

# Entanglement and thermodynamics in non-equilibrium isolated quantum systems

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Cortona, May 23rd 2018

Joint work with Vincenzo Alba

PNAS **114**, 7947 (2017), SciPost Phys. **4**, 017 (2018) & more

# Isolated systems out of equilibrium

## Quantum Quench

- 1) prepare a many-body quantum system in a **pure** state  $|\Psi_0\rangle$  that is **not** an eigenstate of the Hamiltonian
- 2) let it evolve according to quantum mechanics (no coupling to environment)

$$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$$

## Questions:

- How can we describe the dynamics?
- Does it exist a stationary state?
- Can it be thermal? In which sense?

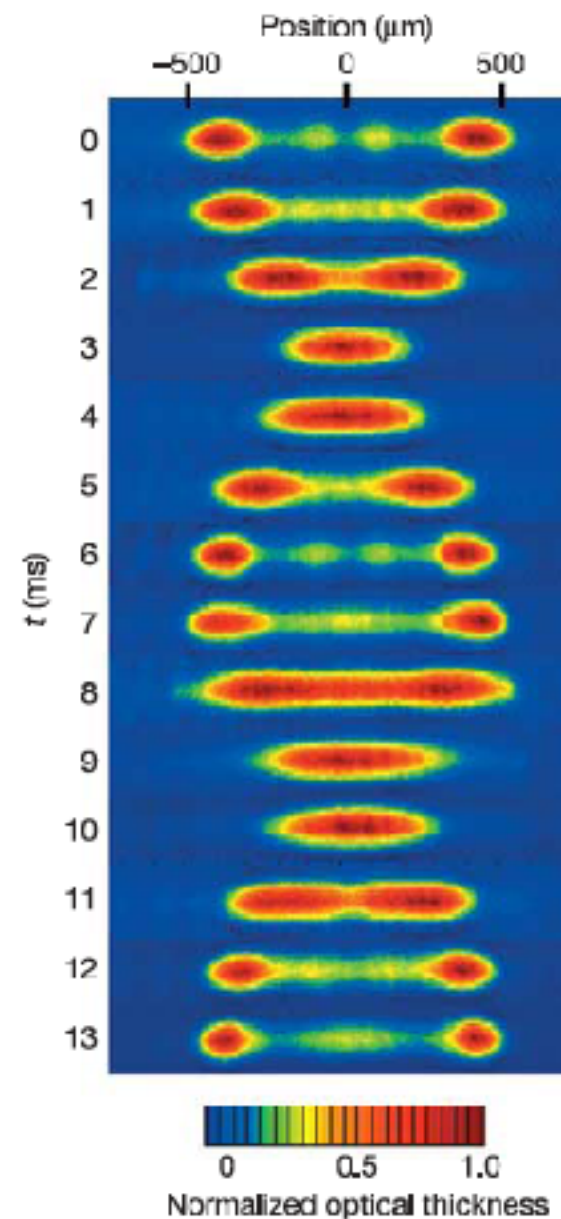
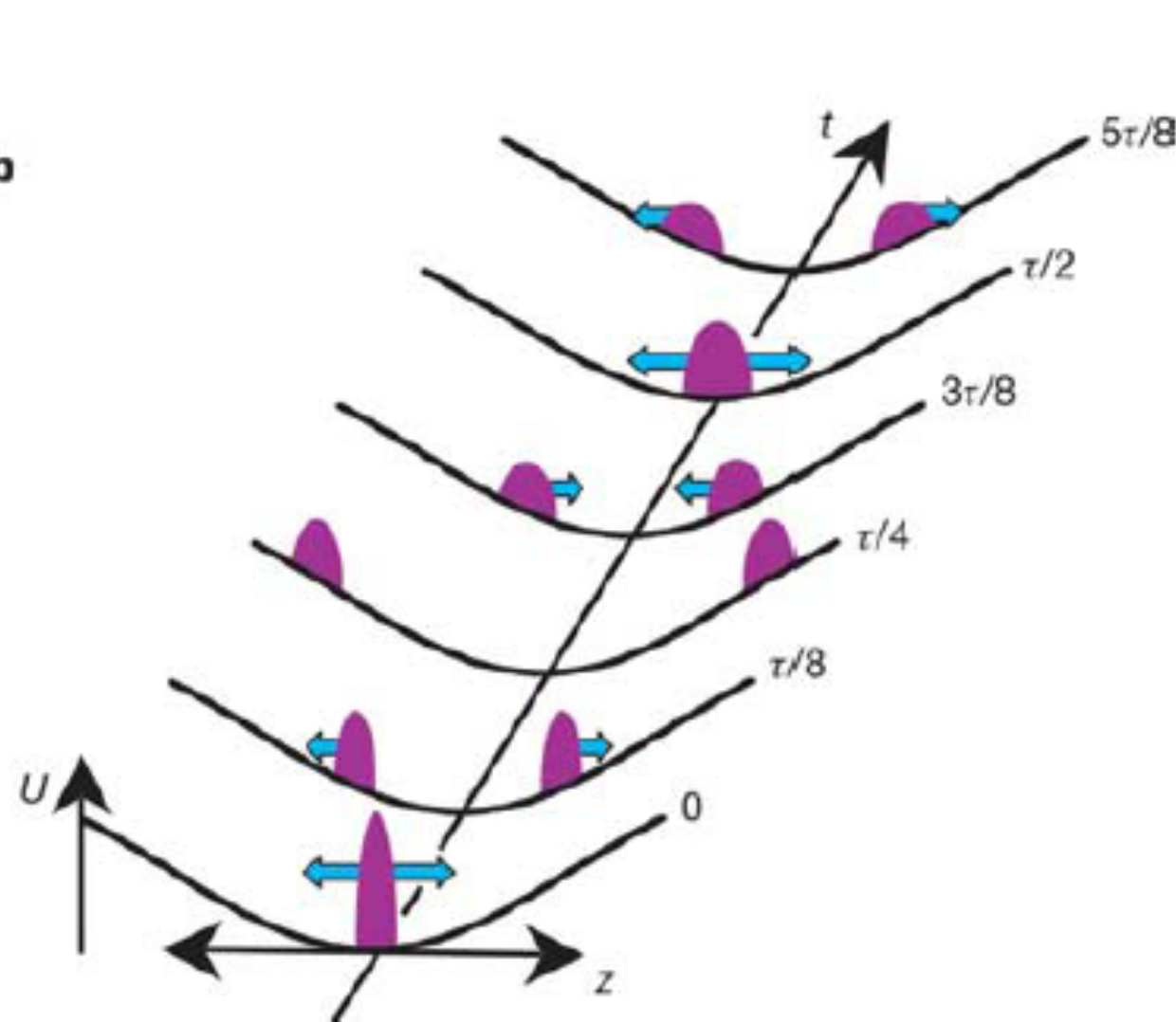
## Don't forget:

$|\Psi(t)\rangle$  is **pure** (zero entropy) for any  $t$  while the thermal **mixed** state has non-zero entropy

