Chapter 3

Equilibrium: KMS states

In a quantum system with Hamiltonian H such that $\mathrm{Tr}\exp(-\beta H)$ is finite for some $\beta > 0$, the Gibbsian rule is as follows: The system in thermal equilibrium is in a state given by a density matrix ρ_β on $\mathcal{H}$,

$$\rho_\beta = Z(\beta)^{-1}\mathrm{e}^{-\beta H}, \qquad Z(\beta) := \mathrm{Tr}\mathrm{e}^{-\beta H}.$$

Among its many properties, we concentrate on an a priori rather coincidental properties. Let ω_β denote the state associated to the density matrix ρ_β, and $\tau_t(A) = \exp(\mathrm{i}tH)A\exp(-\mathrm{i}tH)$. Consider the function $F_\beta(A, B; t) = Z(\beta)^{-1}\mathrm{Tr}(\exp(-\mathrm{i}(t-\mathrm{i}\beta)H)A\exp(\mathrm{i}tH)B)$. Using the cyclicity of the trace, $F_\beta(A, B; t) = \omega_\beta(A\tau_t(B))$. On the other hand, $F_\beta(A, B; t)$ can be analytically continued into the complex plane to $t + \mathrm{i}\beta$ to give $F_\beta(A, B; t + \mathrm{i}\beta) = Z(\beta)^{-1}\mathrm{Tr}(\exp(-\mathrm{i}tH)A\exp(\mathrm{i}(t + \mathrm{i}\beta)H)B) = \omega_\beta(\tau_t(B)A)$. Hence, there is an analytic function $F_\beta(A, B; z)$ defined on the strip $\{z \in \mathbb{C} : 0 \leq \mathrm{Im}z \leq \beta\}$ with boundary values

$$F_\beta(A, B; t) = \omega_\beta(A\tau_t(B)), \qquad F_\beta(A, B; t + \mathrm{i}\beta) = \omega_\beta(\tau_t(B)A). \tag{3.1}$$

This turns our to be the property that extends naturally to the algebraic setting.

3.1 Definition

It will be useful to first introduce some terminology.

Definition 11. *A pair $(\mathcal{A}, \tau_t)$ is a* C*-dynamical system *if $\mathcal{A}$ is a C*-algebra with an identity and $\mathbb{R} \ni t \mapsto \tau_t$ is a strongly continuous group of *-automorphisms of $\mathcal{A}$, namely*

$$\|\tau_{t+\epsilon}(A) - \tau_t(A)\| \to 0 \qquad (\epsilon \to 0)$$

for all $A \in \mathcal{A}$.

It follows from the strong continuity that τ_t is generated by a *-derivation, $\tau_t(A) = \mathrm{e}^{t\delta}A$:

Proposition 22. *Let $\delta_t : \mathcal{A} \to \mathcal{A}, A \mapsto \delta_t(A) = t^{-1}(\tau_t(A) - A)$, let*

$$D(\delta) := \{A \in \mathcal{A} : \lim_{t\to 0^+} \delta_t(A) \text{ exists}\},$$

and define

$$\begin{aligned} \delta : D(\delta) &\to \mathcal{A} \\ A &\mapsto \delta(A) = \lim_{t\to 0^+} t^{-1}(\tau_t(A) - A). \end{aligned}$$

Then, δ is a closed, densely defined map such that

$$\begin{aligned}
&1 \in D(\delta) \text{ and } \delta(1) = 0,\\
&\delta(AB) = \delta(A)B + A\delta(B),\\
&\delta(A^*) = \delta(A)^*.
\end{aligned}$$

In fact, just as there is a one-to-one correspondence between self-adjoint generators and strongly continuous unitary groups on a Hilbert space, there a correspondence between *-derivations and strongly continuous groups of *-automorphisms on a C*-algebra. This is Hille-Yosida's theorem. Recall that A is an analytic element for a derivation δ if $A \in D(\delta^n)$ for all $n \in \mathbb{N}$ and $\sum_{n=0}^{\infty} \frac{t^n}{n!}\|\delta^n A\| < \infty$, for $0 \le t < t_A$.

Theorem 23. *Let $\mathcal{A}$ be a C*-algebra with a unit. A densely defined, closed operator δ on $\mathcal{A}$ generates a strongly continuous groups of *-automorphisms if and only if*

$$\begin{aligned}
&\delta \text{ is a *-derivation}\\
&\delta \text{ has a dense set of analytic elements}\\
&\|A + \lambda\delta(A)\| \ge \|A\|, \forall \lambda \in \mathbb{R}, A \in D(\delta).
\end{aligned}$$

In the case of quantum mechanics with a finite number of degrees of freedom, $\tau_t(A) = \exp(\mathrm{i}tH)A\exp(-\mathrm{i}tH)$ is strongly continuous if and only if H is bounded, in which case it is also norm continuous (see exercises). The associated derivation $\delta := \mathrm{i}[H, \cdot]$ is bounded and everywhere defined. In fact, as a consequence of the closed graph theorem, an everywhere defined derivation necessarily generates a norm-continuous *-automorphism.

Definition 12. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system. A state ω on $\mathcal{A}$ is a* (τ, β)-KMS state *for $\beta > 0$ if, for any $A, B \in \mathcal{A}$, there exists a function $F_\beta(A, B, z)$, analytic in $S_\beta := \{z \in \mathbb{C} : 0 < \mathrm{Im} z < \beta\}$, continuous on $\overline{S_\beta}$, and satisfying the KMS boundary condition (3.1).*

We shall say that A is an analytic element for τ_t if the map $A \mapsto \tau_t(A)$ extends to an analytic function on $\mathbb{C}$.

Theorem 24. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system. A state ω on $\mathcal{A}$ is a* (τ, β)-KMS state *if and only if there exists a dense, τ-invariant *-subalgebra $\mathcal{D}$ of analytic elements for τ_t such that*

$$\omega(BA) = \omega(A\tau_{\mathrm{i}\beta}(B)). \tag{3.2}$$

The following proposition shows that the condition of analyticity is never a true restriction.

