Quantum thermodynamics and sequential measurements

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Talk at the meeting

Mathematical Foundations of Quantum Mechanics in memoriam
Paul Busch, 18th - 19th June 2019, University of York

Introduction 1

- H.-J. S. and J. Gemmer:

A framework for sequential measurements and general Jarzynski equations, arXiv:1905.11069 [quant-ph]

- Work → energy differences →sequential energy measurements → POV measures

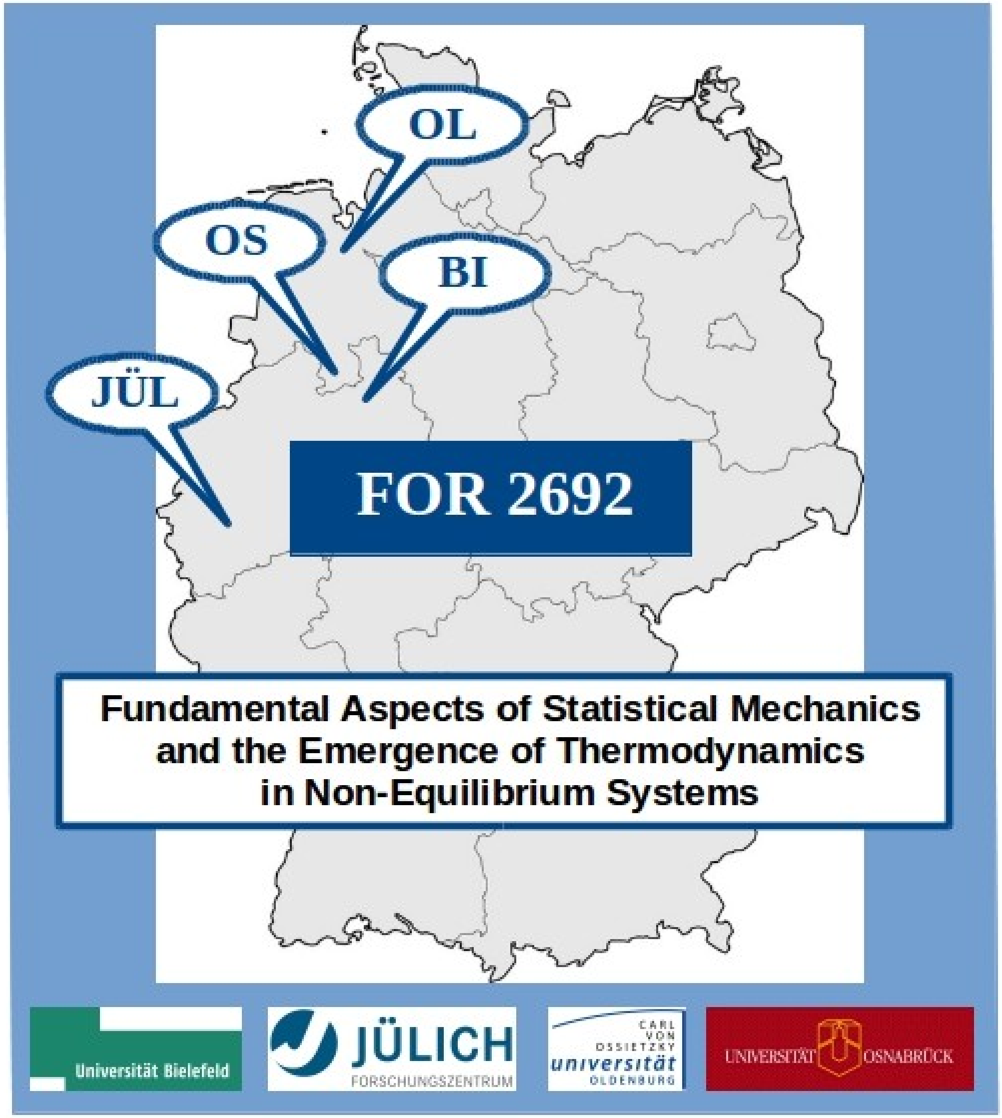
- P. Talkner, E. Lutz, and P. Hänggi,

Fluctuation theorems: Work is not an observable, Phys. Rev. E, **75**, 050102 (2007)