# Quantum Newton cradle

T. Kinoshita, T. Wenger and D.S. Weiss, *Nature* 440, 900 (2006)

few hundreds  $^{87}\text{Rb}$  atoms in a harmonic trap

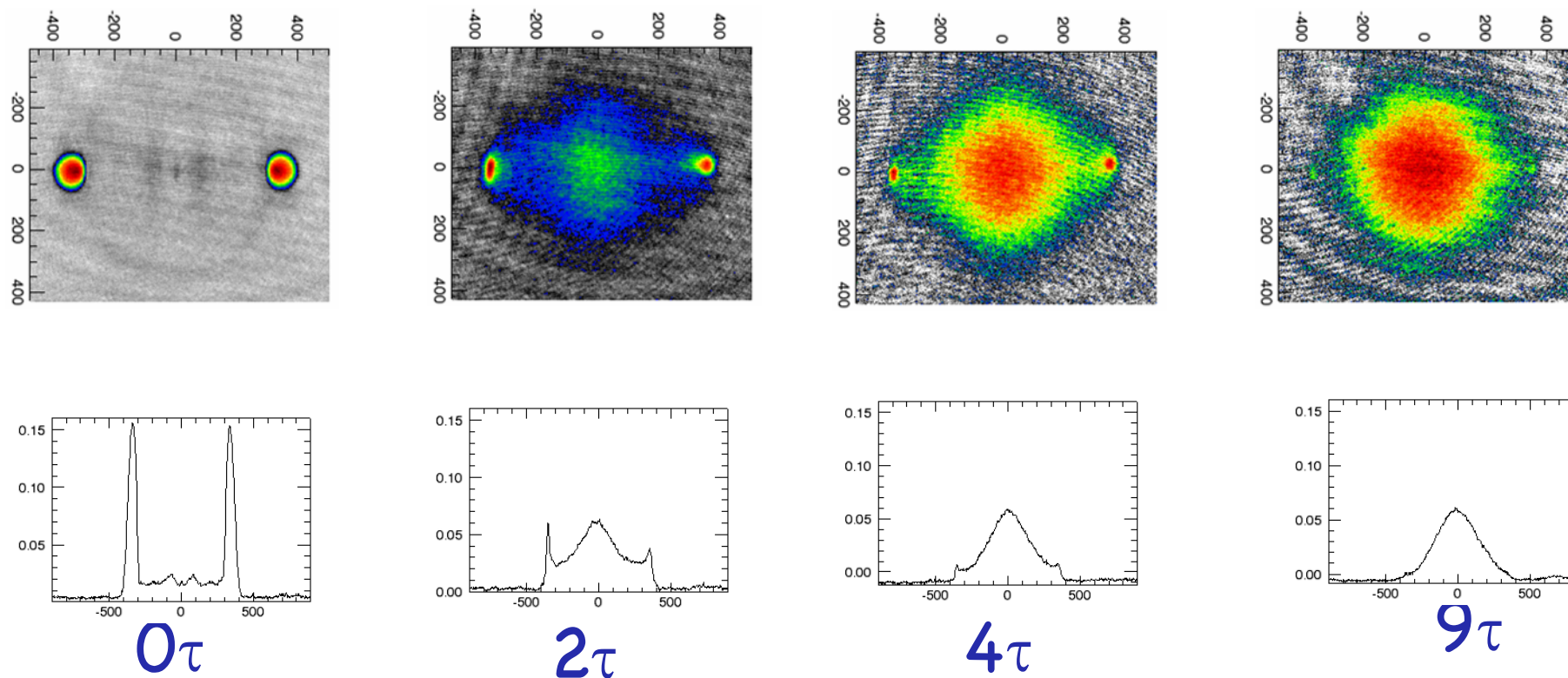


Essentially  
unitary time  
evolution

# Quantum Newton cradle

Kinoshita et al 2006

- 2D and 3D systems relax quickly and thermalize:



- 1D system relaxes slowly in time, to a non-thermal distribution





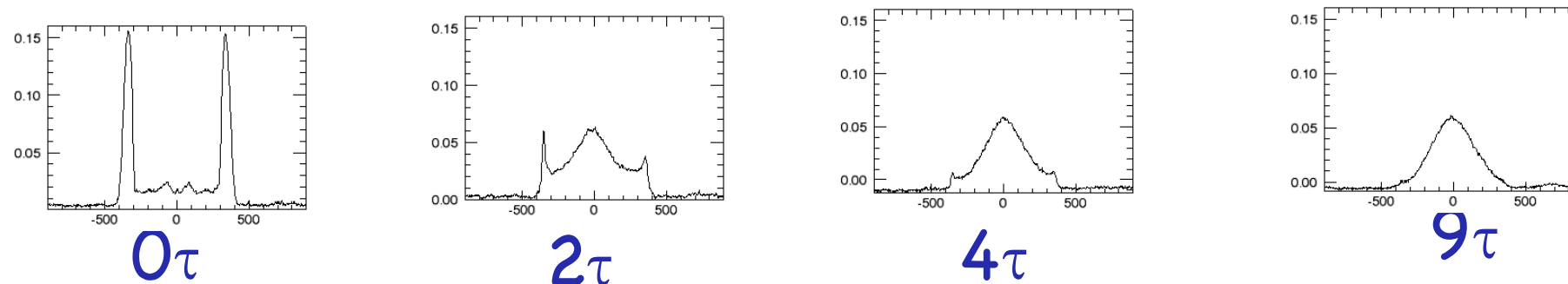
# Quantum Newton cradle

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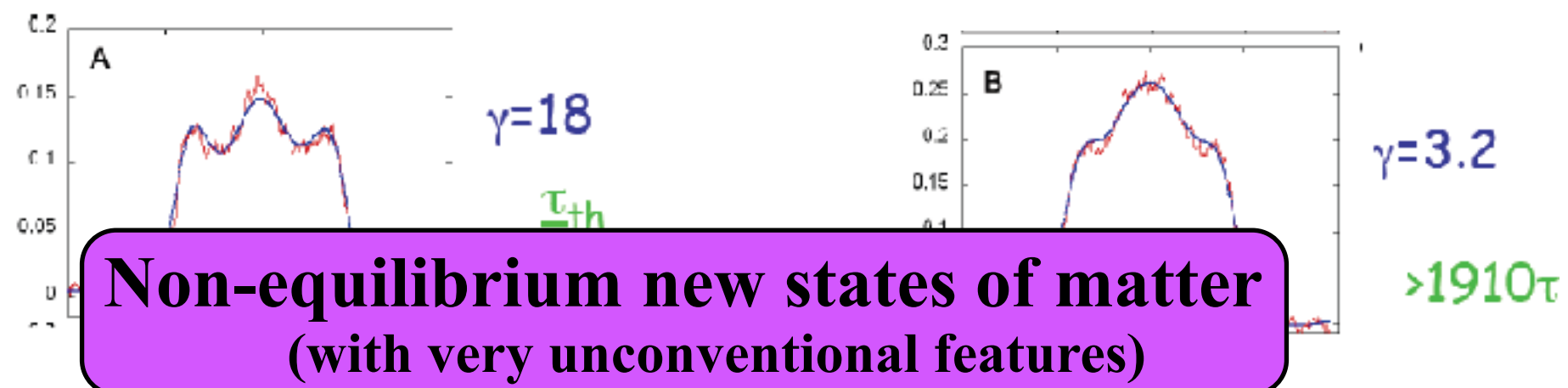
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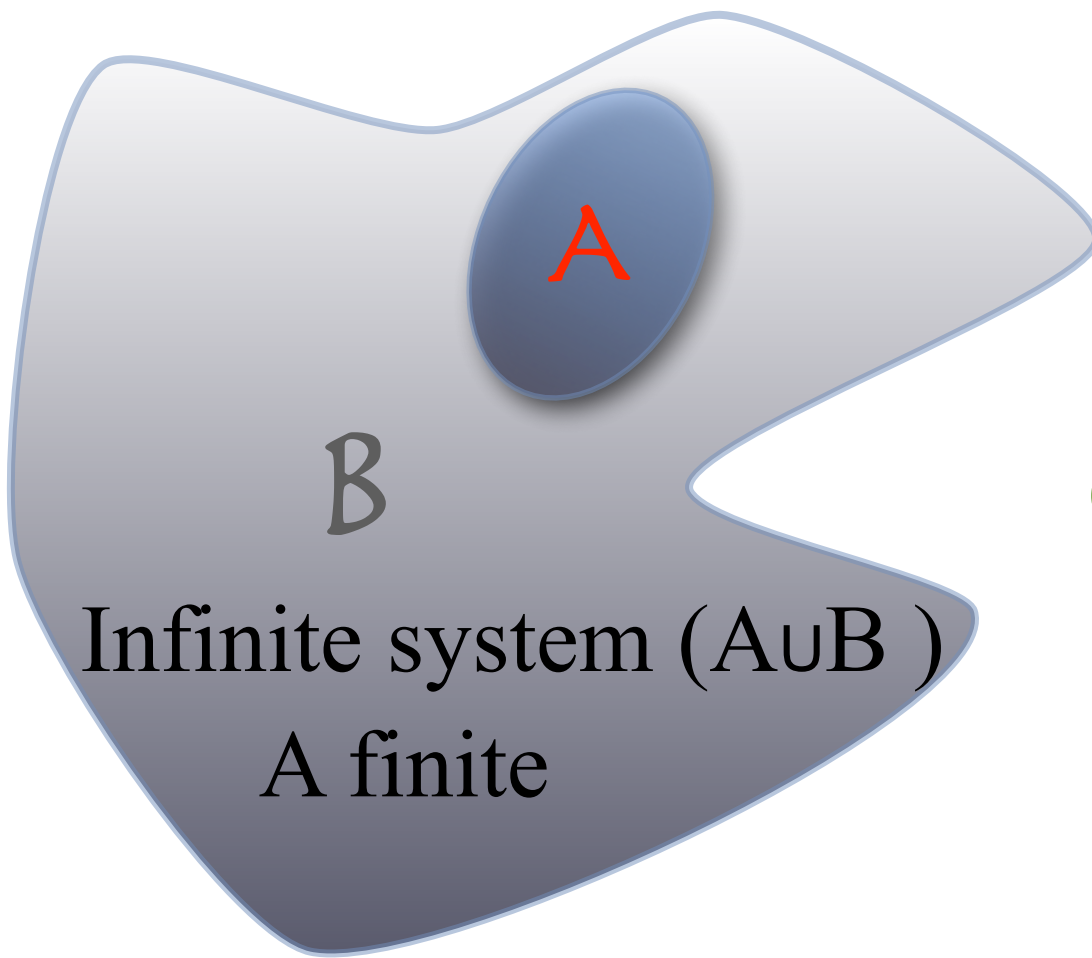
Local observables have the same values as if the entire system was in a thermal ensemble



- 1D system relaxes slowly in time, to a non-thermal distribution



# Entanglement & thermodynamics



● Reduced density matrix:  $\rho_A(t) = \text{Tr}_B \rho(t)$

●  $\rho_A(t)$  corresponds to a mixed state

The **entanglement entropy**  
 $S_A(t) = -\text{Tr}[\rho_A(t) \ln \rho_A(t)]$  measures  
the **bipartite entanglement** between  
A & B

● **Stationary state** exists if for any **finite** subsystem A of an **infinite system**

$$\lim_{t \rightarrow \infty} \rho_A(t) = \rho_A(\infty) \text{ exists}$$

# Thermalization

Consider the Gibbs ensemble for the **entire** system  $A \cup B$

$$\rho_T = e^{-H/T} / Z$$

with

$$\langle \Psi_0 | H | \Psi_0 \rangle = \text{Tr}[\rho_T H]$$

$T$  is fixed by the energy in the initial state: no free parameter!!

