Title: Entropy and energy fluctuations in non-equilibrium quantum statistical mechanics

Speakers: Annalisa Panati

Collection: Women at the Intersection of Mathematics and Theoretical Physics

Date: February 25, 2021 - 11:00 AM

URL: http://pirsa.org/21020047

Abstract: "Non-equilibrium statistical mechanics has seen some impressive developments in the last three decades, thank to the pioneering works of Evans, Cohen, Morris and Searles on the violation of the second law, soon followed by the ground-breaking formulation of the Fluctuation Theorem by Gallavotti and Cohen for entropy fluctuation in the early nineties. Their work was by vast literature, both theoretical and experimental

The extension of these results to the quantum setting has turned out to be surprisingly challenging and it is still an undergoing effort.
Kurchanâ€™s seminal work (2000) showed the measurement role has to be taken in account, leading to the introduction of the so called two-time measurement statistics (also known as full counting statistics).
However in this context, the lack of a trajectory notion leads to both conceptual and technical problems, or phenomena with no classical counterpart, as underlined by some of our recent results.

In this talk I will review some of the key concept involved in the Fluctuation Theorem and its extensions to the quantum setting;
I will present some recent results exploring the role played by ultraviolet regularity conditions (joint work with R.RaquÃ©pas and T.Benoist)."

Entropy and energy fluctuations in non-equilibrium quantum statistical mechanics

joint work with T.Benoist (Toulouse) and R. Raquépas. (McGill and Grenoble)

Annalisa Panati,
CPT, Université de Toulon

Women at the intersection of mathematics and theoretical physics, February 2021

Context: statistical mechanics

Entropy
ρ function on the phase space $\mathcal{M}$ describing particle distribution
$\equiv \rho$ is a measure on $\mathcal{M}$ given by $\rho(x)dx$

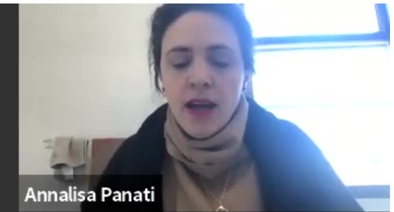
$S(\rho) :=$ ln(number of particle configurations corresponding to ρ / total configurations) encodes how likely the distribution ρ is

Variational principle: the equilibrium distribution ρ is the most likely one i.e. the one that maximize the entropy (between those satisfying energy constraints).

Second law: "Nature evolve from less probable to most probable = entropy of an isolated system tend to increase until it reaches equilibrium"

According to this picture second law is only a statistical one, suggesting that there should always be some nonzero probability that the entropy of an isolated system might spontaneously decrease. Fluctuation relation quantify this probability.

Annalisa Panati, CPT, Université de Toulon



Non-equilibrium and Fluctuation relation

Entropy and Relative entropy $S(\rho) = S(\frac{\mathrm{d}(\rho \mathrm{d}x)}{\mathrm{d}x})$

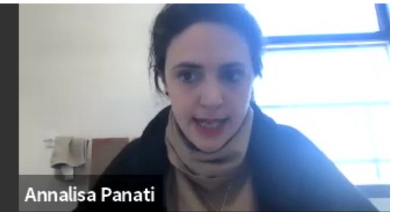
Relative entropy $S(\nu|\mu)$, function of $\frac{\mathrm{d}\nu}{\mathrm{d}\mu}$ encodes increase of entropy, defined when ν absolutely continous with respect to μ

Fluctuation relation If $\mathbb{P}_t^{S,cl}(s)$ is the law of the random variable corresponding to *average entropy production rate* et $\bar{\mathbb{P}}_t^{S,cl}(\phi) = \mathbb{P}_t^{S,cl}(-\phi)$. Under general hypothesis (example: ρ Gibbs, TRI)

$$\frac{\mathrm{d}\bar{\mathbb{P}}_t^{S,cl}}{\mathrm{d}\mathbb{P}_t^{S,cl}}(\phi) = \mathrm{e}^{-t\phi}$$

equivalent to

$$e_t^{cl}(\alpha) = e_t^{cl}(1-\alpha) \qquad e_t^{cl}(\alpha) = \int e^{-t\alpha\phi}\mathrm{d}\mathbb{P}_t^{S,cl}(\phi)$$



