Beyond conventional metallic transport: localization, hydrodynamics, and topology

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Will mention collaborative work with many people, including:
Jens Bardarson, Vir Bulchandani, Christoph Karrasch, Sid Parameswaran, Frank Pollmann, Thomas Scaffidi, Ivo Souza, Romain Vasseur, Shudan Zhong.

Wikipedia image of Berkeley

Main topics

0. Intro: assumptions of the standard treatment of transport in simple metals
Linear response: weak perturbation to equilibrium, which is then restored

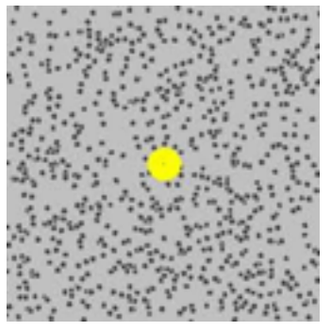
1. What about systems where these assumptions are violated?
Failures of relaxation: localization by disorder; free/integrable systems

Simple guesses:
Localized systems: particles move a localization length, then stop
Conventional (Yang-Baxter) integrable systems: particles move freely
Both simple guesses miss some interesting behavior. Will focus here on cases with *initial inhomogeneity* to observe transport. *Interlude: entanglement and numerics*

2. Are there unexpected ways a system can transport charge/heat?
"Topological" transport in insulators and metals
In insulators, transport can occur by the *ground state*, not quasiparticles
Even metals have some interesting topological effects

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

Standard quantum transport theory

In principle, we want to calculate the Kubo formula for electrical conductivity

$$\sigma_{\alpha\beta} = \frac{ine^2}{m\omega}\delta_{\alpha\beta} + \frac{1}{\hbar\omega V}\int_0^\infty \langle[\hat{j}_\alpha(t)\hat{j}_\beta(0)]\rangle\, dt$$

using the full many-body current operator *j*.

Challenges: for this to be finite, need current to relax (e.g., by disorder scattering, but full quantum theory of disorder scattering is complicated…).

Can do perturbation theory in interactions and disorder (Feynman diagrams). Approximations give Boltzmann transport theory, which we often use in practice as a simple semiclassical picture.

$$\partial_t f_1 + \mathbf{v}\cdot\nabla_{\mathbf{x}} f_1 = \int w'(f_1' f_2' - f_1 f_2) d\mathbf{p}_2\, d\mathbf{p}_1'\, d\mathbf{p}_2'.$$

(This is Boltzmann for collisions in a gas with no external force; in a solid, usually add electron-impurity collisions and applied fields).
A modern reference: J. Rammer, Quantum Transport Theory

Standard quantum transport theory

For the velocity in Boltzmann equation

$$\partial_t f_1 + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_1 = \int w'(f_1' f_2' - f_1 f_2) d\mathbf{p}_2 \, d\mathbf{p}_1' \, d\mathbf{p}_2'.$$

we use the semiclassical velocity of a wave packet (to be discussed in Lecture III).

$$\frac{dx^a}{dt} = \frac{1}{\hbar} \frac{\partial \epsilon_n(\mathbf{k})}{\partial k_a} + \mathcal{F}_n^{ab}(\mathbf{k}) \frac{dk_b}{dt}.$$

Second term is anomalous velocity or "Berry phase" piece.

This Boltzmann approach, while widely used for transport in 3D metals, is only valid under approximations that miss a lot of interesting physics.

Some major developments from past decade

About a decade ago, some key developments occurred in physics that is outside the above "standard model":

The system could fail to relax back to thermal equilibrium

MBL: Basko, Aleiner, Altshuler 2006

Integrable models and CFTs: Calabrese and Cardy "quantum quench", 2006

Transport could occur by something other than quasiparticles

1. Transport could happen in an *insulator* by pumping or edge excitations

Topological insulators, Kane-Mele, 2005; spin quantum Hall effect, 2004; 3D, 2006

2. Transport could occur via strongly interacting fluid without a quasiparticle interpretation

These build on earlier important developments that I will mention briefly but you can find in textbooks. Also, relevant topics such as bosonization will be covered in other lectures (I think).

Examples: non-interacting (Anderson) localization; integer quantum Hall physics (1980s).

Another past-decade development: role of entanglement in quantum statistical mechanics

Theme

Conventional thermodynamics rests on the assumption that initial states thermalize to a "Gibbs ensemble", determined by the conserved quantities (e.g., energy and particle number).

What about systems with infinitely many conservation laws?
(MBL = many-body localization = disorder + interactions)

Simple guesses:
MBL-type systems: particles move a localization length, then stop
Yang-Baxter type systems: particles move freely

Both simple guesses miss some interesting behavior.

Will focus here on cases with *spatial inhomogeneity* and connections to transport.

There is lots of work on homogeneous "quantum quenches" (Cardy and Calabrese, …) that will not be covered.

Outline of non-relaxation material and references

I. Differences between dynamics in MBL phases and in (non-interacting) Anderson localization.

Logarithmic entanglement growth: Jens Bardarson, Frank Pollmann, JEM, PRL 2012
Observation via Poincare "revivals": Siddharth Parameswaran, Romain Vasseur, JEM, PRB 2014

Other work: level statistics and eigenstate properties (with Maksym Serbyn); searching for MBL in translation-invariant systems (with Norman Yao, Chris Laumann, Ignacio Cirac, Mikhail Lukin, PRL 2016)

2. Yang-Baxter systems without disorder also break ergodicity and have infinitely many conserved quantities. How do they evolve in time?

(Examples of Yang-Baxter "integrable" systems: Bose gas with delta-function interaction; Heisenberg spin chain; 1D Hubbard model)

R. Vasseur, C. Karrasch, JEM, PRL 2015; also Vir Bulchandani, R. Vasseur, C. Karrasch, JEM, arXiv 2017.

Lots of recent work on "generalized hydrodynamics" like in classical integrable models;
see in particular Castro-Alvaredo/Doyon/Yoshimura and Bertini/Collura/De Nardis/Fagotti

Anderson localization and MBL

1. For non-interacting systems, we understand essentially completely the effects of disorder, at least away from transitions.
Review of one-particle localization, where numerics are relatively easy.

For the simplest symmetries (orthogonal and unitary ensembles), disorder is localizing for essentially all states in 1D and 2D.

2. The combination of interactions and disorder in closed systems ("many-body localization", Basko et al.) is not nearly as well understood, even in 1D.

Different properties of the MBL phase lead to different possible numerical experiments.
(Until very recently, "numerical experiments" were the only experiments! no longer.
But the current experiments on atomic systems are possibly not in the long-time limit.)

Examples: level statistics; entanglement of eigenstates; dynamics after a quench;…

References and questions to keep in mind

I. How is the MBL state different from ordinary Anderson localization (in entanglement, Bardarson, Pollmann, and JEM, PRL (2012); in random matrix ensemble, Serbyn and JEM, PRB (2016))?

II. How do these differences show up in observable dynamics ("revivals", Parameswaran, Vasseur, JEM, PRB (2014))?

III. How is MBL-type integrability different from Yang-Baxter integrability?

Probably won't get to:

What MBL-like behavior exists in translation-invariant systems? Can look for compact density response to a weak, arbitrarily broad perturbation…

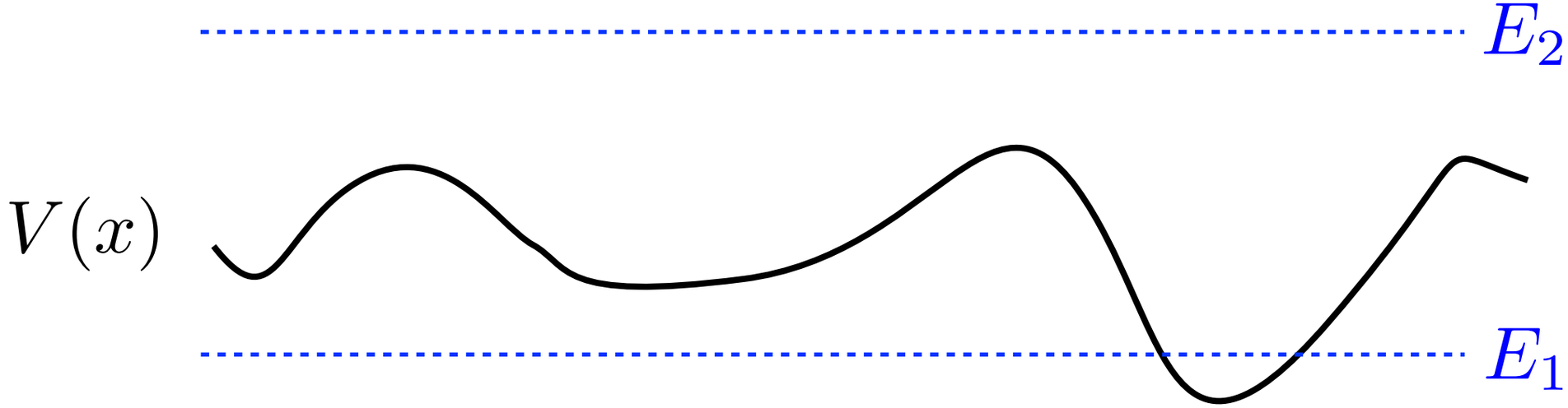
Things that won't be discussed:

higher dimensions; conventional or topological order; response to a *local* quench; theories of thermalizing transition

Intro to disordered electronic systems

Consider a quantum particle, described by the Schrödinger equation, moving in a random potential.

Intuitively, we might expect:
at low energy, eigenstates are trapped ("localized") in potential minima
at high energy, eigenstates are scattering states

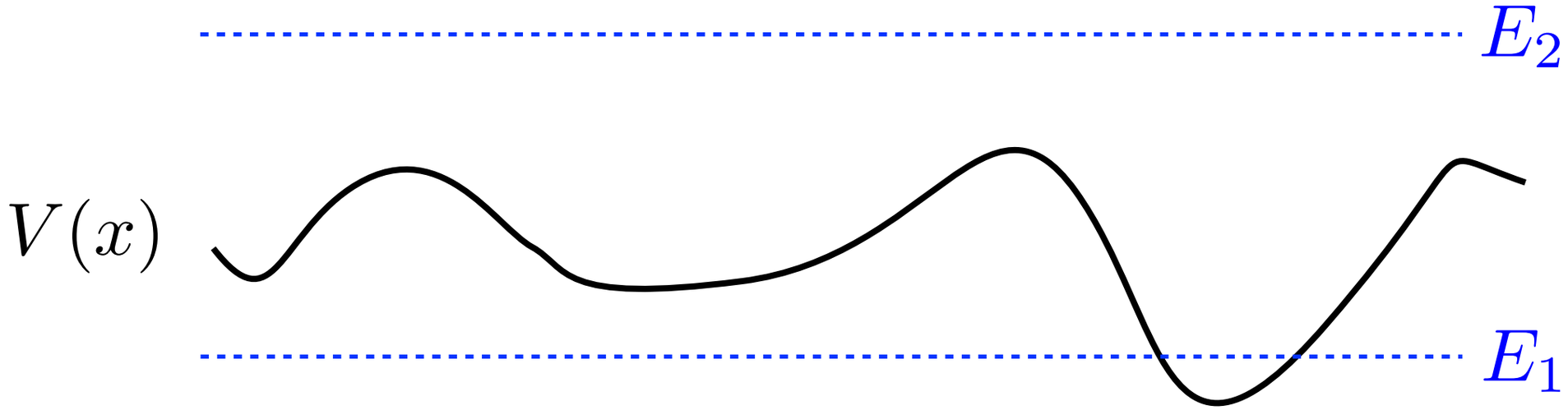


In 3D, this intuition is basically correct, and there is a specific energy (the "mobility edge") that separates localized from disordered states.

Argument for mobility edge: (Mott) coexistence of localized and extended states at same energy is unstable, as a small perturbation will mix and give only extended states.

Intro to disordered electronic systems

This intuition breaks down in one or two dimensions: all electronic states are localized up to arbitrarily high energies, although the localization length increases with *E*.



Why is 2D special (marginal)? Consider the stability of scattering states. We can model the scattering state as a random walk.

A random walk above 2D revisits any point only a finite number of times on average, so a weak potential fluctuation cannot be amplified infinitely. In 2D or below, a point (say the starting point) is visited an infinite number of times, and a "weak" potential can become strong.

Intro to disordered electronic systems

For non-interacting systems, we understand essentially completely the effects of disorder, at least away from transitions.

For the simplest symmetries (orthogonal and unitary ensembles), disorder is localizing for essentially all states in 1D and 2D.

The combination of interactions and disorder in closed systems ("many-body localization") is not well understood even in 1D.

are the only two possibilities diffusive and localized? can there be subdiffusive scaling? (e.g., "glassy": r ~ log t)

CM experimental systems typically have "dephasing" from interactions with phonons, which ultimately leads to a finite diffusion constant.

Systems of atoms in an ultra cold lattice do not have phonons, so may be better.

Intro to disordered electronic systems

How do we see localization experimentally?

Localization in the sense described here requires *interference* (constructive interference of self-intersecting trajectories).

Hence it is a quantum property and disappears if the electrons lose their phase coherence by interacting with a their environment (e.g., a "bath" of phonons).

If that happens on a phase-breaking time scale

τ_ϕ

then this acts as a cutoff on the effects of localization, e.g., on the reduction of conductivity.

Treating localization perturbatively ("weak localization theory") has been very powerful. Interaction effects can be incorporated (Altshuler-Aronov, Finkelstein, others) in this framework.

But in isolated systems (e.g., ultracold atomic systems), or possibly in femtosecond experiments on electrons, the system can be phase-coherent.

Can be treated also using powerful bosonization techniques (Giamarchi-Schulz).

Including the bath also sidesteps some basic questions.

Intro to disordered electronic systems

So one-particle localization is very sensitive to dimensionality.

It is also sensitive to *symmetries*. For example, if we broke time-reversal symmetry with a magnetic field, then in 2D extended states survive at isolated energies.

If we assume that disorder breaks all symmetries except for two discrete symmetries *T* (time reversal) and *C* (chiral/charge conjugation), and that each of these can square to +1 or -1 if present, then there are 10 symmetry classes.

Why 10?

Just considering *T* gives 3 "Wigner-Dyson" classes: orthogonal ($T^2 = +1$), symplectic ($T^2 = -1$), and unitary (*T* broken).

Adding *C* gives 9 classes (3 times 3). There is also the possibility of having *CT* symmetry without either *C* or *T* separately, hence 10 "Altland-Zirnbauer" classes.

How do we see localization experimentally?
Why is it important for some basic physics questions?
Is there more to the story than symmetry and dimensionality?

Periodic table of insulators

Schnyder et al., Kitaev: 10-fold way classification, periodic in dimension
3 Wigner-Dyson cases + particle-hole symmetry in superconductors = 10
Better to think of as 2+8: see Freed and G. Moore, "Twisted Equivariant Matter"

There can be insulator-metal transitions, like the Anderson transition at the mobility edge, and also insulator-insulator transitions, like the quantum Hall plateau transition.

A variety of analytical and numerical results on these transitions, but some are quite difficult.

TABLE II. Topological insulators (superconductors) with an integer ($\mathbb{Z}$) classification, (a) in the complex symmetry classes, predicted from the chiral U(1) anomaly, and (b) in the real symmetry classes, predicted from the gravitational anomaly (red), the chiral anomaly in the presence of background gravity (blue), and the chiral anomaly in the presence of both background gravity and U(1) gauge field (green).

Cartan\d	0	1	2	3	4	5	6	7	8	9	10	11	⋯
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	⋯
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	⋯
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	⋯
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	⋯
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	⋯
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	⋯
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	⋯
CII	0	$\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	⋯
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	⋯
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	⋯

MBL can be motivated by the basic question

Does an isolated quantum system with interactions and disorder show localization?

which is related to the equally basic question

When do isolated quantum systems thermalize?

The connection is that localization is the most plausible physical way to avoid thermalization: localized particles cannot move around and equilibrate. In a delocalized system, we expect that a test particle sees other particles as a thermal "bath".

Will focus on 1D. Besides symmetry and dimensionality, what else controls localization in the interacting case? What are the new properties of the localized phase? Which are interaction-specific?

What about MBL versus ergodic states?

A thermalizing state should have volume-law entanglement of eigenstates according to the eigenstate thermalization hypothesis (ETH).

ETH=local measurements on an eigenstate of a thermalizing system are consistent with a thermal ensemble.

A picture of the MBL state is that it is similar to the ground state of a localized system and has an *area law* for entanglement entropy. (Bauer and Nayak, …)

So far we have three things we can look for to diagnose an MBL transition: vanishing of the conductivity, or absence of thermalization, or the change in the entanglement properties of eigenstates.

Note that the first two are slightly different: we might have a subdiffusive but thermalizing phase, for example.

See Bar Lev et al ’14, Hulin et al ‘90, Agarwal et al ’14, Potter et al ’14, Vosk et al ‘14

Strong MBL and conservation laws

As far as I know, only one model has a rigorously established MBL phase (Imbrie 2014): an Ising model with random couplings and longitudinal & transverse fields

$$H = \sum h_i S_i^z + \sum \gamma_i S_i^x + \sum_i J_i S_i^z S_{i+1}^z$$

What is established is that there is an infinite set of local conserved quantities for a finite range of parameters. Let's call this "Strong MBL".

Immediately implies non-thermalization.

Surprising: a stable range of "integrability", unlike Yang-Baxter case.

Mostly people have studied interacting (Dirac) fermion models instead.

Recent "no-go" work suggests that strong MBL is quite difficult to achieve: specific to 1D; only short-ranged interactions; no SU(2) or other non-Abelian symmetry; … but can get very long time scales for thermalization.

Many-body localization at infinite temperature

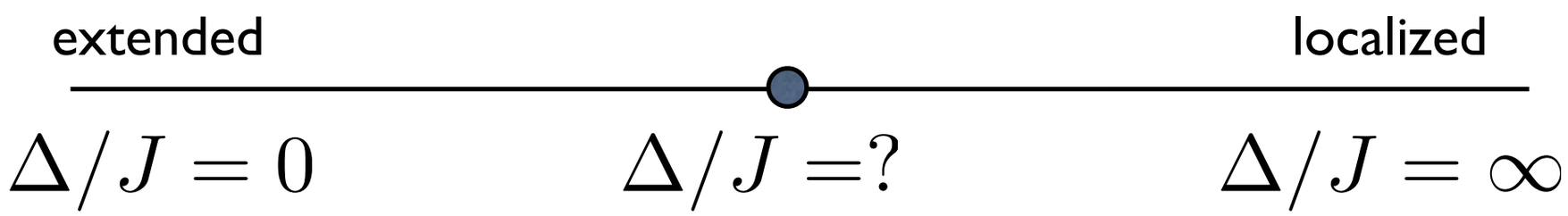
$$H = J_{xx} \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J_z \sum_i S_i^z S_{i+1}^z + \sum_i h_i S_i^z$$

Clean XXZ chain + random z-directed Zeeman field

$$h_i \in (-\Delta, \Delta)$$

Claim: look at "infinite-temperature" dynamics but with no dephasing; evolve an arbitrary initial state by the Schrödinger equation

Heisenberg phase diagram:
(Oganesyan-Huse spin chain version of BAA)



or is there an intermediate "ergodic non-metal"?

Spin and fermonic interpretations

The XXZ chain + z-directed Zeeman fields

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

is canonically equivalent to a model of spinless interacting *fermions*

$$H = -t \sum_i \left(c_{i+1}^\dagger c_i + h.c. \right) + V \sum_i n_i n_{i+1} + \sum_i \mu_i n_i$$

We often present things in spin language to avoid the hassles of sermonic statistics, but in 1D this is not a big problem.

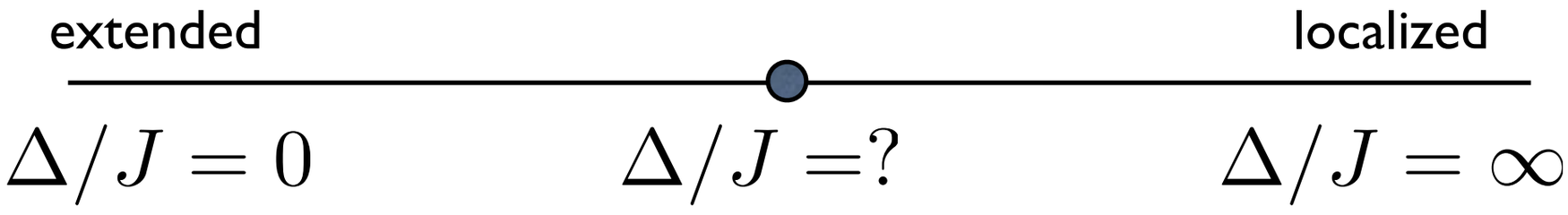
Anderson localization:V = Jz = 0 and

$$H = \sum_i \epsilon_i \tilde{c}_i^\dagger \tilde{c}_i$$

Many-body localization at infinite temperature

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

Heisenberg phase diagram:



Transition(s) should be detectable in:

level statistics: (Wigner-Dyson vs. Poisson) Oganesyan & Huse, 2008
dynamical correlation functions
correlation distributions Pal & Huse, 2010; Reichman et al. 2010
entanglement growth/thermalization (JHB,FP,JEM 2012)
entanglement variance (recent work of Alet et al., Bardarson et al., …)

This spin chain problem is a numerically easier reformulation of many-body localization in continuum Fermi systems at nonzero T (Basko, Aleiner, Altshuler 2007)
Hoped to be generic for 1D local interactions, disorder, U(1) symmetry.

