

Title: Exact thermalization dynamics in the "Rule 54" Quantum Cellular Automaton

Speakers: Katja Klobas

Series: Quantum Fields and Strings

Date: October 26, 2021 - 2:00 PM

URL: <https://pirsa.org/21100007>

Abstract: When a generic isolated quantum many-body system is driven out of equilibrium, its local properties are eventually described by the thermal ensemble. This picture can be intuitively explained by saying that, in the thermodynamic limit, the system acts as a bath for its own local subsystems. Despite the undeniable success of this paradigm, for interacting systems most of the evidence in support of it comes from numerical computations in relatively small systems, and there are very few exact results. In the talk, I will present an exact solution for the thermalization dynamics in the "Rule 54" cellular automaton, which can be considered the simplest interacting integrable model. After introducing the model and its tensor-network formulation, I will present the main tool of my analysis: the space-like formulation of the dynamics. Namely, I will recast the time-evolution of finite subsystems in terms of a transfer matrix in space and construct its fixed-points. I will conclude by showing two examples of physical applications: dynamics of local observables and entanglement growth. The talk is based on a recent series of papers: arXiv:2012.12256, arXiv:2104.04511, and arXiv:2104.04513.

Exact relaxation dynamics in Rule 54 cellular automaton

Katja Klobas

Perimeter Institute (online)

26th October, 2021

Relaxation in closed quantum many-body systems

Quench protocol: the system is initialized in a state $|\psi\rangle$ and let to evolve.

$$|\psi(t)\rangle = U(t) |\psi\rangle$$

Relaxation in closed quantum many-body systems

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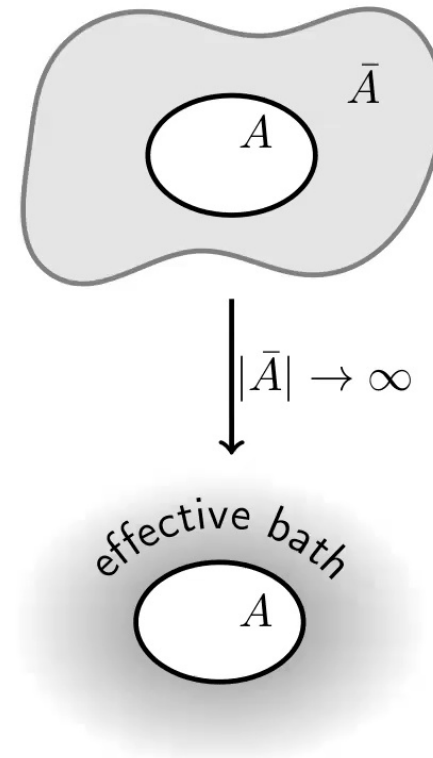
How does the system reach equilibrium?

- equilibrium: mixed state ρ_{th} (e.g. $\frac{1}{Z}e^{-\beta H}$)
- state $|\psi(t)\rangle$ is pure

Thermalization is *local*: the system acts as its own bath.

Expectation values of *local* observables are thermal:

$$\lim_{t \rightarrow \infty} \lim_{|\bar{A}| \rightarrow \infty} \langle \psi(t) | \mathcal{O}_A | \psi(t) \rangle = \text{tr}(\rho_{th} \mathcal{O}_A)$$

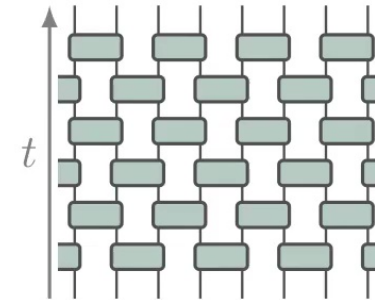


Only a few cases where this can be done explicitly in the presence of interactions.

Integrability does not seem to help!

Surprisingly: possible in certain chaotic circuit models

L. Piroli et al., *Phys. Rev. B* 101, 094304 (2020)



KK, B. Bertini, L. Piroli, *PRL* 126, 160602 (2021): an interacting integrable model where this can be proven exactly

(see also [arXiv:2104.04511](https://arxiv.org/abs/2104.04511), [arXiv:2104.04513](https://arxiv.org/abs/2104.04513))



Bruno Bertini
(Oxford → Nottingham)



Lorenzo Piroli
(Munich → ENS Paris)

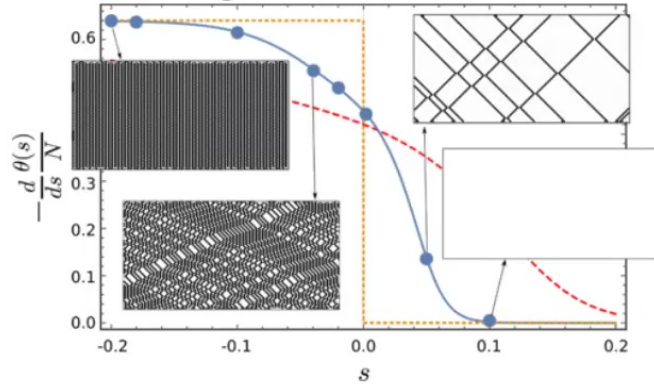
Talk outline

- 1 Motivation
- 2 Definition of the dynamics
- 3 Fixed-points of the transfer matrix in space
 - ▶ Maximum-entropy state
 - ▶ Compatible initial states
 - ▶ Generalisation to Gibbs states
- 4 Expectation values of local observables
 - ▶ Homogeneous case
 - ▶ Inhomogeneous case
- 5 Entanglement growth
- 6 Conclusion

Rule 54 reversible cellular automaton (RCA54) is possibly the simplest *interacting* model.

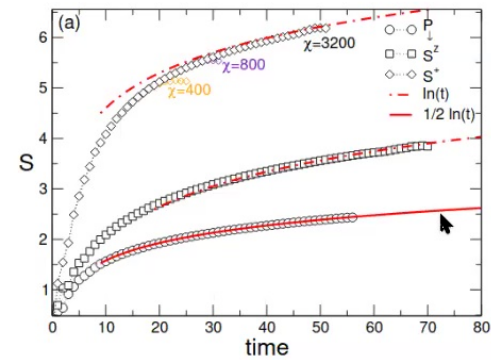
A. Bobenko et al., *Commun. Math. Phys.* 158, 127–134 (1993)