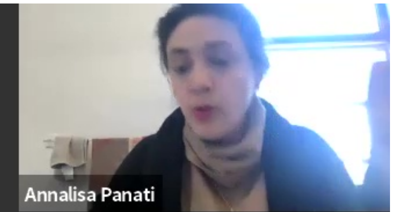
Context: quantum statistical mechanics

Fluctuation relations

Classical case: [Evans-Cohen-Morris '93] numerical experiences
[Evans-Searls '94] [Gallavotti Cohen '94] theoretical explanation

work in driven system [Bochkov-Kuzovlev '70s] [Jaryzinski '97] [Crooks '99] etc

a new area of research was open



Non-equilibrium and Fluctuation relation

Entropy and Relative entropy $S(\rho) = S(\frac{\mathrm{d}(\rho \mathrm{d}x)}{\mathrm{d}x})$

Relative entropy $S(\nu|\mu)$, function of $\frac{\mathrm{d}\nu}{\mathrm{d}\mu}$ encodes increase of entropy, defined when ν absolutely continous with respect to μ

Fluctuation relation If $\mathbb{P}_t^{S,cl}(s)$ is the law of the random variable corresponding to *average entropy production rate* et $\bar{\mathbb{P}}_t^{S,cl}(\phi) = \mathbb{P}_t^{S,cl}(-\phi)$. Under general hypothesis (example: ρ Gibbs, TRI)

$$\frac{\mathrm{d}\bar{\mathbb{P}}_t^{S,cl}}{\mathrm{d}\mathbb{P}_t^{S,cl}}(\phi) = \mathrm{e}^{-t\phi}$$

equivalent to

$$e_t^{cl}(\alpha) = e_t^{cl}(1-\alpha) \qquad e_t^{cl}(\alpha) = \int e^{-t\alpha\phi}\mathrm{d}\mathbb{P}_t^{S,cl}(\phi)$$

Entropy and energy fluctuations in non-equilibrium quantum statistical mechanics

Annalisa Panati, CPT, Université de Toulon

Quantization of fluctuation relation

Quantum case: Simplified setting, S is defined as an operator
Attempt 1: "Naive quantization"
Underlying idea : (in the simplifed setting) define an observable $\Sigma_t = \frac{1}{t}(S_t - S)$ on $\mathcal{H}$ and consider the spectral measure μ_{Σ_t}
—attempted in work related litterature [Bochkov-Kuzovlev '70s-'80s])
—attempted in the '90, called "naive quantization"

leads to *NO-fluctuation relations*!!!!

Attempt 2:
Physcal point of view [Kurchan'00] Measurement has been neglected. Associate to S the *two-time measurment statistics* $\mathbb{P}_t^{S}$ defined as difference between two measurement

leads to *fluctuation relations*

Mathematical point of view family of functionals satisfing the symmetry: the preferred one is the one where $\frac{\mathrm{d}\nu}{\mathrm{d}\mu}$ is replaced by $\triangle_{\nu|\mu}$ [Araki 70s, Jakšić-Pillet since 00s-now]

Quantization of fluctuation relation

Quantum case: Simplified setting, S is defined as an operator
Attempt 1: "Naive quantization"
Underlying idea : (in the simplifed setting) define an observable $\Sigma_t = \frac{1}{t}(S_t - S)$ on $\mathcal{H}$ and consider the spectral measure μ_{Σ_t}
—attempted in work related litterature [Bochkov-Kuzovlev '70s-'80s])
—attempted in the '90, called "naive quantization"

leads to *NO-fluctuation relations*!!!!

Attempt 2:
Physcal point of view [Kurchan'00] Measurement has been neglected. Associate to S the *two-time measurment statistics* $\mathbb{P}_t^S$ defined as difference between two measurement

leads to *fluctuation relations*

Mathematical point of view family of functionals satisfing the symmetry: the preferred one is the one where $\frac{\mathrm{d}\nu}{\mathrm{d}\mu}$ is replaced by $\triangle_{\nu|\mu}$ [Araki 70s, Jakšić-Pillet since 00s-now]

At the level of averages and variances, there is no difference!

