On the foundations of non-equilibrium quantum statistical mechanics

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1967: KMS CONDITION
Haag-Hugenholtz-Winnick

C^*-dynamical system $(\mathcal{O}, \tau^t)$. A state ω on $\mathcal{O}$ is called (τ, β)-KMS, where $\beta \in \mathbb{R}$, if for all $A, B \in \mathcal{O}$

$$F_{A,B}(t) = \omega(A\tau^t(B))$$

$$F_{A,B}(t + \mathrm{i}\beta) = \omega(\tau^t(B)A)$$

The definition is the same in the W^*- case with ω normal.

If $\mathcal{O} = \mathcal{B}(\mathcal{H})$, $\dim \mathcal{H} < \infty$, $\tau^t(A) = \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}$, then

$$\omega(A) = \mathrm{tr}(A\mathrm{e}^{-\beta H})/\mathrm{tr}(\mathrm{e}^{-\beta H})$$

is the unique (τ, β)-KMS state.

1967: MODULAR THEORY
Tomita-Takesaki

$(\mathfrak{M}, \Omega)$, $\mathfrak{M}$ von Neumann algebra on $\mathcal{H}$, Ω cyclic and separating vector.

$$SA\Omega = A^*\Omega$$

Polar decomposition:

$$S = J\Delta^{1/2}$$

J anti-unitary involution (modular conjugation), $\Delta \geq 0$ modular operator. The modular group:

$$\sigma^t(A) = \Delta^{\mathrm{i}t} A \Delta^{-\mathrm{i}t}.$$

Natural cone: $\mathcal{P} = \{AJAJ\Omega : A \in \mathfrak{M}\}^{\mathrm{cl}}$.

Theorem (Tomita-Takesaki)

$$J\mathfrak{M}J = \mathfrak{M}', \qquad \sigma^t(\mathfrak{M}) = \mathfrak{M}.$$

Moreover, the vector state $\omega(A) = (\Omega, A\Omega)$ is $(\sigma, -1)$-KMS state.

KMS Condition and Modular theory $\Rightarrow$ Golden Era of algebraic quantum statistical mechanics (Bratteli-Robinson).

1974: DYNAMICAL STABILITY
Haag–Kastler–Trych-Pohlmeyer

C^*-dynamical system $(\mathcal{O}, \tau^t)$, ω a stationary state.
KMS condition $\Leftrightarrow$ dynamical stability of ω under local perturbations $V = V^* \in \mathcal{O}$.

$\tau^t = \mathrm{e}^{t\delta}$. $\tau^t_\lambda = \mathrm{e}^{t\delta_\lambda}$, $\delta_\lambda(\cdot) = \delta(\cdot) + \mathrm{i}\lambda[V, \cdot]$. Perturbed stationary states:

$$\omega^{\pm}_\lambda(A) = \lim_{t \to \pm\infty} \omega(\tau^t_\lambda(A)).$$

We assume existence and ergodicity of $\omega^{\pm}_\lambda$. Ergodicity $\Rightarrow$ $\omega^+_\lambda \perp \omega^-_\lambda$ or $\omega^+_\lambda = \omega^-_\lambda$. The stability

$$\omega^+_\lambda = \omega^-_\lambda$$

in the first order of λ gives

Stability Criterion (SB)

$$\int_{-\infty}^{\infty} \omega([V, \tau^t(A)]) \mathrm{d}t = 0.$$

Assumption $L^1(\mathcal{O}_0)$ asymptotic abelianness:

$$\int_{-\infty}^{\infty} \|[V, \tau^t(A)]\| \mathrm{d}t < \infty$$

for V, A in the norm dense $*$-subalgebra $\mathcal{O}_0$.

Theorem (Haag–Kastler–Trych-Pohlmeyer, Bratteli–Kishimoto-Robinson)

Suppose in addition that ω is a factor state and that (SB) holds for $V, A \in \mathcal{O}_0$. Then ω is a (τ, β)-KMS state for some $\beta \in \mathbb{R} \cup \{\pm\infty\}$.

