Entropic fluctuations in XY chains and reflectionless Jacobi matrices[1]

Benjamin Landon[2]
Joint work with V. Jakšić[2] and C.-A. Pillet[3]

[2]McGill University
Department of Mathematics and Statistics
[3]Aix-Marseille Université, CNRS UMR 7332, CPT, Marseille
Université du Sud Toulon-Var, CNRS UMR 7332, CPT, La Garde

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Fluctuations in classical statistical mechanics

- Modern fluctuation theorems begin with the works [ECM '93], [ES '94]. They study violations of the second law of thermodynamics in a deterministic system of classical particles.
- Find:

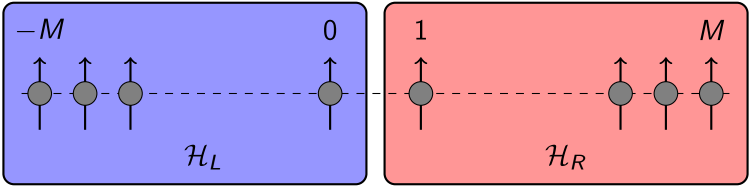
$$\frac{P_t(-\phi)}{P_t(\phi)} = e^{-t\phi},$$

  where $P_t(\phi)$ is the probability of measuring a change of entropy of ϕ over a time interval t.
- Universal; consequence of TRI - see [JPR '11].
- Equivalently, $\mathcal{E}_t(\alpha) = \mathcal{E}_t(1-\alpha)$, with $\mathcal{E}_t(\alpha)$ the cumulant generating function of the mean rate of entropy change w.r.t. the initial state of the system.

Extension to quantum regime; XY chains

- Part of the research program of V. Jakšić and C.-A. Pillet is to extend the theory of entropic fluctuations in classical stat. mech. to quantum case.
- Highly technical (operator algebras, modular theory....).
- XY chain is exactly solvable; can compute the quantities of interest in closed form (entropic functionals, NESS) while avoiding much of the technical machinery.
- Vast literature on XY chains.
- First proofs of NESS and strict positivity of entropy production in an open quantum system in the context of XY chains [AH '00], [AP '03].
- Also [Bernard-Doyon '12], [Bernard et. al. '13].

Finite volume open XY chain



- Two XY chains coupled at an endpoint (sites 0 and 1).
- Initially, each system is at thermal equilibrium; if the temperatures are different, there will be flow of energy and entropy from one chain to the other.
- **Plan**: Write down quantities of interest for finite size chains; take thermodynamic limit ($M \to \infty$) in which each chain becomes semi-infinite. Then take large time limit $t \to \infty$.

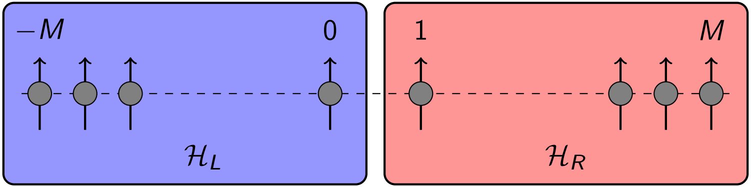
For an interval $[A, B] \subseteq \mathbb{Z}$, define

$$H_{[A,B]} = \frac{1}{2} \sum_{n \in [A,B[} J_n \left(\sigma_n^{(x)} \sigma_{n+1}^{(x)} + \sigma_n^{(y)} \sigma_{n+1}^{(y)} \right) + \frac{1}{2} \sum_{n \in [A,B]} \lambda_n \sigma_n^{(z)}.$$

- Acts on the Hilbert space $\otimes_{n \in [A,B]} \mathbb{C}^2$ (one spin-$\frac{1}{2}$ system at each point in [A, B]).
- J_n, λ_n, $n \in \mathbb{Z}$ are bounded sequences of real numbers, with $J_n \neq 0$ (fixed for the rest of the talk).
- Pauli matrices acting on the site n.

$$\sigma_n^{(x/y/z)} := \mathbb{1}_A \otimes \ldots \otimes \sigma^{(x/y/z)} \otimes \ldots \otimes \mathbb{1}_B$$

$$\sigma^{(x)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma^{(y)} = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}, \qquad \sigma^{(z)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$



- The Hamiltonian acts on $\mathcal{H} = \otimes_{n\in[-M,M]}\mathbb{C}^2$ and is given by

$$H = H_L + H_R + V,$$

where,

$$H = H_{[-M,M]}, \quad H_L = H_{[-M,0]} \otimes \mathbb{1}, \quad H_R = \mathbb{1} \otimes H_{[1,M]},$$
$$V = \frac{1}{2} J_0 \left(\sigma_0^{(x)} \sigma_1^{(x)} + \sigma_0^{(y)} \sigma_1^{(y)} \right).$$

- Initial state is the density matrix

$$\omega := \exp\left[-\beta_L H_L - \beta_R H_R\right]/Z.$$

- ω is steady state for decoupled dynamics $H_0 = H_L + H_R$.

