Jacobi Matrices and Non-Equilibrium Statistical Mechanics of XY-Chains

V. Jaksic, B. Landon, C-A. Pillet
McGill University, Université de Toulon

June 30, 2013

- Research program:

  Entropic fluctuations in quantum statistical mechanics.

- Part of a larger program:

  Large deviations in non-commutative setting (quantum probability).

- This talk:

  Entropic fluctuations and large deviations for XY-chains and their link with spectral/scattering theory of Jacobi matrices.

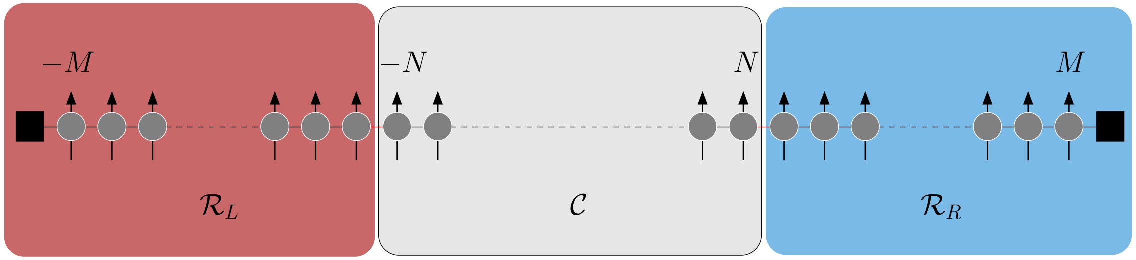
XY–CHAIN OUT OF EQUILIBRIUM

$\Lambda = [A, B] \subset \mathbb{Z}$, Hilbert space $\mathcal{H}_\Lambda = \bigotimes_{x\in\Lambda} \mathbb{C}^2$.
Hamiltonian

$$H_\Lambda = \frac{1}{2} \sum_{x\in[A,B[} J_x \left(\sigma_x^{(1)} \sigma_{x+1}^{(1)} + \sigma_x^{(2)} \sigma_{x+1}^{(2)} \right)$$

$$+ \frac{1}{2} \sum_{x\in[A,B]} \lambda_x \sigma_x^{(3)}.$$

$$\sigma_x^{(1)} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_x^{(2)} = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix}, \quad \sigma_x^{(3)} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$



Central part $\mathcal{C}$: XY-chain on $\Lambda_{\mathcal{C}} = [-N, N]$.

Two reservoirs $\mathcal{R}_{L/R}$: XY-chains on $\Lambda_L = [-M, -N-1]$ and $\Lambda_R = [N+1, M]$. N fixed, thermodynamic limit $M \to \infty$.

Decoupled Hamiltonian $H_0 = H_{\Lambda_L} + H_{\Lambda_{\mathcal{C}}} + H_{\Lambda_R}$.

The full Hamiltonian is

$$H = H_{\Lambda_L \cup \Lambda_{\mathcal{C}} \cup \Lambda_R} = H_0 + V_L + V_R,$$

$$V_L = \frac{J_{-N-1}}{2}\left(\sigma^{(1)}_{-N-1}\sigma^{(1)}_{-N} + \sigma^{(2)}_{-N-1}\sigma^{(2)}_{-N}\right), \text{ etc.}$$

Initial state:

$$\rho = \mathrm{e}^{-\beta_L H_{\Lambda_L}} \otimes \rho_{\mathcal{C}} \otimes \mathrm{e}^{-\beta_R H_{\Lambda_R}} \Big/ Z,$$

$\rho_{\mathcal{C}} = \mathbf{1}/\dim \mathcal{H}_{\Lambda_{\mathcal{C}}}$. Fluxes and entropy production:

$$\Phi_{L/R} = -\mathrm{i}[H, H_{L/R}], \qquad \sigma = -\beta_L \Phi_L - \beta_R \Phi_R.$$

