## 2. KMS-states : A general theory of equilibrium.

- We first discuss the simple case of a quantum system defined on a finite dimensional Hilbert space $\mathcal{H} \simeq \mathbb{C}^n$, with observable algebra $\mathcal{A} = M_n(\mathbb{C})$ and state given by density matrices $\rho \in \mathcal{A}$ : $0 \leq \rho = \rho^* \leq \mathbb{1}$.

The dynamics is generated by the Hamiltonian $H = H^*$ in the Heisenberg picture:

$$\tau_t(A) = \exp(itH) A \exp(-itH)$$

Gibbs variational principle. Among all states, the thermal equilibrium states at $\beta$ are minimizers of the free energy functional

$$F_\beta : \mathcal{E}(\mathcal{A}) \longrightarrow \mathbb{R}$$
$$\rho \longmapsto F[\rho] = E[\rho] - \beta^{-1} S[\rho]$$

where

$$E[\rho] = \mathrm{Tr}(\rho H) \quad ; \quad S[\rho] = -\mathrm{Tr}(\rho \log \rho)$$

"Energy" "Entropy"

Proposition: $F_\beta$ has a unique minimizer

$$\rho_\beta = Z_\beta^{-1} e^{-\beta H} \quad ; \quad Z_\beta := \mathrm{Tr}(e^{-\beta H})$$

with $F_\beta(\rho_\beta) = \beta^{-1} \log Z_\beta =: f_\beta$

• **Lemma**: For any two density matrices $A, B$ such that $\operatorname{Ker} B \subset \operatorname{Ker} A$,

$$\operatorname{Tr}(A(\log A - \log B)) \geq \frac{1}{2}\operatorname{Tr}(A-B)^2$$

**Proof**: W.l.o.g., we assume that $\operatorname{Ker} B = \{0\}$, and let

$$B = \sum \beta_i P_i \qquad 0 < \beta_i \leq 1$$
$$A = \sum \alpha_j Q_j \qquad 0 \leq \alpha_j \leq 1$$

Now: the function $f(x) = \begin{cases} -x\log x & x > 0 \\ 0 & x = 0 \end{cases}$

is $C^2((0,\infty)) \cap C^0([0,\infty))$ and concave with $f''(x) = -\frac{1}{x}$.

Now: $f(y) - f(x) - (y-x)f'(y) = -\frac{1}{2}(x-y)^2 f''(z)$

$$\geq \frac{1}{2}(x-y)^2,$$

for any $0 \leq x < y \leq 1$ and some $z \in (x,y)$.

Hence

$$\operatorname{Tr}\left(P_i Q_j \left(f(B) - f(A) + (A-B)f'(B) - \frac{1}{2}(A-B)^2\right)\right)$$
$$\left(f(\beta_i) - f(\alpha_j) + (\alpha_j - \beta_i)f'(\beta_i) - \frac{1}{2}(\alpha_j - \beta_i)^2\right)\operatorname{Tr}(P_i Q_j) \geq 0$$

Summing over $i, j$ yields

$$\operatorname{Tr}\left(-B\log B + A\log A + (A-B)(-\mathbb{1} - \log B) - \frac{1}{2}(A-B)^2\right) \geq 0$$

which is the claim since $\operatorname{Tr} A = \operatorname{Tr} B = 1$ $\square$

**Proof of the Proposition**: We let $B = Z_\beta^{-1}\exp(-\beta H)$ for which $\operatorname{Ker} B = \{0\}$. Then by the lemma:

$$\beta(F_\beta(A) - f_\beta) = \beta\operatorname{Tr}(AH) + \operatorname{Tr}(A\log A) + \log Z_\beta$$
$$= \operatorname{Tr}(A\log A) - \operatorname{Tr}(A\log(Z_\beta^{-1}\exp(-\beta H)))$$
$$\geq \frac{1}{2}\operatorname{Tr}(A - \rho_\beta)^2$$

Since $(A-\rho_\beta)^2 = (A-\rho_\beta)^*(A-\rho_\beta) \geq 0$, and vanishing trace only if $A = \rho_\beta$, proving that $\rho_\beta$ is the unique minimizer of $F_\beta$. $\square$

- Hence, in the simple case of $\dim \mathcal{H} < \infty$, the equilibrium state is unique and characterized by the fact that it
  - minimizes the free energy, or
  - maximizes the entropy at fixed mean energy.
- Now: Since $H$ is a matrix, $\tau_t(A)$ can be analytically continued to $\tau_z(A)$ for any $z \in \mathbb{C}$. One has

Proposition: The Gibbs state is the unique state satisfying the $(\tau, \beta)$-KMS condition

$$\omega(A\tau_{i\beta}(B)) = \omega(BA) \qquad (+)$$

for all $A, B \in \mathcal{A} = M_n(\mathbb{C})$.

Proof: $\Rightarrow$) $\mathrm{Tr}(e^{-\beta H} A e^{itH} B e^{-itH})|_{t=i\beta} = \mathrm{Tr}(e^{-\beta H} BA)$ by cyclicity.

