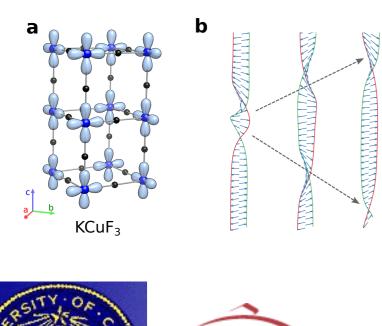
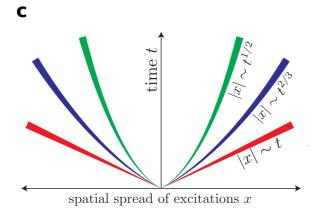
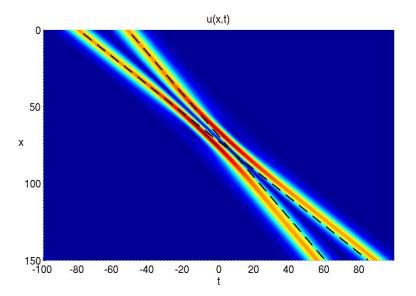
Dynamics in integrable and non-integrable low-dimensional quantum systems

Accademia dei Lincei, 26 January 2023

Joel Moore
University of California, Berkeley,
and Lawrence Berkeley National Laboratory















Acknowledgements

Current Students:
Alex Avdoshkin
Tessa Cookmeyer
Nick Sherman

Postdocs: Maxime Dupont (to Rigetti) Johannes Motruk (Geneva)

Alumni:
Vir Bulchandani (Princeton)
Christoph Karrasch (Braunschweig)
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Alex



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Allen Scheie,
Alan Tennant,
Steve Nagler, et al.



Nick

Thanks also to the Quantum Science Center and TIMES collaborations supported by the US Department of Energy

Topics

- I. Hydrodynamic regimes in the Heisenberg spin chain now realized in materials, emulators, and computers
- 2. Finite-entanglement scaling and the quantum Kibble-Zurek mechanism in one spatial dimension
- (3. Higher dimensions)

References for part I

I. In ID ("spin chains"), we know well the ground states of models like the Heisenberg chain, but basic facts about dynamics were only understood recently. Experiment on KCuF₃.

Examples of theory and numerics in easy-plane case: V. Bulchandani, R. Vasseur, C. Karrasch, JEM, PRL 2018

Does this lead to anything really new and observable about actual spin chains?

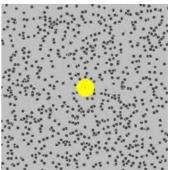
M. Dupont, JEM PRB RC 2020

A. Scheie, N. Sherman, M. Dupont, S. Nagler, G. Granroth, M. Stone, JEM, A. Tennant, Nat. Phys. 2021 M. Dupont, N. Sherman, JEM PRL 2021



How thermalization relates to what we measure in solids: Linear response theory

Einstein's theory of motion of Brownian particles:



the diffusion constant D that appears in Fick's law (which is the restoration to equilibrium from a density perturbation)

$$\mathbf{j} = -D\nabla n$$

is given by the dynamical correlation function of velocity at equilibrium:

$$D = \frac{1}{3} \int_0^\infty \langle \mathbf{v}(0) \cdot \mathbf{v}(t) \rangle_T dt \approx v^2 \tau$$

Philosophy: how a system returns to equilibrium is independent of whether it was driven away or fluctuated away

Kubo formula for electrical conductivity in metals: dynamical correlation function of electrical current

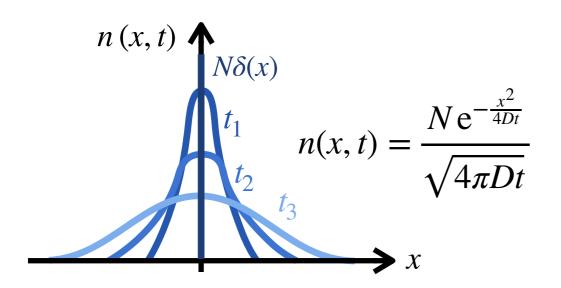
Other possibilities include many-body localization, a failure to thermalize from disorder.

Phenomenological description of most spin chains at high temperatures

The diffusion equation

$$\partial_t n(x,t) - D \nabla^2 n(x,t) = 0$$

of particles N conserved
$$\int_{V} n(x, t) dx = N \forall t$$



Analogy with magnets

$$\hat{M}^z = \sum_n \hat{S}_n^z \equiv \text{# of particles}$$

Conserved
$$\left[\hat{\mathcal{H}}, \hat{M}^z\right] = 0$$

Emergent fluid-like spin diffusion?

$$\lim_{x,t\to+\infty} \left\langle \hat{S}_{x}^{z}(t) \, \hat{S}_{0}^{z}(0) \right\rangle_{k_{\mathrm{B}}T\to+\infty}$$

$$= t^{-1/2} f_{\mathrm{Gaussian}} \left(x^{2}/t \right)$$

Dynamical exponent: z = 2

Different fluid properties are seen in very good crystals where momentum relaxation from impurities and phonons can be avoided.