Reduced density matrix for subsystem A:  $\rho_{A,T} = \text{Tr}_B \rho_T$

The system thermalizes if for any **finite** subsystem A

$$\rho_{A,T} = \rho_A(\infty)$$

In jargon: the infinite part B of the system acts as a heat bath for A

# Generalized Gibbs Ensemble

What about integrable systems?

Proposal by **Rigol et al 2007**: The GGE density matrix

$$\rho_{\text{GGE}} = e^{-\sum \lambda_m I_m} / Z \quad \text{with } \lambda_m \text{ fixed by } \langle \Psi_0 | I_m | \Psi_0 \rangle = \text{Tr}[\rho_{\text{GGE}} I_m]$$

Again no free parameter!!

$I_m$  are the integrals of motion of  $H$ , *i.e.*  $[I_m, H] = 0$

Reduced density matrix for subsystem A:  $\rho_{\text{A,GGE}} = \text{Tr}_B \rho_{\text{GGE}}$

The system is described by GGE if for any **finite** subsystem A of an infinite system

$$\rho_{\text{A,GGE}} = \rho_{\text{A}}(\infty)$$

[Barthel-Schollwock '08]  
[Cramer, Eisert, et al '08] + .....  
[PC, Essler, Fagotti '12]

But, **which integral of motions** must be included in the GGE?

**Too long and technical answer to be discussed here**



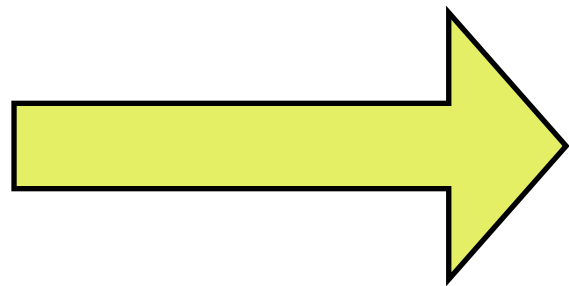
# Entanglement vs Thermodynamics

The equivalence of reduced density matrices

$$\rho_{A,TD} = \rho_A(\infty) \quad \text{TD=Gibbs or GGE}$$

Implies that the subsystem's entropies are the same:  $S_{A,TD} = S_A(\infty)$

The TD entropy  $S_{TD} = -\text{Tr } \rho_{TD} \ln \rho_{TD}$  is extensive



$$\frac{S_{TD}}{L} \simeq \frac{S_{A,TD}}{\ell} = \frac{S_A(\infty)}{\ell}$$

For large time the entanglement entropy becomes thermodynamic entropy

The **entropy** of the stationary state is just the **entanglement** accumulated during time

# Quantum thermalization through entanglement in an isolated many-body system

Adam M. Kaufman, M. Eric Tai, Alexander Lukin, Matthew Rispoli, Robert Schittko, Philipp M. Preiss, Markus Greiner\*

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Science 353, 794 (2016)

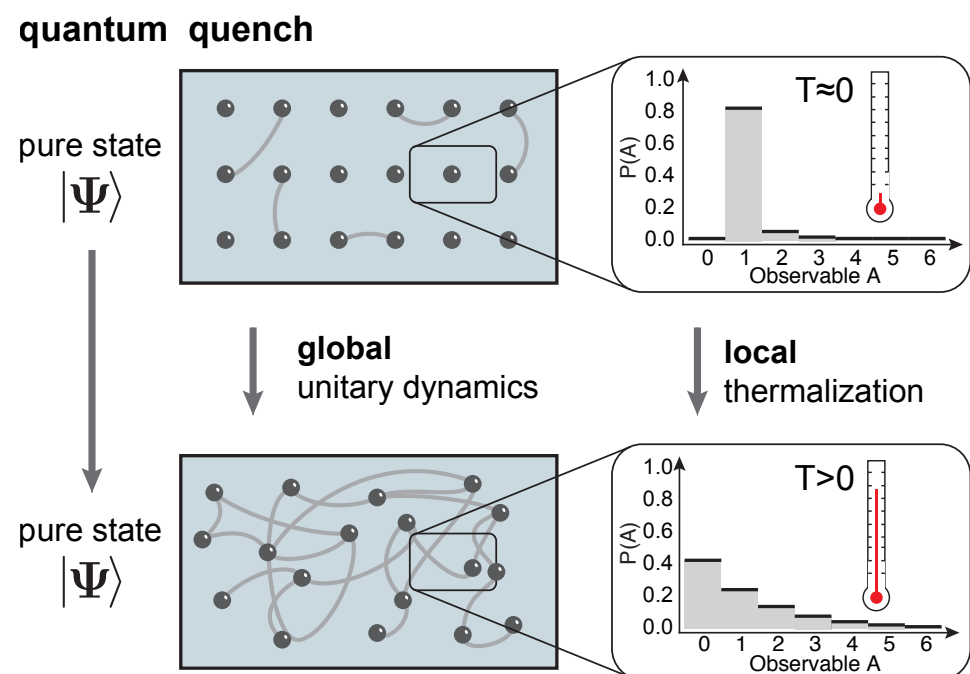
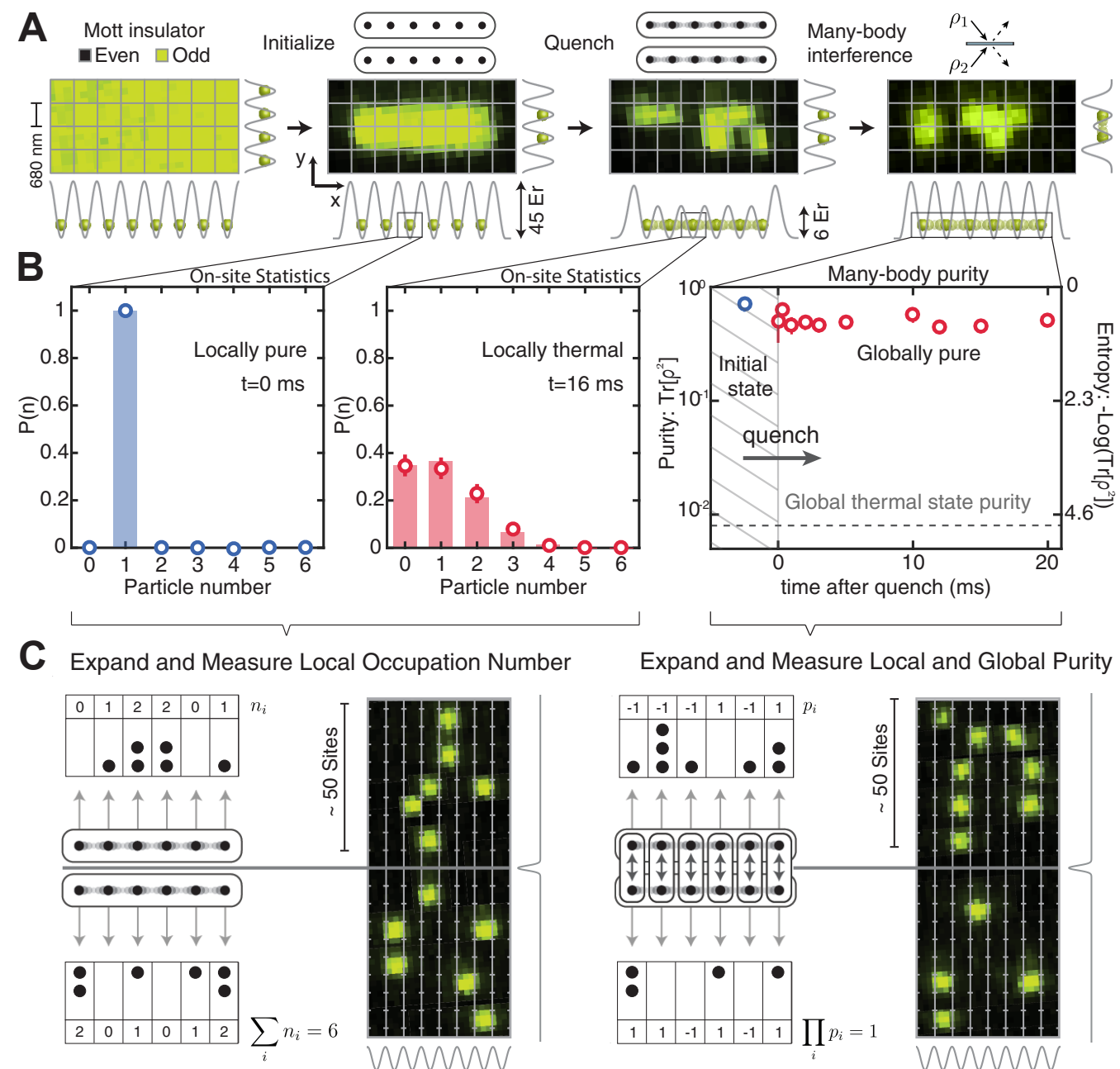


