Equilibrium states ; Quantum Statistical Mechanics

$\mathcal{A} = C^*$-algebra (algebra of observables of QSM system)

time evolution $\sigma : \mathbb{R} \to \mathrm{Aut}(\mathcal{A})$ one-parameter family of automorphisms

$\pi : \mathcal{A} \to B(\mathcal{H})$ is a "covariant representation" if $\exists$ H self-adjoint operator on $\mathcal{H}$ s.t.

$$\pi(\sigma_t(a)) = e^{itH} \pi(a) e^{-itH}$$

H is the Hamiltonian that implements the evolution σ_t in the representation π

(Note: σ_t only depends on $\mathcal{A}$ but H depends also on π)

Example: $\mathcal{H} = \mathbb{C}^N$ $\mathcal{A} = M_N(\mathbb{C})$

$$\varphi(a) = \frac{\mathrm{Tr}(\rho a)}{\mathrm{Tr}(\rho)}$$ states are all of this form for some density matrix $\rho = \eta^*\eta > 0$

time evolution $\sigma_t(a) = e^{itH} a e^{-itH}$ H some self-adj. matrix

then a special choice of state is

$$\varphi_\beta(a) = \frac{\mathrm{Tr}(a e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}$$ for $\beta \in \mathbb{R}_+^*$

These are equilibrium states $\beta = \frac{1}{kT}$ thermodynamic parameter (inverse temperature)

$$\varphi_\beta(\sigma_t(a)) = \varphi_\beta(a)$$

If say diag $a = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{pmatrix}$ so observables are spec(a)

each λ_i weighted with a probability $\frac{e^{-\beta h_i}}{\mathrm{Tr}(e^{-\beta H})}$ $H = \begin{pmatrix} h_1 & & \\ & \ddots & \\ & & h_N \end{pmatrix}$

h_i = energy levels of system (microscopic)

Thermodynamic formalism relating microscopic states of the system to macroscopic thermodyn. quantities like temperature $T \sim \beta^{-1}$

$\beta \to \infty$ $(T \to 0)$ system freezes on vacuum state $\mathrm{Ker}(H)$
while β small (T large) all high energy states count

Internal energy $\quad E = \dfrac{\mathrm{Tr}(He^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}$

note H not bounded; not in alg. $\mathcal{A}$; but if $He^{-\beta H}$ ~~trace class~~ $\mathrm{Tr}(He^{-\beta H}) < \infty$ ~~enough~~
(in more general ∞-dim cases

Principle of maximal entropy

$\varphi(a) = \dfrac{\mathrm{Tr}(a\tilde{\rho})}{\mathrm{Tr}(\tilde{\rho})}$ $\quad$ let $\rho = \dfrac{\tilde{\rho}}{\mathrm{Tr}(\tilde{\rho})}$ normalized

entropy $\quad S = -\mathrm{Tr}(\rho \log \rho)$

$\rho + \delta\rho \qquad \delta S = -\mathrm{Tr}(\delta\rho(\log\rho + 1))$

($\delta \mathrm{Tr}(F(\rho)) = \mathrm{Tr}(\delta\rho\, F'(\rho))$ even when $[\rho, \delta\rho] \neq 0$: perturb. of eigenvalues first order)

with conditions on $\delta\rho$: $\quad \delta\,\mathrm{Tr}(\rho) = 0$ $\quad$ ~~partition~~ remains ~~fcn. same~~ probability ($\mathrm{Tr}(\rho) = 1$)
$\qquad \delta\,\mathrm{Tr}(\rho H) = 0$ $\quad$ (same internal energy)

Lagrange multipliers

$\mathrm{tr}(\delta\rho(\log\rho + \underbrace{1}_{+\alpha} + \beta H)) = 0$ for arbitrary $\delta\rho$

$\Rightarrow \quad \rho = C e^{-\beta H}$

Equilibrium states are also a solution to a variational problem for entropy

Generalizing from $A = M_N(\mathbb{C})$ to arbitrary C^*-algebras

states of the form $\varphi_\beta(a) = \dfrac{Tr(\pi(a) e^{-\beta H})}{Tr(e^{-\beta H})}$
for some covariant rep.
(π, H) $\quad H$ hamiltonian
are called Gibbs states

Condition $Tr(e^{-\beta H}) < \infty$ not always satisfied

Equilibrium states without this trace assumption
KMS states (Kubo-Martin-Schwinger)

$(\mathcal{A}, \sigma_t)$ $\quad \varphi : \mathcal{A} \to \mathbb{C}$ state is KMS_β for $(\mathcal{A}, \sigma_t)$
iff