Proposition 25. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system, and let δ be its generator. For any $A \in \mathcal{A}$ and $m \in \mathbb{N}$, let*

$$A_m := \sqrt{\frac{m}{\pi}} \int_{\mathbb{R}} \tau_t(A) \mathrm{e}^{-mt^2} dt.$$

Then

1. *A_m is analytic for τ_t*
2. *A_m is analytic for δ*
3. *The *-subalgebra $\mathcal{A}_\tau := \{A_m : A \in \mathcal{A}, m \in \mathbb{N}\}$ is dense*

Proof. First of all, $\|\tau_t(A)\| \exp(-mt^2) = \|A\| \exp(-mt^2) \in L^1(\mathbb{R})$, so that A_m is well-defined, $A_m \in \mathcal{A}$ and $\|A_m\| \le \|A\|$. Moreover,

$$\tau_s(A_m) = \sqrt{\frac{m}{\pi}} \int_{\mathbb{R}} \tau_t(A) \mathrm{e}^{-m(t-s)^2} dt.$$

The right-hand-side extends to an analytic function, with $\|\text{r.h.s.}\| \le \|A\| \exp(-m(\mathrm{Im} z)^2)$, which can be used to extend $\tau_s(A_m)$ to $\tau_z(A_m)$ for all $z \in \mathbb{C}$. Moreover, by dominated convergence,

$$\left.\frac{d^n}{ds^n}\tau_s(A_m)\right|_{s=0} = \sqrt{\frac{m}{\pi}} \int_{\mathbb{R}} \tau_t(A) \left.\frac{d^n}{ds^n}\mathrm{e}^{-m(t-s)^2}\right|_{s=0} dt = \sqrt{\frac{m^{1+n}}{\pi}} \int_{\mathbb{R}} \tau_t(A) H_n(t) \mathrm{e}^{-mt^2} dt$$

were H_n are the Hermite polynomials, so that $A_m \in D(\delta^n)$ for all $n \in \mathbb{N}$, and A_m is analytic for δ. Finally,

$$A_n - A = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \left(\tau_{t/\sqrt{n}}(A) - A\right) \mathrm{e}^{-t^2} dt \to 0 \qquad (n \to \infty)$$

by the strong continuity of τ_t and dominated convergence. □

Proof of Theorem 24. Necessity. Let $A \in \mathcal{A}, B \in \mathcal{A}_\tau$ and ω be a (τ, β)-KMS state. Then $z \mapsto G(z) = \omega(A\tau_z(B))$ is analytic and $G(t) = F_\beta(A, B; t)$ for $t \in \mathbb{R}$. Hence $z \mapsto G(z) - F_\beta(A, B; z)$ is analytic on S_β, continuous on $S_\beta \cup \mathbb{R}$ and vanishes on $\mathbb{R}$. By the Schwarz reflection principle, it extends to an analytic function on the double strip $S_\beta \cup S_{-\beta}$ that vanishes on $\mathbb{R}$. Hence it equals zero everywhere, and by continuity also on $\overline{S_\beta}$, that is $F_\beta(A, B; z) = \omega(A\tau_z(B))$ for all $z \in \overline{S_\beta}$. In particular, setting $z = \mathrm{i}\beta$ yields $\omega_\beta(BA) = \omega_\beta(A\tau_{\mathrm{i}\beta}(B))$.
Sufficiency. First, for $A, B \in \mathcal{D}$, $z \mapsto F(A, B; z) := \omega(A\tau_z(B))$ is analytic on $\mathbb{C}$. Since $\tau_t(B) \in \mathcal{D}$,

$$F(A, B; t) = \omega(A\tau_t(B)), \qquad F(A, B; t + \mathrm{i}\beta) = \omega(A\tau_{\mathrm{i}\beta}(\tau_t(B))) = \omega(\tau_t(B)A),$$

by (3.2). Now, $|\omega(A\tau_z(B))| \le \|A\|\|\tau^{\mathrm{i}\mathrm{Im} z}(B)\|$ so that $F(A, B; z)$ is bounded on S_β and Hadamard's three lines theorem yields $\sup_{z \in \overline{S_\beta}} F(A, B; z) \le \|A\|\|B\|$. For arbitrary $A, B \in \mathcal{A}$, let $A_n \to A, B_n \to B$, with $A_n, B_n \in \mathcal{D}$. Since

$$F(A_n, B_n; z) - F(A_m, B_m; z) = F(A_n - A_m, B_n; z) + F(A_m, B_n - B_m; z),$$

so that $F(A_n, B_n; z)$ is uniformly Cauchy in $\overline{S_\beta}$. Its limit is therefore analytic on S_β and continuous on its closure, and it still satisfies the KMS boundary condition. □

Clearly, the Gibbs state on a finite dimensional Hilbert space satisfies the KMS condition. As we shall see later, it is also the unique KMS state in this case[1].

The following theorem shows that a KMS state passes the simplest test for an equilibrium state: it is invariant under time evolution. Mathematically, this is also useful as it implies the unitary implementability of the dynamics in the GNS representation.

Proposition 26. *Let $(\mathcal{A}, \tau_t)$ be a C^*-dynamical system and let ω be a (τ, β)-KMS state. Then $\omega \circ \tau_t = \omega$ for all $t \in \mathbb{R}$.*

Proof. Let $A \in \mathcal{A}_\tau$. The function $z \mapsto g(z) = \omega(\tau_z(A))$ is analytic. By Theorem 24,

$$g(z + \mathrm{i}\beta) = \omega(1\tau_{\mathrm{i}\beta}(\tau_z(A))) = \omega(\tau_z(A)1) = g(z).$$

Hence, g is a periodic function along the imaginary axis, and moreover, $|g(t+\mathrm{i}\alpha)| \le \|\tau_{t+\mathrm{i}\alpha}(A)\| = \|\tau_{\mathrm{i}\alpha}(A)\| \le \sup_{0\le\gamma\le\beta} \|\tau_{\mathrm{i}\gamma}(A)\|$, which is finite. Hence, g is analytic and bounded on $\mathbb{C}$, so that it is constant by Liouville's theorem. This extends to all observables by continuity. □

[1]This shows once again that there cannot be a phase transition for quantum spin systems in finite volume.