Many-body localization at infinite temperature

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

level statistics: (Wigner-Dyson vs. Poisson) Oganesyan & Huse, 2008

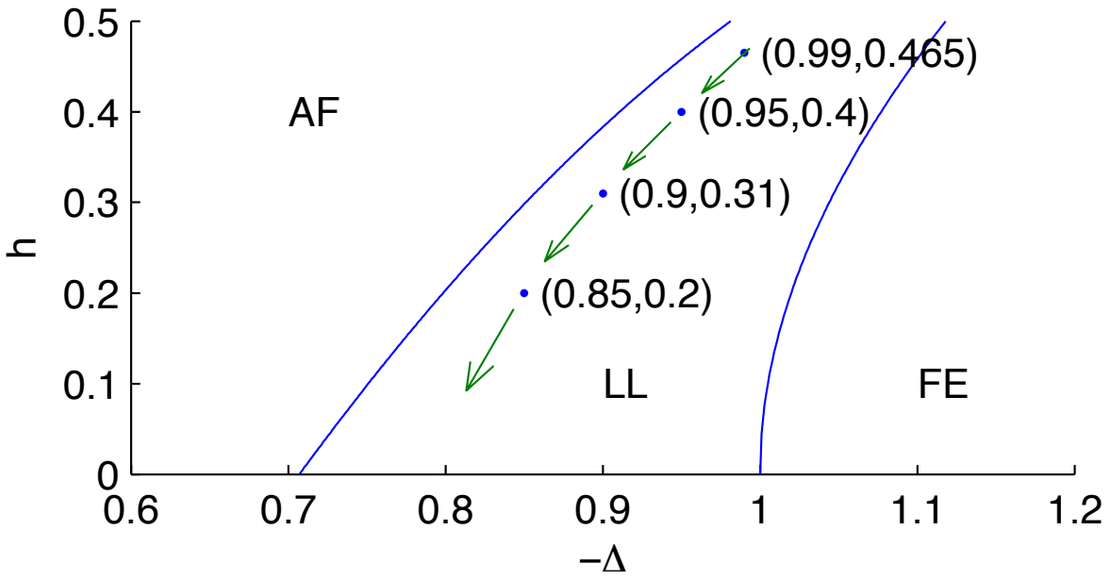
The idea is that diffusive and integrable systems have different level statistics, which is a simple property of the eigenvalues alone.

An MBL system is like an *integrable* system, which normally means a translation-invariant system with a complete set of conservation laws (return to this point in a moment).

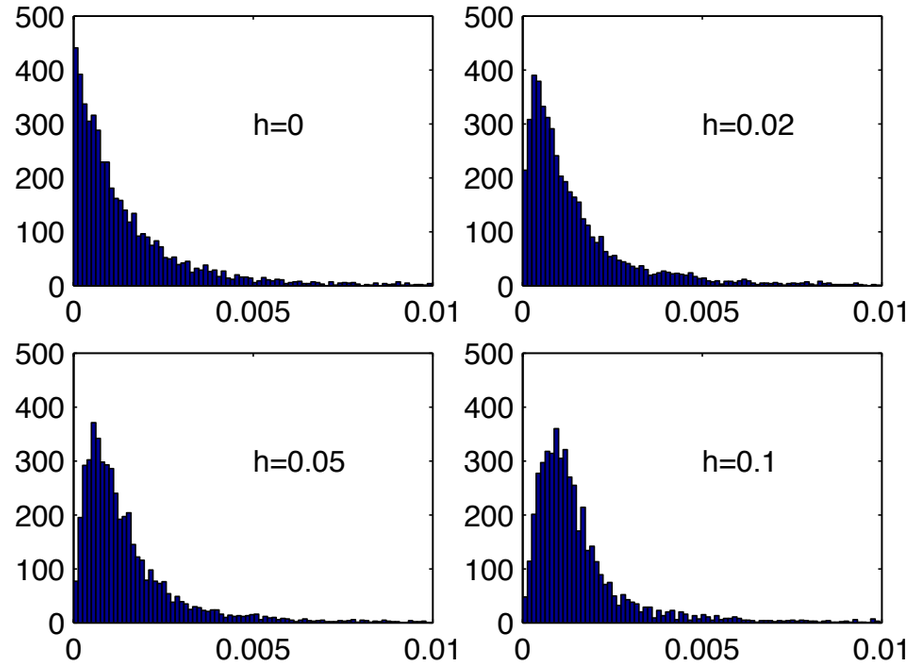
The key difference (and let's look for it numerically) is that the *integrability of an MBL system is stable to disorder, while conventional integrability is not, nor even to translation-invariant perturbations that break the Yang-Baxter equation (factorization of scattering).*

Staggered field and non-integrability

$$H = \sum_{i=1}^{L} \left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z + (-1)^i h S_i^z \right]$$



In one region, of the phase diagram, h is irrelevant (system remains Luttinger liquid), and we can track RG flow

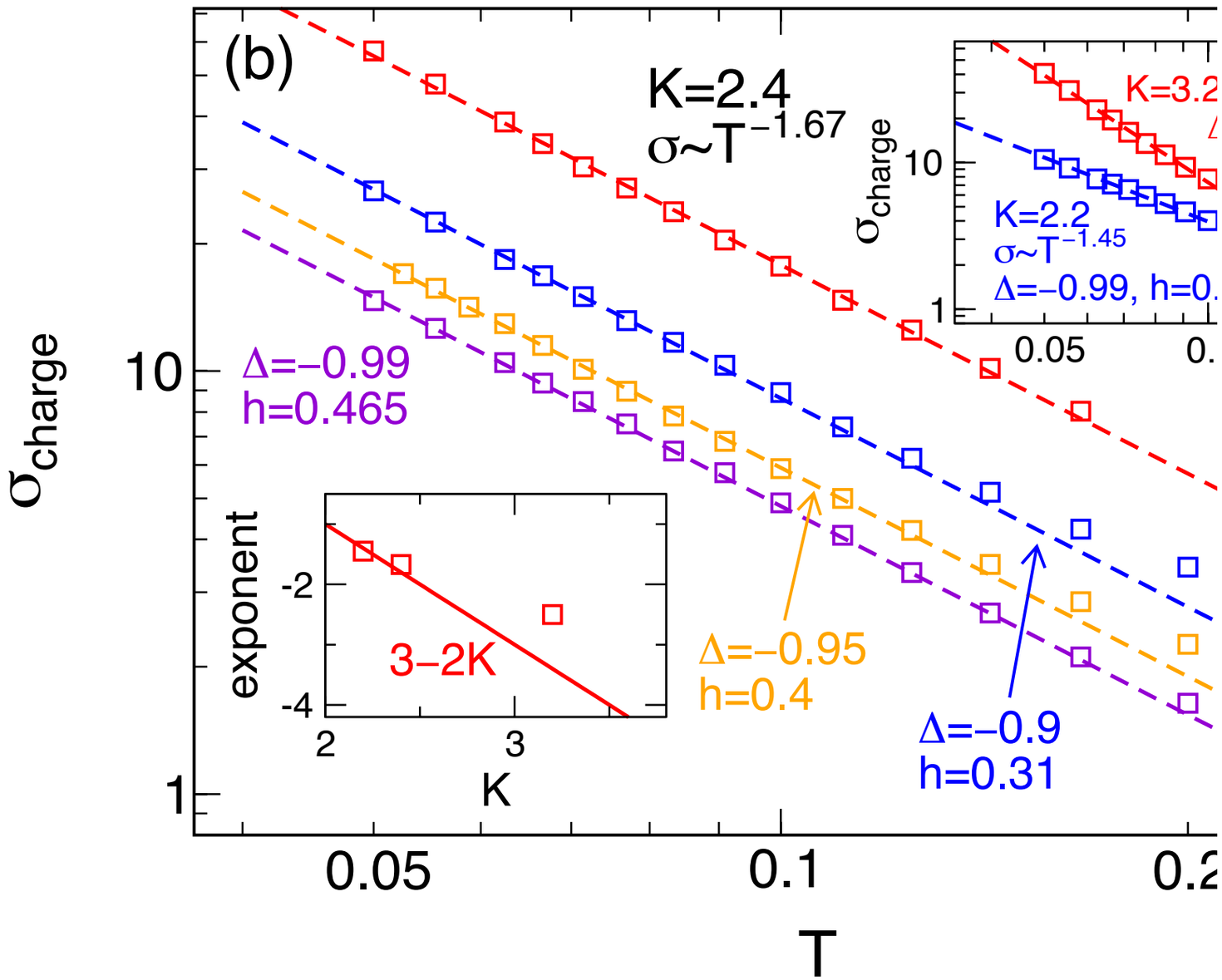


Level statistics become Wigner-Dyson (level repulsion) rather than Poisson

Argument for Poisson statistics: two nearby states are likely to be in different symmetry sectors, and hence do not repel each other as they are not mixed by a perturbation.

Conductivity scaling

$$\sigma = \lim_{t_M \to \infty} \lim_{L \to \infty} \frac{1}{LT} \mathrm{Re} \int_0^{t_M} \langle J(t) J(0) \rangle \, dt.$$



For K not too large, linear prediction is self-consistent and power-laws are observed that are consistent with bosonization predictions.

Conductivity diverges at low temperature as the integrability-breaking perturbation is irrelevant.

(Huang, Karrasch, Moore PRB 2013)

Interlude: entanglement and numerics

Another development in the past decade is that people care a lot more about the quantitative behavior of *entanglement*, usually as measured by entanglement entropy.

Why?

1. Often gives new insight into the structure of a phase (examples to follow).

2. Is related to the difficulty in studying a *quantum* model on a *classical* computer, at least with one method that has become increasingly important in the last decade.

"Density matrix renormalization group" (White, 1992)

Used to produce the conductivity plots in previous slide.
How, in general terms, does it work?

Entanglement entropy

Definition: the entanglement entropy of a pure state,
with respect to a given partition into A and B,
is the von Neumann entropy of the partial density matrices

$$\langle\phi_1|\rho_A|\phi_2\rangle = \sum_j (\langle\phi_1| \times \langle\psi_j|)|\psi\rangle\langle\psi|(|\phi_2\rangle \times |\psi_j\rangle)$$

$$S(\rho) = -\mathrm{Tr}\rho_A \log_2 \rho_A = -\mathrm{Tr}\rho_B \log_2 \rho_B$$

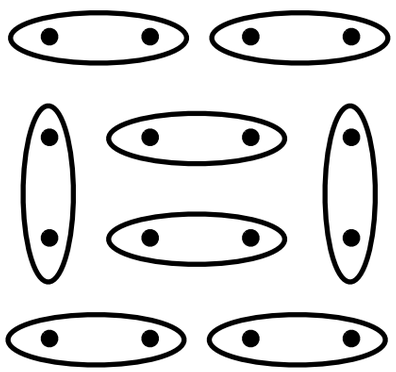
The singlet generates one bit of classical entropy when the two spins are separated

Note that the partial density matrix for subsystem A gives the results of *all* experiments limited to A

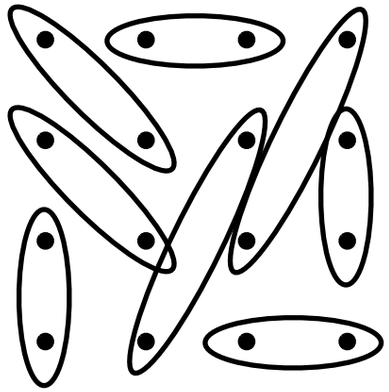
How much entanglement entropy occurs in ground states of local Hamiltonians?

To get some intuition for how entanglement behaves in statistical physics, consider "valence bond states" of $s=1/2$ systems:

Rule: every spin forms a singlet with some other spin



Short-ranged VBS
(= "dimer covering")



Long-ranged VBS

In these states, entanglement entropy S just counts singlets:
S = 1 bit for each singlet crossing the AB boundary. (But real states are usually a bit more complicated.)

How much entanglement entropy occurs in ground states of local Hamiltonians?

Consider partitions of a *d*-dimensional infinite system *AB* into a subregion *A* of linear size *L* and an infinite subregion *B*.

How should entanglement entropy scale with *L*?

If we can ignore entanglement between points farther apart than some length scale ξ, then entanglement entropy should be determined by a shell of thickness ~ ξ around the *AB* boundary:

$$S \sim L^{d-1}\xi \Rightarrow S \sim L^{d-1} \text{as } L \to \infty \text{ with system parameters fixed}$$

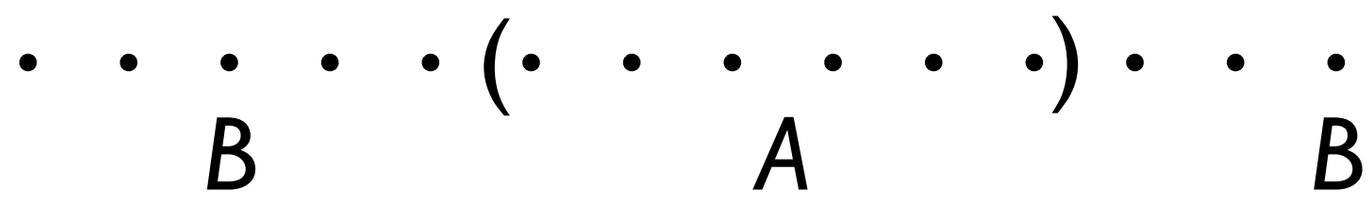
the "area law"

If there is no notion of locality, any site in *A* is as likely to be entangled with a site in *B* as with another site in *A*, and $S \sim L^d$

How much entanglement entropy occurs in ground states of local Hamiltonians?

We start with "pure" (translation-invariant), local Hamiltonians in one dimension.

Consider a partition for which *A* is a contiguous set of *N* spins inside an infinite chain:

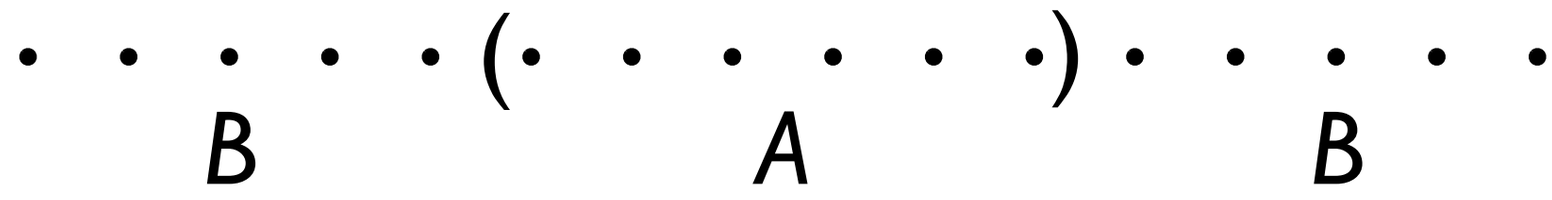


Away from critical points (i.e., when correlations are short-ranged), entanglement is localized in the vicinity of the boundary and the "area law" is satisfied:

$$\lim_{N\to\infty} S = C < \infty$$

But what about quantum critical states? Is there qualitatively more entanglement?

How much entanglement entropy occurs in critical states of local Hamiltonians?



Example of a quantum critical ground state: (c=1) Heisenberg AF

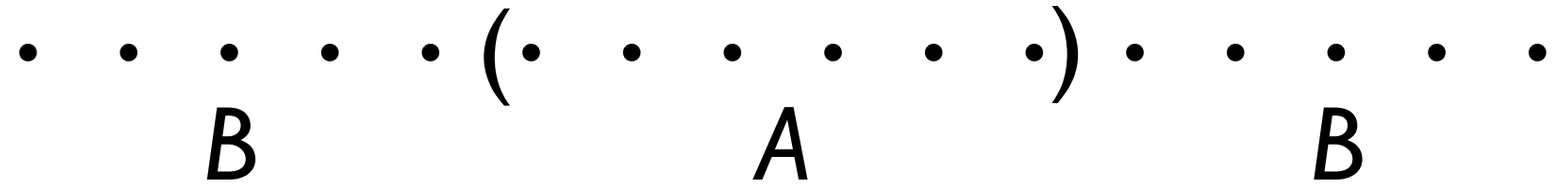
$$H = J \sum_i \mathbf{s}_i \cdot \mathbf{s}_j, \quad J > 0$$

At criticality, the entanglement of a connected subset of N spins, with the remaining spins, is (note: violates area law)

$$\lim_{N \to \infty} S \sim \frac{c}{3} \log N \to \infty$$

At clean and conformally invariant quantum critical points in d=1, there is logarithmically divergent entanglement with a coefficient related to the "central charge" of associated CFT. (Holzhey, Wilczek et al. 94, Vidal 03, Calabrese and Cardy 04).

Uses of entanglement entropy in d=1



For the subset of 1D quantum critical points that are described by 2D conformal field theories:

The appearance of the central charge in the ground-state entanglement is consistent with its appearance in other quantities related to entropy, such as the free energy at finite temperature

$$f = \frac{F}{L} = f_0 - \frac{\pi}{6} c (kT)^2 \hbar v$$

The central charge is an important quantity, but only defined for a subset of quantum critical points.

Entanglement entropy can be defined at *any* quantum critical point. Does it still show similar behavior, with a universal coefficient? *Yes!*

Entanglement entropy beyond conformal invariance

Numerical check of universal coefficient (Refael and Moore, PRL 2004) for simplest case (XX chain) by N. Laflorencie (PRB 2005)

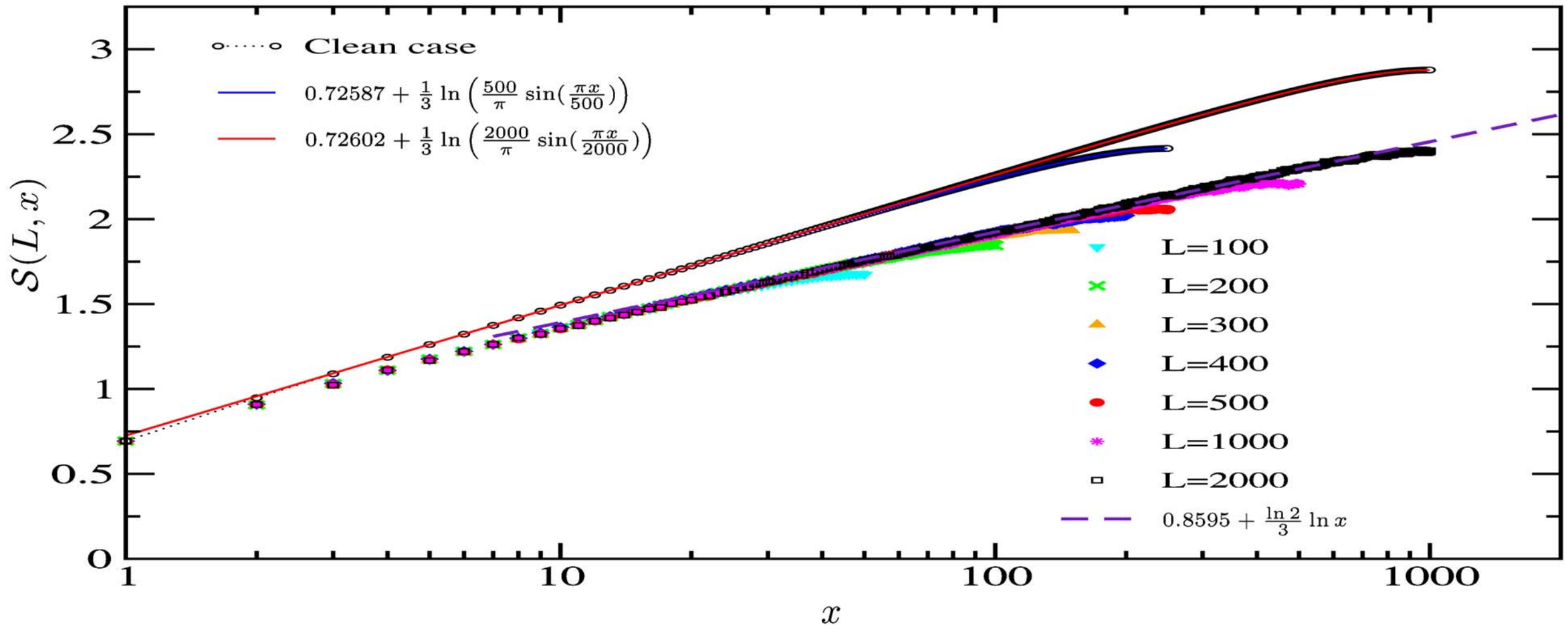


FIG. 2. (Color online) Entanglement entropy of a subsystem of size x embedded in a closed ring of size L, shown vs x in a log-linear plot. Numerical results obtained by exact diagonalizations performed at the XX point. For clean nonrandom systems with $L=500$ and $L=2000$ (open circles), $\mathcal{S}(x)$ is perfectly described by Eq. (3) (red and blue curves). The data for random systems have been averaged over 10^4 samples for $L=500$, 1000, 2000, and 2×10^4 samples for $100\leqslant L\leqslant 400$. The expression $0.8595+(\ln 2/3)\ln x$ (dashed line) fits the data in the regime where finite size effects are absent.