DYNAMICAL INSTABILITY

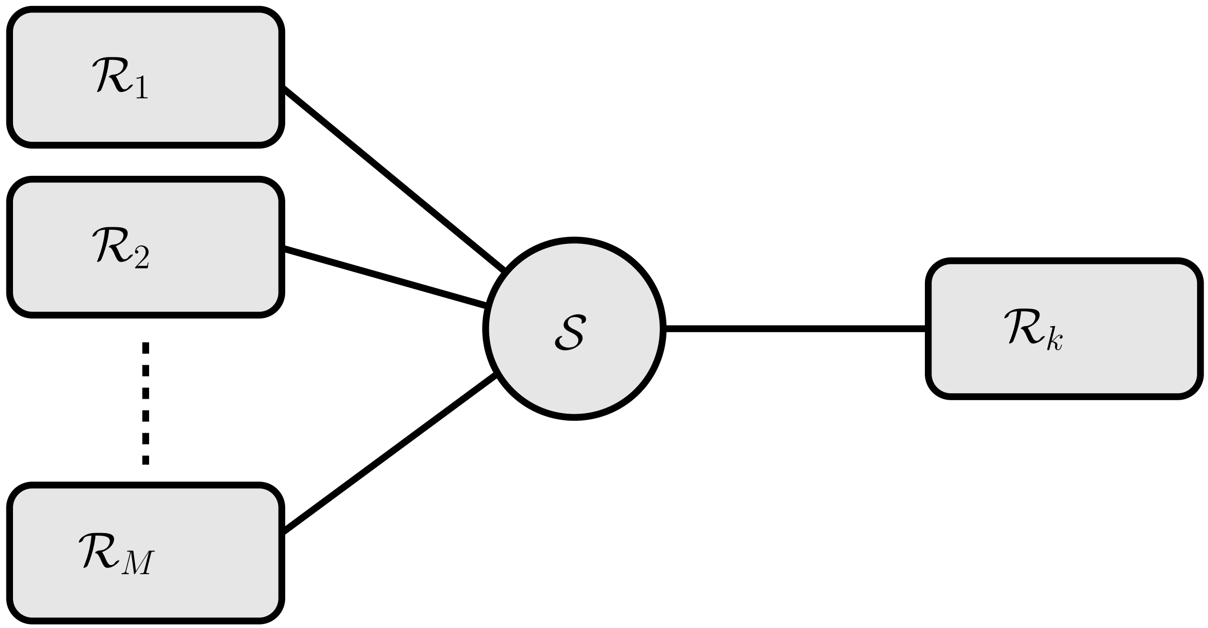
Same setup, but

$$\omega_\lambda^+ \perp \omega_\lambda^-$$

Dynamical instability $\Leftrightarrow$ Non-equilibrium

Quantification of non-equilibrium (our main message):
Degree of separation of the pair of mutually normal states $(\omega \circ \tau_\lambda^t, \omega \circ \tau_\lambda^{-t})$ as they approach the mutually singular limits $(\omega_\lambda^+, \omega_\lambda^-)$ as $t \to \infty$.

PICTURE: OPEN QUANTUM STSTEMS



RELATIVE MODULAR THEORY

Araki

$(\mathcal{H}, \pi, \Omega)$ GNS-representation of $(\mathcal{O}, \tau^t, \omega)$, $\mathfrak{M} = \pi(\mathcal{O})''$, Ω cyclic and separating (assumption), $\omega(A) = (\Omega, A\Omega)$,

$$\tau_\lambda^t(A) = \mathrm{e}^{\mathrm{i}tL_\lambda} A \mathrm{e}^{-\mathrm{i}tL_\lambda}, \qquad \mathrm{e}^{-\mathrm{i}tL_\lambda}\mathcal{P} = \mathcal{P},$$

$\Omega_t = \mathrm{e}^{-\mathrm{i}tL_\lambda}\Omega \in \mathcal{P}$ the vector representative of $\omega \circ \tau_\lambda^t$.

$$SA\Omega = A^*\Omega_t, \qquad S = J\Delta_t^{1/2},$$

$\Delta_t \geq 0$ is the relative modular operator of the pair of states $(\omega \circ \tau_\lambda^t, \omega)$. Non-commutative Radon-Nikodym derivative.

