\tau_{t,s}\}_{s,t\in\mathbb{R}}$ of automorphisms satisfying

$$\forall s, t \in \mathbb{R}: \quad \partial_t \tau_{t,s}(B) = \tau_{t,s} \circ \delta_t(B), \qquad \text{with } \delta_t(B) := i[H_t, B].$$

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# Physical Properties of Quantum Systems

- **Set of states:** Continuous linear functionals $\rho \in \mathcal{X}^*$ that are positive and normalized on some $C^*$-algebra $\mathcal{X}$. For instance, on $\mathcal{X} = \mathcal{B}(\mathcal{H})$ with $\mathcal{H}$ being some Hilbert space, and for $B \in \mathcal{B}(\mathcal{H})$ and some $\psi \in \mathcal{H}$,

$$\rho_\psi(B) = \langle \psi, B\psi \rangle, \qquad B \in \mathcal{B}(\mathcal{H}).$$

  More generally, for $H = H^*$ acting on $\mathcal{H}$ with $\mathrm{Trace}\left(\mathrm{e}^{-\beta H}\right) < \infty$, $\beta > 0$,

$$\rho_{H,\beta}(B) = \frac{\mathrm{Trace}\left(B\mathrm{e}^{-\beta H}\right)}{\mathrm{Trace}\left(\mathrm{e}^{-\beta H}\right)}, \qquad B \in \mathcal{B}(\mathcal{H}).$$

- **Algebra of observables:** Self-adjoint elements of a $C^*$-algebra $\mathcal{X}$, like the self-adjoint elements of $\mathcal{B}(\mathcal{H})$, with $\mathcal{H}$ being some Hilbert space.

$$\Downarrow$$

1. **Hilbert-space formulation of QM:** Fix first a Hilbert space $\mathcal{H}$.
2. **Algebraic formulation of QM:** Fix first a $C^*$-algebra $\mathcal{X}$.

# Heisenberg /Schrödinger Pictures of Quantum Mechanics

(H1) **Heisenberg picture:** One uses a pair constituted of a $C^*$–algebra $\mathcal{X}$ and a group $\{\tau_t\}_{t\in\mathbb{R}}$ of $*$–automorphisms (i.e., a $C^*$–dynamical system). The set $\{\tau_t(A)\}_{t\in\mathbb{R}}$ represents the time-evolution of any element $A \in \mathcal{X}$.

(S2) **Schrödinger picture:** Any physical state of the system is given by a state $\rho \in \mathcal{X}^*$. The expectation value at time $t \in \mathbb{R}$ of an observable $A = A^* \in \mathcal{X}$ is given by

$$A \mapsto \rho \circ \tau_t(A) \in \mathbb{R}$$

and $\rho_t := \rho \circ \tau_t$ defines the time-evolution of the state in the Schrödinger picture.

The Hilbert space formulation is recovered from the GNS–representation $(\pi_\rho, \mathcal{H}_\rho, \Omega_\rho)$:

- $\mathcal{H} \Rightarrow$ Hilbert space $\mathcal{H}_\rho$.
- $\pi_\rho(\mathcal{X}) \subseteq \mathcal{B}(\mathcal{H}_\rho)$.
- The expectation value at time $t \in \mathbb{R}$ of an observable $A = A^* \in \mathcal{X}$ is given by

$$\rho_t = \rho \circ \tau_t(A) = \langle \Omega_\rho, \pi_\rho(\tau_t(A))\Omega_\rho \rangle \in \mathbb{R}.$$

# Towards the Hilbert Space Formulation

The Hilbert space formulation is recovered from the GNS–representation $(\pi_\rho, \mathcal{H}_\rho, \Omega_\rho)$:

- $\mathcal{H} \Rightarrow$ Hilbert space $\mathcal{H}_\rho$ and $\pi_\rho(\mathcal{X}) \subseteq \mathcal{B}(\mathcal{H}_\rho)$.
- The expectation value at time $t \in \mathbb{R}$ of an observable $A = A^* \in \mathcal{X}$ is given by

$$\rho_t = \rho \circ \tau_t(A) = \langle \Omega_\rho, \pi_\rho(\tau_t(A))\Omega_\rho \rangle \in \mathbb{R}.$$