Numerics

Most numerics on MBL so far were done with "exact diagonalization" (ED): find all eigenvalues, or a subset, of the Hamiltonian matrix.

ED is great for small systems as it gives essentially complete information and its implementation and convergence are well understood.

It doesn't scale very well: cost for all eigenvalues goes as the cube of the matrix dimension, so beyond 20 spin-half sites becomes expensive.

Good news: there has been enormous progress 1992-present in DMRG/"matrix product state" methods to solve many-particle quantum problems in low spatial dimensions (especially 1D).

Understanding when these methods work well requires us to understand *entanglement*, which also leads to another useful definition of the MBL state.

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:

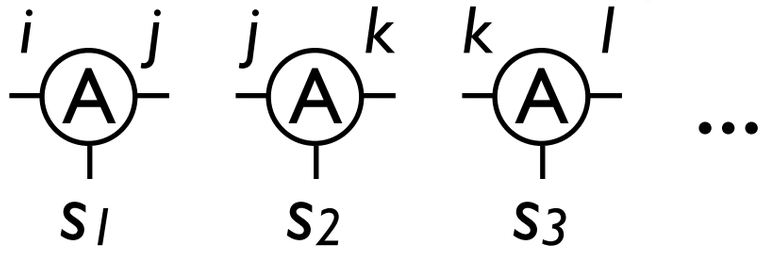
DMRG constructs "matrix product states" that retain local entanglement but throw away long-ranged entanglement.

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)

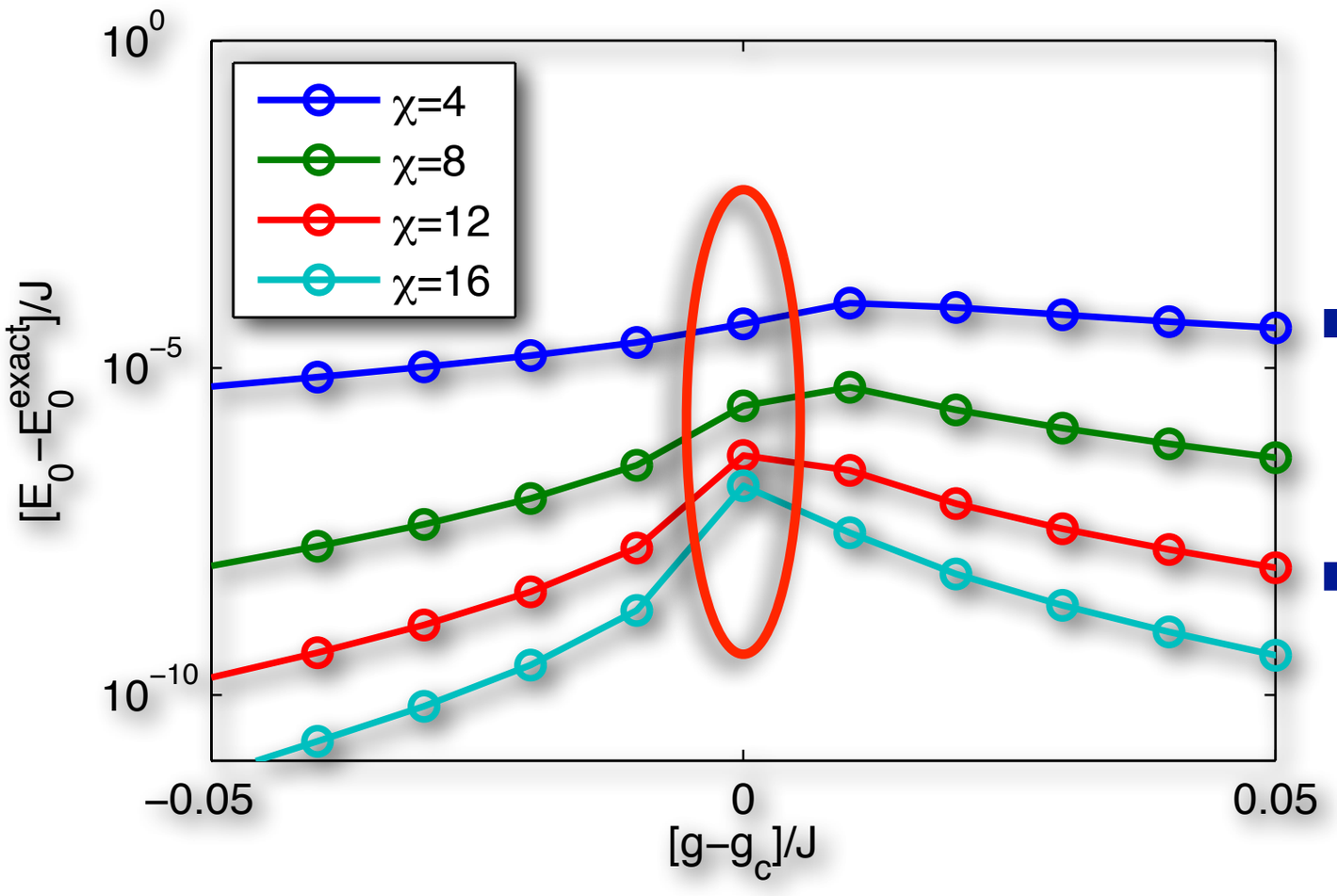
matrix product $$|\psi\rangle = A^{ij}_{s_1} A^{jk}_{s_2} A^{kl}_{s_3} A^{li}_{s_4} |s_1 s_2 s_3 s_4\rangle$$

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. (Gapped uniform systems converge…)
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). $$L_{\text{eff}} \propto \chi^{\kappa}, \quad \chi = \dim A$$

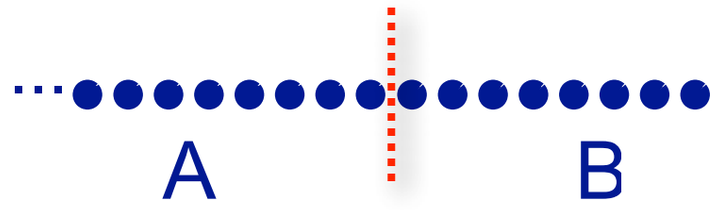
Finite matrix dimension effectively moves the system away from the critical point.

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:**

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

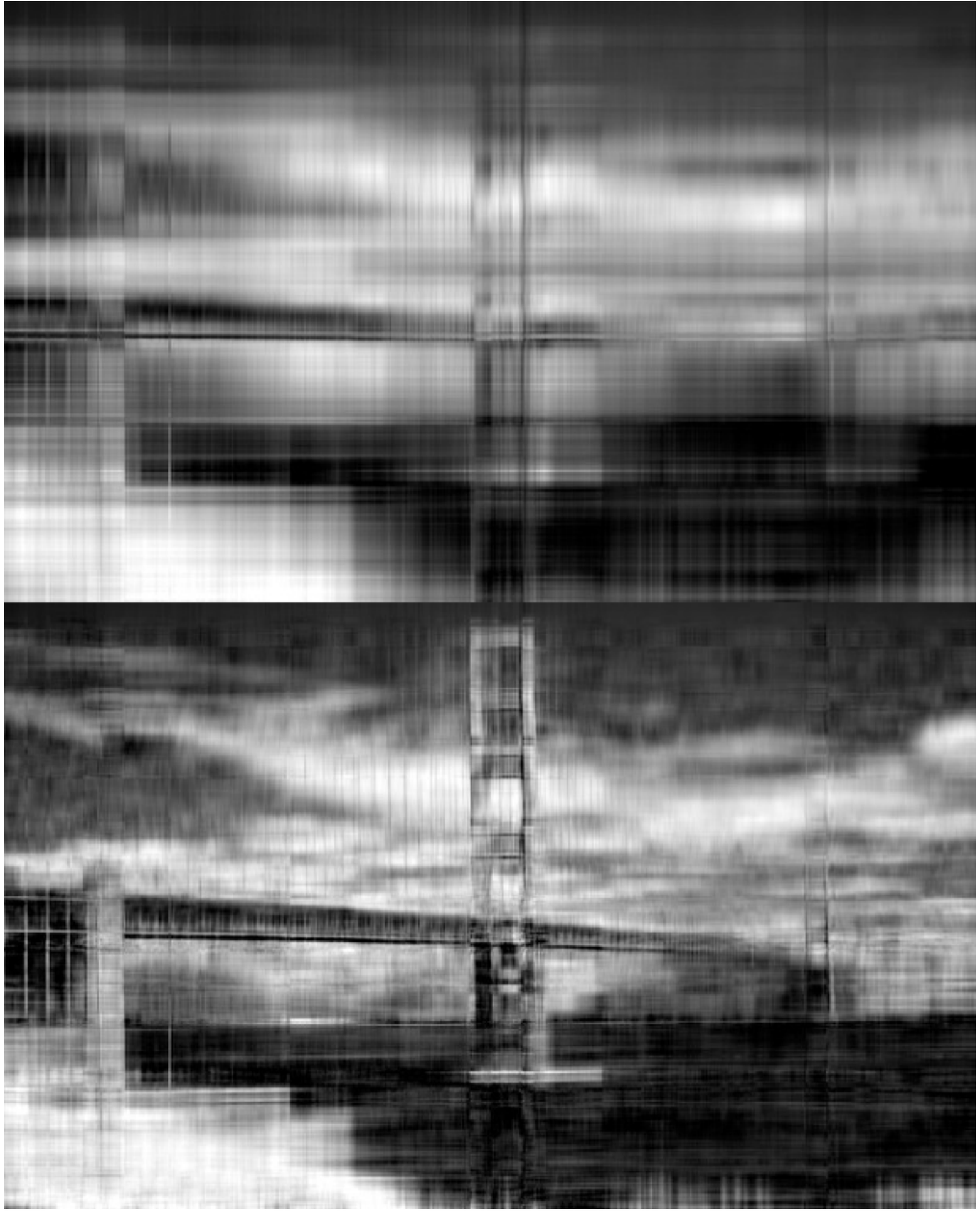
Efficient representation of quantum states?

- 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, ...

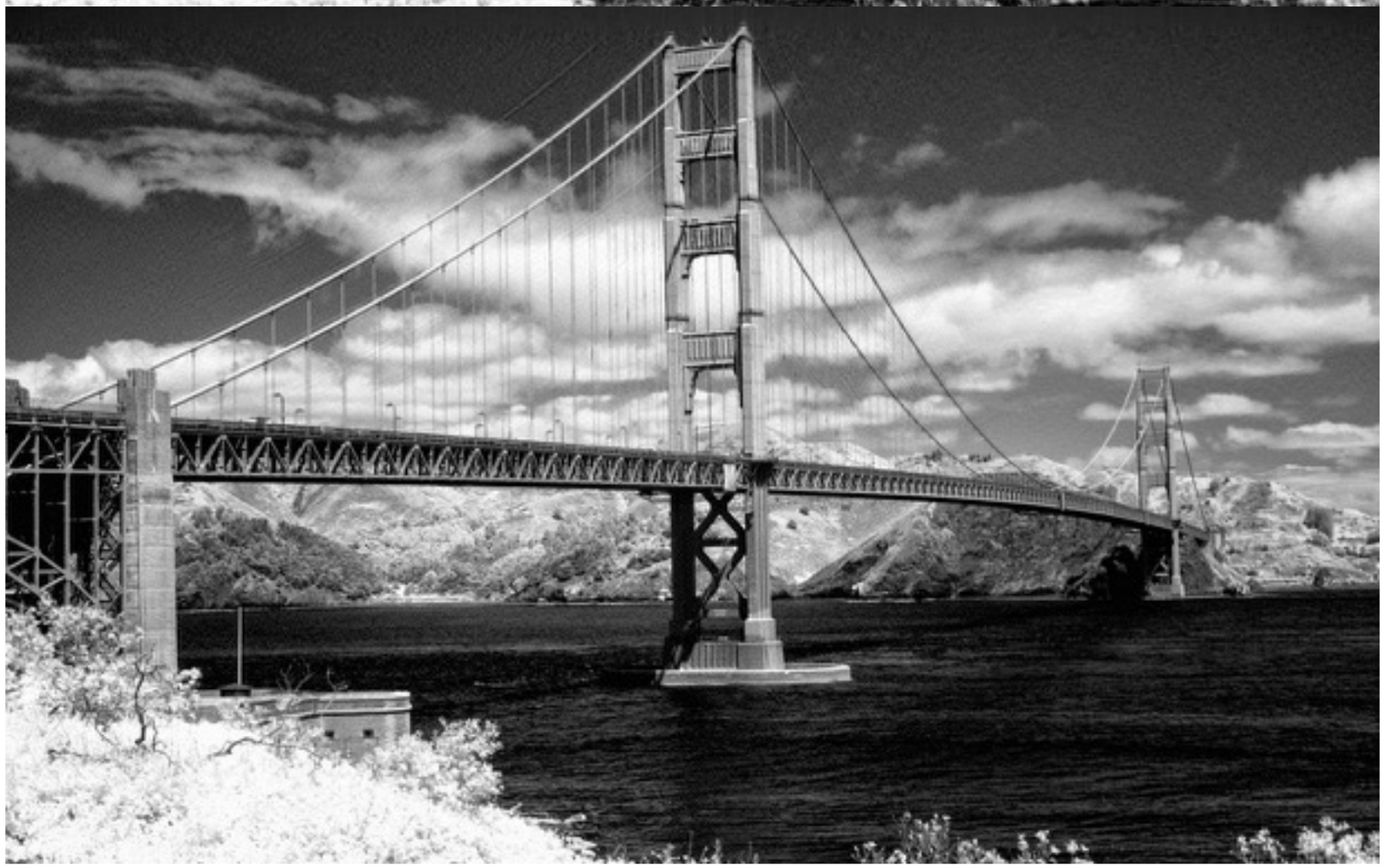
$\chi = 4$



$\chi = 16$

$\chi = 64$

$\chi = 256$



- (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

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

- **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, arXiv:1204.3934

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).

Integrability in MBL

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

Another way to define the MBL phase and explain its lack of thermalization is in terms of a complete set of conserved quantities that are genuinely local (Serbyn, Papic, Abanin; Imbrie)

(i.e., local as in the non-interacting case, not translation-invariant sums of local objects)

We expect to see Poisson statistics in the MBL phase simply because nearby states are likely to be localized in different parts of the sample, and hence not repel each other. Will come back to this.

Many-body localization at infinite temperature

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

Numerical experiment: start with an arbitrary product state (local Sz eigenstate) and evolve under *H*. Can view as a "global quench".

"Extended phase": expect S grows linearly with t (Calabrese and Cardy)

"One-particle localized phase": (Jz = 0) eigenstates are Slater determinants of localized one-particle states; S saturates to a finite value.

What happens if we add interactions to the localized phase?

Note: this is efficiently simulable because for early times the system has small entanglement (Prelovsek et al., 2007; see also De Chiara et al., 2006)

Jens Bardarson, Frank Pollmann, and JEM, PRL **109**, 017202 (2012).

Many-body localization at infinite temperature

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

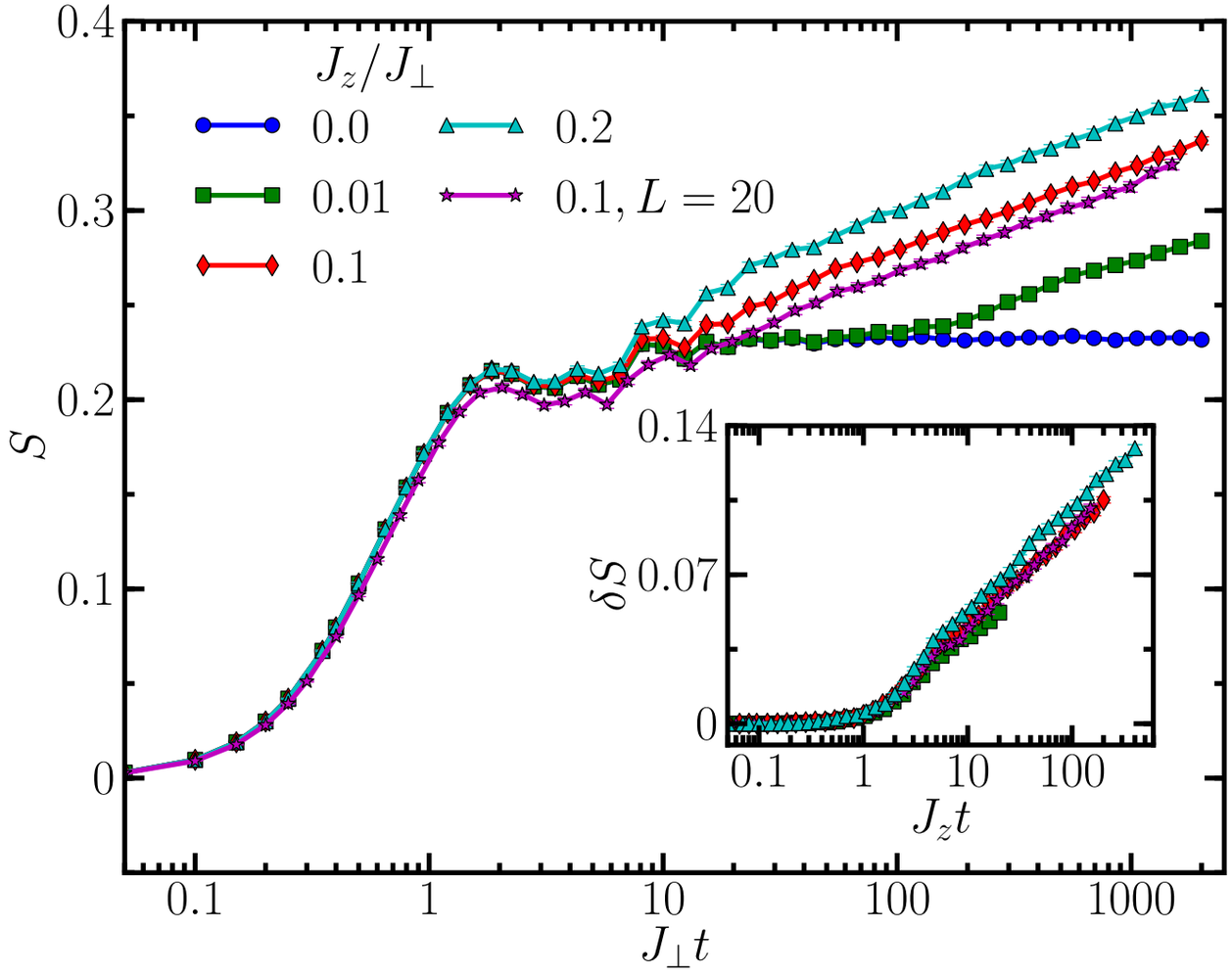
Numerical experiment: start with an arbitrary z-product state (local Sz eigenstate) and evolve under *H*. Can view as a "global quench".

Half-chain entanglement saturates with no interactions.

Interactions increase entanglement growth (consistent with previous work: De Chiara et al., Prelovsek et al.).

Surprise:
Interactions are a singular perturbation.

Even a very weak interaction leads eventually to a *slow* but *unbounded* increase of entanglement.



Many-body localization at infinite temperature

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

Numerical experiment: start with an arbitrary z-product state (local Sz eigenstate) and evolve under *H*. Can view as a "global quench".

