How is quantum many-body physics modified in a world of bounded entanglement?

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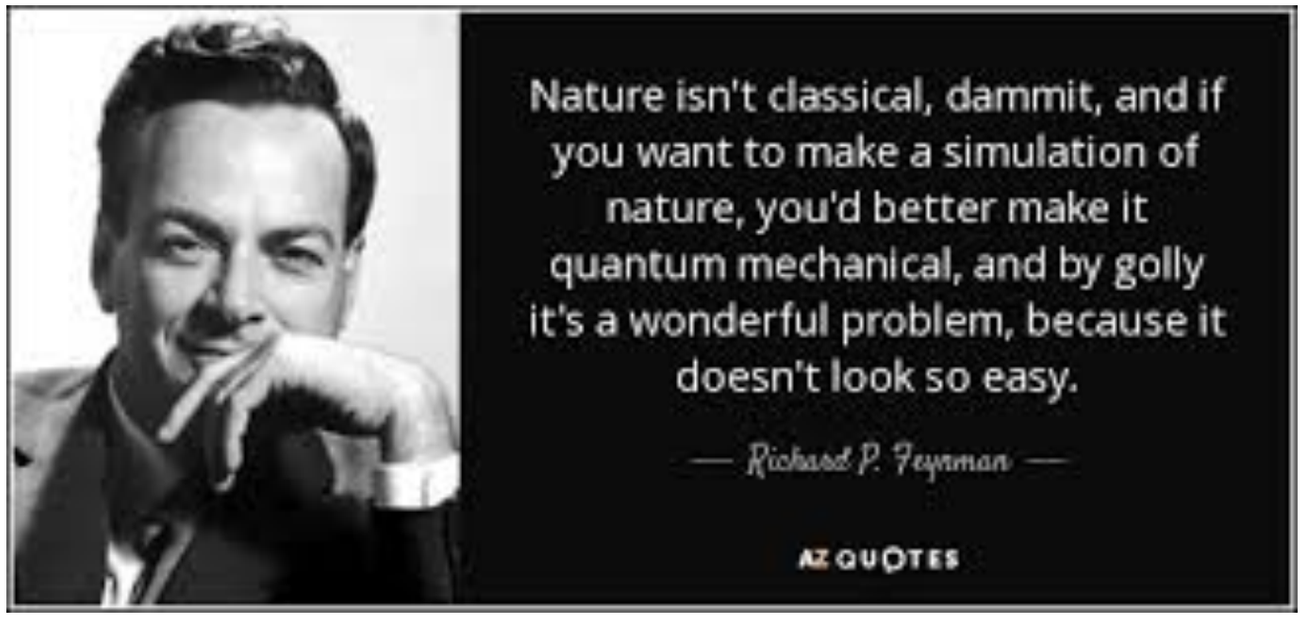
(New part is joint work with Maxime Dupont, UCB)

Physics background and motivation

Feynman, "Simulating Physics with Computers," 1982:

One of the first uses of a quantum computer will be to understand quantum matter (chemistry, materials, nuclei, …).



What do we understand about the classical hardness of that problem?

For "matrix product state" algorithms, difficulty is related to entanglement.

Physics background and motivation

Many old questions about quantum many-body dynamics are now quantitatively accessible in one spatial dimension, either through nonperturbative analytical methods or numerics.

Experimentally, ultracold atomic systems (either in the continuum or in optical lattices) can maintain their quantum phase coherence for many interaction times, unlike "typical" electronic materials.

Transport of energy, charge, or spin is determined by the decay of current-carrying states; either perfect transport or zero transport implies the absence of complete thermalization.

In studying this class of model quantum many-body problems, one is led to think about how physics changes if the full complexity of the quantum wavefunction cannot be retained.

Studying quantum correlations with classical algorithms: applied entanglement entropy

Basic (hazy) concept: "Entanglement entropy determines how much classical information is required to describe a quantum state."

Example:
how many classical real numbers are required to describe a *product* (not entangled) state of N spins?

simple product $$|\psi\rangle = A_{s_1} A_{s_2} A_{s_3} A_{s_4} |s_1 s_2 s_3 s_4\rangle$$

Answer: ~ N (versus exponentially many for a general state)

How do we efficiently manipulate/represent moderately entangled states?

Applied entanglement entropy

The remarkable success of the density-matrix renormalization group algorithm in one dimension (White, 1992; Ostlund and Rommer, 1995) can be understood as follows:

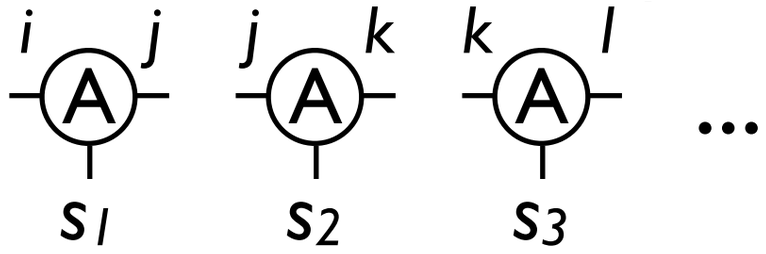
DMRG constructs "matrix product states" that retain local entanglement but throw away long-ranged entanglement.

Example states for four spins:

simple product $$|\psi\rangle = A_{s_1} A_{s_2} A_{s_3} A_{s_4} |s_1 s_2 s_3 s_4\rangle$$

matrix product $$|\psi\rangle = A^{ij}_{s_1} A^{jk}_{s_2} A^{kl}_{s_3} A^{li}_{s_4} |s_1 s_2 s_3 s_4\rangle$$

Graphical tensor network representation:



"Infinite system" methods

Note that we can impose translation invariance simply by requiring constant matrices *A*.

In other words, for quantities in a translation-invariant system,
we just calculate A, rather than a large finite system.
(Idea 1 of renaissance; see Vidal '07, for example)

matrix product $$|\psi\rangle = A^{ij}_{s_1} A^{jk}_{s_2} A^{kl}_{s_3} A^{li}_{s_4} |s_1 s_2 s_3 s_4\rangle$$

