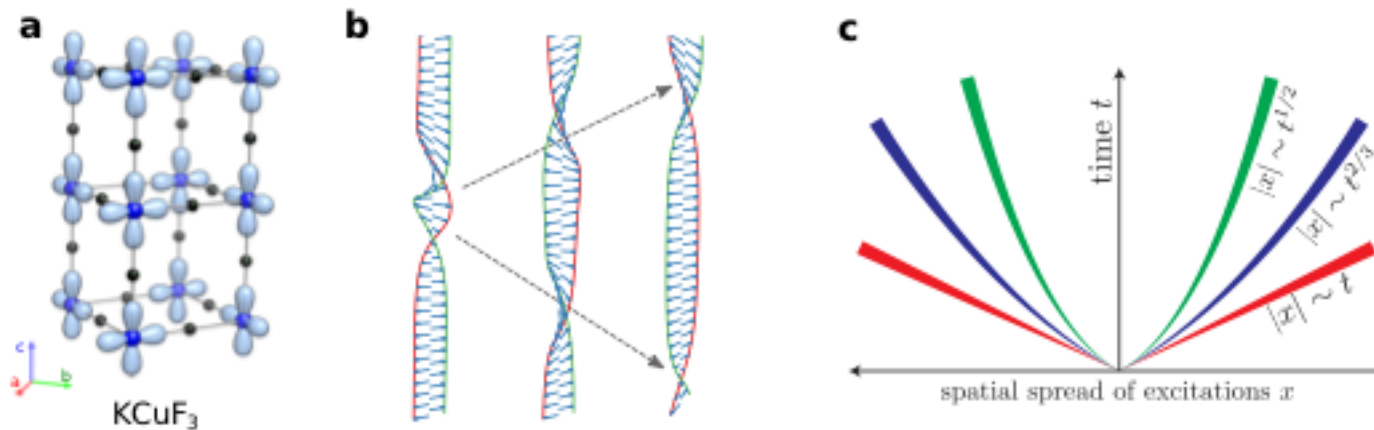


Spin hydrodynamics: from spin chains to neutron scattering

KITP, 1 September 2021

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



SIMONS FOUNDATION



Outline

I. In 1D (“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 KCuF_3 .

Why are there new kinds of hydrodynamics in 1D electron and spin systems?

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 arXiv 2021



Motivation

Conventional thermodynamics of large systems rests on the assumption that initial states thermalize to a “Gibbs ensemble”, determined by the conserved quantities (e.g., energy, particle number, maybe momentum).

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

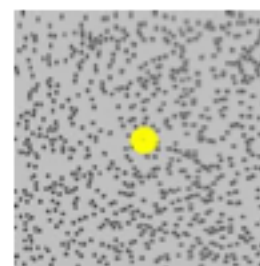
We start with extended quantum interacting systems in $d=1$.

1. What about “integrable” (Yang-Baxter) systems with infinitely many conservation laws?
2. (Real systems are not exactly integrable and there is no “KAM theorem”. Does any of this survive in slightly perturbed $d=1$ systems?)
3. *Does this all have anything to do with experiments on real materials?*

(#1 has been a very active field: see recent review by Bulchandani, Gopalakrishnan, Ilievski, arXiv:2103.01976)

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

Phenomenological description of most spin chains at high temperatures

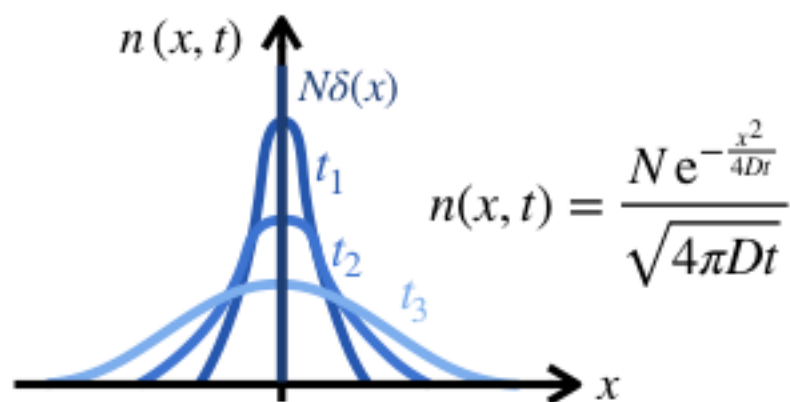
The diffusion equation

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

of particles
N conserved

$$\int_{\mathbf{V}} n(x, t) dx = N \quad \forall t$$

local density



Analogy with magnets

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

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

Emergent fluid-like spin diffusion?

$$\lim_{x, t \rightarrow +\infty} \left\langle \hat{S}_x^z(t) \hat{S}_0^z(0) \right\rangle_{k_B T \rightarrow +\infty} = t^{-1/2} f_{\text{Gaussian}}(x/t^2)$$

Dynamical exponent: $z = 2$

Standard hydrodynamics (0th order)

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

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

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

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

These come from the Boltzmann equation assuming local equilibrium.

Hydrodynamics: how does local equilibrium become global equilibrium?

Models to be studied

Let's start with two examples of Yang-Baxter “integrable” systems:

the 1D Bose gas with delta-function interaction (Lieb-Liniger model);

the 1D “XXZ” spin chain.

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

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 $J_z = J_{xx}$.