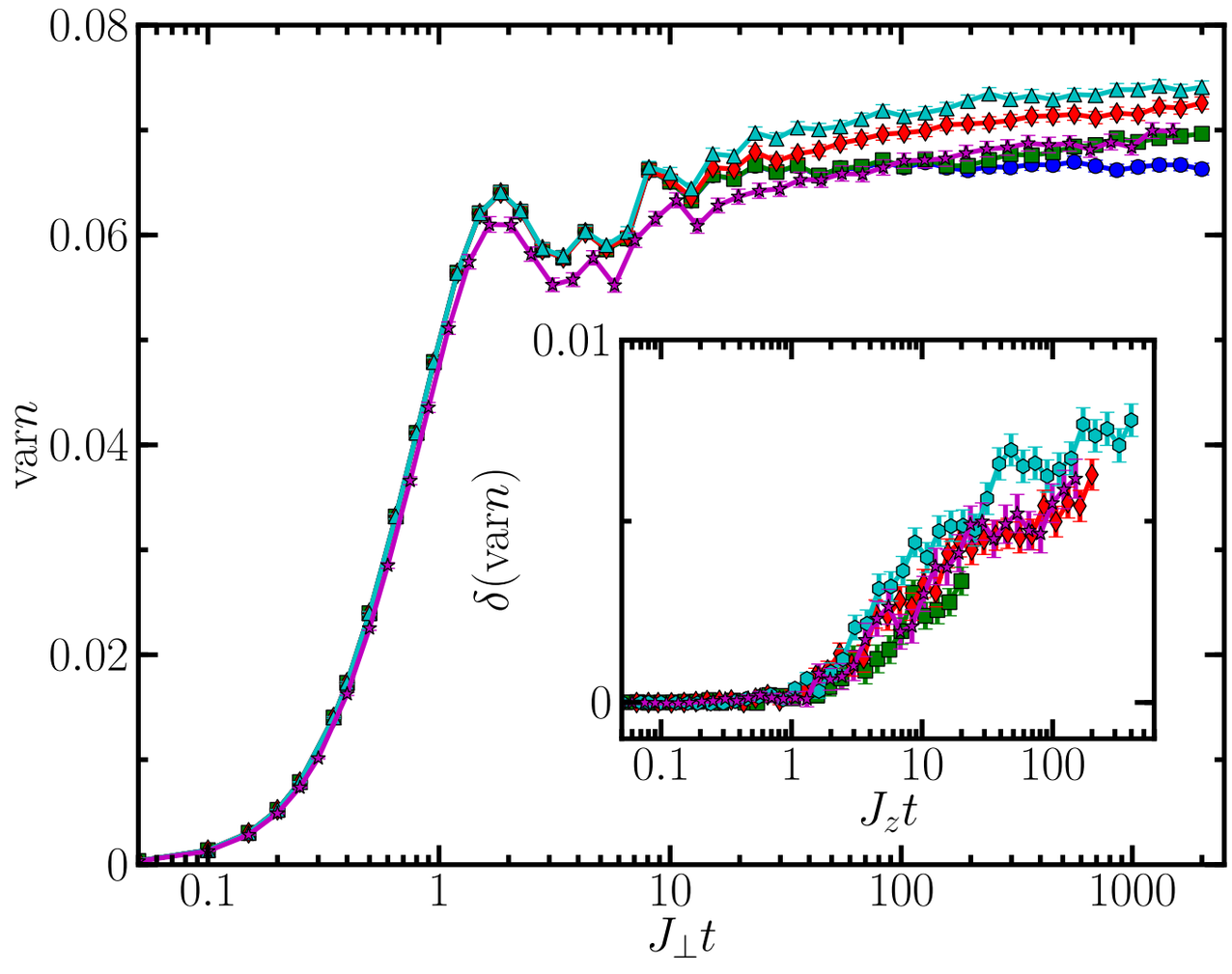
What about transport of the U(1) quantity?

Effect of interactions is less obviously singular--it could be that conductivity is zero.

We cannot rule out that the only physics with interactions is extended and that there is eventually thermalization.

But there is a long, possibly infinite, time range over which dynamics is very slow.

(Slower log log dynamics at low energy in random singlet phase--Igloi et al. PRB 2012)



Question: Is entanglement "physical"?

Yes, but hard to measure (although see Greiner et al. 2015); are other properties sensitive to this logarithmically slow dynamics?

Eigenstates versus dynamics of observables

One way to view the MBL phase: all eigenstates are basically similar, because a slight change in the potential will change which eigenstate is the ground state.

For example, all (or almost all) eigenstates are area-law (cf. Bauer-Nayak).

Different from the diffusive case, where the ground state is special (area law versus volume law, for example).

The arbitrariness in the MBL phase suggests that it may be difficult to prepare a single excited eigenstate; more generally, it is nontrivial to connect dynamics of observables (e.g., after a quench) to the properties of eigenstates.

Testing "dephasing without delocalization"

Favored scenario: (Huse-Oganesyan, Papic-Serbyn,-Abanin, Vosk-Altman, …)

The entanglement increase can be understood in terms of independent pairs with interaction energy scale

$$J_{\text{eff}} = J_0 \exp(-L/\xi_0)$$

which under the (short-time) assumption that pairs contribute independently to entanglement gives

$$S \sim \xi_0 \log(J_0 t)$$

An experimentally practical way to test this log: Romain Vasseur, Siddharth Parameswaran, and JEM, PRB 2015

"Revivals": how often, in a single realization of disorder, does a single spin's expectation return to its original value?

This is basically a probe of how many frequencies are involved in the spin's dynamics. That increases dramatically between Anderson localization and MBL.

The dephasing picture has to break down as we approach the transition to a delocalized phase.

Model: XXZ chain plus "probe spin" at edge

(Rossini, Calarco, Giovannetti, Montangero, Fazio, 2007)

$$
\begin{aligned}
H &= H_{\mathrm{XXZ}}[\{\sigma_i\}] + \frac{\lambda}{2}\left(S^+\sigma_1^- + S^-\sigma_1^+\right) \\
H_{\mathrm{XXZ}} &= \frac{1}{4}\sum_{i=1}^{L-1} J_\perp\left(\sigma_i^+\sigma_{i+1}^- + \sigma_i^-\sigma_{i+1}^+\right) + J_z\sigma_i^z\sigma_{i+1}^z + \frac{h_i}{2}\sigma_i^z
\end{aligned}
$$

Question: "revivals"

If probe spin is initially polarized, how frequently does its polarization return to nearly the initial value?

Qualitative motivation:
already in a classical system, Poincare recurrence time is a measurement of phase space volume.
Larger phase space to explore = lower rate of revivals.

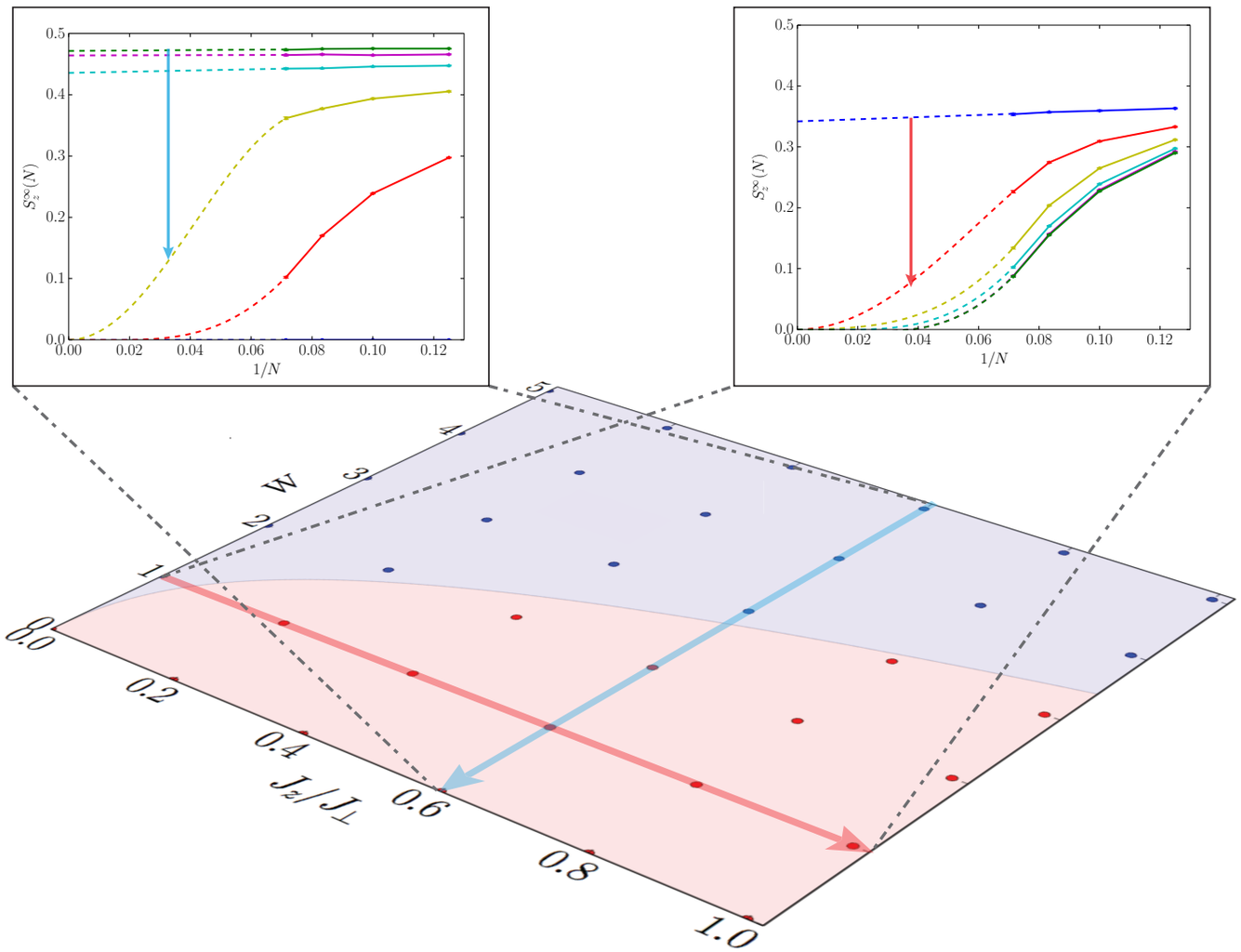
Numerical experiment

Initial state is probe spin up and random initial state of chain (with and without constraint of total Sz = 0).

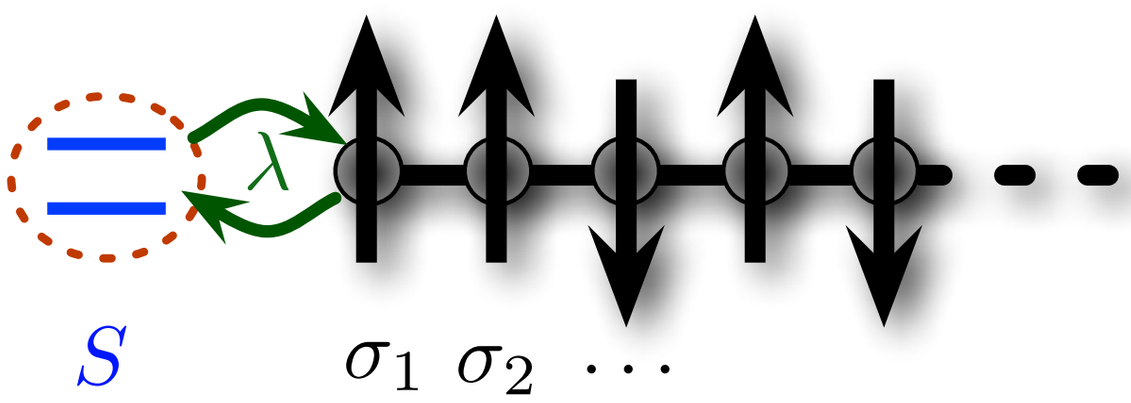
Evolve in time and record a "revival" whenever average probe spin is within (1-epsilon) of initial value.

1. Estimate phase diagram via residual magnetization

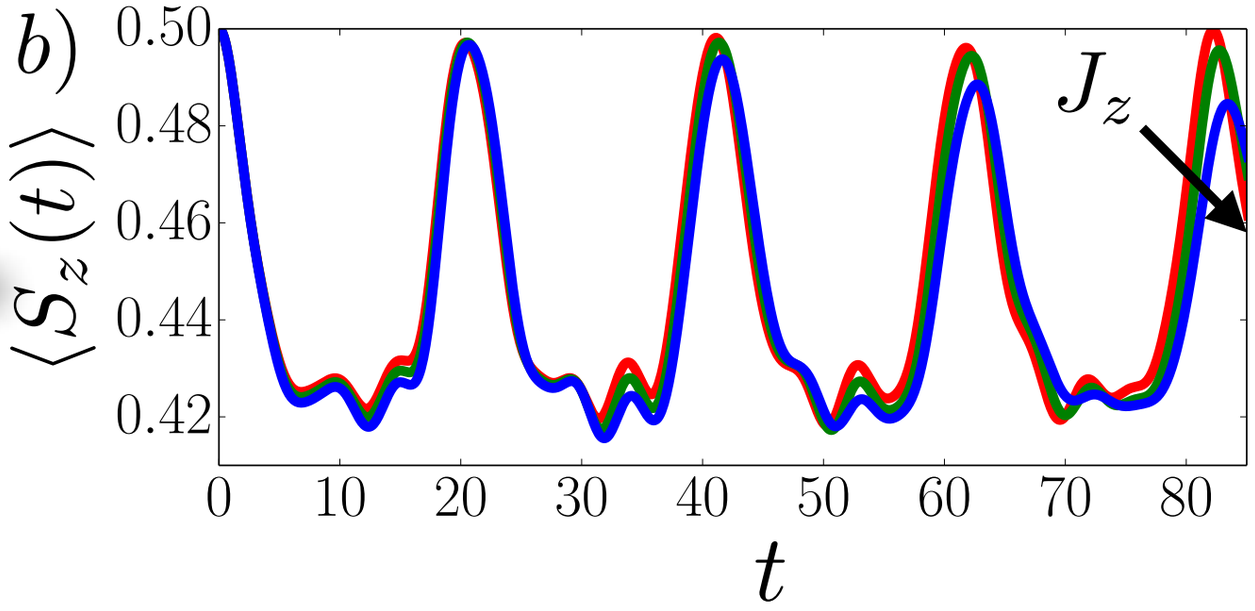
$$\overline{S^z_\infty} \equiv \overline{\sum_\alpha \langle\alpha|S^z|\alpha\rangle \, |\langle\Psi_0|\alpha\rangle|^2},$$



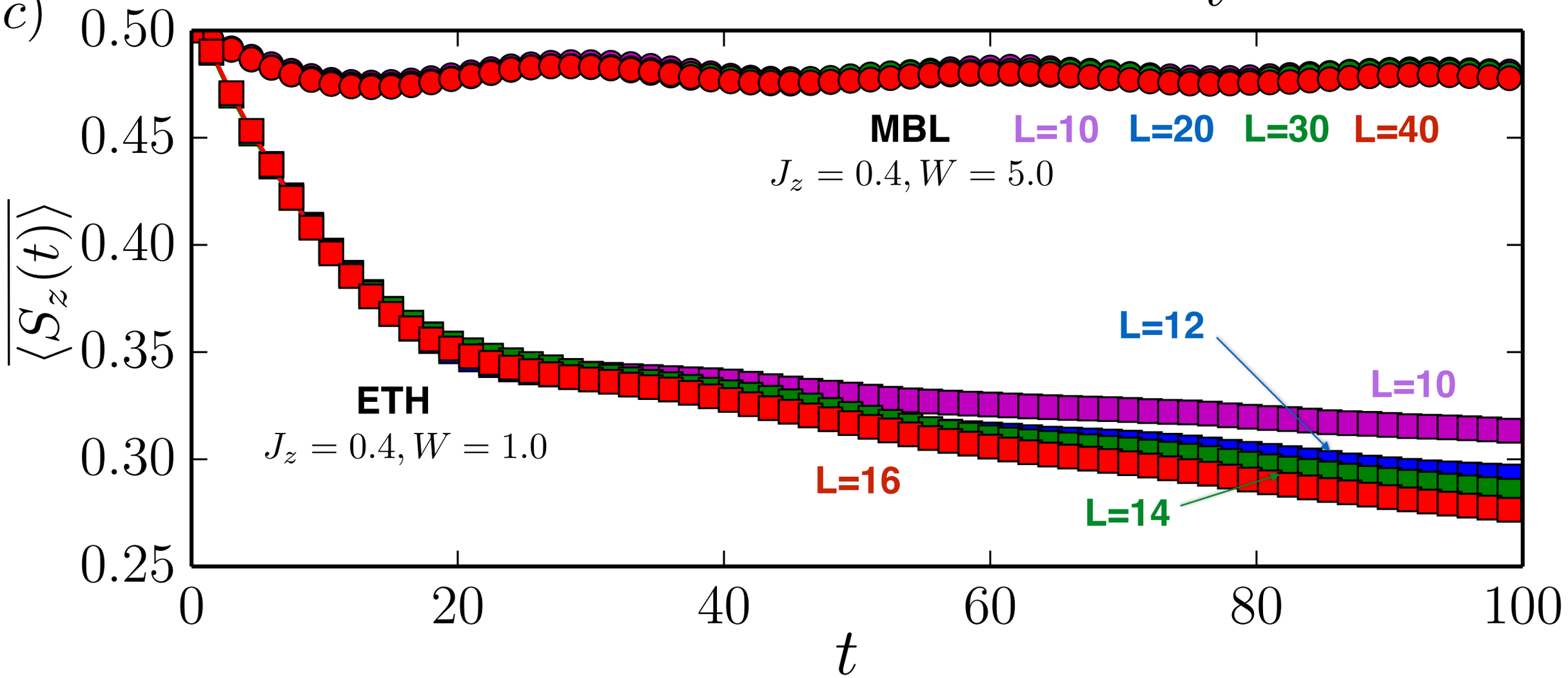
a)


λ
S
σ_1 σ_2 $\cdots$

b)

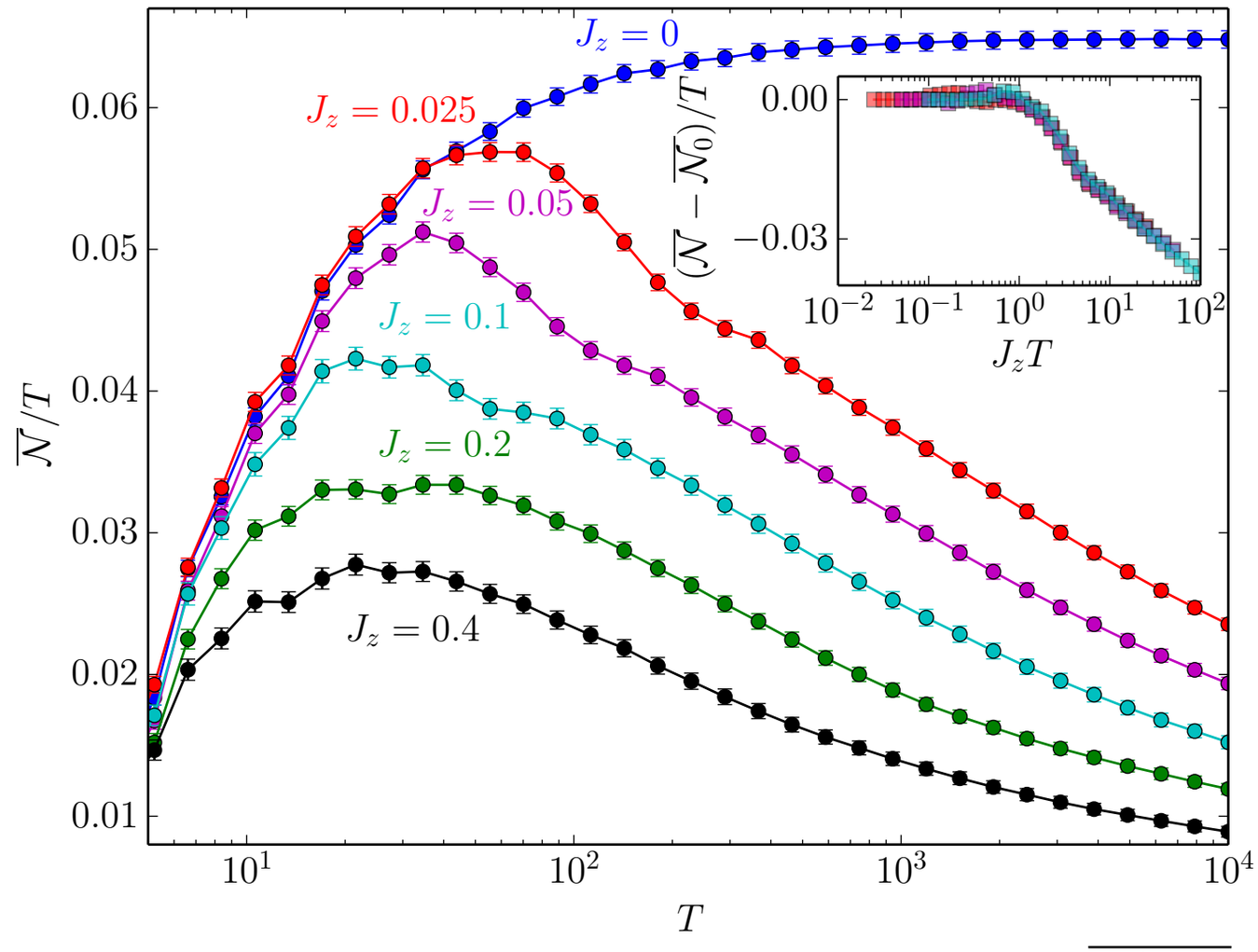

$\langle S_z(t) \rangle$
0.50
0.48
0.46
0.44
0.42
0
10
20
30
40
50
60
70
80
t
J_z

c)


$\overline{\langle S_z(t) \rangle}$
0.50
0.45
0.40
0.35
0.30
0.25
0
20
40
60
80
100
t
MBL
L=10
L=20
L=30
L=40
$J_z = 0.4, W = 5.0$
ETH
$J_z = 0.4, W = 1.0$
L=12
L=10
L=16
L=14

Numerical experiment

2. How does the revival rate show the effects of interactions?



Quantum Revivals. Disorder-averaged revival rate $\overline{\mathcal{N}(T)}/T$ as function of total time, T. Upon adding interactions of strength J_z, revivals are suppressed beyond $T^* \sim J_z^{-1}$. (Inset) The same data collapses onto a universal curve when plotted against J_zT.

