Modular Theory
in Quantum Field Theory

(part 1: The CCR & Araki–Woods representation)

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Introduction

In statistical mechanics, modular theory provides powerful tools that survive the thermodynamic limit. In QFT (also on curved spacetimes) it is the primary ingredient to define measures of entanglement through different notions of entropy. The Araki–Woods '63 construction plays a distinguished role in both.

References:

- O. Brattelli, D. W. Robinson: Operator Algebras and Quantum Statistical Mechanics 2
- V. Jakšic, Y. Ogata, Y. Pautrat, C.-A. Pillet, Entropic fluctuations in quantum statistical mechanics. An introduction *(however focus on fermions there, e.g. Araki–Wyss representation)*
- J. Derezinski, C. Gérard, Mathematics of Quantization and Quantum Fields
- C. Gérard, Microlocal Analysis of Quantum Fields on Curved Spacetimes

Bosonic Fock spaces and CCR

Let complex $\mathcal{K}$ Hilbert space. Bosonic Fock space

$$\Gamma(\mathcal{K}) = \bigoplus_{n\geqslant 0} \Gamma_n(\mathcal{K}), \quad \Gamma_n(\mathcal{K}) = \mathcal{K}^{\otimes_s n},$$

with vacuum vector $\Omega = (1, 0, 0^{\otimes 2}, 0^{\otimes 3}, \dots)$. If $A \in B(\mathcal{K})$, second quantization $\Gamma(A), \mathrm{d}\Gamma(A) \in B(\Gamma(\mathcal{K}))$ defined as direct sums of

$$\Gamma_n(A)(f_1 \otimes_s \cdots \otimes_s f_n) = Af_1 \otimes_s \cdots \otimes_s Af_n,$$

$$\mathrm{d}\Gamma_n(A)(f_1 \otimes_s \cdots \otimes_s f_n) = Af_1 \otimes_s \cdots \otimes_s f_n + \cdots + f_1 \otimes_s \cdots \otimes_s Af_n.$$

Properties:

$$\Gamma(AB) = \Gamma(A)\Gamma(B), \quad \mathrm{d}\Gamma(A) = \frac{\mathrm{d}}{\mathrm{d}t}\Gamma(e^{tA})|_{t=0}, \quad \Gamma(e^A) = e^{\mathrm{d}\Gamma(A)}$$

$$[\mathrm{d}\Gamma(A), \mathrm{d}\Gamma(B)] = \mathrm{d}\Gamma([A, B]).$$

Creation and annihilation operators for $f \in \mathcal{K}$ are symmetrizations and direct sums of

$$a(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = n^{\frac{1}{2}} \langle f | f_1 \rangle f_2 \otimes f_3 \otimes \cdots f_n,$$
$$a^*(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = (n+1)^{\frac{1}{2}} f \otimes f_1 \otimes f_2 \otimes f_3 \otimes \cdots f_n.$$

They satisfy

$$[a(f), a(g)] = 0 = [a^*(f), a^*(g)], \quad [a(f), a^*(g)] = \langle f | g \rangle \mathbf{1}.$$

The field operators are

$$\Phi(f) = \frac{1}{\sqrt{2}}(a(f) + a^*(f)), \quad f \in \mathcal{K}$$

and satisfy the CCR

$$\Phi(f_1)\Phi(f_2) - \Phi(f_2)\Phi(f_1) = i \operatorname{Im}\langle f_1 | f_2 \rangle \mathbf{1} =: i\sigma(f_1, f_2)\mathbf{1}$$

(Non)-equivalent CCR representations $f \mapsto \Phi(f)$ (or $f \mapsto a^\#(f)$):

$$\text{new scalar product } \langle f_1 | f_2 \rangle_j = \sigma(f_1, jf_2) + \sigma(f_1, f_2)$$

provided $(\mathcal{K}_\mathbb{R}, \sigma, j)$ is Kähler, i.e. $j^2 = -\mathbf{1}$ and $\sigma \circ j \geqslant 0$. New Hilbert space by complexification:

$$(\alpha + \beta)f := \alpha h + j\beta f, \quad f \in \mathcal{K}_\mathbb{R}, \ \alpha + \beta \in \mathbb{C}.$$

