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

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On the occasion of Klaus Fredenhagen 70th birthday

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.

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

Basic settings for 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 $\omega(1) = 1$.

  GNS construction permits to represent $\mathcal{A}$ as bounded operators on some Hilbert space up to unitary equivalences: $(\mathfrak{H}_\omega, \pi_\omega, \psi_\omega)$ $\mathfrak{H}_\omega$ is an Hilbert space, $\pi_\omega(A) \in \mathfrak{B}(\mathfrak{H}_\omega)$ is a $*-$homomorphism and $\psi_\omega \in \mathfrak{H}_\omega$ is such that

$$\omega(A) = \langle \psi_\omega, \pi_\omega(A)\psi_\omega \rangle$$

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 a perturbed dynamics α^P,

$$\frac{d}{dt}\alpha_t^P(A)\Big|_{t=0} = \frac{d}{dt}\alpha_t(A)\Big|_{t=0} + i[P, A]$$

$$\alpha_t^P(A) = U_P(t)\alpha_t(A)U_P(t)^*, \qquad \text{where} \qquad -i\frac{d}{dt}U_P(t) = U_P(t)\alpha_t(P)$$

$P = P^* \in \mathcal{A}$ is the perturbation Hamiltonian and $U_P(t)$ is the cocycle gen. by P

Theorem (Araki)

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

$$\omega^P(A) := \frac{\omega(AU_P(i\beta))}{\omega(U_P(i\beta))}$$

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

Stability of KMS states for C^*-dynamical systems

If **strong clustering** holds for ω

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

- **Return to equilibrium property**:

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

[Haag Kastler Trych-Pohlmeyer, Bratteli, 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 **off-shell** field configurations $\varphi \in \mathcal{C} := C^\infty(M;\mathbb{R})$

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

Examples:

$$\Phi(f)(\varphi) := \int_M f(x)\varphi(x) d\mu(x), \qquad F(\varphi) = \int_{M\times M} \varphi(x)\varphi(y) f(x,y) d\mu(x) d\mu(y), \qquad W2(f)(\varphi) := \int_M f(x)\varphi(x)^2 d\mu(x)$$

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

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

- $\mathcal{F}_{\mu c}$ equipped with the pointwise product $F \cdot G(\varphi) := F(\varphi)G(\varphi)$ and with the complex conjugation as involution forms the commutative $*-$algebra of classical observables.

Free quantum theory

- Set $\lambda = 0$

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

- **Deformation Quantization:** pointwise product is deformed to a non-commutative $\star-$product (compatible with the free dynamics):

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

where ω is an Hadamard bidistribution:

(a weak solution of the equation of motion up to smooth functions)

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

its wave front set is such that the product with microcausal functionals is well defined.

  - Δ is the causal propagator (the reatrded minus advanced fundamental solution of the KG eq.)

Introduction to pAQFT

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

  Observables are elements of $\mathcal{F}_{\mu c}[[\lambda]]$ namely **formal power series** in the coupling constant λ with coefficients in $\mathcal{F}_{\mu c}$.
- To construct them explicitly, the time ordered product 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 the ambiguities are renormalization ambiguities).
- The **formal** $S-$**matrix** is the time ordered exp. of the interaction Lagrangian $V \in \mathcal{F}_{loc}$

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

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

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

- Observables of the interacting field theory are represented as elements of the algebra

$$\mathcal{F}_I \subset \mathcal{F}_{\mu c}$$

  generated by elements of $\mathcal{R}_V(\mathcal{F}_{loc})$.

  - $\mathcal{R}_V(\Phi(f))$ satisfies the off shell interacting equation of motion
  - $\mathcal{R}_V(F)$ is compatible with causality thanks to the causal factorisation property of the $S-$matrix

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

- 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

- We would like 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.

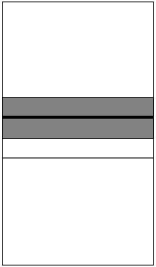
- Insert a cutoff g (a C_0^∞ function equal to 1 in the region where the observables are supported). Eventually remove this cutoff taking a limit where $g \to 1$. (This is called **adiabatic limit**)

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

Question

Can it be done in a reasonable way?

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]

- The **causal factorisation property** implies that

$$\mathcal{F}_I^{V_g}(\Sigma_\epsilon), \qquad \text{and} \qquad \mathcal{F}_I^{V_{g'}}(\Sigma_\epsilon)$$

are unitarily equivalent if $g - g' \cap \Sigma_\epsilon = \emptyset$ and they are equal if $g - g' \cap J^-(\Sigma_\epsilon) = \emptyset$
[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 $t < -2\epsilon$)

- The only limit we have to care about is $h \to 1$ *[Fredenhagen Lindner]*

KMS state and the adiabatic limit

[Fredenhagen Lindner] have constructed KMS state under 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 $V_{\chi h}$.

- Analyze α_t^V and compare it with α_t.
- Although their generators are not at disposal, it holds that

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

- Where

$$U_V(t) := 1+\sum_{n\geq 1} i^n\int_{tS_n} dt_1\ldots dt_n\,\alpha_{t_n}(K_h^\chi)\star\cdots\star\alpha_{t_1}(K_h^\chi)$$

where S_n is the $n-$dimensional simplex and

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

- Having U_V at disposal the Araki construction can be repeated.
- $\omega^{\beta,V}$ 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.