Standard hydrodynamics (0th order)

The "zeroth-order" hydrodynamical equations in three dimensions, which neglect dissipative behavior such as viscosity, are

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{u}) = 0 \tag{1}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \mathbf{u} + \frac{1}{\rho} \nabla P = \frac{\mathbf{F}}{m}.$$
 (2)

$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \tau + \frac{2}{3} (\nabla \cdot \mathbf{u}) \tau = 0. \tag{3}$$

These come from the Boltzmann equation assuming local equilibrium.

Hydrodynamics: how does local equilibrium become global equilibrium?

Simple models with complicated dynamics

Here are two examples of Yang-Baxter "integrable" systems:

the ID Bose gas with delta-function interaction (Lieb-Liniger model);

the ID "XXZ" spin chain.

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

The latter has a more complicated Bethe ansatz formulation, but is easier to compare to microscopic DMRG numerics and to experiments.

By adding a random field (last term), we could obtain a localized phase.

The "Heisenberg chain" we discuss in most detail is just Jz = Jxx.

Some history

The ground state of the Heisenberg chain was solved by Bethe (1931) and the thermodynamics was understood in the 1970s.

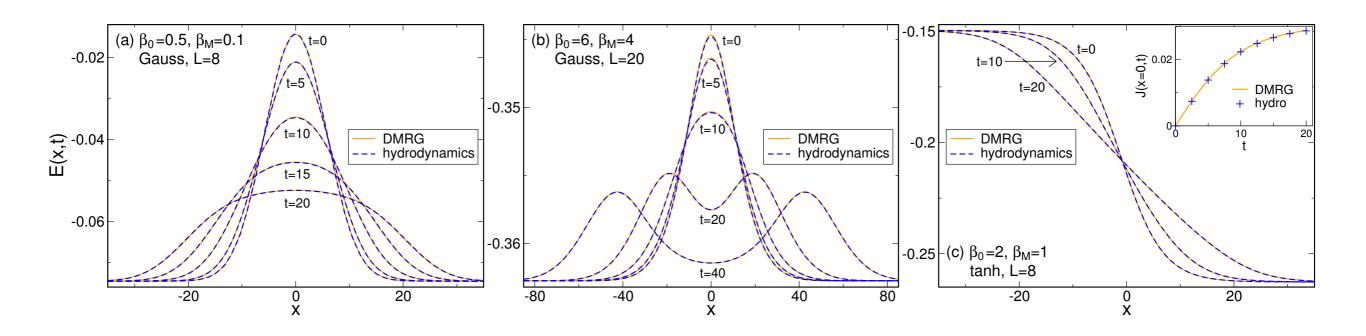
However, dynamical questions such as whether there is a nonzero "Drude weight" remained perplexing

2011: it turns out that *half* of the conserved quantities had been missed, including those that control the spin dynamics (Prosen). This yields a nonzero Drude weight, matching computations that became available at that time.

One can use these conservation laws to get some far-from-equilibrium hydrodynamical results that pass tests against DMRG-type numerical calculations.

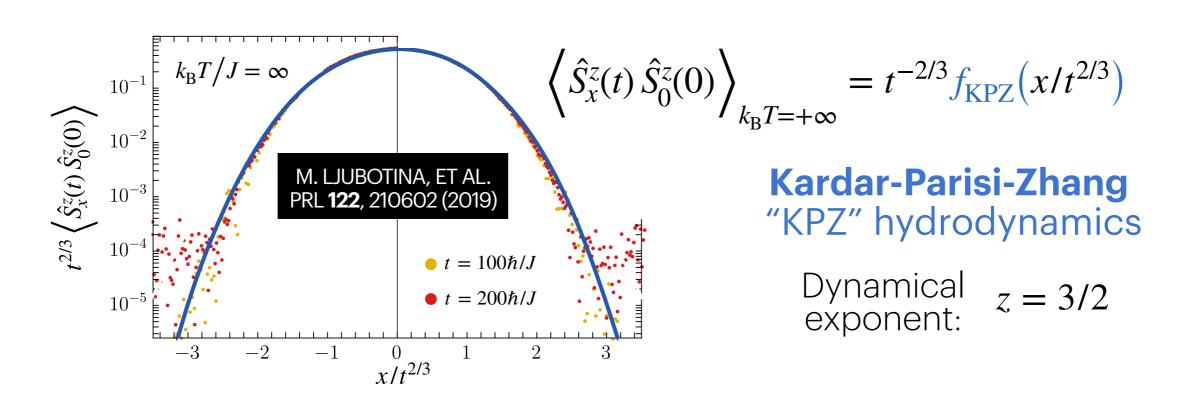
Take XXZ in zero magnetic field. Make a spatial variation of initial temperature. Watch the energy spread out in time.

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, PRL 2018)

Emergent hydrodynamics in Heisenberg spin chain at infinite temperature



What is KPZ?

$$\partial_t h(x,t) - D \nabla^2 h(x,t) = \lambda \left[\nabla h(x,t) \right]^2 + \sigma \eta(x,t)$$

Solution:

$$\langle \nabla h(x,t) \cdot \nabla h(0,0) \rangle \sim t^{-2/3} f_{\text{KPZ}}(x/t^{2/3})$$

Where to find it?