Scaling collapse

We can do better than just saying that interactions = fewer revivals. Actually the same phenomenology that explains entanglement growth appears here as well: the difference in revival rates is

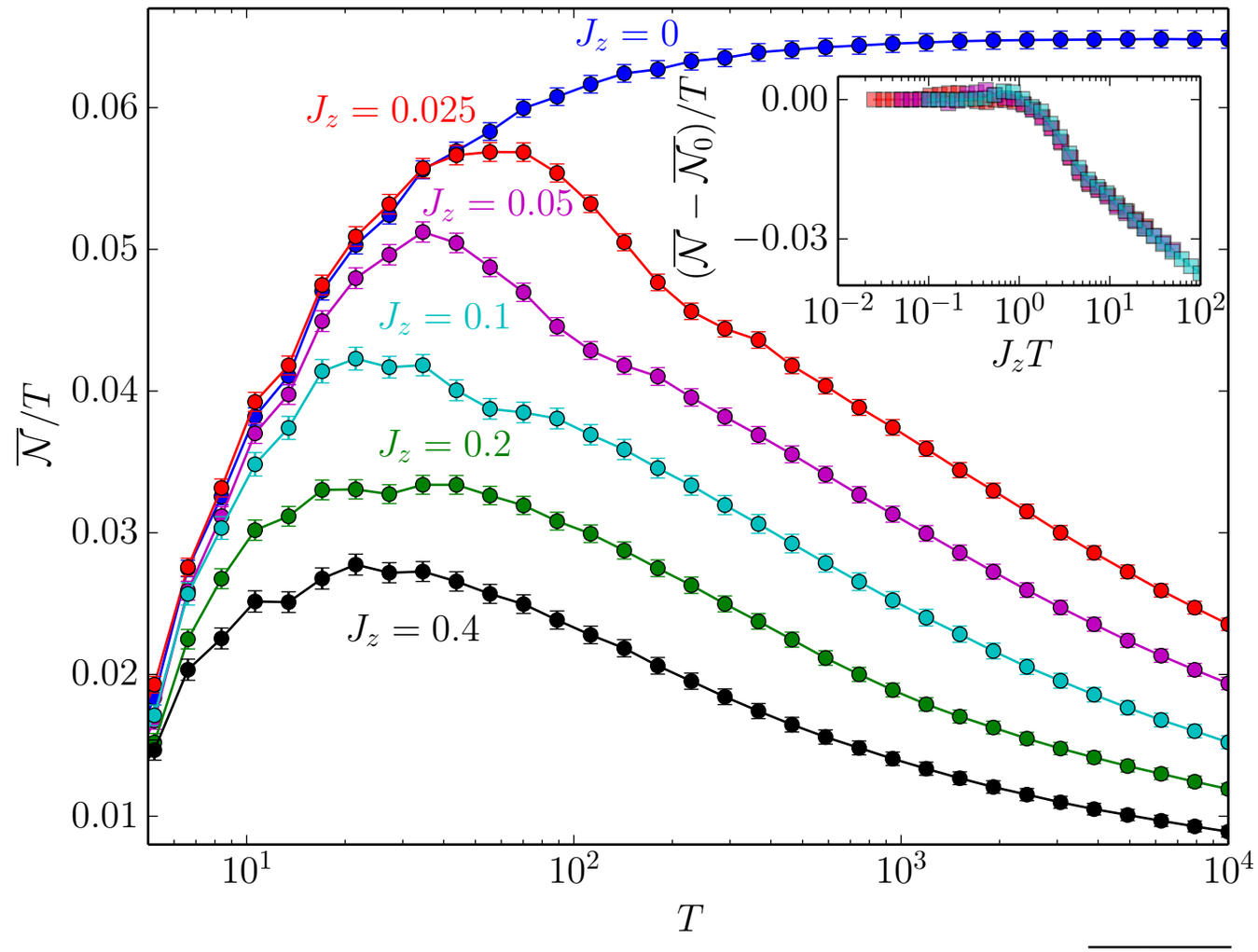
$$\frac{\overline{\mathcal{N} - \mathcal{N}_0}}{T} \approx \nu(N + \alpha \log J_z t) - \nu(N),$$

where \nu(N) is the revival rate when N different frequencies matter (expect an exponential dependence, but details turn out to be irrelevant).

The numerics show that the revival rate indeed shows a collapse with logarithmic time over most of the MBL phase (presumably not all of it)…

Numerical experiment

2. How does the revival rate show the effects of interactions?



Quantum Revivals. Disorder-averaged revival rate $\overline{\mathcal{N}(T)}/T$ as function of total time, T. Upon adding interactions of strength J_z, revivals are suppressed beyond $T^* \sim J_z^{-1}$. (Inset) The same data collapses onto a universal curve when plotted against J_zT.

Result: a simple picture

The "real-space Fermi liquid" form

$$H = \sum_i \epsilon_i n_i + \sum_{i,j} U_{ij} n_i n_j + \dots$$

controls not just entanglement growth but more "physical" observables over a wide range of the MBL phase.

The resulting logarithmic time evolution (assuming U falls off exponentially) is likely to be a generic property of dynamics of observables in the MBL phase. This log scaling may be the most important observable difference between MBL and Anderson phases.

Point: two simple guesses (revival rate saturates as in Anderson case, or as 1/exp(xi)) are wrong.

It would be nice to understand (a) what is the long-time state of a block in the MBL phase starting from some physical preparation process (typically volume law but not ETH); (b) how *H* becomes more complicated (3-body, etc.) close to the transition.

Many-body localization at infinite temperature

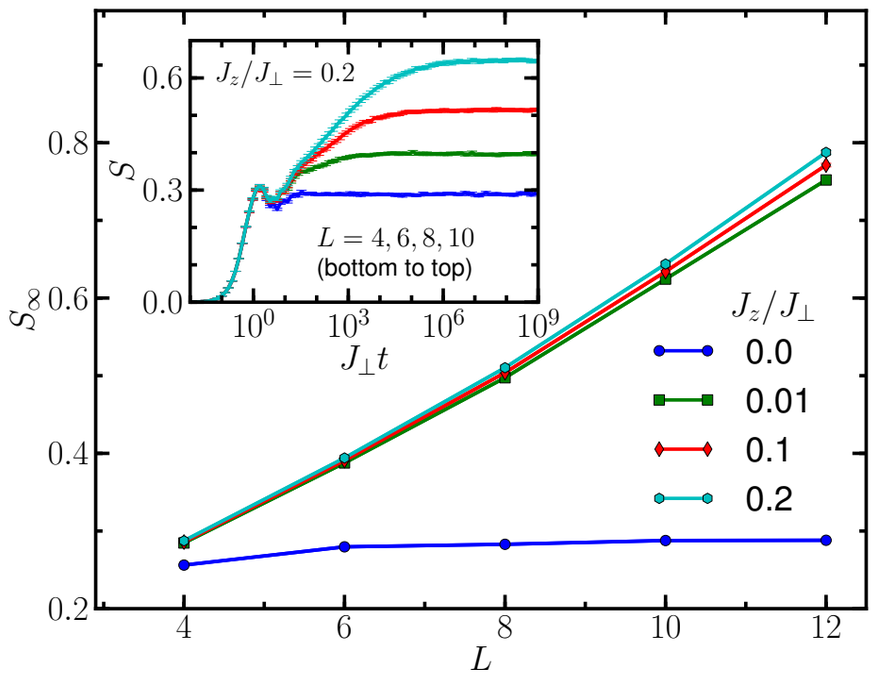
$$H = J_{xx} \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J_z \sum_i S_i^z S_{i+1}^z + \sum_i h_i S_i^z$$

What does entanglement entropy growth mean?

The entanglement entropy comes from the reduced density matrix, which governs any local experiment.

So any measurement of entropy in a subsystem will show that the interacting system is "more thermalized" than the Anderson one.

However, studies of the saturation of small blocks suggest that the full thermal entropy is not reached: O(L) but small.



Long-time behavior: some version of GGE?

A difference from normal GGE in Yang-Baxter integrability:

In something like XXZ or Lieb-Liniger, the conserved quantities are sums of local operators and hence *extensive*. Microcanonical and Gibbs ensembles are equivalent because fluctuations in an extensive operator like energy are relatively small.

This does not hold for the local quantities in MBL; it would be nice to have a useful means to calculate the long-time evolution of a generic initial state (which is related to the question of operators beyond two-spin).

Nature of phase transition

Believed to be "purely dynamical", which we know already from the non-interacting case to be difficult.
(e.g., the Anderson and quantum Hall plateau transition)

Some theories in 1D based on real-space renormalization group (Vosk-Altman-Huse, Vasseur-Parameswaran-Potter)

So far, not perfectly clear agreement between theory and numerics (or even between numerics from different groups!).

Next: no disorder

Remark: what are MBL-like features in translation-invariant systems? (M. Mueller et al., Yao et al., Papic et al.)

Point: can make artificial models that show MBL with translation invariance.

For example, we could interpret a random potential model as resulting from infinitely heavy particles that create a potential for light particles.

Are these stable? For example, if the heavy particles have large finite mass, does MBL still exist?

In our example, it does not, but very long time scales are needed to see it. (Of course, this isn't a general proof.)

Similarly unstable are "conventional" integrable systems. How is their long-time dynamics modified by the existence of infinitely many conservation laws?

Part II: Quantum hydrodynamics in 1D and 2D

1. Outline: start with a model problem: two-reservoir quench in 1D

Simple cases: free bosons; CFTs
Review of ballistic linear response (Drude weight)

In less simple integrable models: exact results for some quantities even arbitrarily far from equilibrium; can compare to DMRG simulations for XXZ
(Vasseur, Karrasch, JEM PRL 2015)
Background to hydrodynamical/kinetic theory approaches for soliton gases, Lieb-Liniger, XXZ.

2. Test of kinetic theory predictions in more general cases: expansions from smooth initial conditions.

When is hydrodynamics (i.e., Bethe-Boltzmann equation) valid? Can compare to *microscopic simulations at nonzero T,* when hydrodynamics should be generic. (At T=0, coarse-graining length diverges at least in CFTs)
What does hydrodynamics miss?

3. (if time permits) Hall viscosity in d=2 hydrodynamics

Standard hydrodynamics (0th order)

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

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

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

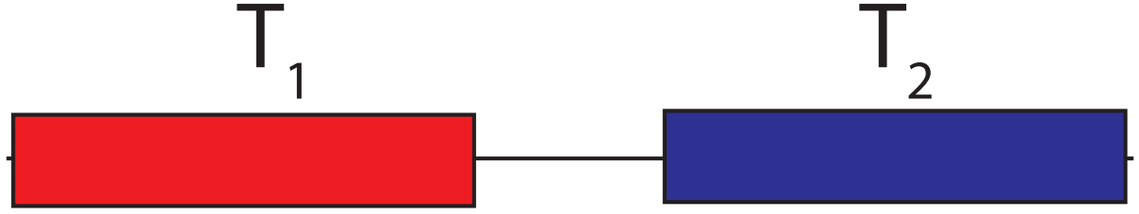
$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right) \tau + \frac{2}{3}(\nabla \cdot \mathbf{u})\tau = 0. \tag{3}$$

These come from the Boltzmann equation assuming local equilibrium.

Non-equilibrium energy 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.



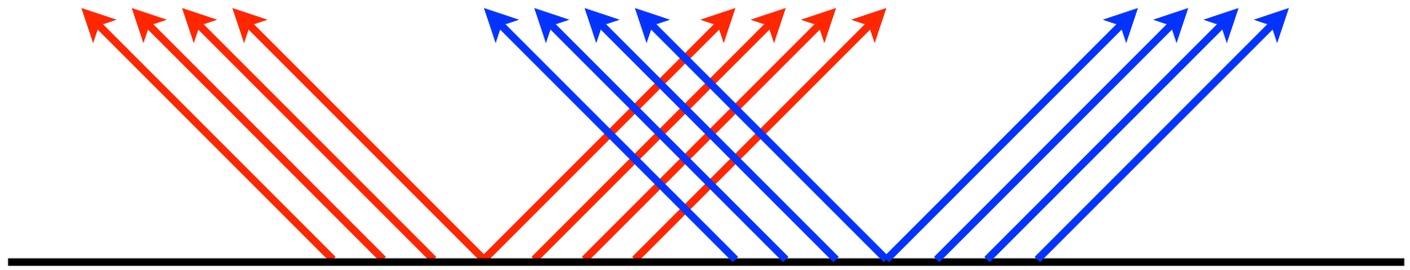
Is a steady-state heat current reached?

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

We observe two different outcomes, depending on integrability of the leads and whether the connected system is homogeneous.

Stefan-Boltzmann picture

Idea: the right lead is prepared at one temperature and the left lead at a different temperature.



In a ballistic system like a CFT, there is no local temperature at x=0 at later times; rather the right-movers are at a different temperature than the left-movers. The thermal current is the difference between total radiation from left and right.
(Sotiriadis-Cardy, Bernard-Doyon)

Warmup: free bosons

We compute the right-moving energy current from a lead at temperature $T+dt$ and subtracting the left-moving energy current from a lead at T. Assume one-dimensional free bosons as in the Schwab et al. experiment mentioned above. Using k for momentum, we have that the total energy current (units of energy per time) is

$$J_E = J_E^R - J_E^L = \int_0^{\pi/a} \frac{dk}{2\pi} \left[f_{T+dt}(\hbar\omega_k) - f_T(\hbar\omega_k) \right] \hbar\omega_k v_k. \tag{1}$$

Here $v_k = d\omega_k/dk$ and $f_T(E)$ is the Bose factor $(e^{E/k_BT} - 1)^{-1}$. So

$$J_E = (dt) \int_0^{\omega_{max}} \frac{d\omega}{2\pi k_B T^2} \frac{e^{\hbar\omega/k_BT}}{(e^{\hbar\omega/k_BT} - 1)^2} \hbar^2\omega^2. \tag{2}$$

Here ω_{max} is the highest phonon frequency. If we assume that the temperature is small compared to this, so that $x = \hbar\omega/k_BT$ runs from 0 to infinity, then we obtain (note that we need to multiply by $(k_BT/\hbar)^3$)

$$J_E = \frac{{k_B}^2 T}{2\pi\hbar}(dt) \int_0^{\infty} dx \, \frac{x^2 e^x}{(e^x - 1)^2}. \tag{3}$$

The dimensionless integral gives $\pi^2/3$, so

$$G_0 = \frac{J_E}{dt} = \frac{\pi^2 {k_B}^2 T}{3h}. \tag{4}$$

An interesting fact about the thermal conductance G_0 is that it is the same for bosons or fermions (or indeed anyons), unlike charge transport. The Schwab et al. experiment observed one thermal conductance quantum G_0 for each low-temperature phonon mode.

Dissipationless transport

When is there a nonzero Drude weight *D*?

$$\sigma(\omega) = D\delta(\omega) + \dots$$

Two easy examples:

I. Superconductors (transport by condensate)

II. Part of the current is conserved: Mazur lower bound

$$D = \frac{1}{2LT} \lim_{t\to\infty} \langle J(t)J(0)\rangle \geq \frac{1}{2LT} \sum_k \frac{\langle JQ_k\rangle^2}{\langle {Q_k}^2\rangle}$$

Dissipationless transport

When is there a nonzero Drude weight *D*?

$$\sigma(\omega) = D\delta(\omega) + \dots$$

Example of Mazur bound: suppose momentum is conserved, and current is proportional to momentum (e.g., if only one kind of particle).

Technical note: the Drude weight is not thermodynamic:

$$D = \frac{1}{L}\left[\langle\Theta\rangle - \hbar\sum_{n,m}(1-\delta_{\epsilon_n,\epsilon_m})\frac{e^{-\beta\epsilon_n}-e^{-\beta\epsilon_m}}{Z(\epsilon_m-\epsilon_n)}|\langle n|J|m\rangle|^2\right], \quad D_m = \frac{1}{L}\left[\langle\Theta\rangle - \hbar\sum_{n,m}\frac{e^{-\beta\epsilon_n}-e^{-\beta\epsilon_m}}{Z(\epsilon_m-\epsilon_n)}|\langle n|J|m\rangle|^2\right]$$

where D_m is "Meissner stiffness" (response to flux). Always $D \geq D_m$. (Mukerjee and Shastry, PRB 2007). Here

$$\Theta = \lim_{k\to 0}\frac{1}{k}[\rho(k), J(-k)]$$

$$\sigma(\omega) = D\delta(\omega) + \dots$$

$$D = \frac{1}{2LT} \lim_{t\to\infty} \langle J(t)J(0)\rangle \geq \frac{1}{2LT} \sum_k \frac{\langle JQ_k\rangle^2}{\langle {Q_k}^2\rangle}$$

What about "integrable" models with an infinite number of conserved local quantities, none of which gives a lower bound?

Actually this happens quite often in 1D--simplest case is spinless interacting fermions (XXZ model in zero magnetic field).

$$H = \sum_i \left[J_{xx}(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \Delta S_i^z S_{i+1}^z + hS_i^z\right]$$

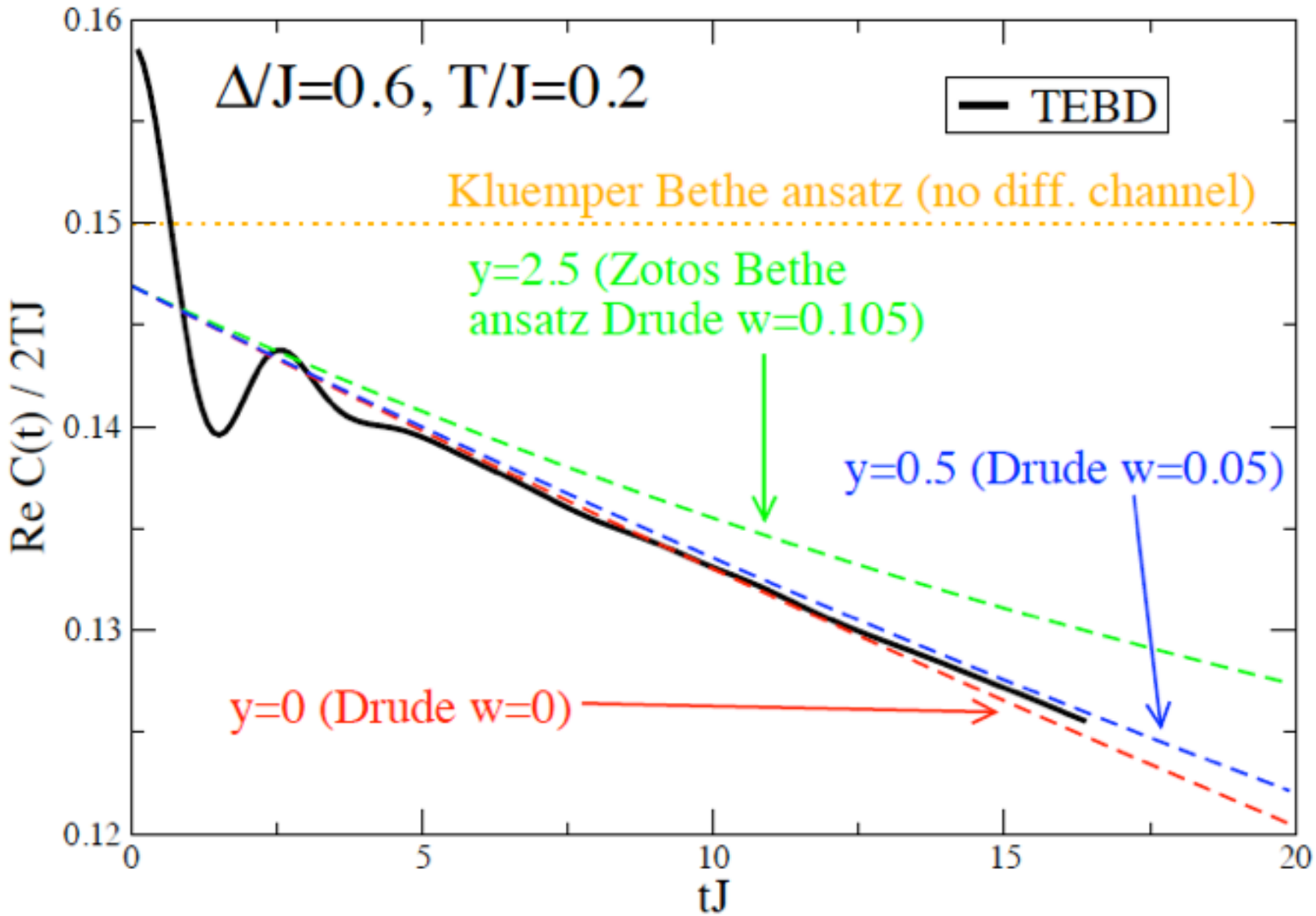
The Drude weight is easy to calculate and nonzero at T=0.
20+ years of efforts to calculate it (or even prove that it is nonzero) at T>0, h=0, by either analytical or numerical methods.

