Thermal states in pAQFT: stability, relative entropy and entropy production

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Joint work with Nicolò Drago and Federico Faldino
[arXiv:1609.01124 in CMP] [arXiv:1710.09747]

Plan of the talk

1. Thermal states for C^*-dynamical systems
2. Perturbative algebraic quantum field theory and KMS states *[Fredenhagen Lindner]*
3. Stability of KMS states for spatially compact interactions
4. Instabilities under the adiabatic limit and non equilibrium steady states NESS
5. Relative entropy and entropy production for these states.

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Basic settings of quantum statistical mechanics

- Let $\mathcal{A}$ be the C^*-algebra describing the **observables** of the theory.

- **Time evolution** (also called **dynamics**) is described by a one-parameter group of $*-$automorphisms $t \mapsto \alpha_t$, $\alpha_t : \mathcal{A} \to \mathcal{A}$.

- A C^*-algebra $\mathcal{A}$ equipped with a continuous time evolution α_τ forms a C^*-**dynamical system**

- A **state** ω over $\mathcal{A}$ is a linear functional which is positive and normalized $\omega(1) = 1$.

C^*-dynamical systems and equilibrium states

Equilibrium states are characterized by the KMS condition

Definition (KMS states)

A state ω for $\mathcal{A}$, invariant under α_t, is a $(\beta, \alpha_t)-$KMS state if $\forall A, B \in \mathcal{A}$ the map

$$t \mapsto \omega(A\alpha_t(B))$$

can be extended to an analytic function in the strip $\Im(t) \in [0, \beta]$ and if

$$\omega(A\alpha_{i\beta}(B)) = \omega(BA).$$

β is the inverse temperature.

- Gibbs states for discrete systems are KMS states
- KMS condition is meaningful for infinitely extended systems
- KMS states are stable under perturbation of the dynamics

Araki construction of perturbed KMS states

Consider $P = P^* \in \mathcal{A}$ the perturbation Hamiltonian.

Then the perturbed dynamics α^P is such that

$$\alpha_t^P(A) = U(t)\alpha_t(A)U(t)^*,$$

where $U(t)$ is the cocycle generated by P

Theorem (Araki)

Let ω be an extremal $(\beta, \alpha)-$KMS state and α^P the perturbed dynamics. Consider

$$\omega^P(A) := \frac{\omega(AU(i\beta))}{\omega(U(i\beta))}$$

where $\omega(AU(i\beta))$ is the analytic continuation of $\omega(AU(t))$, then $\omega^P(A)$ is a $(\beta, \alpha^P)-$KMS state.

Stability of KMS states for C^*-dynamical systems

If **strong clustering** holds for ω

$$\lim_{t\to\pm\infty} \omega(A\alpha_t(B)) = \omega(A)\omega(B)$$

stability - return to equilibrium hold:

$$\lim_{t\to\infty} \omega(\alpha_t^P(A)) = \omega^P(A) \qquad \text{and} \qquad \lim_{t\to\infty} \omega^P(\alpha_t(A)) = \omega(A)$$

[Haag Kastler Trych-Pohlmeyer, Bratteli Robinson, Bratteli Robinson Kishimoto]

Aim

extend the scheme to encompass perturbatively constructed KMS states for interacting quantum field theories

Quantum field theories (PAQFT)

- Real scalar fields on Minkowski space M (with signature $-,+,+,+$)

$$-\Box\phi + m^2\phi + \lambda V^{(1)}(\phi) = 0, \qquad V(\phi) = \int \phi^n(x) f(x) d\mu$$

- Observables are **functionals** over the field configurations $\varphi \in \mathcal{C} := C^\infty(M;\mathbb{R})$ (**off-shell**)

$$\mathcal{F}_{\mu c} := \{F : \mathcal{C} \to \mathbb{C} \mid \text{smooth, compactly supported, microcausal}\}$$

Examples $f \in C_0^\infty$

$$\Phi(f) := \int_M f(x)\varphi(x) d\mu(x), \qquad F(\varphi) = \int_{M\times M} \varphi(x)\varphi(y) f(x,y) d\mu(x) d\mu(y), \qquad \Phi^2(f) := \int_M f(x)\varphi(x)^2 d\mu(x)$$