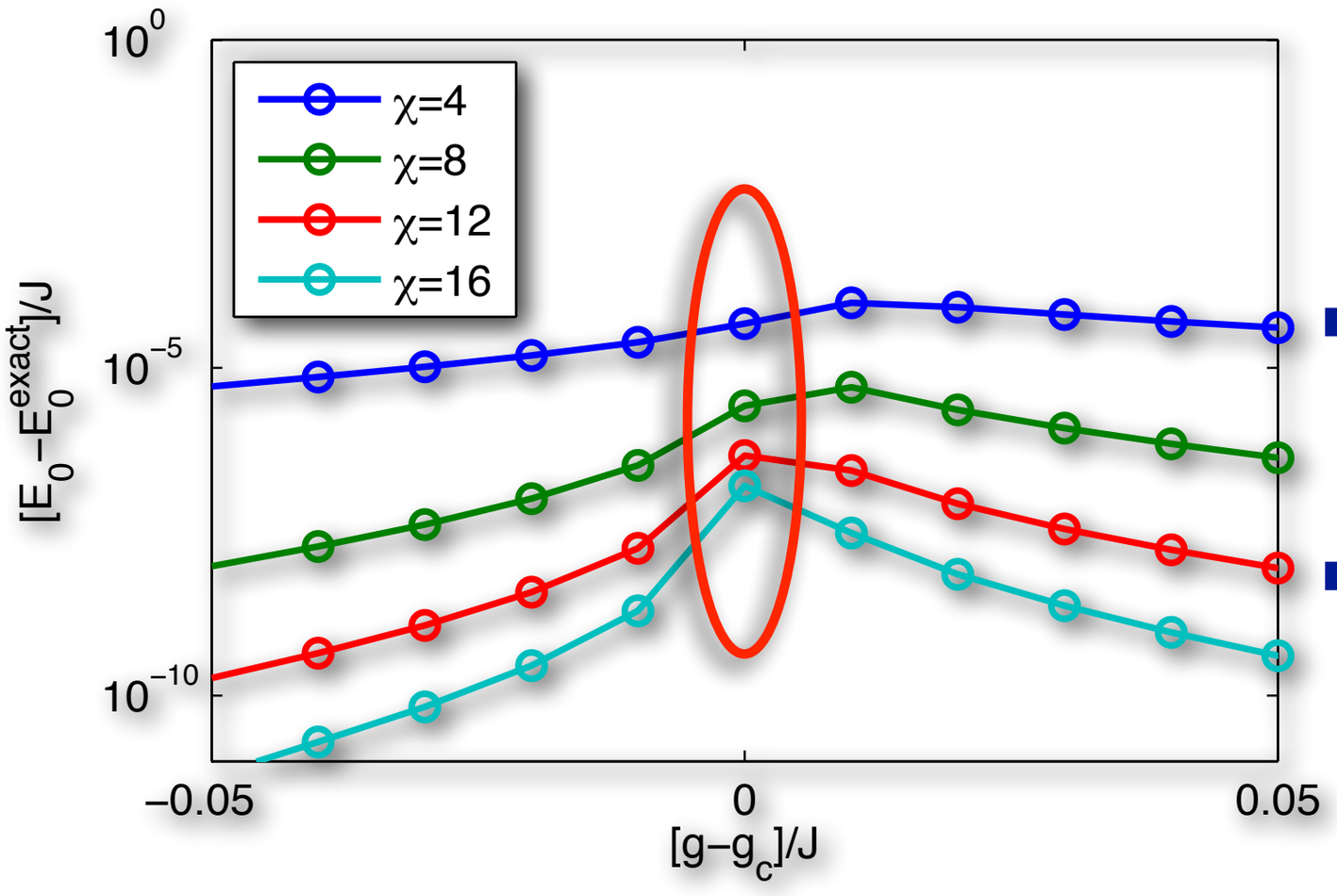
So where is the approximation?

A finite matrix *A* can only capture a finite amount of entanglement.

In the early DMRG days, it was often thought:
1. To study an infinite system, we should study a large finite one.
2. Gapless/critical systems are hard
3. Dynamical properties are hard
4. Finite temperature is hard

But none of these is strictly correct.

- find the ground state of a system by using **imaginary time evolution** (almost unitary for small time steps)
- parallel updates for **infinite/translational invariant** systems: **iTEBD** [Vidal '07]
- **example**, transverse Ising model: $H = \sum_i \left(J\sigma_i^z \sigma_{i+1}^z + g\sigma_i^x \right)$



➡convergence of wave function is worst at the **critical point**

➡**conformal invariance**

Criticality: finite-entanglement scaling

All numerical methods have difficulty with quantum critical points. In DMRG-type approaches, this can be understood from the divergence of entanglement entropy at such points: the entanglement in a matrix product state is limited by dim *A*.

matrix product $$|\psi\rangle = A^{ij}_{s_1} A^{jk}_{s_2} A^{kl}_{s_3} A^{li}_{s_4} |s_1 s_2 s_3 s_4\rangle$$

Quantitatively, it is found that dim *A* plays a role similar to imposing a finite system size:

(Tagliacozzo et al., PRB 2008). $$L_{\text{eff}} \propto \chi^{\kappa}, \quad \chi = \dim A$$

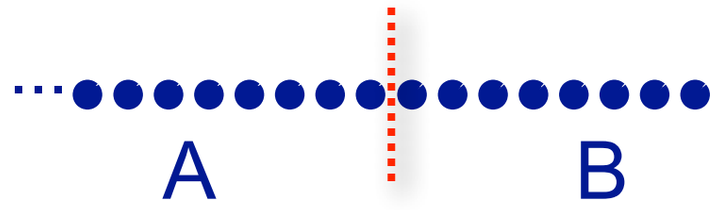
Finite matrix dimension effectively moves the system away from the critical point.

What determines this "finite-entanglement scaling"?
Is it like "finite-size scaling" of CFT's (cf. Blöte, Cardy, & Nightingale)

A way to picture the entanglement of a state

- **Schmidt decomposition** of the state (**SVD**):
-

$$
\begin{aligned}
|\psi\rangle &= \sum_{i=1}^{N_A}\sum_{j=1}^{N_B} C_{ij}|i\rangle_A|j\rangle_B \\
&= \sum_{\alpha=1}^{\min(N_A,N_B)} \lambda_\alpha|\phi_\alpha\rangle_A|\phi_\alpha\rangle_B
\end{aligned}
$$



with $\lambda_\alpha \geq 0$ and $\sum_\alpha \lambda_\alpha^2 = 1$

- a natural measure of the entanglement is the **entropy:**

$$S_A = S_B = S = -\sum_\alpha \lambda_\alpha^2 \log(\lambda_\alpha^2)$$

Efficient representation of quantum states?