Bosonic quasi-free states for finite systems

Let $\dim \mathcal{K} < \infty$. Let $Q \in B(\mathcal{K})$ be such that

$$0 \leqslant Q \leqslant 1, \quad \mathrm{Ker}(\mathbf{1} - Q) = \{0\}.$$

Then, define the operator

$$T := Q(\mathbf{1} - Q)^{-1}, \quad Q = T(\mathbf{1} + T)^{-1}$$

referred to as 1-particle charge density, or in short density. To T we associate the normalization factor $Z_T = \mathrm{Tr}(\Gamma(Q)) = \mathrm{Tr}(\Gamma(T/(\mathbf{1} + T)))$ the density matrix

$$\omega_T = \frac{1}{Z_T} \Gamma\left(\frac{T}{\mathbf{1} + T}\right) = \frac{1}{\mathrm{Tr}(\Gamma(Q))} \Gamma(Q).$$

We denote by the same letter ω_T the corresponding state on $B(\Gamma(\mathcal{K}))$. It is called the quasi-free state associated to the density T.

$$T := Q(\mathbf{1}-Q)^{-1}, \quad Q = T(\mathbf{1}+T)^{-1}, \quad \frac{1}{Z_T}\Gamma\left(\frac{T}{\mathbf{1}+T}\right) = \frac{1}{\mathrm{Tr}(\Gamma(Q))}\Gamma(Q).$$

This applies in particular to the situation when we are given a one-particle Hamiltonian $h = h^* \in B(\mathcal{K})$, and want to consider the Gibbs state

$$\frac{e^{-\beta d\Gamma(h)}}{\mathrm{Tr}\, e^{-\beta \mathrm{d}\Gamma(h)}}$$

at inverse temperature β for the Hamiltonian of the free Bose gas $\mathrm{d}\Gamma(h)$. The corresponding density is

$$T = \frac{1}{e^{\beta h} - \mathbf{1}}$$

and in our notation $Q = e^{-\beta h}$.

No problem for finite systems, but Gibbs density matrix problematic in thermodynamic limit or in QFT.

$$T := Q(\mathbf{1}-Q)^{-1}, \quad Q = T(\mathbf{1}+T)^{-1}, \quad \frac{1}{Z_T}\Gamma\left(\frac{T}{\mathbf{1}+T}\right) = \frac{1}{\mathrm{Tr}(\Gamma(Q))}\Gamma(Q).$$

Theorem

1. *If* $g_1,\dots,g_n, f_1,\dots,f_m \in \mathcal{K}$, *then*

$$\omega_T(a^*(g_n)\cdots a^*(g_1)a(f_1)\cdots a(f_m)) = \delta_{nm}\mathrm{perm}[\langle f_i|Tg_j\rangle],$$

   where perm *defined as* det *but with only* $+$ *signs. In particular* $\omega_T(a^*(g)a(f)) = \langle f|Tg\rangle$.

2. $\log Z_T = \log\det(\mathbf{1}+T) = \mathrm{Tr}(\log(\mathbf{1}+T))$.
3. $\omega_T(\Gamma(A)) = \det(\mathbf{1}+T(\mathbf{1}-A))$.
4. $\omega_T(\mathrm{d}\Gamma(A)) = \mathrm{Tr}(TA)$.
5. $S(\omega_T) = -\mathrm{Tr}(T\log T - (\mathbf{1}+T)\log(\mathbf{1}+T))$, *where* $S(\omega_T) = -\omega_T \ln \omega_T$.
6. $\omega_{T_1} \ll \omega_{T_2}$ *iff* $\mathrm{Ker}\, T_1 \subset \mathrm{Ker}\, T_2$, *and then*

$$S(\omega_{T_1}|\omega_{T_2}) = \mathrm{Tr}\left(T_1(\log T_2 - \log T_1) - (\mathbf{1}+T_1)(\log(\mathbf{1}+T_2) - \log(\mathbf{1}+T_1))\right)$$

Uses a lot formula $\mathrm{Tr}\,\Gamma(A) = \det(1-A)^{-1}$.