(cf. Sirker, Pereira, Affleck, PRB 2011)
(Thermal Drude weight is easier, for reason said later: found by Klumper and Sakai)

$$\sigma(\omega) = D\delta(\omega) + \dots$$

$$D = \frac{1}{2LT} \lim_{t\to\infty} \langle J(t)J(0)\rangle \geq \frac{1}{2LT} \sum_k \frac{\langle JQ_k\rangle^2}{\langle {Q_k}^2\rangle}$$

data from Sirker, Pereira, Affleck, PRB 2011



Drude weight progress, from 2011

$$\sigma(\omega) = D\delta(\omega) + \dots$$

$$D = \frac{1}{2LT} \lim_{t\to\infty} \langle J(t)J(0)\rangle \geq \frac{1}{2LT} \sum_k \frac{\langle JQ_k\rangle^2}{\langle {Q_k}^2\rangle}$$

Prosen: there is an iterative process to construct a nonlocal quantity that gives a lower bound that depends non-analytically on anisotropy, with cusps at $\Delta=\cos(\pi/n)$. (PRL 2011)
(subsequent work generalizing this result: Ilievski-Prosen, …)

Karrasch-Bardarson-JEM: The Drude weight can be calculated numerically for all but the lowest temperatures at positive Δ, and essentially all temperatures at negative Δ.

The lower bound appears to saturate the full value at the cusps.

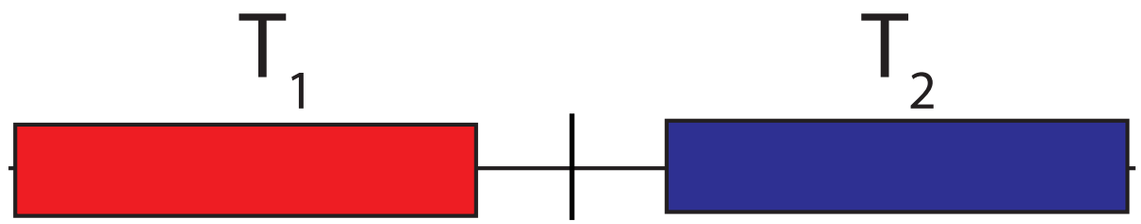
"Non-equilibrium expansions"

Almost everything that follows will be specific to 1D systems, where we have special analytical and numerical tools.

A. "Point current": A natural question about electrons is to compute the (charge or energy) current through a *point*.

Many beautiful works, especially in quantum impurity models. Older works on translation-invariant case: Sotiriadis-Cardy, Bernard-Doyon, Karrasch-Ilan-JEM

Solved (not too easily) by new hydrodynamical methods mentioned earlier



B. "Expansion": with atoms, it is more natural to *imag*e the full distribution of atoms (or conceivably energy). Two nice features:

1. The most natural model of 1D interacting atoms, the Lieb-Liniger model, is integrable.

2. For charge current in Lieb-Liniger, or energy current in the XXZ model, there is conservation of the spatially integrated current, which turns out to have remarkable consequences: expansion is controlled by a form of non-equilibrium thermodynamics.

“Non-equilibrium expansions”

Lieb-Liniger model = Bose gas with delta-function interactions

Thermodynamics (Yang and Yang) interpolates from free bosons to free fermions as interaction strength increases.

Tonks–Girardeau gas of ultracold atoms in an optical lattice

Belén Paredes[1], Artur Widera[1,2,3], Valentin Murg[1], Olaf Mandel[1,2,3], Simon Fölling[1,2,3], Ignacio Cirac[1], Gora V. Shlyapnikov[4], Theodor W. Hänsch[1,2] & Immanuel Bloch[1,2,3]

One experimental example:
Nature, 2004

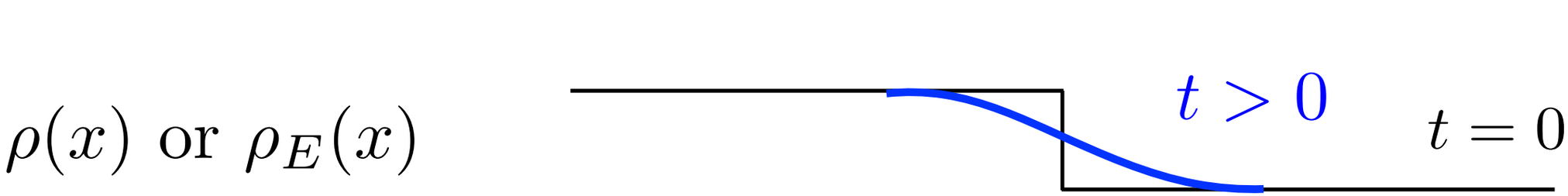
Originally, it was only possible to measure momentum-space distributions; now several groups have achieved imaging of individual sites of an optical lattice (Greiner, Chin, Bloch, …).

How to quantify an expansion?

There is a great deal of theoretical work, especially on the Lieb-Liniger case (~100 papers; Stringari, Caux-Konik, Gangardt,…). Three time scales:

Short time: initial transient, which we ignore

Intermediate time: (becomes infinite if reservoirs are infinite)

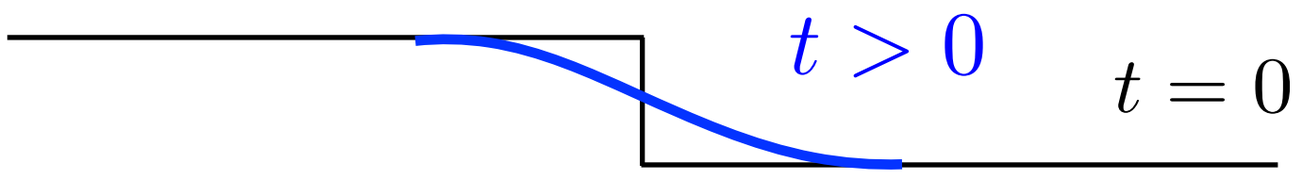


In a ballistic (nonzero Drude weight system), the first moment increases quadratically in time.

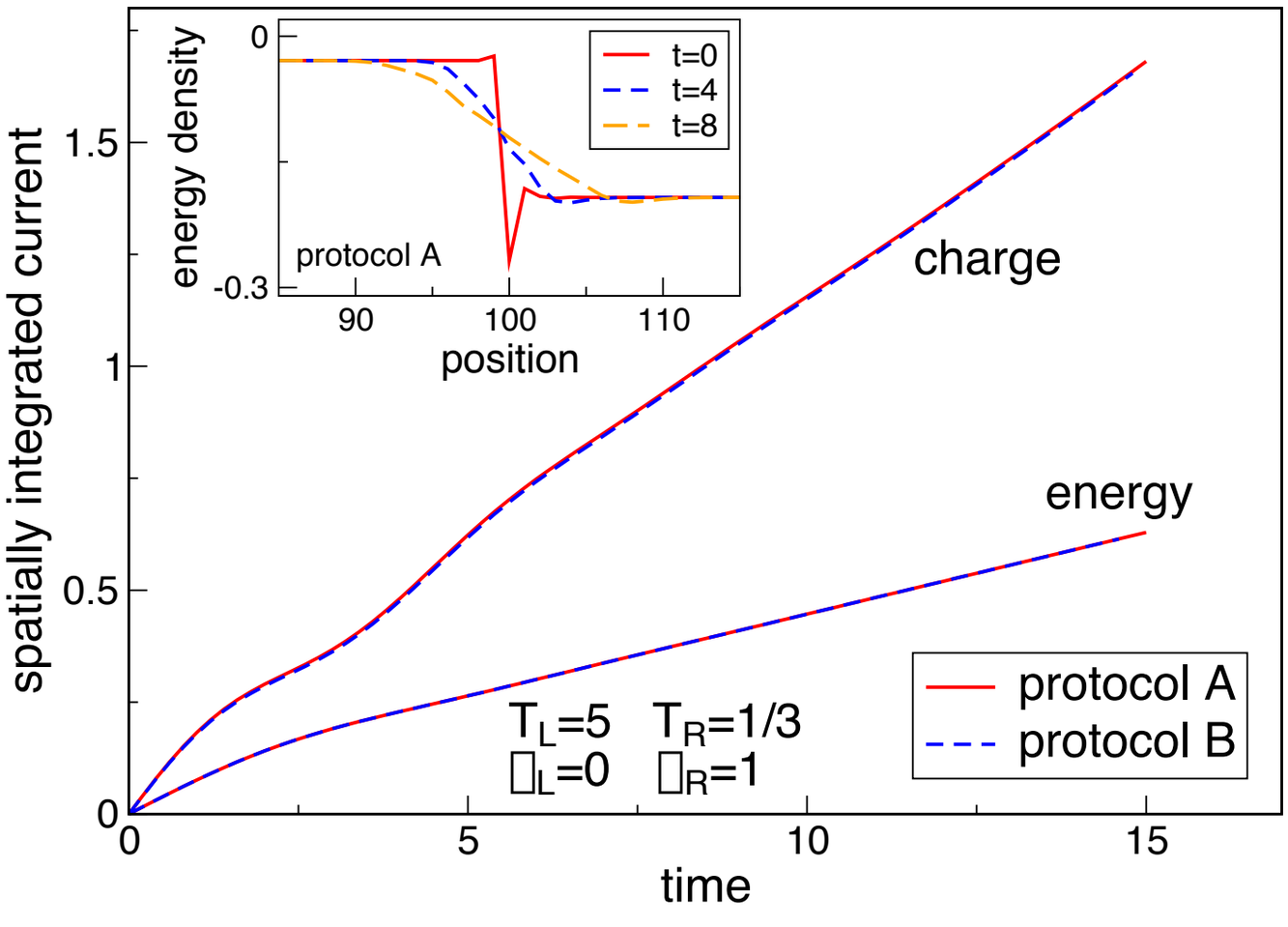
Long time: long-time expansion into vacuum can be analyzed relatively simply in BA because asymptotic density is zero.

How to quantify an expansion?

$\rho(x)$ or $\rho_E(x)$



In a ballistic (nonzero Drude weight system), the first moment increases quadratically in time.



How to quantify an expansion?

At $t = 0$, prepare two leads at (μ_1, T_1) and (μ_2, T_2). The initial state on the boundary between the two leads does not matter after some initial transient. We can quantify the expansion by the time dependence of the first moment of particle density (or similarly for energy)

$$M_1 = \int_{-\infty}^{\infty} n(x) x \, dx. \tag{1}$$

The continuity equation relates density and current:

$$\partial_t n + \partial_x j = 0. \tag{2}$$

Now

$$\partial_t M_1 = \int_{-\infty}^{\infty} x \partial_t n \, dx = -\int_{-\infty}^{\infty} x \partial_x j \, dx = \int_{-\infty}^{\infty} j \, dx, \tag{3}$$

where in the integration by parts we have assumed $j(x)$ vanishes rapidly at $x = \pm\infty$. We will make considerable use of the fact that in many problems of interest

$$\left[\int_{-\infty}^{\infty} j \, dx, H \right] = 0. \tag{4}$$

Now go back to basic ideas of equilibration…

Linear and non-linear response: point current

For the final *H* a homogeneous integrable model, there is numerically a "generalized Stefan-Boltzmann law" to high accuracy (to be defined in a moment), which led us to the idea that this picture can be made exact for expansions.

For final *H* homogeneous and non-integrable, we do not observe a steady state. We believe that the temperature gradient is decreasing and Fourier's law is setting in, but cannot access very long times.

For final H inhomogeneous, there can be a steady state if the leads are integrable and *J* is a function of both temperatures jointly.

We can see the onset of the nontrivial power-laws in tunneling between Luttinger liquids as temperature is lowered.

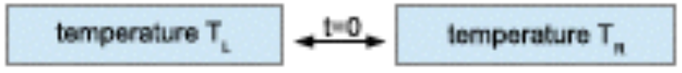
One methodology slide (C. Karrasch)
Time-dependent DMRG at nonzero T

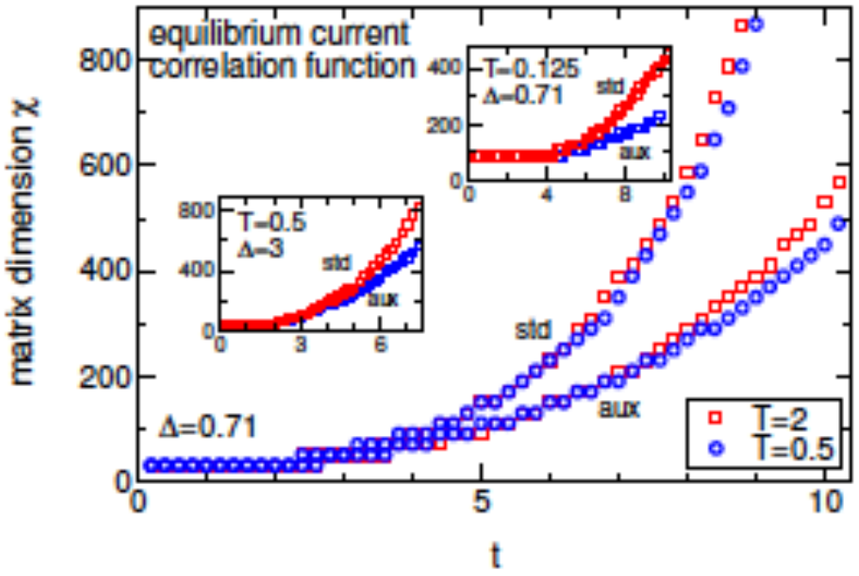
Finite Temperature: Improvement

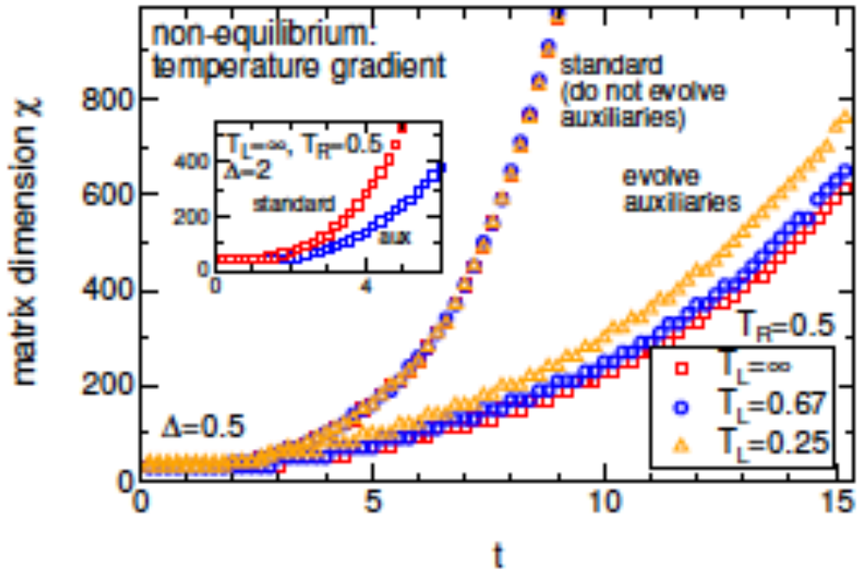
- slower increase of $\chi \Rightarrow$ access longer time scales
- how much longer? depends on model, temperature, ...

  example: spinless fermions, interaction Δ

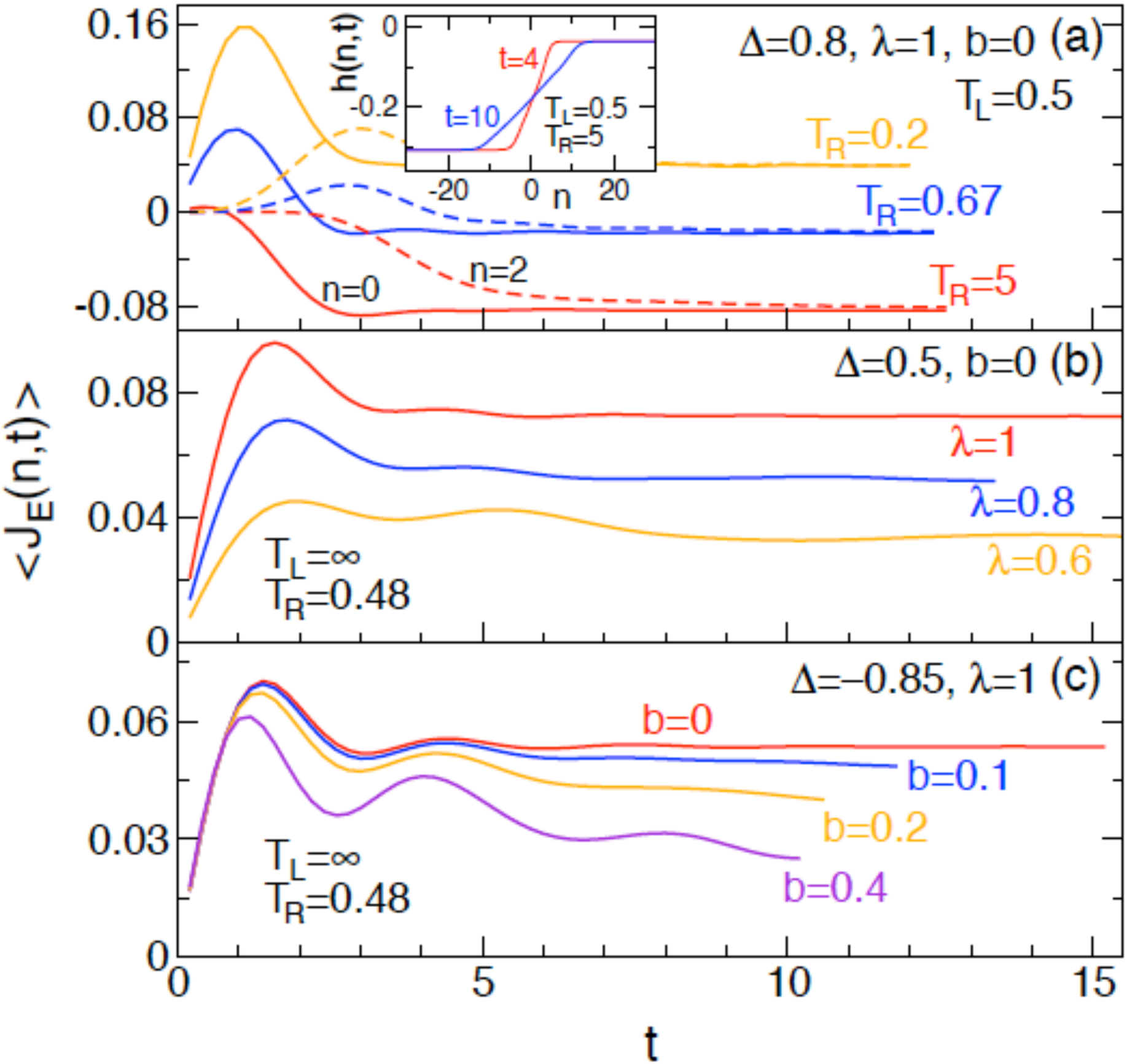
correlation function $\langle J(t)J\rangle_\beta$







(CK, Bardarson, Moore '12 '13)
(Barthel, Schollwöck, Sachdev '12)
(Barthel '13)


Δ=0.8, λ=1, b=0 (a)
T_L=0.5
T_R=0.2
T_R=0.67
T_R=5
n=0
n=2
h(n,t)
t=4
t=10
T_L=0.5
T_R=5
n
Δ=0.5, b=0 (b)
λ=1
λ=0.8
λ=0.6
T_L=∞
T_R=0.48
Δ=–0.85, λ=1 (c)
b=0
b=0.1
b=0.2
b=0.4
T_L=∞
T_R=0.48
<J_E(n,t)>
t

Alternative hydrodynamics: from more conservation laws

Energy transport in XXZ is special: because integrated energy current commutes with the Hamiltonian, we expect an additional continuity equation

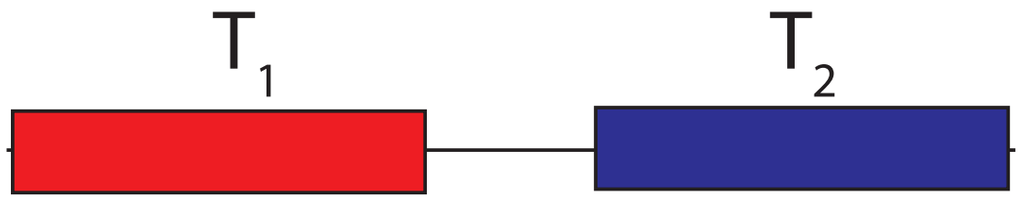
$$\partial_t \rho_E + \partial_x j_E = 0, \quad \partial_t j_E + \partial_x Q_4 = 0$$

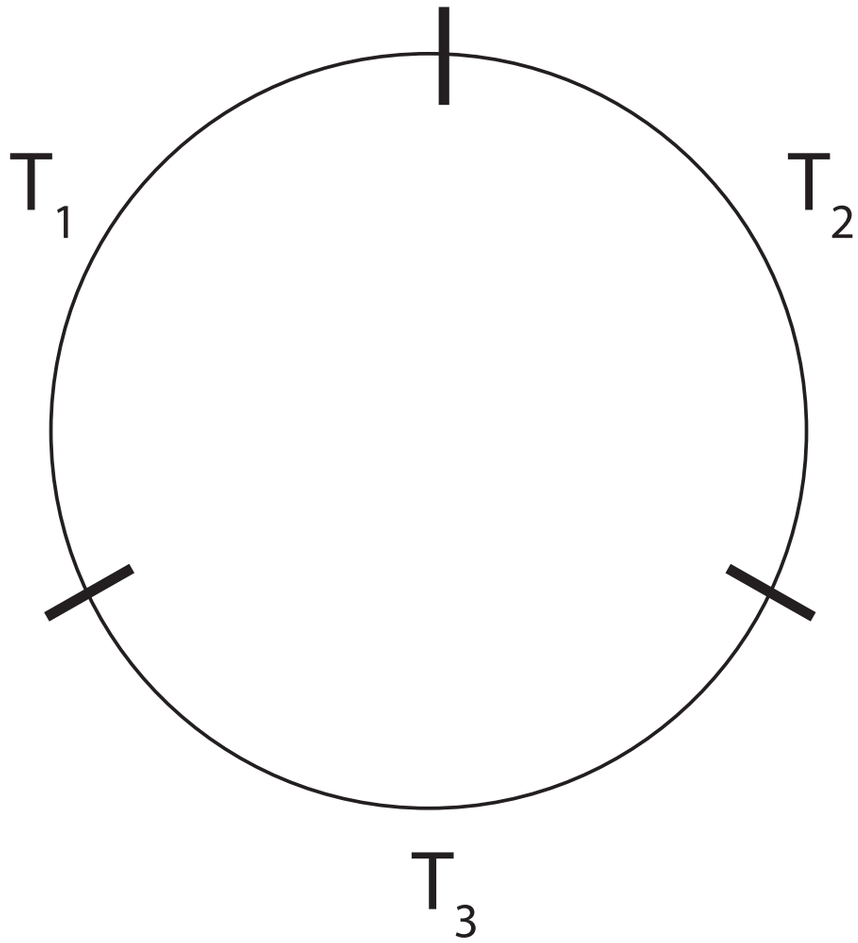
This is familiar from Lorentz-invariant models (cf. Bernard-Doyon): the energy current is itself a conserved density, by symmetry of the stress-energy tensor.

