Quantum Statistical Mechanics

Simplest example (finite dimensional case)

$$\mathcal{H} = \mathbb{C}^n \qquad \mathcal{A} = M_n(\mathbb{C})$$ with ~~~~ repres: on $\mathbb{C}^n$

A state $\varphi(a) = \dfrac{\mathrm{Tr}(\rho a)}{\mathrm{Tr}(\rho)}$ with density matrix $\rho \in M_n(\mathbb{C})$ $\rho > 0$
(i.e. $\rho = \eta^*\eta$)

H self adjoint matrix acting on $\mathbb{C}^n$; ~~~~

$\Rightarrow$ time evolution $\sigma_t(a) = e^{itH} a e^{-itH} \quad \forall t \in \mathbb{R}$

Associated "equilibrium states"

$$\varphi_\beta(a) = \frac{\mathrm{Tr}(a e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})}$$ density $\rho = e^{-\beta H}$

Gibbs states

$\beta \in \mathbb{R}_+^*$ (inverse temperature)

<u>equilibrium</u>: $\varphi(\sigma_t(a)) = \varphi(a) \quad \forall t \in \mathbb{R}$

Another way to see Gibbs states: Solutions of variational problem for energy functional

Generalizing to infinite dimensional case

- Observables of a quantum statistical mechanical system:

  $a \in \mathcal{A}$ $\quad C^*$-algebra

- Time evolution $\quad \sigma : \mathbb{R} \to \mathrm{Aut}(\mathcal{A})$

- Representation $\mathcal{A} \to B(\mathcal{H})$ bounded operators on a Hilbert space $\mathcal{H}$

  – is a <u>covariant</u> representation if
  $\exists\, H$ self-adjoint operator on $\mathcal{H}$ such that

  $$\pi(\sigma_t(a)) = e^{itH}\,\pi(a)\,e^{-itH} \qquad \forall t \in \mathbb{R}$$

  – Positive energy representation if Hamiltonian H can be chosen ~~__~~ with $\mathrm{Spec}(H) \subset [0,\infty)$

- Usually assume $\mathcal{A}$ unital; if not $\rightsquigarrow$ compactifications

  <u>simplest</u>: 1-point compactification

  $$\mathcal{A}^{comp} = \mathcal{A} \oplus \mathbb{C} \quad \text{w/product:}$$

  $$(a,\lambda)(b,\mu) = (ab + \lambda b + \mu a,\ \lambda\mu)$$

  $$a, b \in \mathcal{A} \quad \lambda, \mu \in \mathbb{C}$$

  other compactifications:

  Stone–Čech compactification

Def: $I \subset \mathcal{A}$ essential ideal if

I closed ideal s.t. if $J \subset \mathcal{A}$ any closed ideal $I \cap J \neq \phi$

Def: (Stone-Čech compactification)

$\mathcal{A}$ non-unital C^*-algebra, $\exists$ maximal C^*-algebra $M(\mathcal{A})$ s.t. $\mathcal{A} \subset M(\mathcal{A})$ essential ideal

(unique up to isomorphism

"multiplier algebra"

(idea: $M(\mathcal{A})$ consists of all T s.t. $Ta \in \mathcal{A}$ for all $a \in \mathcal{A}$ and $T(ab) = aT(b)$)
T bounded lin. operators

Sometime useful to consider also "unbounded multipliers"

$T : \mathcal{D}(T) \to \mathcal{A}$ defined on a dense ideal $\mathcal{D}(T) \subset \mathcal{A}$

with $T(ab) = aT(b)$ $\forall a \in \mathcal{A}$ and $b \in \mathcal{D}(T)$

States: $\mathcal{A}$ unital C^*-algebra

$\varphi : \mathcal{A} \to \mathbb{C}$ continuous linear functional with normalization $\varphi(1) = 1$ and positivity