An important consequence of integrability for dynamics and thermalization is that there exists an infinite number of conserved quantities, although these become quite complicated for XXZ. There the conserved *charges* and *currents* are (notation from T. Prosen), after spin and E,

$$\begin{aligned}
q_{[3]} &= -\Delta\sigma^{xyz} + \Delta\sigma^{yxz} - \Delta\sigma^{zxy} + \Delta\sigma^{zyx} + \sigma^{xzy} - \sigma^{yzx}, \\
q_{[4]} &= -2\Delta^2(\sigma^{xxxx} + \sigma^{yyyy}) - (2\Delta^2 + 2)(\sigma^{xx00} + \sigma^{yy00}) + 2\Delta(\sigma^{x0x0} + \sigma^{xyxy} \\
&\quad - \sigma^{xyyx} + \sigma^{xzxz} + \sigma^{y0y0} - \sigma^{yxxy} + \sigma^{yxxy} + \sigma^{yzyz} + \sigma^{z0z0} + \sigma^{zxzx} + \sigma^{zyzy} \\
&\quad - 2\sigma^{zz00}) - 2\sigma^{xzzx} - 2\sigma^{yzzz}, \\
q_{[5]} &= (4\Delta^3 + 14\Delta)(\sigma^{xyz00} - \sigma^{yxz00} + \sigma^{zxy00} - \sigma^{zyx00}) + 6\Delta^2(-\sigma^{x0yz0} + \sigma^{xyxxx} \\
&\quad + \sigma^{xyyyz} + \sigma^{y0xz0} - \sigma^{yxxxx} - \sigma^{yxxyy} - \sigma^{zx0y0} + \sigma^{zxxx} - \sigma^{zxyx} - \sigma^{zxyz} \\
&\quad + \sigma^{zy0x0} + \sigma^{zyyx} - \sigma^{zyyyx} + \sigma^{zyzxx}) + (10\Delta^2 + 8)(-\sigma^{xzy00} + \sigma^{yzx00}) \\
&\quad + 6\Delta(\sigma^{x0zy0} - \sigma^{xy0z0} - \sigma^{yxzx} - \sigma^{xyzy} + \sigma^{xz0y0} - \sigma^{zxxy} + \sigma^{zxxy} + \sigma^{xzzz} \\
&\quad - \sigma^{y0zx0} + \sigma^{yx0z0} + \sigma^{yxzx} + \sigma^{yxzy} - \sigma^{yz0x0} - \sigma^{yzxy} + \sigma^{zyyx} - \sigma^{yzzz} \\
&\quad - \sigma^{z0xy0} + \sigma^{z0yx0} + \sigma^{zxzy} - \sigma^{zyzx}) - 6\sigma^{xzzz} + 6\sigma^{yzzz}, \\
P_{[2]} &= -2q_{[3]}, \\
P_{[3]} &= 2\Delta^2(\sigma^{xxxx} + \sigma^{yyyy}) - (2\Delta^2 + 2)(\sigma^{0xx0} + \sigma^{0yy0}) + 2\Delta(-2\sigma^{0zz0} - \sigma^{xyxy} \\
&\quad + \sigma^{xyyx} - \sigma^{xzxz} + \sigma^{yxxy} - \sigma^{yxxy} - \sigma^{yzyz} - \sigma^{zxxz} - \sigma^{zyzy}) + 2\sigma^{xzzz} + 2\sigma^{yzzz}, \\
P_{[4]} &= (4\Delta^3 + 4\Delta)(\sigma^{0xyz0} - \sigma^{0yxz0} - \sigma^{zxy00} + \sigma^{zyx00}) + 4\Delta^2(-\sigma^{xyxxx} - \sigma^{xyyyz} \\
&\quad + \sigma^{yxxxx} + \sigma^{yxxyy} + \sigma^{zx0y0} - \sigma^{zxxx} + \sigma^{zxyx} + \sigma^{zxyz} - \sigma^{zy0x0} - \sigma^{zyyx} \\
&\quad + \sigma^{zyyyx} - \sigma^{zyzxx}) + (4\Delta^2 + 4)(-\sigma^{0xzy0} + \sigma^{0yzx0} + \sigma^{xzy00} - \sigma^{yzx00}) \\
&\quad + 4\Delta(2\sigma^{0zxy0} - 2\sigma^{0zyx0} + \sigma^{xy0z0} + \sigma^{yxzx} + \sigma^{xyzy} - 2\sigma^{xyz00} - \sigma^{xz0y0} \\
&\quad + \sigma^{zxxy} - \sigma^{zxyx} - \sigma^{xzzz} - \sigma^{yx0z0} - \sigma^{yxzx} - \sigma^{yxzy} + 2\sigma^{yxz00} + \sigma^{yz0x0} \\
&\quad + \sigma^{zyyx} - \sigma^{zyyx} + \sigma^{yzzz} - \sigma^{zxzy} + \sigma^{zyzx}) + 4\sigma^{xzzz} - 4\sigma^{yzzz}, \quad (82)
\end{aligned}$$

Note that these are local in real space; the momentum-space occupancies only work for the non-interacting system.

Some history

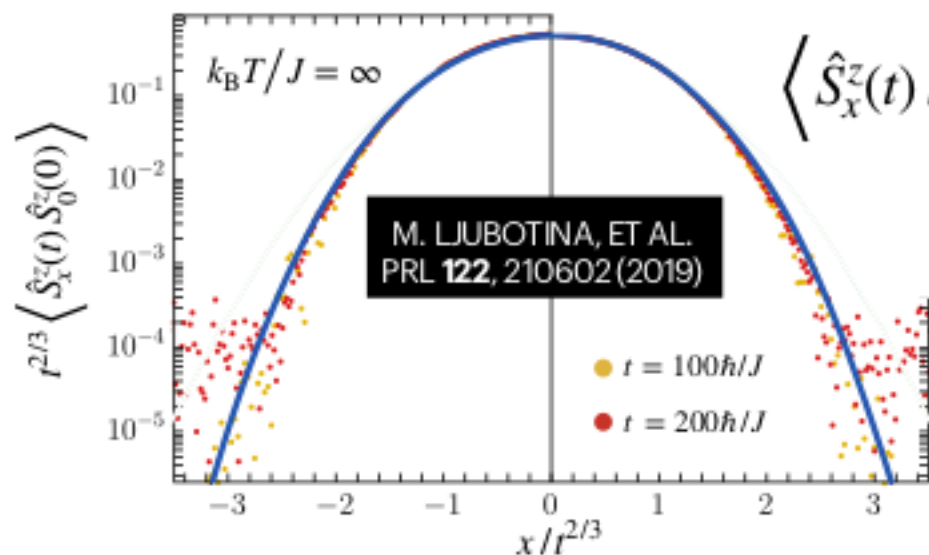
The ground state of the Heisenberg chain was solved by Bethe (1931) and the thermodynamics was understood in the 1970s.

