Entropic Fluctuations of Quantum Dynamical Semigroups

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Joint work with V. Jakšić *and* M. Westrich (McGill University)

Quantum Spectra and Transport
Yosi's 65th Birthday
The Hebrew University of Jerusalem — July 2013

1. Background

2. Thermodynamics of QDS

3. Entropic Fluctuations

Statistics of Current Fluctuations – Fluctuation Relations (FR)

Evans, Cohen, Morriss, PRL 71 (1993)

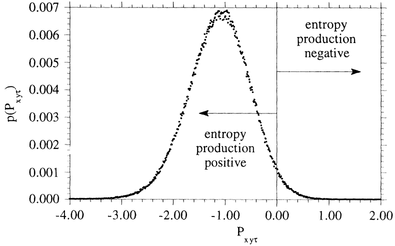

FIG. 1. The probability distribution of segment averages, $\langle P_{xy,i}\rangle_\tau$, of the xy element of the pressure tensor for 56 WCA disks at $H_0/N = 1.560\,32$, $n = 0.8$, a shear rate $\gamma = 0.5$, and a segment time $\tau = 0.1$. For those states where $\langle P_{xy,i}\rangle_\tau = P_{xy\tau}$ is positive the entropy production is negative for a period of time τ, counter to the second law of thermodynamics.

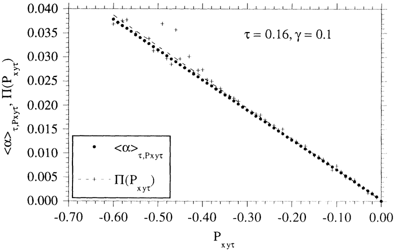

FIG. 2. The logarithmic probability ratio $\Pi(P_{xy\tau})$ and $\langle\alpha\rangle_{\tau,P_{xy\tau}}$ as a function of the segment averaged shear stress $P_{xy\tau} = \langle P_{xy,i}\rangle_\tau$ for $\tau = 0.16$ and $\gamma = 0.1$. As can be seen the two curves are essentially linear [11], with very nearly equal slopes. The agreement between the two slopes becomes progressively better as τ increases. The straight line shows the results of a weighted linear least-squares fit to the logarithmic probability ratio data.

Background 1

Statistics of Current Fluctuations – Fluctuation Relations (FR)

- Transient FR [Evans–Cohen–Morriss '93, Evans–Searles '94+]
- Steady state FR [Gallavotti–Cohen '95]
- FR in stochastic dynamics [Kurchan '98, Lebowitz–Spohn '99]
- FR for Gibbsian measures [Maes '99]

- numerical
- experimental
- theoretical
- mathematical

Including extensions to quantum dynamical systems

- More recent reviews: [Rondoni–Mejia-Monasterio '07, Jakšić–P–Rey-Bellet '11]

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- FR are **structural** (model-independent) properties of dynamical systems
- They are refinements of the **2^{nd} Law of Thermodynamics**
- They reduce to **Fluctuation–Dissipation Relations** (Green-Kubo formula, Onsager reciprocity relations) near equilibrium [Gallavotti '96]

Background 2

Effective Quantum Dynamics of Open Systems (Completely Positive Maps)

Small system $\mathcal{S}$

- Hilbert space $\mathcal{H}_{\mathcal{S}}$(dim $< \infty$)
- Hamiltonian $H_{\mathcal{S}}$
- Observables $\mathcal{O} = \mathcal{B}(\mathcal{H}_{\mathcal{S}})$

Large environment $\mathcal{E}$

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Joint system $\mathcal{S} + \mathcal{R}$

- Hilbert space $\mathcal{H}_\mathcal{S} \otimes \mathcal{H}_\mathcal{E}$
- Coupling $V = \sum_a Q_a \otimes R_a \in \mathcal{O} \otimes \mathcal{A}_\mathcal{E}$
- Hamiltonian $H = H_\mathcal{S} + H_\mathcal{E} + \lambda V$