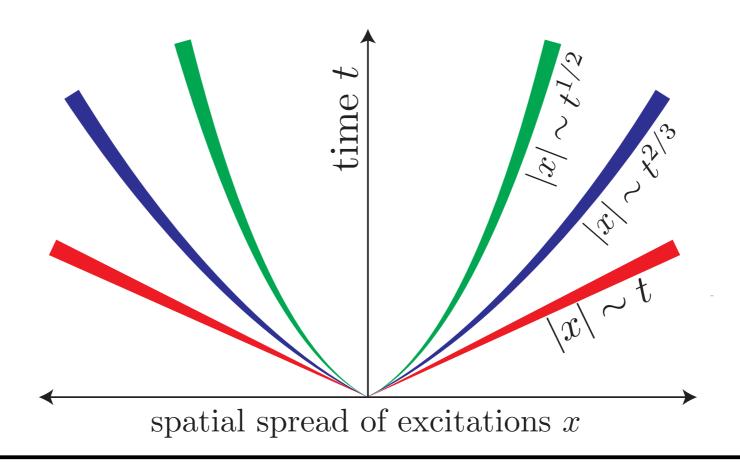
Profile of a growing interface, disordered conductors, traffic flow, spin-1/2 Heisenberg chain...

Kardar-Parisi-Zhang physics

An example of a classical problem with this scaling: interface growth Model below is "Sticky Tetris"



Emergent hydrodynamics in Heisenberg spin chain at infinite temperature



What is KPZ?

$$\partial_t h(x,t) - D \nabla^2 h(x,t) = \lambda \left[\nabla h(x,t) \right]^2 + \sigma \eta(x,t)$$

Solution:

$$\langle \nabla h(x,t) \cdot \nabla h(0,0) \rangle \sim t^{-2/3} f_{\text{KPZ}}(x/t^{2/3})$$

Where to find it?

Profile of a growing interface, disordered conductors, traffic flow, spin-1/2

Heisenberg chain...

Hydrodynamics beyond diffusion

Example:
$$\hat{\mathcal{H}} = J \sum_{n} \hat{S}_{n}^{x} \hat{S}_{n+1}^{x} + \hat{S}_{n}^{y} \hat{S}_{n+1}^{y} + \Delta \hat{S}_{n}^{z} \hat{S}_{n+1}^{z}$$

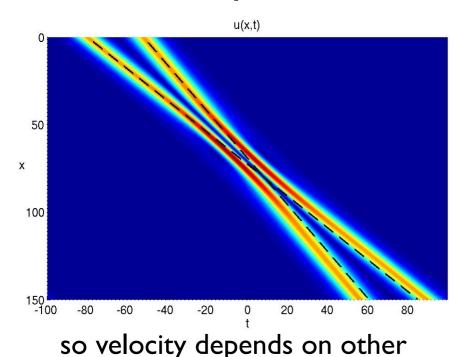
$$\Delta > 1$$

Why Boltzmann equation should get modified in (classical or quantum) integrable systems: quasi-ballistic case

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



solitons at spacetime point

Quantum

Phase shift from Bethe equations

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

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

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

One early classical appearance of this type of equation is

Kinetic Equation for a Dense Soliton Gas

G. A. El^{1,*} and A. M. Kamchatnov^{2,†}

¹Department of Mathematical Sciences, Loughborough University, Loughborough LE11 3TU, United Kingdom

²Institute 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.

Quantum:

Castro-Alvaredo/Doyon/Yoshimura, PRX 2016 (Lieb-Liniger) Bertini/Collura/De Nardis/Fagotti, PRL 2016 (XXZ)

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/generalized HD

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

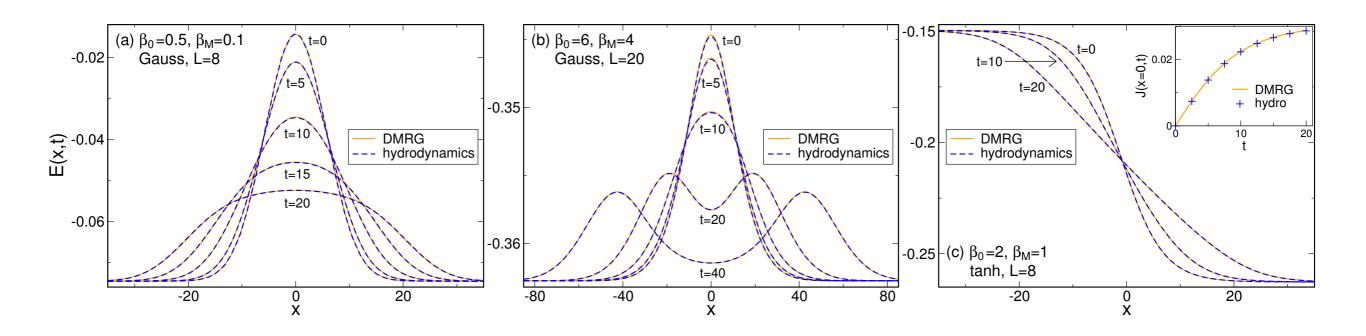
Two-reservoir problem already solved in 2016 papers: solution is function of one variable (x/t).