$\forall a, b \in \mathcal{A} \quad \exists \quad F_{ab}(z)$ function

holomorphic on the strip $\{Im(z) \in (0, \beta)\} = I_\beta$
extends to a continuous function on the boundary ∂I_β
$Im(z) = 0$ & $Im(z) = \beta$

And on ∂I_β it satisfies

$$\begin{cases} F_{ab}(t) = \varphi(a \sigma_t(b)) \\ F_{ab}(i\beta + t) = \varphi(\sigma_t(b) a) \end{cases} \qquad \left(\sup_{I_\beta} |F_{ab}(z)| \leq \|a\| \cdot \|b\| \right)$$

Note: it extends (modifies) the property of being a trace

φ is a trace if $\varphi(ab) = \varphi(ba)$ $\Rightarrow$ a trace is a KMS_0-state

F interpolates holomorphically between $\varphi(ab)$ and $\varphi(ba)$
using an analytic extension of the time evolution

Check that states of Gibbs form are KMS

$$\varphi(a) = \frac{Tr(\pi(a)e^{-\beta H})}{Tr(e^{-\beta H})} \qquad \text{with } Tr(e^{-\beta H}) < \infty$$

is a KMS_β state for $(\mathcal{A}, \sigma_t)$

$$\varphi(a\,\sigma_t(b)) = \frac{Tr(\pi(a)e^{itH}\pi(b)e^{-itH}e^{-\beta H})}{Tr(e^{-\beta H})} \qquad = F_{ab}(t)$$

$$\varphi(\sigma_t(b)a) = \frac{Tr(e^{itH}\pi(b)e^{-itH}\pi(a)e^{-\beta H})}{Tr(e^{-\beta H})} \qquad = F_{ab}(t+i\beta)$$

$$Tr(\pi(a)e^{itH}\pi(b)e^{-itH}e^{-\beta H}) = Tr(e^{itH}\pi(b)e^{-itH}e^{-\beta H}\pi(a)e^{\beta H}e^{-\beta H})$$

$$Tr(e^{itH}\pi(b)e^{-itH}\pi(a)e^{-\beta H}) = Tr(\pi(a)\,e^{(it-\beta)H}\pi(b)\,e^{(-it+\beta H)}e^{-\beta H})$$

$$F_{ab}(z) = \frac{Tr(\pi(a)e^{izH}\pi(b)e^{-izH}e^{-\beta H})}{Tr(e^{-\beta H})}$$

$$\begin{cases} z = t & \varphi(a\,\sigma_t(b)) \\ z = t + i\beta & \varphi(\sigma_t(b)a) \end{cases}$$

$$\pi(\sigma_t(a)) = e^{itH}\pi(a)e^{-itH}$$

analytic continuation to $\sigma_z(a) \qquad z \in I_\beta$

<u>Equivalent definition of KMS condition:</u>

$\exists$ a norm dense σ-invariant subalgebra $\mathcal{B}_\sigma \subset \mathcal{A}$ s.t. $\forall a, b \in \mathcal{B}_\sigma$

$$(*) \qquad \varphi(a\,\sigma_{i\beta}(b)) = \varphi(ba)$$

shows more clearly that generalization of "trace" property

$\mathcal{B}_\sigma$ = algebra of <u>analytic elements</u> i.e. s.t.

$\sigma_t(a)$ extends analytically to $\sigma_z(a)$ for all $z \in \mathbb{C}$ (entire holom. function)

KMS states are equilibrium states

$$\varphi(\sigma_t(a)) = \varphi(a)$$

in fact take for $a \in B_\sigma$

$$F(z) = \varphi(\sigma_z(a))$$ holom. function bounded

by $M = \sup\{ \| \sigma_z(a) \| : \gamma \in [0,\beta] \}$, $z = i\gamma$

because

$$F(z+i\beta) = \varphi(1 \cdot \sigma_{i\beta}(\sigma_z(a))) = \varphi(\sigma_z(a) \cdot 1) = F(z)$$

so F is periodic of period $i\beta$

and
$$|F(z)| \leq \| \sigma_z(a) \| = \| \sigma_{Re(z)}(\sigma_{i\,Im(z)}(a)) \|$$
$$= \| \sigma_{i\,Im(z)}(a) \| .$$

but then F is constant so $\varphi(\sigma_t(a)) = \varphi(a)$

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from (*) to $F_{a,b}$ definition by setting $F_{a,b}(z) = \varphi(a\,\sigma_z(b))$ for $a,b \in B_\sigma$ and more generally approximate $a,b \in \mathcal{A}$ by sequences in B_σ