Exact large-deviation statistics

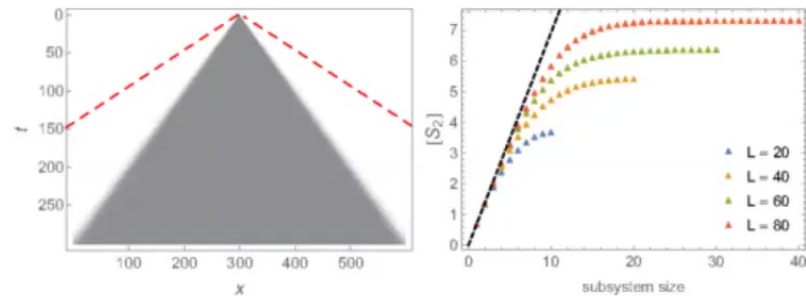


B. Buča et al., *Phys. Rev. E* 100, 020103(R) (2019)

Operator growth



V. Alba, *Phys. Rev. B* 104, 094410 (2021)

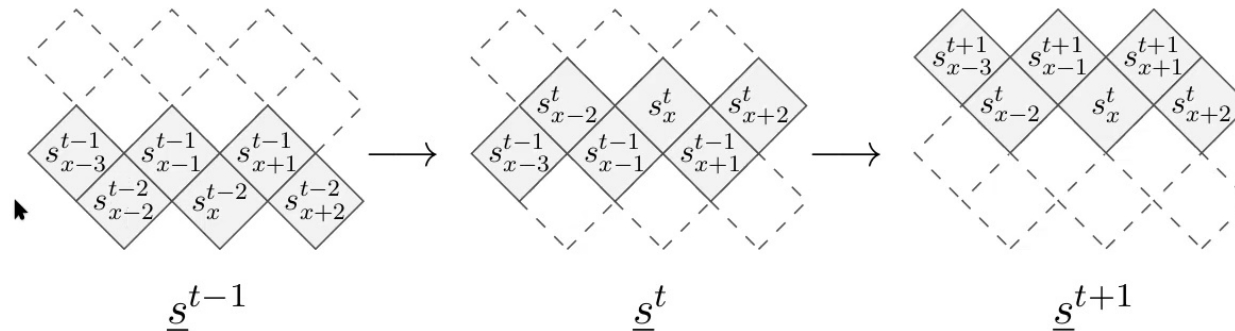


S. Gopalakrishnan, *Phys. Rev. B* 98, 060302(R) (2018)

Definition of dynamics

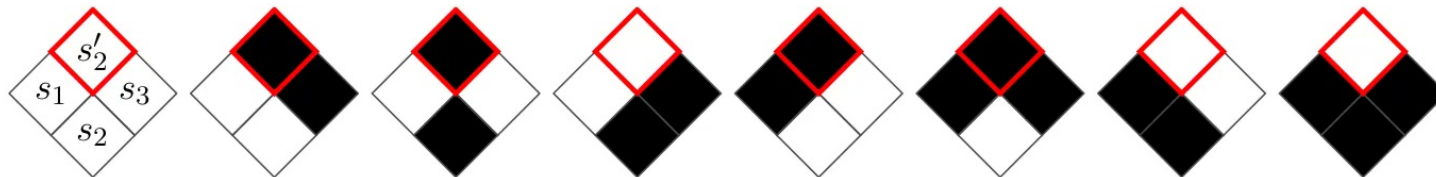
A. Bobenko et al., *Commun. Math. Phys.* 158, 127–134 (1993)

1-dim lattice of binary variables, with staggered time evolution:

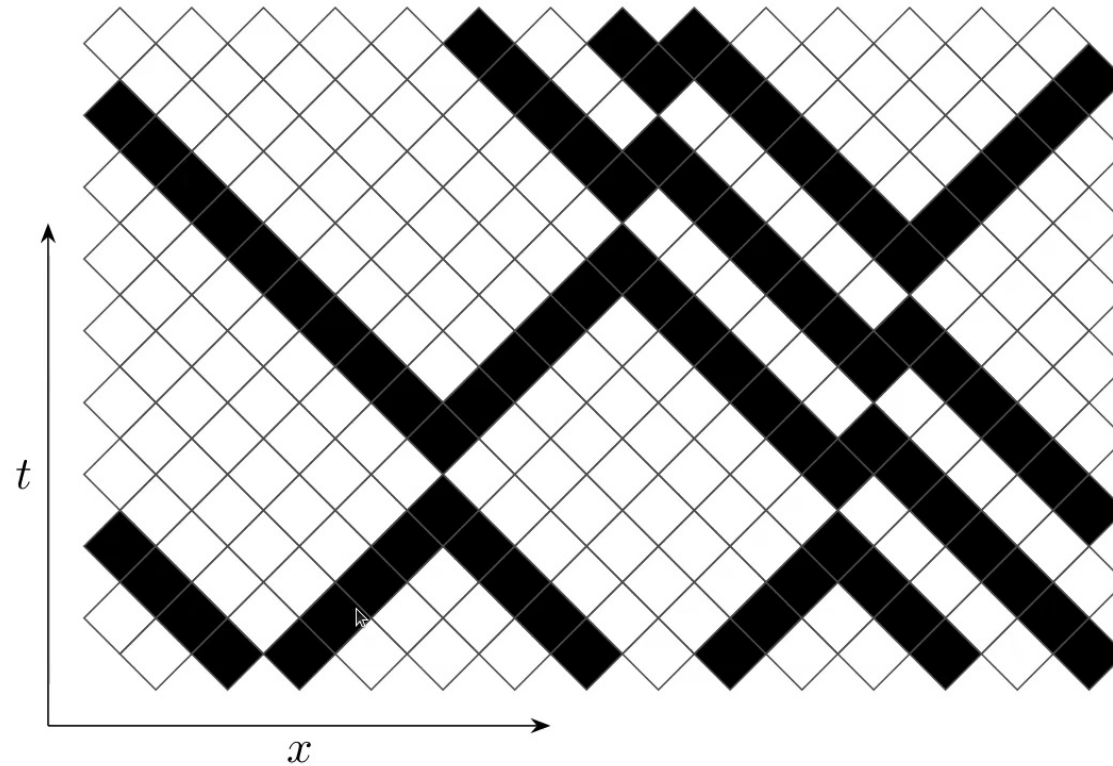


Local time evolution maps:

$$s'_2 = \chi(s_1, s_2, s_3) \equiv s_1 + s_2 + s_3 + s_1 s_3 \pmod{2}$$



Solitons move with fixed velocities ± 1 and obtain a delay while scattering.



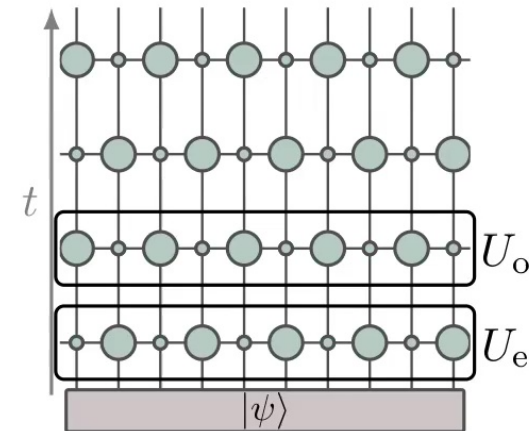
Quantum formulation

Discrete time-evolution on the qubit chain

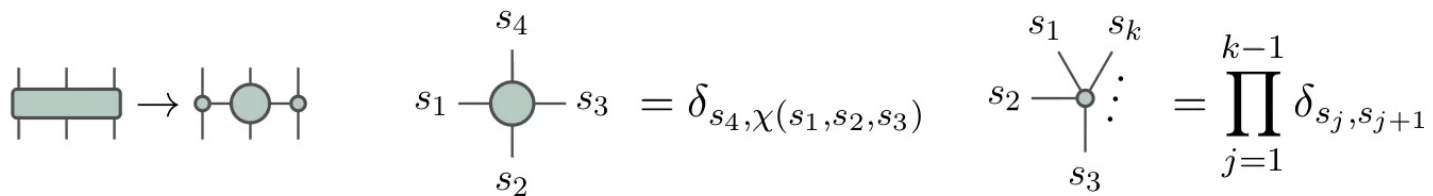
$$|\psi(t+1)\rangle = U_o U_e |\psi(t)\rangle$$

Local 3-site evolution operator

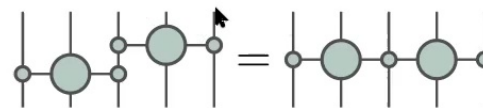
$$U = \text{[box]}, \quad U_{s_1 s_2 s_3}^{s'_1 s'_2 s'_3} = \delta_{s'_1, s_1} \delta_{s'_2, \chi(s_1, s_2, s_3)} \delta_{s'_3, s_3}$$



A convenient representation in terms of two tensors:



Operators at the same step commute:



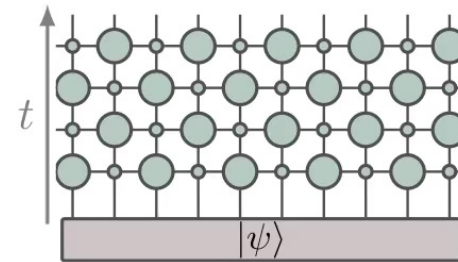
Quantum formulation

Discrete time-evolution on the qubit chain

$$|\psi(t+1)\rangle = U_o U_e |\psi(t)\rangle$$

Local 3-site evolution operator

$$U = \text{[Diagram: a box with three vertical lines]}, \quad U_{s_1 s_2 s_3}^{s'_1 s'_2 s'_3} = \delta_{s'_1, s_1} \delta_{s'_2, \chi(s_1, s_2, s_3)} \delta_{s'_3, s_3}$$