$\Leftarrow$) In a basis $(\psi_j)_{j=1,\dots,n}$ of eigenvectors of $H$ with eigenvalues $\lambda_j$ and choosing $A = \langle \psi_j, \cdot\rangle \psi_i$ ; $B = \langle \psi_l, \cdot \rangle \psi_k$, $(+)$ reads

$$\langle \psi_l, \rho \psi_i \rangle \delta_{jk} e^{-\beta(\lambda_k - \lambda_l)} = \langle \psi_j, \rho \psi_k\rangle \delta_{il}$$

from which it follows that $\rho$ is diagonal with

$$\langle \psi_i, \rho \psi_i \rangle = C e^{-\beta \lambda_i}$$ $\square$

- Note: The KMS condition only relies on the existence and analyticity of $\tau_z$ is a strip

$$S_\beta := \{ z \in \mathbb{C} : 0 < \mathrm{Im}\, z < \beta \}$$

with a continuous extension to $\overline{S_\beta}$.

The cumbersome analytic extension can even be relaxed with the following definition.

- <u>Definition</u>: Let $(\mathcal{A}, \tau)$ be a $C^*$-dynamical system, and $0 < \beta < \infty$. A state $\omega$ on $\mathcal{A}$ is a <u>$(\tau, \beta)$-KMS state</u> if, for any $A, B \in \mathcal{A}$, there exists a function $F_\beta(A, B; z)$, analytic in $S_\beta$, continuous on $\overline{S_\beta}$ and satisfying the KMS boundary conditions

$$\begin{cases} F(A, B; t) = \omega(A \tau_t(B)) \\ F(A, B; t + i\beta) = \omega(\tau_t(B) A) \end{cases} \qquad (t \in \mathbb{R})$$

<u>Remark</u>: For the Gibbs state, we have

$$F(A, B; z) = \mathrm{Tr}(\rho_\beta A \tau_z(B))$$

- An element $A \in \mathcal{A}$ is called analytic for $\tau$ if $t \mapsto \tau_t(A)$ extends to an analytic function on $\mathbb{C}$. And:

<u>Theorem</u>: A state $\omega$ on $\mathcal{A}$ is a $(\tau, \beta)$-KMS state if and only if there is a dense, $\tau$-invariant, $*$-subalgebra $\mathcal{D}$ of analytic elements for $\tau$ such that

$$\omega(A \tau_{i\beta}(B)) = \omega(BA) \qquad (*)$$

- <u>Note</u>: on $\mathcal{A} = M_n(\mathbb{C})$, there is a unique $(\tau, \beta)$-KMS state, the Gibbs state. This is <u>in general not true</u>, as illustrated in the case of the Bose gas in the TDL limit: this non-uniqueness is a key characterisation of a <u>phase transition</u>.

(the TDL of Gibbs states at fixed $\beta$ is always a KMS state as we shall see later, using the Energy-Entropy-Balance Inequality).

- Proof of the theorem.

i) Let $A, B$ be analytic. Then $G(z) = \omega(A\tau_z(B))$ is analytic with $G(t) = F_\beta(A,B;t)$ if $t\in\mathbb{R}$. Hence

$$z \mapsto G(z) - F_\beta(A,B;z)$$

is analytic on $S_\beta$, continuous on $\overline{S_\beta}$ and vanishes on $\mathbb{R}$. Hence (Schwarz reflection) it extends to an analytic function on $\{z\in\mathbb{C} : |\mathrm{Im}\, z| < \beta\}$, which still vanishes on $\mathbb{R}$. Hence it vanishes everywhere, and by continuity $G(i\beta) = F_\beta(A,B;i\beta)$, namely $\omega(A\tau_{i\beta}(B)) = \omega(BA)$ by the KMS boundary condition.

ii) If $A,B\in\mathcal{D}$, $F(A,B;z) := \omega(A\tau_z(B))$ is analytic on $\mathbb{C}$, and since $\tau_t(B)\in\mathcal{D}$:

$$F(A,B;t) = \omega(A\tau_t(B)) \quad ; \quad F(A,B;t+i\beta) = \omega(A\tau_{i\beta}(\tau_t(B)))$$
$$= \omega(\tau_t(B)A) \quad \text{by } (*),$$

which are the KMS boundary conditions. This extends to any $A,B\in\mathcal{A}$ by density of $\mathcal{D}$ and a bit of complex analysis. $\square$

- First physically essential property: A KMS state is invariant under time evolution.

<u>Proposition</u>: If $\omega$ is a $(\tau,\beta)$-KMS state, then $\omega\circ\tau_t = \omega$ for all $t\in\mathbb{R}$.

Proof: Let $A \in \mathcal{A}$ be analytic for $\tau$. Then $g(z) = \omega(\tau_z(A))$ is analytic in $\mathbb{C}$. Hence

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

so that $g$ is periodic in the imaginary direction. Moreover

$$|g(t+i\alpha)| \leq \|\tau_t(\tau_{i\alpha}(A))\| = \|\tau_{i\alpha}(A)\|$$
$$\leq \sup\{\|\tau_{i\gamma}(A)\| : 0 \leq \gamma < \beta\} < \infty.$$

Hence $g$ is analytic and bounded on $\mathbb{C}$, therefore constant by Liouville's theorem. This finally extends to all $A \in \mathcal{A}$ by continuity. $\square$

- Technical aside: there always is a dense set of analytic elements.

Proposition: For any $A \in \mathcal{A}$, $m \in \mathbb{N}$, let

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

Then: (i) $A_m$ is analytic

(ii) $\mathcal{A}_\tau := \{A_m : A \in \mathcal{A}, m \in \mathbb{N}\}$ is a dense $*$-subalgebra.

