Some remarks on entropy production in quantum statistical mechanics

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This talk is an introduction to the recent series of papers by Benoist, Bruneau, J, Panati, Pillet:

A note on two-times measurement entropy production and modular theory, Lett. Math. Phys. 2024.

On the thermodynamic limit of two-times measurement entropy production, to appear in Rev. Math. Phys.

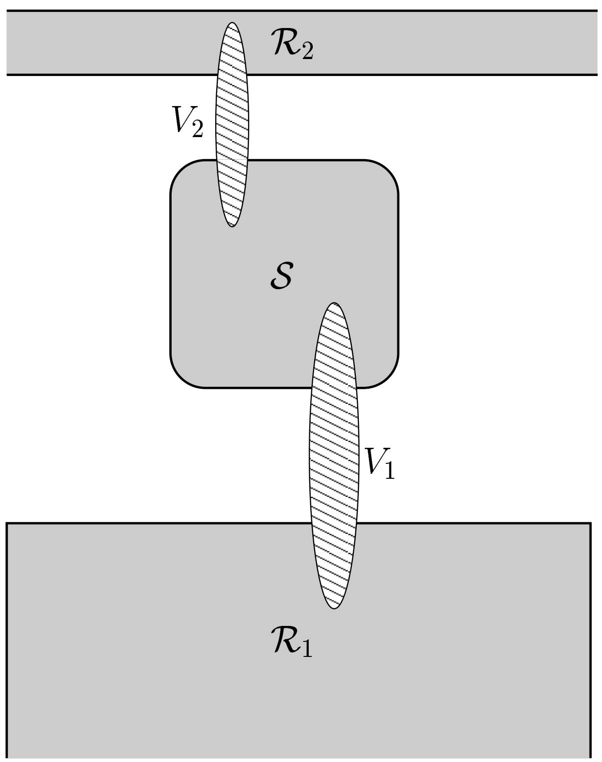
Entropic fluctuations in statistical mechanics II. Quantum dynamical systems, preprint

Entropic fluctuation theorems for spin-fermion model, preprint.

The references can be found therein. Continuation of the story in Laurent's talk.

OPEN QUANTUM SYSTEMS

Ruelle 2001, J-Pillet 2001. Small Hamiltonian system S coupled to two thermal reservoirs R_1 and R_2.



Hilbert space $\mathcal{H}_{R_1} \otimes \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{R_2}$.

Hamiltonians: $H_0 = H_S + H_{R_1} + H_{R_2}$,

$$H = H_0 + V.$$

Initial state:

$$\rho = \frac{1}{Z}\mathrm{e}^{-\beta_1 H_{R_1} - \beta_2 H_{R_2}}.$$

System $\mathcal{S}$ is in a tracial state (for convenience).

$$\Phi_j = \mathrm{i}[H_{R_j}, H] = \mathrm{i}[H_{R_j}, V]$$

the energy flux observable (out of the j-th reservoir).

The entropy production observable is

$$\sigma = -\beta_1 \Phi_1 - \beta_2 \Phi_2.$$

If

$$S = -\log \rho = \beta_1 H_{R_1} + \beta_2 H_{R_2} + \log Z,$$

$$S_t = \mathrm{e}^{\mathrm{i}tH} S \mathrm{e}^{-\mathrm{i}tH}, \qquad \rho_t = \mathrm{e}^{-\mathrm{i}tH} \rho \mathrm{e}^{\mathrm{i}tH},$$

$$\frac{\mathrm{d}}{\mathrm{d}t} S_t \Big|_{t=0} = \sigma$$

Entropic cocycle

$$c^t = S_t - S = \int_0^t \mathrm{e}^{\mathrm{i}sH} \sigma \mathrm{e}^{-\mathrm{i}sH} \mathrm{d}s.$$

Relative entropy $S(\nu|\mu) = \mathrm{tr}(\nu(\log\nu - \log\mu))$. $S(\nu|\mu) \geq 0$ with equality iff $\nu = \mu$.

Entropy balance equation (EBE)

$$S(\rho_t|\rho) = \mathrm{tr}(\rho c^t) = \int_0^t \rho_s(\sigma)\mathrm{d}s$$

$$= -\beta_1 \underbrace{\int_0^t \rho_s(\Phi_1)\mathrm{d}s}_{\text{Energy change of } R_1} -\beta_2 \underbrace{\int_0^t \rho_s(\Phi_2)\mathrm{d}s}_{\text{Energy change of } R_2}$$

$$\geq 0 \iff \text{heat flows from hot to cold}$$

The sign in the ”second law” comes from the choice of initial condition.