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$$T_t(X) = \mathrm{tr}_{\mathcal{H}_\mathcal{E}}\left((\mathbb{1} \otimes \rho_\mathcal{E})\mathrm{e}^{\mathrm{i}tH}(X \otimes \mathbb{1})\mathrm{e}^{-\mathrm{i}tH}\right)$$

$$T_t : \mathcal{O}_\mathcal{S} \to \mathcal{O}_\mathcal{S} \text{ is } \mathrm{CP}_\mathbb{1} \quad : \quad \sum_{j,k} Y_j^* T_t(X_j^* X_k) Y_k \geq 0, \qquad T_t(\mathbb{1}) = \mathbb{1}$$

$$\mathrm{tr}(\rho T_t(X)) = \mathrm{tr}\left((\rho \otimes \rho_\mathcal{E})\mathrm{e}^{\mathrm{i}tH}(X \otimes \mathbb{1})\mathrm{e}^{-\mathrm{i}tH}\right)$$

Background 3

Weak Coupling Limit – QDS – Lindbladians

[Davies '74+]

$\{T_t\}_{t\geq 0}$ is **not** a semigroup, but $[H_\mathcal{E}, \rho_\mathcal{E}] = 0$ and suitable **decay of correlations** in $\mathcal{E}$ imply, for any $\tau > 0$ and $X \in \mathcal{O}$,

$$\lim_{\lambda\to 0} \sup_{\lambda^2 t\in[0,\tau]} \| T_t(X) - \mathrm{e}^{t(\mathcal{L}_\mathcal{S}+\lambda^2\mathcal{L})}(X)\| = 0$$

$\mathcal{L}_\mathcal{S} = \mathrm{i}[H_\mathcal{S}, \cdot\,]$ and $\mathcal{L}$ (=**Davies Generator**) generate **QDS** (=$\mathrm{CP}_\mathbb{1}$-semigroup).

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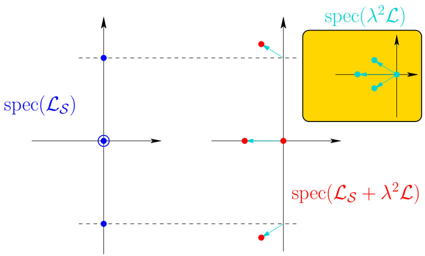

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Remarks.

- For small but finite values of λ
  - [Dereziński–Jakšić '07] To leading order in λ the resonances of the Liouvillian implementing the dynamics of the joint system $\mathcal{S} + \mathcal{E}$ in the GNS representation are given by $\mathrm{spec}(\mathcal{L}_{\mathcal{S}} + \lambda^2 \mathcal{L})$.
  - [de Roeck '07] Systematic expansion of T_t around its leading contribution $\mathrm{e}^{t(\mathcal{L}_{\mathcal{S}} + \lambda^2 \mathcal{L})}$.
- [Dereziński–de Roeck '08] Extended weak coupling limit.
- Scaling limits in extended systems $\Longrightarrow$ Boltzmann and diffusion equations
  - [Erdös–Salmhofer–Yau '02+]
  - [de Roeck–Fröhlich–Pizzo '10+]

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[Lindblad, Gorini–Kossakowski–Sudarshan '76]

Structure of QDS-generators (**Lindbladians**)

$$\mathcal{L}(X) = \mathrm{i}[T, X] + \Phi(X) - \frac{1}{2}\{\Phi(\mathbb{1}), X\}$$

$T = T^* \in \mathcal{O}$ and $\Phi : \mathcal{O} \to \mathcal{O}$ a CP-map.

Remark. T and Φ are uniquely determined if one imposes the conditions $\mathrm{tr}(T) = 0$ and $\mathrm{tr}(\Phi) = 0$.

Thermal Equilibrium & Detailed Balance

Let ρ be a faithful state on $\mathcal{O}$ (strictly positive density matrix)

Hilbert space structures on $\mathcal{O}$ & dualities

$$\langle X|Y\rangle = \mathrm{tr}(X^* Y) \quad \langle X|\mathcal{F}(Y)\rangle = \langle \mathcal{F}^*(X)|Y\rangle$$

$$\langle X|Y\rangle_\rho = \mathrm{tr}(\rho X^* Y) \quad \langle X|\mathcal{F}(Y)\rangle_\rho = \langle \mathcal{F}^\rho(X)|Y\rangle_\rho$$

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[Kossakowski–Frigerio–Gorini–Verri '77]

Lindbladian $\mathcal{L} = \mathrm{i}[T,\cdot\,] + \Phi - \frac{1}{2}\{\Phi(\mathbb{1}),\cdot\,\} \in \mathrm{DB}(\rho)$ if it satisfies **detailed balance** w.r.t. ρ:

$$\mathcal{L}^*(\rho) = 0 \text{ and } \Phi^\rho = \Phi$$

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$\mathcal{L} \in \mathrm{DB}(\rho)$ implies that ρ is a **steady state** of the QDS $\mathrm{e}^{t\mathcal{L}}$

$$\mathrm{tr}(\rho \mathrm{e}^{t\mathcal{L}}(X)) = \langle \rho|\mathrm{e}^{t\mathcal{L}}(X)\rangle = \langle \mathrm{e}^{t\mathcal{L}^*}(\rho)|X\rangle = \langle \rho|X\rangle = \mathrm{tr}(\rho X)$$

for all $t \geq 0$ and $X \in \mathcal{O}$.