Proof. See exercises

- We now turn to an equivalent characterisation of KMS states which is of great practical use: the energy-entropy-balance inequality (EEB). Just as the Gibbs variational principle, it can be seen as characterising equilibrium by a minimisation problem.

• <u>Theorem</u>: A state $\omega$ over $\mathcal{A}$ is a $(\tau, \beta)$-KMS state if and only if

$$-i\beta\omega(A^\dagger\delta(A)) \geq \omega(A^\dagger A)\log\frac{\omega(A^\dagger A)}{\omega(AA^\dagger)}$$

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

• <u>Notes</u>: * $u\log\left(\frac{u}{v}\right) = \begin{cases} 0 & \text{if } u=0,\ v\geq 0 \\ +\infty & \text{if } u>0,\ v=0 \end{cases}$

* $\delta$ in the thm is the generator of $\tau_t$.

• If $\omega$ is a $\tau$-invariant state, $\omega\circ\tau_t = \omega$ for all $t\in\mathbb{R}$, then by the uniqueness of the GNS representation, $\exists\ H_\omega = H_\omega^\dagger$ on $\mathcal{H}_\omega$ s.t. (i) $H_\omega\Omega_\omega = 0$

(ii) $\exp(itH_\omega)\pi_\omega(A)\exp(-itH_\omega) = \pi_\omega(\tau_t(A))$

One says that $\exp(itH_\omega)$ is a <u>unitary implementation</u> of $\tau_t$ in the representation $(\mathcal{H}_\omega, \pi_\omega)$.

For any $A\in\mathcal{A}$, we define the following measures:

$$\mu_A(\Delta) := \langle\pi_\omega(A)\Omega_\omega, P_\omega(\Delta)\pi_\omega(A)\Omega_\omega\rangle\sqrt{2\pi}$$

$$\nu_A(\Delta) := \langle\pi_\omega(A^\dagger)\Omega_\omega, P_\omega(-\Delta)\pi_\omega(A^\dagger)\Omega_\omega\rangle\sqrt{2\pi}$$

for any Borel set $\Delta\subset\mathbb{R}$, where $P$ is the projection valued measure of $H_\omega$: $H_\omega = \int_{\mathbb{R}}\lambda\, dP_\omega(\lambda)$

These measures completely characterize the KMS property:

Let $f$ be an entire function that is the F.T. of a $C_c^\infty(\mathbb{R})$ function. By Paley-Wiener, there is for any $N \in \mathbb{N}$ a $C_N$ s.t.
$$|f(\xi)| \leq \frac{C_N \exp(R\,|\mathrm{Im}(\xi)|)}{(1+|\xi|)^N} \quad \text{for some } R>0.$$
and in particular,
$$\tau_f(A) := \int f(t)\,\tau_t(A)\,dt$$
is well-defined (and an analytic element of $\mathcal{A}$).
$$\omega(A^* \tau_f(A)) = \int \langle \pi_\omega(A)\Omega_\omega, e^{itH_\omega}\pi_\omega(A)\Omega_\omega\rangle f(t)\,dt$$
$$= \int \langle \pi_\omega(A)\Omega_\omega, dP_\omega(\lambda)\pi_\omega(A)\Omega_\omega\rangle e^{it\lambda} f(t)\,dt$$
$$= \int \check{f}(\lambda)\sqrt{2\pi}\langle \pi_\omega(A)\Omega_\omega, dP(\lambda)\pi_\omega(A)\Omega_\omega\rangle$$
$$= \int \check{f}(\lambda)\,d\mu_A(\lambda).$$
Similarly:
$$\omega(\tau_f(A)A^*) = \int \langle \pi_\omega(A^*)\Omega_\omega, dP_\omega(\lambda)\,\pi_\omega(A^*)\Omega_\omega\rangle e^{-it\lambda} f(t)\,dt$$
$$= \int \check{f}(-\lambda)\sqrt{2\pi}\,\langle \pi_\omega(A^*)\Omega_\omega, dP_\omega(\lambda)\,\pi_\omega(A^*)\Omega_\omega\rangle$$
$$= \int \check{f}(\lambda)\,d\nu_A(\lambda)$$
Now: $z \mapsto f(z)\,\omega(A^*\tau_z(A))$ is entire, so that
$$\omega(A^*\tau_f(A)) = \int_{\mathbb{R}} f(t+i\beta)\,\omega(A^*\tau_{t+i\beta}(A))\,dt$$
and if $\omega$ is a $(\tau,\beta)$-KMS state:

$$\omega(A^* \tau_f(A)) = \int f(t+i\beta)\, \omega(\tau_t(A) A^*)\, dt$$
$$= \int \check{f}(\lambda)\, e^{\beta\lambda}\, d\nu_A(\lambda)$$

Since this holds for any test function $f$, we have: $\omega$ is a $(\tau,\beta)$-KMS state iff

$$\frac{d\mu_A}{d\nu_A}(\lambda) = e^{\beta\lambda} \qquad (*)$$

With this, we are in a position to prove the theorem.