TD limit (quantum spin systems, Ruelle 2001) or general abstract framework (J-Pillet 2001): Quantum dynamical system $(\mathcal{O}, \tau^t, \rho)$,

$$\mathcal{O} = \mathcal{O}_{\mathcal{S}} \otimes \mathcal{O}_{R_1} \otimes \mathcal{O}_{R_2},$$

$\tau^t = \mathrm{e}^{t\delta}$, $\delta = \delta_0 + \mathrm{i}[V, \cdot]$, $\delta_0 = \delta_{\mathcal{S}} + \delta_{R_1} + \delta_{R_2}$,

$$\rho = \rho_{\mathcal{S}} \otimes \rho_{R_1} \otimes \rho_{R_2}$$

ρ_{R_j} is β_j-KMS state.

$\Phi_j = \delta_{R_j}(V)$, σ as before, σ, Φ_j, are in $\mathcal{O}$.

Entropic cocycle $c^t \in \mathcal{O}$ = derivative of Connes' cocycle of the pair (ρ_t, ρ), its definition requires modular theory (non-commutative measure theory).

EBE holds with $S(\rho_t|\rho) = \rho(c^t)$ Araki's relative entropy of the pair (ρ_t, ρ).

Non-Equilibrium Steady States (NESS, Ruelle 1999):

$$\rho_+ = \mathrm{w} - \lim_{T\to\infty} \frac{1}{T}\int_0^T \rho\circ\tau^t \mathrm{d}t.$$

ρ_+ is stationary,

$$\rho_+(\Phi_1) + \rho_+(\Phi_2) = 0$$

$$\beta_1\rho_+(\Phi_1) + \beta_2\rho_+(\Phi_2) = -\lim_{t\to\infty}\frac{1}{t}S(\rho_t|\rho) \le 0.$$

The first and the second law. Establishing strict inequality in the second law is crucial!

(QUANTUM) OBJECTIONS

The exposed theory parallels the classical one, with modular structure replacing classical measure theory/probability. We will refer to it as the **direct quantization.**

There are however several objections from the physical perspective.

(a) Finite time fluctuation relation (the fine form of the second law) fails.

(b) The observational status of $\int_0^t \sigma_s \mathrm{d}s$ and of the fluctuations of entropy production along the state trajectory is questionable.

Backed to confined setting.

Entropic cocycle

$$c^t = S_t - S = \int_0^t \tau^s(\sigma)\mathrm{d}s.$$

It has positive and negative eigenvalues ($\mathtt{tr}(c^t) = 0$).

TRI $\Rightarrow$ the eigenvalues of c^t are symmetric wrt 0!

Spectral decomposition

$$c^t = \sum_{s \in \mathrm{sp}(c^t)} s P_s$$

The spectral measure for ρ and c^t is

$$Q_t(s) = \rho(P_s), \qquad s \in \mathrm{sp}(c^t).$$

We have

$$S(\rho_t|\rho) = \rho(c^t) = \int s\mathrm{d}Q_t(s) \geq 0.$$

Q_t favours positive s (”second law”).
However, the fluctuation relation (the fine form of the second law, under TRI, in classical case works of Evans-Searles, Gallavotti-Cohen)

$$\frac{Q_t(-s)}{Q_t(s)} = \mathrm{e}^{-s}$$

fails except in trivial cases.

TWO-TIME MEASUREMENT ENTROPY PRODUCTION

Kurchan, Tasaki, Tasaki-Matsui 2000-2003. Radically different proposal for quantum mechanical entropy production.

$$S = -\log \rho = \beta_1 H_1 + \beta_2 H_2 + \log Z.$$

$\rho = \sum \lambda P_\lambda$. First measurement at $t = 0$, $-\log \lambda$ is observed with probability $\mathtt{tr}(\rho P_\lambda)$. State reduction $\rho \mapsto \rho P_\lambda / \mathtt{tr}(\rho P_\lambda)$.