- Local functionals are contained in $\mathcal{F}_{\mu c}$

$$\mathcal{F}_{loc} := \left\{ F \in \mathcal{F}_{\mu c} \,\middle|\, \text{supp}F^{(n)} \subset \text{Diag}_n \right\}$$

Free quantum theory

- Set $\lambda = 0$

$$P\phi := -\Box\phi + m^2\phi = 0$$

- On $\mathcal{F}_{\mu c}$ acts the following product (compatible with the free dynamics):

$$F \star_\omega G := e^{\langle \omega, \frac{\delta^2}{\delta\varphi\delta\varphi'} \rangle} F(\varphi)G(\varphi')\big|_{\varphi'=\varphi}$$

where ω is an Hadamard bidistribution:

  - ω is a bisolution of the equation of motion up to smooth functions
  - $\omega(x,y) - \omega(y,x) = i\Delta(x,y)$
  - it satisfies the microlocal spectrum condition then the product of microcausal functionals is well defined.

- $(\mathcal{F}_{\mu c}, \star_\omega)$ is the algebra of observable of the free theory.

$$[\Phi(f), \Phi(h)]_\star := \Phi(f) \star \Phi(h) - \Phi(h) \star \Phi(f) = i\Delta(f,h), \qquad f, h \in \mathcal{D}(M)$$

- Local fields are Wick ordered wrt ω
- Different ω produce isomorphic algebras

Introduction to pAQFT

- Interacting fields can be treated perturbatively within the algebraic picture *[Brunetti, Dütch, Fredenhagen, Hollands, Rejzner, Wald]*

  Observables are **formal power series** in the coupling constant λ with coefficients in $\mathcal{F}_{\mu c}$ namely elements of $\mathcal{F}_{\mu c}[[\lambda]]$.
- To construct them explicitly, the time ordering map is needed:

$$T : \mathcal{F}_{loc}^{\otimes n} \to \mathcal{F}_{\mu c}$$

  On **regular functionals**, T is characterised by the **causal factorisation property**

$$T(A, B) = T(A) \star T(B) \qquad \text{if} \qquad A \gtrsim B$$

  where $A \gtrsim B$ if $J^+(\mathrm{supp}(A)) \cap \mathrm{supp}(B) = \emptyset$.
  It can be extended to local functionals (in a non unique way, there are renormalization ambiguities) *[Epstain Glaser, Steinmann, Brunetti Fredenhagen, Hollands Wald]*
- The **formal** $S-$**matrix** of $V \in \mathcal{F}_{loc}$ is the time ordered exponential

$$S(V) := \exp_T \left(\frac{i\lambda}{\hbar} V \right)$$

- The causal factorisation property of the $S-$matrix

$$S(A + B + C) = S(A + B) \star S(B)^{-1} \star S(B + C), \qquad \text{if} \qquad A \gtrsim C$$

- The **Bogoliubov map** is used to construct interacting field theories

$$\mathcal{R}_V(F) := \frac{d}{d\lambda} S_V(\lambda F)\Big|_{\lambda=0} := \frac{d}{d\lambda} S(V)^{-1} \star S(V+\lambda F)\Big|_{\lambda=0}$$

- Observables of the interacting theory $\mathcal{F}_I$ are represented in the free algebra

$$\mathcal{R}_V : \mathcal{F}_I \to \mathcal{F}_{\mu c}.$$

We may think of $\mathcal{F}_I$ as being generated by elements of $S_V(\mathcal{F}_{loc})$ or of $\mathcal{R}_V(\mathcal{F}_{loc})$.

  - $\mathcal{R}_V(\Phi(Pf) + \lambda V^{(1)}(f)) = \Phi(Pf)$
  - $\mathcal{R}_V(F)$ is compatible with causality thanks to the causal factorisation property of the $S-$matrix

$$\mathcal{R}_V(A) = A \qquad \text{if} \qquad V \gtrsim A$$

  - $\text{supp}\mathcal{R}_V(F) \subset J^-(\text{supp}F) \cap J^+(\text{supp}V)$

- An **interacting state** ω is fixed once the correlation functions among local interacting fields are given

$$\omega^I(F_1, \ldots, F_n) := \omega\left(\mathcal{R}_V(F_1) \star \cdots \star \mathcal{R}_V(F_n)\right), \qquad F_i \in \mathcal{F}_{loc}.$$

- **Interacting time evolution**

$$\alpha_t^V \mathcal{R}_V(F) := \mathcal{R}_V(\alpha_t F)$$

Adiabatic limits

- Aim is to have interaction Lagrangians invariant under spacetime translations.