Araki–Woods representation

With $T = Q(\mathbf{1} - Q)^{-1}$ as previously, set

$$\begin{aligned} \mathcal{H}_{\mathsf{AW}} &= \Gamma(\mathcal{K}) \otimes \Gamma(\mathcal{K}), \\ \Omega_{\mathsf{AW}} &= \Omega \otimes \Omega, \\ b^*_{\mathsf{AW}} &= a^*((\mathbf{1} + T)^{\frac{1}{2}} f) \otimes \mathbf{1} + \mathbf{1} \otimes a(\overline{T^{1/2} f}), \\ b_{\mathsf{AW}} &= a((\mathbf{1} + T)^{\frac{1}{2}} f) \otimes \mathbf{1} + \mathbf{1} \otimes a^*(\overline{T^{1/2} f}). \end{aligned}$$

1. $f \mapsto b^\#_{\mathsf{AW}}(f)$ define a representation of the CCR over $\mathcal{K}$ on $\mathcal{H}_{\mathsf{AW}}$.
2. Let π_{AW} be the induced representation of $B(\Gamma(\mathcal{K}))$ on $\mathcal{H}_{\mathsf{AW}}$. Ω_{AW} is a cyclic vector for this representation and

   $$\omega_T(A) = (\Omega_{\mathsf{AW}} | \pi_{\mathsf{AW}}(A) \Omega_{\mathsf{AW}}),$$

   for all $A \in B(\Gamma(\mathcal{K}))$.
3. The modular conjugation is given by

   $$J(\psi_1 \otimes \psi_2) = \overline{\psi_2} \otimes \overline{\psi_1}.$$

4. The modular operator of ω_T is

$$\Delta_{\omega_T} = \Gamma(Q) \otimes \Gamma(\overline{Q^{-1}}).$$

In consequence

$$\log \Delta_{\omega_T} = \mathrm{d}\Gamma(\log Q) \otimes \mathbf{1} - \mathbf{1} \otimes \mathrm{d}\Gamma(\overline{\log Q}).$$

5. If ω_{T_1} is the quasi-free state of density $T_1 > 0$ then the relative Hamiltonian is

$$\ell_{\omega_{T_1}|\omega_T} = \log\det\left((\mathbf{1}+T_1)(\mathbf{1}+T)^{-1}\right) + \mathrm{d}\Gamma(\log Q_1 - \log Q),$$

with $Q_1 = T_1(\mathbf{1}+T_1)^{-1}$, and

$$\log \Delta_{\omega_{T_1}|\omega_T} = \log \Delta_{\omega_T} + \pi_{\mathrm{AW}}(\ell_{\omega_{T_1}|\omega_{T_2}})$$

6. Suppose h commutes with T. Then ω_T is invariant under the dynamics τ^t generated by $H = \mathrm{d}\Gamma(h)$. Moreover

$$K = \mathrm{d}\Gamma(h) \otimes \mathbf{1} - \mathbf{1} \otimes \mathrm{d}\Gamma(\overline{h})$$

is the standard Liouvillean of this dynamics.

Let us abbreviate $\Delta = \Delta_{\omega_T}$. For (1) and (2) it suffices to prove that

$$J\Delta^{\frac{1}{2}} A\Omega_{\mathsf{AW}} = A^* \Omega_{\mathsf{AW}}$$

for any monomial $A = b^{\#}_{\mathsf{AW}}(f_n) \cdots b^{\#}_{\mathsf{AW}}(f_1)$. We do it by induction on n.
We first compute