In other words, energy transport in XXZ is like that in a Lorentz-invariant model, and expansion occurs according to a expansion potential or generalized pressure Q4. ("cyclic law")

The "q-boson" model is a lattice example of similar physics for *charge* current rather than energy current.

When the cyclic law is exact



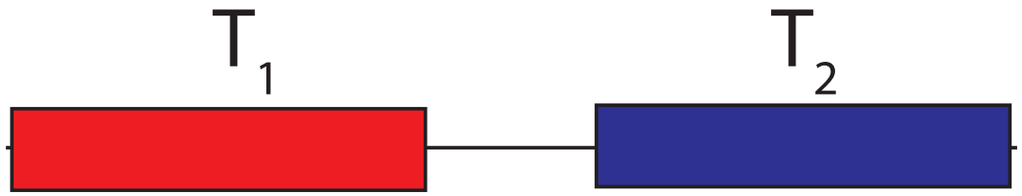


Global energy current conservation connects what happens at 3 interfaces

Cyclic form of existence of f-function:

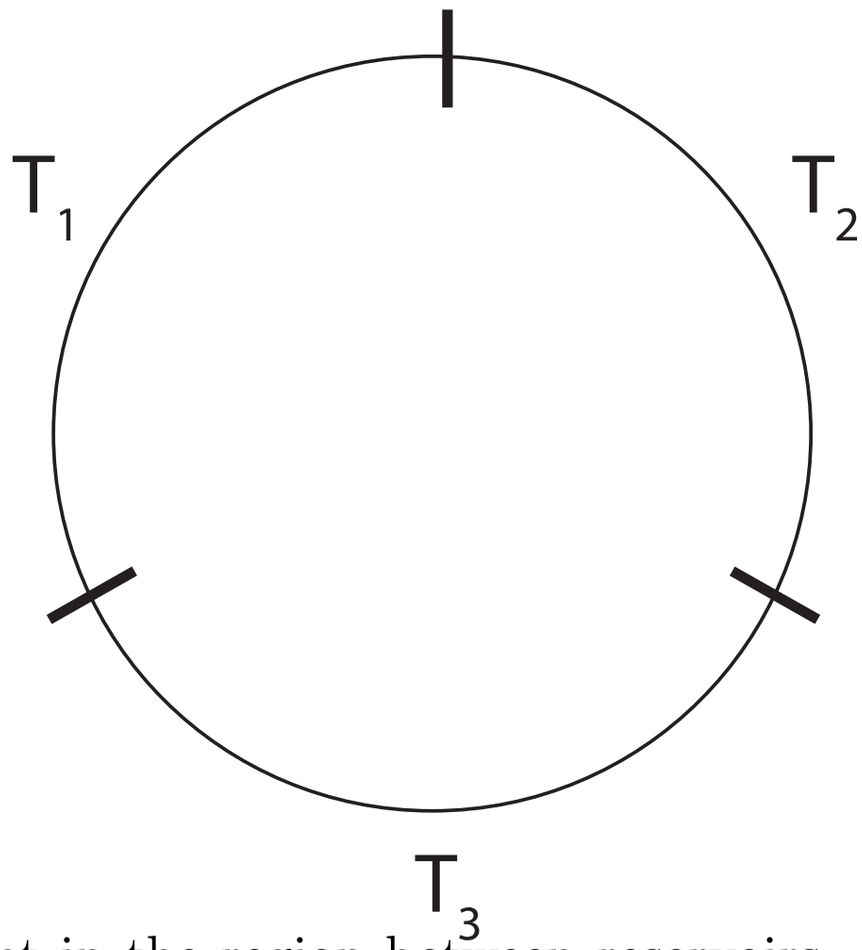
$$j_E^{\infty}(T_1 \to T_2) + j_E^{\infty}(T_2 \to T_3) + j_E^{\infty}(T_3 \to T_1) = 0$$

When the cyclic law is exact



Global energy current conservation links spatial *integrals of current* across each interface, not steady-state current

In a CFT, probably same thing since there is a unique velocity, but they are not obviously connected in general.



Let j_{12} be the spatially integrated current in the region between reservoirs 1 and 2. Then global current conservation means

$$[H, j_{12} + j_{23} + j_{31}] = 0. \tag{1}$$

But this cyclic law implies that at every time j_{12} is of the form $f(t, \mu_1, T_1) - f(t, \mu_2, T_2)$.

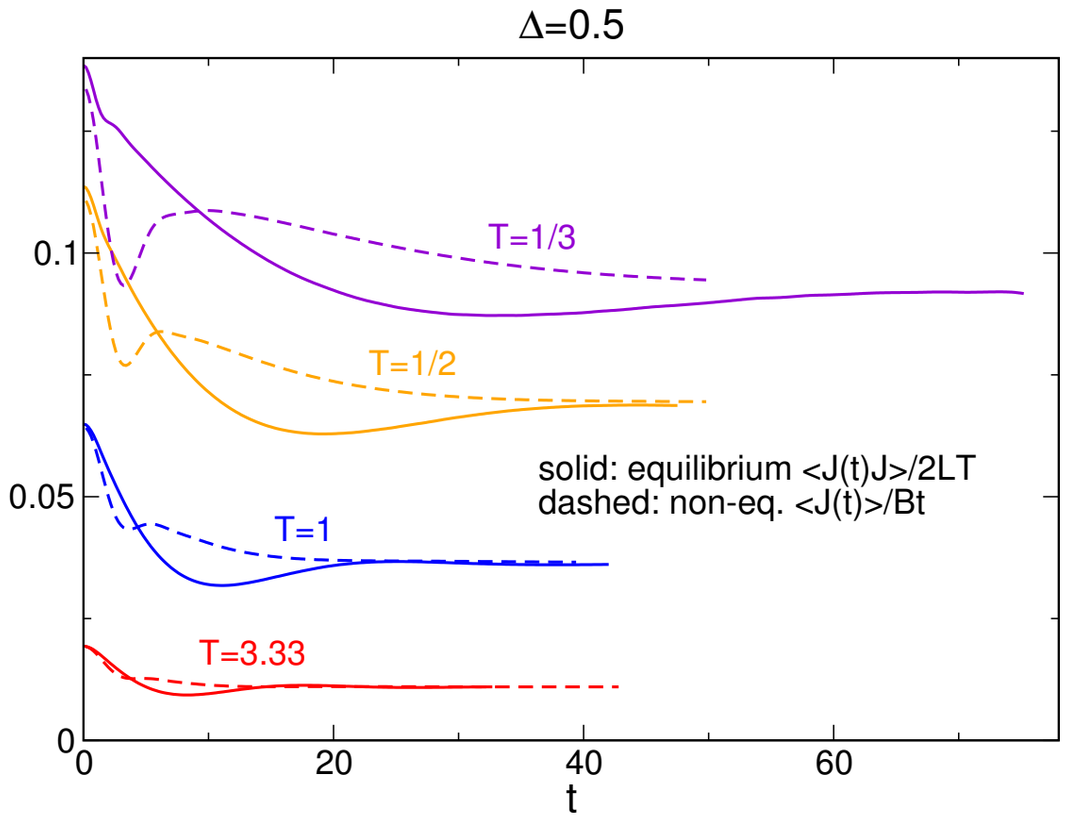
Linear response: Drude weight

The cyclic law means that linear-response is enough to predict non-equilibrium. The increase of the moment at linear-response can be related to the Drude weight: focusing for the moment on energy current and a purely thermal gradient, we find

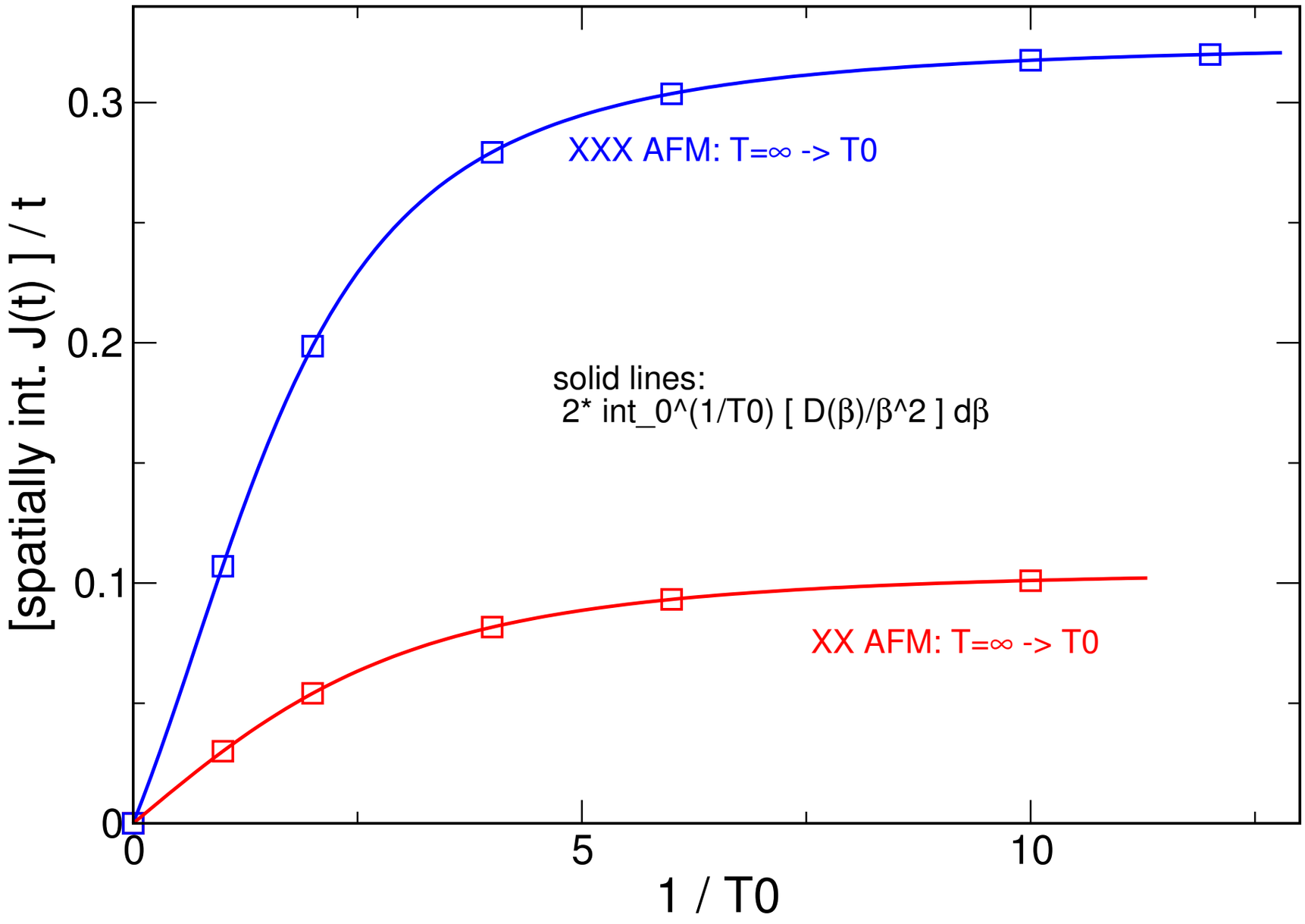
$$\partial_t^2 M_1^{\rm th} = \partial_t \int_{-\infty}^{\infty} j\, dx = G^{\rm th} \times (\Delta T). \qquad (1)$$

This can be checked numerically by comparing the rate of expansion to the thermal Drude weight of the XXZ model computed by Klümper and Sakai.

Actually this connection exists in LR even without current conservation: example is *charge* current in XXZ model



Combine cyclicity with Drude weight:
Exact far-from-equilibrium energy expansion in XXZ



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

Recent progress

The above is a very specialized trick to get some exact results for one model. Can one develop a more general approach for hydrodynamics in integrable models?

Yes: recent work on (almost certainly) asymptotically exact solutions for this initial condition by

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 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"

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

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.

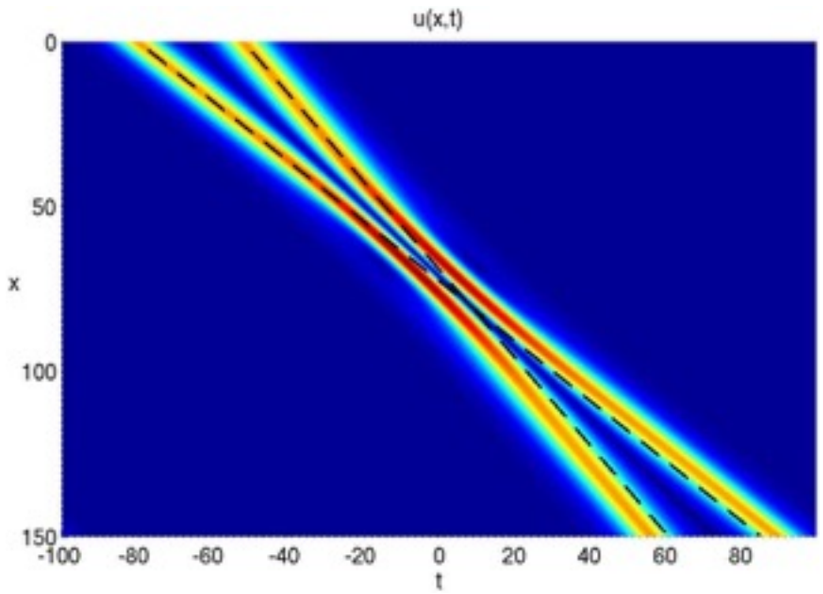
Why Boltzmann equation gets modified in (classical or quantum) integrable systems

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)

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

This derives the equation directly for NLS and KdV solitons as a kinetic theory;
An alternate route is via hydrodynamical equations (cf. Doyon talk)

Different integrable models just differ in the velocity form: three examples are

El and Kamchatnov for NLS solitons (dense generalization of Zakharov 1971):

$$s(\alpha,\gamma) = -4\alpha + \frac{1}{2\gamma}\int_{-\infty}^{\infty}\int_{0}^{\infty} \ln\left|\frac{\lambda-\bar{\mu}}{\lambda-\mu}\right|^2 f(\xi,\eta) \times [s(\alpha,\gamma)-s(\xi,\eta)]d\xi d\eta.$$

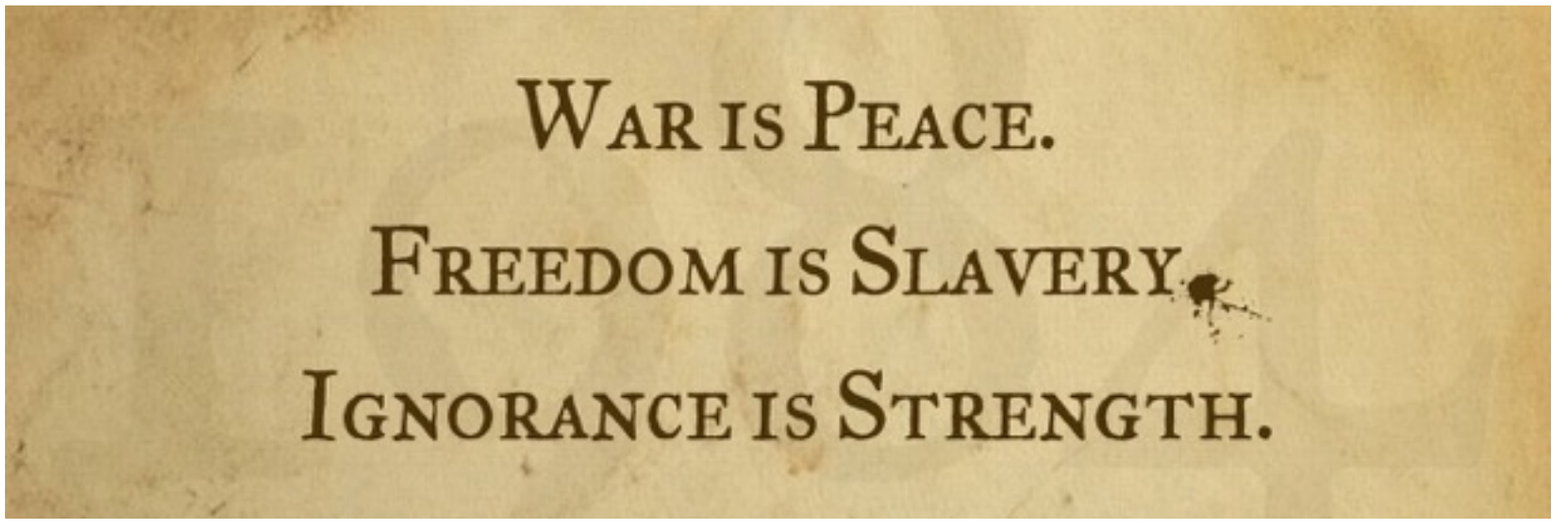
Castro-Alvaredo/Doyon/Yoshimura for Lieb-Liniger

Bertini et al. for XXZ

arXiv:1605.09790 [pdf, other]
Transport in out-of-equilibrium XXZ chains: exact profiles of charges and currents
Bruno Bertini, Mario Collura, Jacopo De Nardis, Maurizio Fagotti

How do kinetic theory (Boltzmann equation) and hydrodynamics (Euler equations) give the same description?

Equivalence is a little surprising, esp. in XXZ.
From *1984*, by Orwell:



For integrable models:
(to at least as good an approximation as above)

TBA is GGE
Kinetic theory is hydrodynamics
One (functional) equation is an infinite hierarchy

Integrable hydrodynamics

Simplest case is Bose gas (Lieb-Liniger; Yang and Yang)
GGE = Generalized Gibbs Ensemble = include 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 so far

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.