FIG. 1. **Schematic of thermalization dynamics in closed systems.** An isolated quantum system at zero temperature can be described by a single pure wavefunction  $|\Psi\rangle$ . Subsystems of the full quantum state appear pure, as long as the entanglement (indicated by grey lines) between subsystems is negligible. If suddenly perturbed, the full system evolves unitarily, developing significant entanglement between all parts of the system. While the full system remains in a pure, zero-entropy state, the entropy of entanglement causes the subsystems to equilibrate, and local, thermal mixed states appear to emerge within a globally pure quantum state.

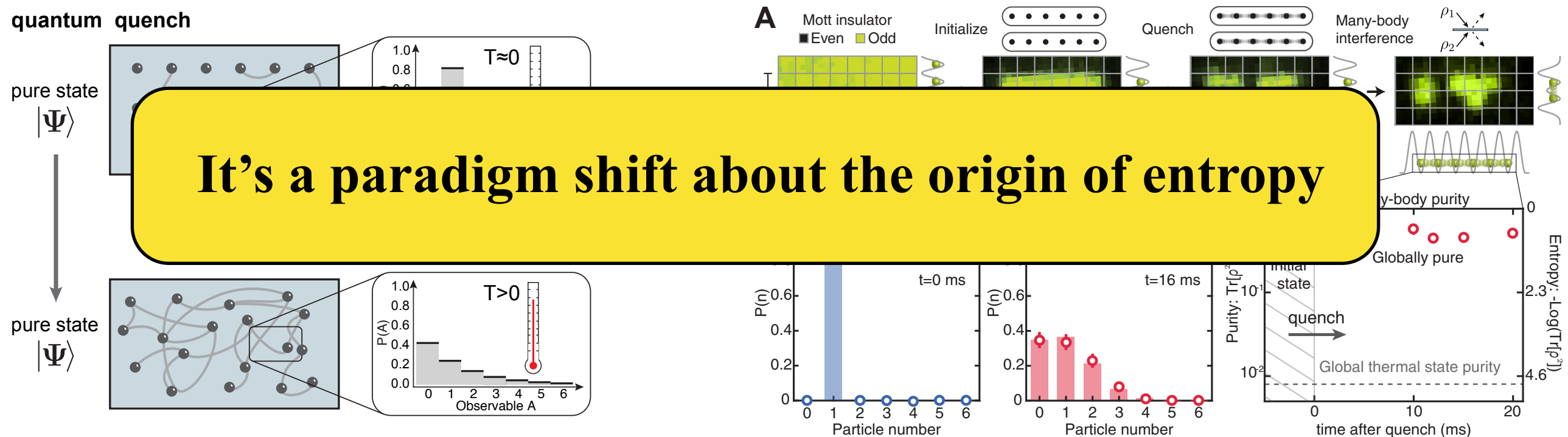


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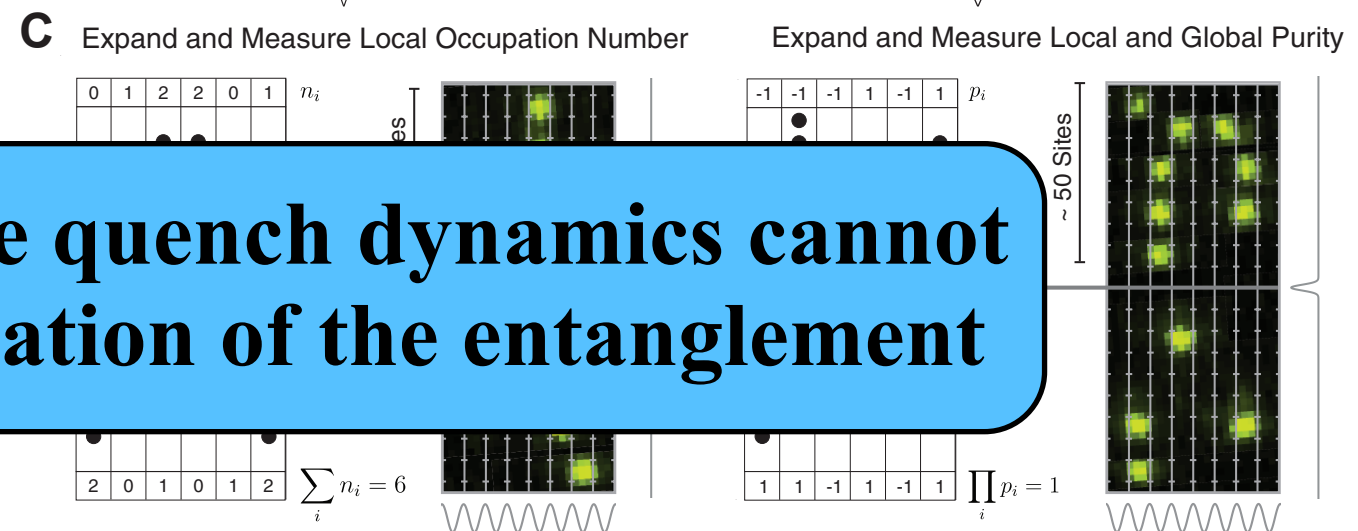
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It's a paradigm shift about the origin of entropy

FIG. 1. **Schematic of thermalization dynamics in closed systems.** An isolated quantum system at zero temperature can be described by a single pure wavefunction  $|\Psi\rangle$ . Subsystems of the system, however, evolve as the entanglement spreads throughout the system. As the entanglement spreads, the subsystems evolve as if they were thermal mixed states. The understanding of the quench dynamics cannot prescind the characterisation of the entanglement.

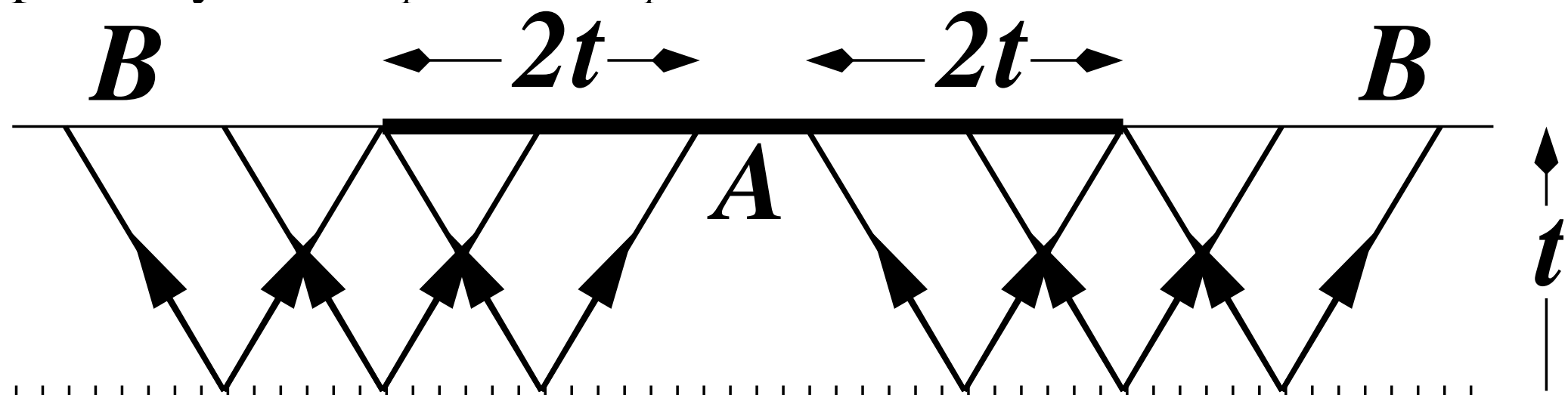
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# Light-cone spreading of entanglement entropy

