Entanglement and thermodynamics in non-equilibrium isolated quantum systems

Pasquale Calabrese

SISSA-Trieste

Rome, Feb 16th 2018

Joint work with Vincenzo Alba

PNAS **114**, 7947 (2017) & 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:

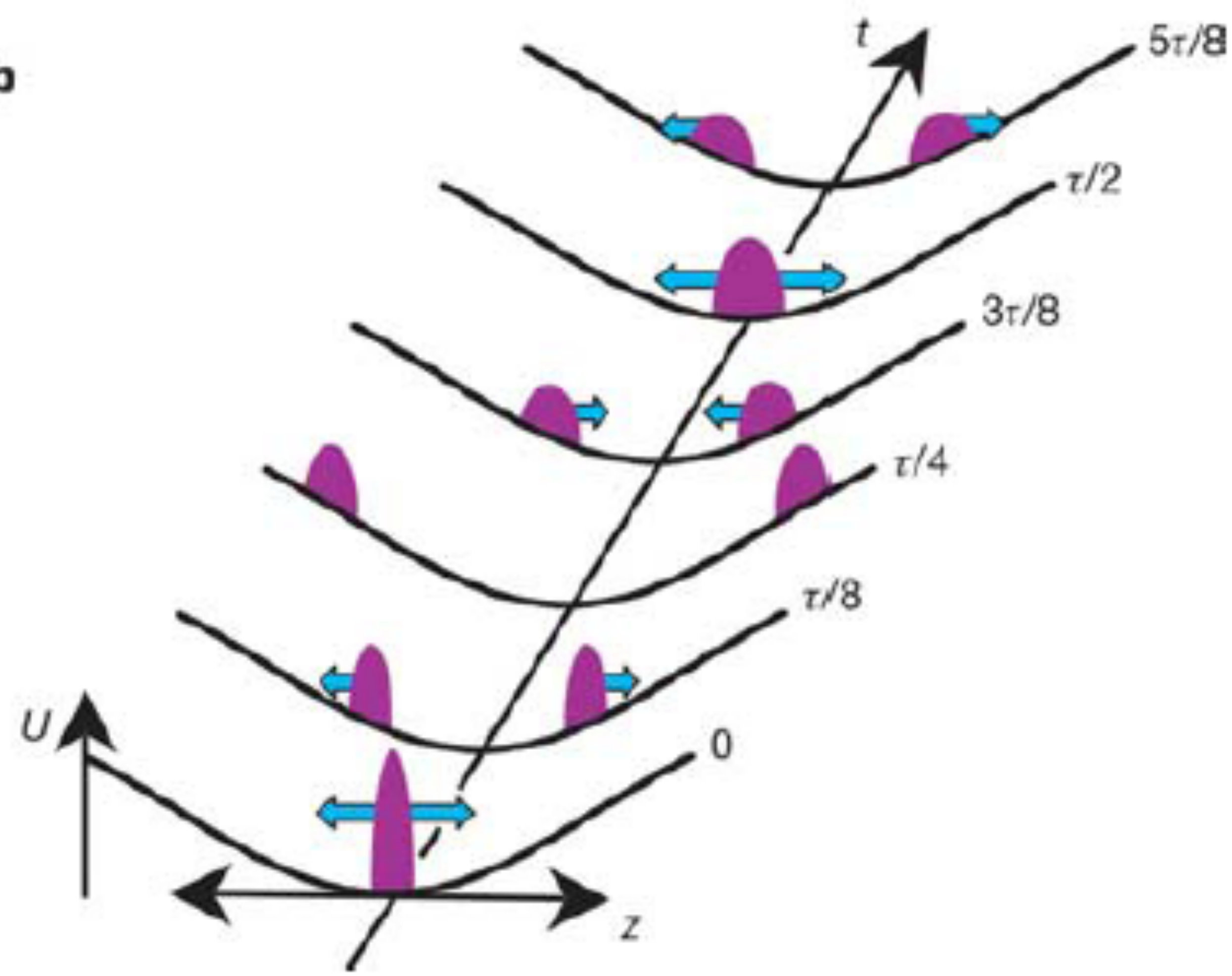
- How can we describe the dynamics?
- Does it exist a stationary state?
- Can it be thermal? In which sense?

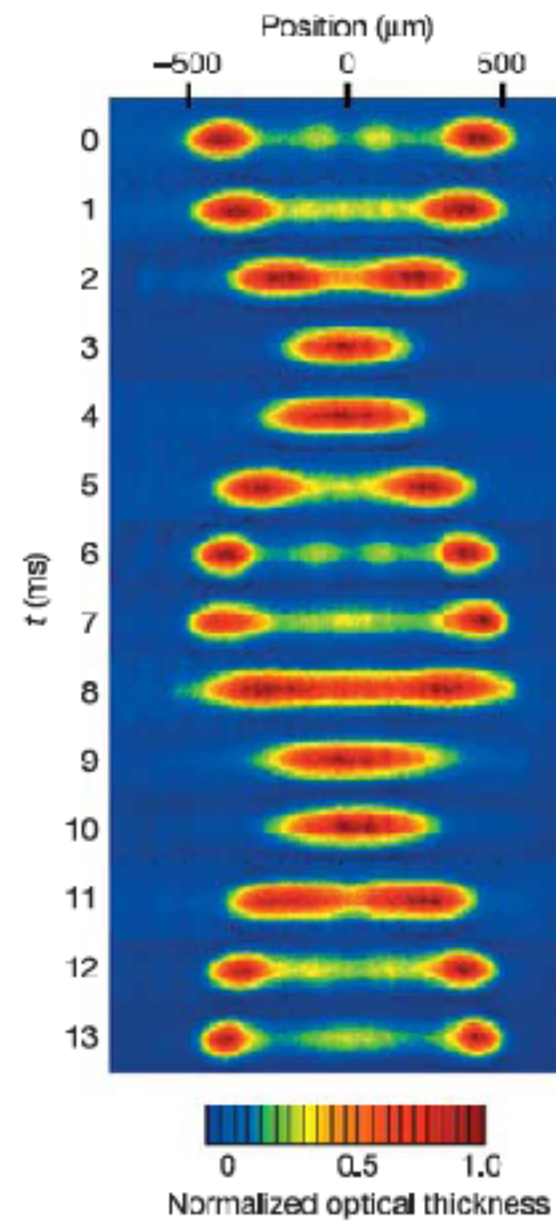
Don't forget: $|\Psi(t)\rangle$ is pure (zero entropy) for any t while the thermal mixed state has non-zero entropy