Proof: $\Rightarrow$) Note:

$$\omega(A^*\delta(A)) = i\langle \pi_\omega(A)\Omega_\omega, H_\omega \pi_\omega(A)\Omega_\omega\rangle$$

so that

$$\frac{-i\beta\,\omega(A^*\delta(A))}{\omega(A^*A)} = \frac{\beta\int\lambda\, d\mu_A(\lambda)}{\int d\mu_A(\lambda)}$$

By Jensen's inequality:

$$\exp\left(-\beta\frac{\int\lambda\, d\mu_A(\lambda)}{\int d\mu_A(\lambda)}\right) \leq \frac{\int e^{-\beta\lambda} d\mu_A(\lambda)}{\int d\mu_A(\lambda)} = \frac{\int d\nu_A(\lambda)}{\int d\mu_A(\lambda)}$$

Taking the inverse:

$$\exp\left(\frac{-i\beta\,\omega(A^*\delta(A))}{\omega(A^*A)}\right) \geq \frac{\omega(A^*A)}{\omega(AA^*)}$$

concluding the proof since log is an increasing function.

$\Leftarrow$) We have

$$\omega(\tau_f(A)^*\tau_f(A)) = \int \bar{f}(t) f(t')\, e^{i(t-t')\lambda} \langle \pi_\omega(A)\Omega, dP_\omega(\lambda)\pi_\omega(A)\Omega_\omega\rangle\, dt\, dt'$$
$$= \int |\check{f}(\lambda)|^2 d\mu_A(\lambda)$$

and similarly $\omega\left(\tau_f(A)\tau_f(A^*)\right) = \int |\check{f}(\lambda)|^2 d\nu_A(\lambda)$

and $-i\beta\omega\left(\tau_f(A)\delta(\tau_f(A^*))\right) = \int |\check{f}(\lambda)|^2(-\beta\lambda)\, d\nu_A(\lambda)$

Applying the lower bound with $A^* \to \tau_f(A)$

$$\nu_A(\varphi \log \omega) \geq \nu_A(\varphi)\log\left(\frac{\nu_A(\varphi)}{\mu_A(\varphi)}\right)$$

where $\varphi(\lambda) = |\check{f}(\lambda)|^2$ and $\omega(\lambda) = \exp(-\beta\lambda)$,

and similarly with $A \to \tau_f(A)$

$$-\mu_A(\varphi\log\omega) \geq \mu_A(\varphi)\log\left(\frac{\mu_A(\varphi)}{\nu_A(\varphi)}\right)$$

Since $\varphi$ is compactly supported : $\operatorname{supp}\varphi \subset [m, M]$

$$-\beta M\varphi(\lambda) \leq \varphi(\lambda)\log\omega(\lambda) \leq -\beta m\,\varphi(\lambda)$$

hence $\quad -\beta m\,\nu_A(\varphi) \geq \nu_A(\varphi)\log\left(\nu_A(\varphi)/\mu_A(\varphi)\right)$

$\quad\quad \beta M\mu_A(\varphi) \geq \mu_A(\varphi)\log\left(\mu_A(\varphi)/\nu_A(\varphi)\right)$

and together $\mu_A(\varphi)e^{-\beta M} \leq \nu_A(\varphi) \leq \mu_A(\varphi)e^{-\beta m}$.

Using a partition of unity on $\varphi$ and by dominated convergence:

$$\int \varphi(\lambda)\, d\nu_A(\lambda) = \int \varphi(\lambda)e^{-\beta\lambda}d\mu_A(\lambda)$$

namely $\quad \frac{d\mu_A}{d\nu_A}(\lambda) = e^{\beta\lambda}$, so that $\omega$ is a $(\tau,\beta)$-KMS state ∵.

- The EEB inequality provides a simple proof of the following :

• <u>Proposition</u>: Let $(\tau^{(n)})_{n\in\mathbb{N}}$ be a sequence of strongly continuous, 1-parameter group of automorphisms of $\mathcal{A}$ s.t. for any $t\in\mathbb{R}$, $A\in\mathcal{A}$:

$$\| \tau_t^{(n)}(A) - \tau_t(A) \| \longrightarrow 0$$

as $n\to\infty$. If $(\omega^{(n)})_{n\in\mathbb{N}}$ is a sequence of $(\tau^{(n)},\beta)$-KMS states, then any weak-* accumulation point is a $(\tau,\beta)$-KMS state.

<u>Proof</u>: exercise!

• <u>Application</u>: The infinite volume limiting states of the free Bose/Fermi gases are KMS states.
In general: states obtained as TDL of Gibbs states are KMS states.

<u>Passivity & Stability</u>: Two fundamental properties of equilibrium. Vaguely put:

i) Passivity. In a cyclic process starting at equilibrium, no work can be extracted from the system, on average.

ii) Stability: (a) Structural: Equilibrium states depend continuously on the Hamiltonian (at least for <u>local</u> perturbations)

(b) Dynamical: A locally perturbed system returns to equilibrium asymptotically at $t \to \infty$.

- Passivity in the case $\dim(\mathcal{H}) < \infty$.

Time-dependent Hamiltonian $H(t) = H(t)^*$, $t \in [0,T]$ with $H(0) = H(T) =: H$.

Initial state: Gibbs state $\omega_\beta = \mathrm{Tr}(\rho_\beta \cdot)$.

