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Ergodic Properties in Quantum Systems

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1 Introduction

Boltzmann's ideas about the time evolution of large systems has developed in two mathematical disciplines, topological dynamics and measure theoretic ergodic theory. In the former one considers a dynamical system consisting of a C^*-algebra $\mathcal{A}$ (the "observables") and an automorphism Θ of $\mathcal{A}$ (the "time evolution" for unit time) whereas in the latter one studies Θ-invariant states over $\mathcal{A}$. In both cases one is interested in the long time behaviour ($\lim_{n\to\infty}\Theta^n$). This framework can be taken over directly to quantum mechanics where $\mathcal{A}$ is not commutative. (We add as standing assumption $\Theta \neq id$ and $1 \in \mathcal{A}$.) However, before generalizing the various classical theorems we have to discuss to which physical situation this framework applies. The system we are interested in is bulk matter which consists of electrons and nuclei. Electrons are fermions and since the difference between various isotopes are of no relevance for us we might as well consider odd mass number isotopes so that all particles are fermions which makes the mathematics much easier. Since we are interested in large systems which are spatially unlimited but have a finite particle density the appropriate description is a quantized fermi field. Thus a minimal algebra $\mathcal{A}$ will be the CAR algebra generated by the annihilation operators $\alpha_f = \int d^3x \bar{f}(x)\alpha(x)$, $f \in L^2(\mathbf{R}^3)$, i.e. the norm closure of the polynomials

$$a = x + \sum_{n,m} \alpha^*_{f_1} \dots \alpha^*_{f_n} \alpha_{g_1} \dots \alpha_{g_m}. \tag{1.1}$$

From the CAR relations

$$[\alpha_f, \alpha^*_g]_+ = \langle f|g\rangle \tag{1.2}$$

one infers $\|\alpha_f\| = \|f\|$. The observable algebra will be the subalgebra where $n = m$. $\mathcal{A}$ is a pleasant C^*-algebra, it is simple (i.e. it has no proper twosided ideal) and it is UHF (i.e. the norm closure of an increasing sequence of matrix algebras). States are positive linear functionals ω over $\mathcal{A}$ and by the GNS construction they give a representation Π_ω of $\mathcal{A}$ in a Hilbert space $\mathcal{H}_\omega$. Popular states are the equilibrium states Φ_ω for a quasifree time evolution $\tilde{f}(k) \to e^{i\varepsilon(k)t}\tilde{f}(k)$. They are defined by

$$\Phi_\beta(\alpha^*_f \alpha_g) = \int \frac{d^3k}{(2\pi)^3} \frac{\tilde{f}(k)\tilde{g}(k)}{1 + e^{\beta(\varepsilon(k)-\mu)}} \tag{1.3}$$

and vanishing reduced $n \geq 3$ point functions. The have the following features:

1. Π_{Φ_β} is a factor (i.e. if $\Pi_\omega(\mathcal{A})'$ is the commutant of $\Pi_\omega(\mathcal{A})$, $\Pi_\omega(\mathcal{A})''$ the commutant of $\Pi_\omega(\mathcal{A})'$, then the center $\Pi_\omega(\mathcal{A})' \cap \Pi_\omega(\mathcal{A})''$ is trivial for a factor).
2. For $\beta \neq \infty$ Φ_β is faithful (i.e. $\Phi_\beta(a^*a) = 0 \leftrightarrow a = 0$, $a \in \mathcal{A}$).
3. Φ_0 is tracial (i.e. $\Phi_0(ab) = \Phi_0(ba)$.
4. Φ_∞ (the Fock state) is pure (i.e. Π_{Φ_∞} is irreducible).

To describe the dynamics of particles interacting via a potential v one usually writes down a Hamiltonian

$$H = \frac{1}{2m}\int dx \nabla\alpha^*(x)\nabla\alpha(x) + \int dx dx' \alpha^*(x)\alpha^*(x')v(x-x')\alpha(x')\alpha(x) =: T + V \tag{1.4}$$

and defines a time evolution by

$$\Theta^t(\alpha(x)) = e^{iHt}\alpha(x)e^{-iHt}. \tag{1.5}$$

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Indeed in the Fock representation Π_{Φ_∞} where one has sectors with finite particle number $N = \int dx \alpha^*(x)\alpha(x)$ there is no doubt that for reasonable v's the restriction H_N will define a time evolution in these sectors. However, in general this will not be a one parameter automorphism group of $\mathcal{A}$ but only of $\Pi_{\Phi_\infty}(\mathcal{A})''$. Having an automorphism of $\mathcal{A}$ means a dynamics independent of the state and this can in general not be expected. Generically potentials are not stable in the sense that there exists $c \in \mathbf{R}^+$ such that

$$H_N > -cN \qquad \forall N. \tag{1.6}$$

This condition ensures that the energy per particle stays finite for $N \to \infty$. If it does not hold the motion gets faster and faster as N increases [1] and a limiting dynamics exists only after rescaling the time. Thus one can hope for an automorphism of $\mathcal{A}$ only for stable potentials. Unfortunately, the situation is worse because of the following argument. $K(\alpha_f) = \alpha^*_{\bar{f}}$ is an automorphism of $\mathcal{A}$, $K^2 = \mathbf{1}$. $K\Theta^t K$ would again be an automorphism of $\mathcal{A}$ generated by KHK. Since $\alpha(x)$ is not bounded we should express H by the a_f's otherwise the time derivative $i[H, a]$ will lead out of $\mathcal{A}$. But regularizing H somehow in the form:

$$T = \sum_f a^*_{\nabla f} a_{\nabla f}, \qquad V = \sum_{f,g} a^*_f a_f v(f,g) a^*_g a_g \tag{1.7}$$

we see $KTK = -T + c_1$, $KVK = V + c_2 N + c_3$, $c_i \in \mathbf{R}$. Removing the regularization the constants c_i become infinite but they have no influence on the time development of gauge invariant quantities. For the existence of the N-independent dynamics we need either $H_N > -cN$ or $H_N < cN$. Since $0 < T \not< cN$ we need therefore

$$T + V > -cN, \qquad T - V > -cN \quad \text{that is } -cN - T < V < cN + T. \tag{1.8}$$