<u>Example:</u> depending on $(\mathcal{A},\sigma)$ KMS_β state may exist or not

Comparison of two cases : $(\mathcal{T}_n,\sigma)$ Toeplitz algebra

$(\mathcal{O}_n,\sigma)$ Cuntz algebra

with compatible time evolutions (<u>ie</u> induced on quotient $1\to \mathcal{I}_n \to \mathcal{T}_n \to \mathcal{O}_n \to 1$)

* Toeplitz : there is at <u>each</u> β a <u>unique</u> KMS_β state
* Cuntz : there is a <u>unique</u> $\beta=\log n$ for which there are KMS_β states : <u>unique</u> one

S_i $i=1,\dots,n$ isometries generators

$S_i^* S_i = 1$ — in Cuntz case also have relation $\sum_i S_i S_i^* = 1$ <u>not</u> in Toeplitz case

$$\sigma_t(S_i) = e^{it} S_i$$ gauge action ($U(1)$-action)

defines a time evolution on both $\mathcal{T}_n$ & $\mathcal{O}_n$ compatibly

Fixed pt. algebra $\mathcal{A}^\sigma$ lin. combin. of elements $S_\mu S_\nu^*$

$$S_\mu = S_{i_1}\cdots S_{i_k} \qquad S_\nu^* = S_{j_r}^*\cdots S_{j_1}^*$$ with $k=|\mu| = |\nu| = r$

$$\sigma_t(S_\mu S_\nu^*) = e^{it(|\mu|-|\nu|)} S_\mu S_\nu^*$$

φ KMS_β state : since $\varphi(\sigma_t(a)) = \varphi(a)$

$$\varphi(\sigma_t(S_\mu S_\nu^*)) = e^{it(|\mu|-|\nu|)}\varphi(S_\mu S_\nu^*)$$

$\Rightarrow \varphi(S_\mu S_\nu^*) = 0$ whenever $|\mu|\neq|\nu|$ while

for $|\mu|=|\nu|$ note that $S_\nu^* S_\mu = \delta_{\mu,\nu}$ so KMS condition * gives $\varphi(S_\mu S_\nu^*) = \delta_{\mu,\nu}\cdot e^{-\beta|\mu|}$

for $\mathcal{O}_n$ $\sum_i \varphi(S_i S_i^*) = n\cdot e^{-\beta} = \varphi(1) =$

$\Downarrow$

$e^\beta = n$

$\beta = \log n$

while for $\mathcal{T}_n$ gives one state for each β

This for $\beta \in (0,\infty)$: $\beta = 0$ traces

What for $\beta = \infty$: physically interesting case $T=0$ zero temperature

Two possibilities:

(1) Define equilibrium states for $\beta = \infty$ using

$\exists\, F_{a,b}(z)$ holom in $\mathbb{H} = \{ \mathrm{Im}(z) > 0 \}$ upper half plane

continuous on $\mathrm{Im}(z)=0$: $F_{a,b}(t) = \varphi(a\,\sigma_t(b))$

<u>Weaker</u> condition than KMS_β $\beta < \infty$

"ground states"

(2) KMS_∞ states defined as weak limits of KMS_β states as $\beta \to \infty$

$$\varphi_\infty(a) := \lim_{\beta\to\infty} \varphi_\beta(a) \qquad \varphi_\beta \in KMS_\beta(\mathcal{A},\sigma)$$

better notion: more similar to KMS_β, smaller set

Better behavior of KMS states as opposed to $\mathfrak{S}(\mathcal{A})$ all states:

KMS_β also a convex <u>compact</u> set (in A^* weak*-top)

Extremal KMS-states $\mathcal{E}_\beta$: pure states in KMS_β

But now KMS_β is also a <u>simplex</u>

hence $\mathcal{E}_\beta$ suff. "small" to be a <u>good</u> set of "classical points"
compared to pure states in $\mathfrak{S}(\mathcal{A})$ <u>but</u> adapted to time evolution and varying with temperature

KMS_∞ as weak-limit still simplex; ground states <u>not</u>

See Chapter 5 of Bratteli–Robinson "Operator Algebras and QSM"

Symmetries of a QSM system $(\mathcal{A},\sigma)$

Automorphisms : $g \in Aut(\mathcal{A})$ s.t. $g\sigma_t = \sigma_t g$

induced action on KMS_β states

pullback $(\vec{g}^*\varphi)(a) = \varphi(g(a))$ $\qquad (g_1 g_2)^*(\varphi) = g_2^* g_1^*(\varphi)$