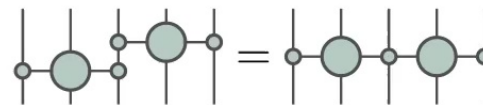


A convenient representation in terms of two tensors:

$$\text{[Diagram: a box with three vertical lines]} \rightarrow \text{[Diagram: a circle with three vertical lines]} \quad s_1 \text{---} \text{[Diagram: a circle with four vertical lines]} \text{---} s_3 = \delta_{s_4, \chi(s_1, s_2, s_3)}$$

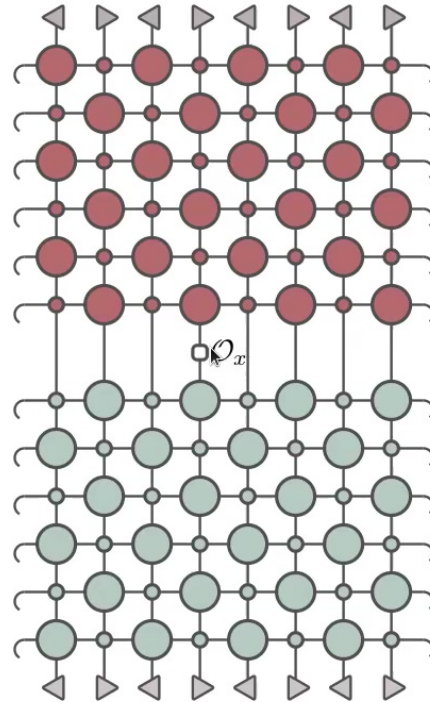
$$s_2 \text{---} \text{[Diagram: a circle with k vertical lines]} \text{---} s_3 = \prod_{j=1}^{k-1} \delta_{s_j, s_{j+1}}$$

Operators at the same step commute:

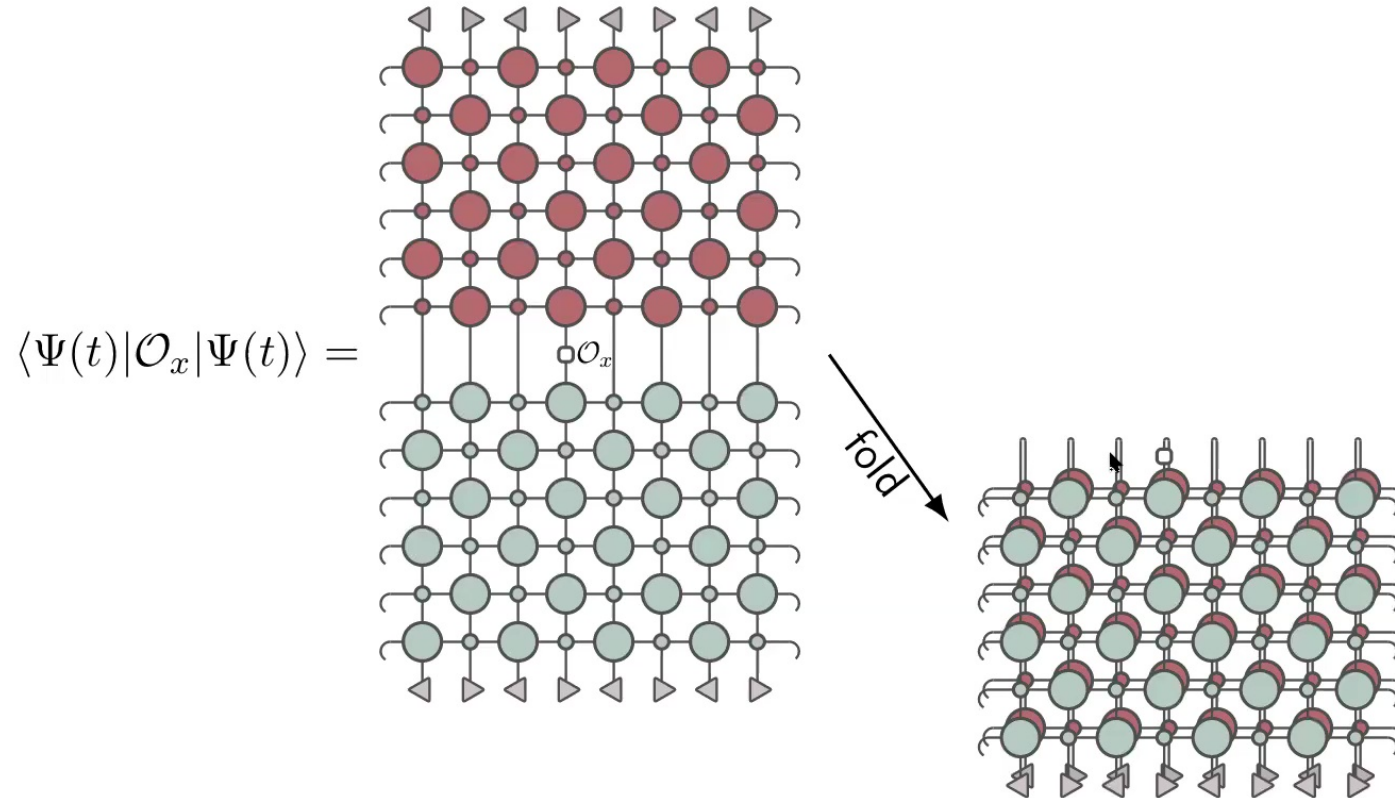


Local observables after a quench

$$\langle \Psi(t) | \mathcal{O}_x | \Psi(t) \rangle =$$

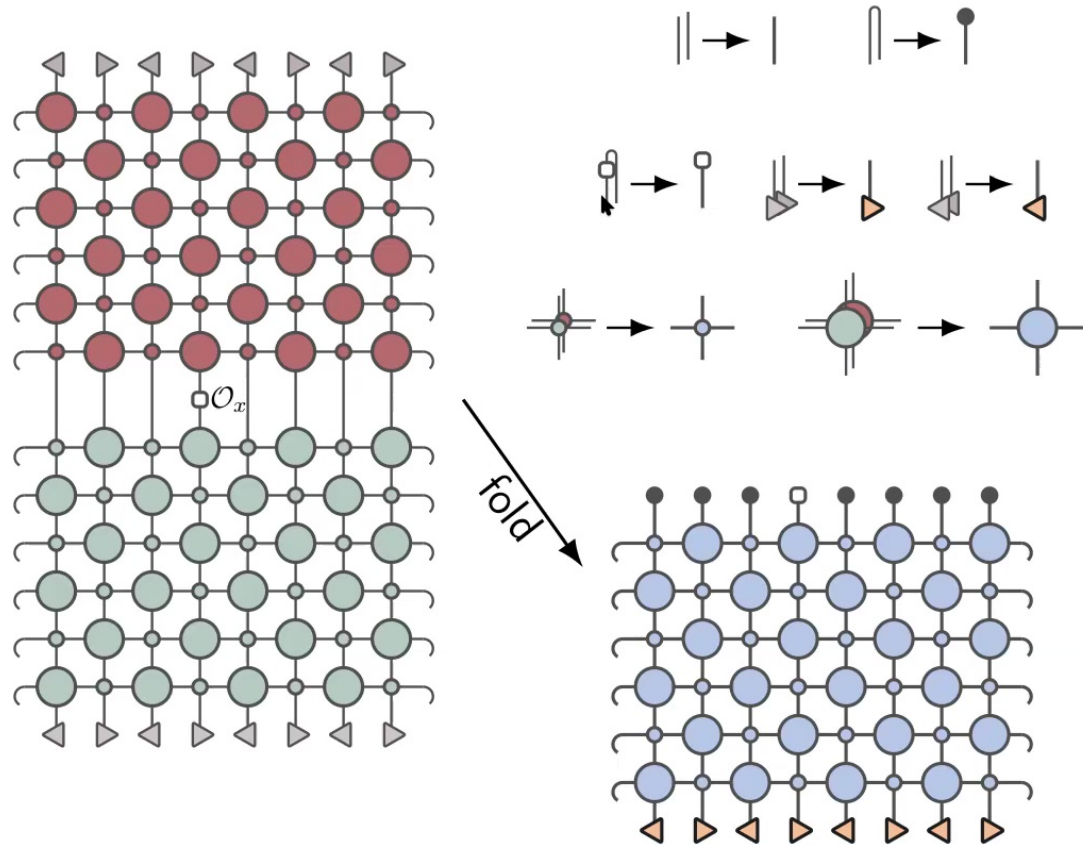


Local observables after a quench



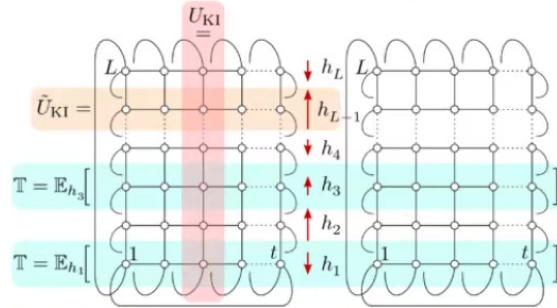
Local observables after a quench

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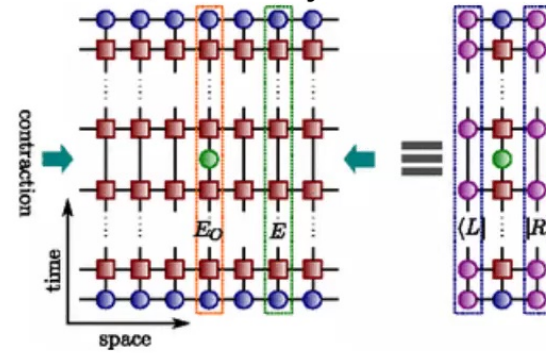
Tool: space-time duality transformation

Quantum many-body chaos



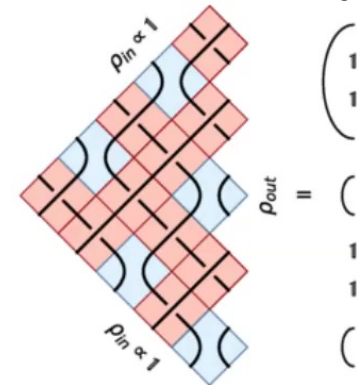
B. Bertini, P. Kos, T. Prosen, Phys. Rev. Lett. 121, 264101 (2018)

Quench dynamics

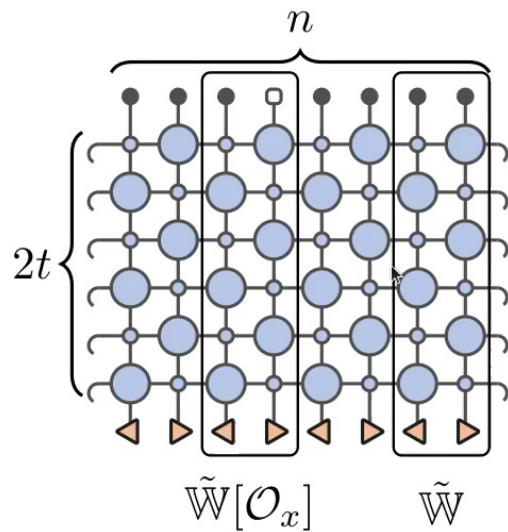


M. C. Bañuls et al., Phys. Rev. Lett. 102, 240603 (2009)

Measurement-induced dynamics



M. Ippoliti, V. Khemani, Phys. Rev. Lett. 126, 060501 (2021)

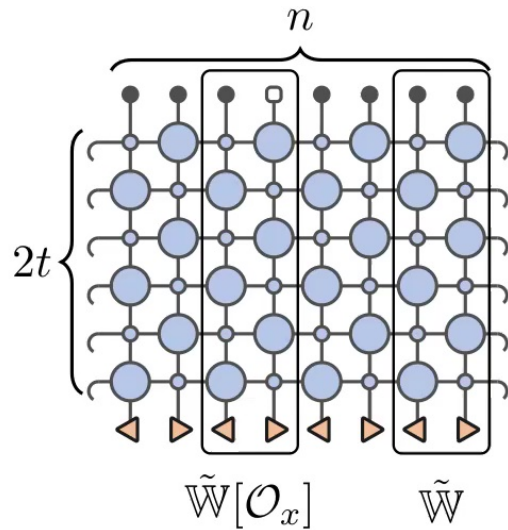


Blue tensors are defined on the *doubled* space ($s_j, b_j \in \{0, 1\}$)

$$\begin{array}{c} s_4 b_4 \\ | \\ s_1 b_1 \text{---} \text{---} \text{---} s_3 b_3 \\ | \\ s_2 b_2 \end{array} = \delta_{s_4, \chi(s_1, s_2, s_3)} \delta_{b_4, \chi(b_1, b_2, b_3)}$$

$$\begin{array}{c} s_4 b_4 \\ | \\ s_1 b_1 \text{---} \text{---} s_3 b_3 \\ | \\ s_2 b_2 \end{array} = \prod_{j=1}^3 \delta_{s_j, s_{j+1}} \delta_{b_j, b_{j+1}}$$

$$\begin{array}{c} \bullet \\ | \\ s_1 b_1 \end{array} = \delta_{s_1, b_1}$$



Expectation value in terms of transverse transfer matrices:

$$\langle \psi(t) | \mathcal{O}_x | \psi(t) \rangle = \text{tr} \left(\tilde{W}^{\frac{n}{2}-1} \tilde{W}[\mathcal{O}_x] \right)$$

$$\stackrel{n \geq 2t}{=} \langle L | \tilde{W}[\mathcal{O}_x] | R \rangle$$

$$\langle L | \tilde{W} = \langle L | \quad \tilde{W} | R \rangle = | R \rangle \quad \langle L | R \rangle = 1$$

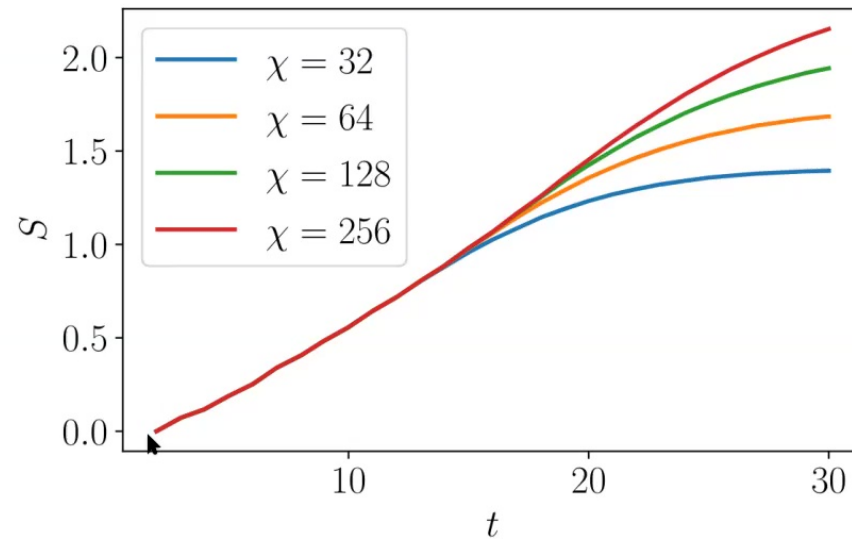
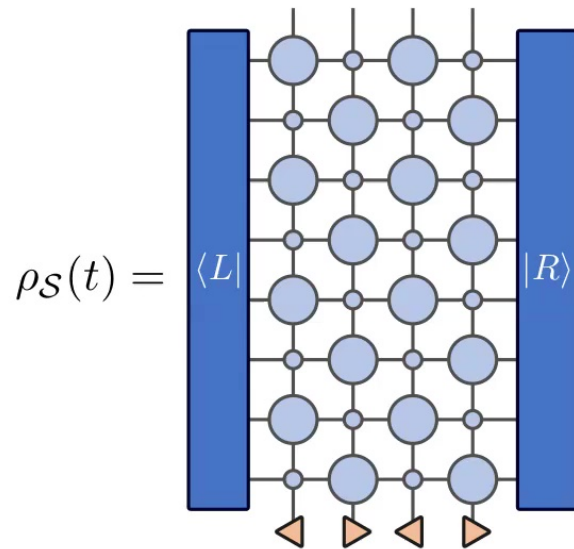
Blue tensors are defined on the *doubled* space ($s_j, b_j \in \{0, 1\}$)

$$\begin{array}{c}
 s_4 b_4 \\
 | \\
 s_1 b_1 \text{---} \text{---} s_3 b_3 \\
 | \\
 s_2 b_2
 \end{array}
 = \delta_{s_4, \chi(s_1, s_2, s_3)} \delta_{b_4, \chi(b_1, b_2, b_3)}$$

$$\begin{array}{c}
 s_4 b_4 \\
 | \\
 s_1 b_1 \text{---} \text{---} s_3 b_3 \\
 | \\
 s_2 b_2
 \end{array}
 = \prod_{j=1}^3 \delta_{s_j, s_{j+1}} \delta_{b_j, b_{j+1}}$$