- A. J. Roncaglia, F. Cerisola, and J. P. Paz,

Work Measurement as a Generalized Quantum Measurement, Phys. Rev. Lett.**113**, 250601 (2014)

Introduction 2



Content

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- Sequential measurements
- Excursion: 1st law
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Sequential measurements 1

ρ

$P_i \rho P_i$

$U P_i \rho P_i U^*$

$P(i,j) = Tr(Q_j U P_i \rho P_i U^*)$

$= Tr(\rho F(i,j))$

$F(i,j) = P_i U^* Q_j U P_i \geqslant 0$

$\Rightarrow \Sigma_{i\,j} F(i,j) = \mathbb{1}$

- initial state
- 1st Lüders measurement
- time evolution
- 2nd measurement
- POV measure

Sequential measurements 2

- Consider two sequential energy measurements of

$$H(t_0) = \sum_i E_i(t_0) P_i \quad \text{and} \quad H(t_1) = \sum_j E_j(t_1) Q_j$$

- Define ``work" as the random variable

$$W(i,j) = E_j(t_1) - E_i(t_0)$$

such that, e.g.,

$$\langle W \rangle = \sum_{i,j} P(i,j) \left(E_j(t_1) - E_i(t_0) \right)$$

- W can also be viewed as a POV-measure and hence as a (generalized) observable

Excursion: 1^{st} law

- Let the total system consist of a system S and a heat bath B such that

$$H(t) = H^S(t) \otimes 1 + 1 \otimes H^B + H^{SB}(t)$$

and

$$H^{SB}(t_0) = H^{SB}(t_1) = 0$$

- It follows that

$$W(i,j) = E_j(t_1) - E_i(t_0) = \left(E_j^S(t_1) - E_i^S(t_0)\right) + \left(E_j^B - E_i^B\right)$$

$$\equiv \Delta U(i,j) + Q(i,j)$$

- Hence the 1^{st} law W=ΔU+Q holds for the observables

ΔU *change in the internal energy* and

Q *heat*

Framework / Simple case 1

$$\Omega = \mathcal{I} \times \mathcal{J}$$

- Outcome set

$$\mathcal{P} : \Omega \longrightarrow [0,1]$$

- Probability function

$$\Sigma_{i\,j}\ \mathcal{P}(i,j) = 1$$

$$p(i) = \Sigma_{j}\ \mathcal{P}(i,j)$$

- 1^{st} marginal probability

$$\pi(\,j \mid i\,)$$

- Conditional probability

$$\mathcal{P}(i,j) = \pi(\,j \mid i\,)\, p(i)$$

Framework / Simple case 2

$Y: \Omega \longrightarrow \mathbb{R}$

- Random variable

p(i) > 0 for all i$\in\mathcal{I}$

- Assumption

$$Y(i,j) = \frac{q(j)}{p(i)}$$

- Special random variable

- J-equation :

$$\left\langle \frac{q(j)}{p(i)} \right\rangle = 1 \text{ for all } q : \mathcal{J} \rightarrow [0,1] \text{ such that } \sum_{j\in\mathcal{J}} q(j) = 1$$

Framework / Simple case 3

- J-equation $\Longleftrightarrow$ π is doubly stochastic
- Proof of $\Leftarrow$:

$$\langle Y \rangle = \sum_{i,j} \mathcal{P}(i,j) Y(i,j) = \sum_{i,j} \pi(j|i) p(i) \frac{q(j)}{p(i)}$$

$$= \sum_{i,j} \pi(j|i) q(j) = \sum_{j} q(j) = 1. \quad \square$$

General assumption: π is doubly stochastic

Framework / Simple case 4

- Choose $q(j)=\Sigma_i \mathcal{P}(i,j)$ (2nd marginal probability)

- log concave ⇒

$$0 = \log 1 \overset{\text{J-eq.}}{=} \log\langle Y\rangle \overset{\text{Jensen}}{\geq} \langle \log Y\rangle$$