$$b'_{\mathsf{AW}}(f) := Jb_{AW}(f)J = a^*(T^{\frac{1}{2}} f) \otimes \mathbf{1} + \mathbf{1} \otimes a(\overline{(\mathbf{1}+T)^{\frac{1}{2}} f}),$$
$$b'^*_{\mathsf{AW}}(f) = Jb^*_{AW}(f)J = a(T^{\frac{1}{2}} f) \otimes \mathbf{1} + \mathbf{1} \otimes a^*(\overline{(\mathbf{1}+T)^{\frac{1}{2}} f}),$$

and check that $[b'_{\mathsf{AW}}(f), b^{\#}_{\mathsf{AW}}(g)] = 0$ for all $f, g \in \mathcal{K}$. Next, we observe that

$$\Delta^{\frac{1}{2}} b_{\mathsf{AW}}(f) \Delta^{-\frac{1}{2}} = b_{\mathsf{AW}}(Q^{-\frac{1}{2}} f), \quad \Delta^{\frac{1}{2}} b^*_{\mathsf{AW}}(f) \Delta^{-\frac{1}{2}} = b^*_{\mathsf{AW}}(Q^{\frac{1}{2}} f).$$

For $n = 1$, the claim follows from the fact that

$$\begin{aligned} J\Delta^{\frac{1}{2}} b_{\mathsf{AW}}(f)\Omega_{\mathsf{AW}} &= J\Delta^{\frac{1}{2}} b_{\mathsf{AW}}(f)\Delta^{-\frac{1}{2}} J\Omega_{\mathsf{AW}} \\ &= b'_{\mathsf{AW}}(Q^{-\frac{1}{2}} f)\Omega_{\mathsf{AW}} \\ &= \big(a^*(Q^{-1} T^{\frac{1}{2}} f) \otimes \mathbf{1}\big)\Omega_{\mathsf{AW}} \\ &= b^*_{\mathsf{AW}}(f)\Omega_{\mathsf{AW}}. \end{aligned}$$

Next, for the induction, let A be a monomial of degree less than n in the $b^\#_{\mathsf{AW}}$ and assume that $J\Delta^{\frac{1}{2}}A\Omega_{\mathsf{AW}} = A^*\Omega_{\mathsf{AW}}$ for all such monomials. Then,

$$\begin{aligned} J\Delta^{\frac{1}{2}} b^\#_{\mathsf{AW}}(f)A\Omega_{\mathsf{AW}} &= (J\Delta^{\frac{1}{2}} b^\#_{\mathsf{AW}}(f)\Delta^{-\frac{1}{2}}J)J\Delta^{\frac{1}{2}}A\Omega_{\mathsf{AW}} \\ &= (Jb^\#_{\mathsf{AW}}(Q^{\mp\frac{1}{2}}f)J)A^*\Omega_{\mathsf{AW}} \\ &= b'^\#_{\mathsf{AW}}(Q^{\mp\frac{1}{2}}f)A^*\Omega_{\mathsf{AW}} \\ &= A^* b'^\#_{\mathsf{AW}}(Q^{\mp\frac{1}{2}}f)\Omega_{\mathsf{AW}} \\ &= A^* J\Delta^{\frac{1}{2}} b^\#_{\mathsf{AW}}(f)\Delta^{-\frac{1}{2}}J\Omega_{\mathsf{AW}} \\ &= A^* J\Delta^{\frac{1}{2}} b^\#_{\mathsf{AW}}(f)\Omega_{\mathsf{AW}} \\ &= A^* b^\#_{\mathsf{AW}}(f)^*\Omega_{\mathsf{AW}}, \end{aligned}$$

which shows that the induction property holds for all monomials of degree $\leqslant n+1$. □

Valid for $\dim \mathcal{K} = \infty$, Araki–Woods representations are valid without trace-class assumptions.

Quasi-free states on Weyl C^*-algebra

Given a symplectic space $(\mathcal{X}, \sigma)$ there is a unique up to *-isomorphism C^*-algebra (the Weyl C^*-algebra) generated by $V(f)$, $f \in \mathcal{X}$, s.t.