Observables of the XY chain

Evolution of observables A and states ρ under the Hamiltonian dynamics is,

$$A_t := \mathrm{e}^{\mathrm{i}tH} A \mathrm{e}^{-\mathrm{i}tH}, \qquad \rho_t := \mathrm{e}^{-\mathrm{i}tH} \rho \mathrm{e}^{\mathrm{i}tH}$$

- The observable describing the flux out of the left/right reservoir is

$$\Phi_{L/R} = -\frac{\mathrm{d}}{\mathrm{d}t} H_{L/R,t} \bigg|_{t=0} = \mathrm{i}[H_{L/R}, V].$$

- The entropy production observable is,

$$\sigma = -\beta_L \Phi_L - \beta_R \Phi_R.$$

- The mean entropy production rate over the time interval $[0, t]$ is

$$\Sigma^t = \frac{1}{t} \int_0^t \sigma_s \mathrm{d}s.$$

Entropic functionals

- The direct ('naive') quantization of the entropic functional appearing in classical statistical mechanics is

$$\mathrm{ES}_t(\alpha) = \log \omega\left(\mathrm{e}^{-t\alpha\Sigma^t}\right).$$

  However, the fluctuation relation $\mathrm{ES}_t(\alpha) = \mathrm{ES}_t(1-\alpha)$ *fails*; i.e., this holds for all t iff $[\omega, H] = 0$.

- Look at the functional

$$\mathrm{FCS}_t(\alpha) = \log \sum_\phi e^{-\alpha t \phi}\mathbb{P}_t(\phi) = \log \mathrm{tr}\left(\omega_t^{1-\alpha}\omega^\alpha\right)$$

  Here, $\mathbb{P}_t(\phi)$ is the measure for the **full counting statistics** for the mean rate of entropy change. Proposed independently by [Kurchan '00], [Tasaki - Matsui, '03].

- Note $\mathrm{FCS}_t(\alpha) = \mathrm{FCS}_t(1-\alpha)$.

Full counting statistics

- System is in initial state ω. Entropy observable is

$$S = -\log \omega.$$

- In order to measure the mean rate of entropy change of the system over a time interval $[0, t]$,
  - measure S at $t = 0$ and obtain the eigenvalue s
  - measure the entropy S again at time t and obtain s'.

  The mean rate of entropy change is

$$\phi = \frac{s' - s}{t}.$$

- The discrete probability measure $\mathbb{P}_t(\phi)$ is the probability of obtaining ϕ for the mean rate of entropy change over the interval $[0, t]$.

Entropic pressure functionals

Define, for $1 \leq p < \infty$,

$$\mathrm{e}_{p,t}(\alpha) = \log \operatorname{tr}\left[\left(\omega^{(1-\alpha)/p}\omega_t^{2\alpha/p}\omega^{(1-\alpha)/p}\right)^{p/2}\right]$$

and

$$\mathrm{e}_{\infty,t}(\alpha) = \log \operatorname{tr}\left(\mathrm{e}^{\log\omega + \alpha(\log\omega_t - \log\omega)}\right).$$

Properties: [Jakšić-Ogata-Pillet-Pautrat '12]

- $\mathrm{FCS}_t(\alpha) = \mathrm{e}_{2,t}(\alpha) = \log \operatorname{tr}\left(\omega_t^{1-\alpha}\omega^{\alpha}\right)$ (from $\alpha \leftrightarrow 1-\alpha$ symmetry)
- $\mathrm{e}_{p,t}(\alpha) = \mathrm{e}_{p,t}(1-\alpha)$; consequence of TRI.
- $\alpha \to \mathrm{e}_{p,t}(\alpha)$ and $\alpha \to \mathrm{ES}_t(\alpha)$ are convex, real analytic; $p \to e_{p,t}(\alpha)$ is continuous, strictly decreasing.
- $\lim_{p\to\infty} e_{p,t}(\alpha) = e_{\infty,t}(\alpha)$.