RENYI AND RELATIVE ENTROPY

$$S_t(\alpha) = \log(\Omega, \Delta_t^\alpha \Omega), \qquad \mathrm{Ent}_t = (\Omega_t, \log \Delta_t \Omega_t).$$

$S_t(0) = S_t(1) = 0$, $\alpha \mapsto S_t(\alpha)$ convex, we assume it is finite, $S_t'(1) = \mathrm{Ent}_t \geq 0$.

$$S_t(\alpha) = \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t s} \mathrm{d}\mathbb{P}_t(s),$$

where $\mathbb{P}_t$ is the spectral measure for $-\frac{1}{t} \log \Delta_t$ and Ω.

Time-reversal invariance (TRI) $\Rightarrow$

$$S_t(\alpha) = S_t(1 - \alpha).$$

BASIC OBJECTS

$$e(\alpha) = \lim_{t\to\infty} \frac{1}{t} S_t(\alpha).$$

Assumption Existence of limit and real-analyticity of $e(\alpha)$.

$\alpha \mapsto e(\alpha)$ is convex, $e(0) = e(1) = 0$.
TRI $\Rightarrow e(\alpha) = e(1-\alpha)$.

Entropy production of $(\mathcal{O}, \tau_\lambda^t, \omega)$ is

$$\Sigma = \lim_{t\to\infty} \frac{1}{t}\mathrm{Ent}_t = \lim_{t\to\infty} \frac{1}{t} S_t'(1).$$

TRI $\Rightarrow \Sigma = 0$ iff $e(\alpha) \equiv 0$.

LARGE DEVIATIONS

Rate function

$$I(\theta) = -\inf_{\alpha \in \mathbb{R}} (\alpha\theta + e(\alpha)).$$

For any $O \subset \mathbb{R}$ open,

$$\lim_{t \to \infty} \frac{1}{t} \log \mathbb{P}_t(O) = -\inf_{\theta \in O} I(\theta).$$

TRI $\Rightarrow$

$$I(-\theta) = \theta + I(\theta)$$

Quantum Gallavotti-Cohen Fluctuation Relation.

BACK TO TIME SEPARATION

Shorthand $\omega^t := \omega \circ \tau_\lambda^t$.
$(\omega^t, \omega^{-t}) \to (\omega^+, \omega^-)$ as $t \to \infty$.

$$\lim_{t\to\infty} \|\omega^t - \omega^{-t}\| = \|\omega^+ - \omega^-\| = 2.$$

$$D_t = \frac{1}{2}\left(2 - \|\omega^t - \omega^{-t}\|\right).$$

Quantum Neyman-Pearson Lemma

$$D_t = \inf_T \left(\omega^t(T) + \omega^{-t}(\mathbf{1} - T)\right),$$

where `inf` is over all orthogonal projections $T \in \mathfrak{M}$.

Quantum Hypothesis Testing

CHERNOFF EXPONENT

Theorem (JOPS)

$$\lim_{t\to\infty} \frac{1}{2t} \log D_t = \min_{\alpha\in[0,1]} e(\alpha)$$

Proof: Based on the estimate

$$\frac{1}{2}\mathbb{P}_t(\mathbb{R}_-) \leq D_t \leq (\Omega, \Delta_t^{\alpha}\Omega), \qquad \alpha \in [0,1]$$

The difficult part is the upper-bound. $\alpha = 1/2$ proven by Araki in 1973. In the case of matrices:

$$\frac{1}{2}(\text{Tr } A + \text{Tr } B - \text{Tr } |A - B|) \leq \text{Tr } A^{1-\alpha}B^{\alpha}$$

K. M. R. Audenaert, J. Calsamiglia, R. Munoz-Tapia, E. Bagan, Ll. Masanes, A. Acin, and F. Verstraete (2007). Simple proof: Ozawa (unpublished). General case: Ogata, JOPS.