Steady state entropy flux:

$$\langle \sigma \rangle_+ = \lim_{T\to\infty} \lim_{M\to\infty} \frac{1}{T} \int_0^T \mathrm{tr}(\rho \mathrm{e}^{\mathrm{i}tH} \sigma \mathrm{e}^{-\mathrm{i}tH}) \mathrm{d}t.$$

Araki-Ho, Ashbacher-Pillet $\sim$ 2000, J-Landon-Pillet 2012:

$$\langle \sigma \rangle_+ = \frac{\Delta\beta}{4\pi} \int_{\mathbb{R}} |T(E)|^2 \frac{E \sinh(\Delta\beta E)}{\cosh \frac{\beta_L E}{2} \cosh \frac{\beta_R E}{2}} \mathrm{d}E > 0.$$

$\langle \sigma \rangle_+ = \Delta\beta \langle \Phi_L \rangle_+ = -\Delta\beta \langle \Phi_R \rangle_+$, $\Delta\beta = \beta_L - \beta_R$.

Beyond ”law of large numbers”: Fluctuations (CLT and LDP).

FLUCTUATIONS

Cummulant generating functions: $\dfrac{1}{t}\displaystyle\int_0^t \sigma_s \mathrm{d}s$, $\sigma_t = \mathrm{e}^{\mathrm{i}tH}\sigma\mathrm{e}^{-\mathrm{i}tH}$.

(I) (Evans-Searles) Fluctuations with respect to the initial state:

$$C_t(\alpha) = \lim_{M\to\infty} \log \mathrm{tr}\left(\rho \mathrm{e}^{-\alpha\int_0^t \sigma_s \mathrm{d}s}\right) = \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \varsigma} \mathrm{d}P_t(\varsigma).$$

(II) (Gallavotti-Cohen) Steady state fluctuations: $\rho_t = \mathrm{e}^{-\mathrm{i}tH}\rho\mathrm{e}^{\mathrm{i}tH}$.

$$C_{t+}(\alpha) = \lim_{T\to\infty} \lim_{M\to\infty} \log \mathrm{tr}\left(\rho_T \mathrm{e}^{-\alpha\int_0^t \sigma_s \mathrm{d}s}\right)$$
$$= \log \int_{\mathbb{R}} \mathrm{e}^{-\alpha t \varsigma} \mathrm{d}P_{t+}(\varsigma)$$

$$C_t(\alpha) = \log \omega\left(\mathrm{e}^{-\alpha\int_0^t \sigma_s \mathrm{d}s}\right), \qquad C_{t+}(\alpha) = \log \omega_+\left(\mathrm{e}^{-\alpha\int_0^t \sigma_s \mathrm{d}s}\right).$$

$P_{t/t+}$ is the spectral measure for ω/ω_+ and $\frac{1}{t}\int_0^t \sigma_s \mathrm{d}s$.

(III) Full counting statistics.

$$F_t(\alpha) = \lim_{M\to\infty} \log \mathrm{tr}\left(\mathrm{e}^{(1-\alpha)\log\rho}\mathrm{e}^{\alpha\log\rho_t}\right) = \log\int_{\mathbb{R}} \mathrm{e}^{-\alpha t\varsigma}\mathrm{d}\mathbb{P}_t(\varsigma).$$

The statistics of the repeated measurement of

$$S = -\log\rho = \beta_L H_{\Lambda_L} + \beta_R H_{\Lambda_R}.$$

Remarks.

$$C_t(\alpha) = \lim_{M\to\infty} \log \mathrm{tr}\left(\mathrm{e}^{\log\rho}\mathrm{e}^{\alpha(\log\rho_t - \log\rho)}\right).$$

Host of other entropic functionals:

$$\log \mathrm{tr}\left(\mathrm{e}^{\frac{1-\alpha}{p}\log\rho}\mathrm{e}^{\frac{2\alpha}{p}\log\rho_t}\mathrm{e}^{\frac{1-\alpha}{p}\log\rho}\right)^{p/2}.$$

Theorem.