Let $U(t,t_0)$, be the solution of

$$\begin{cases} i\dot{U}(t,t_0) = H(t)U(t,t_0) \\ U(t_0,t_0) = \mathbb{1} \end{cases}$$

and denote $U = U(T,0)$ the driven time evolution over one cycle. The work done by the system on the environment is given by

$$W = \mathrm{Tr}(\rho_\beta H) - \mathrm{Tr}(U\rho_\beta U^* H)$$

$$\overset{\dim(\mathcal{H})<\infty}{=} -\mathrm{Tr}\left(\rho_\beta U^*[H,U]\right) = i\omega_\beta(U^*\delta(U)) \qquad (W)$$

Given a $C^*$-dynamical system $(\mathcal{A},\tau)$, a state is called <u>passive</u> if $-i\omega(U^*\delta(U)) \geq 0$ for any unitary $U \in \mathcal{A}$, $U \in D(\delta)$ and $U$ is in the connected component of $\mathbb{1}$.

- <u>Proposition</u>: A $(\tau,\beta)$-KMS state is passive.

Proof: Follows immediately from the EEB-inequality since $UU^* = U^*U = \mathbb{1}$.

Back to $(W)$: Since $\omega_\beta$ is a $(\tau,\beta)$-KMS state and

$\delta$ is the generator of $\tau$, passivity implies that $W \leq 0$.

- We shall now prove that $W \leq 0$ in the general setting of $C^*$-dynamical systems.

If $\delta$ is the generator of $\tau$, one says that

$$\delta_V = \delta + i[V, \cdot\,] \qquad D(\delta_V) = D(\delta)$$

where $V \in \mathcal{A}$ is a <u>local perturbation</u> of $\delta$.

Now:

$$\frac{d}{ds}\tau_{-s}\left(\tau_s^V(A)\right) = \tau_{-s}\left(i\left[V, \tau_s^V(A)\right]\right) \quad \text{so that}$$

$$\tau_t^V(A) - \tau_t(A) = \tau_{t-s}\left(\tau_s^V(A)\right)\Big|_{s=0}^{s=t} = \int_0^t \tau_{t-s}\left(i\left[V, \tau_s^V(A)\right]\right) ds$$

and iterating:

$$\tau_t^V(A) = \tau_t(A) + \sum_{n=1}^{\infty} \int_{0 \leq t_1 \leq \dots \leq t_n \leq t} i\left[\tau_{t_1}(V), i\left[\dots i\left[\tau_{t_n}(V), \tau_t(A)\right]\dots\right]\right] dt_1 \dots dt_n$$

which is norm-convergent.

In fact $\mathbb{C} \ni \lambda \longmapsto \tau_t^{\lambda V}(A) \in \mathcal{A}$ is an entire function.

The unitary $\Gamma_V(t)$ solving

$$\begin{cases} -i\dfrac{d}{dt}\Gamma_V(t) = \Gamma_V(t)\,\tau_t(V) \\ \Gamma_V(0) = \mathbb{1} \end{cases}$$

is the following intertwiner of dynamics

$$\tau_t^V(A)\,\Gamma_V(t) = \Gamma_V(t)\,\tau_t(A)$$

- We now define the work performed by the system along a cycle $V_t$, $t \in [0,T]$, $V_0 = V_T = 0$, where the initial state is an arbitrary $\omega$:

$$W := -\int_0^T \underbrace{(\omega \circ \tau_t^V)}_{\text{state at } t} \underbrace{\left(\frac{dV_t}{dt}\right)}_{\text{change of energy / flux}} dt .$$

Note that $\frac{d}{dt}(\omega \circ \tau_t^V)(V_t) = (\omega \circ \tau_t^V)(\delta_{V_t}(V_t)) + (\omega \circ \tau_t^V)\left(\frac{dV}{dt}\right)$

and $\delta_{V_t}(V_t) = \delta(V_t)$. Hence

$$W = \int_0^T (\omega \circ \tau_t^V)(\delta(V_t))\, dt$$

since $V_0 = V_T = 0$.

We now prove

- **Theorem**: Let $V_t \in C_c^1([0,T]; \mathcal{A})$ and s.t. $V_t \in D(\delta)$, $\delta(dV/dt) = d(\delta V)/dt$.
If $\omega$ is a $(\tau, \beta)$-KMS state, then $W \le 0$.

**Proof**: Since $\omega$ is positive and $\Gamma_V(t)$ is unitary, it suffices to prove that

$$W = i\omega(\Gamma_V(T)\,\delta(\Gamma_V(T)^*)).$$

This follows by calculation:

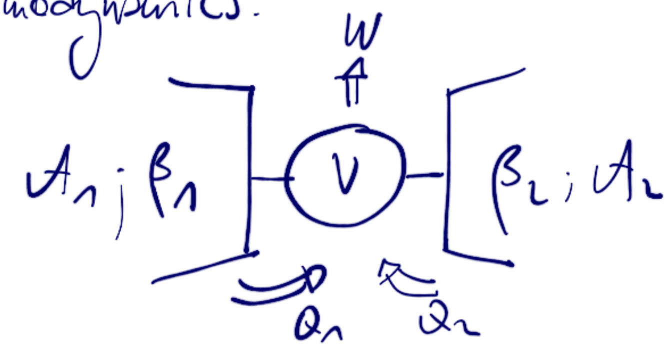
$$i\omega(\Gamma\delta(\Gamma^*)) - \int_0^T \omega\left(i\dot{\Gamma}\delta(\Gamma^*) + i\Gamma\delta(\dot{\Gamma}^*)\right) =$$

$$= \int_0^T \omega\left(-\Gamma_t \tau_t(V)\,\delta(\Gamma_t^*) + \Gamma_t\,\delta(\tau_t(V)\Gamma_t^*)\right) dt$$

$$= \int_0^T \omega\left(\underbrace{\Gamma_t\,\tau_t(\delta(V))\,\Gamma_t^*}_{=\tau_t^V(\delta(V))}\right) dt = W$$

$\square$

- Passivity also implies Carnot's version of the second law of thermodynamics.