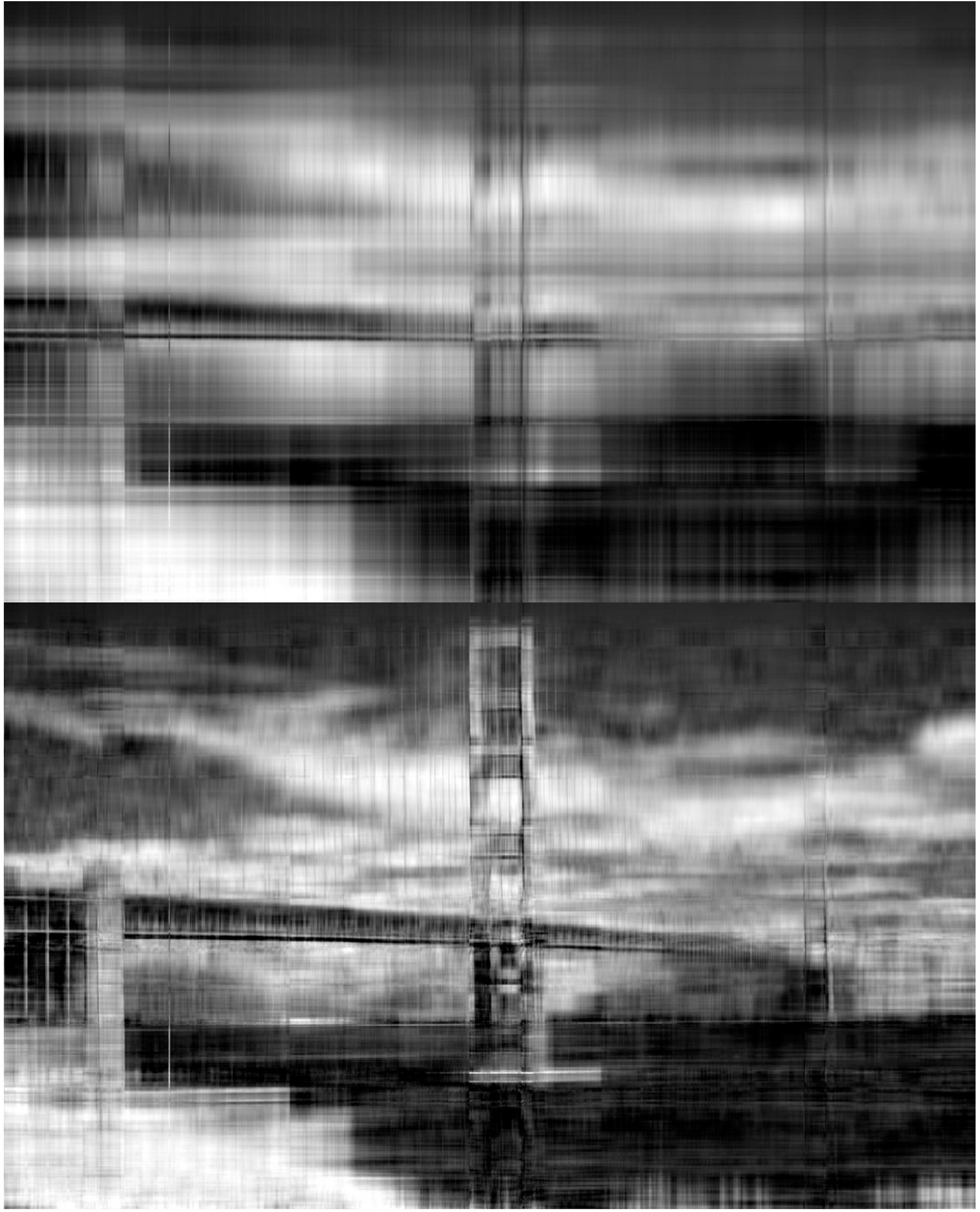
- Hilbert-space dimension of many-body problems increases **exponentially** with number of sites
  example: spin 1/2 system on “classical” computers
  (store **one state** in double precision)

- need an efficient way to “**compress**” quantum states so that the matrices studied remain finite-dimensional

  ➡slightly entangled 1D systems: **Matrix Product States**

  ➡DMRG, TEBD, ...

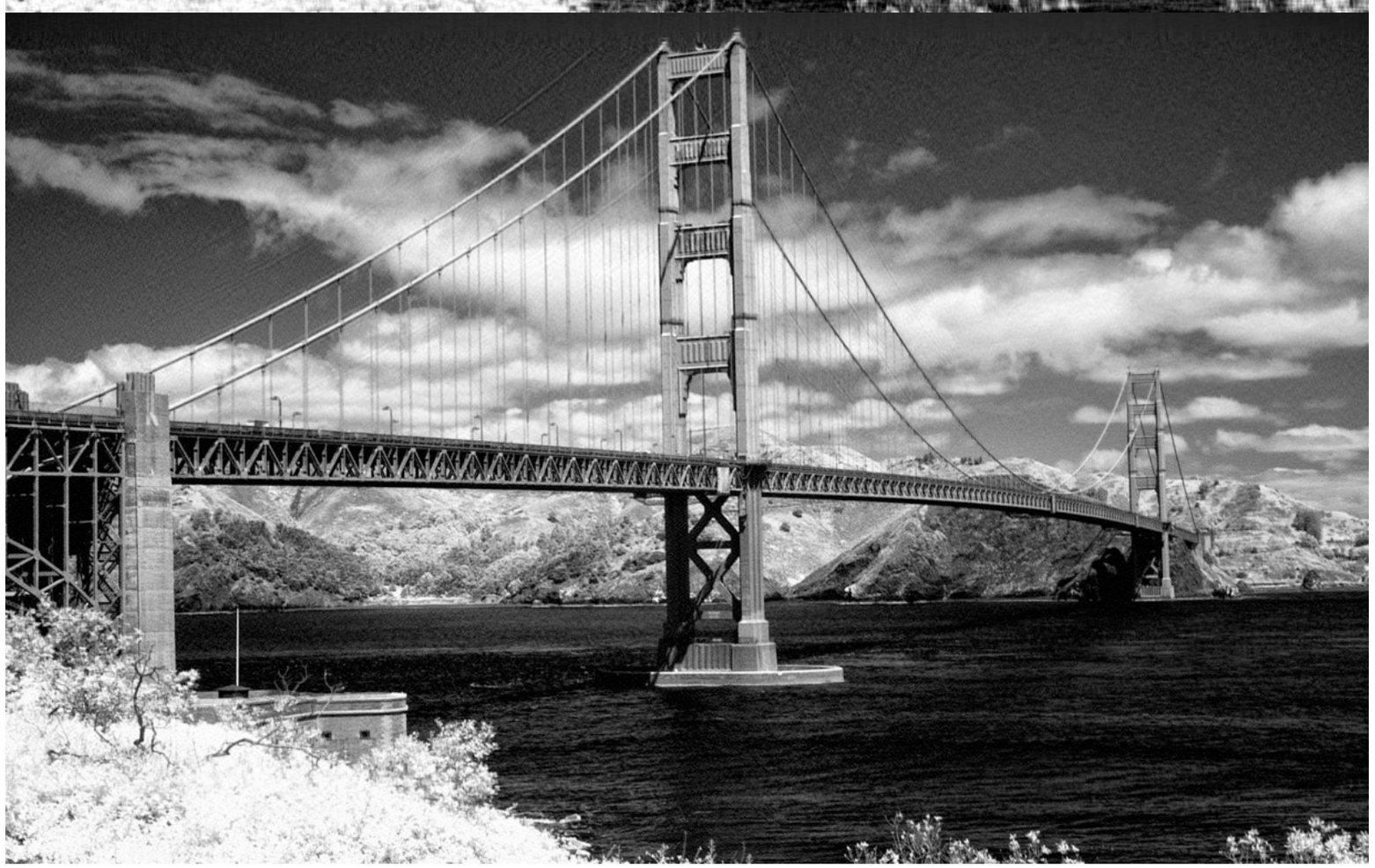
$\chi = 4$



$\chi = 16$

$\chi = 64$

$\chi = 256$



- (Li-Haldane) “entanglement spectrum” [Calabrese et al ‘08]

$$n(\lambda) = I_0\left(2\sqrt{-b^2 - 2b\log\lambda}\right)$$

of $\hat{\lambda}$ ‘s greater than λ

with $b = \dfrac{S}{2} = \dfrac{c}{12}\log\xi = -2\log\lambda_{\max}$

continuum of Schmidt values $|\psi\rangle = \sum_{\alpha=1}^{\infty}\lambda_\alpha|\phi_\alpha\rangle_A|\phi_\alpha\rangle_B$