$\omega^{\beta,V}$ can be given in terms of the truncated $n-$point functions

$$\omega^{\beta,V}(A) = \sum_{n\geq 0}(-1)^n \int_{\beta S_n} \mathrm{d}U\ \omega^{\beta,c}\left(A \otimes \bigotimes_{k=1}^{n} \alpha_{iu_k}(K)\right)$$

$$\omega(F_1 \star \dots \star F_n) = \sum_{P\in \mathrm{Part}\{1,\dots,n\}} \prod_{I\in P} \omega^c\left(\bigotimes_{i\in I} F_i\right),$$

Stability and KMS condition

Aim

Analyze the return to equilibrium properties in these states.

We start with the case of fixed h.

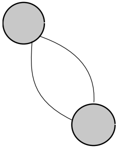
Proposition (Clustering condition for α_t)

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.

Idea of the proof.
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 $\lim_{T\to\infty} \omega^\beta(\alpha^V_T(A)) = \omega^{\beta,V}(A)$ holds we have to work another bit.

The clustering condition established above does not suffice to obtain the sought return to equilibrium to all orders in K.

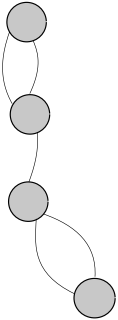
Proposition (Clustering condition for α_t^V)

The following clustering condition,

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

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.

Idea of the proof



Stability

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 - infrared divergences

- Under the adiabatic limit, the clustering condition fails at first order in perturbation theory also when the ergodic mean is considered, i.e.

$$\lim_{T\to\infty}\lim_{h\to 1}\frac{1}{T}\int_0^T dt\ \Big(\omega^\beta(A\star\alpha_t(K))-\omega^\beta(A)\omega^\beta(K)\Big)\neq 0$$

- 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 $T\to\infty$.
  - We do not expect to have the return to equilibrium property.
  - Infrared divergences occur in the large time limit of the ergodic mean $\omega^{V,+}_T(A)$ taken after the adiabatic limit $h\to 1$.

- The expansion of $\lim_{h\to 1}\omega^{\beta,V}$ is free from infrared 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 generators K_i, hence we can define the relative entropy by analogy

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

- In the same manner we get

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

- and

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

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) is at least of second order both in* K_i *and in* λ.
b) *(Positivity) is positive in the sense of formal power series for every* t.
c) *(Convexity) is convex in* V_1, V_2 *and* V_3 *in the sense of formal power series.*
d) *(Continuity) is continuous in* V_i *in the sense of formal power series with respect to the topology of* $\mathcal{F}_{\mu c}$.

Adiabatic limits

Haag's Theorem says 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

- In the case of C^*-dynamical systems, **entropy production** is used to test how far is a NESS from equilibrium. *[Ojima and collaborator, Ruelle, Jacsic Pillet.]*

- For C^*-dynamical systems: Let ω be a KMS state with respect to α_t and α_t^V the dynamics perturbed by V. The entropy production in the state η of α_t^V with respect to α_t is defined as

$$\mathcal{E}_V(\eta) := \eta\left(\sigma_V\right), \qquad \text{where} \qquad \sigma_V := \frac{d}{dt}\alpha_t(-\beta V)\Big|_{t=0} = \frac{d}{dt}\alpha_t^V(-\beta V)\Big|_{t=0}.$$

- If η is an $\alpha_t^{V_2}$ invariant state we may rewrite it

$$\mathcal{E}_{V_1}(\eta) = \frac{d}{dt}\eta(-\alpha_{-t}^{V_2}\alpha_t(\beta V_1))\Big|_{t=0}.$$

- These formulas can be generalized to pAQFT

Properties of the entropy production

Proposition

Consider V_i for $i \in \{1,2,3\}$ three perturbation potentials with spatially compact supports then

$$\mathcal{S}(\omega^{\beta,V_1} \circ \alpha_t^{V_2}, \omega^{\beta,V_3}) = \mathcal{S}(\omega^{\beta,V_1}, \omega^{\beta,V_3}) + \int_0^t \mathcal{E}_{V_1}(\omega^{\beta,V_1} \circ \alpha_s^{V_2}) \, ds$$

where $\mathcal{E}_{V_2}(\omega^{\beta,V_1} \circ \alpha_s^{V_2})$ is the entropy production of $\alpha_t^{V_2}$ relative to the KMS state ω^{β,V_3}.

NESS and entropy production

For the NESS the entropy production per unit volume

$$e(\omega^+_{V_1}) := \lim_{t\to\infty} \lim_{h\to 1} \frac{1}{t} \frac{1}{I(h)} \int_0^t ds\, \mathcal{E}(\omega^{\beta,V_1} \circ \alpha_s)$$

Theorem

The NESS ω^+ discussed above has vanishing entropy production per unit volume.

This means that ω^+ is not so far from being a KMS state.

NESS with vanishing entropy production are called thermodynamically simple.

Summary

- Equilibrium states in perturbative algebraic quantum field theory.
- Proof of the 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

Happy birthday Klaus!