Equilibrium Thermodynamics

Example: The Davies Generator at Equilibrium

If $\rho_{\mathcal{E}}$ is a thermal equilibrium state at inverse temperature $\beta = (k_{\rm B} T)^{-1}$ then the Davies generator

$$\mathcal{L}(X) = \mathrm{i}[T, X] + \Phi(X) - \frac{1}{2}\{\Phi(\mathbb{1}), X\}$$

satisfies

$$\mathcal{L} \in \mathrm{DB}\left(\frac{\mathrm{e}^{-\beta H_{\mathcal{S}}}}{\mathrm{tr}(\mathrm{e}^{-\beta H_{\mathcal{S}}})}\right)$$

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$$T = \sum_{a,b} \sum_{\omega \in \mathrm{spec}(\mathrm{i}\mathcal{L}_{\mathcal{S}})} s_{ab}(\omega) Q_a^{(\omega)*} Q_b^{(\omega)}, \quad \Phi(X) = \sum_{a,b} \sum_{\omega \in \mathrm{spec}(\mathrm{i}\mathcal{L}_{\mathcal{S}})} h_{ab}(\omega) Q_a^{(\omega)*} X Q_b^{(\omega)}$$

where

$$h_{ab}(\omega) = 2\,\mathrm{Im}\,\mathrm{tr}\left(\rho_{\mathcal{E}} R_a (H_{\mathcal{E}} - \omega - \mathrm{i}0)^{-1} R_b\right), \qquad s_{ab}(\omega) = \mathrm{Re}\,\mathrm{tr}\left(\rho_{\mathcal{E}} R_a (H_{\mathcal{E}} - \omega - \mathrm{i}0)^{-1} R_b\right)$$

$$Q_a^{(\omega)} = P_\omega(\mathrm{i}\mathcal{L}_{\mathcal{S}})(Q_a) = \sum_{\mu - \nu = \omega} P_\nu(H_{\mathcal{S}}) Q_a P_\mu(H_{\mathcal{S}})$$

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[Spohn '77]

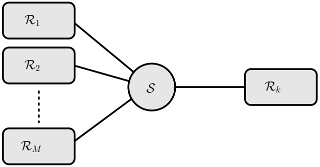
$$\{H_{\mathcal{S}}, Q_a\}' = \mathbb{C}\mathbb{1}, \qquad [h_{ab}(\omega)] > 0 \text{ for all } \omega \in \mathrm{spec}(\mathrm{i}\mathcal{L}_{\mathcal{S}})$$

imply that the QDS $\mathrm{e}^{t\mathcal{L}}$ is positivity improving. It follows that $\mathrm{Ker}(\mathcal{L}) = \mathbb{C}\mathbb{1}$ and

for any state ρ, $\lim_{t\to\infty} \mathrm{e}^{t\mathcal{L}^*}(\rho) = \frac{\mathrm{e}^{-\beta H_{\mathcal{S}}}}{\mathrm{tr}(\mathrm{e}^{-\beta H_{\mathcal{S}}})} =$ the unique state in $\mathrm{Ker}(\mathcal{L}^*)$

QDS for Open Systems Out of Equilibrium

[Lebowitz-Spohn '78]



- $\mathcal{E} = \mathcal{R}_1 + \cdots + \mathcal{R}_M$
- $\mathcal{R}_k$ in thermal equilibrium at inverse temperature β_k
- $V = \sum_{k,a} Q_{k,a} \otimes R_{k,a}$, $Q_{k,a} \otimes R_{k,a} \in \mathcal{O} \otimes \mathcal{A}_{\mathcal{R}_k}$
- Davies generator $\mathcal{L} = \sum_k \mathcal{L}_k$
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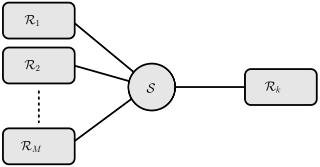