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

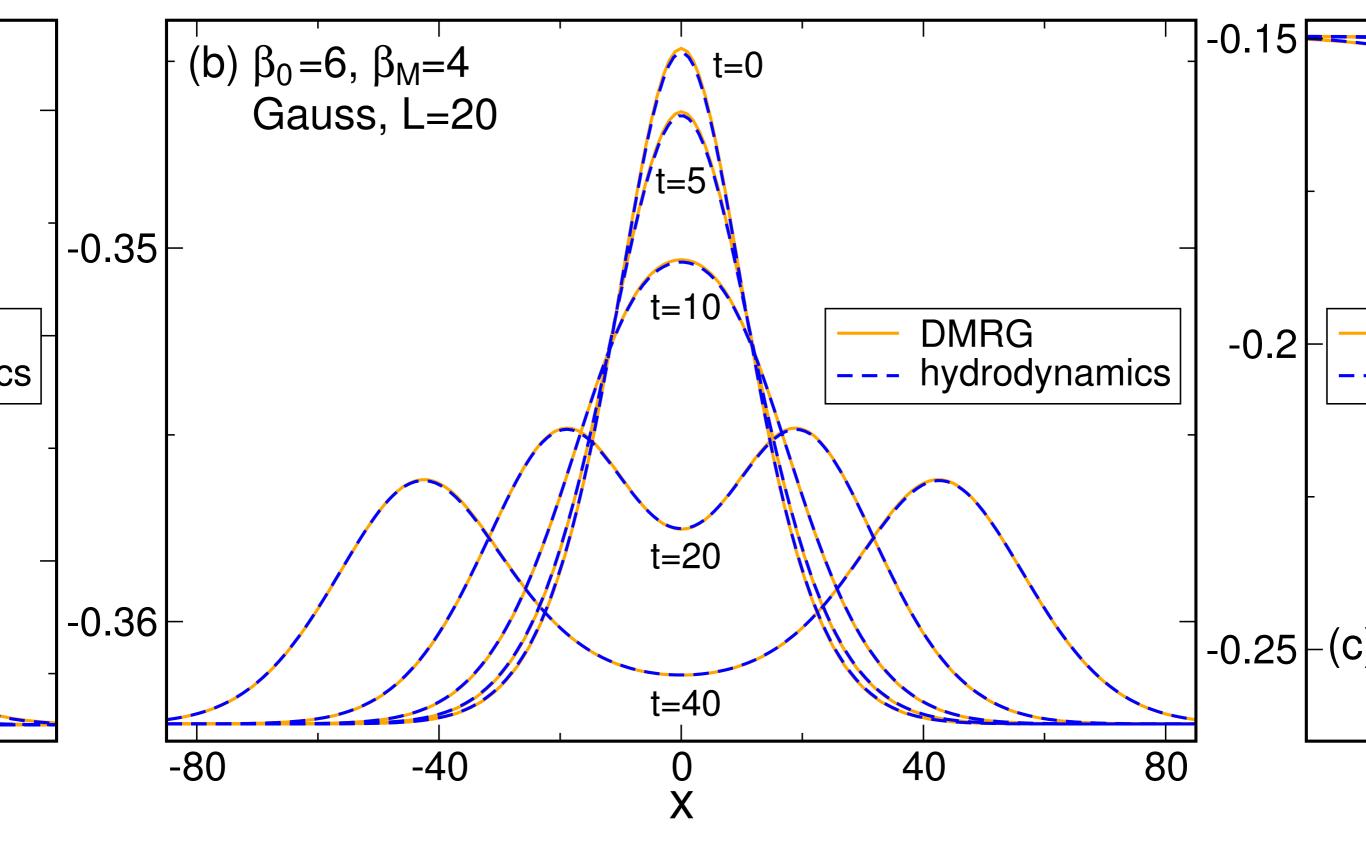
Mathematical properties of solutions ("semi-Hamiltonian structure"): Bulchandani, 2017, as for NLS

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

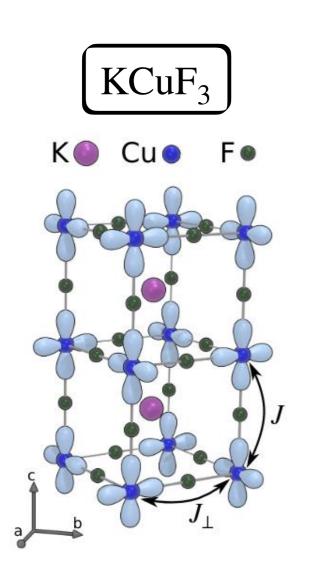
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Experimentally looking for hydrodynamics