$\beta_1 \leq \beta_2$

Dynamics $\tau = \tau_1 \otimes \tau_2$

with generator $\delta = \delta_1 \otimes \mathbb{1} + \mathbb{1} \otimes \delta_2$

Initial state: $\omega = \omega_{\beta_1} \otimes \omega_{\beta_2}$

note: $\omega$ is a $(\sigma, 1)$-KMS state, where

$$\sigma_t = \tau_{1,\beta_1 t} \otimes \tau_{2,\beta_2 t}$$

with generator

$$\gamma = \beta_1 \delta_1 \otimes \mathbb{1} + \mathbb{1} \otimes \beta_2 \delta_2$$

(Cyclic) machine: local perturbation $V_t \in \mathcal{A}$.

Total work performed by the joint system

$$W = i\omega\left(\Gamma_V(T)\,\delta(\Gamma_V(T)^*)\right)$$

$$= i\omega\left(\Gamma_V(T)(\delta_1 \otimes \mathbb{1})(\Gamma_V(T)^*)\right) + i\omega\left(\Gamma_V(T)(\mathbb{1} \otimes \delta_2)(\Gamma_V(T)^*)\right)$$

$$= Q_1 + Q_2$$

where $Q_i$ has the natural interpretation of the heat that has been pumped out of system $i$. Now

$$\beta_1 Q_1 + \beta_2 Q_2 = i\omega\left(\Gamma_V(T)\,\gamma\left(\Gamma_V(T)^*\right)\right) \le 0$$

by passivity. Hence $\beta_1 Q_1 + \beta_2 (W - Q_1) \le 0$, namely

$$W T_1 \le Q_1 (T_1 - T_2)$$

yielding the efficiency of the machine

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

where we assumed that $Q_1 \ge 0$ : the machine pumps heat out of the hot reservoir to produce work.

- Remark: Passivity is not sufficient to ensure that a state is KMS. One needs the stronger condition of complete passivity: for any $n \in \mathbb{N}$ the state $\bigotimes_{i=1}^n \omega$ is passive for the $C^*$-dynamical system $(\otimes \mathcal{A}, \bigotimes_{i=1}^n \tau)$.
- By perturbation theory, KMS states are structurally stable w.r.t. local perturbations: If $\omega$ is a $(\tau, \beta)$-KMS state, then for any local perturbation $V$, there is a $(\tau^V, \beta)$-KMS state $\omega^V$

$$\|\omega - \omega^V\| \le C\|V\|$$

Moreover, $\omega^V$ can be represented by a density matrix in the GNS representation of $\omega$.

In fact, there is a homeomorphism between the set of $(\tau,\beta)$-KMS states and that of $(\tau^V,\beta)$-KMS states.

In other words: local perturbations are thermodynamically irrelevant

- Natural question: Is the structural map $\omega \mapsto \omega^V$ also realized dynamically, i.e. do we have

$$\omega \circ \tau_t^V \longrightarrow \omega^V$$

in some form as $t \to \infty$ ?

("return to equilibrium", "thermalization")

Reciprocally: Does the convergence $\nu \circ \tau_t \longrightarrow \omega$ imply that $\omega$ is a $(\tau,\beta)$-KMS state for some $\beta$ ?

A general theorem:

Assumption (A): for any $V = V^*$ in a dense $*$-subalgebra of $\mathcal{A}$, $\exists\, \lambda_V > 0$ s.t.

$$\int \| [V, \tau_s^{\lambda V}(A)] \| ds < \infty$$

for all $|\lambda| \le \lambda_V$, $A \in \mathcal{A}_0$

Stability (S): for any $V, \lambda_V$ as above,

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

$$\lim_{\lambda \to 0} \| \omega - \omega_+^{\lambda V} \| = 0.$$

Then:

<u>Theorem</u>: Assume that $\omega$ is a factor state and that Assumption (A) holds.
Then (S) holds iff $\omega$ is a $(\tau,\beta)$-KMS state.
In that case, $\omega_+^{\lambda V}$ is a $(\tau^{\lambda V},\beta)$-KMS state.

($\omega$ is a factor state if $\pi_\omega(\mathcal{A})' \cap \pi_\omega(\mathcal{A})'' = \mathbb{C}\cdot\mathbb{1}$).

In other words: If the dynamics is $L^1$-asymptotically abelian (A), then dynamical and local stability (S)

- Easier (partial) result:

<u>Proposition</u>: Let $V = V^* \in \mathcal{A}$, $\omega^V$ a $(\tau^V,\beta)$-KMS state and $\omega_+$ a weak-* limit point of $\omega^V\circ\tau_t$ as $t\to\infty$.
If $\|[V,\tau_t(A)]\| \longrightarrow 0$ $\forall A\in\mathcal{A}$, then $\omega_+$ is a $(\tau,\beta)$-KMS state.