Properties con'd:

- $e'_{p,t}(0) = -t\omega(\Sigma^t), e'_{p,t}(1) = t\omega(\Sigma^t)$. In particular, these derivatives do not depend on p.
- We have,

$$e''_{2,t}(0) = \mathrm{ES}''_t(0) = \int_0^t \int_0^t \omega((\sigma_s - \omega(\sigma_s))(\sigma_u - \omega(\sigma_u)))\mathrm{d}s\mathrm{d}u.$$

- $\mathrm{e}_{\infty,t}(\alpha) = \max_\rho \left(S(\rho|\omega) - \alpha t\rho(\Sigma^t)\right)$. Quantization of variational characterization of ES functional in classical case.
- $e_{p,t}(\alpha)$ are linked with quantization of Ruelle transfer operators, $e_{p,t}(\alpha) = \log \left\|\mathrm{e}^{-\mathrm{i}tL_{p/\alpha}}\xi_\omega\right\|^p_{\omega,p}$. [Jakšić-Pillet '12]

Above, the relative entropy of ρ w.r.t ν is

$$S(\rho|\nu) := \begin{cases} \mathrm{tr}\left(\rho(\log\nu - \log\rho)\right) & \mathrm{Ker}\nu \subseteq \mathrm{Ker}\rho, \\ -\infty & \mathrm{else.} \end{cases}$$

Recap and outline

Done:

- Have described open XY chain: Hamiltonian, initial state, observables.
- Have introduced entropic functionals $\mathrm{ES}_t(\alpha)$, $\mathrm{FCS}_t(\alpha)$, $\mathrm{e}_{p,t}(\alpha)$.

To do:

1. Thermodynamic limit: describe the extended XY chain and its observables. Describe entropic functionals
2. Large time limit: describe NESS, and entropic functionals. Introduce Gallavotti-Cohen functional.
3. Consequences for large deviations.
4. Proof ingredients (only one slide!)

Thermodynamic limit $M \to \infty$

Notation: let the subscript M denote the dependence of the various objects on the size of the XY chain, i.e. ω_M, H_M, etc. The algebra of observables of the XY chain of size M is denoted $\mathcal{O}_M$.
The algebra of observables of the extended XY chain is $\mathcal{O} = \mathrm{closure}(\mathcal{O}_{\mathrm{loc}})$ where,

$$\mathcal{O}_{\mathrm{loc}} = \bigcup_{M>0} \mathcal{O}_M.$$

Above, $\mathcal{O}_{M_1}$ is identified with subalgebra of $\mathcal{O}_{M_2}$, $M_1 < M_2$.

Theorem:

For $A \in \mathcal{O}_{\mathrm{loc}}$, the limits

$$\tau^t(A) = \lim_{M\to\infty} e^{\mathrm{i}tH_M} A e^{-\mathrm{i}tH_M}, \qquad \omega(A) = \lim_{M\to\infty} \omega_M(A)$$

exist, and τ^t and ω extend uniquely to a **dynamics** and **state** on $\mathcal{O}$. The extended XY chain is described by the C^*-dynamical system $(\mathcal{O}, \omega, \tau^t)$.

Entropic functionals in the thermodynamic limit

Proposition: [Jakšić-L-Pillet '13]

1. The limits

$$\mathrm{ES}_t(\alpha) = \lim_{M\to\infty} \mathrm{ES}_{t,M}(\alpha), \qquad e_{p,t}(\alpha) = \lim_{M\to\infty} e_{p,t,M}(\alpha)$$

   exist and are finite.
2. The functions $\alpha \to e_{p,t}(\alpha)$ and $\alpha \to \mathrm{ES}_t(\alpha)$ are real-analytic and convex. The function $p \to e_{p,t}(\alpha)$ is decreasing.
3. $e_{p,t}(\alpha) = e_{p,t}(1-\alpha)$.
4. $e'_{p,t}(0) = \mathrm{ES}'_t(0) = -t\omega\left(\Sigma^t\right)$.
5. $e''_{2,t}(0) = \mathrm{ES}''_t(0) = \int_0^t \int_0^t \omega\left((\sigma_s - \omega(\sigma_s))(\sigma_u - \omega(\sigma_u))\right) \mathrm{d}s\mathrm{d}u$
6. As $M \to \infty$, the sequences of measures $\mathbb{P}_{t,M}$ converges weakly to a Borel probability measure $\mathbb{P}_t$ (FCS of the extended XY chain). Moments of $\mathbb{P}_{t,M} \to \mathbb{P}_t$.