Reduced state evolves to

$$\mathrm{e}^{-\mathrm{i}tH} \left[\rho P_\lambda / \mathtt{tr}(\rho P_\lambda)\right] \mathrm{e}^{\mathrm{i}tH}.$$

The second measurement at time t gives $-\log \mu$ with probability

$$\mathtt{tr}\left(\mathrm{e}^{-\mathrm{i}tH} \left[\rho P_\lambda / \mathtt{tr}(\rho P_\lambda)\right] \mathrm{e}^{\mathrm{i}tH} P_\mu\right).$$

The probability that the pair $(-\log\lambda, -\log\mu)$ is observed is

$$p_t(\lambda,\mu) = \mathrm{tr}\left(\mathrm{e}^{-\mathrm{i}tH}\rho P_\lambda \mathrm{e}^{\mathrm{i}tH} P_\mu\right).$$

The entropy production random variable is

$$\mathcal{E}(\lambda,\mu) = -\log\mu - (-\log\lambda)$$

It describes the entropy produced in the time period $[0,t]$,

$$\mathcal{E}(\lambda,\mu) = s = \beta_1 \Delta E_1 + \beta_2 \Delta E_2$$

where ΔE_j is the measured change of the energy of the j-th reservoir. The distribution $\mathcal{Q}_t$ of $\mathcal{E}$ wrt p_t is

$$\mathcal{Q}_t(s) = \sum_{\mathcal{E}(\lambda,\mu)=s} p_t(\lambda,\mu).$$

$\mathcal{Q}_t$ is physically natural and experimentally accessible (in principle).

$\mathcal{B}(\mathcal{H})$ is Hilbert space with inner product $\langle X, Y\rangle = \mathtt{tr}(X^*Y)$.
Relative modular operator

$$\Delta_{\rho|\nu}(X) = \rho X \nu^{-1}$$

is positive.
Basic fact (TRI) $\Omega_\rho = \rho^{1/2}$,

$$\int_{\mathbb{R}} \mathrm{e}^{-\alpha s} \mathrm{d}\mathcal{Q}_t(s) = \langle \Omega_\rho, \Delta^{\alpha}_{\rho_{-t}|\rho} \Omega_\rho \rangle = \mathtt{tr}(\rho_t^{1-\alpha} \rho^{\alpha}).$$

$\mathcal{Q}_t$ = spectral measure of $-\log \Delta_{\rho_{-t}|\rho}$ for Ω_ρ (Tasaki-Matsui 2003 definition!).
Its characteristic function is Renyi's relative entropy of (ρ_t, ρ).

Observational status of the modular structure!

Of particular importance is further link of $\mathcal{Q}_t$ with Ruelle Quantum Transfer Operators and Araki-Masuda theory of non-commutative L^p-spaces.

Comparison with the direct quantization (Q_t spectral measure for ρ and c^t) under TRI.

$$\int_{\mathbb{R}} s \mathrm{d}\mathcal{Q}_t(s) = \int_0^t \rho(\sigma_s)\mathrm{d}s = S(\rho_t|\rho) = \int_{\mathbb{R}} s\mathrm{d}Q_t(s),$$

$$\int_{\mathbb{R}} s^2 \mathrm{d}\mathcal{Q}_t(s) = \int_{\mathbb{R}} s^2 \mathrm{d}Q_t(s).$$

However, the third moments of $\mathcal{Q}_t$ and Q_t are typically different.

This time Fluctuation Relation holds:

$$\frac{\mathcal{Q}_t(-s)}{\mathcal{Q}_t(s)} = \mathrm{e}^{-s}.$$

A physically and mathematically beautiful setting for qm entropy production.

But there are objections.

(a) The experiments are done only on the models with small $\mathrm{dim}\mathcal{H}$. The 2TMEP is obviously only a thought experiment if $\mathrm{dim}\mathcal{H}$ is large. But in the thermodynamic limit $\mathrm{dim}\mathcal{H} \to \infty$!

(b) Even worse, how to implement/interpret two-times measurement protocol wrt NESS ρ_+? This is necessary for the Gallavotti-Cohen theory of entropic fluctuations.

(c) The conceptual difficulty regarding the role of quantum measurements in development of quantum statistical mechanics.

We will discuss recently proposed solution to (a). For (b) and (c) see the series.

ENTROPIC ANCILLA STATE TOMOGRAPHY (2013-onwards)

The ancilla's Hilbert space is $\mathbb{C}^2$ and its initial state is the density matrix

$$\rho_{\mathrm{a}} = \begin{bmatrix} \rho_{++} & \rho_{+-} \\ \rho_{-+} & \rho_{--} \end{bmatrix},$$

with $\rho_{+-} \neq 0$.