Weakly coupled spin-1/2 chains

$$J = 33.5 \text{ meV} \gg J_{\perp} = -1.6 \text{ meV}$$

Well described by the 1D Heisenberg model $\hat{\mathcal{H}} = J \sum_{n} \hat{S}_{n} \cdot \hat{S}_{n+1}$

$$\hat{\mathcal{H}} = J \sum_{n} \hat{\mathbf{S}}_{n} \cdot \hat{\mathbf{S}}_{n+1}$$

Superdiffusive Kardar-Parisi-Zhang "KPZ" hydrodynamics expected

$$\left\langle \hat{S}_{x}^{z}(t)\,\hat{S}_{0}^{z}(0)\right\rangle$$
 Fourier transforms $S\left(Q,\omega\right)$

Corresponds to the <u>neutron</u> scattering intensity

Neutron scattering measurements

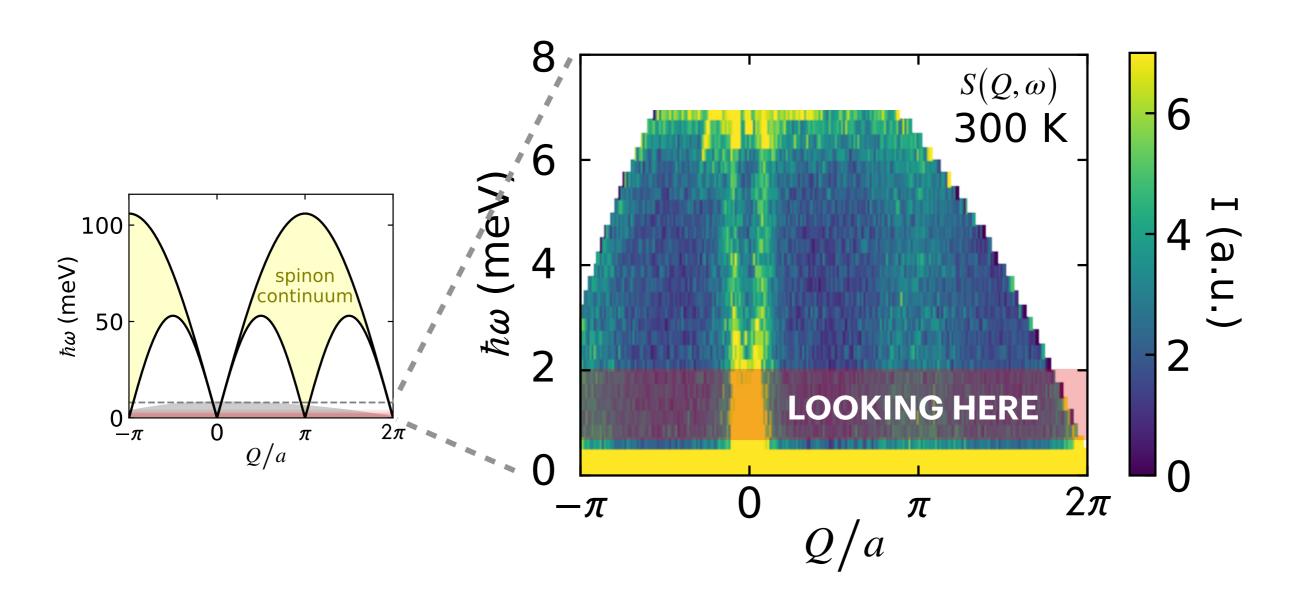
Where to look for hydrodynamics?

$$S(Q \to 0, \omega \approx 0) \sim Q^{-3/2}$$

Dynamical exponent z

It emerges in the long time and wavelength limits

$$Q \rightarrow 0, \omega \rightarrow 0$$



Additional experimental insight from a very different system

RESEARCH ARTICLE

QUANTUM SIMULATION

Quantum gas microscopy of Kardar-Parisi-Zhang superdiffusion

David Wei^{1,2}, Antonio Rubio-Abadal^{1,2}†, Bingtian Ye³, Francisco Machado^{3,4}, Jack Kemp³, Kritsana Srakaew^{1,2}, Simon Hollerith^{1,2}, Jun Rui^{1,2}‡, Sarang Gopalakrishnan^{5,6}, Norman Y. Yao^{3,4}, Immanuel Bloch^{1,2,7}, Johannes Zeiher^{1,2}*

The Kardar-Parisi-Zhang (KPZ) universality class describes the coarse-grained behavior of a wealth of classical stochastic models. Surprisingly, KPZ universality was recently conjectured to also describe spin transport in the one-dimensional quantum Heisenberg model. We tested this conjecture by experimentally probing transport in a cold-atom quantum simulator via the relaxation of domain walls in spin chains of up to 50 spins. We found that domain-wall relaxation is indeed governed by the KPZ dynamical exponent z = 3/2 and that the occurrence of KPZ scaling requires both integrability and a nonabelian SU(2) symmetry. Finally, we leveraged the single-spin-sensitive detection enabled by the quantum gas microscope to measure an observable based on spin-transport statistics. Our results yield a clear signature of the nonlinearity that is a hallmark of KPZ universality.

~50 spins in an **isolated** chain, with control over the XXZ anisotropy.