- The dynamics can be unitarily implemented when the state is stationary:

## Theorem

*Let $\mathcal{X}$ be a unital $C^*$–algebra and a group $\{\tau_t\}_{t\in\mathbb{R}}$ of $*$–automorphisms.*
*(i) Then, there is has at least one stationary state $\rho \in \mathcal{X}^*$, i.e., $\rho \circ \tau_t = \rho$ for all $t \in \mathbb{R}$.*
*(ii) Let $(\mathcal{H}_\rho, \pi_\rho, \Omega_\rho)$ be its GNS–representation. Then, there is a unique family $(U_t)_{t\in\mathbb{R}}$ of unitary operators $\mathcal{H}_\rho \to \mathcal{H}_\rho$ such that, for all $A \in \mathcal{X}$ and $t \in \mathbb{R}$,*

$$\Omega_\rho = U_t\Omega_\rho \quad \text{and} \quad \pi_\rho(\tau_t(A)) = U_t\pi_\rho(A)U_t^*.$$

*(iii) $(U_t)_{t\in\mathbb{R}}$ is strongly continuous, i.e., for all $\psi \in \mathcal{H}_\rho$, the mapping $t \mapsto U_t\psi$ is a continuous function from $\mathbb{R}$ to $\mathcal{H}_\rho$. In particular, $U_t = \mathrm{e}^{itH}$ with $H = H^*$ acting on $\mathcal{H}_\rho$.*

# Outline

# Hilbert-Space of Quantum Particles

- Consider one quantum particle in $\Omega = \mathbb{R}^d$, $\mathbb{Z}^d$, etc.:

$$\mathcal{H}_1 = L^2(\Omega).$$

- Consider $N$ *different* quantum particles in $\Omega = \mathbb{R}^d$, $\mathbb{Z}^d$, etc.:

$$\mathcal{H}_N = \left(L^2(\Omega)\right)^{\otimes N} = L^2(\Omega^N).$$

- Consider $N$ *identical* quantum particles in $\Omega = \mathbb{R}^d$, $\mathbb{Z}^d$, etc.:

$$\mathcal{H}_N = \left\{\psi \in L^2(\Omega^N) : \forall \text{permutation } \pi,\ \psi(x_1, \ldots, x_N) = \varepsilon_\pi \psi\left(x_{\pi(1)}, \ldots, x_{\pi(N)}\right)\right\}.$$

There are basically two choices:

1. **Bosons:** $\varepsilon_\pi = 1$.
2. **Fermions:** $\varepsilon_\pi = \mathrm{sgn}(\pi)$ is the sign of the permutation $\pi$.

# Finite Number of Identical Particles

- Consider $N$ *identical* quantum in $\Omega = \mathbb{R}^d$, $\mathbb{Z}^d$, etc.:

$$\mathcal{H}_N = \left\{ \psi \in L^2(\Omega^N) : \forall \text{permutation } \pi,\ \psi(x_1, \ldots, x_N) = \varepsilon_\pi \psi\left(x_{\pi(1)}, \ldots, x_{\pi(N)}\right) \right\}$$

- Hamiltonian of the system: for external potential $V : \Omega \to \mathbb{R}$ and some pair (interaction) potential $v : \mathbb{R}^+ \to \mathbb{R}$,

$$H_N = \sum_{i=1}^{N} \left(-\Delta_i + V(x_i)\right) + \sum_{1 \leq i < j \leq N} v\left(|x_i - x_j|\right)$$

1. Ground state $\varphi_N$ (if it exists):

$$E_N := \inf_{\psi \in \mathcal{H}_N} \langle \psi, H_N \psi \rangle_{\mathcal{H}_N} = \langle \varphi_N, H_N \varphi_N \rangle_{\mathcal{H}_N} .$$

2. Schrödinger equation:

$$i\partial_t \psi(t) = H_N \psi(t), \qquad \psi(0) \in \mathcal{H}_N.$$

# Many-Boson Systems

- Consider $N$ *bosons* in $\Omega = \mathbb{R}^3$:

$$\mathcal{H}_N = \left\{ \psi \in L^2(\mathbb{R}^{3N}) : \forall \text{permutation } \pi,\ \psi(x_1, \ldots, x_N) = \psi\left(x_{\pi(1)}, \ldots, x_{\pi(N)}\right) \right\}$$