Quantum Newton cradle

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

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



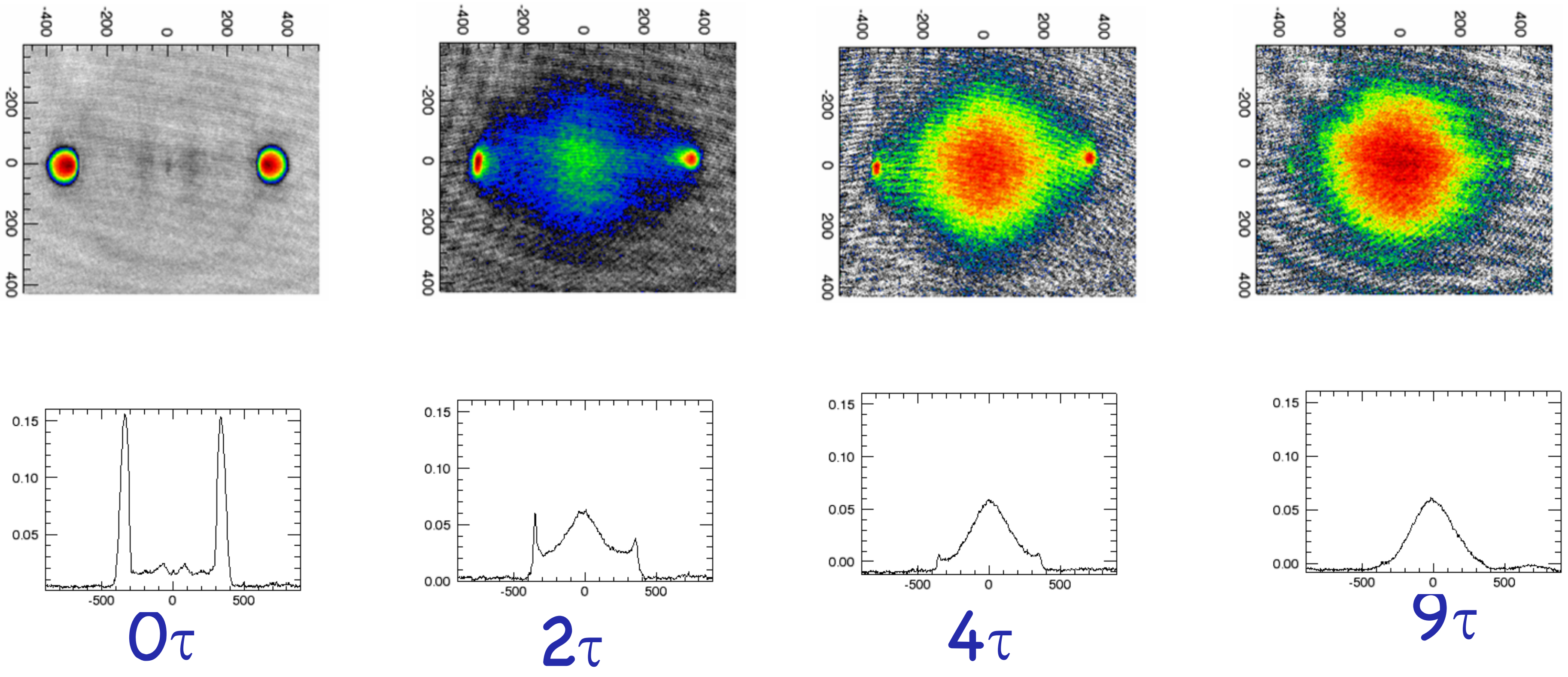


Essentially unitary time evolution

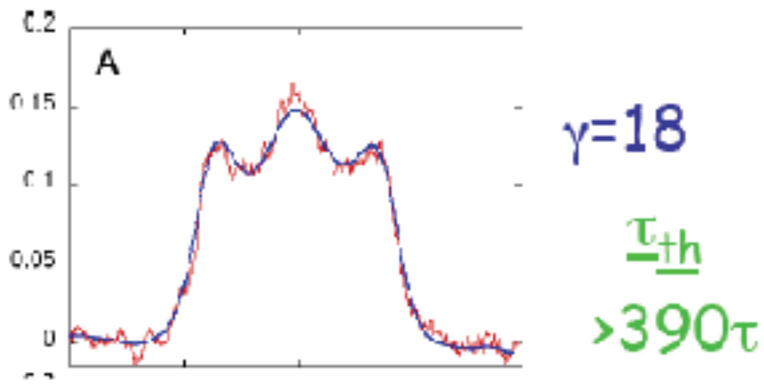
Quantum Newton cradle

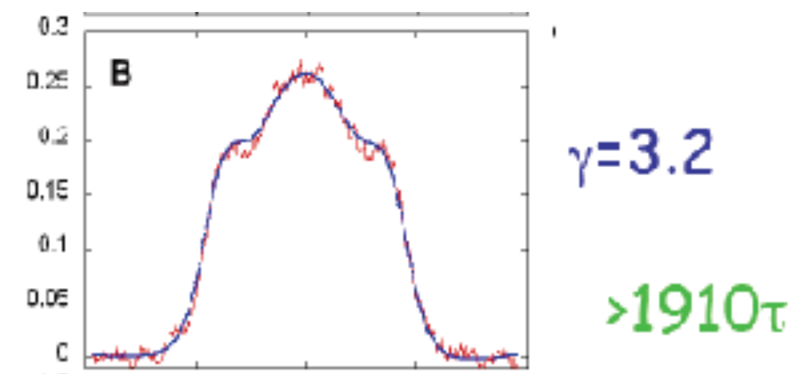
Kinoshita et al 2006

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



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





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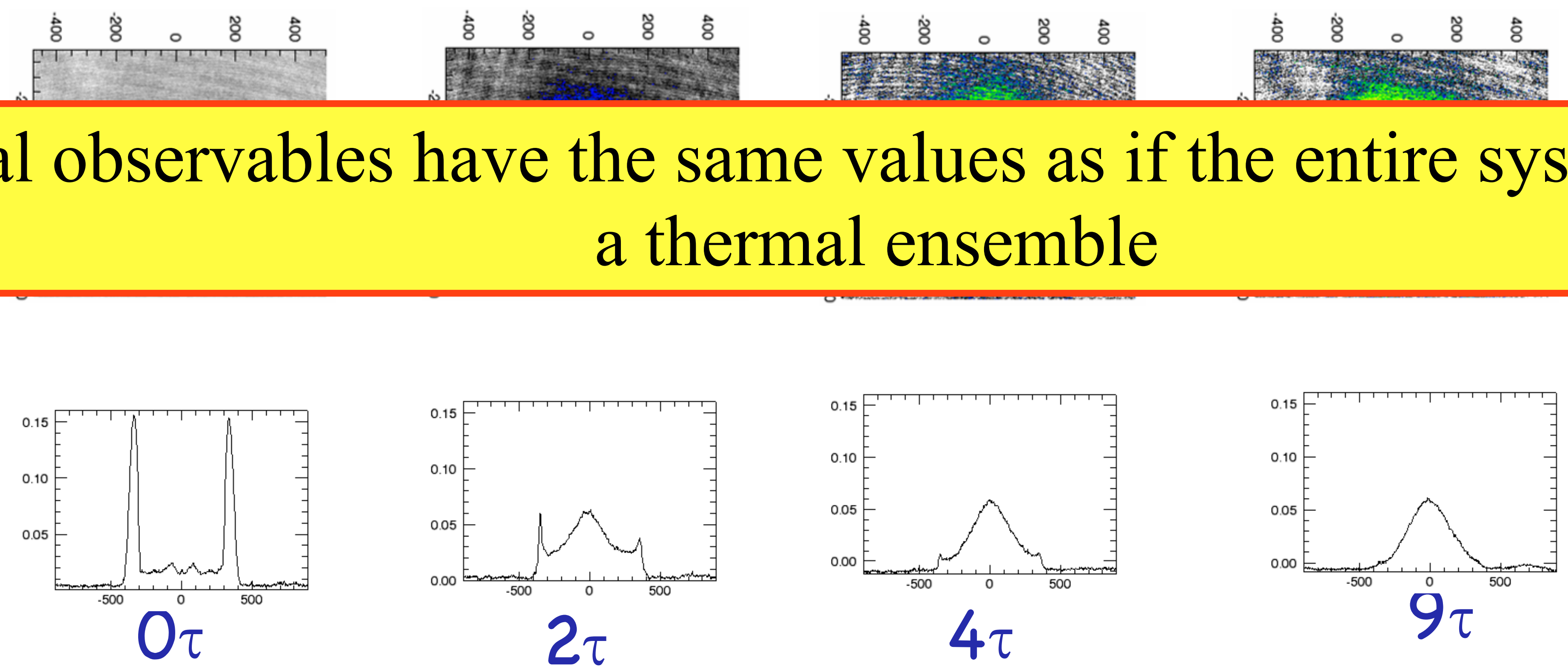
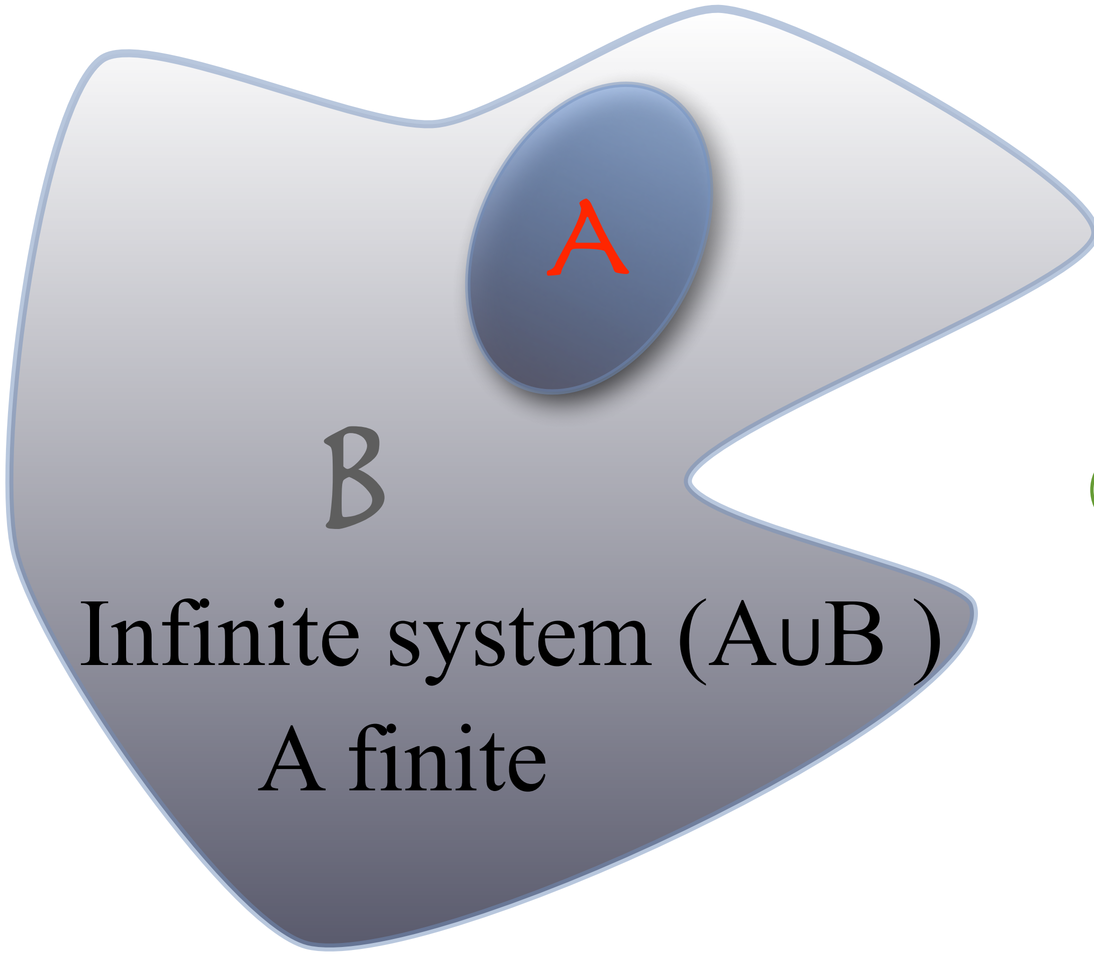