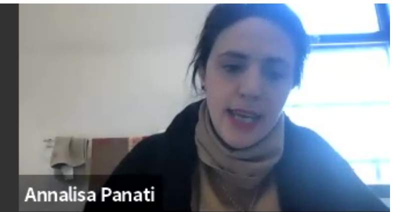
Two-time measurment statistics

Confined systems: described by $(\mathcal{H}, H, \rho)$ $dim\mathcal{H} < \infty$
Given an observable A: $A = \sum_j a_j P_{a_j}$ where $a_j \in \sigma(A)$ P_{a_j} associated spectral projections
Procedure:
- $t = 0$, we measure A (outcome a_j)
- evolve for time t
- measure again at time t (outcome a_k)

Two-time measurement distribution of A:
$\mathbb{P}_{A,t}(\phi)$= probability of measuring a change in A equal to ϕ.

Pagina 29 di 64

Annalisa Panati, CPT, Université de Toulon



Two-time measurment statistics

Procedure:

- $t = 0$, we measure A (outcome a_j)
- evolve for time t
- measure again at time t (outcome a_k)

$\mathbb{P}_{A,t}(\phi)$= probability of measuring a change in A equal to ϕ

In confined system:

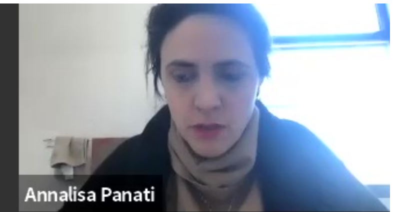
$$\mathbb{P}_{A,t}(\phi) = \sum_{a_k - a_j = \phi} \mathrm{tr}(\rho P_{a_j}) \mathrm{tr}(e^{-\mathrm{i}tH} \rho_{am} e^{\mathrm{i}tH} P_{a_k})$$

$$= \sum_{a_k - a_j = \phi} \mathrm{tr}(e^{-\mathrm{i}tH} P_{a_j} \rho P_{a_j} e^{\mathrm{i}tH} P_{a_k})$$

with

$$\rho_{am} = \frac{1}{\mathrm{tr}(\rho P_{a_j})} P_{a_j} \rho P_{a_j}.$$

Fact/Problem: *the measurment perturbes the state, the intial state reduces to* ρ_{am}



Two-time measurment statistics

Procedure:

- $t = 0$, we measure A (outcome a_j)
- evolve for time t
- measure again at time t (outcome a_k)

$\mathbb{P}_{A,t}(\phi)$= probability of measuring a change in A equal to ϕ

In confined system:

$$\mathbb{P}_{A,t}(\phi) = \sum_{a_k - a_j = \phi} \mathrm{tr}(\rho P_{a_j}) \mathrm{tr}(e^{-\mathrm{i}tH} \rho_{am} e^{\mathrm{i}tH} P_{a_k})$$

$$= \sum_{a_k - a_j = \phi} \mathrm{tr}(e^{-\mathrm{i}tH} P_{a_j} \rho P_{a_j} e^{\mathrm{i}tH} P_{a_k})$$

with

$$\rho_{am} = \frac{1}{\mathrm{tr}(\rho P_{a_j})} P_{a_j} \rho P_{a_j}.$$

Fact/Problem: *the measurment perturbes the state, the intial state reduces to ρ_{am}*

Remark: $\mathrm{supp}(\mathbb{P}_{A,t})$ is included on the set of possible A-differences

Two-time measurement statistics

Conservation laws

Classical system:$(\mathcal{M}, H, \rho)$
Two-time measurement statistics is equivalent to the law $\mathbb{P}_{\triangle A_t}$ associated to $\triangle A_t := A_t - A$. [1]

Assume $A + B$ is conserved. The identity as classical observables $\triangle A_t = A_t - A = -(B_t - B) = -\triangle B_t$ yiels the identity

$$\mathbb{P}_{\triangle A_t} = \mathbb{P}_{-\triangle B_t}$$

Quantum system $A_t - A = -(B_t - B)$ as operators yields identity between all spectral measures

$$\mu_{\triangle A_t} = \mu_{-\triangle B_t} \quad \text{but} \quad \mathbb{P}_{A,t} \neq \mathbb{P}_{-B,t}$$