3.2 The energy-entropy balance inequality

Just as the Gibbs state is characterised by the variational principle as being a minimiser of the free energy, general KMS states are equivalently defined by satisfying the *energy-entropy balance inequality* (EEB). In this section, $(\mathcal{A}, \tau_t)$ is a C*-dynamical system, and δ is the generator of τ_t. We start with a simple observation.

Lemma 27. *If a state ω over $\mathcal{A}$ is such that $-\mathrm{i}\omega(A^*\delta(A)) \in \mathbb{R}$ for all $A \in D(\delta)$, then $\omega \circ \tau_t = \omega$.*

Proof. Since $\omega(B^*\delta(B))$ is purely imaginary, and $\delta(B^*) = \delta(B)^*$, $\omega(\delta(B^*B)) = \omega(B^*\delta(B)) + \overline{\omega(B^*\delta(B))} = 0$. Hence, with the continuity of ω,

$$\omega(\tau_t(A^*A)) - \omega(A^*A) = \int_0^t \omega(\delta(\tau_s(A^*A)))ds = 0.$$

Hence, the statement holds for all positive elements of $\mathcal{A}$, and further extends to all of $\mathcal{A}$ by noting that any observable is a linear combination of four positive elements. $\square$

Let f be the Fourier transform of $\check{f} \in C_c^\infty(\mathbb{R})$. By Paley-Wiener's theorem, f is analytic in $\mathbb{C}$ and $|f(z)| \leq C_n(1 + |z|^n)\exp(R|\mathrm{Im}(z)|)$ for all $n \in \mathbb{N}$. Let

$$\tau_f(A) := \int_{\mathbb{R}} f(t)\tau_t(A)dt \in D(\delta)$$

since it is analytic for δ. Let ω be a τ_t-invariant state and $H = \int_{\mathbb{R}} \lambda dP(\lambda)$ is the GNS Hamiltonian satisfying $H\Omega = 0$. We have

$$\omega(A^*\tau_f(A)) = \int_{\mathbb{R}} f(t)\langle \pi(A)\Omega, \mathrm{e}^{\mathrm{i}tH}\pi(A)\Omega\rangle dt = \int_{\mathbb{R}} \check{f}(\lambda)d\mu_A(\lambda) \tag{3.3}$$

where $d\mu_A(\lambda) = \langle \pi(A)\Omega, dP(\lambda)\pi(A)\Omega\rangle$ is the spectral measure associated with $\pi(A)\Omega$. Similary, $\omega(\tau_f(A)A^*) = \int_{\mathbb{R}} \check{f}(\lambda)d\nu_A(\lambda)$ where $d\nu_A(\lambda) = \langle \pi(A^*)\Omega, dP(-\lambda)\pi(A^*)\Omega\rangle$. Moreover, the analyticity of $z \mapsto f(z)\omega(A^*\tau_z(A))$ and the KMS condition yield

$$\omega(A^*\tau_f(A)) = \int_{\mathbb{R}} f(t + \mathrm{i}\beta)\omega(\tau_t(A)A^*)dt.$$

The right hand side is also equal to $\int_{\mathbb{R}} \check{f}(\lambda)\exp(\beta\lambda)d\nu_A(\lambda)$. Since this and (3.3) hold for any test function $\check{f}$, we obtain

$$\frac{d\mu_A}{d\nu_A}(\lambda) = \mathrm{e}^{\beta\lambda}. \tag{3.4}$$

Theorem 28. *A state ω over $\mathcal{A}$ is a (τ, β)-KMS state if and only if*

$$-\mathrm{i}\beta\omega(A^*\delta(A)) \geq \omega(A^*A)\ln\frac{\omega(A^*A)}{\omega(AA^*)}$$

for all $A \in D(\delta)$.

Proof. We only prove $\Rightarrow$. First observe that $\omega(A^*\delta(A)) = \mathrm{i}\langle \pi(A)\Omega, H\pi(A)\Omega\rangle$ and

$$\beta\frac{\langle \pi(A)\Omega, H\pi(A)\Omega\rangle}{\langle \pi(A)\Omega, \pi(A)\Omega\rangle} = \frac{\int_{\mathbb{R}} \beta\lambda d\mu_A(\lambda)}{\int_{\mathbb{R}} d\mu_A(\lambda)}.$$

By Jensen's inequality,

$$\exp\left(-\frac{\int_{\mathbb{R}} \beta\lambda d\mu_A(\lambda)}{\int_{\mathbb{R}} d\mu_A(\lambda)}\right) \leq \frac{\int_{\mathbb{R}} \exp(-\beta\lambda)d\mu_A(\lambda)}{\int_{\mathbb{R}} d\mu_A(\lambda)} = \frac{\int_{\mathbb{R}} d\nu_A(\lambda)}{\int_{\mathbb{R}} d\mu_A(\lambda)} = \frac{\omega(AA^*)}{\omega(A^*A)}$$

if ω is a (τ, β)-KMS state by (3.4). Hence, $\exp(\mathrm{i}\beta\omega(A^*\delta(A))/\omega(A^*A)) \leq \omega(AA^*)/\omega(A^*A)$. $\square$

Corollary 29. *Let $\mathcal{A}$ be a C^*-algebra with a unit and $\{\tau^n\}_{n\in\mathbb{N}}$ be a sequence of strongly continuous one-parameter groups of automorphisms of $\mathcal{A}$ such that*

$$\tau_t^n(A) \to \tau_t(A) \qquad (n \to \infty)$$

for all $A \in \mathcal{A}, t \in \mathbb{R}$, where τ_t is a strongly continuous one-parameter group of automorphisms of $\mathcal{A}$. If $\{\omega_n\}_{n\in\mathbb{N}}$ is a sequence of (τ^n, β)-KMS states, then any weak- limit point of $\{\omega_n\}$ is a (τ, β)-KMS state.*

Proof. See exercises. □

Simple example. $\tau^n = \tau^{\Lambda_n}$ the dynamics of a quantum spin system in a finite volume Λ_n, such that $\Lambda_n \to \Gamma$ as $n \to \infty$[2], generated by a Hamiltonian H_{Λ_n}. The unique KMS state is the Gibbs state with density matrix $Z_n(\beta)^{-1}\exp(-\beta H_{\Lambda_n})$. If the infinite volume dynamics exists, $\tau^{\Lambda_n}(A) \to \tau^{\Gamma}(A)$, then the limiting thermodynamic states are (τ^{Γ}, β)-KMS states.