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. 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 results that pass tests against DMRG-type numerical calculations.

Emergent hydrodynamics in Heisenberg spin chain at infinite temperature



$$\langle \hat{S}_x^z(t) \hat{S}_0^z(0) \rangle_{k_B T = +\infty} = t^{-2/3} f_{\text{KPZ}}(x/t^{2/3})$$

Kardar-Parisi-Zhang
“KPZ” hydrodynamics

Dynamical exponent: $z = 3/2$

What is KPZ?

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

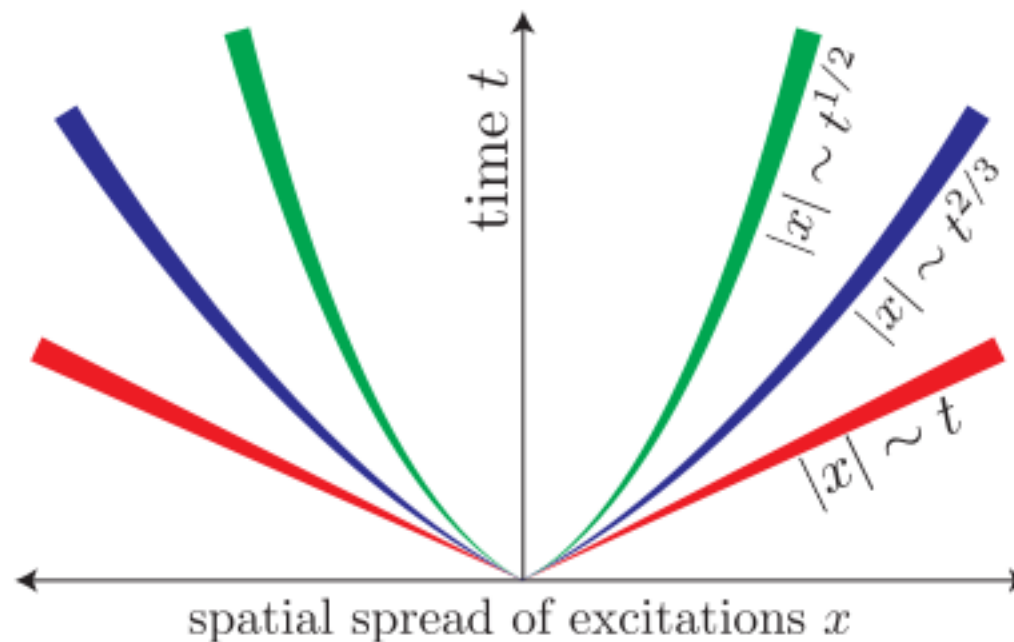
Solution:

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

Where to find it?

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

Emergent hydrodynamics in Heisenberg spin chain at infinite temperature



What is KPZ?

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

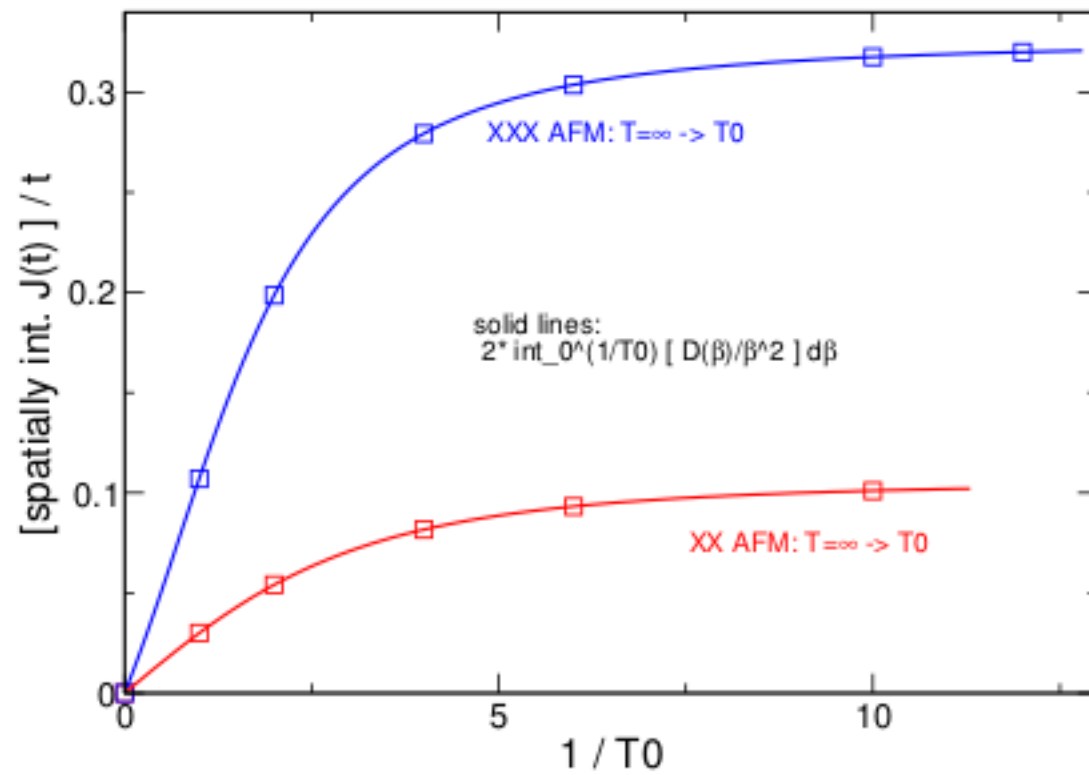
Solution:

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

Where to find it?