  Example: we would like to treat

  $$\text{“}V(\varphi) = \int \varphi(x)^4 d\mu(x)\text{”}$$

  however, this is not compatible with the scheme discussed above.

- Insert a **cutoff** g
  (a C_0^∞ function equal to 1 in the region where the observables are supported).
- Eventually remove the cutoff taking the limit where $g \to 1$. (This is called **adiabatic limit**)

  $$V_g(\varphi) = \int g(x)\mathcal{L}_I(x)d\mu(x)$$

Question

Can it be done when a state is constructed?

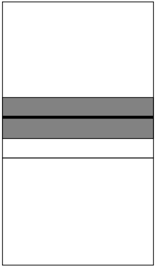
Strategy

- Thanks to the **Time-slice axiom** it is sufficient to define the state on interacting observables $\mathcal{F}_I(\Sigma_\epsilon)$ supported in some neighborhood of a Cauchy surface:

$$\Sigma_\epsilon = \{(t, \mathbf{x}) \in M | -\epsilon < t < \epsilon\}$$

($\mathcal{F}_I(\Sigma_\epsilon)$ is generated by $\mathcal{R}_V(F)$ with F local and supp$F \subset \Sigma_\epsilon$)

[Chilian Fredenhagen, Hollands Wald]



- The **causal factorisation property** implies that

$$\mathcal{F}_I^{V_g}(\Sigma_\epsilon) = W \star \mathcal{F}_I^{V_{g'}}(\Sigma_\epsilon) \star W^{-1}$$

if $\mathrm{supp}(g - g') \cap J^+(\Sigma_\epsilon) = \emptyset$ where $W = S_{V_g}(V_{g'-g})$ is unitary and

$$\mathcal{F}_I^{V_g}(\Sigma_\epsilon) = \mathcal{F}_I^{V_{g'}}(\Sigma_\epsilon)$$

if $\mathrm{supp}(g - g') \cap J^-(\Sigma_\epsilon) = \emptyset$

[Hollands Wald, Brunetti Fredenhagen]

- Hence, select $g(t, \mathbf{x}) = \chi(t)h(\mathbf{x})$ where χ is equal to 1 on $J^+(\Sigma_\epsilon)$ and it is past compact ($\chi(t) = 0$ for $t < -2\epsilon$)

KMS state and the adiabatic limit

[Fredenhagen Lindner] have obtained KMS states in the adiabatic limit extending the Araki construction to pAQFT.

It exists an unique free quasifree extremal KMS state ω^β at inverse temperature β wrt α_t.

$$\widehat{\omega_2^\beta}(p) = \frac{1}{2\pi}\frac{1}{1-e^{-\beta p_0}}\delta(p^2+m^2)\mathrm{sign}(p_0)$$

Fix the cutoff χh in $V_{\chi h}$.

- Analyze α_t^V and compare it with α_t

$$\alpha_t^V(S_V(F)) = S_V(F_t), \qquad \alpha_t(S_V(F)) = S_{V_t}(F_t),$$

- Although the generator is not at disposal, the **causal factorisation property** of S implies that

$$\alpha_t^V(A) = U_V(t) \star \alpha_t(A) \star U_V(t)^{-1}$$

- The cocycle

$$U_V(t) = S(V)^{-1} \star S(V_t)$$

  Differentiating wrt time we get the generator

$$K_h^\chi := \mathcal{R}_V(H(h\dot\chi)), \qquad H(h\dot\chi) = \int h\dot\chi \mathcal{L}_I d\mu$$

- Notice that support of K is before Σ_ϵ

- Having, K and thus U_V at disposal the Araki construction can be repeated.

$$\omega^{\beta,V}(F) = \frac{\omega^\beta(F \star U_V(i\beta))}{\omega^\beta(U_V(i\beta))}$$

- $\omega^{\beta,V}$ depends on h through U_V. Exploiting the decaying properties of the free KMS state 2-pt function for large spatial separation *[Fredenhagen Lindner]* have shown that the limit $h \to 1$ can be taken.