3.3 Passivity and stability

Definition 13. *Let $(\mathcal{A}, \tau_t)$ be a C^*-dynamical system. A state ω on $\mathcal{A}$ is a* passive state *if $-\mathrm{i}\omega(U^*\delta(U)) \geq 0$ for any $U \in \mathcal{U}_0(\mathcal{A}) \cap D(\delta)$. Here, $\mathcal{U}_0(\mathcal{A})$ is the connected component of the identity in the set of all unitary elements of $\mathcal{A}$.*

Proposition 30. *If ω is a (τ, β)-KMS state, then ω is passive.*

Proof. Choose $A = U \in \mathcal{U}_0(\mathcal{A}) \cap D(\delta)$ in the EEB inequality. □

In order to have equivalence in the proposition above, one needs to require *complete passivity*, namely that $\otimes_{i=1}^N \omega$ is passive as a state on the tensored system $(\otimes_{i=1}^N \mathcal{A}, \otimes_{i=1}^N \tau_t)$ for all $N \in \mathbb{N}$.

Interpretation in the case $\dim(\mathcal{H}) < \infty$, where $\omega(A) = \mathrm{Tr}(\rho_\beta A)$ where $\rho_\beta = Z(\beta)^{-1}\exp(-\beta H)$ with $Z(\beta) = \mathrm{Tr}\exp(-\beta H)$, the Gibbs state. Consider a time dependent Hamiltonian $H(t) = H(t)^*, t \in [0, T]$ such that $H(0) = H(T) = H$, an let U be the associated unitary evolution on $[0, T]$. The change in energy between $t = 0$ and $t = T$ is given by

$$W_\beta := \mathrm{Tr}(U\rho_\beta U^* H) - \mathrm{Tr}(\rho_\beta H) = \mathrm{Tr}(\rho_\beta U^*[H, U]) = -\mathrm{i}\omega_\beta(U^*\delta(U)) \geq 0$$

since the KMS state is passive. Passivity expresses a basic thermodynamic fact: the total work done by the system on the environment in an arbitrary cyclic process, $-W_\beta$, is non-positive on average.

Definition 14. *Let $(\mathcal{A}, \tau_t)$ be a C^*-dynamical system with generator δ^0. A* local perturbation *δ^V of δ^0 is given by*

$$\delta^V = \delta^0 + \mathrm{i}[V, \cdot], \qquad D(\delta^V) = D(\delta^0),$$

for a $V = V^* \in \mathcal{A}$.

Using Thm 23, one can show that δ^V generates a strongly continuous group of automorphisms τ^V. Since $\frac{d}{ds}\tau_{-s}^0(\tau_s^V(A)) = \tau_{-s}^0(\mathrm{i}[V, \tau_s^V(A)])$, we have Duhamel's formula

$$\tau_t^V(A) = \tau_t^0(A) + \int_0^t \tau_{t-s}^0(\mathrm{i}[V, \tau_s^V(A)])ds,$$

[2] $\Lambda_n \subset \Lambda_m$ if $n \leq m$, and $\forall x \in \Gamma$, $\exists n_0 \in \mathbb{N}$ such that $x \in \Lambda_n$ $\forall n \geq n_0$

which can be solved iteratively yielding Dyson's expansion

$$\tau_t^V(A) = \tau_t^0(A) + \sum_{k=1}^{\infty} \int_{0\le t_1\le\cdots\le t_k\le t} \mathrm{i}[\tau_{t_1}^0(V), \mathrm{i}[\tau_{t_2}^0(V), \cdots \mathrm{i}[\tau_{t_k}^0(V), \tau_t^0(A)]\cdots]]dt_1\cdots dt_k. \quad (3.5)$$

In fact, writing λV for $\lambda \in \mathbb{C}$, the series is norm convergent for all $\lambda \in \mathbb{C}, t \in \mathbb{R}, A \in \mathcal{A}$ and defines an analytic function $\lambda \mapsto \tau_t^{\lambda V}(A)$.

The unitary element solving

$$-\mathrm{i}\partial_t \Gamma_t^V = \Gamma_t^V \tau_t^0(V), \qquad \Gamma_0^V = 1,$$

has the following intertwining property $\tau_t^V(A)\Gamma_t^V = \Gamma_t^V \tau_t^0(A)$. Solving the differential equation iteratively again yields the expansion

$$\Gamma_t^V = 1 + \sum_{k=1}^{\infty} \mathrm{i}^k \int_{0\le t_1\le\cdots\le t_k\le t} \tau_{t_1}^0(V)\cdots\tau_{t_k}^0(V)dt_1\cdots dt_k.$$

In fact, all above results continue to hold for a time dependent perturbation V_t. A cyclic perturbation of a C*-dynamical system is a norm-differentiable family $[0,T] \ni t \mapsto V_t = V_t^* \in \mathcal{A}$ such that $V_0 = V_T = 0$, $V_t \in D(\delta)$ and $\delta(dV_t/dt) = d\delta V_t/dt$.

Definition 15. *The* work performed on the system *along a cyclic V_t, $t \in [0,T]$ is*

$$W := \int_0^T \omega \circ \tau_t^V \left(\frac{dV_t}{dt} \right) dt.$$

where ω is the initial state of the system.