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

Qid: exact far-from-equilibrium energy expansion in $\lambda\lambda\lambda$ (Vasseur, Karrasch, JEM 2015)



Comparison is rate of increase of energy current versus temperature integral of Drude weight



Recent progress

We had some specialized tricks to get exact far-from-equilibrium results for a few models. Can one develop a more general approach for hydrodynamics in integrable models?

Yes: started from work on (almost certainly) asymptotically exact solutions for the two-reservoir initial condition in

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

1. Key steps of approach (in one language)
Physical picture of kinetic theory (Boltzmann equation):
same *classical spirit* as El and Kamchatnov, PRL 2005
2. Does it pass XXZ numerical comparisons that previous similar ansatzes failed?

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

“Bethe-Boltzmann equation”

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

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.

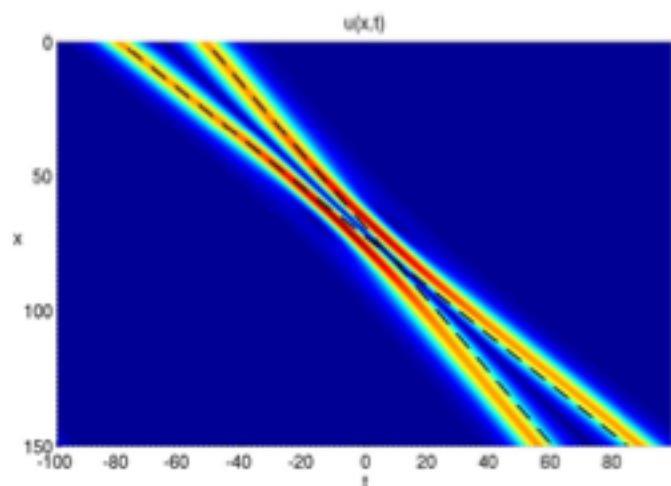
Why Boltzmann equation gets modified in (classical or quantum) integrable systems

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)

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

Summary of when this is useful

Normal fluid:

Initial state \rightarrow Local equilibrium \rightarrow Hydrodynamics

Integrable fluid:

Initial state \rightarrow Local GGE \rightarrow 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).

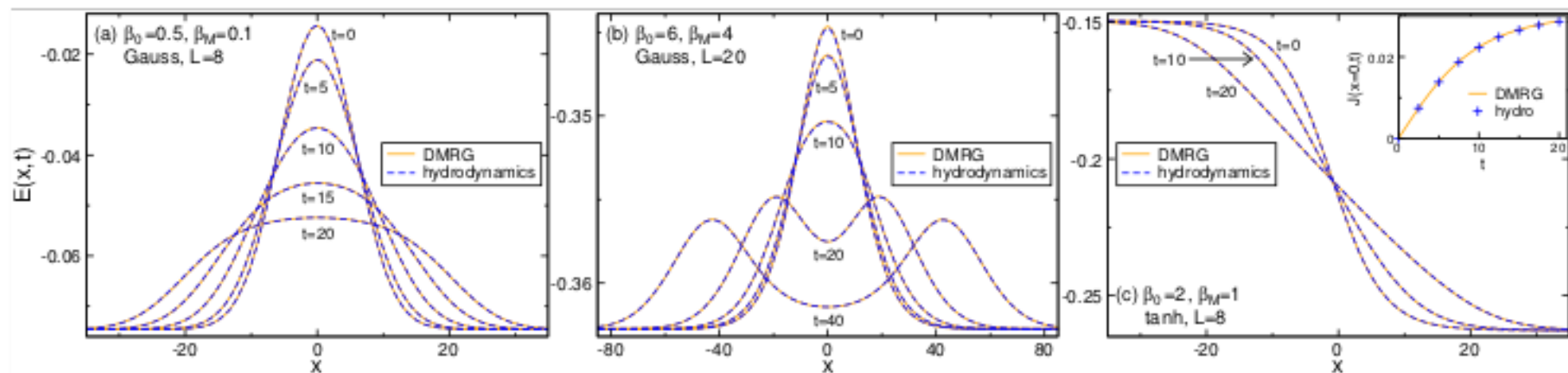
Let’s look for full (x,t) solutions: are quantum dynamics really describable by these classical particle equations?

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

Take XXZ in zero magnetic field. Make a spatial variation of initial temperature.

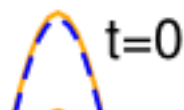
Watch the energy spread out in time.

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.)