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- $\mathcal{L}_k \in \mathrm{DB}\left(\rho_k = \mathrm{e}^{-\beta_k H_\mathcal{S}} / \mathrm{tr}(\mathrm{e}^{-\beta_k H_\mathcal{S}})\right)$

- Under Spohn's Conditions $\dim \mathrm{Ker}(\mathcal{L}) = 1$ and $\mathrm{Ker}(\mathcal{L}^*)$ contains a unique **NESS** ρ_+, s.t. for any state ρ on $\mathcal{O}$

$$\lim_{t\to\infty} \mathrm{e}^{t\mathcal{L}^*}(\rho) = \rho_+$$

- The **Heat/Entropy flux** observable

$$\phi_k = \mathcal{L}_k(H_\mathcal{S}), \qquad \psi_k = \mathcal{L}_k(-\log \rho_k) = \beta_k \phi_k$$

  describes the energy/entropy current out of heat reservoir $\mathcal{R}_k$
- **1st Law**:

$$\sum_k \mathrm{tr}(\rho_+ \phi_k) = \langle \rho_+ | \mathcal{L}(H_\mathcal{S}) \rangle = \langle \mathcal{L}^*(\rho_+) | H_\mathcal{S} \rangle = 0$$

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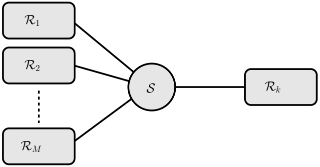

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- The von Neumann entropy $S(\rho) = -\mathrm{tr}(\rho \log \rho)$ satisfies the balance equation

$$\frac{\mathrm{d}}{\mathrm{d}t} S(\mathrm{e}^{t\mathcal{L}^*}(\rho))\Big|_{t=0} = \underbrace{\sigma(\rho)}_{\textbf{entropy production}} + \underbrace{j(\rho)}_{\textbf{entropy current}}$$

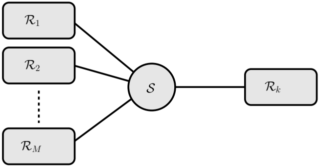
- Entropy current is $j(\rho) = \sum_k \mathrm{tr}(\rho\psi_k)$
- Entropy production $\sigma(\rho)$ is a non-negative lsc convex function of ρ
- In the NESS

$$\sigma(\rho_+) = -j(\rho_+) = -\sum_k \mathrm{tr}(\rho_+\psi_k) > 0$$

Nonequilibrium Thermodynamics

QDS for Open Systems Out of Equilibrium

[Lebowitz-Spohn '78]



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- $\sigma(\rho) = 0 \Longleftrightarrow \beta_1 = \cdots = \beta_M = \beta_{\mathrm{eq}}$ and $\rho = \rho_{\mathrm{eq}} = \mathrm{e}^{-\beta_{\mathrm{eq}} H_{\mathcal{S}}} / \mathrm{tr}(\mathrm{e}^{-\beta_{\mathrm{eq}} H_{\mathcal{S}}})$
- $\beta_1 = \cdots = \beta_M = \beta_{\mathrm{eq}} \Longrightarrow \rho_+ = \rho_{\mathrm{eq}}$
- The Onsager matrix

$$L_{jk} = \frac{\partial}{\partial \beta_k} \mathrm{tr}(\rho_+ \phi_j)\Big|_{\beta_1 = \cdots = \beta_M = \beta_{\mathrm{eq}}}$$

satisfies Green-Kubo (fluctuation–dissipation) relation

$$L_{jk} = \int_0^\infty \mathrm{tr}\left(\rho_{\mathrm{eq}} \mathrm{e}^{t\mathcal{L}}(\phi_j)\phi_k\right) \mathrm{d}t \quad (j \neq k)$$

- Time reversal invariance implies Onsager's reciprocity relations

$$L_{jk} = L_{kj}$$

Entropic Fluctuations

Let $\mathcal{L} = \sum_k \mathcal{L}_k$ with $\mathcal{L}_k \in \mathrm{DB}(\rho_k)$ and for $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_M) \in \mathbb{R}^M$ set

$$\mathcal{L}_{\boldsymbol{\alpha}}(X) = \sum_k \mathcal{L}_k(X\rho_k^{-\alpha_k})\rho_k^{\alpha_k}$$

Theorem 1. [de Roeck, Maes, Dereziński, Jakšić–P–Westrich]

Assume that the QDS $\mathrm{e}^{t\mathcal{L}}$ is positivity improving (e.g., that Spohn's criterion holds).