In general, there is no such operator inequality since $V \sim N^2$. For fermions there is a way out by observing that the particle density in configuration space $\alpha^*(x)\alpha(x)$ is unbounded in spite of the exclusion principle because by going to high momenta we can pack arbitrarily many fermions in any volume. However, the fermion density in phase space $\rho(z)$ is bounded by 1 (in units $\hbar = 1$) if

$$z = (x,p) \in \mathbf{R}^6, \qquad \rho(z) = a^*_z a_z, \qquad a_z = \int \frac{d^3x}{\pi^{3/4}} e^{ipy} e^{-(x-y)^2/2} \alpha(y).$$

We have $0 < \rho(z) < 1$ and if we use a velocity dependent potential which cuts off high momenta, then (1.8) should be satisfied. Indeed we have

Proposition (1.9)
The potential $V = \int d^6z d^6z' a^*_z a^*_{z'} v(z-z') a_{z'} a_z$ satisfies $-\|v\|_1 N \le V \le \|v\|_1 N$, $\|v\|_1 = \int d^6z |v(z)|$.

Proof: We have the operator inequality

$$a^*_z a^*_{z'} a_{z'} a_z \le a^*_z a_z \|a^*_{z'} a_{z'}\| = a^*_z a_z$$

and thus

$$V \le \int dz dz' |v(z-z')| a^*_z a_z = \|v\|_1 N$$

and similarly the left inequality.

Once the obstacle of instability is removed we get indeed an automorphism of the CAR algebra. This is stated by the next theorem, the proof of which is based on expansion in the coupling constant and clearly too involved to be given here [2].

Theorem (1.10)
$H = T + V$, v from (1.9) with $\|v\| < \infty$ defines by $\Theta^t a_f = e^{iHt} a_f e^{-iHt}$ a one parameter group of automorphisms of the CAR algebra which is norm continuous and Galilei invariant.

Remarks (1.11)

1. Norm continuous means $\lim_{t\to 0} \|\Theta^t a - a\| = 0 \ \forall a \in \mathcal{A}$. There is no uniformity, $\lim_{t\to 0} \sup_{a\in\mathcal{A},\|a\|=1} \|\Theta^t a - a\| = 0$ would imply bounded H.

2. Galilei invariant means that together with the shift σ: $\sigma^x a_f = a_{f_x}$, $f_x(y) = f(x+y)$, the boost γ: $\gamma^p a_f = a_{e^{ipx}f}$, and the gauge transformation (first kind) ν: $\nu^\alpha a_f = e^{i\alpha} a_f$ the time evolution Θ satisfies

$$\sigma^x \circ \nu^\alpha = \nu^\alpha \circ \sigma^x, \quad \gamma^p \circ \nu^\alpha = \nu^\alpha \circ \gamma^p, \quad \gamma^p \circ \sigma^x = \sigma^x \circ \gamma^p \circ \nu^{-px}$$

$$\Theta^t \circ \nu^\alpha = \nu^\alpha \circ \Theta^t, \quad \Theta^t \circ \sigma^x = \sigma^x \circ \Theta^t, \quad \Theta^t \circ \gamma^p = \Theta^t \circ \sigma^{-pt} \circ \nu^{-p^2 t/2}.$$

   This expresses that Θ, σ, γ, ν give a realization of the central extension of the Galilei group by norm continuous automorphisms of the CAR algebra.

3. A local potential means v is p-independent in which case $\|v\|_1 = \infty$ and (1.10) does not apply. However, there is no limit on the momentum cut-off and one can hope that for stable systems where high momenta do not occur in a reasonable subset of states, then (1.10) gives a physically acceptable description of the time evolution.

When we develop the general theory in the next section we shall always have this model in mind since it exists mathematically and is relevant for physics.

2 Topological Dynamics

The knowledge of an observer about the system is contained in the state. Thus the properties of $(\mathcal{A}, \Theta)$ are objective in the sense that they do not depend on any observer. On the other hand, $(\mathcal{A}, \Theta, \omega)$ reflects how the situation appears to a particular observer. Similar elements from $\Pi_\omega(\mathcal{A})'' \setminus \Pi_\omega(\mathcal{A})$ are extrapolations from some observer and are different for different ω [3]. Thus we shall first study properties of $(\mathcal{A}, \Theta)$ alone and in the next section the additional information contained in invariant states. It turns out that there is a close interplay between these points of view. From some states we can draw conclusions about $(\mathcal{A}, \Theta)$ and sufficient algebraic structure of $(\mathcal{A}, \Theta)$ implies some feature of all invariant states.