$\varphi(a^* a) \geq 0 \quad \forall a \in \mathcal{A}$

In the non-unital case:

instead of condition $\varphi(1)=1$ have

$\|\varphi\| = 1$ where

$$\|\varphi\| = \sup_{\substack{a \in \mathcal{A} \\ \|a\| \leq 1}} |\varphi(a)|$$

GNS representation associated to a state:

given $\rho : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ a repres

$\Rightarrow$ state $\varphi(a) = \langle \xi, \pi(a) \xi \rangle$ for a given $\xi \in \mathcal{H}$ $\|\xi\| = 1$

Conversely: given a state $\varphi : \mathcal{A} \to \mathbb{C}$

define

$$\langle a, b \rangle = \varphi(a^* b)$$

induces an inner product on the vector space

$$\mathcal{H} = \mathcal{A}/I \qquad I = \text{left ideal } \{a : \varphi(a^* a) = 0\}$$

$\mathcal{A}$ acts on $\mathcal{H}$ by left multiplication

$$a \cdot (b \bmod I) = ab \bmod I$$

$$\xi = 1 + I \qquad 1 \in \mathcal{A} \text{ unit}$$

$$\varphi(a) = \langle \xi, a \xi \rangle$$

Equilibrium states for $(\mathcal{A}, \sigma_t)$

β (inverse temperature)

$$I_\beta = \{ z \in \mathbb{C} \mid 0 < \mathrm{Im}(z) < \beta \}$$

$$\partial I_\beta = \{ z \in \mathbb{C} \mid \mathrm{Im}(z) = 0 \text{ or } \mathrm{Im}(z) = \beta \}$$

$\varphi : \mathcal{A} \to \mathbb{C}$ satisfies the KMS condition
(Kubo-Martin-Schwinger)
at inverse temperature β if

$\forall a, b \in \mathcal{A}$ $\exists$ $F_{a,b}(z)$ holomorphic function
on I_β
extending continuously to ∂I_β

Such that

$$F_{a,b}(t) = \varphi(a \, \sigma_t(b))$$

$$F_{a,b}(t + i\beta) = \varphi(\sigma_t(b) \, a)$$

Observations:

- $\varphi_\beta(\sigma_t(a)) = \varphi_\beta(a)$ equilibrium states

- topology on set of KMS_β states Σ_β

  $\varphi_n \to \varphi$ iff $\varphi_n(a) \to \varphi(a)$ $\forall a \in \mathcal{A}$

  (weak convergence)

  $\Rightarrow$ Σ_β compact convex set

  $\Rightarrow$ $\mathcal{E}_\beta \subset \Sigma_\beta$ set of <u>extremal</u> points (extremal KMS states)

- $\mathcal{A}$ commutative, $\sigma_t = id$ trivial

  $\Rightarrow$ KMS states measures on X $\quad C(X) = \mathcal{A}$

  extremal: measures supported on points

- Gibbs states $\varphi(a) = \dfrac{Tr(a e^{-\beta H})}{Tr(e^{-\beta H})}$ are KMS_β-states

  but <u>NOT</u> all KMS_β states are of this form

- $\beta = 0$ case: traces i.e.

  $\varphi(ab) = \varphi(ba)$

Zero temperature KMS-states

Two different notions

<u>Stronger:</u> $\varphi : \mathcal{A} \to \mathbb{C}$ KMS_∞ if

$\exists \; \varphi_\beta \quad \beta < \infty$ (large) s.t.

$$\varphi(a) = \lim_{\beta \to \infty} \varphi_\beta(a) \qquad \forall a \in \mathcal{A}$$

Weak limits of positive temperature KMS states

<u>Weaker:</u> (ground states) $\varphi : \mathcal{A} \to \mathbb{C}$

$\forall a, b \in \mathcal{A} \quad \exists \; F_{a,b}(z)$ holomorphic on

$I = \{ z \in \mathbb{C} \mid \mathrm{Im}(z) > 0 \}$

such that $F_{a,b}(t) = \varphi(a \sigma_t(b))$

too coarse (too many ground states as opposed to KMS_∞-states) not nice convex etc.