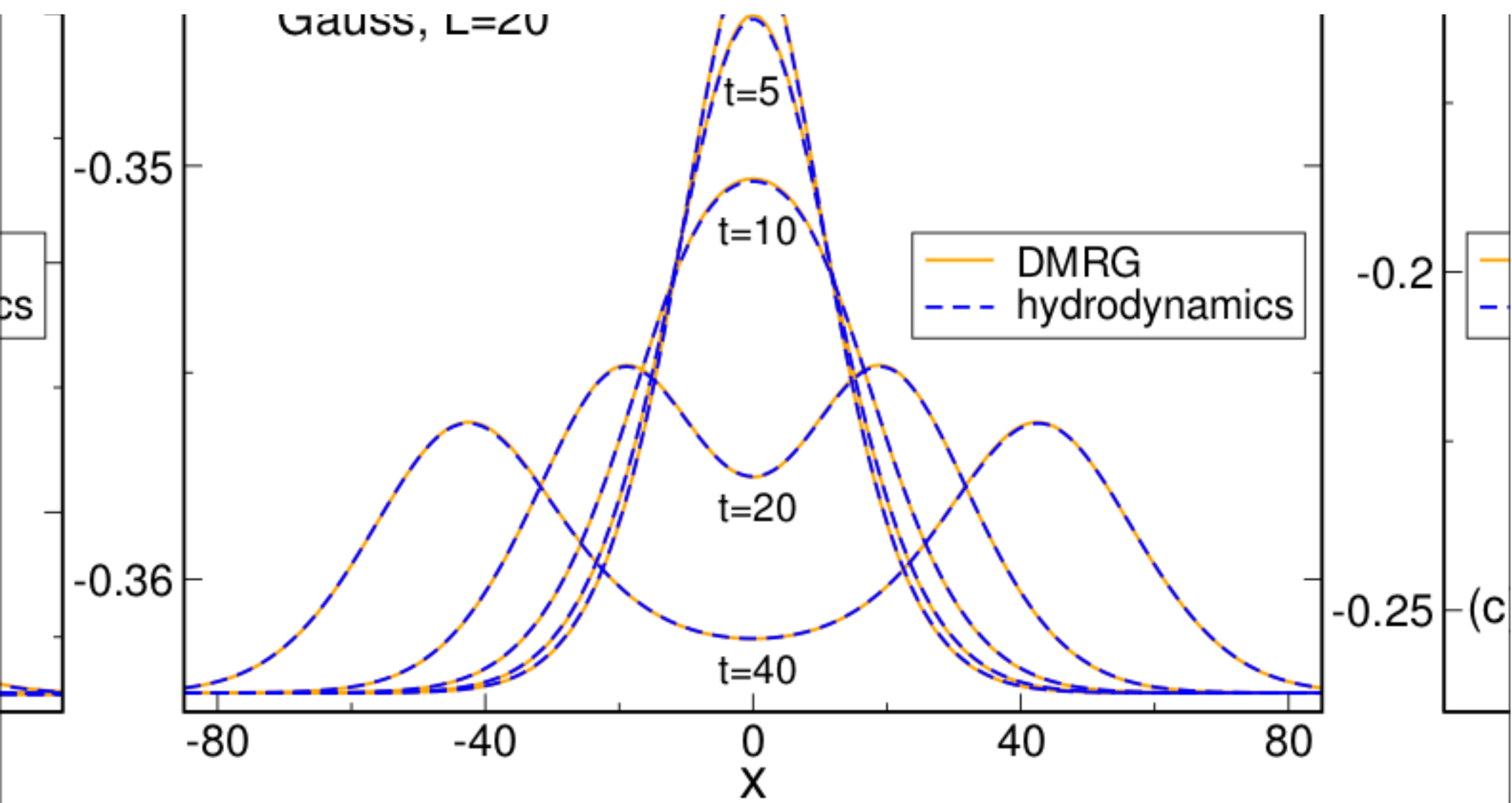
These are comparisons for interacting spinless fermions (XXZ) between backwards Euler solution of Bethe-Boltzmann and microscopic DMRG simulations. (figure from "Solvable quantum hydrodynamics", V. Bulchandani, R. Vasseur, C. Karrasch, and JEM, arXiv April 2017)

(b) $\beta_0=6, \beta_M=4$



-0.15

Gauss, L=20



What else can happen?

The previous examples were for the gapless regime, with ultimately ballistic scaling.
The gapped, easy-axis regime is diffusive.

What about the last gapless point, the Heisenberg point?

Another reason people care about spin chains and DMRG:

They are an example of a physical system that we can understand “beyond the diagonalization limit”, and simulate on quantum hardware

Hydrodynamics beyond diffusion

Example:

$$\hat{\mathcal{H}} = J \sum_n \hat{S}_n^x \hat{S}_{n+1}^x + \hat{S}_n^y \hat{S}_{n+1}^y + \Delta \hat{S}_n^z \hat{S}_{n+1}^z$$



$\mathfrak{D}(T) > 0$	$\mathfrak{D}(T) = 0$ but $\langle \hat{J}(t)\hat{J}(0) \rangle \sim t^{-2/3}$	$\mathfrak{D}(T) = 0$
Ballistic dynamics $z = 1$	Superdiffusion Kardar-Parisi-Zhang $z = 3/2$	Diffusion $z = 2$
Integrable	Integrable + spin isotropy	Integrable + easy-axis anisotropy <i>Or absence of integrability</i>

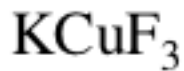
M. DUPONT AND J.E. MOORE
PRB **101**, 121106(R) (2020)

Are there experimental consequences of this

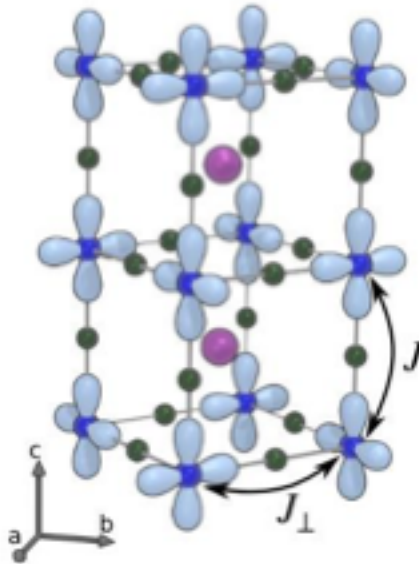
“generalized hydrodynamics” structure?