Proposition (2.1)
Between the properties of a dynamical system $(\mathcal{A}, \Theta)$

(i) all Θ-invariant elements of $\mathcal{A}$ are $\sim \mathbf{1}$,

(ii) all Θ-quasiperiodic elements of $\mathcal{A}$ are $\sim \mathbf{1}$,

(iii) $(\mathcal{A}, \Theta)$ is a K-system,

(iv) $\mathcal{A}$ has only trivial Θ-invariant closed subalgebras,

there are the implications

$$\begin{array}{ccc} \text{(iv)} & \Longrightarrow & \text{(i)} \\ & & \Uparrow \\ \text{(iii)} & \Longrightarrow & \text{(ii)} \end{array}$$

Explanations (2.2)

ad (i) This is usually called ergodicity and is too weak a property since it does not imply mixing. Nevertheless it excludes systems where Θ is an inner automorphism (i.e. $\Theta(a) = U^{-1}aU, U \in \mathcal{A}$) and in particular finite quantum systems (where $U = e^{iH}$). It also excludes finite Θ-invariant subalgebras $\mathcal{A}_0$ since Θ restricted to $\mathcal{A}_0$ would be an automorphism of $\mathcal{A}_0$ and they always have invariant elements.

ad (ii) Quasiperiodicity for an element $a \in \mathcal{A}$ means $\forall \varepsilon > 0$, $N \in \mathbf{Z}^+ \; \exists |n| > N$ with $\|\Theta^n a - a\| < \varepsilon$. This property is of interest in connection with Poincaré's recurrence theorem which says that classically almost all orbits keep coming arbitrarily close to their origin. Nevertheless classical systems may have property (ii) since the observables are smooth functions on phase space and they may never regain their original form.

ad (iii) K-system [4] means that $\mathcal{A}$ has a C^*-subalgebra $\mathcal{A}_0$ with the properties

(a) $\Theta^n \mathcal{A}_0 \supset \mathcal{A}_0 \; \forall n \in \mathbf{Z}^+$

(b) $\bigvee_{n=0}^{\infty} \Theta^n \mathcal{A}_0 = \mathcal{A}$ (V means norm completion of algebra generated by the $\Theta^n \mathcal{A}_0$)

(c) $\bigwedge_{n=0}^{\infty} \Theta^{-n} \mathcal{A}_0 = c \cdot \mathbf{1}$ ($\bigwedge$ is the intersection).

Rephrased it means that Θ^{-1} gives an isomorphism between $\mathcal{A}_1 := \Theta\mathcal{A}_0$ and its proper subalgebra $\mathcal{A}_0$ but this isomorphism has no proper invariant subalgebra (this would remain in the "tail" $\bigwedge_{n=0}^{\infty} \Theta^{-n} \mathcal{A}_0$). (b) might be considered as definition of $\mathcal{A}$ such that the isomorphism $\Theta : \mathcal{A}_n \to \mathcal{A}_{n+1}$ extends to an automorphism $\mathcal{A} \to \mathcal{A}$.

ad (iv) This is equivalent to requiring that $\forall z \cdot \mathbf{1} \neq a \in \mathcal{A}$ the C^*-algebra generated by $\{\Theta^n a, n \in \mathbf{Z}\}$ is all of $\mathcal{A}$. For our purposes it is too strong a condition since the particle number conserving time evolutions (1.10) of the CAR algebra leave the subalgebras

$$\mathcal{A}_{n_0} = \{z + \sum_{n > n_0} a^*(f_1)a^*(f_2)\ldots a^*(f_n)a(g_1)\ldots a(g_n)\}$$

$\forall n_0 \in \mathbf{Z}^+$ invariant. (iv) is not related to (iii) since these time evolutions may nevertheless generate K-systems. On the other hand, the tensor product of two K-systems $(\mathcal{A}, \Theta_1)$ and $(\mathcal{A}, \Theta_2)$ can be endowed naturally with a K-structure but $(\mathcal{A}_1 \otimes \mathcal{A}_2, \Theta_1 \otimes \Theta_2)$ has $(\mathcal{A}_1 \otimes \mathbf{1})$ and $(\mathbf{1} \otimes \mathcal{A}_2)$ as invariant subalgebras, thus (iii) $\not\Rightarrow$ (iv). Furthermore (iv) is too weak to imply (ii) since there are trivial examples of periodic systems with only trivial subalgebras.

Proof of (2.1)

(ii) $\Rightarrow$ (i). Invariant elements are quasiperiodic.

(iv) $\Rightarrow$ (i). The invariant elements form a closed invariant subalgebra.

(iii) $\Rightarrow$ (ii). Let b be a quasiperiodic element. Because of property (b) $\forall \varepsilon > 0$ we can find an $n(\varepsilon) \in \mathbf{Z}^+$ with $\inf_{a\in\mathcal{A}_{n(\varepsilon)}} \|b - a\| < \varepsilon$, $\mathcal{A}_n = \Theta^n \mathcal{A}_0$. As the norm is invariant under Θ we have $\forall N \in \mathbf{Z}^+$ $\inf_{a\in\mathcal{A}_{n(\varepsilon)-N}} \|\Theta^{-N} b - a\| < \varepsilon$ and because b is quasiperiodic $\inf_{a\in\mathcal{A}_{n(\varepsilon)-m}} \|b - a\| \leq 2\varepsilon$ for some $m > N$ and thus $\forall N \in \mathbf{Z}^+$ $\inf_{a\in\mathcal{A}_{n(\varepsilon)-N}} \|b - a\| \leq 2\varepsilon$. This means $\forall \varepsilon > 0$, $n \in \mathbf{Z}$, $\inf_{a\in\mathcal{A}_n} \|b - a\| < \varepsilon$ and since the $\mathcal{A}_n$ are norm-closed $b \in \mathcal{A}_n$ $\forall n \in \mathbf{Z}$. Thus the property (c) requires $b = c \cdot \mathbf{1}$, $c \in C$.