- Confining external potential $V : \mathbb{R}^3 \to \mathbb{R}$: $V(\lambda x) \sim \lambda^n V(\lambda x)$, as $\lambda \to \infty$.
- Fix some compactly supported pair potential $v : \mathbb{R}^+ \to \mathbb{R}^+$ and define

$$v_N(r) := N^3 v(N^\alpha r) \geq 0, \qquad \alpha \in [0, 1].$$

- Hamiltonian of the system:

$$H_N = \sum_{i=1}^{N} (-\Delta_i + V(x_i)) + \frac{1}{N} \sum_{1 \leq i < j \leq N} v_N(|x_i - x_j|)$$

1. Ground state $\varphi_N$ as $N \to \infty$ and

$$\lim_{N\to\infty} \frac{E_N}{N} := \lim_{N\to\infty} \frac{1}{N} \min_{\psi \in \mathcal{H}_N} \langle \psi, H_N \psi \rangle_{\mathcal{H}_N} = \lim_{N\to\infty} \frac{1}{N} \langle \varphi_N, H_N \varphi_N \rangle_{\mathcal{H}_N} \ ?$$

2. Schrödinger equation: As $N \to \infty$, what is

$$i\partial_t \psi(t) = H_N \psi(t), \qquad \psi(0) \in \mathcal{H}_N \ ?$$

# Ground State of Many-Boson Systems (1957-2023)

Cf. Dyson, Lieb, Yngvason, Seiringer, Nam, Rougerie, Serfaty, Lewin, Solovej, etc.

- As $N \to \infty$, the ground state energy of $H_N$ converges to

$$\lim_{N\to\infty} \frac{E_N}{N} = \lim_{N\to\infty} \frac{1}{N} \min_{\psi\in\mathcal{H}_N} \langle \psi, H_N \psi \rangle_{\mathcal{H}_N} = \min_{\varphi\in L^2(\mathbb{R}^3), \|\varphi\|_2=1} \mathcal{E}_{\mathrm{GP}}(\varphi) = \mathcal{E}_{\mathrm{GP}}(\varphi_{\mathrm{GP}})$$

with

$$\mathcal{E}_{\mathrm{GP}}(\varphi) := \int_{\mathbb{R}^3} \left\{ |\nabla\varphi(x)|^2 + V(x_i)\,|\varphi(x)|^2 + 4\pi a(\alpha)\,|\varphi(x)|^4 \right\} \mathrm{d}x$$

- If $\varphi_N$ is the ground state of $H_N$ and

$$\gamma_N^{(1)} = \int_{\mathbb{R}^3} |\varphi_N\rangle \langle\varphi_N| \, \mathrm{d}x_2 \cdots \mathrm{d}x_N \in \mathcal{B}(L^2(\mathbb{R}^3))$$

denotes the one-particle reduced density associated with $\varphi_N$, then

$$\gamma_N^{(1)} \to |\varphi_{\mathrm{GP}}\rangle \langle\varphi_{\mathrm{GP}}|$$

- The next order term of $E_N N^{-1}$ is also studied (cf. Bogoliubov spectrum), etc...

# Dynamics of Many-Boson Systems (1957-2023)

Cf. Dyson, Erdös, Schlein, Yau, Pickl, etc.

- Let $\varphi_N(t)$ be the solution of the Schrödinger equation

$$i\partial_t \varphi_N(t) = H_N \varphi_N(t), \qquad \varphi_N(0) = \varphi_N \in \mathcal{H}_N$$

  with initial state being in the ground state of $H_N$. Here, $\alpha = 1$ and, at time $t = 0$, the confining potential $V$ is switched off.