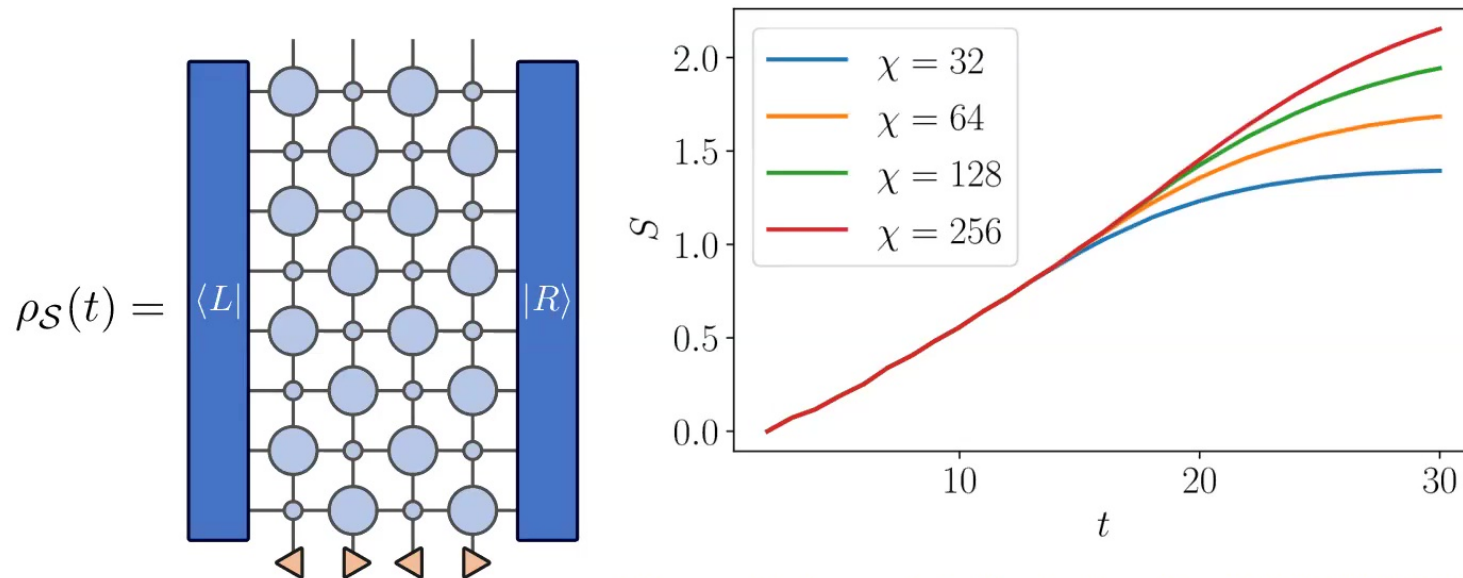
$$\begin{array}{c}
 \bullet \\
 | \\
 s_1 b_1
 \end{array}
 = \delta_{s_1, b_1}$$

Motivation: $\langle L|$ and $|R\rangle$ completely characterise thermalisation



A. Lerose, M. Sonner, D. A. Abanin, Phys. Rev. X 11, 021040 (2021)

Motivation: $\langle L|$ and $|R\rangle$ completely characterise thermalisation



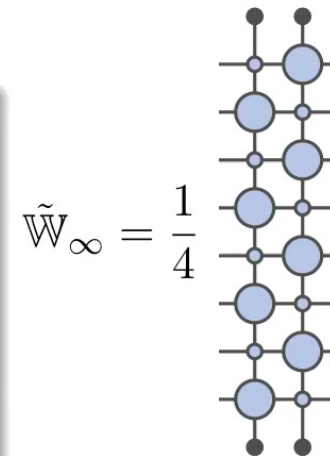
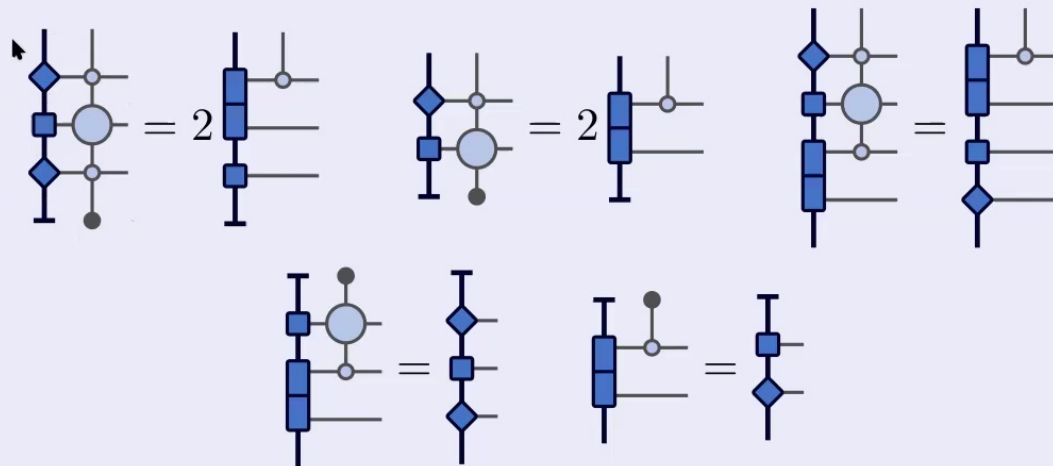
A. Lerose, M. Sonner, D. A. Abanin, Phys. Rev. X 11, 021040 (2021)

Our case: MPS with *finite* bond-dimension

Detour: maximum-entropy state

Let us consider the transfer matrix \tilde{W}_∞

Algebraic relations



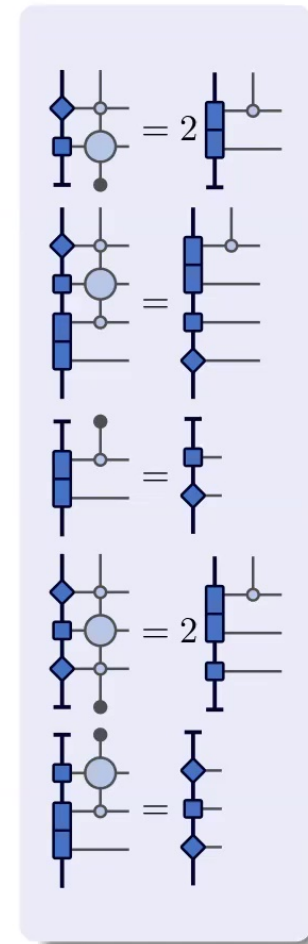
We introduce one- and two-site tensors:

$$A_{sb} = \text{diamond}(sb) \quad B_{sb} = \text{square}(sb) \quad C_{s_1 b_1 s_2 b_2} = \text{square}(s_1 b_1, s_2 b_2) \quad |b\rangle = \perp$$

Using these tensors we can build $\langle L_\infty |$ and $|R_\infty \rangle$

$$\langle L_\infty | \tilde{W}_\infty = \frac{1}{4} \left[\text{Diagram 1} \right] = \frac{1}{2} \left[\text{Diagram 2} \right] = \langle L_\infty |$$