[1] Given a classical observable C and an intial state ρ, we call C-statistics the probability measure $\mathbb{P}_C$ such that $\int f(s)\mathrm{d}\mathbb{P}_C(s) = \int f(C)\mathrm{d}\rho$ for all $f \in \mathcal{B}(\mathbb{R})$

Two-time measurement statistics

Conservation laws-energy balance

Classical system $(\mathcal{M}, H, \rho)$

$H = H_0 + V$ $\quad \rho$ is invariant for the dynamics associated to H_0

(H_0 interpreted as heat)

Energy conservation:

$\triangle H_{0,t} = H_{0,t} - H_0 = -(V_t - V) = (-V)_t - (-V)$ as function on $\mathcal{M}$

In particular if V is bounded by C then

$\sup_t |\triangle H_{0,t}| < 2C$ and $supp(\mathbb{P}_{\triangle H_{0,t}})$ bounded

Quantum system $(\mathcal{H}, H, \rho)$ $\quad H = H_0 + V$

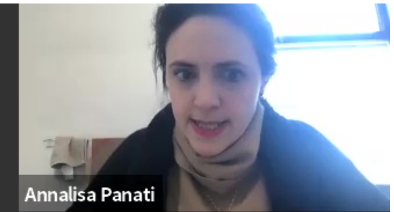
Energy conservation: $H_{0,t} - H_0 = -V_t + V = (-V)_t - (-V)$ as operator on $\mathcal{H}$ yields an identity between all spectral measures but

$$\mathbb{P}_{H_0,t} \neq \mathbb{P}_{-V,t}$$

A priori one can have: $supp(\mathbb{P}_{V,t})$ bounded but

$$\mathbb{E}_t(\phi^{2n}) = \int \phi^{2n} \mathrm{d}\mathbb{P}_{H_0,t}(\phi) = +\infty$$

Annalisa Panati, CPT, Université de Toulon



Heat fluctuations

Perturbation V bounded

Regularity condition optimality

Quantum impurity in a free Fermi gas

$\mathcal{H} = \Gamma_a(\mathbb{C}) \otimes \Gamma_a(L^2(\mathbb{R}_+, \mathrm{d}e)) = \mathbb{C}^2 \otimes \Gamma_a(L^2(\mathbb{R}_+, \mathrm{d}e))$

$H_0 = \mathrm{d}\Gamma(\varepsilon_0) \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\hat{e}) \qquad \varepsilon_0 > 0$

$H = H_0 + (a^*(1) \otimes \mathbb{1})(\mathbb{1} \otimes a(f)) + (a(1) \otimes \mathbb{1})(\mathbb{1} \otimes a^*(f))$

$f \in L^2(\mathbb{R}_+, \mathrm{d}e)$

ω is a (τ_0, β) KMS state

Theorem (Benoist, P., Raquépas 2017)

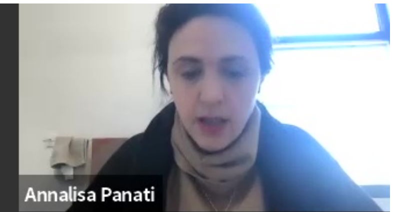
For the above model the following are equivalent:

1. $\sup_{t\in\mathbb{R}} \mathbb{E}_t[\phi^{2n+2}] < \infty$;
2. *for a non-trivial time interval* $[t_1, t_2]$ $\int_{t_1}^{t_2} \mathbb{E}_t[\phi^{2n+2}]\mathrm{d}t < \infty$;
3. (nD)

For this model (nD) is equivalent to $\mathbb{R} \ni s \mapsto \mathrm{e}^{\mathrm{i}s\hat{e}} f \in L^2(\mathbb{R}_+, \mathrm{d}e)$ is n times norm- differentiable i.e $f \in \mathrm{Dom}(\hat{e}^n)$