- Let

$$\gamma_N^{(1)}(t) = \int_{\mathbb{R}^3} |\varphi_N(t)\rangle \langle \varphi_N(t)| \, \mathrm{d}x_2 \cdots \mathrm{d}x_N \in \mathcal{B}(L^2(\mathbb{R}^3))$$

  be the one-particle reduced density associated with $\varphi_N(t)$. Then, for any $t \geq 0$,

$$\gamma_N^{(1)}(t) \to |\varphi_{\mathrm{GP}}(t)\rangle \langle \varphi_{\mathrm{GP}}(t)|$$

  with $\varphi_{\mathrm{GP}}(0) \in L^2(\mathbb{R}^3)$ being the ground state of the GP functional and

$$i\partial_t \varphi_{\mathrm{GP}}(t) = -\Delta \varphi_{\mathrm{GP}}(t) + 4\pi a(1) |\varphi_{\mathrm{GP}}(t)|^2 \varphi_{\mathrm{GP}}(t).$$

- Many other results for different initial states, $\alpha \in [0,1]$ or with $V \neq 0$.

# General Observations

- Results for $N \to \infty$ are basically at **zero temperature** on "mean-field" models for which the interaction term $\frac{1}{N} \sum_{1 \leq i < j \leq N} v_N \left( |x_i - x_j| \right)$ has a $N^{-1}$ coupling constant with often repulsive interactions $(v \geq 0)$.

- For a system in a box $\Lambda$, one usually fixes the **particle density** $N / |\Lambda|$ and let $|\Lambda| \to \infty$ to get a macroscopic system (thermodynamic limit).

  Previous results are for $N \to \infty$ but with either "$|\Lambda| < \infty$" (confining potential) or for $|\Lambda| = \infty$ (on full space).

- Many open questions: study of models with Lennard-Jones potentials (crystallization), non-zero temperature effects, etc.

- Note that semiclassical analysis is referred to as "putting quantum flesh on classical bones," where classical mechanics provides the skeletal framework on which quantum quantities are constructed.

- As observed by Haag in 1962 with the BCS model no reasonable microscopic theory of first order phase transitions is possible within the Hilbert space based approach, and the use of the algebraic setting is imperative.

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# Outline

# Algebraic Formulation of QM

- Unital $C^*$-algebra: $\mathcal{X} \equiv (\mathcal{X}, +, \cdot_{\mathbb{C}}, \times, ^*, \|\cdot\|_{\mathcal{X}})$, that is, a Banach algebra, with a unit $\mathfrak{1}$, endowed with an involution $A \mapsto A^*$ such that

$$\|A^*A\|_{\mathcal{X}} = \|A\|_{\mathcal{X}}^2 , \qquad A \in \mathcal{X} .$$

- **Observables.** The (real) Banach subspace of all self-adjoint elements $A = A^* \in \mathcal{X}$.
- **States.** Weak$^*$-compact convex set of states:

$$E := \bigcap_{A \in \mathcal{X}} \{\rho \in \mathcal{X}^* : \rho(A^*A) \geq 0, \ \rho(\mathfrak{1}) = 1\}$$

- **Heisenberg picture**. The dynamics is given by a strongly continuous group $\tau \doteq \{\tau_t\}_{t \in \mathbb{R}}$ of $*$–automorphisms generated by a symmetric derivation $\delta$ acting on $\mathcal{X}$:

$$\forall t \in \mathbb{R} : \quad \partial_t \tau_t = \tau_t \circ \delta = \delta \circ \tau_t , \qquad \tau_0 = 1_{\mathcal{X}} .$$

- **Schrödinger picture:** The dynamics for any initial state $\rho \in E$ is given by

$$\forall t \in \mathbb{R} : \quad \rho_t = \rho \circ \tau_t \in E , \qquad \rho_0 = \rho \in E .$$

# Importance of the Algebraic Approach for Infinite Systems

- A *representation* on the Hilbert space $\mathcal{H}$ of $\mathcal{X}$ is a $*$-homomorphism $\pi$ from $\mathcal{X}$ to $\mathcal{B}(\mathcal{H})$. Injective representations are called faithful.
- By the Gelfand-Naimark theorem, each $C^*$-algebra has, at least, one faithful representation: $\mathcal{X}$ can be identified with a $C^*$-subalgebra of some $\mathcal{B}(\mathcal{H})$.
- For any representation $\pi : \mathcal{X} \to \mathcal{B}(\mathcal{H})$, one constructs another one by doubling the Hilbert space $\mathcal{H}$ and the map $\pi$, via $\mathcal{H}_1 \oplus \mathcal{H}_2$ with $\mathcal{H}_1, \mathcal{H}_2$ being two copies of $\mathcal{H}$.