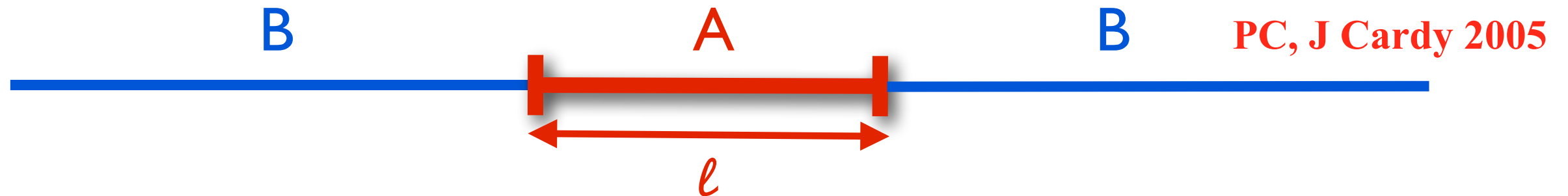
PC, J Cardy 2005

- After a global quench, the initial state  $|\psi_0\rangle$  has an extensive excess of energy
- It acts as a source of quasi-particles at  $t=0$ . A particle of momentum  $p$  has energy  $E_p$  and velocity  $v_p = dE_p/dp$
- For  $t > 0$  the particles move semiclassically with velocity  $v_p$
- particles emitted from regions of size of the initial correlation length are entangled, particles from far points are incoherent
- The point  $x \in A$  is entangled with a point  $x' \in B$  if a left (right) moving particle arriving at  $x$  is entangled with a right (left) moving particle arriving at  $x'$ . This can happen only if  $x \pm v_p t \sim x' \mp v_p t$





# Light-cone spreading of entanglement entropy



- The entanglement entropy of an interval  $A$  of length  $\ell$  is proportional to the total number of pairs of particles emitted from arbitrary points such that at time  $t$ ,  $x \in A$  and  $x' \in B$
- Denoting with  $f(p)$  the rate of production of pairs of momenta  $\pm p$  and their contribution to the entanglement entropy, this implies

$$S_A(t) \approx \int_{x' \in A} dx' \int_{x'' \in B} dx'' \int_{-\infty}^{\infty} dx \int f(p) dp \delta(x' - x - v_p t) \delta(x'' - x + v_p t)$$

$$\propto t \int_0^{\infty} dp f(p) 2v_p \theta(\ell - 2v_p t) + \ell \int_0^{\infty} dp f(p) \theta(2v_p t - \ell)$$

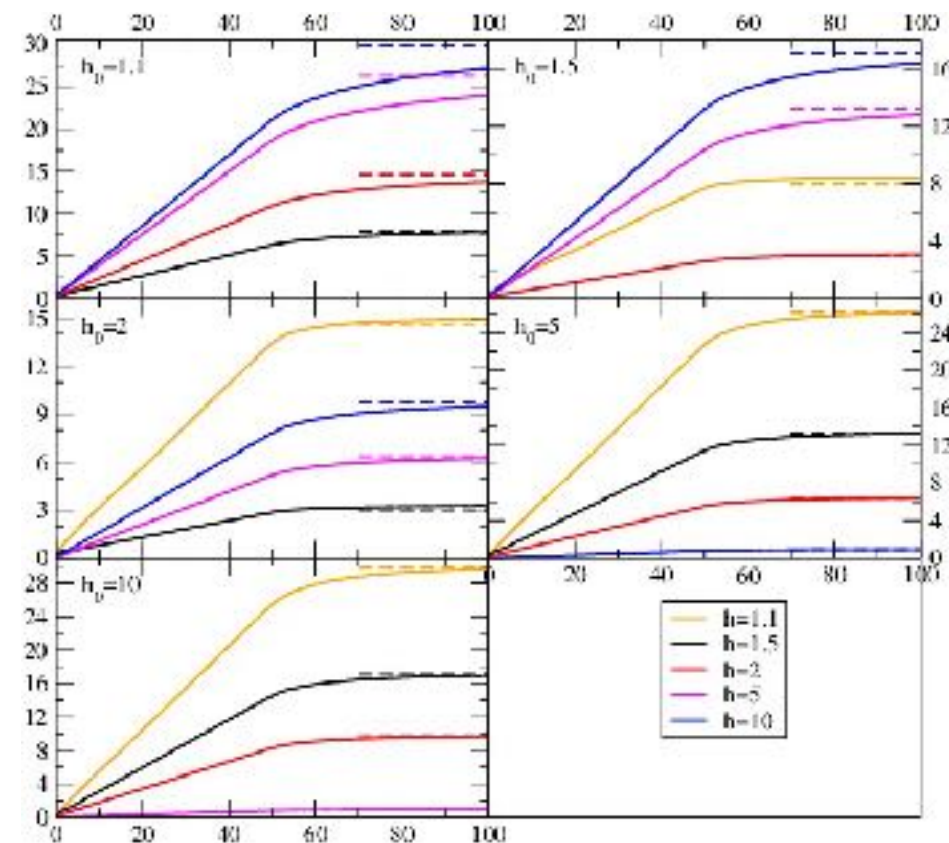
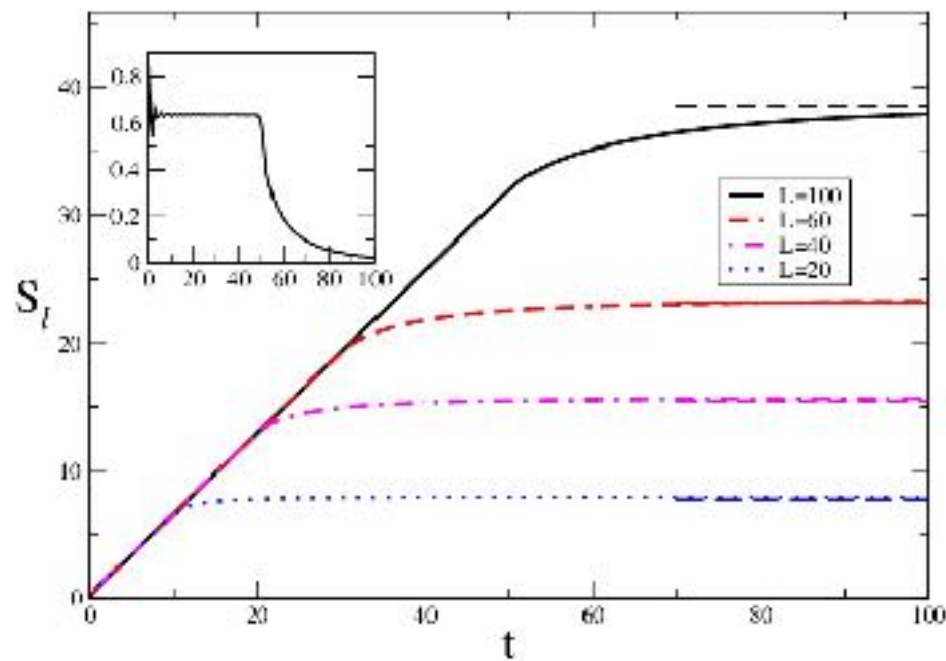
- When  $v_p$  is bounded (e.g. Lieb-Robinson bounds)  $|v_p| < v_{\max}$ , the second term is vanishing for  $2 v_{\max} t < \ell$  and the entanglement entropy grows linearly with time up to a value linear in  $\ell$