In classical topological dynamics there is the important notion of topologically mixing [5] which we generalize to the noncommutative case as follows [6,7,8,9]:

Definition (2.3)
A dynamical system $(\mathcal{A}, \Theta)$ is called

(i) weakly mixing if $\forall a, b \in \mathcal{A}\ \exists N, \varepsilon >$ such that $\|a\Theta^n b\| > \varepsilon\|a\|\|b\|\ \forall n > N$,

(ii) strongly mixing if $\lim_{n\to\infty} \|a\Theta^n b\| = \|a\|\|b\|$.

Remarks (2.4)

1. The intuitive meaning of mixing is visualized best in the classical case where a and b are continuous functions on phase space. Even if they have disjoint supports such that $ab = 0$ if one is time translated their supports will eventually overlap. (i) says that b is dispersed so finely that eventually its support keeps overlapping with the one of a forever. (ii) says that even the part close to the maximum of b will eventually meet the maximum of a and keep overlapping it.

2. Classically (i) and (ii) are equivalent since (i) must hold for all functions supported near the maxima of a and b. Obviously (ii) $\Rightarrow$ (i) but whether generally (i) $\Rightarrow$ (ii) is an open question.

3. Since $\|a\Theta^n b\| = \|b^*\Theta^{-n} a^*\|$ there is no distinction between $n \to \infty$ and $n \to -\infty$.

Proposition (2.5)
(2.3,ii) $\Rightarrow$ (2.1,ii).

Proof: Suppose b is a quasiperiodic element $\neq c \cdot \mathbf{1}$. Then either $B = b + b^*$ or $B = i(b - b^*)$ has at least two different spectral values and is hermitian and also quasiperiodic. Suppose $f_\pm$ are two smooth functions with disjoint support having their maxima at the two spectral values, respectively. Then $f_\pm(B)$ are $\neq 0$ and $f_+(B)f_-(B) = 0$. Suppose there were some ε with $\|f_+(B)\Theta^n f_-(B)\| > \varepsilon\|f_+\|\|f_-\|\ \forall n > N$. Since $f_- f_-^*$ is quasiperiodic there is some $m > N$ with $\|\Theta^m f_- f_-^* - f_- f_-^*\| \leq \varepsilon^2\|f_-\|^2/4$ and we have

$$\|f_+\Theta^m f_-\| = \|f_+(\Theta^m(f_- f_-^*) - f_- f_-^*)f_+^*\|^{1/2} \leq \frac{\varepsilon}{2}\|f_+\|\|f_-\|$$

contradicting our assumption.

3 Representations by Invariant States

Each invariant state ω gives a GNS representation Π_ω of $(\mathcal{A},\Theta)$ in a Hilbert space $\mathcal{H}_\omega = \overline{\Pi_\omega(\mathcal{A})|\Omega\rangle}$ where Θ is unitarily implemented by U, $U\Pi_\omega(a)|\Omega\rangle = \Pi_\omega(\Theta a)|\Omega\rangle$ [10,11]. The ergodic properties of $(\mathcal{A},\Theta)$ have their counterpart in properties for ω. The following proposition shows that in a pure quantum situation automatically one gets mixing.

Proposition (3.1)
Let ω be a Θ-invariant state of $(\mathcal{A},\Theta)$ (i.e. $\omega\circ\Theta = \omega$) such that ω is faithful on $\Pi_\omega(\mathcal{A})''$ (i.e. $\langle\Omega|a^*a|\Omega\rangle = 0 \Leftrightarrow a = 0\ \forall\, a \in \Pi_\omega(\mathcal{A})''$) and $\mathcal{Z}_\omega = \Pi''_\omega(\mathcal{A}) \cap \Pi_\omega(\mathcal{A})' = c\cdot\mathbf{1}$.

Then the following properties are equivalent:

(i) ω is mixing,

(ii) $\text{w-lim}_{n\to\infty} U^n = |\Omega\rangle\langle\Omega|$.

(iii) $\text{w-lim}_{n\to\infty} \Pi_\omega(\Theta^n a) = \omega(a)\cdot\mathbf{1}\ \forall\, a \in \Pi_\omega(\mathcal{A})$,

(iv) $(\mathcal{A},\Theta,\omega)$ is weakly asymptotic abelian.

Remarks (3.2)

1. Faithful states are dense and so this requirement does not leave us with exceptions only. There are examples of states faithful on $\Pi_\omega(\mathcal{A})$ and not on $\Pi_\omega(\mathcal{A})''$ but they do not seem to be important in physics. The advantage of faithfulness is that they supply the modular automorphism σ_t^ω which satisfies the KMS condition [10,11] $\langle\Omega|ab|\Omega\rangle = \langle\Omega|b\sigma_i^\omega(a)|\Omega\rangle$. If ω is Θ-invariant σ^ω and Θ commute.