Local observables have the same values as if the entire system was in a thermal ensemble

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

Non-equilibrium new states of matter
(with very unconventional features)

Entanglement & thermodynamics



- Reduced density matrix: $\rho_A(t) = \mathrm{Tr}_B\, \rho(t)$

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

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

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

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

Thermalization

Consider the Gibbs ensemble for the entire system A∪B

$\boxed{\rho_T = e^{-H/T}/Z}$ with $\boxed{\langle\Psi_0|\, H\, |\Psi_0\rangle = \mathrm{Tr}[\rho_T\, H]}$

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

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

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 an heat bath for A

Generalized Gibbs Ensemble

What about integrable systems?

Proposal by Rigol et al 2007: The GGE density matrix

$$\boxed{\rho_{\mathrm{GGE}} = e^{-\sum \lambda_m I_m} / Z}$$

with λ_m fixed by $\langle \Psi_0 | I_m | \Psi_0 \rangle = \mathrm{Tr}[\rho_{\mathrm{GGE}} I_m]$

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: $\rho_{A,\mathrm{GGE}} = \mathrm{Tr}_B\, \rho_{\mathrm{GGE}}$

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

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

[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

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

TD=Gibbs or GGE

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

The TD entropy S_{TD}=-Tr ρ_{TD} ln ρ_{TD} is extensive

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

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

Science 353, 794 (2016)

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

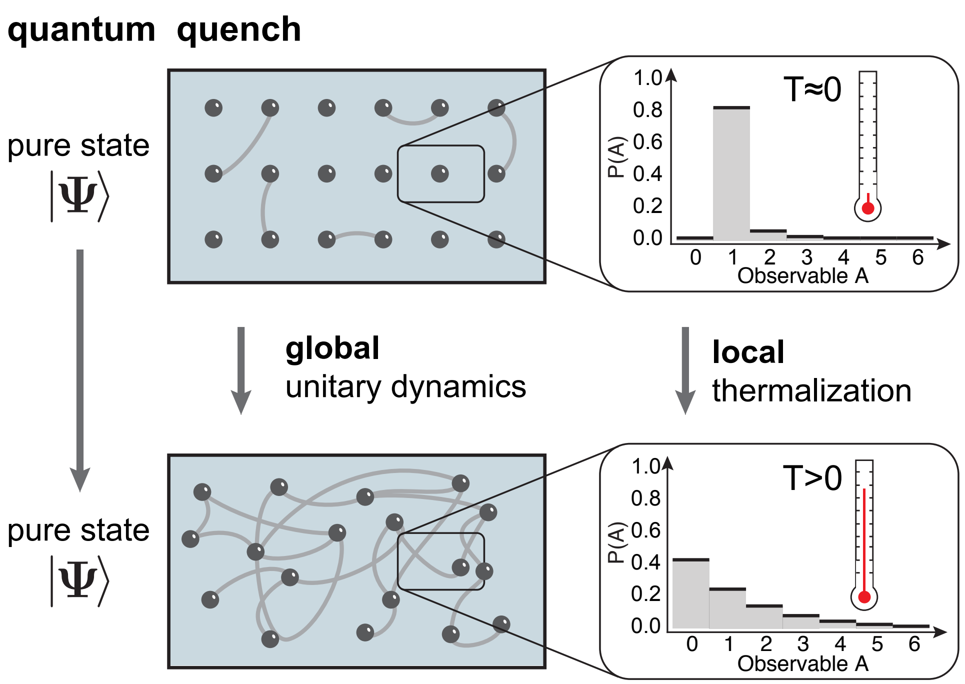
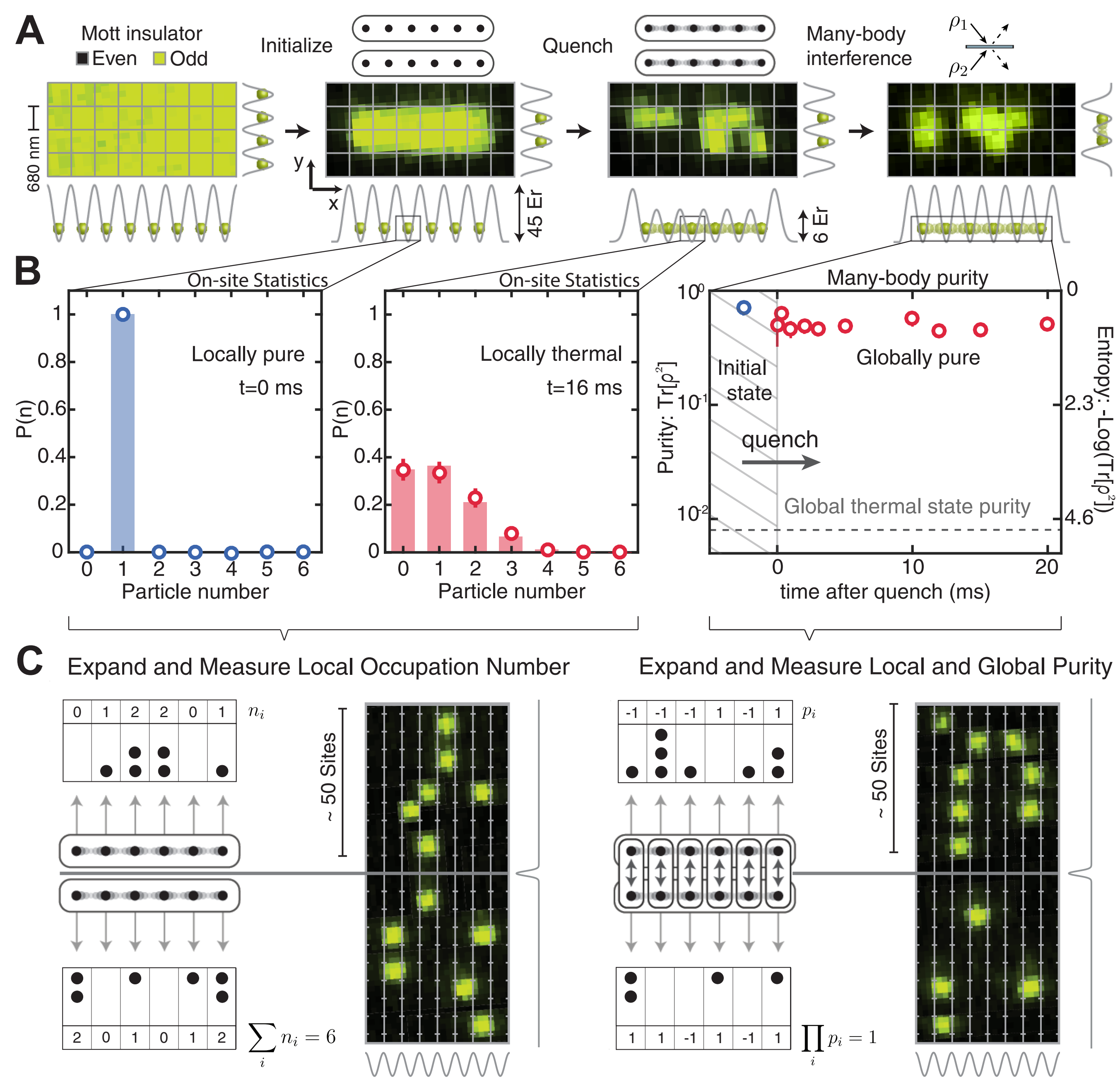