Entropy and energy fluctuations in non-equilibrium quantum statistical mechanics

Annalisa Panati, CPT, Université de Toulon



Heat fluctuations

Perturbation V bounded

Regularity condition optimality

Quantum impurity in a free Fermi gas

$\mathcal{H} = \Gamma_a(\mathbb{C}) \otimes \Gamma_a(L^2(\mathbb{R}_+, \mathrm{d}e)) = \mathbb{C}^2 \otimes \Gamma_a(L^2(\mathbb{R}_+, \mathrm{d}e))$

$H_0 = \mathrm{d}\Gamma(\varepsilon_0) \otimes \mathbb{1} + \mathbb{1} \otimes \mathrm{d}\Gamma(\hat{e}) \qquad \varepsilon_0 > 0$

$H = H_0 + (a^*(1) \otimes \mathbb{1})(\mathbb{1} \otimes a(f)) + (a(1) \otimes \mathbb{1})(\mathbb{1} \otimes a^*(f))$

$f \in L^2(\mathbb{R}_+, \mathrm{d}e)$

ω is a (τ_0, β) KMS state

Theorem (Benoist, P., Raquépas 2017)

For the above model the following are equivalent:

1. $\sup_{t\in\mathbb{R}} \mathbb{E}_t[\phi^{2n+2}] < \infty$;
2. *for a non-trivial time interval* $[t_1, t_2]$ $\int_{t_1}^{t_2} \mathbb{E}_t[\phi^{2n+2}]\mathrm{d}t < \infty$;
3. (nD)

For this model (nD) is equivalent to $\mathbb{R} \ni s \mapsto \mathrm{e}^{\mathrm{i}s\hat{e}} f \in L^2(\mathbb{R}_+, \mathrm{d}e)$ is n times norm- differentiable i.e $f \in \mathrm{Dom}(\hat{e}^n)$

Remark: decay of f controls how high energy frequencies contribute to the interaction (ultraviolet regularity)

Conclusions: underlying picture

Classical VS Quantum two-time measurement

Classical

trajectory picture
$V \approx 0 \Rightarrow \Delta H_0 \approx 0$
supp($\mathbb{P}_{t,-V}$) bounded
$\Rightarrow$ supp($\mathbb{P}_{t,H_0}$)
bounded **no large fluctuations exist when the interaction is bounded**

2nd law

fluctuation relations
"probability of negative entropy production decays exponentially in time"

Quantum TTM

jumps picture
$V \approx 0 \not\Rightarrow \Delta H_0 \approx 0$
ex:supp($\mathbb{P}_{t,-V}$) and $\mathbb{P}_{t,H_0}$
heavy-tailed
energy transitions induced by the interaction ,large fluctuations may exists even if the interaction is bounded

2nd law

fluctuation relations
picture unchanged
without UV conditions

Entropy and energy fluctuations in non-equilibrium quantum statistical mechanics

Annalisa Panati, CPT, Université de Toulon

Two-time measurment statistics

Conservation laws-energy balance

Classical system $(\mathcal{M}, H, \rho)$

$H = H_0 + V \qquad \rho$ is invariant for the dynamics associated to H_0 (H_0 interpreted as heat)

Energy conservation:

$\triangle H_{0,t} = H_{0,t} - H_0 = -(V_t - V) = (-V)_t - (-V)$ as function on $\mathcal{M}$

In particular if V is bounded by C then $\sup_t |\triangle H_{0,t}| < 2C$ and $supp(\mathbb{P}_{\triangle H_{0,t}})$ bounded

Quantum system $(\mathcal{H}, H, \rho) \qquad H = H_0 + V$

Energy conservation: $H_{0,t} - H_0 = -V_t + V = (-V)_t - (-V)$ as operator on $\mathcal{H}$ yields an identity between all spectral measures but

$$\mathbb{P}_{H_0,t} \neq \mathbb{P}_{-V,t}$$

A priori one can have: $supp(\mathbb{P}_{V,t})$ bounded but

$$\mathbb{E}_t(\phi^{2n}) = \int \phi^{2n} \mathrm{d}\mathbb{P}_{H_0,t}(\phi) = +\infty$$

We want to study the behaviour of $\mathbb{P}_{H_0,t}$ tails