- For all $\boldsymbol{\alpha} \in \mathbb{R}^M$, $\mathrm{e}^{t\mathcal{L}_{\boldsymbol{\alpha}}}$ is a positivity improving CP-semigroup.
- For all $\boldsymbol{\alpha} \in \mathbb{R}^M$, $e(\boldsymbol{\alpha}) = \max \mathrm{Re}(\mathrm{spec}(\mathcal{L}_{\boldsymbol{\alpha}}))$ is a simple eigenvalue of $\mathcal{L}_{\boldsymbol{\alpha}}$ and its only eigenvalue on the line $\mathrm{Re}(z) = e(\boldsymbol{\alpha})$.
- For any state ρ there exists a probability measure P_ρ^t on $\mathbb{R}^M$ such that

$$\mathrm{tr}\left(\rho \mathrm{e}^{t\mathcal{L}_{\boldsymbol{\alpha}}}(\mathbb{1})\right) = \int_{\mathbb{R}^M} \mathrm{e}^{-t\boldsymbol{\alpha}\cdot\boldsymbol{\varsigma}} \mathrm{d}P_\rho^t(\boldsymbol{\varsigma})$$

- $e(\boldsymbol{\alpha})$ is a real-analytic convex function of $\boldsymbol{\alpha}$ and

$$\lim_{t\to\infty} \frac{1}{t} \log \int_{\mathbb{R}^M} \mathrm{e}^{-t\boldsymbol{\alpha}\cdot\boldsymbol{\varsigma}} \mathrm{d}P_\rho^t(\boldsymbol{\varsigma}) = e(\boldsymbol{\alpha})$$

holds for $\boldsymbol{\alpha}$ in a complex neighborhood of $\mathbb{R}^M$.

Entropic Fluctuations

Unraveling – Quantum Trajectories

$$\mathcal{L}_k = \mathcal{L}_{k,\text{no jumps}} + \Phi_k, \qquad \mathcal{L}_{k,\text{no jumps}} = \mathrm{i}[T_k, \cdot\,] - \frac{1}{2}\{\Phi_k(\mathbb{1}), \cdot\,\}$$

Detailed balance ($\mathcal{L}_k \in \mathrm{DB}(\rho_k)$) implies the **spectral decomposition**

$$\Phi_k = \sum_{\omega \in \Omega_k} \Phi_{k,\omega}, \qquad \Phi_{k,\omega}(X\rho_k^{-\alpha})\rho_k^{\alpha} = \mathrm{e}^{-\alpha\omega}\Phi_{k,\omega}(X)$$

with $\Omega_k = \mathrm{spec}(\log \rho_k) - \mathrm{spec}(\log \rho_k)$ (=spectrum of the modular group of ρ_k)

Set $\mathcal{L}_{\text{no jumps}} = \sum_k \mathcal{L}_{k,\text{no jumps}}$

The Dyson expansion of $\mathrm{e}^{t\mathcal{L}_{\boldsymbol{\alpha}}}$ around $\mathrm{e}^{t\mathcal{L}_{\text{no jumps}}}$ leads to

$$\langle \rho | \mathrm{e}^{t\mathcal{L}_{\boldsymbol{\alpha}}}(\mathbb{1})\rangle = \int \mathrm{e}^{-t\sum_j \alpha_j \varsigma_j(\xi)} \mathrm{d}\mu_\rho^t(\xi)$$

where μ_ρ^t is a probability measure on the set of **Quantum Trajectories** $\xi = [\xi_1, \ldots, \xi_N]$

$$N \in \mathbb{N}, \xi_k = (j_k, \omega_k, s_k), j_k \in \{1, \ldots, M\}, \omega_k \in \Omega_k, 0 \le s_1 \le \cdots \le s_N \le t$$

P_ρ^t is the joint distribution of the RV $\varsigma_j(\xi) = t^{-1}\sum_{k:j_k=j} \omega_k$ under μ_ρ^t