1. $V(-f) = V(f)^*$,
2. $V(f)V(g) = e^{-i\sigma(f,g)/2} V(f+g)$

A state is a positive unital functional ω. A state ω is quasi-free if there is a symmetric form η (called covariance) s.t.

$$\omega(V(f)) = e^{-\eta(f,f)/2}$$

Our next goal: The GNS representation of ω is an Araki–Woods representation, with density Q identified with a complexification of $\eta - \frac{i}{2}\sigma$.

Proposition

Suppose η is a covariance as above, η is non-degenerate and $\mathcal{X}$ is complete for η. If $\dim \operatorname{Ker} \sigma$ is even or infinite, then there exists an anti-involution j such that (η, j) is Kähler.

(roughly, polar decomposition of $\frac{1}{2}\eta^{-1}\sigma$)

For many purposes we can replace the Weyl C^*-algebra by a "polynomial" $*$-algebra $\mathsf{CCR}(\mathcal{X}, \sigma)$ finitely spanned by abstract field elements $\mathcal{X} \ni f \mapsto \Phi(f)$ satisfying the CCR

$$[\Phi(f), \Phi(g)] = i\sigma(f, g)\mathbf{1}$$

formally, $\Phi(f) = \frac{\mathrm{d}}{\mathrm{d}t} W(tf)|_{t=0}$.

A quasi-free state ω on $\mathsf{CCR}(\mathcal{X}, \sigma)$ is characterized by:

$$\omega(\Phi(f_1) \cdots \Phi(f_n)) = 0,$$

$$\omega(\Phi(f_1) \cdots \Phi(f_n)) = \sum_{s \text{ pair}} \prod_{j=1}^{m} \omega(\Phi(f_{s(2j-1)}\Phi(f_{s(2j)})))$$

and η is equivalently characterized by two-point function

$$\omega(\Phi(f)\Phi(g)) = \eta(f, g) + \frac{i}{2}\sigma(f, g).$$

The GNS representation associated to ω is **equivalent to the Araki–Woods representation** based on the Hilbert space $\mathcal{K} := \mathcal{X}$ with complex structure j and

$$\langle f|g\rangle := \sigma(f, jg) + i\sigma(f, g),$$

with density Q computed from $\langle f|Qf\rangle = \eta(f, f)$.

Kay doubling

Our representation was actually the left Araki–Woods representation $b^{\#}_{\mathsf{AW}}$, and it comes with the right Araki–Woods representation (which appeared already!):

$$b'_{\mathsf{AW}}(f) := Jb_{AW}(f)J = a^*(T^{\frac{1}{2}}f) \otimes \mathbf{1} + \mathbf{1} \otimes a(\overline{(\mathbf{1}+T)^{\frac{1}{2}}f}).$$

In terms of the field operators $\Phi_{\mathsf{AW}}(f)$, $\Phi'_{\mathsf{AW}}(f)$,

$$[\Phi_{\mathsf{AW}}(f), \Phi_{\mathsf{AW}}(g)] = i\sigma(f,g)\mathbf{1}, \quad [\Phi'_{\mathsf{AW}}(f), \Phi'_{\mathsf{AW}}(g)] = -i\sigma(f,g)\mathbf{1}$$

Doubling procedure (by Kay '85 in QFT context):

$$(\mathcal{X}_{\mathsf{d}}, \sigma_d) := (\mathcal{X}, \sigma) \oplus (\mathcal{X}, -\sigma), \quad \Phi_{\mathsf{d}}((f,g)) := \Phi_{\mathsf{AW}}(f) + \Phi'_{\mathsf{AW}}(g).$$

The vacuum vector Ω induces a quasi-free state ω_{d} on $\mathsf{CCR}(\mathcal{X}_{\mathsf{d}}, \sigma_{\mathsf{d}})$, formally by

$$\omega_{\mathsf{d}}(\Phi((f_1,g_1))\Phi((f_2,g_2))) := \langle \Omega | \Phi_{\mathsf{d}}((f_1,g_1))\Phi_{\mathsf{d}}((f_2,g_2))\Omega\rangle$$

This state is a pure state.

Modular conjugation exchanges σ and $-\sigma$ ("time reversal") and creation/annihilation processes.