Dynamics of the quantum spin-1/2 Heisenberg chain

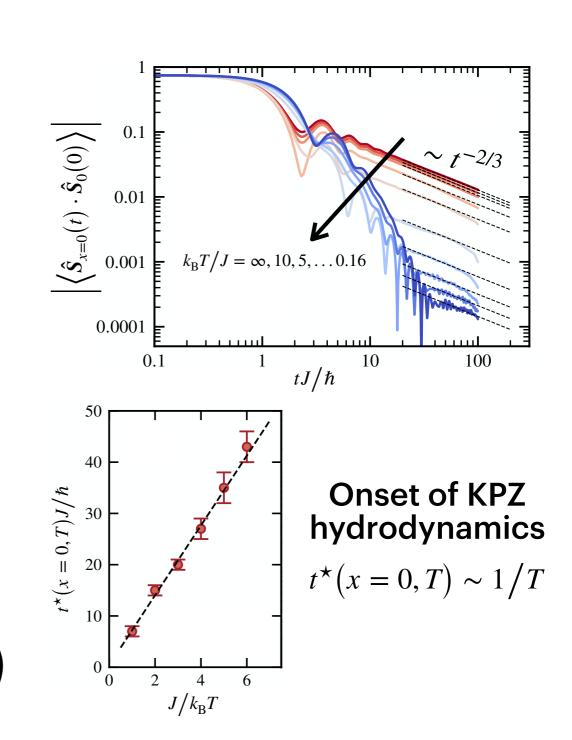
High-temperature

Kardar-Parisi-Zhang "KPZ" Hydrodynamics

> M. DUPONT, ET AL. ARXIV:2104.13393 (2021)

Tomonaga-Luttinger liquid physics

Low-temperature



Part 2: Why do classical numerics work so well for that problem? Try to understand in a more general case

Universal quantum behavior out of equilibrium

At ground state phase transitions (``quantum phase transitions''), an energy gap closes.

At second-order phase transitions, this gap closing involves a diverging correlation length and universal critical exponents.

Now imagine a parameter in the Hamiltonian to sweep through this gap closing. The failure of adiabaticity ("quantum Kibble-Zurek mechanism") gives a way to measure some properties of the quantum critical point.

Very suitable for quantum hardware, e.g., in Harvard Rydberg system to measure critical exponents of 2D quantum Ising model.

Universal quantum behavior out of equilibrium

The scaling exponents can be deduced from a simple reasoning. The adiabaticity is lost when $t \approx -\tau$, where τ is determined by Eq. (1), this corresponds to

$$\tau_{KZ} \sim v^{-\frac{v_z}{1+v_z}}, \; \xi_{KZ} \sim v^{-\frac{v}{1+v_z}},$$
 (2)

thus defining the Kibble-Zurek time and length, correspondingly. Since the adiabaticity is restored after $t = \tau$ and we expect the generated exitations to freeze out and the average density of excitations and energy will be

$$n_{ex} \sim 1/\xi_{KZ} \sim v^{\frac{\nu}{1+z\nu}},\tag{3}$$

$$\epsilon_{ex} \sim 1/\xi_{KZ}^2 \sim v^{\frac{2\nu}{1+z\nu}}.\tag{4}$$

This is a very simple argument, but the result has been confirmed by numerics and experiments. There's also an exact solution for the transverse-field Ising model [36].

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
$$|\psi\rangle=A_{s_1}A_{s_2}A_{s_3}A_{s_4}|s_1s_2s_3s_4\rangle$$
 matrix product
$$|\psi\rangle=A_{s_1}^{ij}A_{s_2}^{jk}A_{s_3}^{kl}A_{s_4}^{li}|s_1s_2s_3s_4\rangle$$

matrix product

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 I of renaissance; see Vidal '07, for example)

matrix product
$$|\psi\rangle=A_{s_1}^{ij}A_{s_2}^{jk}A_{s_3}^{kl}A_{s_4}^{li}|s_1s_2s_3s_4\rangle$$

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 (solved pre-2005)

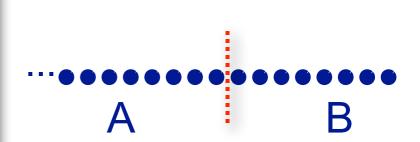
But none of these is strictly correct. Going above one dimension is expensive, but not impossible. Long-range interactions very hard.