## Definition (notion of “minimal” representations)

If $\pi : \mathcal{X} \to \mathcal{B}(\mathcal{H})$ is a representation of $\mathcal{X}$ on $\mathcal{H}$, we say that it is *irreducible*, whenever $\{0\}$ and $\mathcal{H}$ are the only closed subspaces of $\mathcal{H}$ which are invariant w.r.t. to any operator of $\pi(\mathcal{X}) \subseteq \mathcal{B}(\mathcal{H})$.

## Definition (Unitarly equivalence)

Two representations $(\pi_1, \mathcal{H}_1)$ and $(\pi_2, \mathcal{H}_2)$ of $\mathcal{X}$ are equivalent if there is a unitary map $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $\pi_1(A) = U^* \pi_2(A) U$ for $A \in \mathcal{X}$.

## Theorem (Rosenberg, 1953)

*If a $C^*$-algebra $\mathcal{X}$ has a faithful representation on a separable Hilbert space, then its irreducible representation is unique (up to unitary equivalence) iff $\mathcal{X}$ is isomorphic to some $C^*$-algebra of compact operators on some Hilbert space.*

- The question whether all $C^*$-algebras with a unique (up to unitary equivalence) irreducible representation is isomorphic to an algebra of compact operators on a non-separable Hilbert space is known as "Naimark's problem". It depends on the continuum hypothesis and not only on the axioms of the Zermelo-Fraenkel set theory with the axiom of choice (ZFC).

## Corollary

*Let $\mathcal{X}$ be a unital $C^*$-algebra with faithful representation on a separable Hilbert space $\mathcal{H}$.*
*(i) $\dim \mathcal{H} < \infty$: Irreducible representations of $\mathcal{X}$ are unique, up to unitary equivalence.*
*(ii) $\dim \mathcal{H} = \infty$: $\mathcal{X}$ has more than one unitarily non-equivalent irreducible representation.*

- $\dim \mathcal{H} < \infty \Rightarrow$ **Algebraic and Hilbert-space formulations are equivalent.**
- $\dim \mathcal{H} = \infty \Rightarrow$ **Algebraic formulation more general than the other one.**

# Many-Body Problem in Fock Spaces

- $\mathfrak{h}$ is the one-particle Hilbert space. E.g., $\mathfrak{h} := L^2(\Omega)$ with $\Omega = \mathbb{R}^d, \mathbb{Z}^d$.
- The Fock space is the *Hilbert space* defined by

$$\mathcal{F} := \mathbb{C} \oplus \bigoplus_{n\in\mathbb{N}} \mathfrak{h}^{\otimes n}.$$

$\psi \in \mathcal{F}$ is a sequence $(\psi_n)_{n\geq 0}$ of vectors. $\mathfrak{h}^{\otimes n}$ is identified as the closed subspace of $\mathcal{F}$ formed by the vectors with all components except the $n$th equal to zero.

- Let $P_\pm : \mathcal{F} \to \mathcal{F}$ be defined by

$$P_\pm (f_1 \otimes \cdots \otimes f_n) := \frac{1}{n!} \sum_{\text{permutation } \pi} \varepsilon_{\pi,\pm} f_{\pi(1)} \otimes \cdots \otimes f_{\pi(n)}$$

with $\varepsilon_{\pi,+} = 1$ (bosons), $\varepsilon_{\pi,-} = \operatorname{sgn}(\pi)$ (fermion) is the sign of the permutation $\pi$.

## Definition (Creation and annihilation operators)

For $f \in \mathfrak{h}$, we define $a(f), a^*(f) : \mathfrak{h} \to \mathcal{F}$ by $a(f)\psi_0 = 0$, $a^*(f)\psi_0 = f$ and

$$\begin{aligned} a(f) f_1 \otimes \cdots \otimes f_N &= \sqrt{n} \langle f, f_1 \rangle_{\mathfrak{h}} f_2 \otimes \cdots \otimes f_N \\ a^*(f) f_1 \otimes \cdots \otimes f_N &= \sqrt{n+1} \langle f, f_1 \rangle_{\mathfrak{h}} f_1 \otimes f_2 \otimes \cdots \otimes f_N \end{aligned}$$