- In this way one obtains the KMS state for the interacting theory under the adiabatic limit.

- The limiting state does not depend on χ.

- The case $m = 0$ can be treated with the use of the thermal mass. *[Drago, Hack, np]*.

Comparison with other approaches

[Le Bellac, Altherr, Landsman van Weert]

- **Realtime formalism**. A direct comparison requires a bit of work. Notice in particular that

$$S_V(F) \star U_V(t) = S_V\left(F + \int_0^t \alpha_s \dot{V} ds\right)$$

hence,

$$S_V(F) \star U_V(i\beta) = \tilde{S}\left(F + \int_C \alpha_s \dot{V} ds\right)$$

where C is related to the known Keldysh contour and $\tilde{S}$ is the time ordered exponential with respect to the contour C.

- **Matsubara method**. Imaginary time formalism. Not suited to compute space dependent correlation functions.

Stability and KMS condition

Aim

Analyze the return to equilibrium properties in these states.

We start with an h of compact spatial support.

Proposition (Clustering condition for α_t)

Consider A and B two elements of $\mathcal{F}_I(\mathcal{O})$, ($\mathcal{O} \subset \Sigma_\epsilon$), it holds that

$$\lim_{t\to\infty} \omega^\beta(A \star \alpha_t(B)) = \omega^\beta(A)\omega^\beta(B)$$

in the sense of formal power series in the coupling constant.

At fixed x, y, $\omega_2^\beta(x, y + te)$ decays as $1/t^{3/2}$ for large t. *[Bros Buchholz]*

The clustering condition implies the following **return to equilibrium**

$$\lim_{T\to\infty} \omega^{\beta,V}(\alpha_T(A)) = \lim_{T\to\infty} \frac{\omega^\beta(\alpha_T(A) \star U_V(i\beta))}{\omega^\beta(U_V(i\beta))} = \omega^\beta(A)$$

where the limit is taken in the sense of perturbation theories.

To check if $\lim_{T\to\infty} \omega^\beta(\alpha_T^V(A)) = \omega^{\beta,V}(A)$ we need the following

Proposition (Clustering condition for α_t^V)

The limit,

$$\lim_{t\to+\infty} \left[\omega^\beta(A \star \alpha_t^V(B)) - \omega^\beta(A)\omega^\beta(\alpha_t^V(B))\right] = 0,$$

for A and B in $\mathcal{F}_I(\mathcal{O})$, holds in the sense of formal power series in the coupling constant whenever the perturbation Lagrangian $V_{\chi,h}$ has spatial compact support.

Theorem (Stability)

If $V_{\chi,h}$ is a spatially compact interaction Lagrangian

$$\lim_{T\to\infty} \omega^\beta(\alpha_T^V(A)) = \omega^{\beta,V}(A)$$

where A is an element of $\mathcal{F}_I(\Sigma_\epsilon)$.

Instabilities in the adiabatic limit - secular effects

- Under the adiabatic limit, the clustering condition fails at first order

$$\lim_{t\to\infty}\lim_{h\to 1}\left(\omega^{\beta}(A\star\alpha_t(K))-\omega^{\beta}(A)\omega^{\beta}(K)\right)\neq 0$$

- We study the **ergodic mean** of $\omega^{\beta}\circ\alpha^{V}_{\tau}$ to smoothen oscillations

$$\omega^{V,+}_{T}(A):=\lim_{h\to 1}\frac{1}{T}\int_0^T\omega^{\beta}(\alpha^{V}_{\tau}(A))d\tau$$

  and eventually we analyze the limit $T\to\infty$.

  - The clustering condition fails also in this case $\Longrightarrow$ no return to equilibrium is expected to hold.
  - Higher orders in $\omega^{V,+}_{T}(A)$ grow polynomially in T at large time.