1. There are Lieb-Liniger atomic experiments (Bouchoule et al.). Here: how neutron scattering on a model Heisenberg chain compound shows Kardar-Parisi-Zhang superdiffusive behavior as a consequence of extra conservation laws.
2. (The generic state of 1D metals is a “Luttinger liquid” but with irrelevant, integrability-breaking perturbations. We can realize this by adding integrability-breaking terms that retain lattice translation invariance. Conclusion: there are at least *two* different mechanisms for adjustable power-laws in LL transport, and a surprising consequence for experiments.)

Experimentally looking for hydrodynamics



K ● Cu ● F ●



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

**Superdiffusive Kardar-Parisi-Zhang
“KPZ” hydrodynamics expected**

A. SCHEIE, ET AL.
NAT. PHYS. (2021)

$$\langle \hat{S}_x^z(t) \hat{S}_0^z(0) \rangle \xrightarrow{\text{Fourier transforms}} S(Q, \omega)$$

Corresponds to the neutron scattering intensity

Neutron scattering measurements

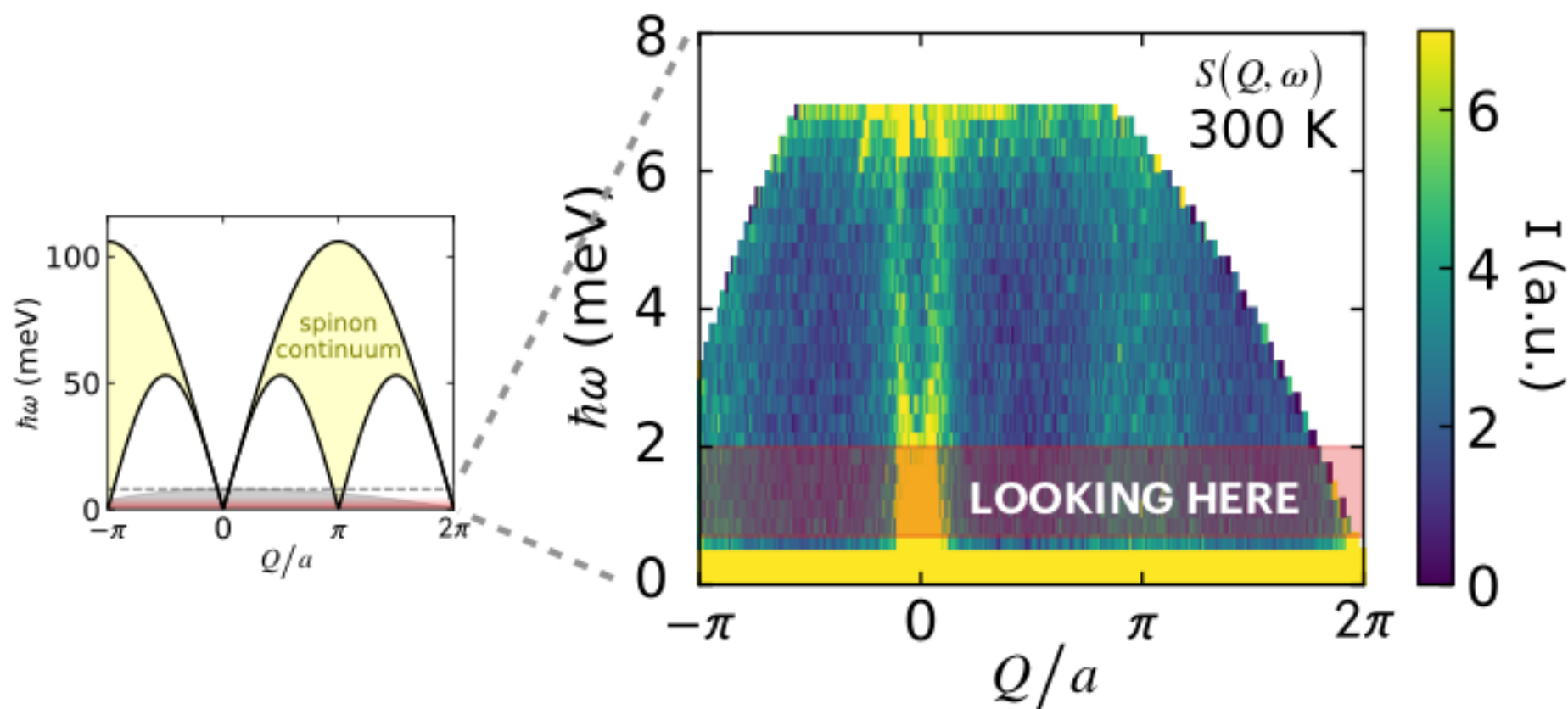
Where to look for hydrodynamics?

It emerges in the long time
and wavelength limits

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

Dynamical exponent z

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



Kardar-Parisi-Zhang universality at *high*

temperatures in the Heisenberg spin chain

In XXZ, the Heisenberg point separates diffusion from ballistic behavior...

Numerical observation: (starting c. 2017;
most convincing is Ljubotina, Znidaric, Prosen, 2019)

At infinite temperature, the spin correlations in the quantum spin-half Heisenberg chain are in a famous classical stochastic universality class.

(This is not true for the non-integrable classical Heisenberg model.)

$$\frac{\partial h(x, t)}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x, t)$$

Diffusion, another classical stochastic description, is thought to emerge in purely quantum systems, so why not others?