**Note:** This is only valid in the space-time scaling limit  $t, \ell \rightarrow \infty$ , with  $t/\ell$  constant

# One example

## Transverse field Ising chain

PC, J Cardy 2005



Analytically for  $t, \ell \gg 1$  with  $t/\ell$  constant

M Fagotti, PC 2008

$$S(t) = t \int_{2|\epsilon'| < t < \ell} \frac{d\varphi}{2\pi} 2|\epsilon'| H(\cos \Delta_\varphi) + \ell \int_{2|\epsilon'| > \ell} \frac{d\varphi}{2\pi} H(\cos \Delta_\varphi)$$

$$\cos \Delta_\varphi = \frac{1 - \cos \varphi (h + h_0) + h h_0}{\epsilon_\varphi \epsilon_\varphi^0}$$

$$H(x) = -\frac{1+x}{2} \log \frac{1+x}{2} - \frac{1-x}{2} \log \frac{1-x}{2}$$

# In the experiment

Kaufmann et al 2016

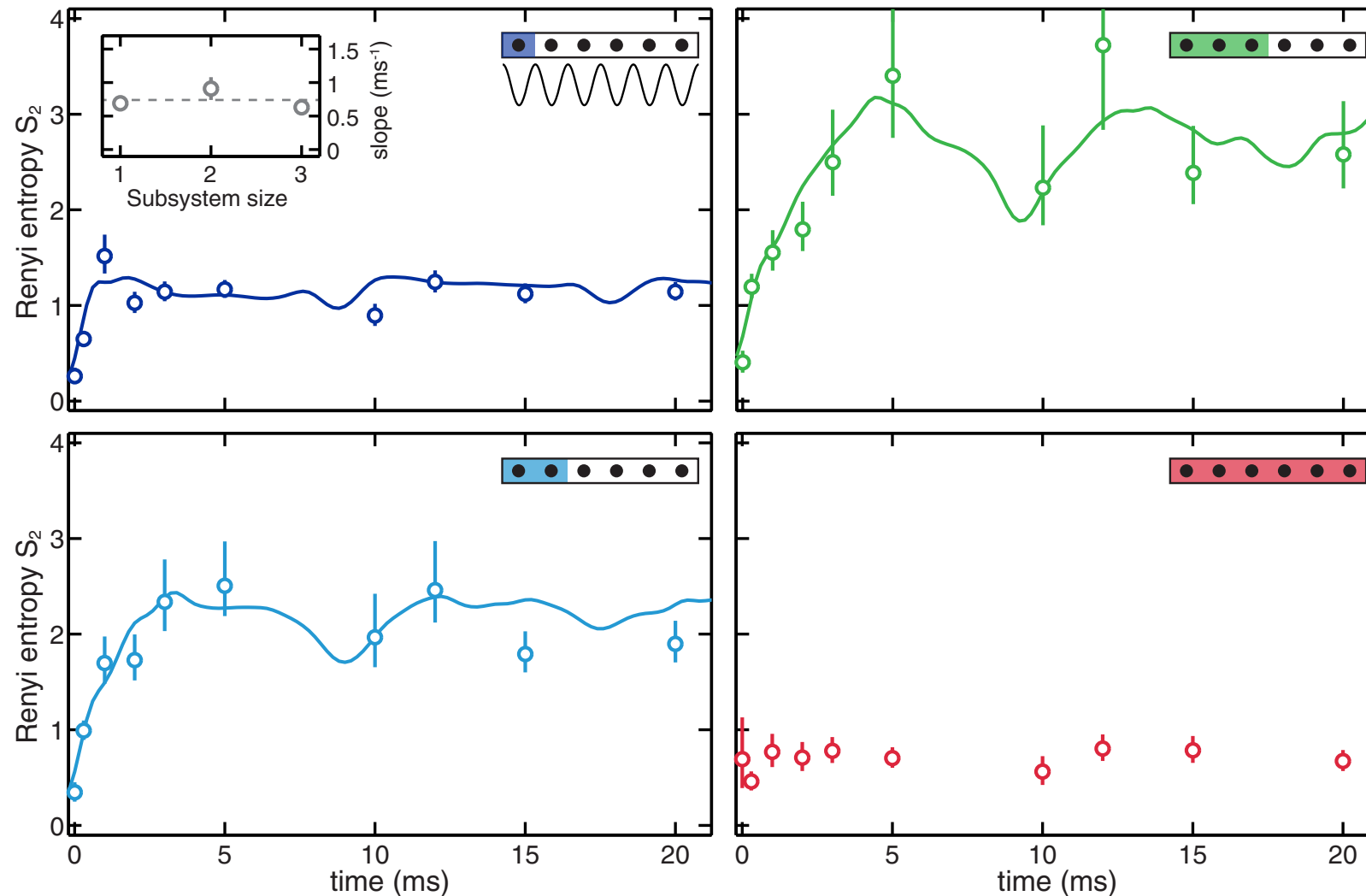
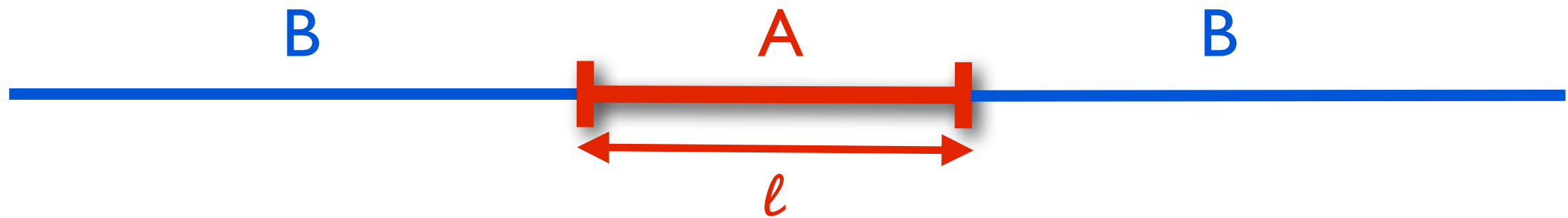


FIG. 3. **Dynamics of entanglement entropy.** Starting from a low-entanglement ground state, a global quantum quench leads to the development of large-scale entanglement between all subsystems. We quench a six-site system from the Mott insulating product state ( $J/U \ll 1$ ) with one atom per site to the weakly interacting regime of  $J/U = 0.64$  and measure the dynamics of the entanglement entropy. As it equilibrates, the system acquires local entropy while the full system entropy remains constant and at a value given by measurement imperfections. The dynamics agree with exact numerical simulations with no free parameters (solid lines). Error bars are the standard error of the mean (S.E.M.). For the largest entropies encountered in the three-site system, the large number of populated microstates leads to a significant statistical uncertainty in the entropy, which is reflected in the upper error bar extending to large entropies or being unbounded. Inset: slope of the early time dynamics, extracted with a piecewise linear fit (see Supplementary Material). The dashed line is the mean of these measurements.

# What is the evolution of the entanglement entropy for a generic integrable models?



- In a generic integrable model, there are infinite species of quasiparticles, corresponding to bound states of an arbitrary number of elementary excitations
- These must be treated independently

$$S(t) = \sum_n \left[ 2t \int_{2|v_n|t < \ell} d\lambda v_n(\lambda) s_n(\lambda) + \ell \int_{2|v_n|t > \ell} d\lambda s_n(\lambda) \right],$$

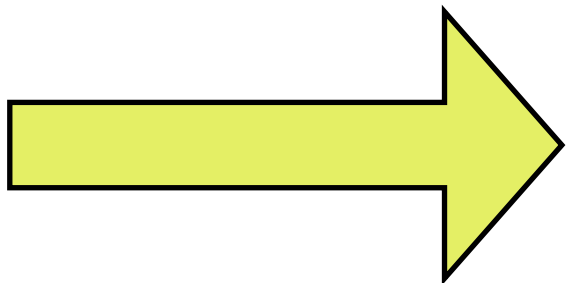
- To give predictive power to this equation, we should devise a way to determine  $v_n$  and  $s_n$



**Idea:** We can use the knowledge of the thermodynamic entropy in the stationary state to go back in time for the entanglement

Alba & PC, 2016

$$S(t) = \sum_n \left[ 2t \int_{2|v_n|t < \ell} d\lambda v_n(\lambda) s_n(\lambda) + \ell \int_{2|v_n|t > \ell} d\lambda s_n(\lambda) \right],$$



$$S(t = \infty) = \ell \sum_n \int d\lambda s_n(\lambda)$$

We need an expression of the stationary entropy written in terms of the quasi-momenta of entangling quasiparticles

# Elementary example: free fermions

It exists a basis in which the Hamiltonian is  $\mathcal{H} = \sum_k \epsilon_k b_k^\dagger b_k$

Given a statistical ensemble  $\rho_{\text{TD}}$ , the TD entropy can be written as

$$S_{\text{TD}} = L \int \frac{dk}{2\pi} H(n_k)$$

with

$$n_k = \langle b_k^\dagger b_k \rangle_{TD} \equiv \text{Tr}[\rho_{TD} b_k^\dagger b_k]$$

$$H(n) = -n \ln n - (1 - n) \ln(1 - n)$$

(i.e. each fermionic modes is independent and has probability  $n_k$  to be occupied and  $1-n_k$  to be empty)

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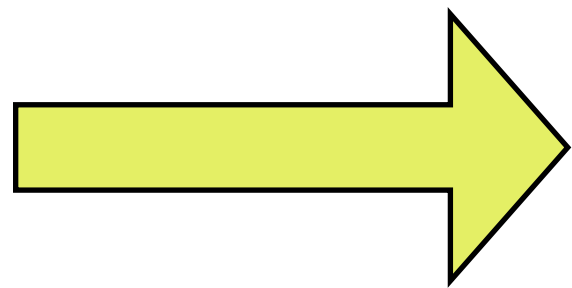
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(i.e. each fermionic modes is independent and has probability  $n_k$  to be occupied and  $1-n_k$  to be empty)



$$S_A(t) = 2t \int_{2|v_k|t < \ell} \frac{dk}{2\pi} v_k H(n_k) + \ell \int_{2|v_k|t > \ell} \frac{dk}{2\pi} H(n_k)$$

generally valid

$$v_k = \epsilon'_k$$

For the quench in the Ising model  $n_k = \frac{1 - \cos \Delta_k}{2}$   
and the above reproduce the Toeplitz result by **M Fagotti, PC 2008**



# Let's get technical





# A slide on Thermodynamic Bethe Ansatz (TBA)

What I cannot create,  
I do not understand.