- The expansion of $\lim_{h\to 1}\omega^{\beta,V}$ is free from divergences. We thus analyze

$$\omega^{+}(A):=\lim_{T\to\infty}\lim_{h\to 1}\frac{1}{T}\int_0^T dt\,\omega^{\beta,V}(\alpha_t(A))$$

A non-equilibrium steady state for the free field theory

Consider the ergodic mean of $\omega^{\beta,V}$ with respect to the free time evolution α_τ

$$\omega^+(A) := \lim_{T\to\infty} \lim_{h\to 1} \frac{1}{T}\int_0^T \omega^{\beta,V}(\alpha_\tau(A))\mathrm{d}\tau$$

which is seen as a state (defined as a formal power series) for the unperturbed theory.

Proposition

The functional ω^+ defined in the sense of formal power series, is a state for the free algebra $\mathcal{F}$. Furthermore, ω^+ is invariant under the free evolution α_t.

Theorem

ω^+ does not satisfy the KMS condition with respect to α_t.

ω^+ is thus a non equilibrium steady states (NESS)

Question

How far is ω^+ from equilibrium?

Relative Entropy

- **Relative entropy** can be used to measure the "distance" between two states.
- Other thermodynamic quantities can be obtained from it.

In the case of a von Neumann algebra $\mathfrak{A} \subset \mathfrak{B}\mathcal{H}$ and two normal states Ψ and Φ.

The **Araki relative entropy**

$$\mathcal{S}(\Psi, \Phi) := -(\Psi, \log(\Delta_{\Psi,\Phi})\Psi).$$

where the relative modular operator is obtained as

$$\Delta_{\Psi,\Phi} := S^* S, \qquad SA\Psi = A^*\Phi, \qquad A \in \mathfrak{A}.$$

Problem

$\Delta_{\Psi,\Phi}$ is not directly available in pAQFT

Relative entropy and perturbations in W^*−dyn. systems

- $(\mathfrak{M}, \alpha_t)$ a W^*−dynamical system on the Hilbert space $\mathfrak{H}$, α_t is generated by H.
- Let $\Omega_0 \in \mathfrak{H}$ be the GNS vector of the KMS state at inverse temperature β wrt α_t.
- Consider a **perturbation** P which is a self-adjoint element of $\mathfrak{M}$. Let $\Omega_1 \in \mathfrak{H}$ be the GNS vector of the Araki KMS state over Ω_0. It holds that

$$\Omega_1 = \frac{1}{N} U\Omega_0, \qquad U = e^{\frac{\beta}{2}H} e^{-\frac{\beta}{2}(H+P)}, \qquad N^2 = (\Omega_0, U^* U\Omega_0).$$

- The **relative modular operator** between Ω_1 and Ω_0 is

$$\Delta_{\Omega_1\Omega_0} = N^2 e^{-\beta H}$$

- **The relative entropy** *[Bratteli Robinson]*

$$\mathcal{S}(\Omega_1, \Omega_0) = \beta(\Omega_1, H\Omega_1) - \log(N^2) = -\beta(\Omega_1, P\Omega_1) - \log(N^2).$$

Relative entropy for perturbatively constructed KMS states

- In pAQFT we do not have the relative modular operator at disposal.
- But if h is of compact support we have the generator K, hence we can define the relative entropy by analogy

$$\mathcal{S}(\omega^{\beta,V},\omega^{\beta}) := -\omega^{\beta,V}(\beta K) - \log(\omega^{\beta}(U(i\beta)))$$

- In the same manner we get

$$\mathcal{S}(\omega^{\beta,V_1},\omega^{\beta,V_3}) := -\omega^{\beta,V_1}(\beta K_1) + \omega^{\beta,V_1}(\beta K_3) - \log(\omega^{\beta}(U_1(i\beta))) + \log(\omega^{\beta}(U_3(i\beta)))$$

$$\mathcal{S}(\omega^{\beta,V_1}\circ\alpha_t^{V_2},\omega^{\beta,V_3}) := \mathcal{S}(\omega^{\beta,V_1},\omega^{\beta,V_3}) + \omega^{\beta,V_1}(\alpha_t^{V_2}(\beta K_3 - \beta K_2)) - \omega^{\beta,V_1}(\beta K_3 - \beta K_2)$$