2. The center $\mathcal{Z}_\omega$ is the classical part of the system and may be nontrivial even if $\mathcal{A}$ is simple and therefore its center is trivial. Our requirement means that Π_ω is a factor representation, there the classical observables have fixed values.

ad (i) Mixing means $\lim_{n\to\infty}\omega(a\Theta^n(b)c) = \omega(ac)\omega(b)$. Since ω is Θ-invariant the limits $n\to\infty$ and $n\to-\infty$ are equivalent:

$$\omega(a\Theta^n(b)c) = \omega(b\Theta^{-n}(c\sigma_i^\omega(a))) = \omega(d^{-1}b\Theta^{-n}(c\sigma_i^\omega(a))\sigma_i^\omega d).$$

ad (ii) w-lim means weak limit in the Hilbert space $\overline{\Pi_\omega(\mathcal{A})|\Omega\rangle}$. Strong limit is impossible since strong limits of unitaries must be isometries.

ad (iii) Again strong limits are impossible:

$$\begin{aligned} 0 &= \text{s-}\lim\Pi_\omega(\Theta^n(a^* - \omega(a^*)))\cdot\text{s-}\lim\Pi_\omega(\Theta^n(a-\omega(a))) \\ &= \text{s-}\lim\Pi_\omega(\Theta^n(a^*-\omega(a^*))(a-\omega(a)) = \omega((a^*-\omega(a))(a-\omega(a)). \end{aligned}$$

Faithfulness requires $a = \omega(a)$ and thus strong convergence holds only for multiples of $\mathbf{1}$ (which are invariant under Θ).

ad (iv) Weak asymptotic abelianness means

$$\lim_{n\to\infty}\omega(a[b,\Theta^n c]d) = 0 \quad \forall\, a,b,c,d \in \mathcal{A}.$$

It is not possible for inner automorphisms $\Theta(a) = U^{-1}aU$ since $\Theta(U) = U$ and thus the condition would make $[b,U] = 0\ \forall\, b \Leftrightarrow \Theta = id$.

Proof of (3.1)

(i) ⇔ (ii) Both require

$$\omega(a\Theta^n(b)c) = \langle\Omega|\sigma^\omega_{-i}(c)aU^n b|\Omega\rangle \to \langle\Omega|ac|\Omega\rangle\langle\Omega|b|\Omega\rangle.$$

(i) ⇔ (iii) Both require

$$\langle\Omega|a\Theta^n(b)c|\Omega\rangle \to \langle\Omega|ac|\Omega\rangle \cdot \langle\Omega|b|\Omega\rangle.$$

(iv) ⇒ (iii) Since in the von Neumann algebra $\Pi_\omega(\mathcal{A})''$ bounded sets are weakly compact, so $\Pi_\omega(\Theta^n a)$ will have weak cluster points $a'' \in \Pi_\omega(\mathcal{A})''$. Asymptotic abelianness requires $a'' \in \Pi_\omega(\mathcal{A})'$ and thus $a'' \in \mathcal{Z}_\omega = c \cdot \mathbf{1}$. Weak continuity of ω tells us $\Pi_\omega(\Theta^{n_i} a) \rightharpoonup a''$ which implies $\omega(a) = \langle\Omega|\Pi_\omega(\Theta^{n_i} a)|\Omega\rangle \to \langle\Omega|a''|\Omega\rangle$ and thus $a'' = \omega(a) \cdot \mathbf{1}$.

(iii) ⇒ (iv)

$$\lim_{n\to\infty} \omega(ab\Theta^n(c)d) = \lim_{n\to\infty} \omega(a\Theta^n(c)bd) = \omega(abd)\omega(c).$$

Remarks (3.3)

1. Note that (i), (iii) and (iv) hold even for all elements from $\Pi_\omega(\mathcal{A})''$. For this to happen faithfulness is crucial. In the Fock state $\Pi_\omega(\mathcal{A})'' = \mathcal{B}(\mathcal{H})$ and the unitary generators of rotations are time invariant but do not commute. Thus there $\Pi_\omega(\mathcal{A})$ is asymptotic abelian but $\Pi_\omega(\mathcal{A})''$ is not.

2. The properties (3.1) imply that ω is extremal invariant (i.e. $\omega = \lambda\omega_1 + (1-\lambda)\omega_2$, $\lambda \in (0,1)$, $\omega_{1,2}$ invariant, implies $\omega_1 = \omega_2 = \omega$). The reason is that in such a decomposition ω_i can be written $\omega_i(a) = \langle\Omega|\Pi_\omega(\mathcal{A})a'|\Omega\rangle$, a' an invariant positive element from $\Pi_\omega(\mathcal{A})'$. For faithful states $\Pi_\omega(\mathcal{A})'$ and $\Pi_\omega(\mathcal{A})''$ are antiisomorphic, and invariance of ω implies this antiisomorphism for their invariant elements. Since the only invariant element from $\Pi_\omega(\mathcal{A})''$ is $c \cdot \mathbf{1}$ the same holds for $\Pi_\omega(\mathcal{A})'$ and thus $a' = \mathbf{1}$. Extremal invariance implies in turn that (i), (iii), and (iv) hold in the mean (ergodicity).

Proposition (3.4)
If (3.1) holds $(\mathcal{A}, \Theta)$ is weakly mixing.

Proof:

$$\|a\Theta^n(b)\| = \|a\Theta^n(bb^*)a^*\|^{1/2} \geq (\omega(a\Theta^n(bb^*)a^*))^{1/2} \to \omega(aa^*)^{1/2}\omega(bb^*)^{1/2} > \varepsilon > 0$$

since ω is faithful.

In some cases pure states are more convenient and even if they are not faithful $\Pi_\omega(\mathcal{A})$ will be if $\mathcal{A}$ is simple. In this case a strengthening of (3.1,i) gives an even stronger result.

Proposition (3.5)
If $\mathcal{A}$ is simple and Π_ω is hyperclustering, $(\mathcal{A}, \Theta)$ is strongly mixing.

Explanations (3.6)

1. Simplicity implies that the center of $\Pi_\omega(\mathcal{A})$ is trivial because a nontrivial twosided ideal can be constructed with nontrivial elements of the center. This does not yet mean that $\Pi_\omega(\mathcal{A})''$ has trivial center.