- Want to explain how at a critical point, finite matrix size χ effectively moves the system away from criticality, leading to universal relations like

$$L_{\text{eff}} \propto \chi^{\kappa}, \quad \chi = \dim\ A$$

- let's look at the **effect of the truncation** at **one** bond

$$|\psi^{\xi}\rangle = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\phi_\alpha\rangle_A |\phi_\alpha\rangle_B \Rightarrow |\psi^{\xi}_{\chi,1}\rangle = \frac{\sum_{\alpha=1}^{\chi} \lambda_\alpha |\phi_\alpha\rangle_A |\phi_\alpha\rangle_B}{\sum_{\alpha=1}^{\chi} \lambda_\alpha^2}$$

- **energy difference** to the non-truncated wavefunction

$$\delta E_{\chi,1} = \left(E^{\rm ex}_\xi - E_\xi\right)\left(1 - |\langle\psi^{\xi}|\psi^{\xi}_{\chi,1}\rangle|^2\right)$$

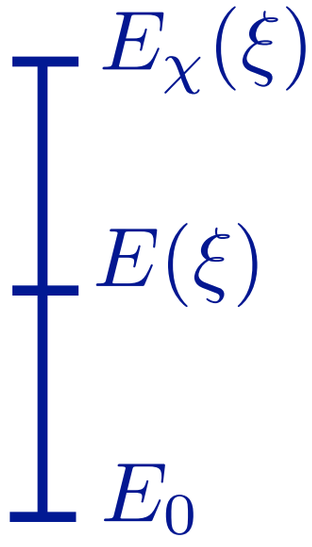
and $\left(E^{\rm ex}_\xi - E_\xi\right) = \Delta \propto 1/\xi$

$E^{\rm ex}_\xi$ = measure of energy of the excited states

- $$\delta E_\chi = \frac{B}{\xi} P_r(\xi,\chi),\ P_r(\xi,\chi) = \sum_{n=\chi+1}^{\infty} \lambda_n^2$$

- energy density of a truncated state

$$E_\chi(\xi) = E_0 + \frac{A}{\xi^2} + \frac{B}{\xi} P_r(\xi, \chi)$$



- $E_\chi(\xi)$ is a non-monotonic function

➡minimize the energy and find the **optimal correlation length for a fixed matrix dimension**

➡scaling relation $S = (c/6) \log \xi$ yields the entropy, etc.

- **we can find the best approximation of the critical state for a given number of states we keep**

- **analytical solution** for the asymptotic case
  (using a continuum of Schmidt values and $\chi \to \infty$)

  ➡**universal finite-entanglement scaling relations**

$$\kappa = \frac{6}{c\left(\sqrt{\frac{12}{c}+1}\right)} \Rightarrow S = \frac{1}{\sqrt{\frac{12}{c}+1}} \log \chi$$

We believe this finite-entanglement scaling will result in any approach with finite matrix dimension, in the same way that finite-size scaling is "universal".

Now we try to check this nonlinear *c* dependence:

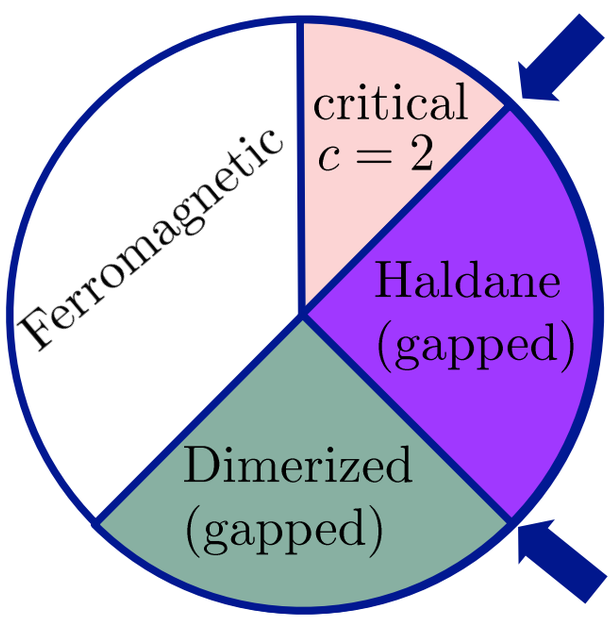
(some more checks are in

[F. Pollmann, S. Mukerjee, A. Turner, and J.E. Moore, arXiv:0812.2903, PRL to appear])

- test the scaling relation on various critical points using the **iTEBD** method
- transverse Ising model: $H = \sum_i \left(\sigma_i^z \sigma_{i+1}^z + g\sigma_i^x\right)$

  ➡critical at $\mathrm{g}{=}1$ with $c = 1/2$
- XXZ model: $H = \sum_i \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta\sigma_i^z \sigma_{i+1}^z\right)$

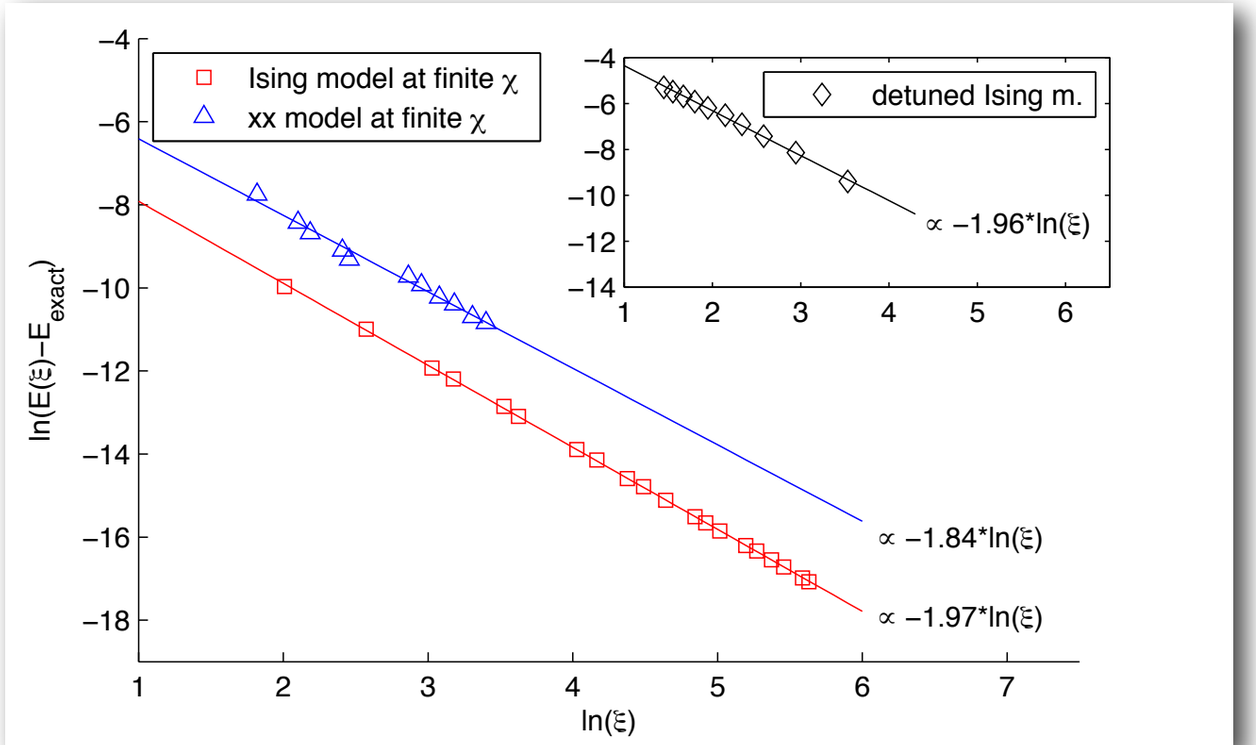
  ➡critical at $\Delta = 1$ with $c = 1$
- spin-1 model: $H = \sum_i \left(\cos\theta(\vec{\tau}_i.\tau_{i+1}^{\rightarrow}) + \sin\theta(\vec{\tau}_i.\tau_{i+1}^{\rightarrow})^2\right)$