Large time limit: NESS

Theorem [Ashbacher-Pillet '03]

Suppose that h has purely a.c. spectrum (see next slide).

1. Then $\forall A \in \mathcal{O}$, the limit

$$\langle A \rangle_+ = \lim_{t\to\infty} \omega\left(\tau^t(A)\right)$$

exists. $\langle \cdot \rangle_+$ is the NESS of the extended XY chain.

2. The steady state heat fluxes are

$$\langle \Phi_L \rangle_+ = -\langle \Phi_R \rangle_+ = \frac{1}{4\pi} \int_{\mathbb{R}} E|s_{lr}(E)|^2 \frac{\sinh(\Delta\beta E/2)}{\cosh(\beta_R E/2)\cosh(\beta_L E/2)} \mathrm{d}E,$$

where $\Delta\beta = \beta_R - \beta_L$.

3. Steady state entropy production is

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

and is strictly positive for "non-trivial" models.

What are s_{lr} and h?

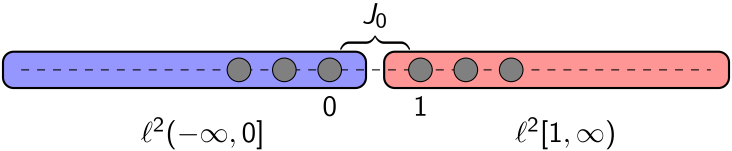
The Jordan-Wigner transformation 'associates' to the XY chain the Jacobi matrix $h : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ given by

$$(hu)_n = J_n u_{n+1} + J_{n-1} u_{n-1} + \lambda_n u_n.$$

where $\{u_n\}_n \in \ell^2(\mathbb{Z})$. Define the left and right half-line restrictions of h by

$$h_L = h \restriction_{\ell^2(-\infty,0]}, \qquad h_R = h \restriction_{\ell^2[1,\infty)}$$

and $h_0 = h_L + h_R$.



Then $h - h_0 = J_0 \left(|\delta_0\rangle\langle\delta_1| + |\delta_1\rangle\langle\delta_0| \right)$.

By the spectral theorem, the absolutely continuous subspace for h_0 is unitarily equivalent to

$$\mathcal{H}_{\mathrm{ac}}(h_0) = \mathcal{H}_{\mathrm{ac}}(h_L) \oplus \mathcal{H}_{\mathrm{ac}}(h_R) \cong L^2(\mathbb{R}, \mathrm{d}\nu_L) \oplus L^2(\mathbb{R}, \mathrm{d}\nu_R).$$

The **scattering matrix** s is a unitary operator on $\mathcal{H}_{\mathrm{ac}}(h_0)$ which acts by multiplication by a (symmetric, unitary) 2×2 matrix,

$$s(E) = \begin{pmatrix} s_{ll}(E) & s_{lr}(E) \\ s_{rl}(E) & s_{rr}(E) \end{pmatrix}.$$

Here,

$$s = w_+^* w_-, \qquad w_\pm = \operatorname*{s-lim}_{t \to \pm\infty} \mathrm{e}^{\mathrm{i}th} e^{-\mathrm{i}th_0} P_{\mathrm{ac}}(h_0),$$

$w_\pm$ are the **wave operators**.
$|s_{ll}(E)|^2 = |s_{rr}(E)|^2$ are the **reflection** probabilities.
$|s_{lr}(E)|^2 = |s_{rl}(E)|^2$ are the **transmission** probabilities.

Gallavotti-Cohen functional

The Gallavotti-Cohen functional

$$\mathrm{GC}_t(\alpha) = \left\langle \mathrm{e}^{-\alpha t \boldsymbol{\Sigma}^t} \right\rangle_+$$

describes fluctuations of the mean rate of entropy production w.r.t. the NESS.

In classical statistical mechanics, goes back to [Gallavotti-Cohen '95].

Compare with Evans-Searles functional

$$\mathrm{ES}_t(\alpha) = \omega\left(e^{-\alpha t \boldsymbol{\Sigma}^t} \right)$$

which describes fluctuations of the mean rate of entropy production w.r.t. the initial state of the system.