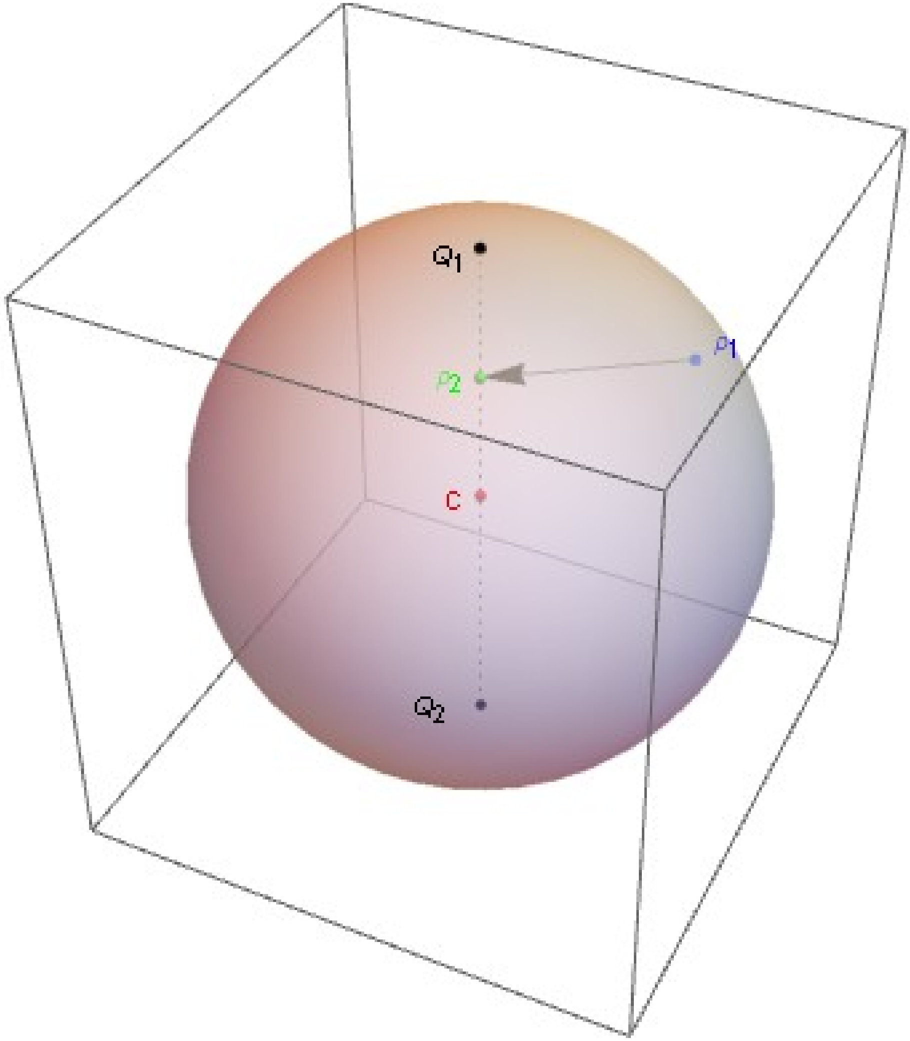
$$= \left\langle \log \frac{q(j)}{p(i)} \right\rangle = \langle \log q(j)\rangle - \langle \log p(i)\rangle = \sum_j q(j) \log q(j) - \sum_i p(i) \log p(i)$$

That means:

The Shannon entropy $S(p) = -\Sigma_i\, p(i) \log p(i)$ does not decrease between two measurements.