FIG. 1. **Schematic of thermalization dynamics in closed systems**. An isolated quantum system at zero temperature can be described by a single pure wavefunction $|\Psi\rangle$. Subsystems of the full quantum state appear pure, as long as the entanglement (indicated by grey lines) between subsystems 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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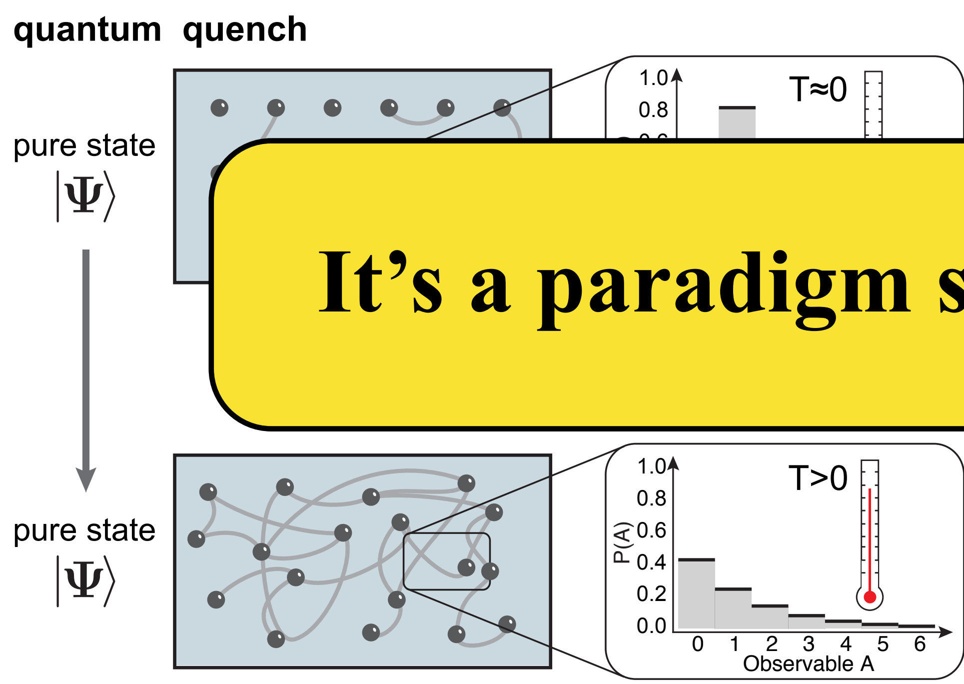

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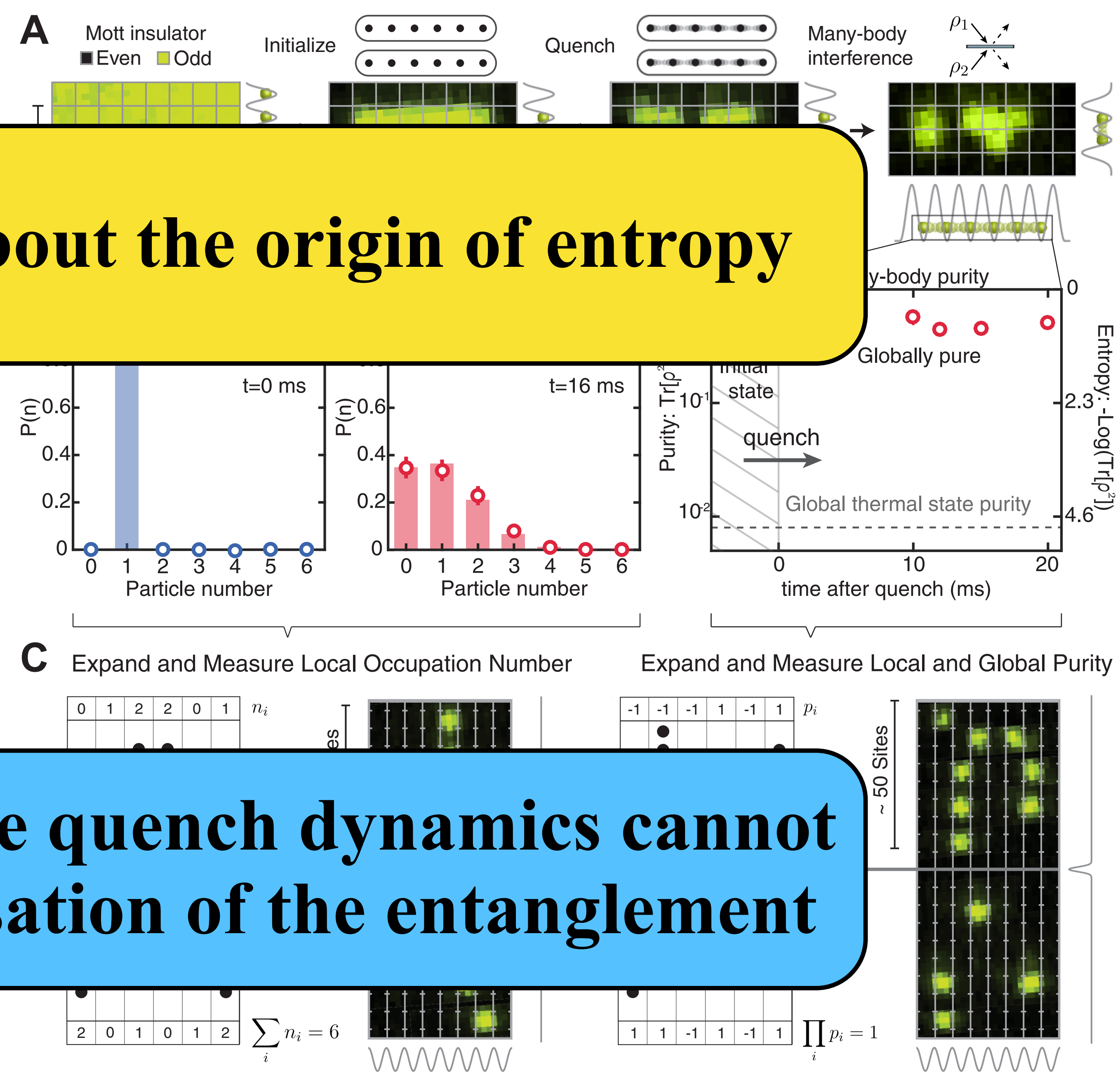