<u>Prop:</u>
- $\varphi \in KMS_\beta$ extremal iff GNS rep. is a factor (trivial center)
- Σ_β convex compact Choquet simplex w/ extremal points $\mathcal{E}_\beta$
- Σ_∞ also convex compact (not a simplex in general)

Extension of states to multiplier algebra:

Given $(\mathcal{A}, \sigma_t)$ define $M(\mathcal{A})_\sigma \subset M(\mathcal{A})$

multipliers such that $t \mapsto \sigma_t(m)$ norm continuous
$m \in M(\mathcal{A})_\sigma$

$\varphi : \mathcal{A} \to \mathbb{C}$ state then admits an extension
$\varphi : M(\mathcal{A})_\sigma \to \mathbb{C}$

If $\varphi \in KMS_\beta$ then its extension is still a KMS_β-state on $M(\mathcal{A})_\sigma$

If $\mathcal{C} \subset M(\mathcal{A})_\sigma$ s.t. $\mathcal{A} \subset \mathcal{C}$ and
$\mathcal{C}$ is σ_t-invariant then

then $K_\beta(\mathcal{C}) = KMS_\beta(\mathcal{C})$ can be thought of as a compactification of $KMS_\beta(\mathcal{A})$

<u>Note</u>: not all $\varphi \in KMS_\beta(\mathcal{C})$ restrict to elements in $KMS_\beta(\mathcal{A})$ on $\mathcal{A}$: restrict to positive linear functionals of
$\|\varphi\| \leq 1$ (not nec $=1$)

"quasi-states"

Symmetries:

$\alpha : G \to \mathrm{Aut}(\mathcal{A}, \sigma_t)$

$\alpha \in \mathrm{Aut}(\mathcal{A})$ s.t. $\alpha \sigma_t = \sigma_t \alpha \quad \forall t \in \mathbb{R}$

induced action on KMS states

$$g^* \varphi(a) = \varphi(g(a))$$

$\mathrm{Inn}(\mathcal{A}, \sigma_t)$ inner automorphisms

$u \in \mathcal{U}(\mathcal{A})$ unitaries $u \in \mathcal{A}$ $u^* u = u u^* = 1$

such that $\sigma_t(u) = u \quad \forall t \in \mathbb{R}$

Acting on $\mathcal{A}$ by

$$\mathrm{ad}(u)\, a = u a u^*$$

induced action of $\mathrm{Inn}(\mathcal{A}, \sigma_t)$ on KMS states is trivial:

$\varphi \in KMS_\beta$ satisfies $\varphi(b \sigma_{i\beta}(a)) = \varphi(ab)$ (*)

$\forall a, b$ in a norm-dense σ-invariant subalgebra ("analytic elements")

(*) is equivalent to KMS condition

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

Symmetries by endomorphisms

("superselection sectors")

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

$$\rho \sigma_t = \sigma_t \rho$$

$\rho(1) \neq 1$ in general $\rho(1) = e$ idempotent
such that $\sigma_t(e) = e$

Given $\varphi \in KMS_\beta$ such that $\varphi(e) \neq 0$

$$\rho^*(\varphi)(a) := \frac{\varphi(\rho(a))}{\varphi(e)}$$

divide to restore normalization
$\rho^*(\varphi)(1) = 1$

Action of endomorphism ρ on KMS states

Inner: $\mathrm{Inn}(\mathcal{A}, \sigma_t)$ endomorphisms case

~~[illegible]~~ $u \in \mathcal{A}$ such that

$u^* u = 1$ (but not $u u^*$ in general now) $uu^* = e$

and $\sigma_t(u) = \lambda^{it} u$ for some $\lambda \in \mathbb{R}_+^*$

isometries eigenvectors of time evolution

$$ad(u)(a) = u a u^* \quad \forall a \in \mathcal{A}$$

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

Pf: $\varphi(uu^*) = \lambda^{-\beta} > 0$ so $ad(u)^*(\varphi)$ well defined and then use KMS_β condition as in automorphism case.