Properties Relative Entropy

Proposition

The generalized relative entropy $\mathcal{S}(\omega^{\beta,V_1} \circ \alpha_t^{V_2}, \omega^{\beta,V_3})$ *satisfies the following properties:*

a) *(Quadratic quantity) it is at least of second order both in* K_i *and in* λ*.*

b) *(Positivity) it is positive in the sense of formal power series for every* t*.*

c) *(Convexity) it is convex in* V_1*,* V_2 *and* V_3 *in the sense of formal power series.*

d) *(Continuity) it is continuous in* V_i *in the sense of formal power series with respect to the topology of* $\mathcal{F}_{\mu c}$*.*

Adiabatic limits

From Haag's Theorem it is expected that under the adiabatic limit the relative entropy diverges

$$\mathcal{S}(\omega^{\beta,V_1},\omega^{\beta}) = -\omega^{\beta,V_1}(\beta K_1) - \log(\omega^{\beta}(U_1(i\beta)))$$

Let V_i for $i \in \{1,2,3\}$ be three interaction potentials with a common spatial cutoff h, the relative entropy per unit volume is

$$s(\omega^{\beta,V_1}\circ\alpha_t,\omega^{\beta,V_3}) := \lim_{h\to 1}\frac{1}{I(h)}\,\mathcal{S}(\omega^{\beta,V_1}\circ\alpha_t,\omega^{\beta,V_3})$$

where $I(h)$ is the integral of the cutoff function over the volume $\mathbb{R}^3$

$$I(h) := \int_{\mathbb{R}^3} h(\mathbf{x})d\mathbf{x}$$

Proposition

The relative entropy per unit volume $s(\omega^{\beta,V_1}\circ\alpha_t,\omega^{\beta,V_3})$ is

- *finite*
- *positive*

Entropy production and its property in pAQFT

$$s(\omega^+, \omega^{\beta,V}) = ??$$

$$\omega^+(A) := \lim_{T\to\infty} \lim_{h\to 1} \frac{1}{T} \int_0^T \omega^{\beta,V}(\alpha_\tau(A))\mathrm{d}\tau$$

In the case of C^*-dynamical systems, $\mathcal{S}(\omega^+, \omega^{\beta,V})$, diverges hence **entropy production** is used to test how far is a NESS from equilibrium.
[Ojima and collaborators, Ruelle, Jaksic Pillet]

Let η be a state invariant under $\alpha_t^{V_1}$. The entropy production in the state $\eta \circ \alpha_t$ of α_t relative to $\alpha_t^{V_3}$ (or to ω^{β,V_3}) is defined as

$$\mathcal{E}^{V_3}(\eta \circ \alpha_s) := \frac{d}{dt}\eta\left(\alpha^{V_1}_{-t}\alpha_t(\beta(K_3))\right)\Big|_{t=s}.$$

It has been also used in another context in *[Hack Verch]*

Proposition

Consider V_i for $i \in \{1,3\}$ two perturbation potentials with spatially compact supports then

$$\mathcal{S}(\omega^{\beta,V_1} \circ \alpha_t, \omega^{\beta,V_3}) = \mathcal{S}(\omega^{\beta,V_1}, \omega^{\beta,V_3}) + \int_0^t \mathcal{E}^{V_3}(\omega^{\beta,V_1} \circ \alpha_s)\, ds$$

NESS and entropy production

For the NESS the entropy production per unit volume wrt $\omega^{\beta,V}$

$$e^V(\omega^+) := \lim_{t\to\infty} \lim_{h\to 1} \frac{1}{t} \frac{1}{l(h)} \int_0^t ds\, \mathcal{E}^V(\omega^{\beta,V} \circ \alpha_s)$$

Theorem

The NESS ω^+ discussed above has vanishing entropy production per unit volume wrt $\omega^{\beta,V}$.

NESS with vanishing entropy production are interpreted to be thermodynamically simple.

This means that $s(\omega^+, \omega^{\beta,V})$ is finite. Hence we can say that ω^+ is not so far from being a KMS state.

Summary

- Equilibrium states in perturbative algebraic quantum field theory.
- Return to equilibrium for interaction Lagrangian compact in space.
- Failure of the return to equilibrium in the adiabatic limit.
- Relative entropy and entropy production among these states can be computed.

Thanks a lot for your attention