A way to picture the entanglement of a state

Schmidt decomposition of the state (SVD):

$$|\psi\rangle = \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} C_{ij} |i\rangle_A |j\rangle_B$$

$$= \sum_{\alpha=1}^{\min(N_A, N_B)} \lambda_\alpha |\phi_\alpha\rangle_A |\phi_\alpha\rangle_B$$



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

a natural measure of the entanglement is the entropy:

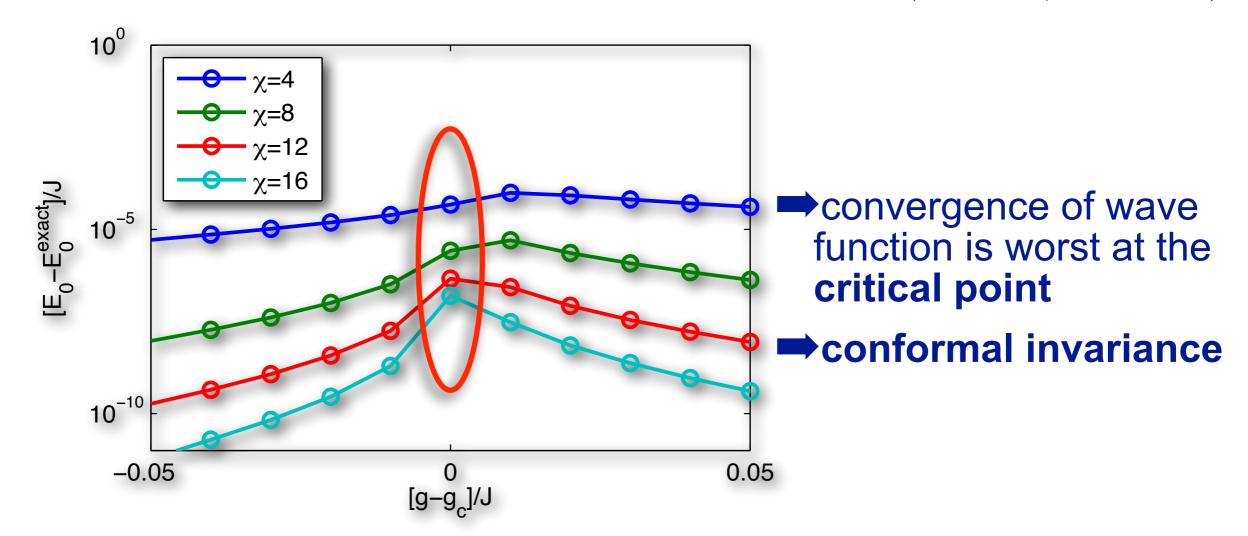
$$S_A = S_B = S = -\sum_{\alpha} \lambda_{\alpha}^2 \log(\lambda_{\alpha}^2)$$

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 fixed-dimensional
 - ⇒slightly entangled 1D systems: Matrix Product States
 - →DMRG, TEBD, ...

- 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: $H = \sum_{i} \left(J \sigma_i^z \sigma_{i+1}^z + g \sigma_i^x \right)$



Good news: can make "finite-entanglement" theory of convergence at critical points; they are hardly inaccessible.

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
$$|\psi\rangle=A_{s_1}^{ij}A_{s_2}^{jk}A_{s_3}^{kl}A_{s_4}^{li}|s_1s_2s_3s_4\rangle$$

Quantitatively, it is found that dim A plays a role similar to imposing a finite system size: $L_{\infty} \propto v^{\kappa} \qquad v = \dim A$

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

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)

• (Li-Haldane) "entanglement spectrum" [Calabrese et al '08]

$$n(\lambda) = I_0 \left(2 \sqrt{-b^2 - 2b \log \lambda} \right) \qquad \text{$\#$ of $\hat{\lambda}$'s greater}$$
 with $b = \frac{S}{2} = \frac{c}{12} \log \xi = -2 \log \lambda_{\max}$ than λ 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

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

- A heuristic argument for the asymptotic case (using a continuum of Schmidt values and $\chi \to \infty$)
 - universal finite-entanglement scaling relations

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

F. Pollmann, S. Mukerjee, A. Turner, and J.E. Moore, PRL 2009 Some checks for various critical theories are in that paper, and the recent work B. Pirvu, G. Vidal, F. Verstraete, L. Tagliacozzo, PRB 2012

So critical points are worse than gapped points, but in a controlled way. What does this mean in practice?

Remark: Entanglement spectra are qualitatively different for random critical spin chains than for pure ones, though entanglement entropies similar (M. Fagotti, P. Calabrese, JEM).

What about a Kibble-Zurek sweep?

The scaling exponents can be deduced from a simple reasoning. The adiabaticity is lost when $t \approx -\tau$, where τ is determined by Eq. (1), this corresponds to

$$\tau_{KZ} \sim v^{-\frac{v_z}{1+v_z}}, \; \xi_{KZ} \sim v^{-\frac{v}{1+v_z}},$$
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thus defining the Kibble-Zurek time and length, correspondingly. Since the adiabaticity is restored after $t=\tau$ and we expect the generated exitations to freeze out and the average density of excitations and energy will be