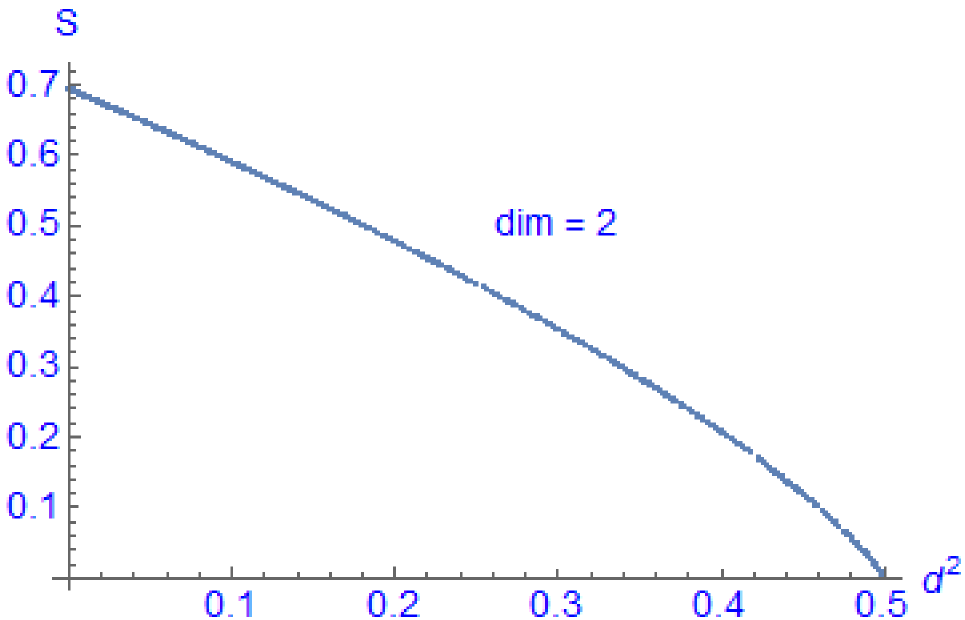
Framework / Simple case 5

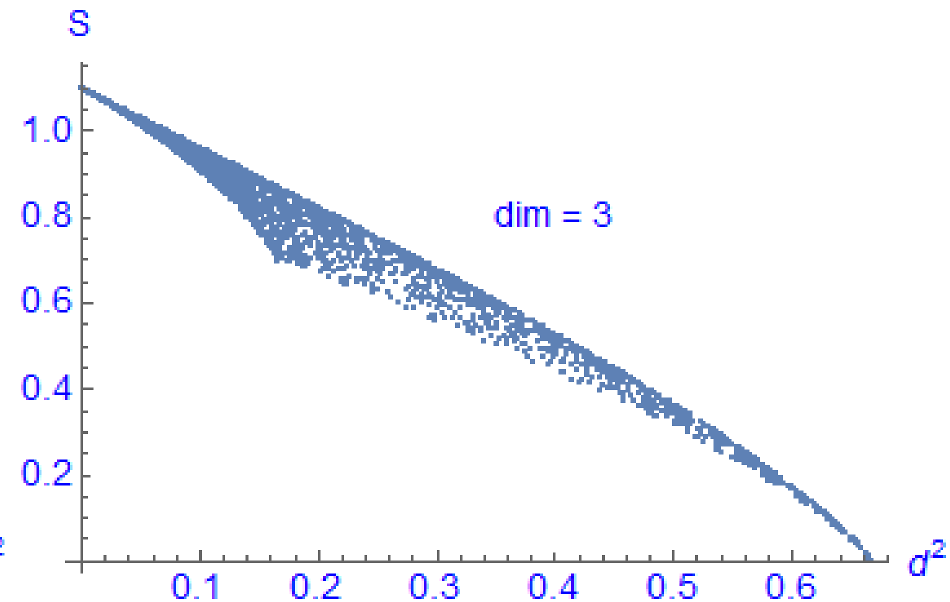
- Qubit measurements:
- The Shannon entropy is a monotonically decreasing function of the distance to the center of the Bloch sphere



Framework / Simple case 6

Shannon entropy vs. distance^2 to the uniform mixed state $\mathbb{1}$/dim:





Framework / Modified case 1

- Is the assumption of π being doubly stochastic satisfied in QT ?

$$\pi(j|i) = \frac{\mathcal{P}(i,j)}{p(i)} = \frac{\mathrm{Tr}\, Q_j U P_i \rho P_i U^*}{\mathrm{Tr}\, \rho P_i} \stackrel{?}{=} \mathrm{Tr}\, Q_j U P_i U^*$$

Only if $d(i) \equiv \mathrm{Tr}\, P_i = D(j) \equiv \mathrm{Tr}\, Q_j = 1$. Too restrictive !