$\theta = \pi/4, SU(3)_1$ with $\mathrm{c}{=}2$

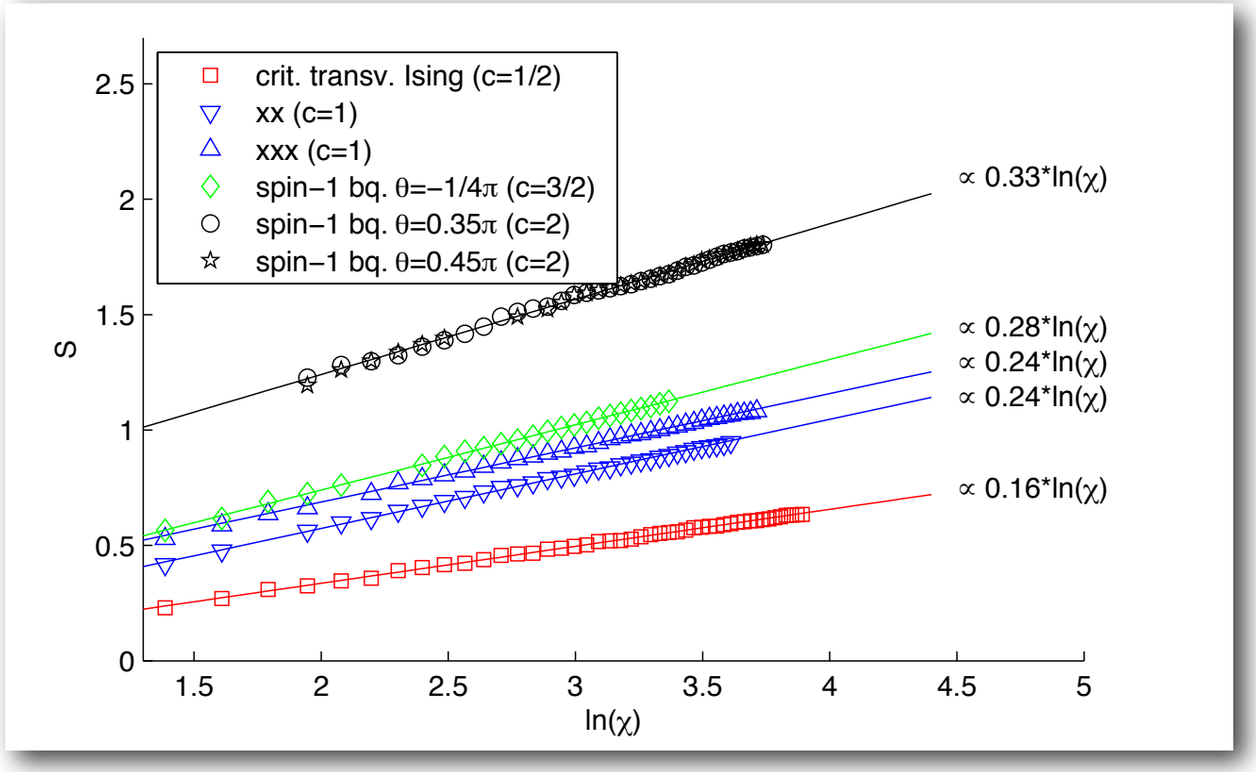
$\theta = -\pi/4, SU(2)_2$ with $\mathrm{c}{=}3/2$

- scaling of the **energy** and **entanglement entropy:**



$$E_\chi(\xi) = E_0 + \frac{A}{\xi^2} + \frac{B}{\xi} P_r(\xi, \chi)$$

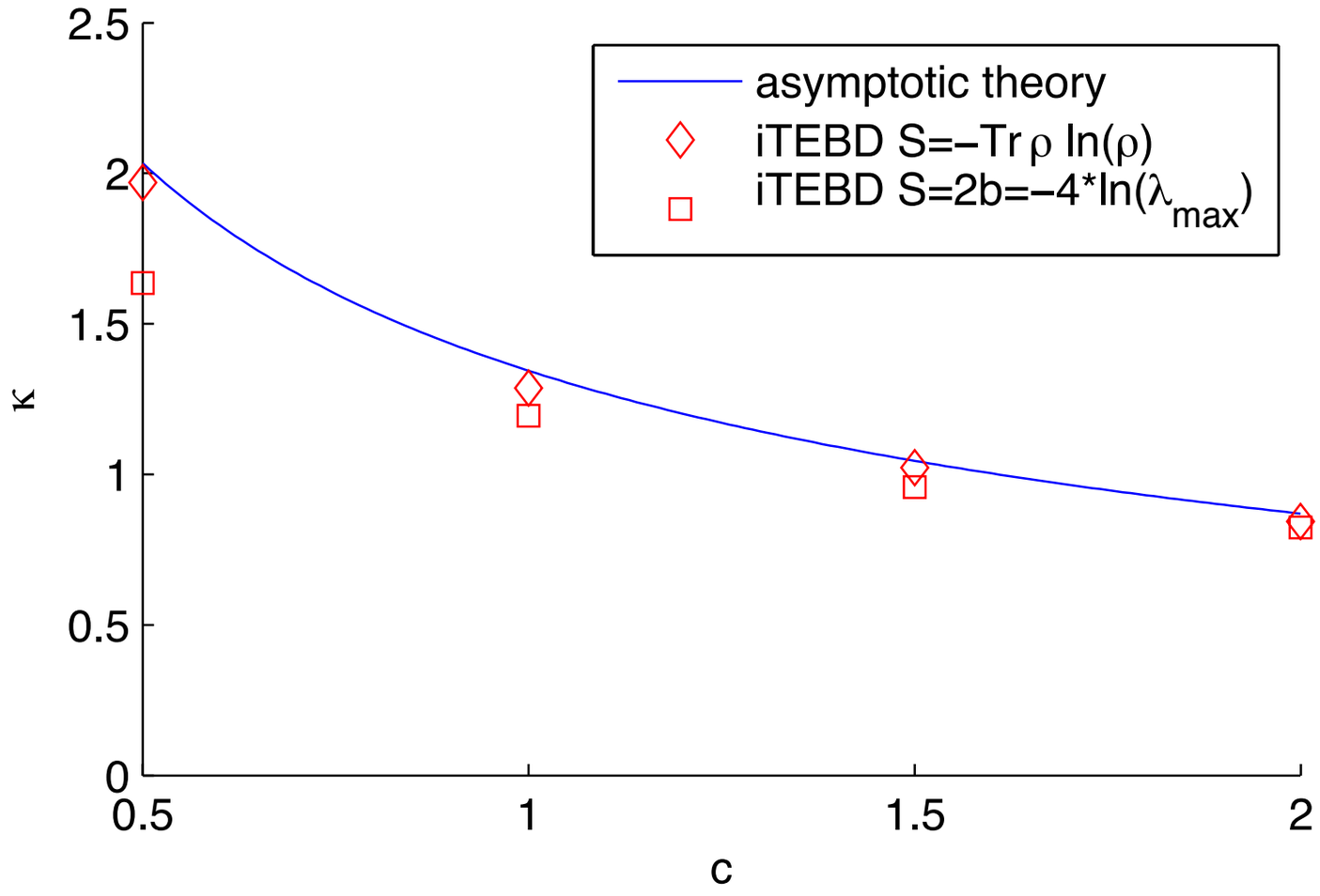
➡scales as $\propto 1/\xi^2$ for $\xi = \xi_{\text{opt}}$ ✔