<u>Proof</u>: $(u,v)\longmapsto v\log u/v$ is lower semicontinuous, so that

$$\omega_+(A^*A)\log\frac{\omega_+(A^*A)}{\omega_+(AA^*)} \le \liminf_{t\to\infty} \omega^V\circ\tau_t(A^*A)\log\frac{\omega^V\circ\tau_t(A^*A)}{\omega^V\circ\tau_t(AA^*)}$$

$$\le \liminf -i\beta\,\omega^V\Big(\tau_t(A^*)\underbrace{\delta_V(\tau_t(A))}_{=\delta(\tau_t(A))+i[V,\tau_t(A)]}\Big)$$

first term $= -i\beta\,\omega_+\big(A^*\delta(A)\big)$ since $\delta\circ\tau_t = \tau_t\circ\delta$

$|\text{second term}| \le \liminf \beta\|[V,\tau_t(A)]\| = 0$

Hence $\omega_+$ solves the EEB for $\delta$, so that $\omega_+$ is a $(\tau,\beta)$-KMS state. $\square$

## Symmetries

**Def**: A $*$-automorphism $\alpha$ of $\mathcal{A}$ is a symmetry of $(\mathcal{A}, \tau)$ if
$$\alpha \circ \tau_t = \tau_t \circ \alpha$$
for all $t \in \mathbb{R}$.

**Proposition**: Let $\omega$ be a faithful $(\tau, \beta)$-KMS state, i.e. $\omega(A^*A) > 0$ for all $A \in \mathcal{A}$. Let $\alpha$ be a $*$-automorph.

(i) $\omega \circ \alpha$ is a $(\alpha^{-1} \circ \tau \circ \alpha, \beta)$-KMS state

(ii) if $\omega \circ \alpha = \omega$, then $\alpha$ is a symmetry

(iii) if $\alpha$ is a symmetry, then $\omega \circ \alpha$ is a $(\tau, \beta)$-KMS state.

**Proof**: (i) If $F$ is the analytic function associated to $\omega$, let
$$F_\alpha(A, B; z) := F(\alpha(A), \alpha(B); z),$$
which is an analytic function on $S_\beta$ with continuous extension to $\overline{S_\beta}$, and
$$\begin{aligned} F_\alpha(A, B; t) &= \omega(\alpha(A) \tau_t(\alpha(B))) \\ &= (\omega \circ \alpha)(A (\alpha^{-1} \circ \tau_t \circ \alpha)(B)) \end{aligned}$$
$$\begin{aligned} F_\alpha(A, B; t + i\beta) &= \omega(\tau_t(\alpha(A)) \alpha(B)) \\ &= (\omega \circ \alpha)((\alpha^{-1} \circ \tau_t \circ \alpha)(A) B) \end{aligned}$$
proving (i).

(ii) A fundamental result of modular theory is the uniqueness of the dynamics w.r.t. which a state is KMS. Now if $\omega \circ \alpha = \omega$, $\omega$ is simultaneously a $(\tau, \beta)$ and by (i) a $(\alpha^{-1} \circ \tau \circ \alpha, \beta)$-

KMS state. Hence $\tau = \alpha^{-1} \circ \tau \circ \alpha$.

(iii) follows from (i) and $\tau = \alpha^{-1} \circ \tau \circ \alpha$.

Remark: In the case $\dim(\mathcal{H}) < \infty$ a faithful state $\rho > 0$ determines a unique Hamiltonian by $H := -\beta^{-1} \log \rho$.

- (iii) above indicates that the set of $(\tau, \beta)$-KMS states is always invariant under the action of a symmetry. If this is not the case for every single state, one speaks of symmetry breaking. This is a typical reason for the existence of many KMS states at a given $\beta$: $SU(2)$-broken equilibrium states of magnets below the critical temperature. Reciprocally, uniqueness of a $(\tau, \beta)$-KMS state implies that the symmetry is unbroken.

Proving symmetry breaking in the case of a continuous symmetry group is a notoriously hard problem. For its absence, here is a general criterion:

Assumption (A): $\alpha$ is "almost inner": $\exists\, (U_n)_{n \in \mathbb{N}}$, $U_n \in \mathcal{A}$ unitary s.t. $U_n \in D(\delta)$ and

$$\lim_{n \to \infty} \| U_n^* A U_n - \alpha(A) \| = 0$$

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

Assumption (B): $\| \delta(U_n) \| \le M$ for all $n \in \mathbb{N}$.

Typically $U_n$ is labeled by increasing volumes $\Lambda_n$, in which case $\delta(U_n) \sim i[H_{\Lambda_n}, U_n]$ is typically supported along the boundary of $\Lambda_n$: for outside, $U_n$ acts trivially, while by the symmetry assumption $H_{\Lambda_n}$ commutes with $U_n$. (B) is a condition on being able to implement the symmetry "smoothly enough" comparing to the dimension.

<u>Theorem</u>: Let $\alpha$ be a symmetry of $(\mathcal{A}, \tau)$. If (A, B) hold, then <u>all</u> $(\tau, \beta)$-KMS states are $\alpha$-invariant for all $0 < \beta < \infty$.