By the boundary condition, $0 = \int_0^T \partial_t \left(\omega \circ \tau_t^V (V_t) \right) dt$, so that

$$W = -\int_0^T \omega \circ \tau_t^V \left(\delta^0 (V_t) \right) dt \quad (3.6)$$

since $\delta^V(V_t) = \delta^0(V_t)$. Also note that by the first law of thermodynamics, this also equals the total heat given by the system to the environment.

Lemma 31. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system with generator δ^0 and $\mathbb{R} \ni t \mapsto V_t = V_t^* \in \mathcal{A}$ be a norm-differentiable local perturbation such that $V_t = 0$ if $t \in (-\infty, 0] \cup [T, \infty)$, $V_t \in D(\delta^0)$ and $\delta^0(dV_t/dt) = d\delta^0 V_t/dt$. Then $W = -\mathrm{i}\omega(\Gamma_T^V \delta^0(\Gamma_T^{V*}))$.*

Proof. Under the given assumption, $\Gamma_t^V \in D(\delta^0)$, and $\delta^0(\Gamma_t^V)$ is differentiable with $d\delta^0(\Gamma_t^V)/dt = \delta^0(d\Gamma_t^V/dt)$ (without proof). But then

$$\begin{aligned} -\mathrm{i}\omega(\Gamma_T^V \delta^0(\Gamma_T^{V*})) &= \int_0^T \omega \left(-\mathrm{i}\partial_t(\Gamma_t^V)\delta^0(\Gamma_t^{V*}) + \Gamma_t^V \delta^0 \left(-\mathrm{i}\partial_t(\Gamma_t^{V*}) \right) \right) \\ &= \int_0^T \omega \left(\Gamma_t^V \tau_t^0(V)\delta^0(\Gamma_t^{V*}) - \Gamma_t^V \delta^0(\tau_t^0(V)\Gamma_t^{V*}) \right) = -\int_0^T \omega \left(\Gamma_t^V \tau_t^0(\delta^0(V))\Gamma_t^{V*} \right). \end{aligned}$$

Conclude by (3.6). ☐

Theorem 32. *Under the assumptions of the previous lemma, if ω is a (τ, β)-KMS state for some β, then $W \geq 0$.*

Proof. By Lemma 31, $W = -\mathrm{i}\omega(\Gamma_T^V \delta^0(\Gamma_T^{V*}))$. Since Γ_T^V is unitary and ω is a (τ, β)-KMS state, $W \geq 0$ by passivity, Proposition 30. □

We now consider a cyclic machine working between two reservoirs at inverse temperature $\beta_1 \leq \beta_2$. The C*-dynamical system is given by $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2$ and $\tau^0 = \tau_1 \otimes \tau_2$, with generator $\delta^0 = \delta_1 \otimes 1 + 1 \otimes \delta_2$. The initial state is $\omega = \omega_1 \otimes \omega_2$ where ω_i is a (τ_i, β_i)-KMS state, and it is a $(\sigma, 1)$-KMS state for the dynamics $\sigma_t := \tau_{1,\beta_1 t} \otimes \tau_{2,\beta_2 t}$ with generator $\gamma = \beta_1\delta_1 \otimes 1 + 1 \otimes \beta_2\delta_2$. The machine is represented by a cyclic perturbation $V_t \in \mathcal{A}$ temporarily coupling the reservoirs. The total work on the system decomposes in $W = Q_1 + Q_2$ where

$$Q_1 = -\mathrm{i}\omega(\Gamma_T^V(\delta_1 \otimes 1)(\Gamma_T^{V*})), \qquad Q_2 = -\mathrm{i}\omega(\Gamma_T^V(1 \otimes \delta_2)(\Gamma_T^{V*}))$$

are the amounts of heat given to both reservoirs. Now,

$$\beta_1 Q_1 + \beta_2 Q_2 = -\mathrm{i}\omega(\Gamma_T^V(\beta_1\delta_1 \otimes 1 + 1 \otimes \beta_2\delta_2)(\Gamma_T^{V*})) = -\mathrm{i}\omega(\Gamma_T^V \gamma(\Gamma_T^{V*})) \geq 0,$$

or $Q_1(T_2 - T_1) \geq -WT_1$. Assuming now that $Q_1 < 0$ (heat pumped out of the hot reservoir)

$$\frac{-W}{-Q_1} \leq \frac{T_1 - T_2}{T_1}$$

which is Carnot's statement of the second law of thermodynamics, namely a bound on the efficiency of a cyclic machine initially at equilibrium (ratio of the work performed by the system to the heat pumped out of the hot reservoir).

Stability of the thermal equilibrium refers to a number of results revolving around the fact that the dynamics applied to a state 'close to thermal' drives the system back to equilibrium. In fact, under additional assumption, it can be shown that this property is equivalent to the KMS condition.

The first result is about *structural stability*, and can be proved by perturbation theory in the line of (3.5).

Proposition 33. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system, and ω a (τ, β)-KMS state on $\mathcal{A}$. Then, for every local perturbation V, there is a (τ^V, β)-KMS state ω^V and*

1. *ω^V is ω-normal*
2. *there is $C > 0$ such that $\|\omega - \omega^V\| \leq C\|V\|$*
3. *the map $\omega \mapsto \omega^V$ is a bijection from the set of (τ, β)-KMS states onto the set of (τ^V, β)-KMS states*

See exercises for a proof in the finite dimensional case. Note in particular that local perturbations cannot induce a phase transition.

Dynamical stability needs more assumptions to hold, usually in the form of asymptotic abelianness of the dynamical system, namely $[A, \tau_t(B)] \to 0$ in some sense.

