KMS states

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The KMS condition plays a fundamental role in quantum statistical mechanics where it provides a general abstract definition of equilibrium state. It is also deeply rooted in the mathematical structure of von Neumann algebras (see [Tomita-Takesaki theory]). Consequently, there is an enormous literature on the subject and the following article only provides a crude and very condensed introduction. We refer the reader to Chapter 5.3, 5.4 in [BR2] and Chapter 5 in [H] for a more elaborate introduction. We also recommend reading the pioneering article [HHW].

1 Motivation and definition

Consider a quantum system with finite dimensional Hilbert space $\mathcal{H}$ (e.g. a N-level atom). Such a system is described by a C^*-dynamical system $(\mathcal{B}(\mathcal{H}), \tau)$ where

$$\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH},$$

and $H = H^*$ denotes the Hamiltonian. For any $\beta \in \mathbb{R}$ this system has a unique thermal equilibrium state ω_β at inverse temperature β given by the Gibbs-Boltzmann prescription

$$\omega_\beta(A) = \frac{\mathrm{tr}(\mathrm{e}^{-\beta H} A)}{\mathrm{tr}(\mathrm{e}^{-\beta H})}.$$

Note that the equilibrium correlation function

$$F_\beta(A, B; t) = \omega_\beta(A\tau^t(B)), \tag{1}$$

is an entire function of t. The cyclicity of the trace yields the identity

$$\mathrm{tr}(\mathrm{e}^{-\beta H} A \tau^t(B)) = \mathrm{tr}(\mathrm{e}^{-\beta H} A \mathrm{e}^{\mathrm{i}tH} B \mathrm{e}^{-\mathrm{i}tH}) = \mathrm{tr}(\mathrm{e}^{-\mathrm{i}(t-\mathrm{i}\beta)H} A \mathrm{e}^{\mathrm{i}tH} B).$$

Analytic continuation from $t \in \mathbb{R}$ to $t \in \mathbb{R} + \mathrm{i}\beta$ further gives

$$\mathrm{tr}(\mathrm{e}^{-\beta H} A \tau^{t+\mathrm{i}\beta}(B)) = \mathrm{tr}(\mathrm{e}^{-\mathrm{i}tH} A \mathrm{e}^{\mathrm{i}(t+\mathrm{i}\beta)H} B) = \mathrm{tr}(\mathrm{e}^{-\beta H} \tau^t(B) A),$$

from which we conclude that

$$F_\beta(A, B; t + \mathrm{i}\beta) = \omega_\beta(\tau^t(B)A). \tag{2}$$

Relations (1), (2) relate the values of the analytic function $F_\beta(A, B; z)$ on the boundary of the strip

$$S_\beta = \{z \in \mathbb{C} \,|\, 0 < \mathrm{Im}(z\,\mathrm{sign}\beta) < |\beta|\},$$

to the state ω_β. They are called Kubo-Martin-Schwinger (KMS) boundary conditions. It is a simple exercise in linear algebra to show that the Gibbs state ω_β is the only state on $\mathcal{B}(\mathcal{H})$ satisfying the KMS boundary conditions (1), (2) for all $A, B \in \mathcal{B}(\mathcal{H})$. This fact motivates the following general definition.

Definition 1 *Let $(\mathcal{O}, \tau)$ be a C^*- or W^*-dynamical system. A state ω on $\mathcal{O}$, supposed to be normal in the W^*-case, is (τ, β)-KMS for some $\beta \in \mathbb{R}$ if the following holds. For any $A, B \in \mathcal{O}$ there exists a function $F_\beta(A, B; z)$ analytic in the strip S_β, continuous on its closure and satisfying the Kubo-Martin-Schwinger conditions (1), (2) on its boundary.*

Remarks. 1. KMS states for negative temperatures have no physical meaning, except for very special systems like the above one. However, for historical reasons, they are widely used in the mathematical literature. For example any modular state on a von Neumann algebra is a KMS state at inverse temperature $\beta = -1$ for its modular group (see [Tomita-Takesaki theory]).
2. In the special case $\beta = 0$ the KMS conditions degenerate to $\omega(AB) = \omega(BA)$. In mathematics such states are called *tracial*. Physicists sometimes call *stochastic* these infinite temperature equilibrium states.
3. If ω is (τ^t, β)-KMS then it is also $(\tau^{\gamma t}, \beta/\gamma)$-KMS. Note however that there is no simple connection between KMS states at different temperatures for the same dynamics τ^t.
4. If ω is a β-KMS state for the C^*- or W^*-dynamical system $(\mathcal{O}, \tau)$ then its normal extension $\tilde{\omega}$ to the enveloping von Neumann algebra $\mathcal{O}_\omega$ is a β-KMS state for the induced W^*-dynamical system $(\mathcal{O}_\omega, \tilde{\tau})$ defined in Section 3 of [Quantum dynamical systems].