<u>Notes</u>: • The symmetry can still be broken in the ground state, at $\beta = \infty$.

• (B) can be replaced by

(B'): all $(\tau, \beta)$-KMS state are $\alpha^2$-invariant (e.g. $\alpha^2 = id$).

and $\| U_n^* \delta(U_n) + U_n \delta(U_n^*) \| \leq M$ for all $n \in \mathbb{N}$.

• We will use this to prove the absence of symmetry breaking for compact Lie groups in dimension 1, 2.

Sketch <u>of proof</u>: By some abstract arguments, it suffices to prove that

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

Apply EEB for $U_m A$ (remark: $U_m \in \mathcal{A}$!).

$$\omega(A^* A) \log \frac{\omega(A^* A)}{\omega(U_m A A^* U_m^*)} \leq -i\beta\, \omega\left(A^* U_m^* \delta(U_m) A\right)$$
$$-i\beta\, \omega\left(A^* \delta(A)\right) \qquad (*)$$

on the l.h.s:

$$\log\frac{\omega(A^*A)}{\omega(U_m AA^* U_m^*)} = \log\frac{\omega(A^*A)}{\omega(AA^*)} + \log\frac{\omega(AA^*)}{\omega(U_m AA^* U_m^*)}$$

use $\frac{d\mu_A(\lambda)}{d\nu_A(\lambda)} = e^{\beta\lambda}$ asymptotically : $\omega(AA^*)/\omega\circ\alpha(AA^*)$

⇝ Need upper bounds on

a) $-i\beta\omega(A^* U_m^* \delta(U_m) A)$

b) $-i\beta\omega(A^*\delta(A)) - \omega(A^*A)\log\frac{\omega(A^*A)}{\omega(AA^*)}$

(a) By Assumption (B):

$$|-i\beta\omega(A^* U_m^* \delta(U_m) A)| \le \|U_m^*\|\,\|\delta(U_m)\|\,\beta\,\omega(A^*A) \le \beta M \omega(A^*A)$$

(b) Trickier as $\omega(A^*\delta(A)) = \langle \pi(A)\Omega, H\pi(A)\Omega\rangle$ is unbounded.

So: Cover $\mathbb{R}$ by intervals $[a_n, b_n]$, $|b_n - a_n| < 1$, let $\check{h}_n \in C_c^\infty(\mathbb{R})$ with $\operatorname{supp}\check{h}_n \subset [a_n, b_n]$, $\sum_n \check{h}_n(\lambda)^2 = 1$ and let

$$A_n := T_{h_n}(A)$$

(formally $A_n = P_n A P_n$, $P_n = \int_{a_n}^{b_n} dP(\lambda)$)

Now:

$$-i\beta\omega(A_n^*\delta(A_n)) = \int \beta\lambda\,\check{h}_n(\lambda)^2\,d\mu_A(\lambda)$$

$$\le \beta b_n\,\omega(A_n^* A_n)$$

Furthermore: $\omega(A_n^* A_n) = \int |h_n^\vee(\lambda)|^2 \, d\mu_A(\lambda)$

$$= \int |h_n^\vee(\lambda)|^2 e^{\beta\lambda} \, d\nu_\beta(\lambda)$$

$$\geq e^{\beta a_n} \omega(A_n A_n^*)$$

so that $-\omega(A_n^* A_n) \log \dfrac{\omega(A_n^* A_n)}{\omega(A_n A_n^*)} \leq -\beta a_n \omega(A_n^* A_n)$

Altogether (from (**)):

$$\omega(A_n^* A_n) \log \frac{\omega(A_n A_n^*)}{\omega(U_m^* A_n A_n^* U_m)} \leq \beta \omega(A_n^* A_n) \Big[ \Pi + \underbrace{(b_n - a_n)}_{<1} \Big].$$

yielding $\quad \omega(A_n A_n^*) \leq e^{\beta(\Pi+1)} \omega(U_m A_n A_n^* U_m^*)$

Letting $m \to \infty$ : $\quad \omega(A_n A_n^*) \leq \exp(\beta(\Pi+1)) (\omega \circ \alpha^{-1})(A_n A_n^*)$

The claim follows by summing over $n$, and replacing $AA^*$ by $\alpha^{-1}(AA^*)$ $\square$

- With assumption (B'): repeat with $U_m \leftrightarrow U_m^*$ and add two bounds:

$$\omega(A_n^* A_n) \log \frac{\omega(A_n A_n^*)^2}{\omega(U_m A_n A_n^* U_m^*) \omega(U_m^* A_n A_n^* U_m)}$$

$$\leq \beta \omega\big(A_n^* (U_m^* \delta(U_m) + U_m \delta(U_m^*)) A_n\big) + 2\beta \omega(A_n^* A_n)$$

$\Rightarrow \omega(A_n A_n^*)^2 \leq e^{\beta(\Pi+2)} (\omega \circ \alpha^{-1})(A_n A_n^*) (\omega \circ \alpha)(A_n A_n^*)$

and since $(\omega \circ \alpha^{-1})$ is also a $(\tau, \beta)$-KMS state, it is $\alpha^2$-invariant by assumption, so that $(\omega \circ \alpha^{-1}) = (\omega \circ \alpha)$.

Taking the square root concludes the proof. $\square$