Theorem 34. *Let $V = V^* \in \mathcal{A}$ and let ω be a (τ^V, β)-KMS state, and let $\tilde{\omega}$ be a weak-* accumulation point of $\omega \circ \tau_t^0$ as $t \to \infty$. If $\lim_{t\to\infty} \|[V, \tau_t^0(A)]\| = 0$ for all $A \in \mathcal{A}$, then $\tilde{\omega}$ is a (τ^0, β)-KMS state.*

Proof. By lower semicontinuity of $(u, v) \mapsto u \ln(u/v)$, we have

$$\begin{aligned}\tilde{\omega}(A^*A) \ln \frac{\tilde{\omega}(A^*A)}{\tilde{\omega}(AA^*)} &\leq \liminf_{t\to\infty} \omega \circ \tau_t^0(A^*A) \ln \frac{\omega \circ \tau_t^0(A^*A)}{\omega \circ \tau_t^0(AA^*)} \leq \liminf_{t\to\infty} -\mathrm{i}\beta\omega(\tau_t^0(A)^* \delta^V(\tau_t^0(A))) \\ &= -\mathrm{i}\beta\tilde{\omega}(A^*\delta^0(A)) + \beta \liminf_{t\to\infty} \omega(\tau_t^0(A)^*[V, \tau_t^0(A)]) = -\mathrm{i}\beta\tilde{\omega}(A^*\delta^0(A))\end{aligned}$$

by the EEB inequality, the decomposition $\delta^V = \delta^0 + \mathrm{i}[V, \cdot]$ and $\delta^0 \circ \tau^0 = \tau^0 \circ \delta^0$. □

Note that the theorem does not state whether the limit of $\omega \circ \tau_t^0$ exists. However, it does so in two simple cases. Firstly, if there is a unique (τ^0, β)-KMS state, since then all accumulation points of $\omega \circ \tau_t^0$ must be equal. Secondly, if $[V, \tau_t^0(A)]$ decays fast enough:

Proposition 35. *Let $V = V^* \in \mathcal{A}$ and let ω be a τ^V-invariant state. Then $\omega_\pm := \lim_{t\to\pm\infty} \omega\circ\tau_t^0$ exists (in the weak*-topology) if and only if $\mathbb{R} \ni t \mapsto \omega([V, \tau_t^0(A)])$ is integrable at $\pm\infty$ for all $A \in \mathcal{A}$.*

Proof. Integrating $\frac{d}{ds}\tau_{-s}^V(\tau_s^0(A)) = -\tau_{-s}^V(\mathrm{i}[V, \tau_s^0(A)])$ and using the invariance of ω yields

$$\omega(\tau_{t_2}^0(A)) - \omega(\tau_{t_1}^0(A)) = -\mathrm{i} \int_{t_1}^{t_2} \omega([V, \tau_s^0(A)]) ds$$

for all $A \in \mathcal{A}$. □

In particular, a sufficient condition for the existence of the limit is the integrability of the map $\mathbb{R} \ni t \mapsto \|[V, \tau_t^0(A)]\|$. We finally state a sharp result. Let ω be an arbitrary reference state.

(A) For any self-adjoint element V of a norm-dense *-subalgebra $\mathcal{A}_0 \subset \mathcal{A}$, there is a $\lambda_V > 0$ such that

$$\int_{\mathbb{R}} \|[V, \tau_s^{\lambda V}(A)]\| ds < \infty, \qquad |\lambda| \le \lambda_V, A \in \mathcal{A}_0.$$

(S) For any self-adjoint element V of a norm-dense *-subalgebra $\mathcal{A}_0 \subset \mathcal{A}$, there is a $\lambda_V > 0$ such that if $|\lambda| \le \lambda_V$, there exists a $\tau^{\lambda V}$-invariant, ω-normal state such that

$$\omega_+^{\lambda V} := \lim_{t\to\infty} \frac{1}{T} \int_0^T \omega \circ \tau_t^{\lambda V} dt \text{ exists,} \quad \text{and} \quad \lim_{\lambda\to 0} \|\omega - \omega^{\lambda V}\| = 0$$

Theorem 36. *Assume that ω is a factor state and that (A) holds. Then (S) holds if and only if ω is a (τ^0, β)-KMS state for some β.*

In that case, by a variant of Theorem (34), $\omega_+^{\lambda V}$ is a $(\tau^{\lambda V}, \beta)$-KMS state.

3.4 On the set of KMS states

Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system with an identity. For any $\beta > 0$, let $\mathcal{S}_\beta(\mathcal{A})$ be the set of all (τ, β)-KMS states. The physical intuition is as follows: for small β, there is a unique thermal state, corresponding to the high temperature phase. As β grows, the set of $\mathcal{S}_\beta(\mathcal{A})$ becomes non trivial, and any state can be decomposed into pure thermodynamic phases. This picture is made mathematically precise in the following theorem:

Theorem 37. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system with an identity, and let $\mathcal{S}_\beta(\mathcal{A})$ be the set of all (τ, β)-KMS states, for $\beta > 0$. Then,*

1. *$\mathcal{S}_\beta(\mathcal{A})$ is convex and weakly-* compact*
2. *The normal extension of ω to $\pi(\mathcal{A})''$ is a KMS state*
3. *$\omega \in \mathcal{S}_\beta(\mathcal{A})$ is an extremal point if and only if ω is a factor state,*
   and if ω' is an ω-normal, extremal KMS state, then $\omega = \omega'$
4. *$\pi(A)' \cap \pi(A)''$ consists of time-invariant elements*

5. *If $\omega \in \mathcal{S}_\beta(\mathcal{A})$ is such that the GNS Hilbert space is separable, there is a unique probability measure μ on $\mathcal{S}_\beta(\mathcal{A})$, which is concentrated on the extremal points, such that $\omega = \int_{\mathcal{S}_\beta(\mathcal{A})} \nu d\mu(\nu)$*

Proof. (Sketch, incomplete) (1). If $\omega_1, \omega_2 \in \mathcal{S}_\beta(\mathcal{A})$, $A, B \in \mathcal{A}$, with associated analytic functions $F_{\beta,1}(A, B, \cdot)$, $F_{\beta,1}(A, B, \cdot)$, then the analytic function $\lambda F_{\beta,1}(A, B, \cdot) + (1-\lambda) F_{\beta,2}(A, B, \cdot)$ has boundary values associated to $\lambda\omega_1 + (1-\lambda)\omega_2$ so that $\mathcal{S}_\beta(\mathcal{A})$ is convex. Moreover, the EEB inequality implies that $\mathcal{S}_\beta(\mathcal{A})$ is a weakly-* closed subset of the weakly-* compact set $\mathcal{E}(\mathcal{A})$, hence $\mathcal{S}_\beta(\mathcal{A})$ is weakly-* compact.