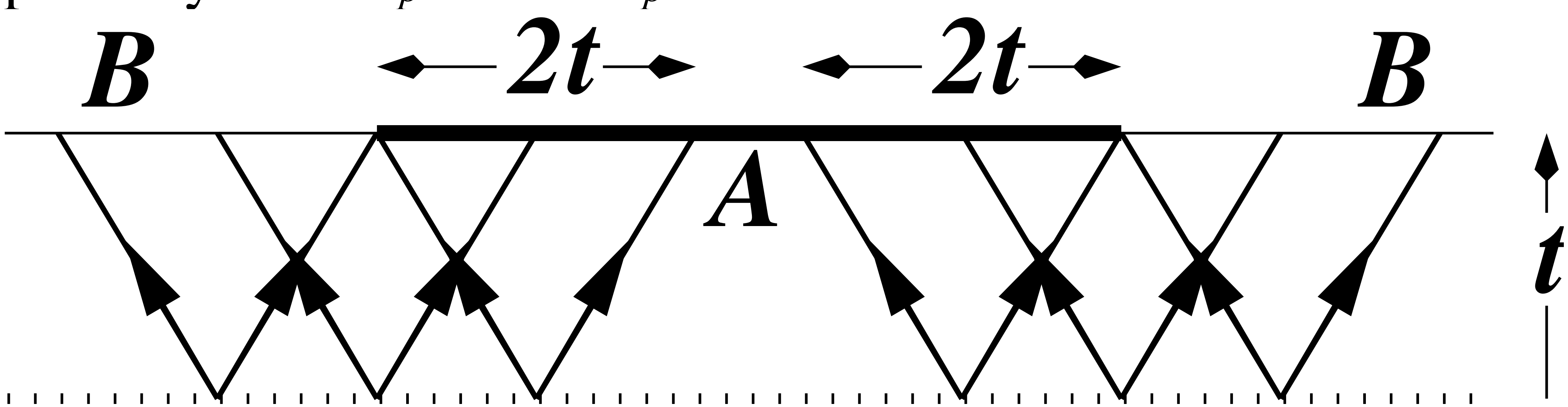
It's a paradigm shift about the origin of entropy

The understanding of the quench dynamics cannot prescind the characterisation of the entanglement

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 moves 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 $x \pm v_p t \sim x' \mp v_p t$



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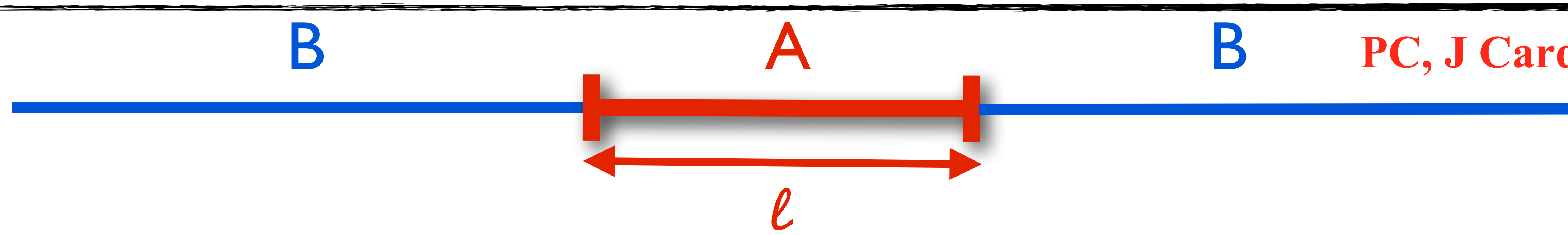


PC, J Cardy 2005

- The entanglement entropy of an interval A of length ℓ 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

$$S_A(t) \approx \int_{x'\in A} dx' \int_{x''\in B} dx'' \int_{-\infty}^{\infty} dx \int f(p) dp \delta\big(x' - x - v_p t\big)\delta\big(x'' - x + v_p t\big)$$
$$\propto t \int_0^{\infty} dp f(p) 2v_p \theta(\ell - 2v_p t) + \ell \int_0^{\infty} dp f(p) \theta(2v_p t - \ell)$$

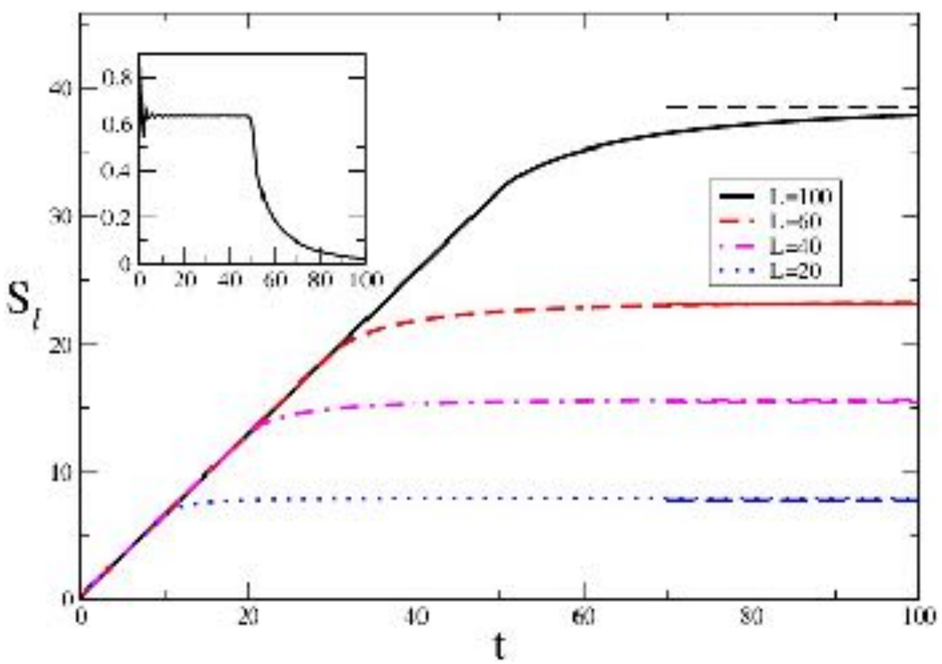
- When v_p is bounded (e.g. Lieb-Robinson bounds) $|v_p|<v_{\max}$, the second term is vanishing for $2\, v_{\max}\, t<\ell$ and the entanglement entropy grows linearly with time up to a value linear in ℓ