Similarly: $|R_\infty \rangle =$

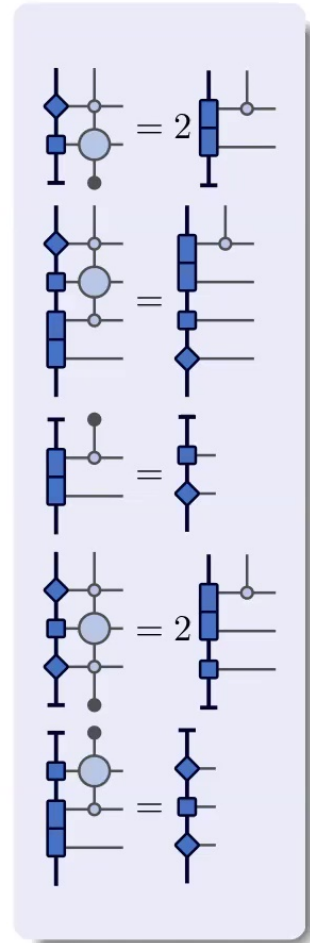


Using these tensors we can build $\langle L_\infty |$ and $|R_\infty \rangle$

$$\langle L_\infty | \tilde{W}_\infty = \frac{1}{4} \left[\begin{array}{c} \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \\ \text{---} \text{---} \text{---} \end{array} \right] = \frac{1}{2} \left[\begin{array}{c} \text{---} \text{---} \\ \text{---} \text{---} \\ \text{---} \text{---} \\ \text{---} \text{---} \\ \text{---} \text{---} \\ \text{---} \text{---} \\ \text{---} \text{---} \end{array} \right] = \langle L_\infty |$$

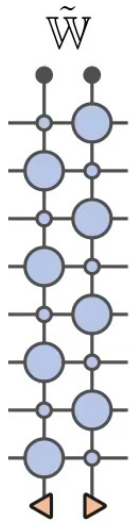
Similarly: $|R_\infty \rangle = \left[\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \end{array} \right]$

The solution exists for 3×3 matrices!!

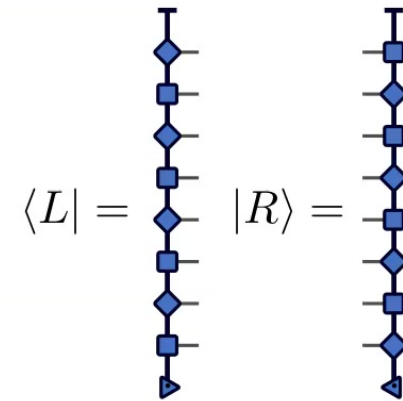
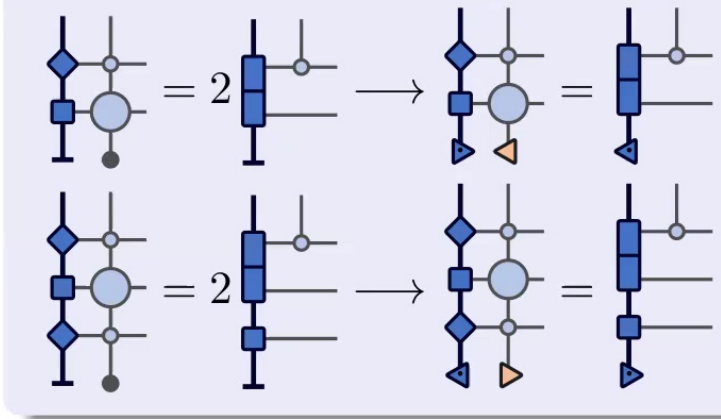


Compatible initial product states

Ansatz: $\langle L|$ and $|R\rangle$ differ from $\langle L_\infty|$ and $|R_\infty\rangle$ only at the very bottom



New boundary algebraic relations:



Solution:

$$\triangleleft = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ e^{i\varphi} \end{bmatrix} \quad \triangleleft = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Generalisation to Gibbs states

This straightforwardly generalises to Gibbs states.

$$\rho_{th} = \frac{1}{Z} e^{-\mu(N_+ + N_-)}, \quad N_{\pm} = \# \text{ of left/right movers}$$

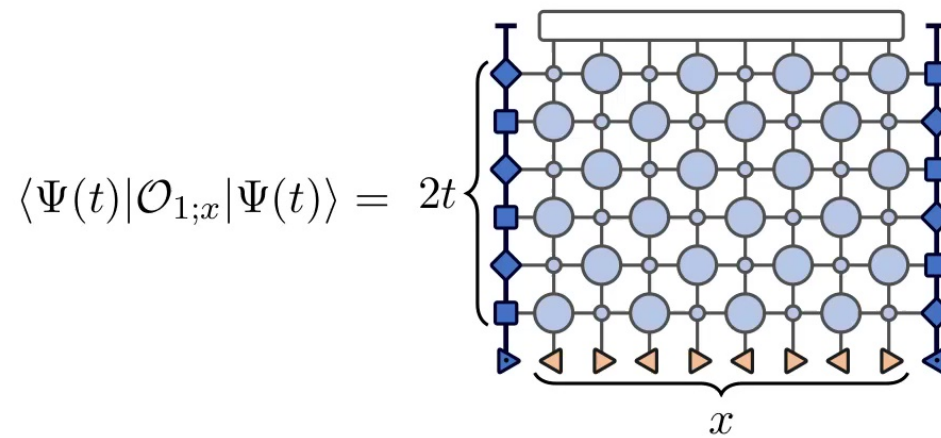
Fixed-point tensors become dependent on $\vartheta \in (0, 1)$ (still 3×3 matrices).

$$\vartheta = \frac{1}{1 + e^{-\mu}}$$

Compatible initial states:

$$\leftarrow = \begin{bmatrix} \sqrt{1 - \vartheta} \\ e^{i\varphi} \sqrt{\vartheta} \end{bmatrix} \quad \rightarrow = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

Expectation values of local observables



Expectation values of local observables

$$\langle \Psi(t) | \mathcal{O}_{1;x} | \Psi(t) \rangle = 2t \left\langle \Phi[\mathcal{O}_{1;x}] \middle| \mathcal{C}_x^t | \Phi_x \right\rangle$$

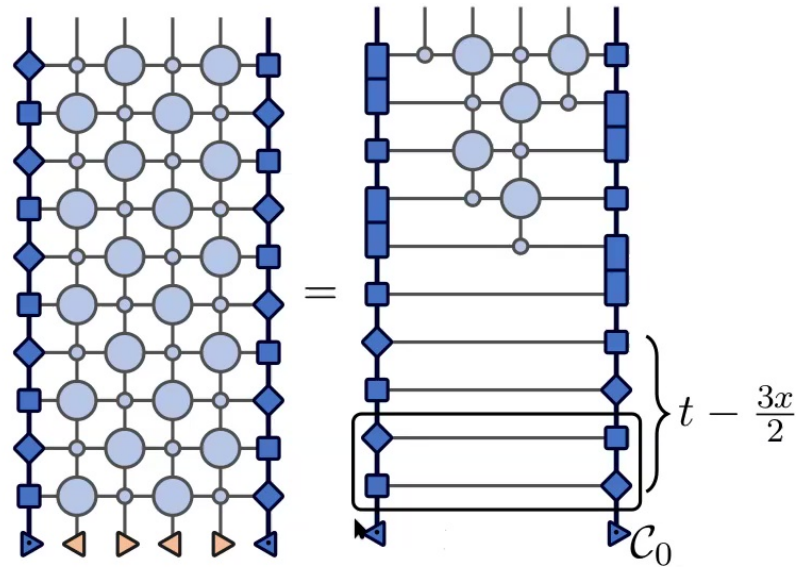
The diagram illustrates a tensor network for calculating the expectation value of a local observable $\mathcal{O}_{1;x}$ at time t . The network is a grid of blue circles (sites) and blue diamonds (time slices). The top boundary is labeled $\langle \Phi[\mathcal{O}_{1;x}] |$. The bottom boundary is labeled $| \Phi_x \rangle$. The horizontal axis is labeled x . The vertical axis is labeled $2t$. The central part of the network is labeled \mathcal{C}_x .