Modified assumption:

$$P_i \rho P_i = \frac{\mathrm{Tr}\, \rho P_i}{\mathrm{Tr}\, P_i} P_i \equiv \frac{p(i)}{d(i)} P_i$$

$$\Rightarrow \ \pi(j|i) = \mathrm{Tr}\left(Q_j U \frac{P_i}{d(i)} U^* \right)$$

Framework / Modified case 2

$\longrightarrow \pi$ is of *modified doubly stochastic* type, i.e.

$$\boxed{\sum_i \pi(j|i)d(i) = D(j)}$$

$\Leftrightarrow$ modified J-equation:

$$\left\langle \frac{d(i)}{D(j)} \frac{q(j)}{p(i)} \right\rangle = 1 \text{ for all } q : \mathcal{J} \to [0,1] \text{ such that} \sum_j q(j) = 1$$

$\Rightarrow$ Non-decrease of modified Shannon entropy S'(p)between two measurements:

$$S'(p) \equiv -\sum_i p(i) \log \frac{p(i)}{d(i)} \leq -\sum_j q(j) \log \frac{q(j)}{D(j)} \equiv S'(q)$$

Framework / Modified case 3

- W. Pauli:

Über das H-Theorem vom Anwachsen der Entropie vom Standpunkt der neuen Quantenmechanik (1928)

- Proof of S'(p)≤S'(q)

using the symmetry condition

$$\frac{\pi(j|i)}{D(j)} = \frac{\pi(i|j)}{d(i)}$$

following from Fermi's Golden Rule

Framework / Modified case 4

- Is entropy a (sharp) observable ?

$$\rho \xrightarrow{\text{Ass.}} \rho_1 = \sum_i \frac{p(i)}{d(i)} P_i$$

$$\Rightarrow S'(p) \equiv -\sum_i p(i) \log \frac{p(i)}{d(i)} = -\mathrm{Tr}\,(\rho_1 \log \rho_1) = -\mathrm{Tr}\,(\rho \log \rho_1)$$

- Fix the self-adjoint operator $\mathcal{S} \equiv -\log \rho_1$ and let ρ run through all density operators. But then the expectation value of $\mathcal{S}$

$\mathrm{Tr}\,(\rho\,\mathcal{S}) = -\mathrm{Tr}(\rho \log \rho_1)$ is the ``cross entropy"

and only reduces to the usual entropy if $\rho \longrightarrow \rho_1$

Jarzynski equations 1

- Recall the assumption

$$P_i \rho P_i = \frac{\mathrm{Tr}\, \rho P_i}{\mathrm{Tr}\, P_i} P_i \equiv \frac{p(i)}{d(i)} P_i$$

- It is satisfied for $\rho = \mathcal{G}\left(H(t_0)\right)$

where $H(t_0) = \sum_i E_i(t_0) P_i$, hence $\frac{p(i)}{d(i)} = \mathcal{G}\left(E_i(t_0)\right)$

Let $H(t_1) = \sum_j E_j(t_1) Q_j$ and $\frac{q(j)}{D(j)} = \mathcal{G}\left(E_j(t_1)\right)$

Jarzynski equations 2

- Then the (modified) J-equation entails

$$\left\langle \frac{\mathcal{G}\left(E_j(t_1)\right)}{\mathcal{G}\left(E_i(t_0)\right)} \right\rangle = 1$$

- Upon choosing the canonical ensemble

$$\mathcal{G}\left(E_i(t_0)\right) = e^{-\beta(E_i(t_0)-F(t_0))}$$

the standard Jarzynski equation

$$\left\langle e^{-\beta W} \right\rangle = e^{-\beta \Delta F}$$

follows, where W denotes the random variable „work“

$W(i,j) = E_j(t_1) - E_i(t_0)$ and $\Delta F \equiv F(t_1) - F(t_0)$

Jarzynski equations 3

- Other choices of $\mathcal{G}$ yield modified Jarzynski equations describing systems in local equilibrium given by
    - microcanonical,
    - canonical, or
    - grand canonical ensembles.
- Application of Jensen's inequality gives 2nd law-like eqs., e.g.,

$$\beta\left(\langle W \rangle - \Delta F\right) \geq 0$$

- But note that S=β(U-F) only holds in the thermal equilibrium and the Jarzynski equation applies to the non-equilibrium case

Summary

Framework for SM^2

J-equation

q(j) 2nd marginal prob.

``Pauli-scenario“

$S'(p) \leqslant S'(q)$

$$\frac{q(j)}{D(j)} = \mathcal{G}\left(E_j(t_1)\right)$$

``Jarzynski-scenario“

$$\beta\left(\langle W\rangle - \Delta F\right) \geq 0$$

- Thank you for your attention !