2. Hyperclustering means
$$\omega(a\Theta^n(b)d\Theta^n(c)) \to \omega(ad)\omega(bc).$$
It implies $\omega(c[a,\Theta^n b][a^*,\Theta^n b^*]d) \to 0$ and thus strengthens (3.1,iii) to
$$\text{s-}\lim_{n\to\infty}[\Pi_\omega(a),\Pi_\omega(\Theta^n b)] = 0$$
(strong asymptotic abelianness). Together with mixing this implies conversely hyperclustering.

Proof of (3.5): For simplicity we write $\Theta^n a = a_n$, etc. Consider the operator inequality
$$cd_n ab_n b_n^* a^* d_n^* c^* \le \|ab_n\|^2 cd_n d_n^* c^*$$
which gives us
$$\frac{\omega(cd_n ab_n b_n^* a^* d_n^* c^*)}{\omega(cd_n d_n^* c^*)} \le \|ab_n\|^2.$$
Let n tend to infinity and remember that commutators go strongly to zero. Thus the left hand side tends to
$$\frac{\omega(caa^*c^*)}{\omega(cc^*)}\frac{\omega(dbb^*d^*)}{\omega(dd^*)}.$$
Now take the sup over d and c and take into account that faithfulness of Π_ω means
$$\sup_{c\in\mathcal{A}}\frac{\omega(caa^*c^*)}{\omega(cc^*)} = \|a\|^2$$
thus $\lim_{n\to\infty}\|ab_n\| \ge \|a\|\|b\|$, but generally $\|ab_n\| \le \|a\|\|b\|$ and thus
$$\lim_{n\to\infty}\|a\Theta^n b\| = \|a\|\|b\|.$$

Corollary (3.7)
Let $\mathcal{A}$ be an UHF algebra and $(\mathcal{A},\Theta)$ norm asymptotic abelian, then $(\mathcal{A},\Theta)$ is strongly mixing.

Remark (3.8)
Norm asymptotic abelian means $\lim_{n\to\infty}\|[a,\Theta^n b]\| = 0$. This is in particular satisfied when Θ is a quasifree automorphism of the CAR algebra $\Theta(a_f) = a_{Uf}$ where the unitary operator U has apart from the eigenvector $|\Omega\rangle$ an absolutely continuous spectrum and $\mathcal{A}$ is the even part of this algebra. In this case $\|[a_f,\Theta^n a_g^*]_+\| = \langle f|U^n g\rangle$ which goes to zero.

Proof of (3.7): The unique tracial state τ is invariant under all automorphisms α ($\tau\circ\alpha$ would be another tracial state and thus equals τ). It is known to be faithful over $\Pi_\tau(\mathcal{A})''$ which is a type II_1 factor and has trivial center. Thus by (3.1) τ is mixing and even hyperclustering since it is norm asymptotic abelian. Thus (3.5) applies.

Corollary (3.9)
Let Θ of the CAR algebra $\mathcal{A}$ be Galilei invariant. Then $(\mathcal{A}, \Theta)$ is weakly mixing.

Proof: The tracial state τ qualifies for (3.1) and from the representation theory of the Galilei group one knows that apart from the invariant vector the U_t which generates the time translation has absolutely continuous spectrum [12]. One knows that $|\Omega\rangle$ is the only translation invariant vector in $\mathcal{H}_\tau$ and therefore the only Galilei invariant vector. Thus $U_n \rightharpoonup |\Omega\rangle\langle\Omega|$ and the conditions of (3.1) are satisfied.

Remarks (3.10)

1. Even without appeal to the representation theory of the Galilei group one can show that τ is mixing using only its multiplication law [13]. One uses the fact that in faster and faster moving Galilei frames the time translation looks more and more like a space translation and the latter is mixing.

2. For the Galilei invariant interactions mentioned in Sect. 1 one can show strong asymptotic abelianness in the Fock representation [12,14]. Thus (3.5) tells us that $(\mathcal{A}, \Theta)$ is even strongly mixing.

So far we have used properties of particular invariant states to deduce state independent features of $(\mathcal{A}, \Theta)$. They do not guarantee ergodic properties of other Θ-invariant states. However, with stronger algebraic structures of $(\mathcal{A}, \Theta)$ one can make statements for all invariant states [15,16].

Proposition (3.11)
For a K-system all faithful invariant states are mixing.

Proof: Denote by $P_n \in \Pi_\omega(\mathcal{A}_n)'$ the orthogonal projector projecting onto $\overline{\mathcal{A}_n|\Omega\rangle}$. Since weak convergence of projections to projections implies strong convergence the K-properties (2.2,iii) are equivalent to

(a) $U_{-n'} P_n U_{n'} = P_{n+n'} \supset P_n \; \forall n' \in N,\ n \in \mathbf{Z}$,

(b) $\text{s-lim}_{n\to\infty} P_n = \mathbf{1}$,

(c) $\text{s-lim}_{n\to\infty} P_n = |\Omega\rangle\langle\Omega|$.