(2) Follows by density of $\pi(\mathcal{A})$ in $\pi(\mathcal{A})''$ in the weak topology, Corollary 7.

(3) If ω is not a factor state, then there exists a projection $1 \neq P \in \pi(A)' \cap \pi(A)''$. We first claim that $\omega(P) \neq 0$. Otherwise $0 = \omega(P) = \|P\Omega\|^2$ so that $P\Omega = 0$. But then, for any $A, B \in \mathcal{A}$, $\omega(A^*PB) = \langle \pi(A)\Omega, P\pi(B)\Omega\rangle = 0$ since $P \in \pi(A)'$, and hence $P = 0$ by cyclicity of Ω. Now, $\omega = \omega(P)\omega_1 + \omega(1-P)\omega_2$, where $\omega_1(A) = \omega(PA)/\omega(P)$ and $\omega_2(A) = \omega((1-P)A)/\omega(1-P)$, is a non-trivial decomposition of ω. Moreover, $\omega(P)\omega_1(BA) = \omega(PBA) = \omega(BPA) = \omega(PA\tau_{\mathrm{i}\beta}(B)) = \omega(P)\omega_1(A\tau_{\mathrm{i}\beta}(B))$ so that ω is not extremal in $\mathcal{S}_\beta(\mathcal{A})$.

(4). Let $C \in \pi(A)' \cap \pi(A)''$ and consider the normal extension of ω to $\pi(A)''$. Repeating the proof of Proposition 26, $t \mapsto \omega(\tau_t(A^*B)C)$ is constant. Hence, $t \mapsto \omega(\tau_t(A^*)C\tau_t(B)) = \langle \pi(A)\Omega, U_t^*\pi(C)U_t\pi(B)\Omega\rangle = \omega(A^*\tau_t(C)B)$ is constant for all $A, B \in \mathcal{A}$.

(5). That any KMS state can be decomposed into extremal KMS states follows from convexity and Krein-Milman's theorem. Uniqueness is more involved. □

The algebra $\pi(A)'' \supset \pi(A)$ contains both microscopic and macroscopic observables. Elements in the centre $\pi(A)' \cap \pi(A)''$ induce 'superselection rules': If $S = S^* \in \pi(A)' \cap \pi(A)''$ with $S \neq \lambda \cdot 1$, the Hilbert space decomposes into components on which S is a constant multiple of the identity, while these components with different 'quantum numbers' are not connected by any observable. In the case of KMS states, (3) above states that such observables associated with quantum numbers are constant in time. Furthermore, in a factor, any such S is a constant multiple of the identity. Hence, by (2) above, extremal KMS states associate fixed, non-fluctuating values to all quantum numbers: they are 'macroscopically pure' states.

Theorem 38. *Let $(\mathcal{A}, \tau_t)$ be a C*-dynamical system, and let ω be a faithful (τ, β)-KMS state, for $\beta > 0$. Let α be a *-automorphism of $\mathcal{A}$. Then,*

1. *$\omega \circ \alpha$ is a $(\alpha^{-1} \circ \tau \circ \alpha, \beta)$-KMS state*
2. *If $\omega \circ \alpha = \omega$, then $\alpha \circ \tau_t = \tau_t \circ \alpha$ for all $t \in \mathbb{R}$*
3. *If $\alpha \circ \tau_t = \tau_t \circ \alpha$ for all $t \in \mathbb{R}$, then $\omega \circ \alpha$ is a (τ, β)-KMS state*

Proof. Let F be the analytic function associated to ω. Then $F_\alpha(A, B; z) := F(\alpha(A), \alpha(B); z)$ is an analytic function in S_β, continuous on $\overline{S_\beta}$ and such that, for $t \in \mathbb{R}$,

$$
\begin{aligned}
F_\alpha(A, B; t) &= \omega(\alpha(A)\tau_t(\alpha(B))) = (\omega \circ \alpha)(A(\alpha^{-1} \circ \tau_t \circ \alpha)(B)) \\
F_\alpha(A, B; t + \mathrm{i}\beta) &= \omega(\tau_t(\alpha(B))\alpha(A)) = (\omega \circ \alpha)((\alpha^{-1} \circ \tau_t \circ \alpha)(B)A)
\end{aligned}
$$

which shows that $\omega \circ \alpha$ is a $(\alpha^{-1} \circ \tau \circ \alpha, \beta)$-KMS state. In order to prove (2), we use the fact that the τ-group with respect to which a ω is a KMS state is unique[3]. But ω is simultaneously a (τ, β)-KMS state and by (1) a $(\alpha^{-1} \circ \tau \circ \alpha, \beta)$-KMS state, hence $\tau_t = \alpha^{-1} \circ \tau_t \circ \alpha$. Finally, (3) follows immediately from (1). □

[3] In the case $\dim(\mathcal{H}) < \infty$, a faithful state is given by a $\rho > 0$, which determines uniquely $H := -\beta^{-1} \ln \rho$ and hence the dynamics.