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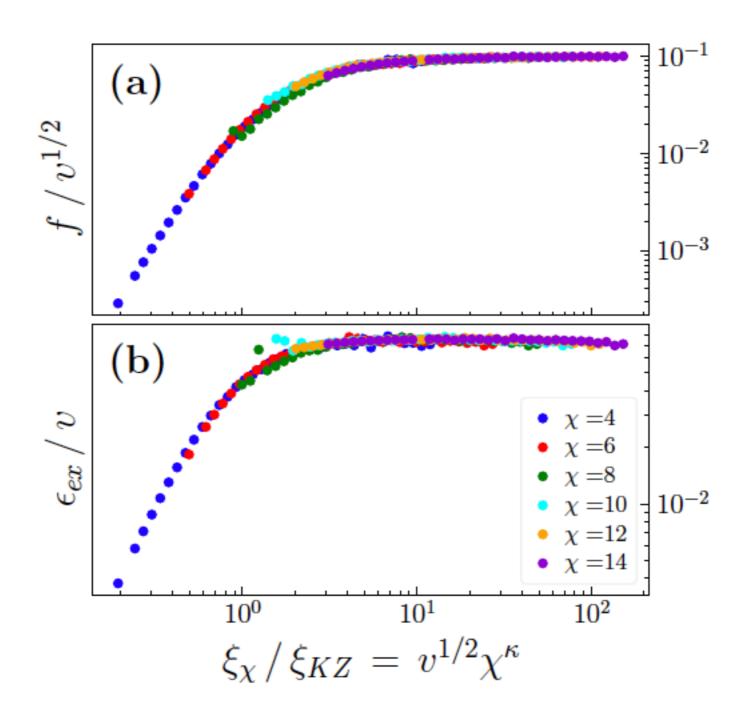
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This is a very simple argument, but the result has been confirmed by numerics and experiments. There's also an exact solution for the transverse-field Ising model [36].

N. Sherman, A. Avdoshkin, JEM, Universality of critical dynamics with finite entanglement, arXiv:2301.09681

What about a Kibble-Zurek sweep at finite entanglement? Double scaling hypothesis

$$n_{ex} = v^{\frac{\nu}{1+\nu}} f(\xi_{KZ}/\xi_{\chi}), \quad \epsilon = v^{\frac{2\nu}{1+\nu}} g(\xi_{KZ}/\xi_{\chi}),$$

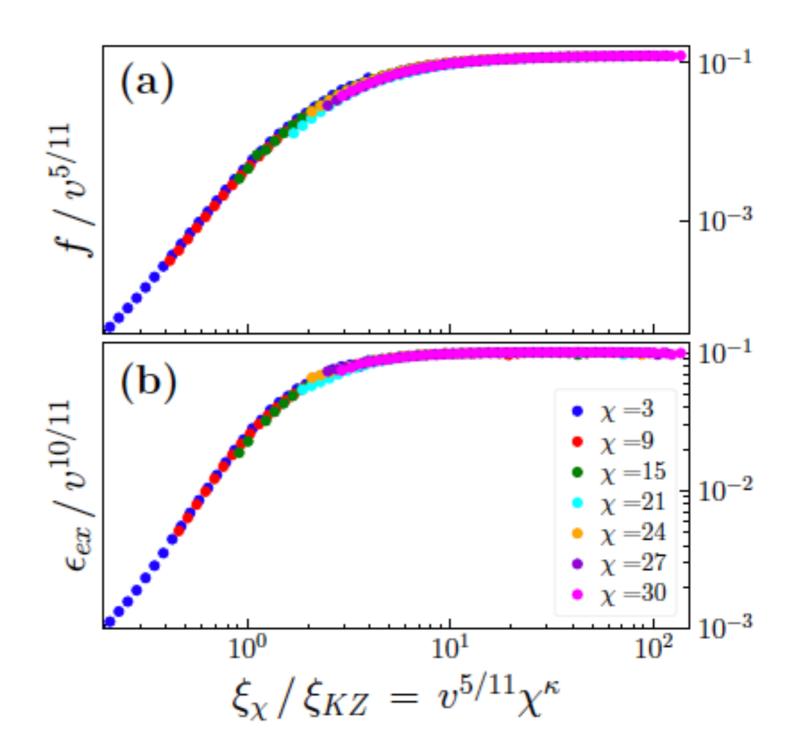


TFIM

What about a Kibble-Zurek sweep? Double scaling hypothesis

$$n_{ex} = v^{\frac{\nu}{1+\nu}} f(\xi_{KZ}/\xi_{\chi}), \quad \epsilon = v^{\frac{2\nu}{1+\nu}} g(\xi_{KZ}/\xi_{\chi}),$$

3-state Potts, More stringent test



Some conclusions/questions

We have some new approaches, experimental and theoretical, to many-body quantum problems in one dimensional systems.

Some of this is actually tested in experiments on ordinary crystals near room temperature, or with ultracold atoms.

The heuristic concept that "finite entanglement" (i.e., finite bond dimension) induces a length scale at quantum critical points describes not just ground states (~2009) but even dynamical processes like the Kibble-Zurek mechanism, with universal scaling functions.

Current questions:

Q: What are the unusual non-diffusive "fluids" of electrons and spins in higher dimensions?

Q: Are other non-standard perturbations, for example those relevant to quantum computers, also still captured within scaling frameworks?

Acknowledgements

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Nick Sherman

Postdocs: Maxime Dupont (to Rigetti) Johannes Motruk (Geneva)

Alumni:
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Christoph Karrasch (Braunschweig)
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Nick



Nick

ORNL

Allen Scheie,

Alan Tennant,

Steve Nagler, et al.

Maxime

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