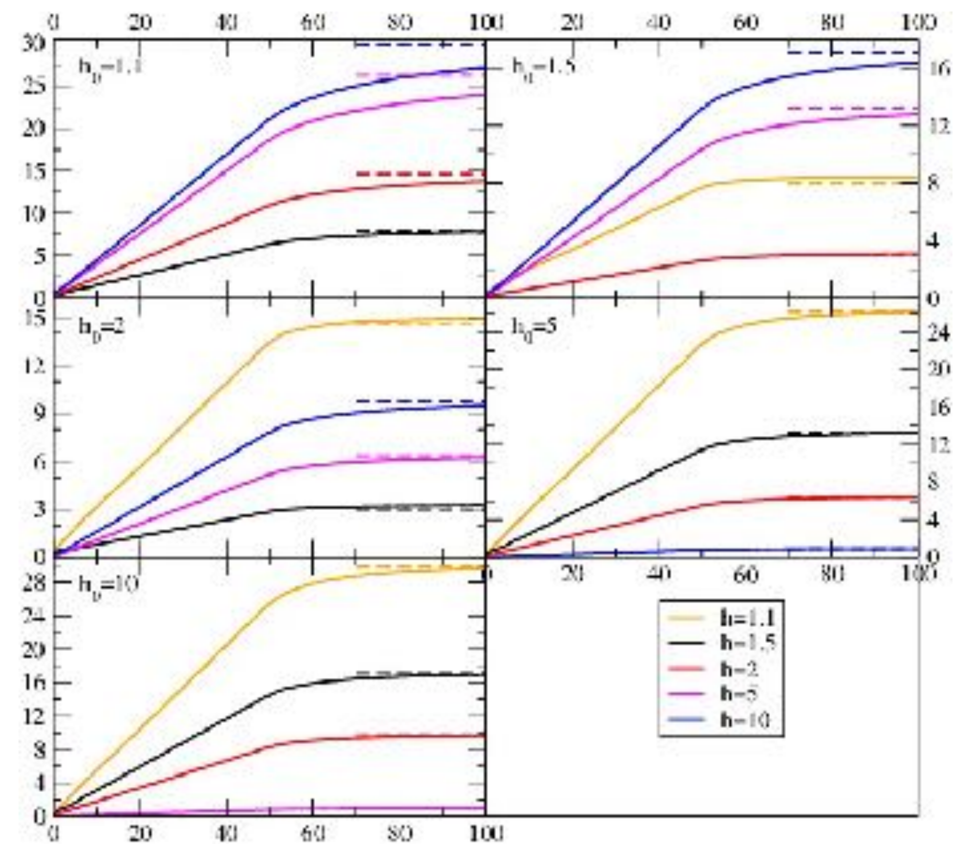
Note: This is only valid in the space-time scaling limit $t,\ell\rightarrow\infty$, with t/ℓ constant

One example

Transverse field Ising chain

PC, J Cardy 2005





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

M Fagotti, PC 2008

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

$$\cos\Delta_\varphi = \frac{1-\cos\varphi(h+h_0)+hh_0}{\epsilon_\varphi \epsilon^0_\varphi} \qquad H(x) = -\frac{1+x}{2}\log\frac{1+x}{2} - \frac{1-x}{2}\log\frac{1-x}{2}$$

In the experiment

Kaufmann et al 2016

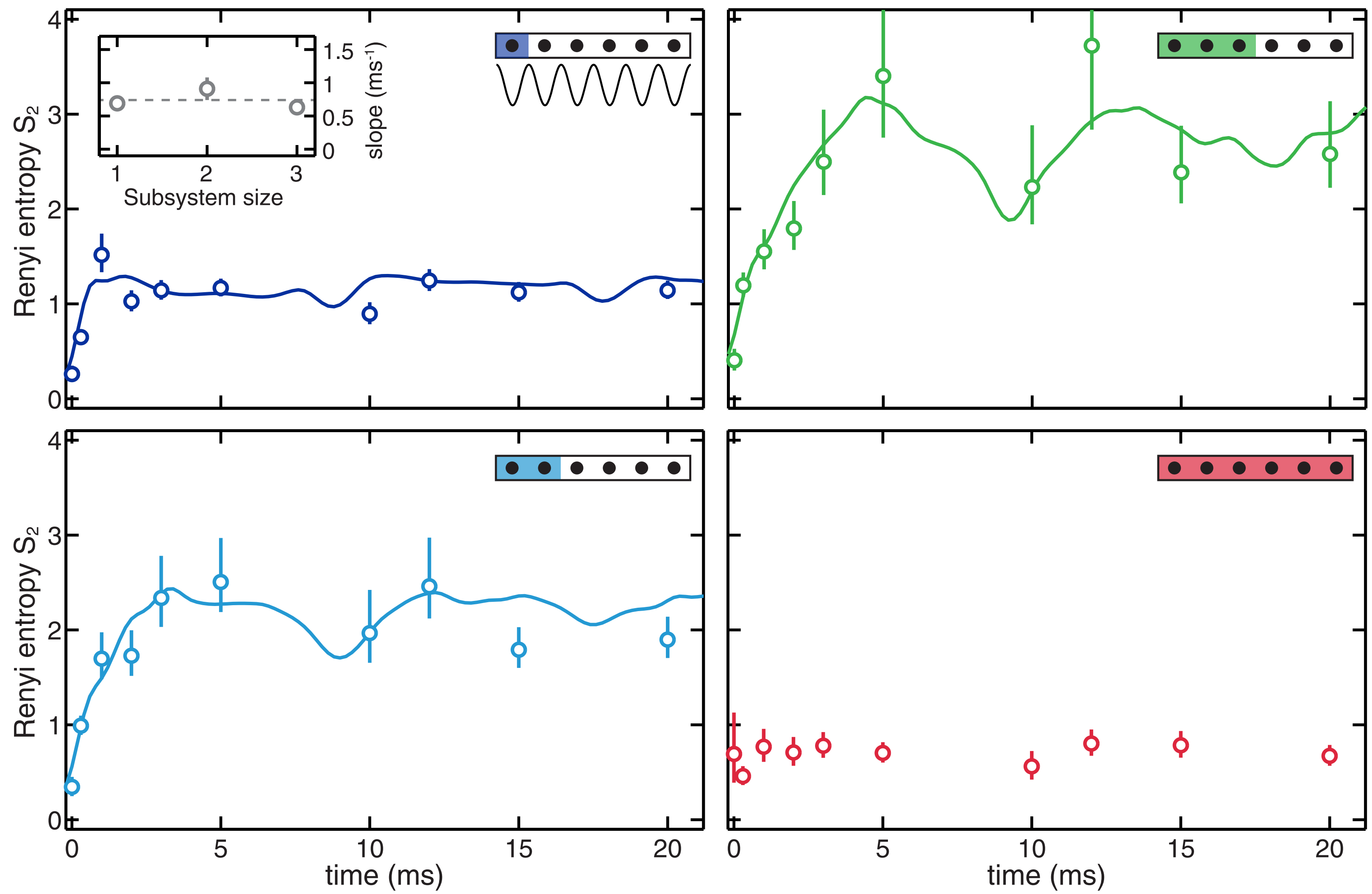
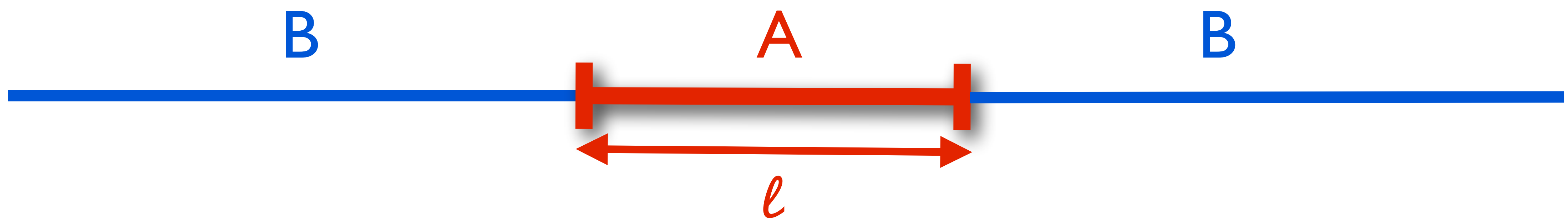