Main results I: explicit formulas

Theorem: [Jakšić-L-Pillet '13]

Suppose h has purely a.c. spectrum. Then,

$$e_{p,+}(\alpha) = \lim_{t\to\infty} \frac{1}{t} e_{p,t}(\alpha) = \int_{\mathbb{R}} \log\left(\frac{\det(1+K_{\alpha,p}(E))}{\det(1+K_{0,p}(E))}\right) \frac{\mathrm{d}E}{2\pi}$$

$$\lim_{t\to\infty} \frac{1}{t}\mathrm{ES}_t(\alpha) = \lim_{t\to\infty} \frac{1}{t}\mathrm{GC}_t(\alpha) = e_+(\alpha) = \int_{\mathbb{R}} \log\left(\frac{\det(1+K_\alpha(E))}{\det(1+K_0(E))}\right) \frac{\mathrm{d}E}{2\pi}$$

where

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

$$K_{\alpha,p}(E) = \left(e^{k_0(E)(1-\alpha)/p} s(E) e^{k_0(E)2\alpha/p} s^*(E) e^{k_0(E)(1-\alpha)/p}\right)^{p/2},$$

$$K_{\alpha,\infty}(E) = \lim_{p\to\infty} K_{\alpha,p}(E) = e^{(1-\alpha)k_0(E)+\alpha s(E)k_0(E)s^*(E)},$$

and $k_0(E) = \mathrm{diag}\{-\beta_L E, -\beta_R E\}$.

Main results II

Assume $s_{lr}(E)$ is not a.e. 0 and $\beta_L \neq \beta_R$. Then,

1. $e'_{p,+}(0) = -\langle\sigma\rangle_+$, and $e_{p,+}(\alpha) = e_{p,+}(1-\alpha)$.
2. The function $\mathbb{R} \ni \alpha \mapsto e_+(\alpha)$ is real-analytic and strictly convex. Moreover, it satisfies $e'_+(0) = -\langle\sigma\rangle_+$, and

$$\begin{aligned} & e''_+(0) = e''_{2,+}(0) \\ = & \lim_{T\to\infty} \frac{1}{T}\int_0^T \left\{ \frac{1}{2}\int_{-t}^t \langle(\sigma_s - \langle\sigma\rangle_+)(\sigma - \langle\sigma\rangle_+)\rangle_+ \,\mathrm{d}s \right\} \mathrm{d}t. \end{aligned}$$

Main results III

Let $\mathcal{E} = \{E : s_{lr}(E) \neq 0\}$. A Jacobi operator h is called **reflectionless** iff

$$|s_{ll}(E)|^2 = |s_{rr}(E)|^2 = 0 \text{ for a.e. } E \in \mathcal{E}.$$

3. If h is **reflectionless**, than all the functionals are identical: $e_{p,+}(\alpha) = e_+(\alpha)$ for every p, and,

$$e_+(\alpha) = \int_{\mathbb{R}} \log\left(\frac{\cosh((\beta_l(1-\alpha)+\beta_r\alpha)E/2)\cosh((\beta_r(1-\alpha)+\beta_l\alpha)E/2)}{\cosh(\beta_l E/2)\cosh(\beta_r E/2)}\right)\frac{\mathrm{d}E}{2\pi},$$

and $e_+(\alpha) = e_+(1-\alpha)$.

4. If h is not **reflectionless**, then all the functionals $e_{p,+}(\alpha)$ are different and e_+ does not have the $\alpha \leftrightarrow 1-\alpha$ symmetry.

Large Deviations

The following formulas hold:

$$e_{2,t}(\alpha) = \mathrm{FCS}_t(\alpha) = \log \int_{\mathbb{R}} e^{-\alpha t \phi} \mathrm{d}\mathbb{P}_t(\phi),$$

$$\mathrm{ES}_t(\alpha) = \log \int_{\mathbb{R}} e^{-\alpha t \phi} \mathrm{d}\mathbb{P}_{\mathrm{ES},t}(\phi), \quad \mathrm{GC}_t(\alpha) = \log \int_{\mathbb{R}} e^{-\alpha t \phi} \mathrm{d}\mathbb{P}_{\mathrm{GC},t}(\phi),$$

with $\mathbb{P}_{\mathrm{ES}/\mathrm{GC},t}$ the spectral measures for ω/ω_+ and Σ^t. Rate functions are,

$$I_{\mathrm{FCS}+}(\theta) = -\inf_{\alpha \in \mathbb{R}} (\alpha\theta + e_{2,+}(\alpha)), \qquad I_+(\theta) = -\inf_{\alpha \in \mathbb{R}} (\alpha\theta + e_+(\alpha)).$$