# Bosonic and Fermionic Fock Spaces

- Note that $a^*(f) = a(f)^*$, $a(f)(\mathfrak{h}^{\otimes n}) \subseteq \mathfrak{h}^{\otimes(n-1)}$ and $a^*(f)(\mathfrak{h}^{\otimes n}) \subseteq \mathfrak{h}^{\otimes(n+1)}$.
- $P_+\mathfrak{h}^{\otimes n}$ is $n$-boson Hilbert space and $P_-\mathfrak{h}^{\otimes n}$ is the $n$-fermion Hilbert space. Let $\mathcal{F}_\pm := P_\pm\mathcal{F}$, which is either the bosonic $(+)$ or fermionic $(-)$ Fock space.

## Definition (Creation and annihilation operators)

$$\forall f \in \mathfrak{h}, \qquad a_\pm(f) := P_\pm a(f) P_\pm, \qquad a_\pm^*(f) := P_\pm a^*(f) P_\pm = a_\pm(f)^* .$$

- (Anti-)symmetry of functions are replaced by commutation relations between $a_\pm(f), a_\pm^*(g)$ for $f, g \in \mathfrak{h}$:

$$\begin{aligned} a_\pm(f) a_\pm(g) \mp a_\pm(g) a_\pm(\varphi) &= 0, \\ a_\pm^*(f) a_\pm(g) \mp a_\pm(g) a_\pm^*(f) &= \langle g, f\rangle 1_{\mathcal{F}} . \end{aligned}$$

**Bosonic case $(+)$:** $a(f), a^*(f)$ are unbounded on $\mathcal{F}_+$. The above equalities $(+)$ are the Canonical Commutation Relations (CCR).

**Fermionic case $(-)$:** $a(\psi), a^*(f) \in \mathcal{B}(\mathcal{F}_-)$. The above equalities $(-)$ are the Canonical Anti–commutation Relations (CAR).

# The Second Quantization

- If $H = H^*$ on $\mathfrak{h}$, $H_0 = 0$ and for $n \in \mathbb{N}$, $H_n$ is defined on $P_\pm(\mathfrak{h}^{\otimes n})$ by

$$H_n P_\pm (f_1 \otimes \cdots \otimes f_n) := P_\pm \left( \sum_{i=1}^{n} f_1 \otimes \cdots \otimes H_n f_i \otimes \cdots \otimes f_n \right)$$

- The second quantization of $H$ is the operator defined on $\mathcal{F}_\pm$ by

$$d\Gamma(H) := \overline{\bigoplus_{n \geq 0} H_n}$$

- E.g., $\mathfrak{h} = L^2(\Omega)$ with $\Omega \subseteq \mathbb{Z}^3$ and $H = -\Delta_d$ (discrete laplacian). Then,

$$H_n = \sum_{i=1}^{n} -(\Delta_d)_i \quad \text{and} \quad d\Gamma(H) = \sum_{x,y\in\Omega} \langle \delta_{\cdot,y}, (-\Delta_d)\, \delta_{\cdot,x} \rangle\, a(\delta_{\cdot,y})^*\, a(\delta_{\cdot,x})$$

- In general, **all families** of $n$-body Hamiltonians can be encoded on the fermionic or bosonic Fock spaces $\mathcal{F}_\pm$ as polynomials in terms of $a_\pm(f), a_\pm^*(g)$ for $f, g \in \mathfrak{h}$.

# Example of Fermion Systems

- $\mathfrak{h}$ is the so-called one-particle Hilbert space. For instance, $\mathfrak{h} = \ell^2\left(\mathbb{Z}^d \times \mathrm{S}\right)$ where $\mathrm{S}$ is a finite (spin) set.
- The CAR algebra
$$\mathcal{X} = \left(\mathrm{CAR}\left(\mathfrak{h}\right), +, \cdot, *\right)$$
associated with the Hilbert space $\mathfrak{h}$ is the $C^*$-algebra generated by a unit $\mathfrak{1}$ and a family $\{a(f) \equiv a_-(f)\}_{f\in\mathfrak{h}}$ of elements satisfying Conditions (a)-(b):

  (a) The map $f \mapsto a(f)^*$ is (complex) linear.