Know how to solve every  
problem that has been solved

Why const  $\times$  sort. Po

TO LEARN:

Bethe Ansatz Probs.

Kondo

2-D Hall

accel. Temp

Non linear Critical Hydro

$$(A) f = u(r, a)$$

$$g = 4(r, z) u(r, z)$$

$$(B) f = 2|r \cdot a|(u \cdot a)$$



Caltech Archives

# A slide on Thermodynamic Bethe Ansatz (TBA)

An eigenstate of an interacting integrable model in the TD limit is characterised by **TBA data**

'70: Yang-Yang, Takahashi...

$\rho_{n,p}$  is the **particle density** ( $n_k/2\pi$  for free fermions)

$\rho_{n,h}$  is the **hole density** ( $(1-n_k)/2\pi$  for free fermions)

$\rho_{n,t} = \rho_{n,p} + \rho_{n,h}$  is the total density  $\neq 1/2\pi$  because of interactions

$\rho_{n,p}$  and  $\rho_{n,h}$  are related by the (TD limit of) Bethe equations

Each set of  $\rho$ s defines a single macrostate, corresponding to many microstates in a generalised microcanonical ensemble

The TD entropy has the Yang-Yang form

$$S_{YY} = L \sum_{n=1}^{\infty} \int d\lambda [\rho_{n,t}(\lambda) \ln \rho_{n,t}(\lambda) - \rho_{n,p}(\lambda) \ln \rho_{n,p}(\lambda) - \rho_{n,h}(\lambda) \ln \rho_{n,h}(\lambda)]$$

Yang-Yang interpretation:

$\exp(S_{YY})$  counts the number of equivalent micro-states with the same densities

# Quench Action Approach

Caux & Essler 2013

Making a long story short: the stationary state may be represented by a **Bethe eigenstate (representative state)** with calculable (but still challenging)  $\rho$ 's.

The Yang-Yang entropy:

$$S_{YY} = L \sum_{n=1}^{\infty} \int d\lambda [\rho_{n,t}(\lambda) \ln \rho_{n,t}(\lambda) - \rho_{n,p}(\lambda) \ln \rho_{n,p}(\lambda) - \rho_{n,h}(\lambda) \ln \rho_{n,h}(\lambda)]$$

$s_n(\lambda)$

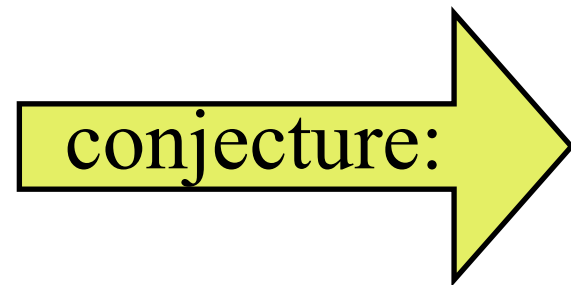
is the corresponding TD entropy

This has the desired form as an integral over quasi-momenta to use it in the quasi-particle picture.

# Final conjecture

Alba & PC, 2016

Assuming that the Bethe excitations are the entangling quasi-particles:



$$S(t) = \sum_n \left[ 2t \int_{2|v_n|t < \ell} d\lambda v_n(\lambda) s_n(\lambda) + \ell \int_{2|v_n|t > \ell} d\lambda s_n(\lambda) \right],$$

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Assuming that the Bethe excitations are the entangling quasi-particles:

conjecture:

$$S(t) = \sum_n \left[ 2t \int_{2|v_n|t < \ell} d\lambda v_n(\lambda) s_n(\lambda) + \ell \int_{2|v_n|t > \ell} d\lambda s_n(\lambda) \right],$$

**Warning:** The determination of the velocity  $v_n(\lambda)$  is a challenge because in integrable models the velocities depend on the state (there is a dressing of the bare velocities due to interaction).

We (reasonably) **conjecture** that the correct ones are the group velocities of the excitations built on top of the stationary state

This is the very same working assumption as in

- Light-cone spreading of correlation **Bonnes, Essler, Lauchli PRL 2013**
- Integrable hydrodynamics **Castro-Alveredo, Doyon, Yoshimura, PRX 2016**  
**Bertini, Collara, De Nardis, Fagotti, PRL 2016**

Calculating these velocities is cumbersome, but doable



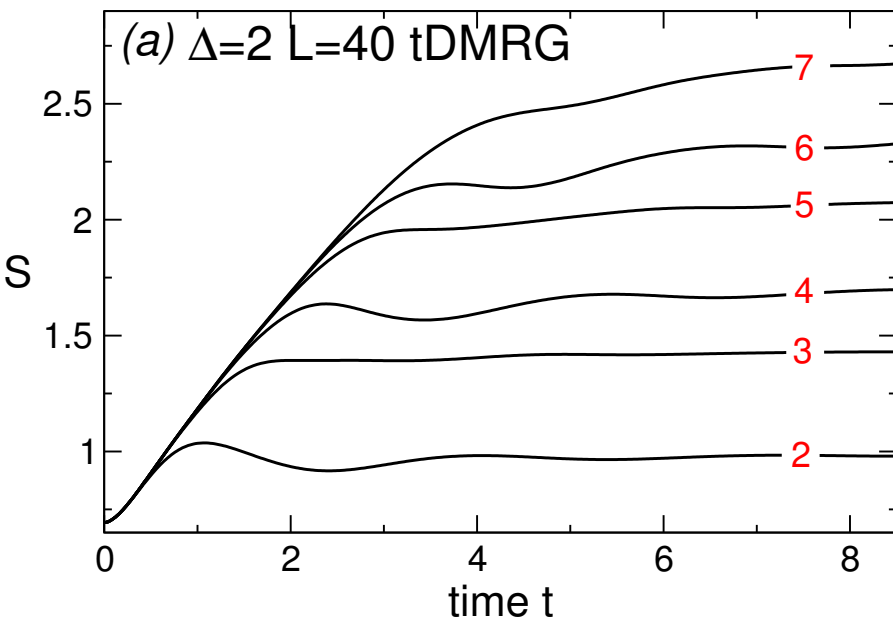
# Test I

conjecture:

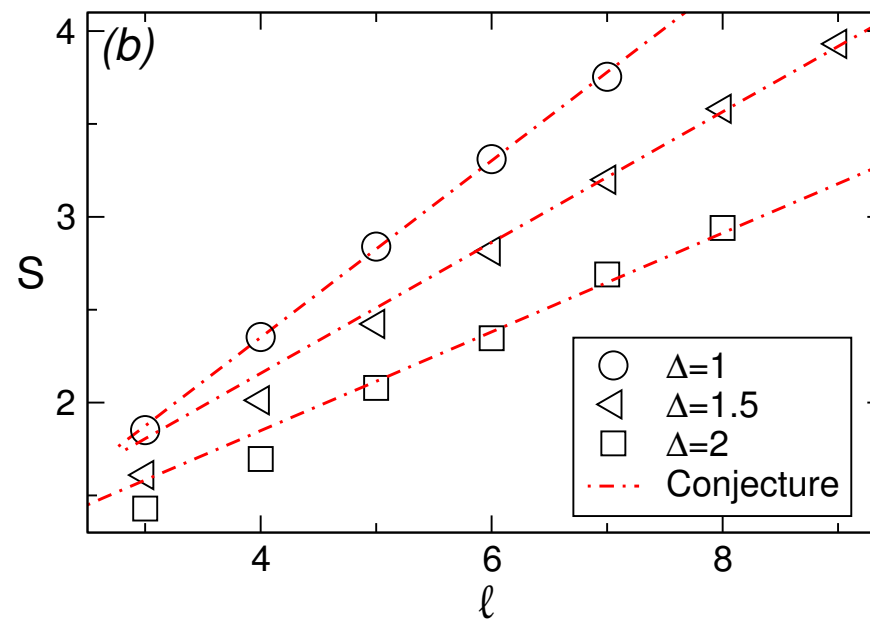
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Conjecture vs tDMRG