3.5 Symmetries

Definition 16. *Let $(\mathcal{A}, \tau_t)$ be a C^*-dynamical system. A $*$-automorphism α of $\mathcal{A}$ is a* symmetry *if $\alpha \circ \tau_t = \tau_t \circ \alpha$ for all $t \in \mathbb{R}$.*

In this case, and by 1 above, if ω is a (τ, β)-KMS state, then so is $\omega \circ \alpha$. Hence, in the presence of a symmetry the set $\mathcal{S}_\beta(\mathcal{A})$ is invariant under τ for any fixed $\beta > 0$. In particular, if there is a unique (τ, β)-KMS state, then it is itself invariant and one says that the symmetry is unbroken at β. If, on the other hand, there is a (τ, β)-KMS state which is not invariant, then the symmetry is said to be broken and there is more than one equilibrium state at β, indicating a phase transition. Examples are the breaking of rotational $SU(2)$-symmetry in magnetic transitions, translational $\mathbb{R}^d$ symmetry in liquid-solid transitions. Here is a general criterion for the absence of symmetry breaking:

(A) There is a sequence $U_n \in \mathcal{A}$ of unitary elements of the algebra such that $U_n \in D(\delta)$ and

$$\lim_{n\to\infty} \|\alpha(A) - U_n^* A U_n\| = 0, \qquad A \in \mathcal{A}.$$

(Bi) There is M such that $\|\delta(U_n)\| \leq M$

(Bii) All (τ, β)-KMS states are α^2-invariant and there is M such that $\|U_n^*\delta(U_n) + U_n\delta(U_n^*)\| \leq M$

If (A) holds, one says that α is almost inner.

Theorem 39. *Let α be a symmetry of $(\mathcal{A}, \tau_t)$. If (A) and either (Bi) or (Bii) are satisfied, then all (τ, β)-KMS states are α-invariant for all $\beta > 0$.*

Note that the symmetry can still be broken in the ground state, $\beta = \infty$.

Proof. Let ω be a (τ, β)-KMS state, H the associated Hamiltonian such that $H\Omega = 0$ and let $H = \int \lambda dP(\lambda)$. For any bounded interval $I \subset \mathbb{R}$, let $\{\check{h}_n\}_{n\in\mathbb{N}}$ be a sequence of real-valued C_c^∞ functions supported on intervals $[a_n, b_n]$, with $|b_n - a_n| \leq 1$ and such that $\sum_n \check{h}_n(\lambda)^2 = 1$ for all $\lambda \in I$. Let $A_n := \tau_{h_n}(A)$, which is analytic for τ_t. First of all,

$$\omega(A_n^* A_n) = \int h_n(t) h_n(-s) \langle e^{iHs}\pi(A)\Omega, e^{iHt}\pi(A)\Omega\rangle dt ds = \int_{a_n}^{b_n} \check{h}_n(\lambda)^2 d\mu_A(\lambda)$$

as well as $\omega(A_n A_n^*) = \int_{a_n}^{b_n} \check{h}_n(\lambda)^2 d\nu_A(\lambda)$. Hence, by the measure-theoretic KMS property, $\omega(A_n^* A_n) \geq \exp(\beta a_n)\omega(A_n A_n^*)$ and further

$$\omega(A_n^* A_n) \ln \frac{\omega(A_n^* A_n)}{\omega(A_n A_n^*)} \geq \beta a_n \omega(A_n^* A_n).$$

Similarly, $-i\omega(A_n^*\delta(A_n)) = \int_{a_n}^{b_n} \lambda \check{h}_n(\lambda)^2 d\mu_A(\lambda)$, and hence,

$$-i\omega(A_n^*\delta(A_n)) \leq b_n \omega(A_n^* A_n)$$

We further write the EEB inequality for the observable $U_m^* A_n$, $n, m \in \mathbb{N}$, namely

$$\omega(A_n^* A_n) \ln \frac{\omega(A_n^* A_n)}{\omega(U_m^* A_n A_n^* U_m)} \leq -i\beta\omega(A_n^* U_m \delta(U_m^*) A_n) - i\beta\omega(A_n^*\delta(A_n))$$

and use the two inequalities above to obtain (note the position of * in the numerator!)

$$\omega(A_n^* A_n) \ln \frac{\omega(A_n A_n^*)}{\omega(U_m^* A_n A_n^* U_m)} \leq -i\beta\omega(A_n^* U_m \delta(U_m^*) A_n) + \beta(b_n - a_n)\omega(A_n^* A_n) \tag{3.7}$$

and $b_n - a_n \leq 1$.
Assumption (Bi). Since $|\omega(A_n^* U_m \delta(U_m^*) A_n)| \leq \|\delta(U_m)\| \omega(A_n^* A_n) \leq M\omega(A_n^* A_n)$, (3.7) yields

$$\omega(A_n A_n^*) \leq \mathrm{e}^{\beta(M+1)} \omega(U_m^* A_n A_n^* U_m)$$

and letting $m \to \infty$, $\omega(A_n A_n^*) \leq \mathrm{e}^{\beta(M+1)} (\omega \circ \alpha)(A_n A_n^*)$. Summing over n, we have proved that there exists a constant $C = C(\beta, M)$ such that

$$\omega(AA^*) \leq C(\omega \circ \alpha)(AA^*),$$

which extends to all $A \in \mathcal{A}$. By the remark after Lemma 9, there is a $T \in \pi_{\omega\circ\alpha}(\mathcal{A})'$ such that $\omega(A) = \langle T\Omega_{\omega\circ\alpha}, \pi_{\omega\circ\alpha}(A) T\Omega_{\omega\circ\alpha}\rangle$, which shows that ω is $(\omega \circ \alpha)$-normal. If ω is an extremal KMS state, then $\omega \circ \alpha$ is also extremal so that they must be equal by Theorem 37(3). Since this holds for all extremal KMS state, the general result holds by decomposition, Theorem 37(5).
Assumption (Bii). We repeat the procedure above with the state $\omega \circ \alpha$, sum (3.7) and the similar bound with $U_m \leftrightarrow U_m^*$, proceed as above and obtain

$$((\omega \circ \alpha)(A_n A_n^*))^2 \leq \mathrm{e}^{\beta(M+2)} \omega(A_n A_n^*)(\omega \circ \alpha^2)(A_n A_n^*). \tag{3.8}$$

Hence, $(\omega \circ \alpha)(A) \leq \tilde{C}\omega(A)$. Hence $(\omega \circ \alpha)$ is ω-normal and the conclusion holds as above. $\square$