2 Characterizations

Let $(\mathcal{O}, \tau)$ be a C^*- or W^*-dynamical system. An element $A \in \mathcal{O}$ is τ-analytic if the function $t \mapsto \tau^t(A)$ extends to an entire function of $t \in \mathbb{C}$. The set $\mathcal{O}_\tau$ of τ-analytic elements is a dense $*$-subalgebra of $\mathcal{O}$ in the appropriate topology (uniform in the C^*-case, σ-weak in the W^*-case). If ω is a (τ, β)-KMS state and $A, B \in \mathcal{O}_\tau$ then the function $F_\beta(A, B; z)$ of Definition 1 is given by $F_\beta(A, B; z) = \omega(A\tau^z(B))$. In particular one has $\omega(A\tau^{\mathrm{i}\beta}(B)) = \omega(BA)$. The following result shows that this property is characteristic of KMS states.

Theorem 2 *Let $(\mathcal{O}, \tau)$ be a C^*- or W^*-dynamical system. A state ω on $\mathcal{O}$, supposed to be normal in the W^*-case, is (τ, β)-KMS for some $\beta \in \mathbb{R}$ if and only if the following holds. There exists a dense, τ-invariant $*$-subalgebra $\mathcal{M} \subset \mathcal{O}$ of τ-analytic elements such that $\omega(A\tau^{\mathrm{i}\beta}(B)) = \omega(BA)$ for all $A, B \in \mathcal{M}$.*

The main property of KMS states, namely the invariance under time evolution, is a simple corollary of Theorem 2.

Theorem 3 *If ω is a (τ, β)-KMS state then it is τ-invariant, i.e., $\omega \circ \tau^t = \omega$ holds for all $t \in \mathbb{R}$.*

Remarkably enough, Definition 1 which involves global properties of the dynamics τ can be rephrased in terms of its infinitesimal generator. To formulate this result let us set

$$s(x, y) = \begin{cases} x(\log x - \log y) & x, y > 0, \\ 0 & x = 0, y \geq 0, \\ +\infty & x > 0, y = 0. \end{cases}$$

Theorem 4 (Araki [A]) *Let $(\mathcal{O}, \tau)$ be a C^*-dynamical system and denote by δ the infinitesimal generator of τ. A state ω is (τ, β)-KMS if and only if it is τ-invariant and satisfies the so called differential β-KMS condition*

$$-\mathrm{i}\beta\omega(A^*\delta(A)) \geq s(\omega(A^*A), \omega(AA^*)), \tag{3}$$

for all $A \in \mathrm{Dom}\,\delta$.

KMS states satisfy various correlation inequalities of the type (3), some of which are characteristic (see [Fannes-Verbeure inequalities], [Bogoliubov correlation inequality], as well as [BR2], [FV]). They play an important role in proving other characterizations of KMS states: Araki's *Gibbs condition* (a quantum substitute for the DLR equation) and variational principle for lattice spin systems (Chapter 6.2 in [BR2]) and lattice fermions ([AM]), see also [Quantum Gibbs-states].

3 Perturbation theory

As thermodynamic equilibrium states, KMS states enjoy a number of stability properties. We shall only discuss one of them here: Structural stability with respect to local perturbations of the dynamics. The reader should consult [Stability and passivity of quantum states] and [Return to equilibrium] as well as [BR2] for more such properties.

Let $(\mathcal{O}, \tau)$ be a C^*- or W^*-dynamical system and ω a (τ, β)-KMS state. Consider the local perturbation τ_V of τ by a self-adjoint element $V \in \mathcal{O}$ (see Section 5 in [Quantum dynamical systems]). In the GNS representation $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$ the perturbed dynamics is unitarily implemented by

$$\pi_\omega(\tau_V^t(A)) = \mathrm{e}^{\mathrm{i}t(L_\omega+Q)}\pi_\omega(A)\mathrm{e}^{-\mathrm{i}t(L_\omega+Q)},$$

where L_ω is the ω-Liouvillean and $Q = \pi_\omega(V)$.

Theorem 5 (Araki's perturbation theory) *The cyclic vector Ω_ω belongs to the domain of $\mathrm{e}^{-\beta(L_\omega+Q)/2}$ and*

$$\omega^V(A) = (\Psi_V|\pi_\omega(A)\Psi_V), \qquad \Psi_V = \frac{\mathrm{e}^{-\beta(L_\omega+Q)/2}\Omega_\omega}{\|\mathrm{e}^{-\beta(L_\omega+Q)/2}\Omega_\omega\|},$$

is a (τ_V, β)-KMS state. The GNS representation of $\mathcal{O}$ induced by ω_V is $(\mathcal{H}_\omega, \pi_\omega, \Psi_V)$. Moreover, the map $\omega \mapsto \omega^V$ is a bijection between the set of (τ, β)-KMS states and the set of (τ_V, β)-KMS states.

In the W^*-case, Araki's theorem extends to perturbed dynamics generated by unbounded perturbations Q affiliated to $\pi_\omega(\mathcal{O})$, see [DJP].

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