FIG. 3. **Dynamics of entanglement entropy.** Starting from a low-entanglement ground state, a global quantum quench leads to the development of large-scale entanglement between all subsystems. We quench a six-site system from the Mott insulating product state ($J/U \ll 1$) with one atom per site to 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 $\rho_{\rm TD}$, the TD entropy can be written as

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

with

$$n_k = \langle b_k^\dagger b_k \rangle_{TD} \equiv \mathrm{Tr}[\rho_{TD} b_k^\dagger b_k] \qquad H(n) = -n \ln n - (1-n)\ln(1-n)$$

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

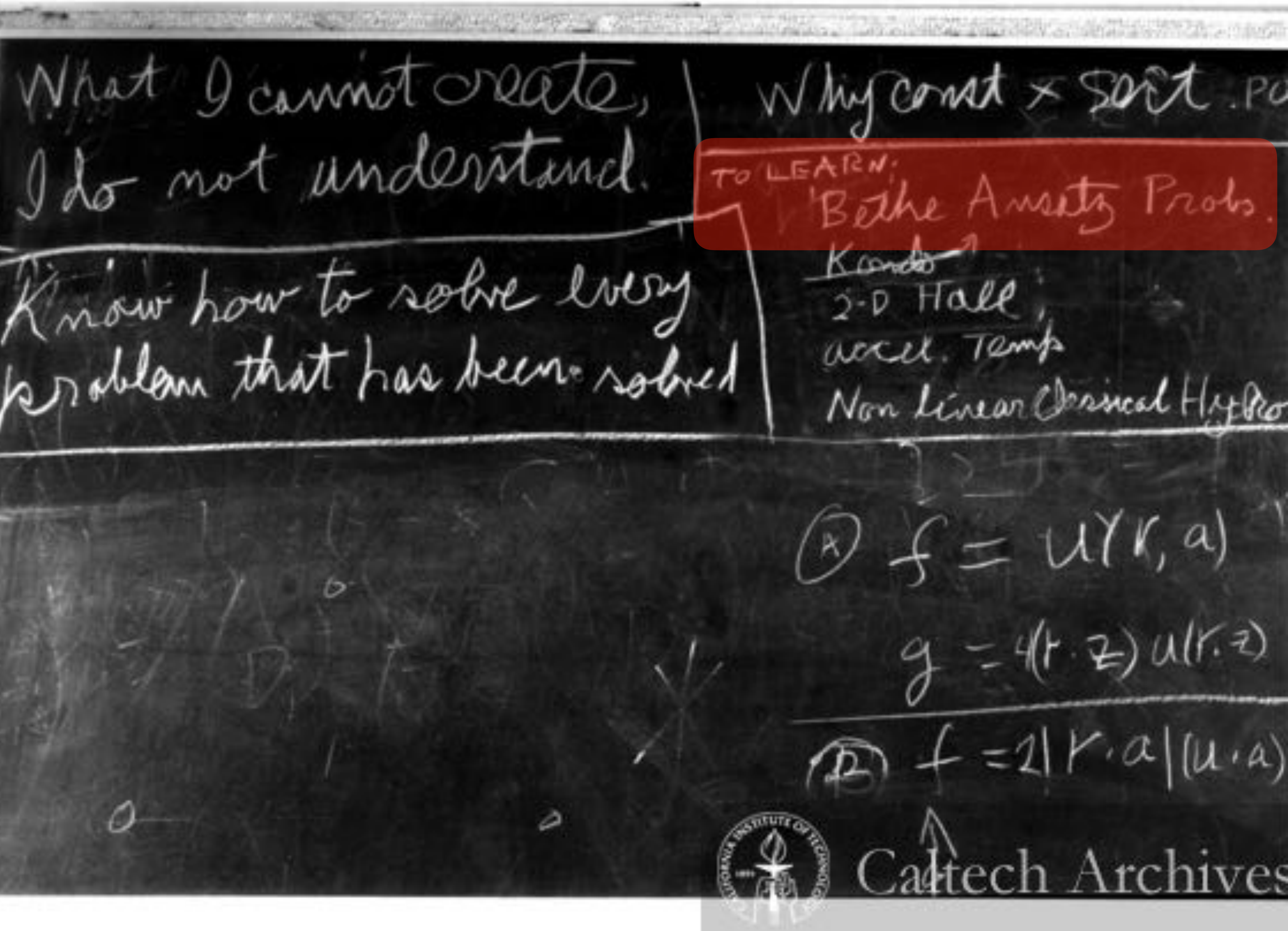
generally valid

$$v_k = \epsilon'_k$$

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 × sort. PC
TO LEARN:
Bethe Ansatz Probs.
~~Kondo~~
2-D Hall
accel. Temp
Non Linear Classical Hydro
Ⓐ f = u(r, a)
g = 4(r·z) u(r·z)
Ⓑ f = 2|r·a|(u·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 ρs defines a single macrostate, corresponding to many microstates in a generalised microcanonical ensemble

The TD entropy has the Yang-Yang form

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

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) ρ's.

The Yang-Yang entropy:

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

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:

conjecture:

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

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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

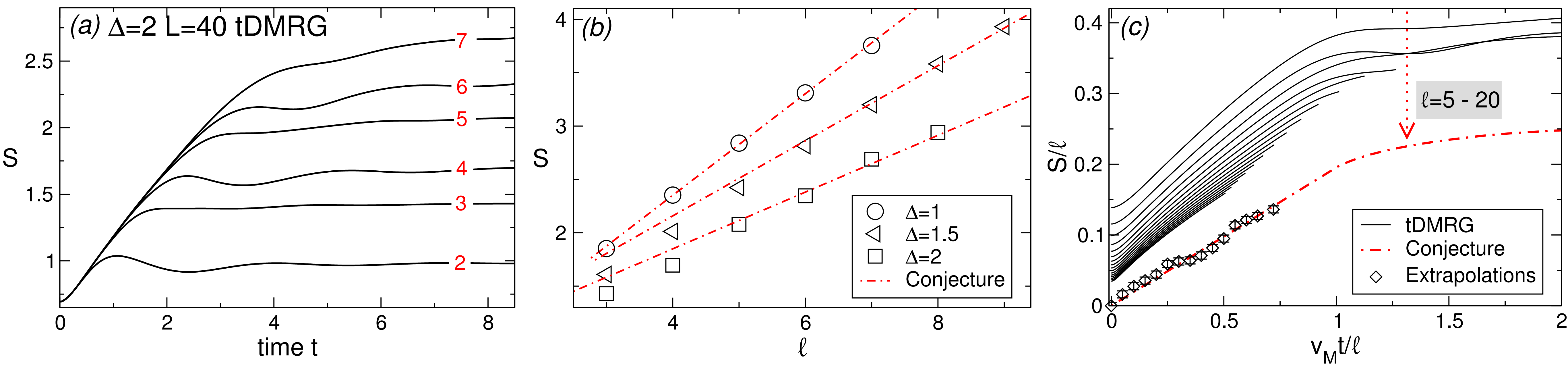
Test I

conjecture:

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

Conjecture vs tDMRG

row data | large t | extrapolation

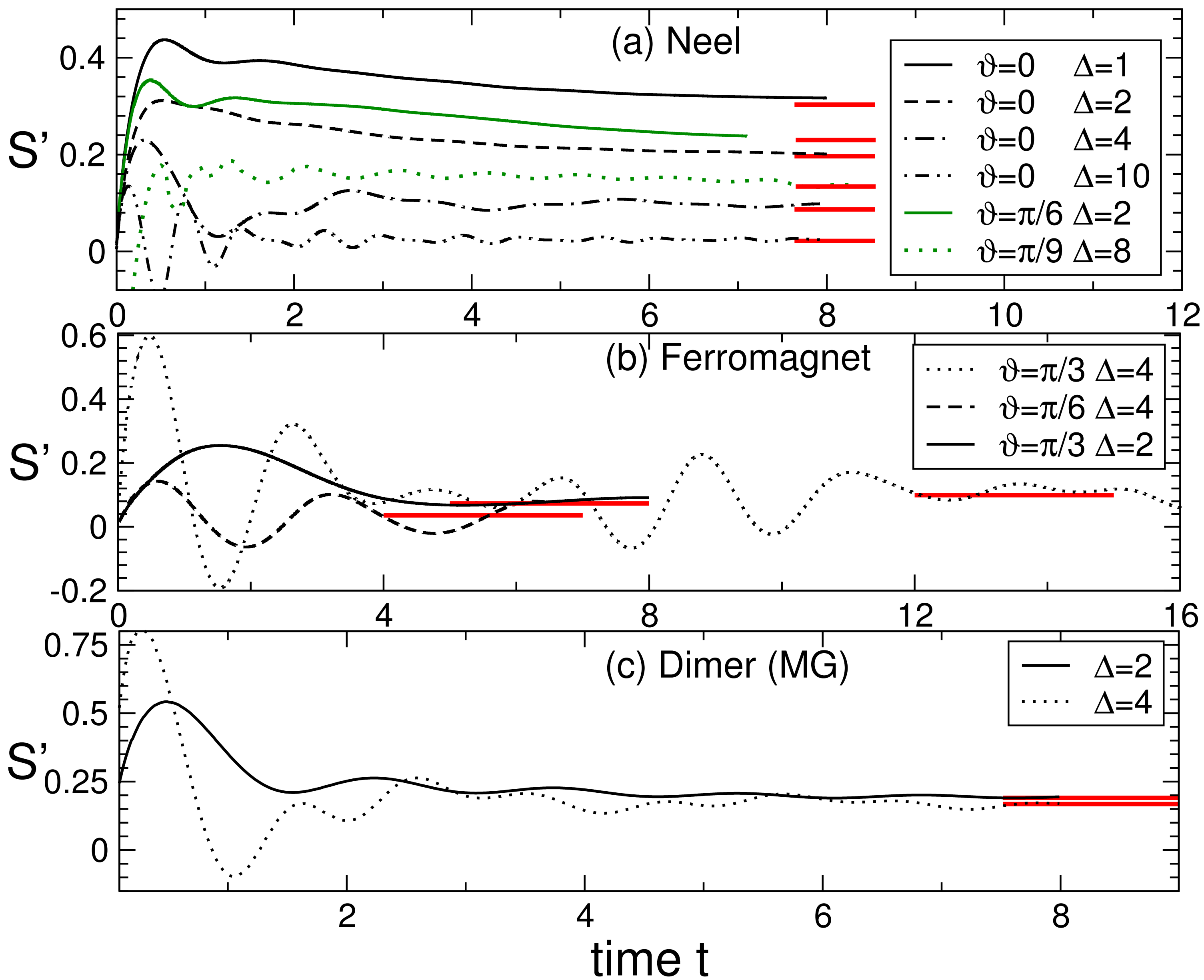


Test II

conjecture:

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

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

Vincenzo Alba[a,1] and Pasquale Calabrese[a]

[a]International School for Advanced Studies, Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, 34136 Trieste, Italy

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 λ 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

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

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

❶ **This is a conjecture, search for proof**

❷ **Valid for arbitrary integrable models**

❸ **Show in a simple formula the crossover from entanglement to thermodynamics**

Entanglement and thermodynamics after a quantum quench in integrable systems

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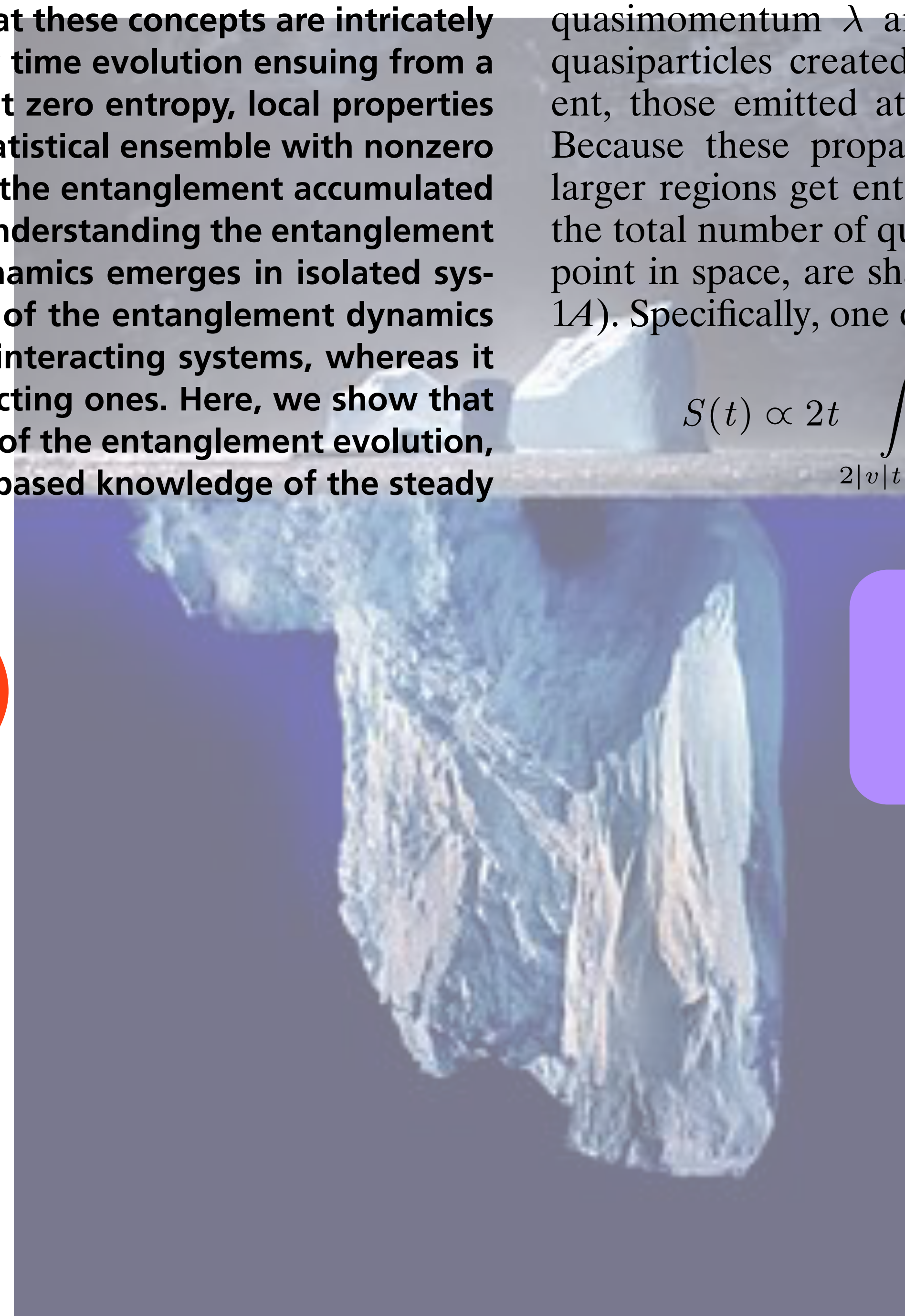

Different multiplets of quasiparticles (triplets…)

Bertini, Tartaglia & PC

Renyi entropy & Entanglement spectrum

Alba, Mestyan & PC

Transport

Bertini, Fagotti, Piroli & PC

Breaking of integrability

Too many people