  (b) The family $\{a(f)\}_{f\in\mathfrak{h}}$ satisfies the CAR: For all $f_1, f_2 \in \mathfrak{h}$,
$$a(f_1)a(f_2) + a(f_2)a(f_1) = 0, \quad a(f_1)a(f_2)^* + a(f_2)^* a(f_1) = \langle f_1, f_2\rangle_{\mathfrak{h}}\mathfrak{1}.$$
- $\{a(f)\}_{f\in\mathfrak{h}}$ can be viewed as operators acting on the fermionic Fock space $\mathcal{F}$ associated with $\mathfrak{h}$. Also, $\mathfrak{1} = 1_{\mathcal{F}} \in \mathcal{B}(\mathcal{F}_-)$ and $\mathcal{X} \subseteq \mathcal{B}(\mathcal{F}_-)$.

# Finite-Volume Systems

- Let $\mathfrak{h} = \ell^2\left(\mathbb{Z}^d \times \mathrm{S}\right)$ and $\mathfrak{h}_L = \ell^2\left(\Lambda_L \times \mathrm{S}\right) \subseteq \mathfrak{h}$ with $\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$, $L \in \mathbb{N}_0$ and $\mathrm{S}$ being any finite (spin) set. Then,

$$\mathrm{CAR}\left(\mathfrak{h}_L\right) \subseteq \mathrm{CAR}\left(\mathfrak{h}\right) = \overline{\bigcup_{L\in\mathbb{N}} \mathrm{CAR}\left(\mathfrak{h}_L\right)}.$$

- Using $a_{x,\mathrm{s}} := a\left(\delta_{\cdot,(x,\mathrm{s})}\right)$ we use the Hamiltonian

$$H_L := \underbrace{\sum_{x,y\in\Lambda_L,\mathrm{s}\in\mathrm{S}} h\left(|x-y|\right) a^*_{x,\mathrm{s}} a_{y,\mathrm{s}}}_{\text{kinetic term}} + \underbrace{\sum_{x,y\in\Lambda_L,\mathrm{s},\mathrm{t}\in\mathrm{S}} v\left(|x-y|\right) a^*_{y,\mathrm{t}} a_{y,\mathrm{t}} a^*_{x,\mathrm{s}} a_{x,\mathrm{s}}}_{\text{interparticle interaction}}$$

  $h : \mathbb{R}_0^+ \to \mathbb{R}$ is the hopping term and is assumed to decay at large distances.
  $v : \mathbb{R}_0^+ \to \mathbb{R}$ is a pair potential. It is usually assumed to be fast decaying.

- Equilibrium states: For any inverse temperature $\beta \in \mathbb{R}^+$, the Gibbs states is the state on the finite-dimensional $\mathrm{CAR}\left(\mathfrak{h}_L\right)$ defined by

$$\rho_L\left(A\right) := \frac{\mathrm{Trace}(A\mathrm{e}^{-\beta H_L})}{\mathrm{Trace}(\mathrm{e}^{-\beta H_L})}, \qquad A \in \mathrm{CAR}\left(\mathfrak{h}_L\right).$$

  It can be extended as a state on $\mathrm{CAR}\left(\mathfrak{h}\right)$.

# Thermodynamic Limit

- For any inverse temperature $\beta \in \mathbb{R}^+$, the Gibbs states is the **unique** solution to a variational problem:

$$P_L \doteq \frac{1}{\beta|\Lambda_L|} \ln \mathrm{Trace}(\mathrm{e}^{-\beta H_L}) = - \inf_{\text{state } \rho \text{ on } \mathrm{CAR}(\mathfrak{h}_L)} \left\{ \frac{\rho(H_L)}{|\Lambda_L|} - \frac{S(\rho)}{\beta|\Lambda_L|} \right\}$$

with $S(\rho)$ being the so-called von Neumann entropy.