STEIN EXPONENT

$\epsilon \in]0,1[$,

$$s_\epsilon = \inf_{\{T_t\}} \left\{ \lim_{t\to\infty} \frac{1}{t} \log \omega^{-t}(T_t) \;\middle|\; \omega^t(T_t) \geq \epsilon \right\}$$

Theorem (JOPS)

$$s_\epsilon = -\Sigma$$

HOEFFDING EXPONENT

$r > 0$,

$$h(r) = \inf_{\{T_t\}} \left\{ \lim_{t\to\infty} \frac{1}{t} \log \omega^{-t}(\mathbf{1} - T_t) \;\middle|\; \limsup_{t\to\infty} \frac{1}{t} \log \omega^{t}(T_t) < -r \right\}$$

Theorem (JOPS)

$$\psi(r) = -\sup_{\alpha\in[0,1[} \frac{-r\alpha - e(\alpha)}{1-\alpha}.$$

THE MEANING OF $\mathbb{P}_t$

Consider a confined quantum system on $\mathcal{H}$, $\dim \mathcal{H} < \infty$.
$\mathcal{O} = \mathcal{B}(\mathcal{H})$,

$$\tau_\lambda^t(A) = \mathrm{e}^{\mathrm{i}tH_\lambda} A \mathrm{e}^{-\mathrm{i}tH_\lambda}, \qquad H = H + \lambda V.$$

The state $\omega =$ density matrix on $\mathcal{H}$, $\omega > 0$, $\omega(A) = \mathrm{tr}(\omega A)$,

$$\omega_\lambda^t = \mathrm{e}^{-\mathrm{i}tH_\lambda} \omega \mathrm{e}^{\mathrm{i}tH_\lambda}.$$

Assume TRI.

Entropy observable

$$\mathcal{S} = -\log \omega.$$

Confined open quantum systems:

$$\mathcal{S} = \beta_S H_S + \sum_k \beta_k H_k.$$

$$\mathcal{S} = \sum sP_s$$

Measurement at $t = 0$ yields s with probability $\mathsf{tr}(\omega P_s)$.

State after the measurement:

$$\omega P_s / \mathsf{tr}(\omega P_s).$$

State at later time t:

$$\mathsf{e}^{-\mathsf{i}tH_\lambda} \omega P_s \mathsf{e}^{\mathsf{i}tH_\lambda} / \mathsf{tr}(\omega P_s).$$

Another measurement of $\mathcal{S}$ yields value s' with probability

$$\mathsf{tr}(P_{s'} \mathsf{e}^{-\mathsf{i}tH} \omega P_s \mathsf{e}^{\mathsf{i}tH}) / \mathsf{tr}(\omega P_s).$$

Probability distribution of the mean change of entropy

$$\phi = (s' - s)/t$$

$$\mathbb{P}_t(\phi) = \sum_{s'-s=t\phi} \mathrm{tr}(P_{s'} \mathrm{e}^{-\mathrm{i}tH} P_s \mathrm{e}^{\mathrm{i}tH}).$$

$$S_t(\alpha) = \log \mathrm{tr}([\omega]^{1-\alpha}[\omega^t]^{\alpha}) = \log \sum_{\phi} \mathrm{e}^{-\alpha t\phi} \mathbb{P}_t(\phi).$$

$S_t(\alpha) = S_t(1-\alpha)$ is equivalent to

$$\frac{\mathbb{P}_t(-\phi)}{\mathbb{P}_t(\phi)} = \mathrm{e}^{-t\phi}.$$

$\mathbb{P}_t$, spectral measure of $-\frac{1}{t}\log \Delta_t$, is identified with so called full statistics of the energy/entropy change in a repeated measurement protocol described above. Thermodynamic limit gives physical interpretation of $\mathbb{P}_t$ of extended systems.

CONCLUSION

Equlibrium. KMS-condition, dynamical stability, equivalence of the two directions of time.

Non-equilibrium. Dynamical instability, the directions of time are not-equivalent. The separation of time directions is quantified by entropic exponents. The exponents are in turn related to LDP for suitable spectral measure of relative modular Hamiltonian. This spectral measure is linked to full statistics of repeated measurements of energy/entropy. TRI implies Fluctuation Relations.

Entropy production. Σ, the Stein exponent, related to expected value of heat/charge fluxes in non-equilibrium steady state. $\Sigma = 0$ for sufficently many V''s + AA $\Rightarrow$ dynamical stability and KMS condition (J, Pillet).

TOPICS NOT DISCUSSED

(1) Concrete physically relevant models.

(2) Onsager reciprocity relations, Fluctuation-Dissipation Theorem.

(3) Host of other entropic functionals

(4) Quantum transfer operators and Ruelle's resonance picture of $e(\alpha)$