(1)

$$C(\alpha) = \lim_{t\to\infty} \frac{1}{t} C_t(\alpha) = \lim_{t\to\infty} \frac{1}{t} C_{t+}(\alpha)$$
$$= \int_{\mathbb{R}} \log\left(\frac{\det(1 + K_\alpha(E))}{\det(1 + K_0(E))}\right) \frac{\mathrm{d}E}{2\pi},$$

$$K_\alpha(E) = \mathrm{e}^{k_0(E)/2} \mathrm{e}^{\alpha(s^*(E)k_0(E)s(E) - k_0(E))} \mathrm{e}^{k_0(E)/2},$$

$$k_0(E) = \begin{bmatrix} -\beta_L E & 0 \\ 0 & -\beta_R E \end{bmatrix}, \; s(E) = \begin{bmatrix} A(E) & T(E) \\ T(E) & B(E) \end{bmatrix}$$

$s(E)$ is unitary.

(2)

$$F(\alpha) = \lim_{t\to\infty} \frac{1}{t} F_t(\alpha) = \int_{\mathbb{R}} \log\left(\frac{\det(1+\widehat{K}_\alpha(E))}{\det(1+\widehat{K}_0(E))}\right)\frac{\mathrm{d}E}{2\pi},$$

$$\widehat{K}_\alpha(E) = \mathrm{e}^{k_0(E)(1-\alpha)/2} s(E) \mathrm{e}^{k_0(E)\alpha} s^*(E) \mathrm{e}^{k_0(E)(1-\alpha)/2}.$$

(3) The functions $C(\alpha), F(\alpha)$ are real-analytic, strictly convex, $C(0) = F(0) = 0$,

$$C'(0) = F'(0) = -\langle\sigma\rangle_+$$

(4)

$$C''(0) = F''(0) = \frac{1}{2}\int_{-\infty}^{\infty} \Big\langle (\sigma_t - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+) \Big\rangle_+ \mathrm{d}t.$$

(5) The CLT holds. For any Borel set $B \subset \mathbb{R}$, let

$$B_t = \{\varsigma \,|\, \sqrt{t}(\varsigma - \langle\sigma\rangle_+) \in B\}.$$

Then

$$\lim_{t\to\infty} P_t(B_t) = \lim_{t\to\infty} \mathbb{P}_{t+}(B_t) = \frac{1}{\sqrt{2\pi D}} \int_B \mathrm{e}^{-\varsigma^2/2D} \mathrm{d}\varsigma,$$

where $D = C''(0) = F''(0)$.

(6) Quantum ES-GC symmetry.

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

$F(1) = 0$

(7) $C(\alpha) = F(\alpha)$ iff $|T(E)| \in \{0, 1\}$ for a.e. E (reflectionless). Otherwise $C(1) > 0$.
Phenomenon: ”Entropic triviality.”

LARGE DEVIATIONS

$P_{t/t_+} \to \delta_{\langle\sigma\rangle_+}$, $\mathbb{P}_t \to \delta_{\langle\sigma\rangle_+}$. Gärtner-Ellis theorem.

$$P_t(B) \simeq P_{t+}(B) \simeq \mathrm{e}^{-t\,\inf_{\varsigma\in B} I(\varsigma)},$$
$$\mathbb{P}_t(B) \simeq \mathrm{e}^{-t\,\inf_{\varsigma\in B} \mathbb{I}(\varsigma)}$$

$$I(\varsigma) = -\inf_{\alpha\in\mathbb{R}^M} (\alpha\cdot\varsigma + C(\alpha)),$$
$$\mathbb{I}(\varsigma) = -\inf_{\alpha\in\mathbb{R}^M} (\alpha\cdot\varsigma + F(\alpha)).$$

Fluctuation Relation: $F(\alpha) = F(1-\alpha)$ implies

$$\mathbb{I}(-\varsigma) = \varsigma + \mathbb{I}(\varsigma).$$

For large t,

$$\frac{\mathbb{P}_t(\{\varsigma\in\mathbb{R}\,|\,\varsigma\simeq-\varphi\})}{\mathbb{P}_t(\{\varsigma\in\mathbb{R}\,|\,\varsigma\simeq\varphi\})} \simeq \mathrm{e}^{-t\varphi}.$$