Experiment: look for KPZ scaling in frequency integrations near $\mathbf{q}=\mathbf{0}$

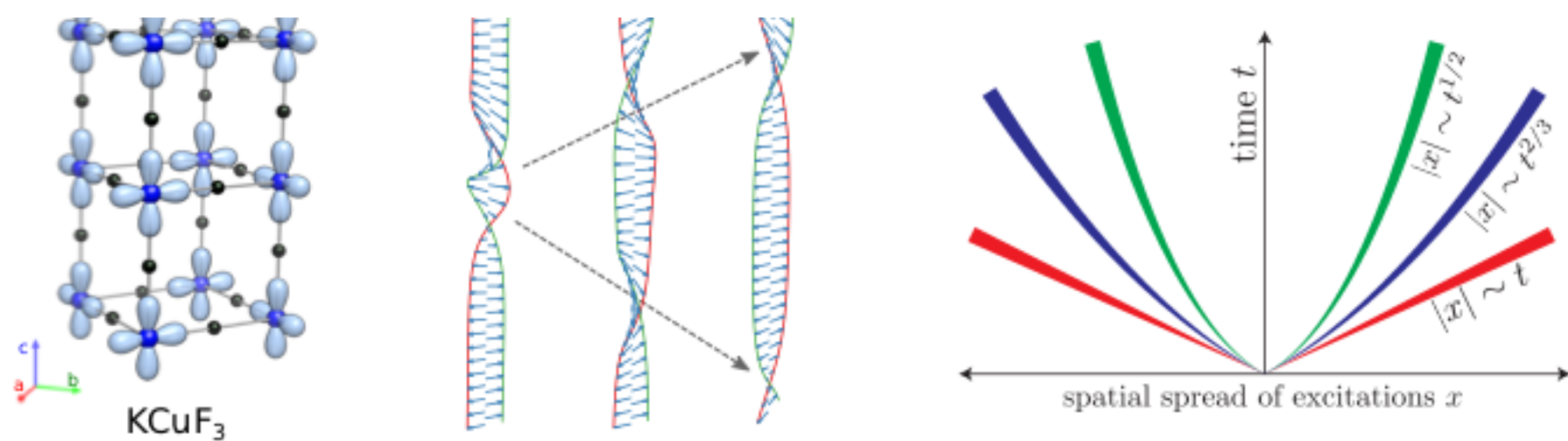
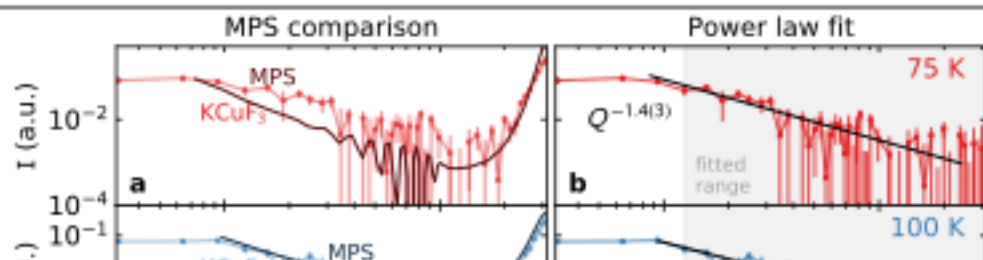


Figure 1: **a** Crystal structure of KCuF_3 , showing the orbital order of the $\text{Cu } x^2 - y^2$ orbitals. This order leads to strong magnetic exchange interactions along the c (vertical) axis and weak exchange interactions along a and b , such that the Cu^{2+} ions effectively make 1D chains. **b** Schematic illustration of spinon excitations in a 1D Heisenberg antiferromagnet (based on Ref. ⁷). **c** Schematic illustration of three possible length-time scaling behaviors $|x| \sim t^{1/z}$ observed at high temperature in 1D quantum magnets, classified by the dynamical exponent z : $z = 2$ corresponds to diffusion (green curve), $z = 3/2$ to superdiffusive (blue curve) and $z = 1$ to ballistic dynamics.