Inner automorphisms : $u \in \mathcal{U}(\mathcal{A})$ with $\sigma_t(u) = u$

$\Rightarrow \quad ad(u)\,a = u a u^*$ inner automorphism of $\mathcal{A}$

$ad(u)^*(\varphi) = \varphi$ acts trivially on KMS states

$$\varphi(uau^*) = \varphi(a u^* \sigma_{i\beta}(u)) = \varphi(a)$$

More general types of symmetries of QSM given by endomorphisms :

$\rho : \mathcal{A} \to \mathcal{A}$ $*$-homomorphism

$\sigma_t \rho = \rho \sigma_t$ compatible w/ time evolution

$\Rightarrow \rho(1) = e \quad e^2 = e = e^*$ with $\sigma_t(e) = e$

can define $\rho^*(\varphi)$ for $\varphi \in KMS_\beta$ provided $\varphi(e) \neq 0$

then $\rho^*(\varphi)(a) = \dfrac{\varphi(\rho(a))}{\varphi(e)}$ normalized again so that $\rho^*(\varphi)(1) = 1$

inner endomorphisms $u \in I(A)$ isometry

$u^* u = 1$ but $u u^* = e (= e^2 = e^*)$ idempotent

$ad(u)(a) = u a u^*$ defines an endomorphism because $u^* u = 1$

$\sigma_t(u) = \lambda^{it} u$ not fixed by σ_t but eigenvectors of σ_t $(\lambda \geq 1)$

Act trivially on KMS_β states (when action defined) if $\varphi(u u^*) \neq 0$

$$ad(u)^*(\varphi)(a) = \frac{\varphi(u a u^*)}{\varphi(u u^*)}$$

$$\varphi(u a u^*) = \varphi(a u^* \sigma_{i\beta}(u)) = \lambda^{-\beta} \varphi(a u^* u) = \lambda^{-\beta} \varphi(a)$$

while $\varphi(u u^*) = \lambda^{-\beta}$

$$\Rightarrow ad(u)^*(\varphi) = \varphi$$

Induced action for KMS_∞ states (at $T=0$)

$$\varphi_\infty(a) = \lim_{\beta \to \infty} \varphi_\beta(a)$$

but in general cannot ensure that $\varphi_\infty(e) \neq 0$ if $\varphi_\beta(e) \neq 0$

so $\rho^*(\varphi_\beta)$ need not induce action for $\beta \to \infty$

$$\varphi_\infty \mapsto \rho^*(\varphi_\infty)$$

Warming up + cooling down process!

works when set of extremal KMS states "stabilizes"

$\forall \beta \geq \beta_0 \quad \Sigma_\beta \simeq \Sigma_{\beta_0}$ so also Σ_∞ and all states for $\beta \geq \beta_0$ Gibbs states

$W_\beta : \Sigma_\infty \to \Sigma_\beta \qquad W_\beta(\varphi)(a) = \dfrac{Tr(\pi_\varphi(a) e^{-\beta H})}{Tr(e^{-\beta H})}$

i.e. assuming W_β homeomorphism $\quad \rho^*(\varphi_\infty) := \lim_{\beta \to \infty} W_\beta^{-1} \rho^*(W_\beta(\varphi))$ gives induced action

Example of time evolutions :

$A \rtimes_\alpha G$ crossed product algebra

given $\pi : G \to GL(V)$ representation of G
$\dim V = n$
as $GL_n^+(\mathbb{C})$ matrices with $\det \pi(g) \geq 0$

$f \in A \rtimes_\alpha G$ $\quad f(a,g)$ finite support

$a \xrightarrow{(a,g)} \alpha_g(a)$ groupoid

$$(f_1 * f_2)(a,g) = \sum_{g = g_1 g_2} f_1(\alpha_{g_2}(a), g_1)\, f_2(a, g_2)$$

Convolution product

$$\sigma_t(f)(a,g) = \det(\pi(g))^{it} f(a,g)$$

check $\quad \sigma_t(f_1 * f_2) = \sigma_t(f_1) * \sigma_t(f_2)$

$$\det(\pi(g))^{it} (f_1 * f_2)(a,g) \qquad \sum_{g = g_1 g_2} \det \pi(g_1)^{it} f_1(\alpha_{g_2}(a), g_1) \det \pi(g_2)^{it} f_2(a, g_2)$$

then $\quad \sigma_t(f^*) = \sigma_t(f)^*$

$$f^*(a,g) = \overline{f(\alpha_g(a), g^{-1})}$$

$$\sigma_t(f^*)(a,g) = \det(\pi(g))^{it} f^*(a,g)$$

$$(\sigma_t(f))^*(a,g) = \det \pi(g^{-1})^{-it}\, \overline{f(\alpha_g(a), g^{-1})}$$

$$\| \quad \overline{\sigma_t(f)(\alpha_g(a), g^{-1})}$$