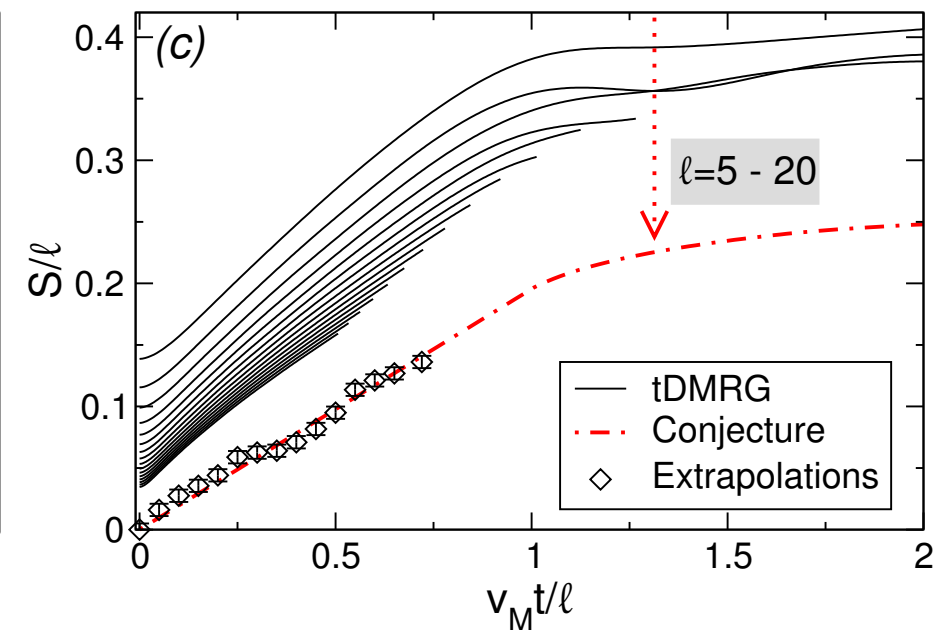
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large t



extrapolation



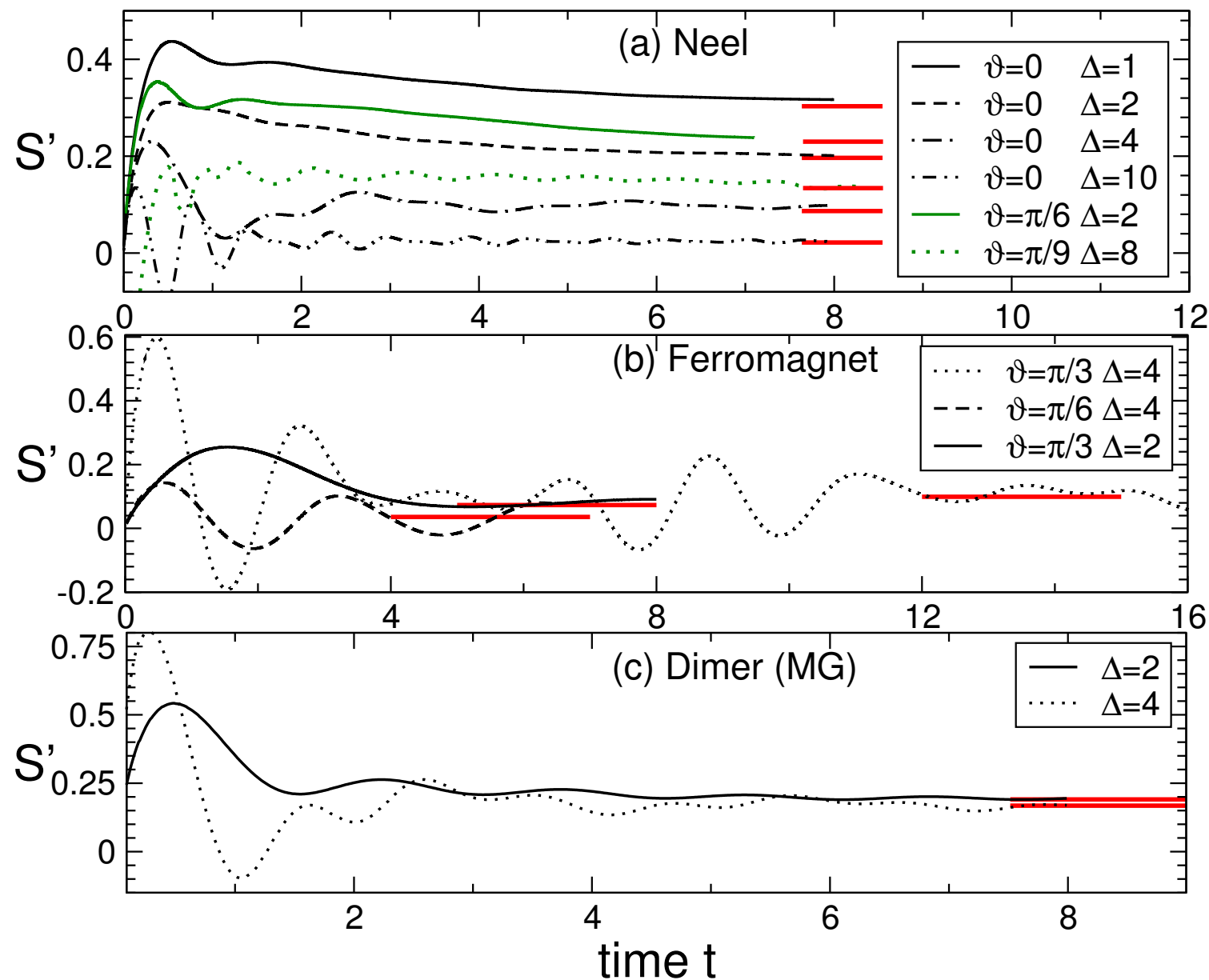
# Test II

conjecture:

$$S(t) = \sum_n \left[ 2t \int d\lambda v_n(\lambda) s_n(\lambda) + \ell \int d\lambda s_n(\lambda) \right],$$

$2|v_n|t < \ell$   $2|v_n|t > \ell$

Conjecture vs iTEBD



Half-chain entanglement

$$S'(t) = \sum_n \int d\lambda v_n(\lambda) s_n(\lambda)$$

# Entanglement and thermodynamics after a quantum quench in integrable systems

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Edited by Subir Sachdev, Harvard University, Cambridge, MA, and approved June 6, 2017 (received for review March 3, 2017)

Entanglement and entropy are key concepts standing at the foundations of quantum and statistical mechanics. Recently, the study of quantum quenches revealed that these concepts are intricately intertwined. Although the unitary time evolution ensuing from a pure state maintains the system at zero entropy, local properties at long times are captured by a statistical ensemble with nonzero thermodynamic entropy, which is the entanglement accumulated during the dynamics. Therefore, understanding the entanglement evolution unveils how thermodynamics emerges in isolated systems. Alas, an exact computation of the entanglement dynamics was available so far only for noninteracting systems, whereas it was deemed unfeasible for interacting ones. Here, we show that the standard quasiparticle picture of the entanglement evolution, complemented with integrability-based knowledge of the steady

source of pairs of quasiparticle excitations. Let us first assume that there is only one type of quasiparticles identified by their quasimomentum  $\lambda$  and moving with velocity  $v(\lambda)$ . Although quasiparticles created far apart from each other are incoherent, those emitted at the same point in space are entangled. Because these propagate ballistically throughout the system, larger regions get entangled. At time  $t$ ,  $S(t)$  is proportional to the total number of quasiparticle pairs that, emitted at the same point in space, are shared between  $A$  and its complement (Fig. 1A). Specifically, one obtains

$$S(t) = \sum_n \left[ 2t \int_{2|v_n|t < \ell} d\lambda v_n(\lambda) s_n(\lambda) + \ell \int_{2|v_n|t > \ell} d\lambda s_n(\lambda) \right], \quad [1]$$

- 1 This is a conjecture, search for proof
- 2 Valid for arbitrary integrable models
- 3 Show in a simple formula the crossover from entanglement to thermodynamics

# Entanglement and thermodynamics after a quantum quench in integrable systems

Vincenzo Alba<sup>a,1</sup> and Pasquale Calabrese<sup>a</sup>

<sup>a</sup>International School for Advanced Studies, Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, 34136 Trieste, Italy

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$$S(t) \propto 2t \int_{2|v|t < \ell} d\lambda v(\lambda) f(\lambda) + \ell \int_{2|v|t > \ell} d\lambda f(\lambda), \quad [1]$$

Different multiplets of quasiparticles (triplets...)

Bertini, Tartaglia & PC

Transport

Bertini, Fagotti, Piroli & PC

Renyi entropy & Entanglement spectrum

Alba, Mestyan & PC

Breaking of integrability

Too many people