$$S_\chi = \frac{1}{\sqrt{\frac{12}{c} + 1}} \log \chi$$

➡$S_\chi \propto \log \chi$ and depends only on c ✔

- reasonable agreement of the **asymptotic theory** and **numerical results**

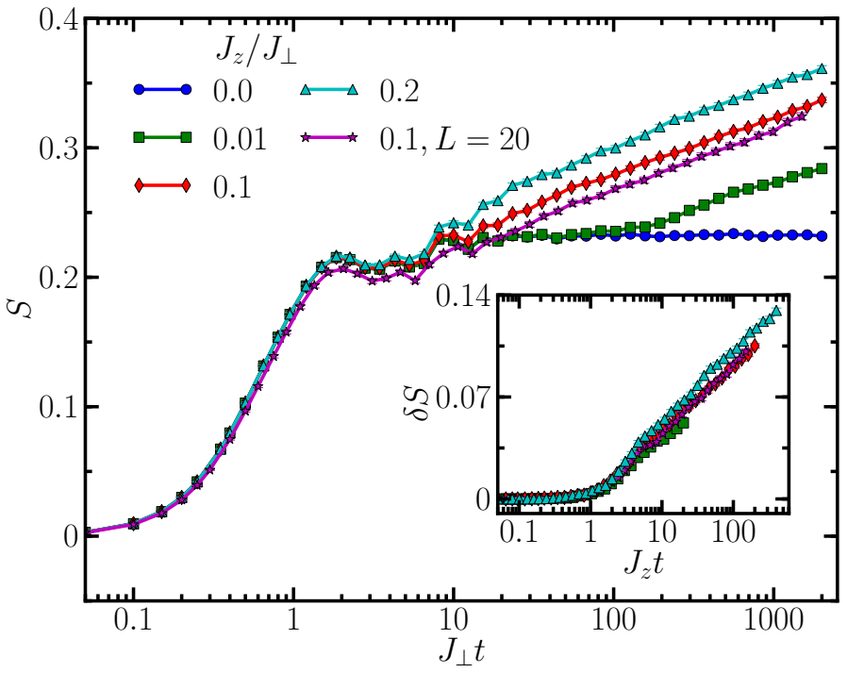


- Errors are no larger than differences between different definitions of entropy
- Another check: combine non-interacting copies; still get nonlinear dependence on total *c*

What about dynamics?

What about dynamics?

- Starting from a product state, entanglement is rapidly generated, and this growth sets a strict limit on microscopically faithful simulation.
- In an MBL state, the entanglement generated in a subregion typically grows as log t.
- In a thermalizing state, the entanglement must scale with subregion size in order to reproduce the thermal entropy.
- Is the final state really that complicated?



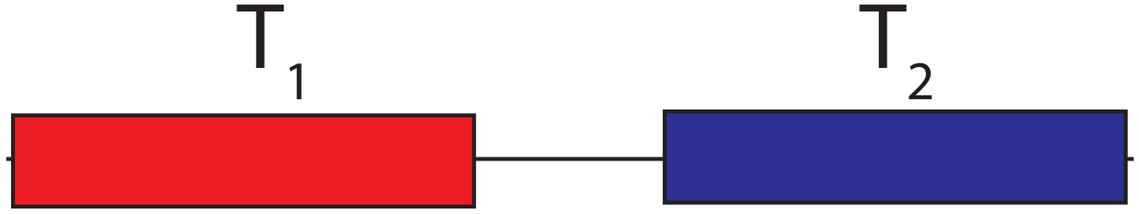
What about dynamics?

- Intuitively we have the idea that the long-time dynamics of a thermalizing system is scrambled. Exact microscopic fidelity is difficult or impossible. Are there some purposes for which it isn't necessary?
- Another way to look at this: for quantum computation we probably want non-generic behavior that depends strongly on the initial state.
- But for physical simulation of hydrodynamics, etc., final states are "simple". Can simulations at finite bond dimension capture these phenomena correctly? ("Get over the complexity hump")
- (Is there any universal sense of robustness to decoherence, other errors, etc.?)

Test: Non-equilibrium transport in XXZ

$$H = J_{xx} \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J_z \sum_i S_i^z S_{i+1}^z + \sum_i h_i S_i^z$$

1. Create two different temperatures in two disconnected, infinite 1D "leads".
2. Connect them by a finite region (e.g., one bond).
3. Evolve in time for as long as possible.



Is a steady-state heat current reached?

Is non-equilibrium (finite bias) thermal transport determined by linear-response thermal conductance?

Can be solved in easy-plane case with "generalized hydrodynamics"
(Castro Alvaredo, Doyon, Yoshimura; Bertini et al., 2016)

Our starting point: think of particles in an integrable model as streaming (with self-consistent velocity) but not colliding

"Bethe-Boltzmann equation"

$$\partial_t \rho(k,x,t) + \partial_x \left[v(\{\rho(k',x,t)\}) \rho(k,x,t) \right] = 0$$

No collision term since quasiparticles retain their identity; however, they modify each other's velocities via phase shifts

This type of equation was written down in various older contexts: I think the most relevant for the models here is

Kinetic Equation for a Dense Soliton Gas

G. A. El[1,*] and A. M. Kamchatnov[2,†]

[1]*Department of Mathematical Sciences, Loughborough University, Loughborough LE11 3TU, United Kingdom*
[2]*Institute of Spectroscopy, Russian Academy of Sciences, Troitsk, Moscow Region, 142190, Russia*
(Received 5 July 2005; published 7 November 2005)

We propose a general method to derive kinetic equations for dense soliton gases in physical systems described by integrable nonlinear wave equations. The kinetic equation describes evolution of the spectral distribution function of solitons due to soliton-soliton collisions. Owing to complete integrability of the soliton equations, only pairwise soliton interactions contribute to the solution, and the evolution reduces to a transport of the eigenvalues of the associated spectral problem with the corresponding soliton velocities modified by the collisions. The proposed general procedure of the derivation of the kinetic equation is illustrated by the examples of the Korteweg–de Vries and nonlinear Schrödinger (NLS) equations. As a simple physical example, we construct an explicit solution for the case of interaction of two cold NLS soliton gases.