Thus, if $b \in \mathcal{A}_0$ and using $U_n|\Omega\rangle = |\Omega\rangle$, we have

$$\begin{aligned} |\omega(a\Theta^n b) - \omega(a)\omega(b)| &= |\langle\Omega|aU_{-n}(P_0 - |\Omega\rangle\langle\Omega|)b|\Omega\rangle| \\ &= |\langle\Omega|a(P_n - |\Omega\rangle\langle\Omega|)U_{-n}b|\Omega\rangle| \\ &\leq \|\langle\Omega|a(P_n - |\Omega\rangle\langle\Omega|)\| \cdot \|b|\Omega\rangle\| \end{aligned}$$

and consequently c) tells us $\forall\, \varepsilon\, \exists N$ such that

$$|\omega(a\Theta^n b) - \omega(a)\omega(b)| < \varepsilon\omega(b^* b) \quad \forall\, n < -N,\ b \in \mathcal{A}_0.$$

Clearly the same holds for b from any $\mathcal{A}_n$ and since the $\mathcal{A}_n$ are norm dense in $\mathcal{A}$ we have $\forall\, a, b \in \mathcal{A},\ \varepsilon\, \exists N$ such that

$$|\omega(a\Theta^n b) - \omega(a)\omega(b)| < \varepsilon \qquad \forall\, n < -N.$$

Faithfulness comes in when we want to treat $n \to \infty$. Since $\omega(a\Theta^n b) = \omega(\Theta^{-n}(a)b) = \omega(\sigma^{\omega}_{-i}(b)\Theta^{-n}a)$ and the image of σ^{ω}_{-i} is norm dense in $\mathcal{A}$ we reach the same conclusion for $n > N$.

Corollary (3.12)
If $\mathcal{A}$ is UHF and $(\mathcal{A}, \Theta)$ a K-system, then for the tracial state all conditions (3.1) are satisfied and $(\mathcal{A}, \Theta)$ is weakly mixing.

Corollary (3.13)
If $\mathcal{A}$ is UHF, then (2.1) can be sharpened to: $(\mathcal{A}, \Theta)$ is a K-system $\Rightarrow$ $(\mathcal{A}, \Theta)$ is weakly mixing $\Rightarrow$ all quasiperiodic elements of $\mathcal{A}$ are $\sim \mathbf{1}$, $\Rightarrow$ all invariant elements of $\mathcal{A}$ are $\sim \mathbf{1}$.

Remark (3.14)
K-systems are not only mixing but even K-mixing which is the maximally possible uniformity in mixing. Wheras complete uniformity in clustering in the sense that $\forall\, a \in \mathcal{A}$, $\|a\| = 1$, $\varepsilon > 0\, \exists N$ such that $|\omega(a\Theta^n b) - \omega(a)\omega(b)| < \varepsilon\|b\|\ \forall\, b \in \mathcal{A}$, $n > N$, is for faithful ω impossible (take $b = \Theta^{-n}a^*$) we found in the proof (3.11) $\forall\, a \in \mathcal{A}$, $m \in \mathbf{Z}$, $\varepsilon > 0\, \exists N$ such that

$$|\omega(a\Theta^n b) - \omega(a)\omega(b)| < \varepsilon\|b\| \quad \forall\, b \in \mathcal{A}_m,\ n < -N.$$

Since the $\mathcal{A}_m$ are dense that is the best one can hope for. It is related to the strong convergence of the P_n and is equivalent to saying that all states when restricted to one of the "strictly local" algebras $\mathcal{A}_m$ converge for $n \to \infty$ strongly to the equilibrium ω. Such states φ can be written $\varphi(b) = \omega(ab)$, $a \in \mathcal{A}$, $\omega(a) = \mathbf{1}$, and we have

Proposition (3.15)
In the Schrödinger representation $\forall\, \varepsilon > 0\ \exists\, N \in \mathbf{Z}^+$ such that

$$\|\varphi_{n|\mathcal{A}_m} - \omega_{|\mathcal{A}_m}\| = \sup_{b \in \mathcal{A}_m, \|b\|=1} |\omega(a\Theta^n b) - \omega(b)| < \varepsilon \quad \forall\, n < -N.$$

4 The Increase of Entropy with Time

One of the key formulas of quantum statistical mechanics is von Neumann's expression for the entropy of a state over $\mathcal{B}(\mathcal{H})$ given by a density matrix ρ

$$S = -\operatorname{Tr} \rho \ln \rho \tag{4.1}$$

This relation has been generalized for states over arbitrary von Neumann algebras $\mathcal{A}$ [17] but one always meets with the same difficulties when one discusses the question of entropy increase.

1. All these expressions have to be invariant under automorphisms and therefore cannot change with time. Furthermore, for infinite system S is infinite.

2. The entropy of the state restricted to a subalgebra $\mathcal{A}_0$, $\Theta\mathcal{A}_0 \neq \mathcal{A}_0$ may change with time but it may increase or decrease. Furthermore, if the state is time invariant – $\omega \circ \Theta = \omega$ – even for a subalgebra the entropy does not change:

$$S(\omega_{|\Theta\mathcal{A}_0}) = S(\omega \circ \Theta_{|\mathcal{A}_0}) = S(\omega_{|\mathcal{A}_0}). \tag{4.2}$$

The following two ways around these difficulties have been proposed:

1. Dynamical Entropy

For some infinite algebras $\mathcal{A}_0$ one can give a well defined meaning for the entropy increase per unit time

$$S(\omega_{|\Theta\mathcal{A}_0}) - S(\omega_{|\mathcal{A}_0}) = \infty - \infty.$$

If $\mathcal{A}_0 = \bigvee_{n=-\infty}^{0} \Theta^n \mathcal{B}_0$, $\mathcal{B}_0$ = finite, then classically

$$h_\omega(\mathcal{B}_0, \Theta) \equiv S(\omega_{|\Theta\mathcal{A}_0}) - S(\omega_{|\mathcal{A}_0}) = \lim_{m\to\infty} (S(\omega_{|\bigvee_{n=-m}^{1} \Theta^n\mathcal{B}_0}) - S(\omega_{|\bigvee_{n=-m}^{0} \Theta^n\mathcal{B}_0}) \tag{4.3}$$

is well defined. The dynamical (or Kolmogorov-Sinai [18]) entropy is the maximal increase (per unit time) of the entropy of these algebras

$$h_\omega(\Theta) = \sup_{\mathcal{B}_0 = \text{finite}} h_\omega(\mathcal{B}_0, \Theta). \tag{4.4}$$

In quantum theory the union $\bigvee_{n=-m}^{0} \Theta^n \mathcal{B}_0$ may be too big and S is not monotonic so the definition (4.3) is no good. Here one needs a more refined theory which has been elaborated in the past years [19]. One now disposes of a dynamical entropy of an automorphism of an arbitrary C^*-algebra [20] for which almost all the desired properties have been demonstrated. The theory is too extensive to be given here.