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



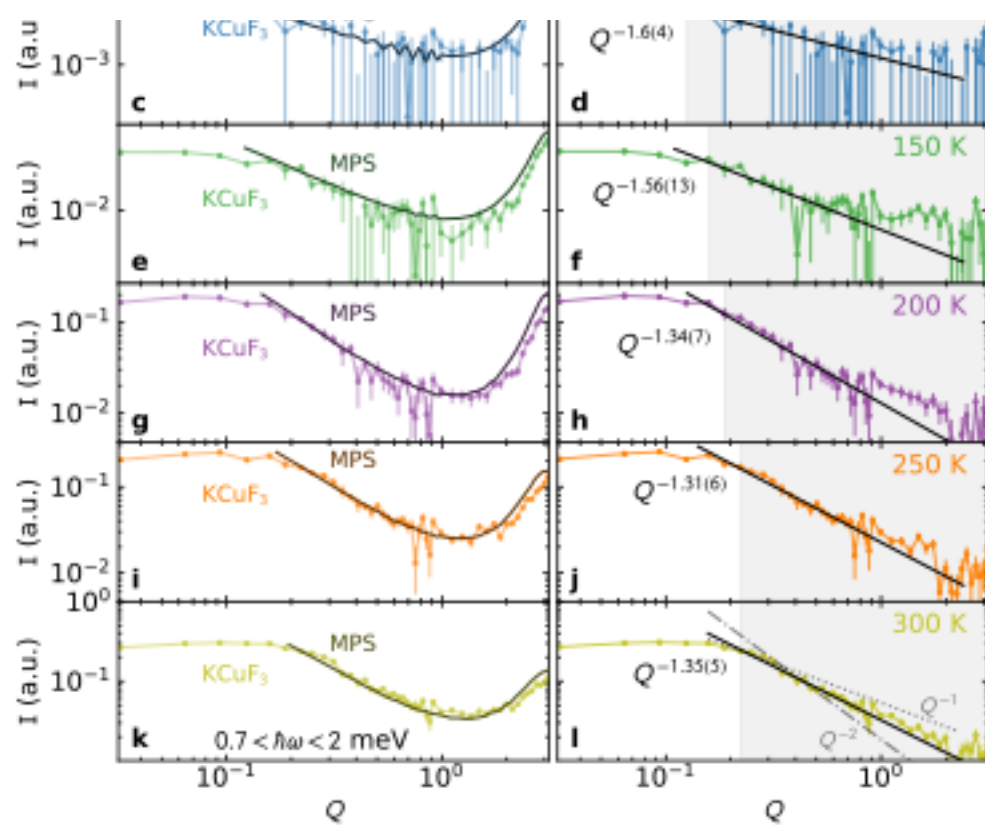


Figure 3: Power law behavior of KCuF_3 around $Q = 0$. The left column shows experimental data integrated over $0.7 < \hbar\omega < 2$ meV (cut a in Fig. 2) symmetrized about $Q = 0$ compared with the MPS simulations. The same multiplicative scaling factor is used for all temperatures, and the agreement is quite good above $Q \approx 0.2$, below which finite-size effects are significant for MPS (See the Supplementary Information). The right column shows the data fitted to a phenomenological power law. As a part of the fit, the $Q = \pi$ peak was also fitted to a power law and subtracted off as background. The fitted power is very close to $-3/2$ at all temperatures. Comparison to $z = 2$ and $z = 1$ exponents are given in panel l. (Note that Q is unitless $0 \rightarrow 2\pi$ as in Fig. 2.)

A. Scheie, N. Sherman, M. Dupont, S. Nagler, G. Granroth, M. Stone, JEM, A. Tennant, arXiv:2009.13535

Dynamics of the quantum spin-1/2 Heisenberg chain

Heisenberg chain

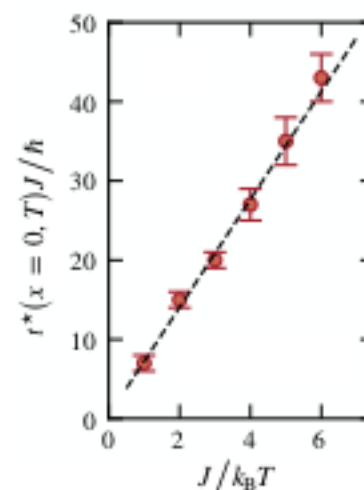
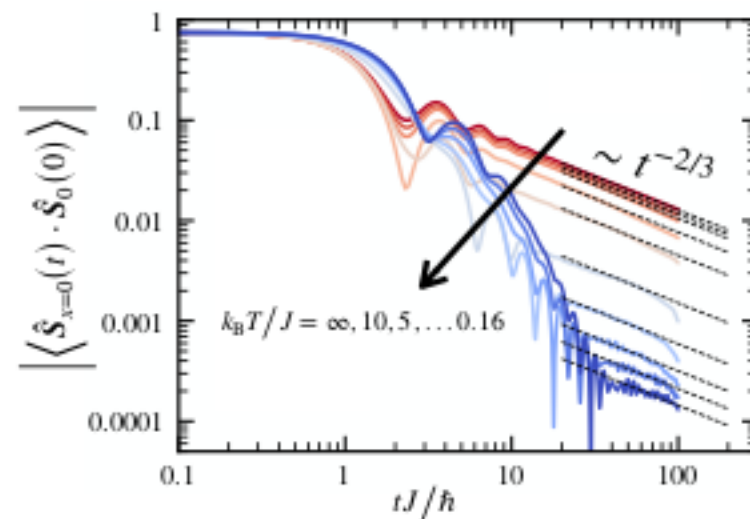
High-temperature

Kardar-Parisi-Zhang "KPZ"
Hydrodynamics

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

Tomonaga-Luttinger
liquid physics

Low-temperature



Onset of KPZ
hydrodynamics

$$t^*(x=0, T) \sim 1/T$$

Conclusion: the data are strong evidence for $z=1.5$ rather than $z=1$ or $z=2$

(Can't directly probe the full KPZ spectral function with neutrons, but can see it in the MPS calculation)

Current work: details of finite-T crossover, B fields, ...

Status of related theory:

1. There is an understanding of which spin chains have the KPZ universality class behavior, and which do not. Both integrability and “isotropy” are crucial. (Dupont and JEM, PRB RC 2020; confirmed analytically in paper below)
2. It is possible to compute $z=3/2$ using integrability (Ilievski et al., arXiv 2020), but not yet the full KPZ scaling function.
3. There are some ideas for how the KPZ universality class might emerge (Bulchandani, PRB RC 2020, ...)

Acknowledgements

Current Students:
Tessa Cookmeyer
Nick Sherman



Nick

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

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



Maxime

EPIQS (GBMF)
Simons Foundation

Alumni:
Vir Bulchandani (Princeton)
Christoph Karrasch (Braunschweig)
Romain Vasseur (UMass)

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

Kardar-Parisi-Zhang universality at *high*

temperature in the Heisenberg spin chain

temperatures in the Heisenberg spin chain

In XXZ, the Heisenberg point separates diffusion from ballistic behavior...

Numerical observation: (starting c. 2017;
most convincing is Ljubotina, Znidaric, Prosen, 2019)

At infinite temperature, the spin correlations in the quantum spin-half Heisenberg chain are in a famous classical stochastic universality class.

(This is not true for the non-integrable classical Heisenberg model.)

$$\frac{\partial h(x, t)}{\partial t} = \nu \nabla^2 h + \frac{\lambda}{2} (\nabla h)^2 + \eta(x, t)$$

Diffusion, another classical stochastic description, is thought to emerge in purely quantum systems, so why not others?

Experiment: look for KPZ scaling in frequency integrations near $\mathbf{q}=\mathbf{0}$

What observables are related to KPZ?

Derivatives of height are like spin

Why? Simple reason: boundary between easy-plane and easy-axis

More complicated reason: nonlinearity of the sigma-model on the sphere. But the role of integrability doesn't come out so clearly here—it gives the right “partial” noise in the noisy Burgers equation that I wrote before

Later: systematics of Zaletel-Pollmann stuff