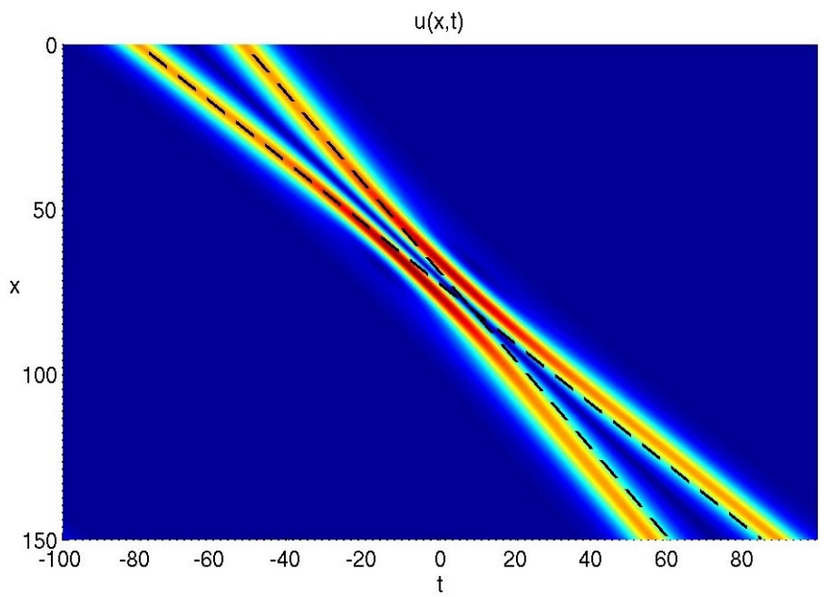
Why Boltzmann equation gets modified in (classical or quantum) integrable systems

Solitons/particles pass through each other even in dense system; no randomization of momentum and no collision term.

However, there is an interaction:

Classical

Solitons delay each other



so velocity depends on other solitons at spacetime point

Quantum

Phase shift from Bethe equations

but semiclassically an energy-dependent phase shift is also just a time delay (Wigner)

$$\tau = 2\hbar \frac{d\delta}{dE}$$

Integrable hydrodynamics

Simplest case is Bose gas with delta-function repulsion.

GGE = Generalized Gibbs Ensemble = includes an infinite number of conservation laws:

$$\int \rho(k,x,t)\,dk = n(x,t)$$

$$\int k\rho(k,x,t) = mv(x,t)$$

$$\int k^2\rho(k,x,t) = 2m\epsilon(x,t)$$

$$\vdots$$

$$\int k^n\rho(k,x,t)$$

Kinetic theory: might as well work with

$$\rho(k,x,t)$$

instead of its moments.

GGE (conserved quantities) is equivalent to distribution function, rather than containing less information.

Somewhat surprising for XXZ, where the charges are quite complicated; somehow Takahashi's old TBA and Bertini et al. backflow leads to Drude weight, i.e., it "knows about" the deep quasilocal charges.

Summary of when this is useful

Normal fluid:
Initial state → Local equilibrium → Hydrodynamics

Integrable fluid:
Initial state → Local GGE → Boltzmann/hydrodynamics

So, for non-local-GGE initial conditions, still need to solve difficult "quench" problem, at least locally.

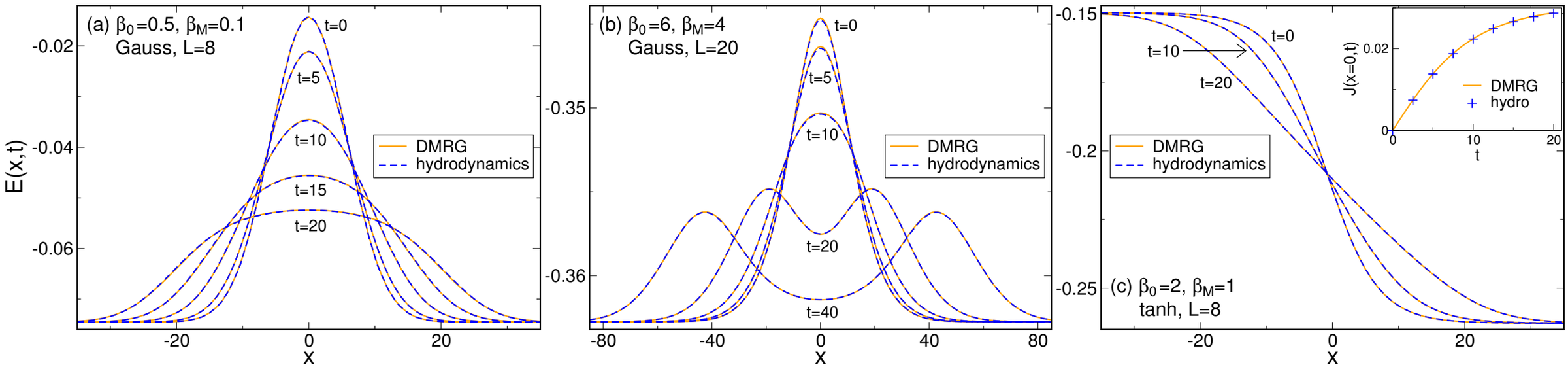
Two-reservoir problem already solved in 2016 papers: solution is function of one variable (x/t).

Let's look for full (x,t) solutions: are quantum dynamics really describable by these classical particle equations?

Mathematical properties of solutions ("semi-Hamiltonian structure"): Bulchandani, 2017, arXiv, as for NLS

Take XXZ in zero magnetic field. Make a spatial variation of initial temperature. Watch the energy spread out in time.

Note: nonzero temperature is required for coarse-graining time to be finite, according to basic principle that systems can't relax faster than hbar/kT.
(Hence more physically generic than T=0 or Bethe-Bethe comparisons.)



These are comparisons for interacting spinless fermions (XXZ) between backwards Euler solution of Bethe-Boltzmann and microscopic DMRG simulations.
(figure from "Solvable quantum hydrodynamics", V. Bulchandani, R. Vasseur, C. Karrasch, and JEM, arXiv April 2017)

(b) β_0=6, β_M=4
Gauss, L=20

t=0
t=5
t=10
t=20
t=40

DMRG
hydrodynamics

-0.35
-0.36
-0.15
-0.2
-0.25
-80
-40
0
40
80
x

Challenging cases: isotropic and easy-axis

There now seems to be a growing consensus that the isotropic point, at infinite temperature, shows "superdiffusive" dynamics with z=3/2.

This is in between z=1 (ballistic) and z=2 (diffusive) and has been argued to reflect the Kardar-Parisi-Zhang universality class (Ljubotina et al., 2019).

We (M. Dupont and JEM, arXiv 2019) have been working on trying to understand the necessary criteria for this behavior, as a way to test models of its origin.