The symmetry $e_{2,+}(\alpha) = e_{2,+}(1-\alpha)$ implies,

$$I_{\mathrm{FCS}+}(\theta) = I_{\mathrm{FCS}+}(-\theta) + \theta.$$

If $I_+(\theta)$ satisfies this relation, then the symmetry $e_+(\alpha) = e_+(1-\alpha)$ must hold and so h is reflectionless.

Corollary: [Jakšić-L-Pillet '13]

Suppose that h has purely absolutely continuous spectrum.

1. The Large Deviation Principle holds: for any open set $O \subseteq \mathbb{R}$,

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mathrm{ES},t}(O) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mathrm{GC},t}(O) = -\inf_{\theta\in O} I_+(\theta),$$

$$\lim_{t\to\infty} \frac{1}{t} \log \mathbb{P}_{\mathrm{FCS},t}(O) = -\inf_{\theta\in O} I_{\mathrm{FCS}+}(\theta).$$

2. The Central Limit Theorem holds: for any Borel set $B \subseteq \mathbb{R}$, let $B_t = \{\phi \mid \sqrt{t}(\phi - \langle\sigma\rangle_+) \in B\}$. Then

$$\lim_{t\to\infty} \mathbb{P}_{\mathrm{ES},t}(B_t) = \lim_{t\to\infty} \mathbb{P}_{\mathrm{GC},t}(B_t) = \lim_{t\to\infty} \mathbb{P}_{\mathrm{FCS},t}(B_t)$$
$$= \frac{1}{\sqrt{2\pi D_+}} \int_B e^{-\phi^2/2D_+} \mathrm{d}\phi,$$

where the variance is $D_+ = e_+''(0)$.

Reflectionless Jacobi operators

Let $\mathcal{E} = \{E : s_{lr}(E) \neq 0\}$. A Jacobi operator h is called **reflectionless** iff

$$|s_{ll}(E)|^2 = |s_{rr}(E)|^2 = 0 \text{ for a.e. } E \in \mathcal{E}.$$

Consider the case $J_n = 1$ for every n. Then $h = -\Delta + V$, a discrete 1-d Schrödinger operator. Does there exist a potential V s.t. $-\Delta + V$ has purely absolutely continuous spectrum and is **not** reflectionless? Open problem. In the general Jacobi case, it is easy to construct such examples.

Main point: all the $e_{p,+}(\alpha) = e_+(\alpha)$ iff h is reflectionless. In particular, $I_{\mathrm{FCS}+} = I_+$ iff h is reflectionless.

Proof ingredients

1. JW transformation + algebra gives

$$\mathrm{ES}_{t,M}(\alpha) = t \int_0^\alpha \mathrm{d}\gamma \int_0^1 \mathrm{d}u \, \mathrm{tr}\left(\mathcal{K}_{\mathrm{ES},t,M}(\gamma, u) \mathrm{i}[k, h]\right).$$

   with $k = -\beta_L h_L - \beta_R h_R$, and $\mathcal{K}_{\mathrm{ES},t,M}$ converges strongly as $M \to \infty$, $t \to \infty$.

2. Theorem of [Aschbacher-Jakšić-Pautrat-Pillet, '07]:

$$\mathrm{tr}\left(\mathcal{K}_{\mathrm{ES},+} \mathrm{i}[k, h]\right) = \int_{\mathbb{R}} \mathrm{tr}_{\mathbb{C}^2}\left(\mathcal{K}_{\mathrm{ES},+}(E)(s^*(E) k_0(E) s(E) - k_0(E))\right) \mathrm{d}E,$$

   from which explicit formulas are obtained.

3. $\det(\mathbb{1} + A) = 1 + tr(A) + \det(A)$ for 2×2 matrices.
4. Golden-Thompson inequality, for A, B self-adjoint:

$$\mathrm{tr}\left(e^A e^B\right) \geq \mathrm{tr}\left(e^{A+B}\right)$$

   with equality iff $[A, B] = 0$.