Expectation values of local observables

$$\langle \Psi(t) | \mathcal{O}_{1;x} | \Psi(t) \rangle = 2t \left\{ \begin{array}{l} \langle \Phi[\mathcal{O}_{1;x}] | \\ \mathcal{C}_x \\ | \Phi_x \rangle \end{array} \right\} = \langle \Phi[\mathcal{O}_{1;x}] | \mathcal{C}_x^t | \Phi_x \rangle$$

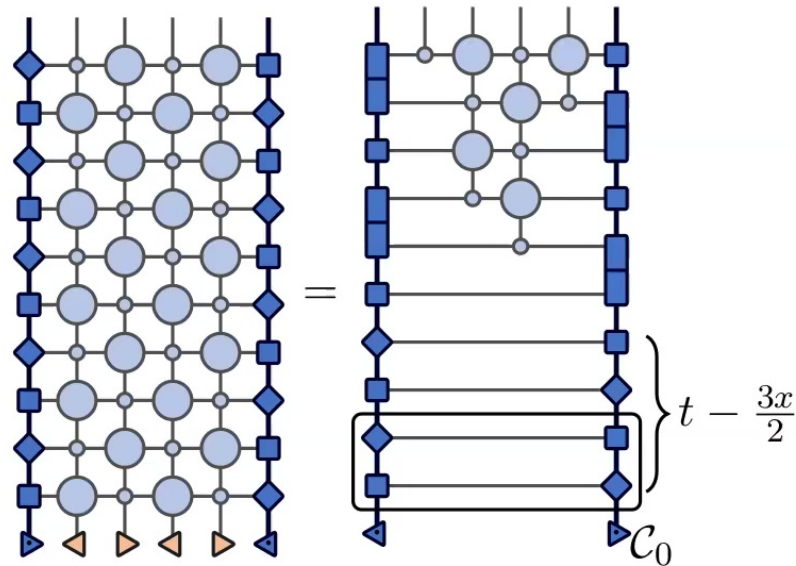
Expectation values are exponentially costly in support x rather than time t .

Long-time behaviour of $\langle \Psi(t) | \mathcal{O}_{1;x} | \Psi(t) \rangle$ is given by the spectrum of \mathcal{C}_0 :



$$\langle \Psi(t) | \mathcal{O}_{1;x} | \Psi(t) \rangle - \text{tr}(\rho_{th} \mathcal{O}_{1;x}) \sim e^{-t/\tau}, \quad \tau = \tau(\vartheta) > 0$$

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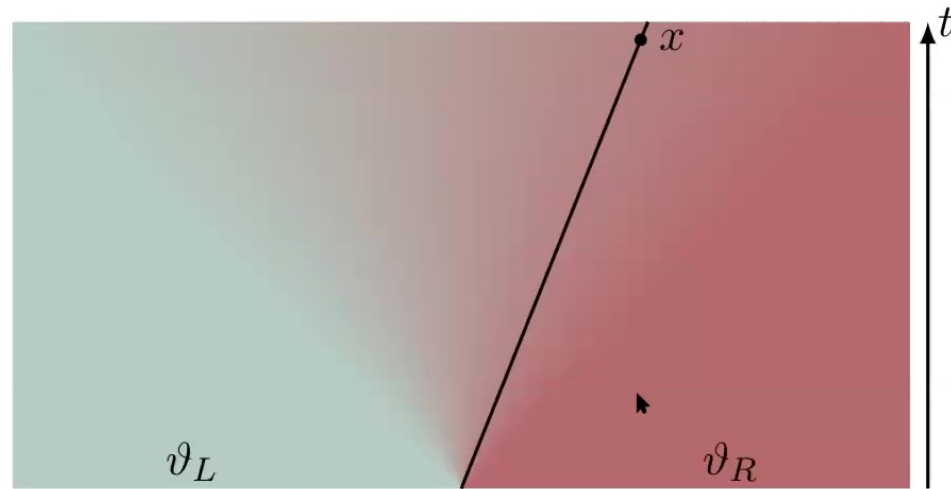


$$\langle \Psi(t) | \mathcal{O}_{1;x} | \Psi(t) \rangle - \text{tr}(\rho_{th} \mathcal{O}_{1;x}) \sim e^{-t/\tau}, \quad \tau = \tau(\vartheta) > 0$$

Expectation values of *all* local observables decay *exponentially*.

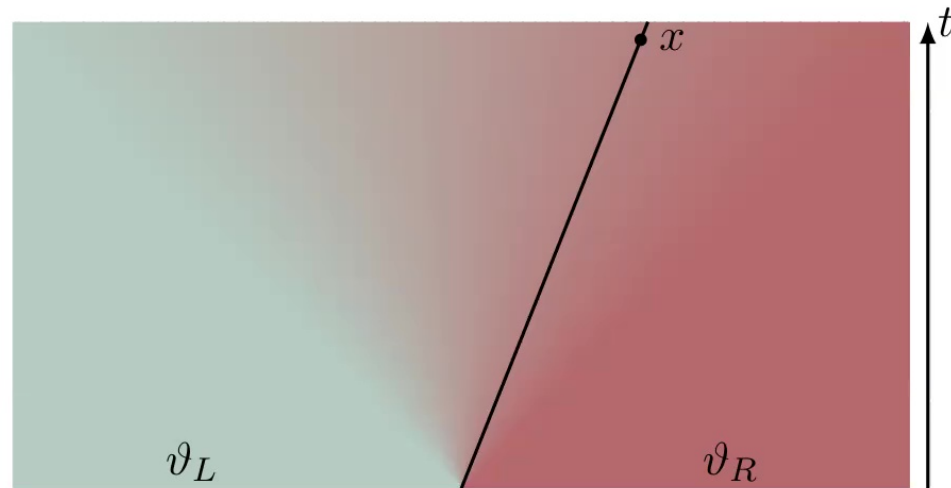
"Non-generic" behaviour for integrable systems

Inhomogeneous quenches



Scaling limit: $x/t = \zeta, x, t \rightarrow \infty$

Inhomogeneous quenches



Scaling limit: $x/t = \zeta$, $x, t \rightarrow \infty$

← described by GHD

Close to the junction ($|\zeta| < \frac{2}{3}$):

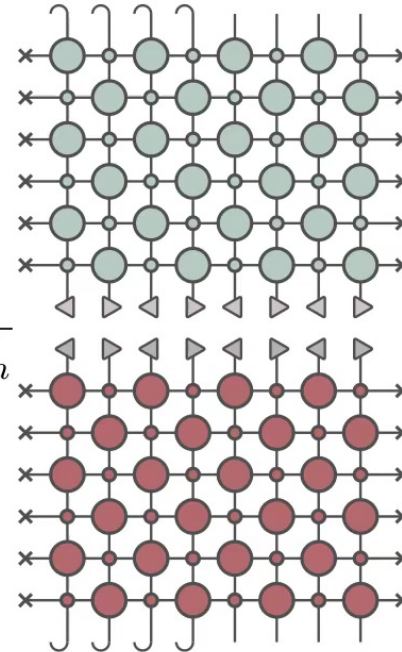
$$\rho_{GGE} = \frac{1}{Z} e^{-\mu_+ N_+ - \mu_- N_-}$$

Confirms GHD!