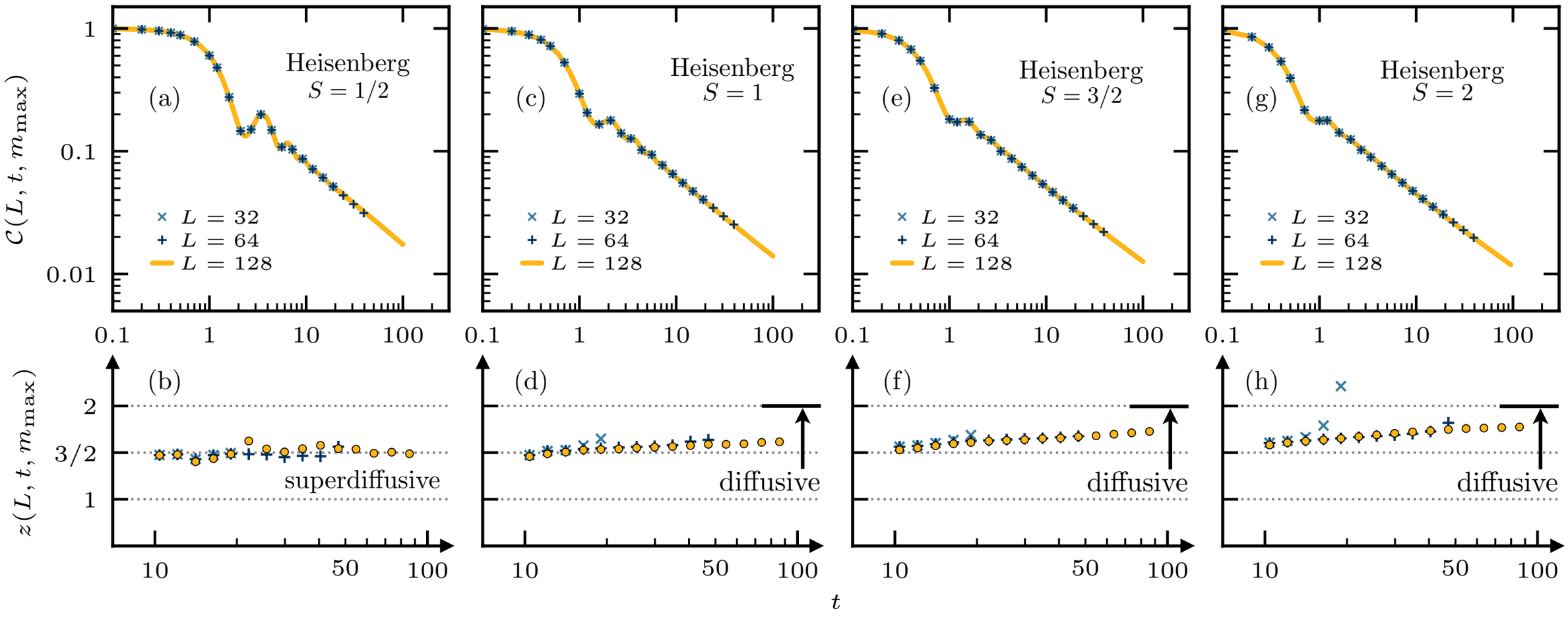
1. We find that a wide variety of ***integrable, isotropic models*** seem to show the z=3/2 behavior.

2. Non-integrable models appear to be diffusive, which is unsurprising and yet apparently controversial.

3. However, the difference between the two classes of behavior onsets at long times where DMRG is not microscopically faithful.

Long-time spin autocorrelators: power laws

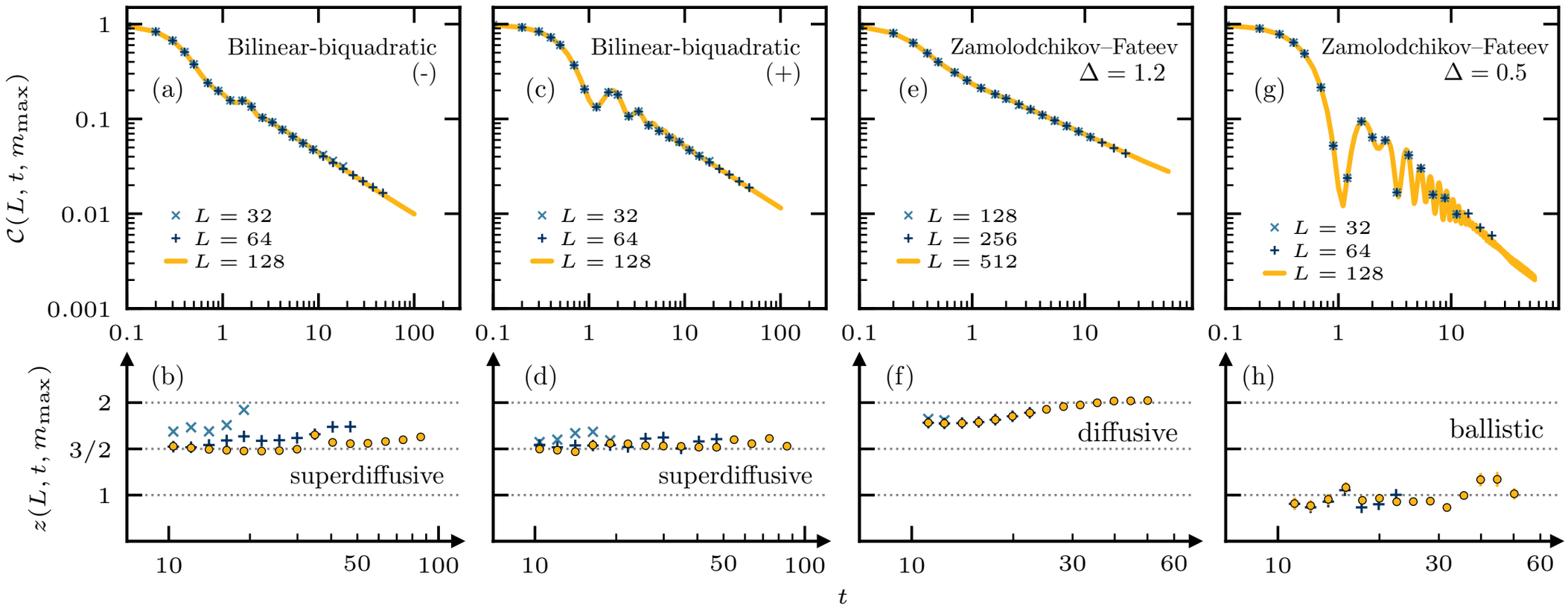
Nearest-neighbor models of various spins: (only s=1/2 is integrable)



Long-time spin autocorrelators: power laws

A variety of integrable s=1 models:

isotropic z=3/2
easy-axis diffusive
easy-plane ballistic



Conclusions

Somehow, reasonably large bond dimension seems to be capturing subtle physics at long times, *even after the simulated state no longer has overlap of order unity with the*

This suggests that, at least for some non-thermalizing many-body systems, the long-time physics has a degree of robustness to finite entanglement.

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This suggests that, at least for some non-thermalizing many-body systems, the long-time physics has a degree of robustness to finite entanglement.

Does this give a reasonably positive prognosis for simulations of quantum dynamics in the NISQ era?

It suggests that things we might try to simulate, like dynamics of the Hubbard model, will be qualitatively correct even if not microscopically correct—they are "easy" quantum computations in that sense.

Clearly this can't be true in all cases—disordered systems are a ready counterexample. When is it true?