Entropic Fluctuations

Full Counting Statistics

Let $\mathcal{L}$ be a Davies generator ($\rho_k = \mathrm{e}^{-\beta_k \mathcal{H}_\mathcal{S}}/\mathrm{tr}(-)$) and $\Pi_\mathbf{s}$ denote the joint spectral projection of $\mathbf{S} = (\beta_1 H_{\mathcal{R}_1}, \ldots, \beta_M H_{\mathcal{R}_M})$ for **finite reservoirs**. The Positive Operator Valued Measure

$$A \subset \mathrm{spec}(\mathbf{S}) \times \mathrm{spec}(\mathbf{S}) \mapsto \mathcal{P}_A(\,\cdot\,) = \sum_{(\mathbf{s},\mathbf{s}')\in A} \Pi_{\mathbf{s}'}\mathrm{e}^{-\mathrm{i}tH}\Pi_\mathbf{s}(\,\cdot\,)\Pi_\mathbf{s}\mathrm{e}^{\mathrm{i}tH}\Pi_{\mathbf{s}'}$$

describes two sets of subsequent measurements of the reservoir energies separated by a time interval t.

Full Counting Statistics of entropy transport = thermodynamic limit of the measure

$$\mathbb{P}_\rho^t(\varsigma) = \mathrm{tr}\left(\mathcal{P}_{\{(\mathbf{s},\mathbf{s}')\,|\,\mathbf{s}'-\mathbf{s}=t\varsigma\}}(\rho \otimes \rho_{\mathcal{R}_1} \otimes \cdots \otimes \rho_{\mathcal{R}_M})\right)$$

The measure P_ρ^t of Theorem 1 is the **weak coupling limit** of FCS

$$\int f(\varsigma)\mathrm{d}P_\rho^t(\varsigma) = \lim_{\lambda\to 0}\int f(\lambda^{-2}\varsigma)\mathrm{d}\mathbb{P}_\rho^{t\lambda^{-2}}(\varsigma)$$

Entropic Fluctuations

LDP – CLT

Theorem 1 + Gärtner–Ellis $\Longrightarrow$ **Large Deviation Principle**

$$P_\rho^t(\Sigma) \simeq \exp\left(-t \inf_{\varsigma\in\Sigma} I(\varsigma)\right) \qquad (\Sigma \subset \mathbb{R}^M, t \to \infty)$$

with rate function

$$I(\varsigma) = -\inf_{\boldsymbol{\alpha}\in\mathbb{R}^M}(\boldsymbol{\alpha}\cdot\varsigma + e(\boldsymbol{\alpha}))$$

Theorem 1 + Bryc $\Longrightarrow$ **Central Limit Theorem**

$$\lim_{t\to\infty} P_\rho^t\left(\left\{\varsigma \,\middle|\, \sqrt{t}(\varsigma - \langle\varsigma\rangle_\rho^t) \in A\right\}\right) = \mu_D(A)$$

centered Gaussian on $\mathbb{R}^M$ with covariance

$$D_{ij} = \left.\frac{\partial^2 e(\boldsymbol{\alpha})}{\partial\alpha_i\partial\alpha_j}\right|_{\boldsymbol{\alpha}=0}$$

Fluctuation Relations

Theorem 2

If **Time-Reversal Invariance** holds ($\mathcal{L}_k \circ \Theta = \Theta \circ \mathcal{L}_k^{\rho_k}$, $\Theta^*(\rho_k) = \rho_k$) then

$$e(\mathbf{1} - \boldsymbol{\alpha}) = e(\boldsymbol{\alpha}), \qquad e(\boldsymbol{\alpha} + \kappa \boldsymbol{\beta}^{-1}) = e(\boldsymbol{\alpha})$$

with $\mathbf{1} = (1, \ldots, 1)$, $\boldsymbol{\beta}^{-1} = (\beta_1^{-1}, \ldots, \beta_M^{-1})$ and for any $\boldsymbol{\alpha} \in \mathbb{R}^M$ and $\kappa \in \mathbb{R}$.

- The first identity is the **Evans–Searles symmetry**. It implies $I(-\varsigma) = I(\varsigma) + \mathbf{1} \cdot \varsigma$, i.e.,

$$\frac{P_\rho^t(\varsigma = -\mathbf{s})}{P_\rho^t(\varsigma = \mathbf{s})} \simeq \mathrm{e}^{-t \sum_k s_k}$$

- The translation symmetry displayed in the second identity is a consequence of energy conservation [Andrieux et al., '09]. It implies that the rate function enforces the **1st Law**

$$I(\varsigma) = +\infty \text{ unless } \boldsymbol{\beta}^{-1} \cdot \varsigma = 0$$

and that the Gaussian measure μ_D is concentrated on the hyperplane $\boldsymbol{\beta}^{-1} \cdot \varsigma = 0$.