2. Relative Entropy

We all have learned in thermodynamics that for part of a system which exchanges energy with the rest, it is not the entropy which tends to a maximum but the free energy which tends to a minimum. Again the free energy of an infinite system may be infinite but the difference between energies of a locally disturbed equilibrium ν and the equilibrium state ω may be finite.

The relative entropy $S(\nu|\omega)$ is precisely this difference. For finite quantum systems where states can be described by density matrices it is

$$S(\nu|\omega) = \text{Tr } \nu(\ln\nu - \ln\omega) \tag{4.5}$$

and if ω is a canonical state (for $\beta = 1$) $\omega = e^{-H+F_\omega}$, F_ω = equilibrium free energy, we find

$$S(\nu|\mu) = \text{Tr } \nu(\ln\nu + H - F_\omega) = \langle H\rangle_\nu - S(\nu) - F_\omega \equiv F_\nu - F_\omega.$$

There is a general definition of $S(\nu|\omega)$ for arbitrary states of C^*-algebras [19,21]. For infinite systems $S(\nu|\mu)$ is finite if $\nu < c\omega$ and ν is a local perturbation of ω. Again the definition is invariant under automorphisms so that $S(\nu|\omega)$ does not change with time. For subsystems it may change but not necessarily monotonically. We shall see that this monotonicity is a special feature of K-systems.

Theorem (4.6)
Let $(\mathcal{A}, \mathcal{A}_0, \Theta)$ be a K-system, ω an invariant state and φ a normal state for $\Pi_\omega(\mathcal{A})''$ with $\lambda_1 \omega \leq \varphi \leq \lambda_2 \omega$, $\lambda_i \in \mathbf{R}^+$. Then for any $m \in \mathbf{Z}$, $\mathcal{A}_m = \Theta^m \mathcal{A}_0$,

$$\Delta F(n) = S(\varphi \circ \Theta^n_{|\mathcal{A}_m} | \omega_{|\mathcal{A}_m})$$

converges monotonically for $-\infty < n < \infty$ from 0 to $S(\varphi|\omega)$.

Remarks (4.7)

1. Even in finite dimensions $S(\varphi|\omega)$ is not continuous and becomes infinite where ω is zero but φ greater zero. Thus we need a condition on the states.
2. We have seen that for mixing systems any normal state converges weakly towards equilibrium. However, $\varphi \rightharpoonup \omega$ does not imply $S(\varphi|\omega) \to 0$ since $S(\varphi|\omega) > \frac{1}{2}||\varphi - \omega||^2$. Thus it is only the strong convergence (3.12) of the restriction of φ which ensues the convergence of the free energy of the subsystems $\mathcal{A}_n$.
3. In general, even if the free energy converges towards its equilibrium value it will not be monotonic because of thermal fluctuations. It is a special feature of K-systems that there are subalgebras where this does not happen.
4. The thoughtful reader will be perplexed by the fact that ΔF converges away from its equilibrium value 0 to its maximal value $S(\varphi|\omega)$. However, it is not yet said whether Θ or Θ^{-1} is the real time devlopment. The physical K-systems are actually time reversal invariant in the sense that there is an antiautomorphism K, $K^2 = 1$, with $K\Theta K = \Theta^{-1}$. Then for $K(\mathcal{A}_0)$ the free energy decreases if it increases for $\mathcal{A}_0$. For time reversal invariant systems there are necessarily as many subsystems with increasing free energy as there are with decreasing free energy.

Proof of (4.6)

(i) Monotonicity

$$\varphi \circ \Theta^n{}_{|\mathcal{A}_m} = \varphi_{|\mathcal{A}_{m+n}}$$

and for $n < n'$ $\mathcal{A}_{m+n} \subset \mathcal{A}_{m+n'}$. The relative entropy has the monotonicity [19]

$$S(\varphi_{|\mathcal{A}}|\omega_{|\mathcal{A}}) \leq S(\varphi_{|\mathcal{B}}|\omega_{|\mathcal{B}}) \quad \text{if } \mathcal{A} \subset \mathcal{B}.$$

(ii) The limit $n \to -\infty$
We have seen in (3.12) that

$$\lim_{n \to -\infty} ||\varphi_{|\mathcal{A}_n} - \omega_{|\mathcal{A}_n}|| \to 0$$

and for states satisfying the hypothesis [16] of (4.6) this implies

$$S(\varphi_{|\mathcal{A}_n}|\omega_{|\mathcal{A}_n}) \to 0 \quad \text{for } n \to -\infty.$$

(iii) S can be written as sup over an expression linear and therefore weak*-continuous in φ and ω [19]. Thus it is weak*-lower semicontinuous and this implies

$$\lim_{n \to \infty} S(\varphi_{|\mathcal{A}_n}|\omega_{|\mathcal{A}_n}) \geq S(\varphi|\omega).$$

However, monotonicity insures the opposite inequality.

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