Entanglement entropy

Reduced density matrix of half of the system with open boundary conditions:

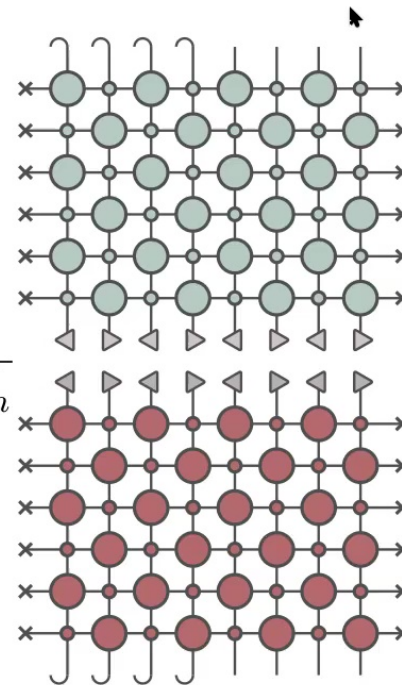
$$\rho_H(t) = \text{tr}_{[1; \frac{n}{2}]} |\Psi(t)\rangle\langle\Psi(t)| = \frac{1}{\mathcal{N}_n}$$



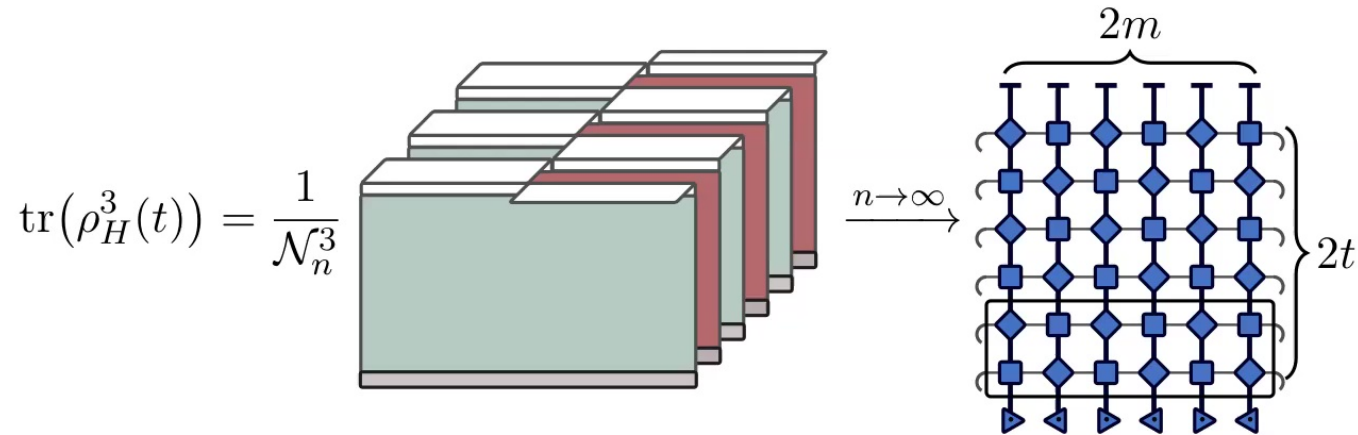
Entanglement entropy

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$$\rho_H(t) = \text{tr}_{[1; \frac{n}{2}]} |\Psi(t)\rangle\langle\Psi(t)| = \frac{1}{\mathcal{N}_n}$$



Rényi- m entanglement entropy: $S_m(t) = \frac{1}{1-m} \log \text{tr}(\rho_H^m(t))$

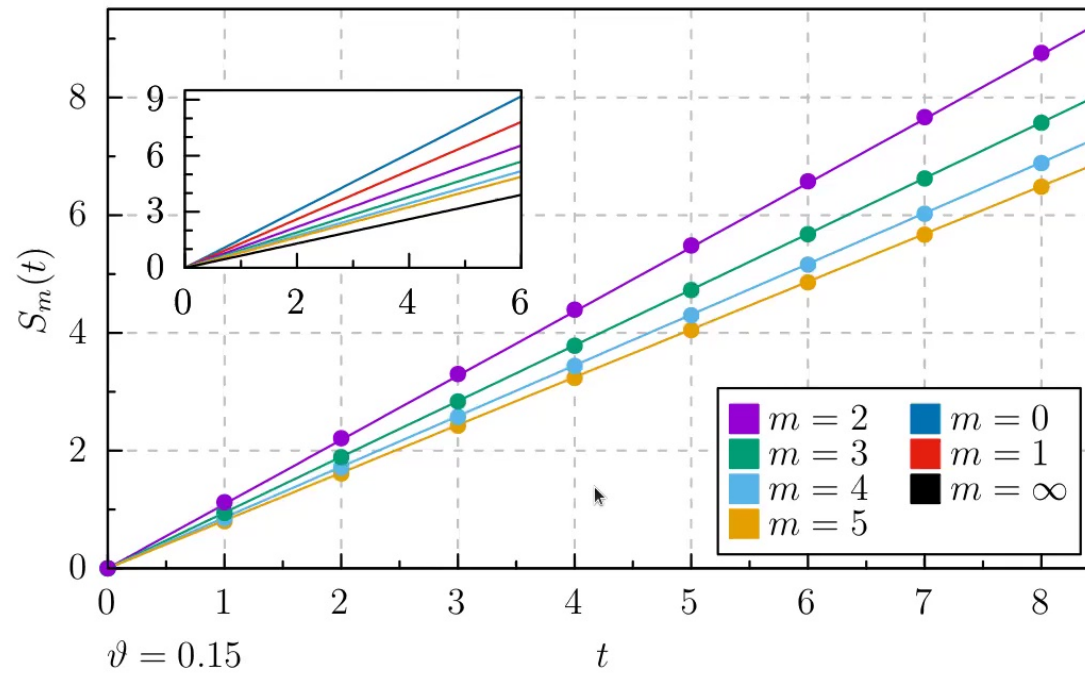


Unfolded tensors: $s \text{---} \diamond \text{---} b = \diamond \text{---} s b$ $s \text{---} \square \text{---} b = \square \text{---} s b$

Rate of entanglement growth: $s_m = \lim_{t \rightarrow \infty} \lim_{n \rightarrow \infty} \frac{S_m(t)}{t} = \frac{1}{1-m} \log \lambda_m$,
 λ_m is the leading solution to

$$x^3 - ((1 - \vartheta)^m x + \vartheta^m)^2 = 0$$

Example:



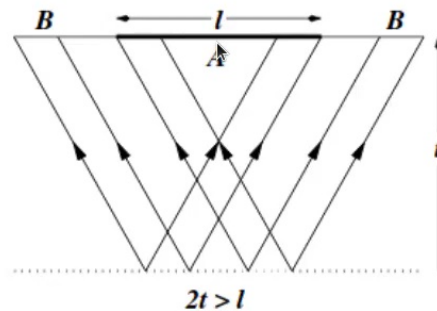
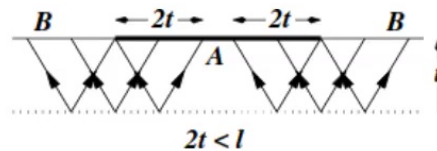
Entanglement growth in integrable systems

P. Calabrese, J. Cardy, J. Stat. Mech. 2005, P04010 (2005)

An effective quasiparticle picture:

- quench produces pairs of oppositely moving particles
- each pair "carries" some amount of entanglement
- pairs shared between the subsystem and the rest contribute to entanglement

$$S(t) = \int d\lambda \min\{v(\lambda)t, l\} s(\lambda)$$



Entangling quasi-particles are the excitations on the stationary state ρ_{th}
 \Rightarrow fixes $v(\lambda), s(\lambda)$

V. Alba, P. Calabrese, PNAS 114, 7947–7951 (2017)

Quantitative prediction:

$$S(t) = -(\vartheta \log \vartheta + (1 - \vartheta) \log(1 - \vartheta)) \min \left\{ \frac{2t}{1 + 2\vartheta}, l \right\}$$

Agrees with expression $\lim_{m \rightarrow 1} s_m$.

First exact confirmation of quasi-particle picture for an *interacting* system.

Also for inhomogeneous quenches

V. Alba, B. Bertini, M. Fagotti, SciPost Phys. 7 (2019)

What about higher Rényi?

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No consistent quasi-particle description.

Summary and outlook

Using simple algebraic identities we find fixed points of the transverse transfer matrix and provide the microscopic description of the effective bath.

Open questions:

- What happens with entanglement entropies in the finite system?
Motivation: quasi-particle vs. entanglement membrane

[A. Nahum et al., Phys. Rev. X 7, 031016 \(2017\)](#)

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[A. Nahum et al., Phys. Rev. X 7, 031016 \(2017\)](#)
- Extensions to richer stationary states (more conservation laws)
- Generalisations to other models Not hopeless!
[J. W. P. Wilkinson et al., Phys. Rev. E 102, 062107 \(2020\)](#)
[T. Iadecola, S. Vijay, Phys. Rev. B 102, 180302 \(2020\)](#)
- Approximate solutions to algebraic relations