Linear Response Theory à la Gallavotti

Theorem 3

- The expected heat/entropy fluxes in the NESS are given by

$$\mathrm{tr}(\rho_+\phi_j) = \frac{1}{\beta_j}\frac{\partial e(\boldsymbol{\alpha})}{\partial \alpha_j}\bigg|_{\boldsymbol{\alpha}=0}, \qquad \mathrm{tr}(\rho_+\psi_j) = \frac{\partial e(\boldsymbol{\alpha})}{\partial \alpha_j}\bigg|_{\boldsymbol{\alpha}=0} \tag{1}$$

- If time-reversal invariance holds then the Onsager matrix is given by

$$L_{jk} = \partial_{\beta_k}\mathrm{tr}(\rho_+\phi_j)\big|_{\boldsymbol{\beta}=\beta_{\mathrm{eq}}\mathbf{1}} = -\frac{1}{2\beta_{\mathrm{eq}}^2}\frac{\partial^2 e(\boldsymbol{\alpha})}{\partial\alpha_k\partial\alpha_j}\bigg|_{\boldsymbol{\beta}=\beta_{\mathrm{eq}}\mathbf{1},\boldsymbol{\alpha}=0} \tag{2}$$

- Combining the two symmetries of Theorem 2, Relation (1) gives

$$\mathrm{tr}(\rho_+\phi_j) = \frac{1}{\beta_j}(\partial_{\alpha_j}e)(0) = -\frac{1}{\beta_j}(\partial_{\alpha_j}e)(1-\beta_{\mathrm{eq}}\boldsymbol{\beta}^{-1})$$

  and (2) follows from differentiation w.r.t. β_k at $\boldsymbol{\beta} = \beta_{\mathrm{eq}}\mathbf{1}$.
- The Green–Kubo formula follows from direct evaluation of the right hand side of (2).

Main Ingredients of the Proofs of Theorem 1 & 2

Non-Commutative Perron-Frobenius Theory

Theorem 4. $\Longleftarrow$ [Evans–Høegh-Krohn '78, Schrader '01]

If the CP semigroup $\mathrm{e}^{t\mathcal{L}}$ is positivity improving and $\ell = \max \mathrm{Re}(\mathrm{spec}(\mathcal{L}))$ then

- ℓ is a simple eigenvalue of $\mathcal{L}$, and the only one on the line $\mathrm{Re}z = \ell$.
- For any state ρ and any non-zero $X \geq 0$

$$\ell = \lim_{t\to\infty} \frac{1}{t} \log \mathrm{tr}\left(\rho \mathrm{e}^{t\mathcal{L}}(X)\right)$$

- If $\mathcal{L}(\mathbb{1}) = 0$ then $\ell = 0$ and there is a faithful state $\rho_+ \in \mathrm{Ker}(\mathcal{L}^*)$ such that

$$\left|\mathrm{tr}\left(\rho \mathrm{e}^{t\mathcal{L}}(X)\right) - \mathrm{tr}(\rho_+ X)\right| \leq C\mathrm{e}^{-\gamma t}\|X\|$$

for some constants C, $\gamma > 0$, all states ρ and all $X \in \mathcal{O}$.

Structural properties of CP semigroups

- $\mathcal{L}_k \in \mathrm{DB}(\rho_k) \Longrightarrow \mathcal{L}_k$ commutes with the modular group of ρ_k
- Time reversal invariance $\Longrightarrow \mathcal{L}_{\boldsymbol{\alpha}} \circ \Theta = \Theta \circ \mathcal{L}^*_{\mathbf{1}-\boldsymbol{\alpha}}$
- $\mathrm{e}^{\kappa H_{\mathcal{S}}/2}\mathcal{L}_{\boldsymbol{\alpha}}(X)\mathrm{e}^{\kappa H_{\mathcal{S}}/2} = \mathcal{L}_{\boldsymbol{\alpha}+\kappa\boldsymbol{\beta}^{-1}}(\mathrm{e}^{\kappa H_{\mathcal{S}}/2} X \mathrm{e}^{\kappa H_{\mathcal{S}}/2})$
- Elementary calculations

Happy Birthday Yosi !