- In the thermodynamic limit $L \to \infty$ ($\to$ dimension $\infty$), one proves [Araki-Moriya, 2003] that

$$P := \lim_{L\to\infty} P_L = - \inf_{\rho \in E_1} \left\{ e(\rho) - \beta^{-1} s(\rho) \right\} < \infty \qquad (1)$$

where $E_1$ is the weak$^*$ compact set of translation invariant states, $e : E_1 \to \mathbb{R}$ is the energy density and $s : E_1 \to \mathbb{R}$ is the entropy density, defined by

$$e(\rho) := \lim_{L\to\infty} \frac{\rho(H_L)}{|\Lambda_L|} \qquad \text{and} \qquad s(\rho) := \lim_{L\to\infty} \frac{S(\rho)}{|\Lambda_L|}$$

$e$ and $s$ are weak$^*$ lower semicontinuous and equilibrium states are solutions to (1).

$\Rightarrow$ **Uniqueness can be broken, cf. 1st order phase transitions, BCS model of superconductivity (Haag, 1962).**

# Example of Lattice Fermion Systems

- Let $\mathfrak{h} = \ell^2(\mathbb{Z}^d \times \mathrm{S})$ and $\mathfrak{h}_L = \ell^2(\Lambda_L \times \mathrm{S}) \subseteq \mathfrak{h}$ with $\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$ and $\mathrm{S}$ being any finite (spin) set. For $L \in \mathbb{N}_0$, the fermionic Fock space is

$$\mathcal{F}_-^{(L)} := \mathbb{C} \oplus \bigoplus_{n=1}^{|\Lambda \times \mathrm{S}|} \{\text{antisymmetric } \psi \in \mathfrak{h}_L^{\otimes n}\}, \quad \dim \mathcal{F}_-^{(L)} = 2^{|\Lambda_L \times \mathrm{S}|}.$$

- For $L \in \mathbb{N}_0$, let $\mathrm{CAR}(\mathfrak{h}_L) \subseteq \mathrm{CAR}(\mathfrak{h})$ be the unital $C^*$–algebra generated by elements $\{a(f)\}_{f \in \mathfrak{h}_L}$ satisfying the CAR.
- $\exists!$ *faithful* and *irreducible* representation $\pi$ of $\mathrm{CAR}(\mathfrak{h})$ on $\mathcal{F}_-^{(\infty)}$ so that

$$\pi(\mathrm{CAR}(\mathfrak{h}_L)) = \mathcal{B}(\mathcal{F}_-^{(L)}), \qquad L \in \mathbb{N}_0 .$$

- The Fock space $\mathcal{F}_-^{(\infty)}$ has infinite dimension and is separable $\Rightarrow$ Algebraic formulation more general than the Hilbert-space one.
- One proves that

$$\pi(\mathrm{CAR}(\mathfrak{h})) = \overline{\bigcup_{L \in \mathbb{N}_0} \mathcal{B}(\mathcal{F}_-^{(L)})} \subsetneq \mathcal{B}(\mathcal{F}_-^{(\infty)})$$

and the state space of $\pi(\mathrm{CAR}(\mathfrak{h}))$ is **strictly larger** than the one of $\mathcal{B}(\mathcal{F}_-^{(\infty)})$.

- In infinite volume, we study the variational problem

$$\inf_{\rho \in E_1} F(\rho) \leq \inf_{\rho \in E_1 : \rho \circ \pi \text{ extends to a state on } \mathcal{B}(\mathcal{F}_-^{(\infty)})} F(\rho)$$

with $F := e - \beta^{-1} s$. Here, $E_1$ is the weak$^*$ compact convex set of translation invariant states, $e : E_1 \to \mathbb{R}$ is the energy density and $s : E_1 \to \mathbb{R}$ is the entropy density.

- The set of **equilibrium** states is defined by

$$M := \{\omega \in E_1 : F(\omega) = \inf F(E_1)\} \neq \emptyset$$

- GNS: For each $\omega \in M$, there is a unique (up to a unitary transformation) cyclic representation $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega)$ such that

$$\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle_{\mathcal{H}_\omega}, \qquad A \in \mathrm{CAR}(\mathfrak{h}).$$

- $(\pi_\omega, \mathcal{H}_\omega)$ is not necessarily unitarily equivalent to $(\pi, \mathcal{F}_-^{(\infty)})$, in particular if

$$\inf_{\rho \in E_1} F(\rho) < \inf_{\rho \in E_1 : \rho \circ \pi \text{ extends to a state on } \mathcal{B}(\mathcal{F}_-^{(\infty)})} F(\rho)$$