The Hilbert space of the coupled system is $\widehat{\mathcal{H}} = \mathcal{H} \otimes \mathbb{C}^2$ and its initial state is $\widehat{\rho} = \rho \otimes \rho_{\mathrm{a}}$.

The coupling between the system and the ancilla is given by the Hamiltonian

$$\widehat{H}_\alpha = \mathrm{e}^{\frac{\alpha}{2}\log\rho\otimes\sigma_z}\,(H\otimes\mathbf{1})\,\mathrm{e}^{-\frac{\alpha}{2}\log\rho\otimes\sigma_z}$$

parametrized by $\alpha \in \mathrm{i}\mathbb{R}$.

Since $H = H_0 + V$ with $[H_0, \rho] = 0$,

$$\widehat{H}_\alpha = H\otimes\mathbf{1} + \widehat{W}_\alpha,$$

$$\widehat{W}_\alpha = \frac{1}{2}W_\alpha\otimes(\mathbf{1}+\sigma_z) + \frac{1}{2}W_\alpha\otimes(\mathbf{1}-\sigma_z),$$

$$W_\alpha = \rho^\alpha(V) - V.$$

The ancilla's state at time t is given by

$$\rho_{\mathsf{a}}(t) = \mathsf{tr}_{\mathcal{H}}(\mathsf{e}^{-\mathsf{i}t\widehat{H}_\alpha}\widehat{\rho}\mathsf{e}^{\mathsf{i}t\widehat{H}_\alpha}) = \begin{bmatrix} \rho_{++} & \mathcal{F}_t(\alpha)\rho_{+-} \\ \overline{\mathcal{F}_t(\alpha)}\rho_{-+} & \rho_{--} \end{bmatrix}.$$

where

$$\mathcal{F}_t(\alpha) = \int_{\mathbb{R}} \mathsf{e}^{-\alpha s}\mathsf{d}\mathcal{Q}_t(s).$$

Ancilla state tomography (projective measurements on $\mathbb{C}^2$) gives the access to $\rho_{\mathsf{a}}(t)$ and hence to $\mathcal{F}_t$!

These observations are of theoretical and experimental importance and resolve objection (a).

What is the series about?

Described two-times measurement protocol: The first measurement of $S = -\log \rho$ at time $t = 0$ when the system was in the state ρ.

What if the state of the system at $t = 0$ is some other state ν? Of particular interest is $\nu = \rho_T$ for large T.

It turned out that due to the decoherence effect induced by the first measurement, the two-times measurement entropy production is (under an ergodicity assumption on the reservoirs) essentially independent of the state of the system at the instant of the first measurement.

Paper I.

The strength of this conclusion requires a careful thermodynamical limit justification of certain formulas that naturally arise through modular theory description of the two-times measurement protocol.

This TDL justification touches on some foundational open problems of quantum statistical mechanics related to Araki-Gibbs condition (quantum analog of DLR).

An unusual thermodynamic limit argument (dynamical assumption that reservoirs are ergodic plays key role).

Paper II.

The direct relation with entropic ancila state tomography is broken as soon as the state at the instant of the first measurement is different from ρ. It is however restored in the asymptotic regimes relevant for Large Deviation Theory and quantum Evans-Searles/Gallavotti-Cohen Fluctuation Theorems.

Key to this restoration: connection with complex resonances of quantum transfer operators.

Strong parallel with classical entropic fluctuation theory of Evans-Searls and Gallavotti-Cohen.

Papers III and IV.

BRUNEAU-PANATI FORMULA

With $\varsigma_\rho^\theta(A) = \mathrm{e}^{\mathrm{i}\theta \log \rho}(A)\mathrm{e}^{-\mathrm{i}\theta \log \rho}$ (modular dynamics),

$$\mathfrak{F}_{t,T}(\alpha) = \lim_{R\to\infty} \frac{1}{R}\int_0^R \rho_T\left(\varsigma_\rho^\theta\left([D\rho_{-t} : D\rho]_\alpha\right)\right) \mathrm{d}\theta$$
$$= \int \mathrm{e}^{-\alpha s}\mathrm{d}\mathcal{Q}_{t,T}(s).$$

Remarkable and unexpected.

Survives thermodynamic limit/infinite system extension.

Modular dynamics ergodic $\Rightarrow \mathcal{Q}_{t,T}$ does not depend on the time of the first measurement and is constant along the state trajectory.