JACOBI MATRIX

The Jacobi matrix of our XY chain is

$$(hu)(x) = J_x u(x+1) + J_{x-1}u(x-1) + \lambda_x u(x).$$

Our main theorem holds under the assumption:

h **has purely absolutely continuous spectrum**

The matrix $s(E)$ arises through the scattering theory of h.

$$h_0 = h_L + h_{\mathcal{C}} + h_R,$$

$$\ell^2(\mathbb{Z}) = \ell^2(]-\infty, -N-1]) \oplus \ell^2([-N, N]) \oplus \ell^2([N+1, \infty[),$$

$$h = h_0 + v_L + v_R,$$

$$v_L = J_{-N-1}(|\delta_{-N-1}\rangle\langle\delta_{-N}| + \text{h.c}), \;\; v_R = J_N(|\delta_{N+1}\rangle\langle\delta_N| + \text{h.c})$$

The wave operators

$$w^{\pm} = \mathrm{s}-\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}th}\mathrm{e}^{-\mathrm{i}th_0}\mathbf{1}_{\mathrm{ac}}(h_0)$$

exist and are complete.

The scattering matrix:

$$s = w_+^* w_- : \mathcal{H}_{\mathrm{ac}}(h_0) \to \mathcal{H}_{\mathrm{ac}}(h_0),\ s(E) = \begin{bmatrix} A(E) & T(E) \\ T(E) & B(E) \end{bmatrix}.$$

$$T(E) = \frac{2\mathrm{i}}{\pi} J_{-N-1} J_N \langle \delta_N | (h - E - \mathrm{i}0)^{-1} \delta_{-N} \rangle \sqrt{F_L(E) F_R(E)}$$

$$F_{L/R}(E) = \mathrm{Im}\, \langle \delta_{L/R} | (h_{L/R} - E - \mathrm{i}0)^{-1} \delta_{L/R} \rangle,$$

$\delta_L = \delta_{-N-1}$, $\delta_R = \delta_{N+1}$.

h is reflectionless iff $|T(E)| \in \{0, 1\}$ for a.e. E.
Examples: Volberg-Yuditskii 2002.

ON THE NOTION OF REFLECTIONLESS

h is reflectionless on a Borel set $B \subset \mathbb{R}$ iff for all x,

$$\text{Re}\,\langle \delta_x | (h - E - \text{i}0)^{-1} \delta_x \rangle = 0 \text{ for a.e. } E \in B.$$

Remling 2011. Notions of reflectionless:

Measure-theoretic $\Leftrightarrow$ Spectral $\Leftrightarrow$ Dynamical

Breuer-Ryckman-Simon 2010.
Stationary scattering reflectionless (J-Landon-Panati):

$$|T(E)| = 1 \text{ for a.e. } E \in B.$$

Equivalent to the above + a simpler proof of Breuer-Ryckman-Simon result.
Open problem: $J_x = const$, pure ac spectrum and not reflectionless.

REMARKS

The fluctuation relations are structural model independent features of classical non-equilibrium statistical mechanics (Evans-Searles, Gallavotti-Cohen). They can be viewed as a refinement of the second law of thermodynamics. In the linear regime near equilibrium the fluctuation relations reduce to familiar fluctuation-dissipation formulae (Green-Kubo, Onsager). During the last decade (starting with works of Kurchan and Tasaki-Matsui) the fluctuation relation have been extended to quantum domain. The extension led to novel entropic functionals (most notable of which is full counting statistics), a novel large deviation theory, and a deep link with modular theory of operator algebras. The results described in this talk concern a simple but instructive example of non-equilibrium XY-chains that allows for a sharp differentiation between the ”naive” quantization and the ”full counting statistics” quantization.