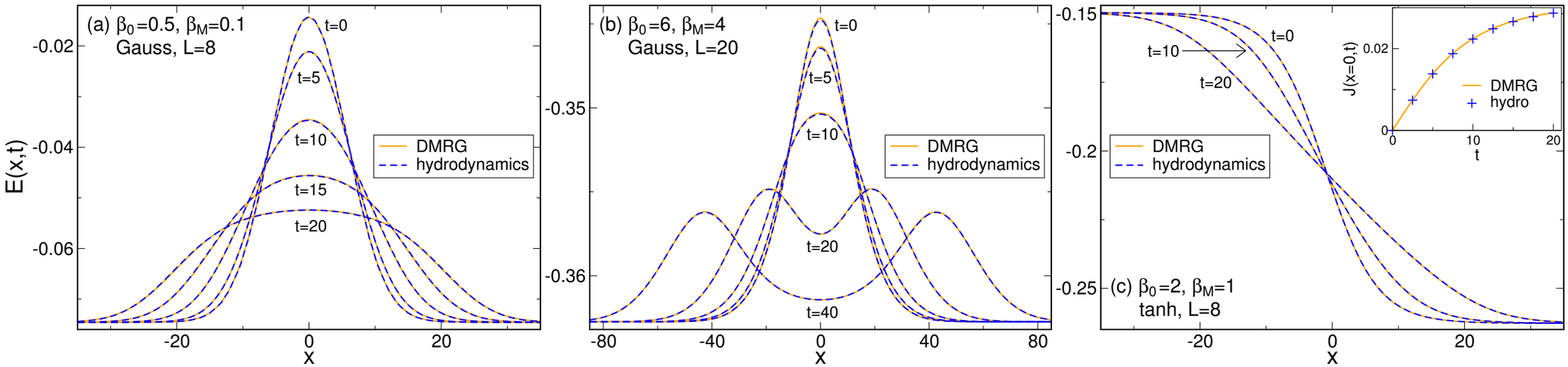
Two-reservoir problem already solved in 2016 papers: solution is function of one variable (x/t).

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

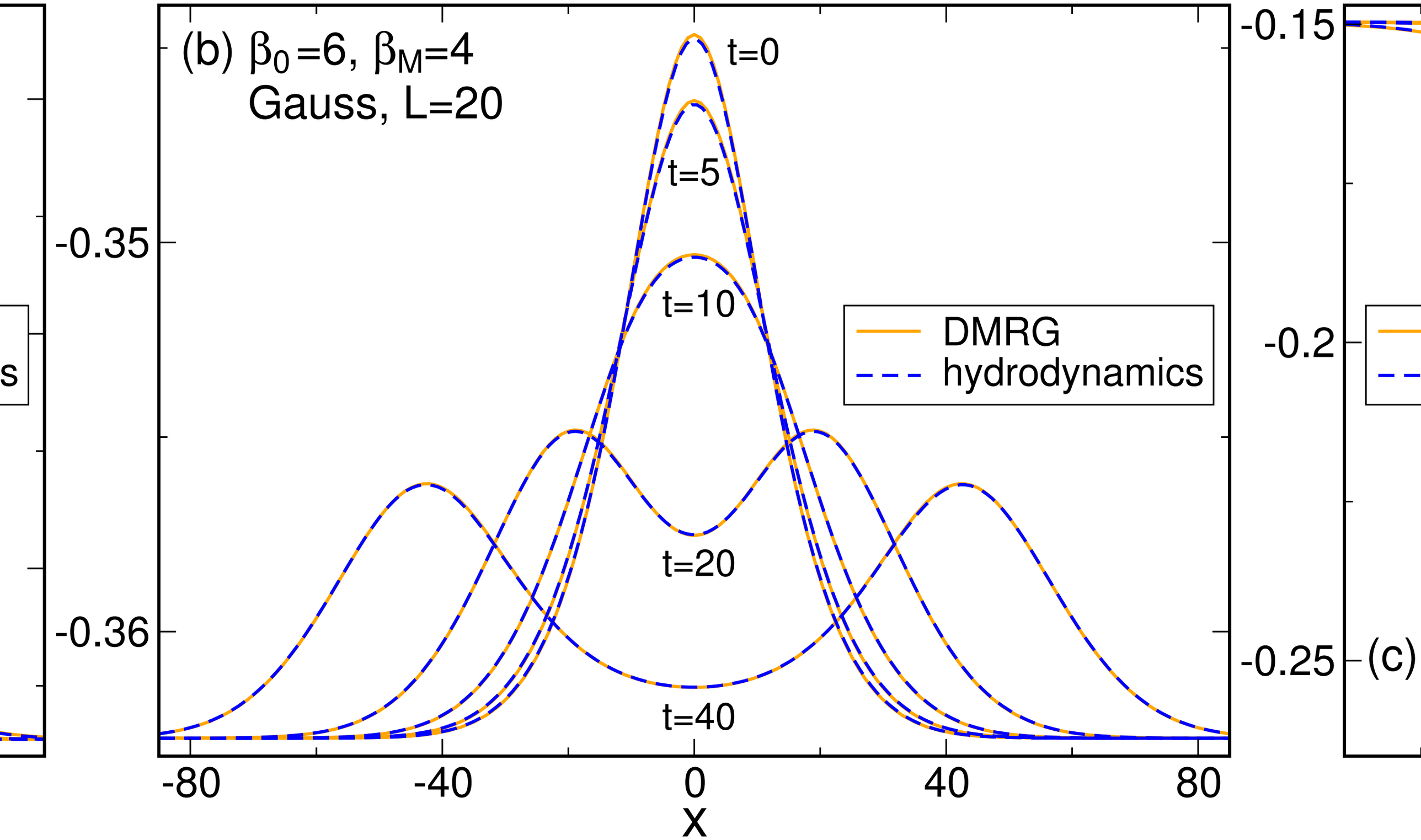
Take XXZ in zero magnetic field. Make a spatial variation of initial temperature. Watch the energy spread out in time.

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)

Zoom in!


(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
(c)
-80
-40
0
40
80
x

Summary

1. The two-reservoir quench is now pretty well understood in various approaches.

2. For that and more general problems, it is useful to think about the Boltzmann equation for quasiparticles, whose only interaction is via delays (Bethe ansatz phase shifts), a.k.a. GHD.

3. This type of equation has a long history in classical integrable systems (El and Kamchatnov). Even for fairly small quantum systems, it can be remarkably successful in comparison to microscopics.

What is left out: for other initial states, need to solve initial GGE problem;
possible singularities;
corrections from integrability-breaking terms;
non-ballistic behavior (e.g., in gapped XXZ regions)
subleading terms (e.g., Schwarzian in Sotiriadis-Cardy)

Brief intro to quantum hydrodynamics above 1D: near-equilibrium

An example of recent progress on a long-standing question:

Are there intrinisic limits on how fast a system can relax to equilibrium?

Related to conductivity via the Kubo formula: how rapidly does the current-current correlation decay in time?

Also related to existence of “hydrodynamical” regimes of electron transport where quasiparticle scattering is not the right picture.

Some past formulations:

Mott-Ioffe-Regel: mean free path must be at least the lattice spacing

Sachdev: $\tau \geq \frac{\hbar}{k_B T}$ $\qquad$ quantum $e^{-iHt/\hbar} \leftrightarrow e^{-H/(k_B T)}$ thermal

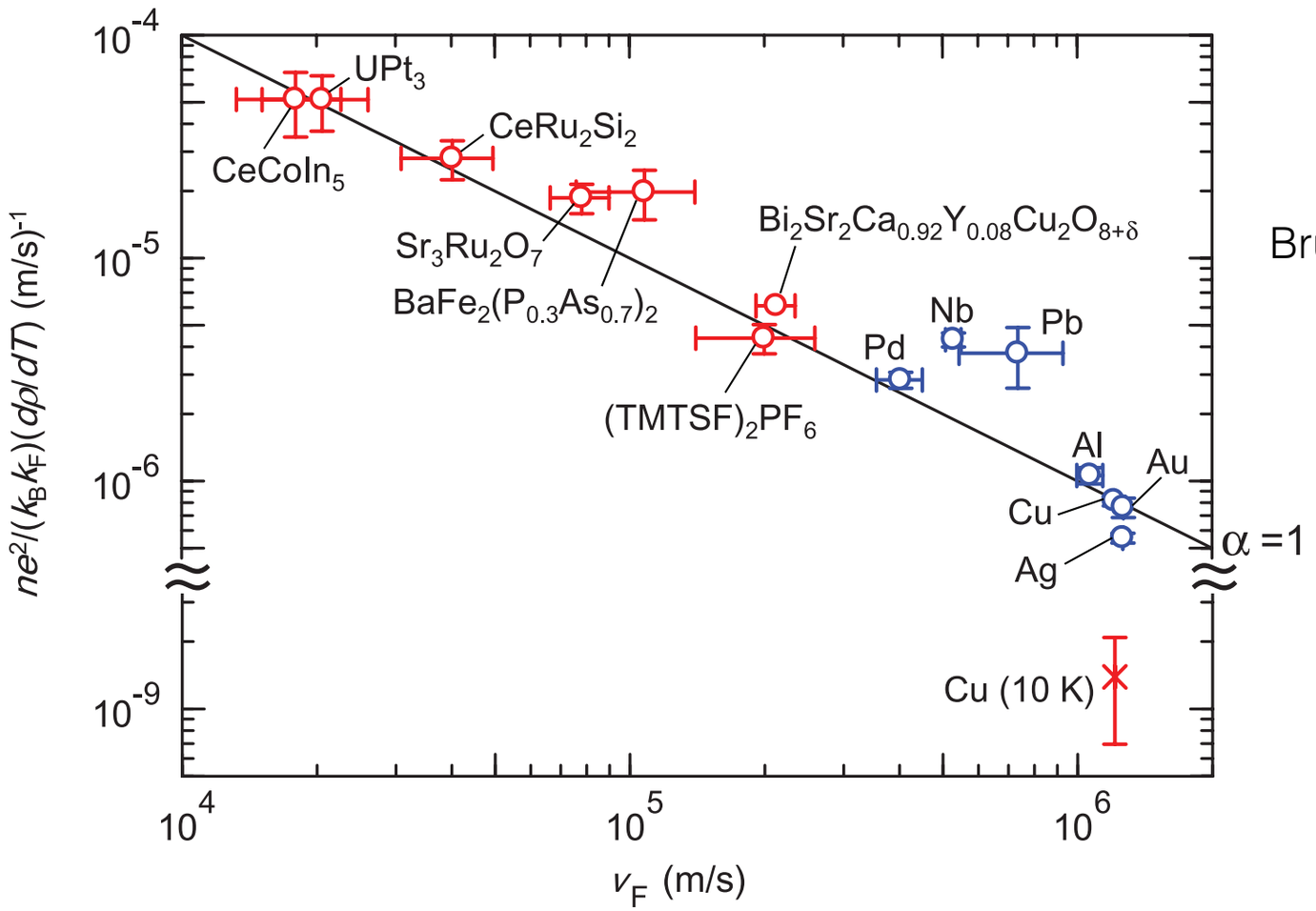
Kovtun-Son-Starinets: the viscosity is bounded below* $\qquad \frac{\eta}{s} \geq \frac{\hbar}{4\pi k_B}$

Hartnoll: reinterpret viscosity bound as a lower limit on diffusion constant

Near-equilibrium

Why these bounds matter: nature seems to contain such behavior

$$\tau \geq \frac{\hbar}{k_B T}$$



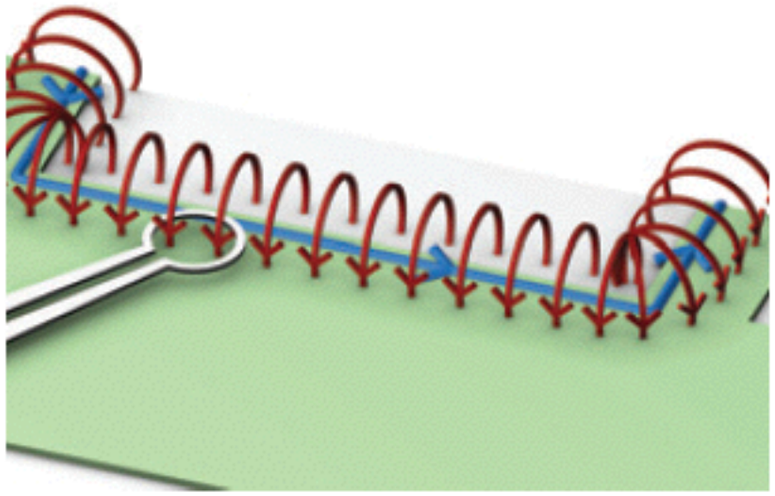
Bruin et al. (Mackenzie), Science 2013

$$\frac{\eta}{s} \geq \frac{\hbar}{4\pi k_B}$$

is satisfied (I believe) in all experimental liquids, and within ~10 of saturation in helium and QGP, but there exist violations in exotic theories

Hydrodynamics of electrons

In materials that are very clean, momentum relaxation may take a relatively long time. It might be better to view electrons as a *fluid* rather than as independently scattering quasiparticles.



Nowack et al., Nat. Mat. 2013

Solid-state electrons where fluid properties measured

2DEGs (Molenkamp & others, 1990s)
Graphene (P. Kim; A. Geim)
Layered crystals (A. Mackenzie)
…

Near-equilibrium

New work, originally motivated by AdS but derivable without gravity dual:
(Kitaev, Maldacena-Shenker-Stanford, 2015):

The Lyapunov exponent for short-time onset of chaos is bounded

$$\lambda_L \leq \frac{2\pi k_B T}{\hbar}$$

Other ways quantum mechanics modifies hydrodynamics:

"Hall viscosity" in topological states: (Avron; Read; Gurarie…) stress tensor is

$$T_{ij} = p\delta_{ij} - \lambda_{ijkl}\xi_{kl} - \eta_{ijkl}\dot{\xi}_{kl}$$

and T-breaking allows an odd contribution $\eta^{(A)}_{ijkl} = -\eta^{(A)}_{klij}$

What is Hall viscosity in T-breaking gapless systems?
Allowed by symmetry.

Hydrodynamics of electrons

What makes electron fluids different from classical fluids?

In 2D and 3D, can induce broken T by a magnetic field
and have a new kind of viscosity, "Hall viscosity"

Is significant, and could be observable, in simple *metals*:
T. Scaffidi, N. Nandi, B. Schmidt, AP Mackenzie, JEM, PRL 17

In the quantum Hall regime there are two contributions in the q^2 correction to Hall conductance

$$\sigma_{xy}(q) = \sigma_{xy}(0) + O(q^2)$$

that are comparable (Hoyos-Son): one from Hall viscosity and one from (inverse) internal compressibility. In a metal, the internal compressibility part is small and the Hall viscosity follows from a Boltzmann calculation.

Hydrodynamics of electrons

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In a metal, the internal compressibility part is small and the Hall viscosity follows from a kinetic theory calculation. (work mentioned above)

Topology (part III)

What are (insulating) topological phases of matter?
How do some of them support quantized transport?

What is a "Berry phase"?
How do Berry phases give a unified approach to insulators, metals, …

Topological insulators: theory 2005-present
New topological semimetals: 2012-present

What are the unique transport properties of topological metals?
Does it help to go to nonzero frequency or nonlinear effects?

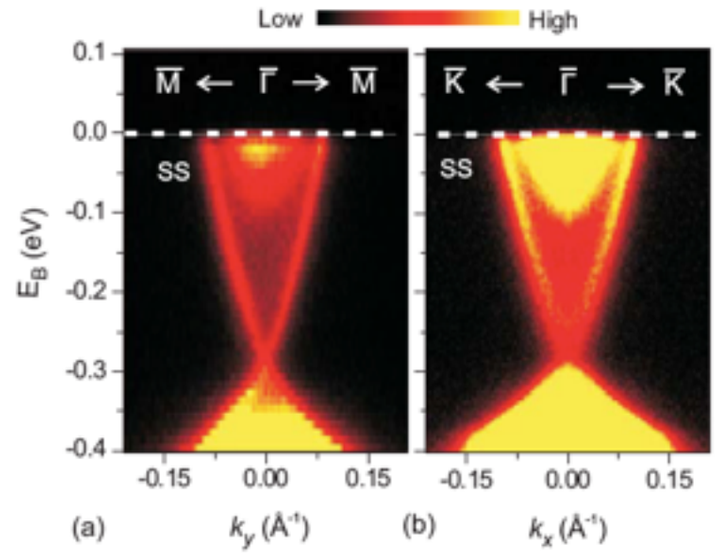
Berry phase in solids

Every simple gauge-invariant object made from A and F seems to mean something physically. We can identify several types of Berry-phase phenomena of nearly free electrons:

Insulators:

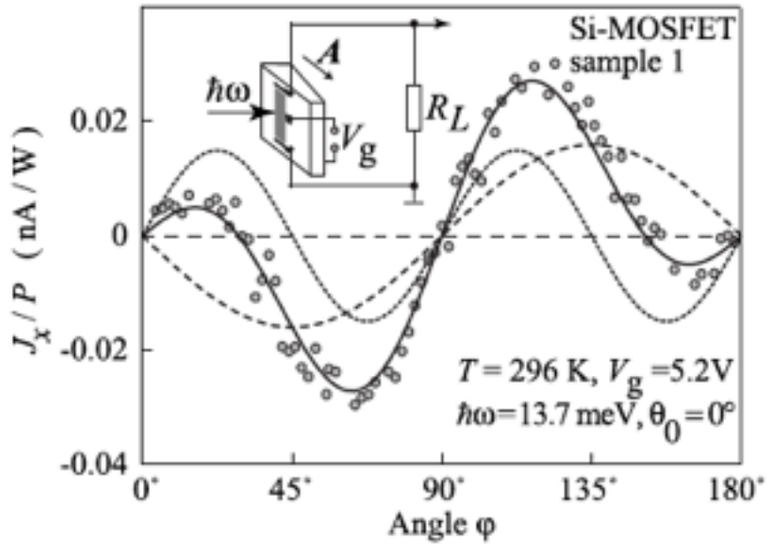
Topological phases independent of symmetry:
Examples: 2D and 4D QHE (1982,1988)

Topological phases dependent on symmetry
Examples: 2D and 3D Z2 topological insulators (2005,2007)



The Berry-phase approach to understanding these leads to expressions that are physically meaningful without symmetries:

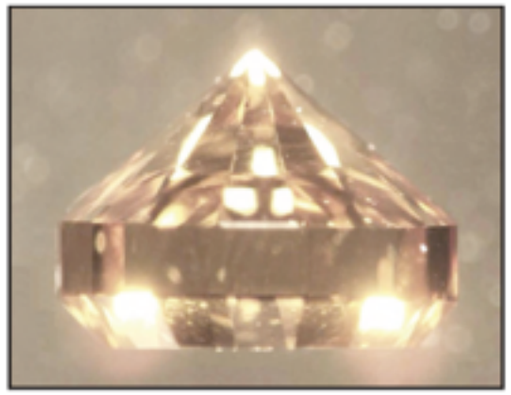
Examples: electrical polarization (1987-1990);
magnetoelectric effect (~2010) non-Abelian Berry phase

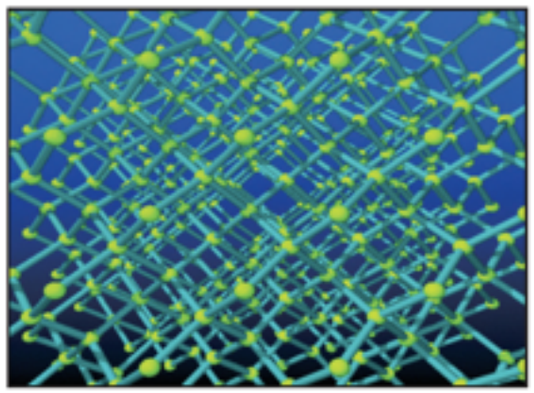


Metals: Several long-observed phenomena in metals are now believed to be Berry-phase effects. (AHE, CPGE,)
Are there other wave function properties that could matter?

Types of order

Much of condensed matter is about how different kinds of order emerge from interactions between many simple constituents.





Until 1980, all ordered phases could be understood as "symmetry breaking":

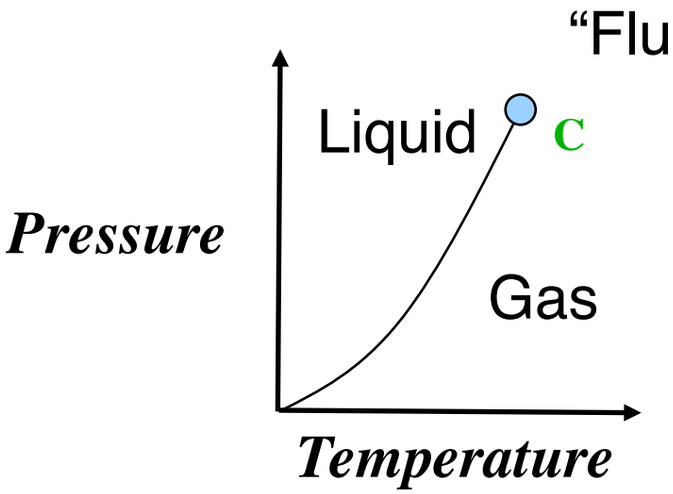
an ordered state appears at low temperature when the system spontaneously loses one of the symmetries present at high temperature.

Examples:
Crystals break the *translational* and *rotational* symmetries of free space.
The "liquid crystal" in an LCD breaks *rotational* but not *translational* symmetry.
Magnets break time-reversal symmetry and the rotational symmetry of spin space.
Superfluids break an internal symmetry of quantum mechanics.

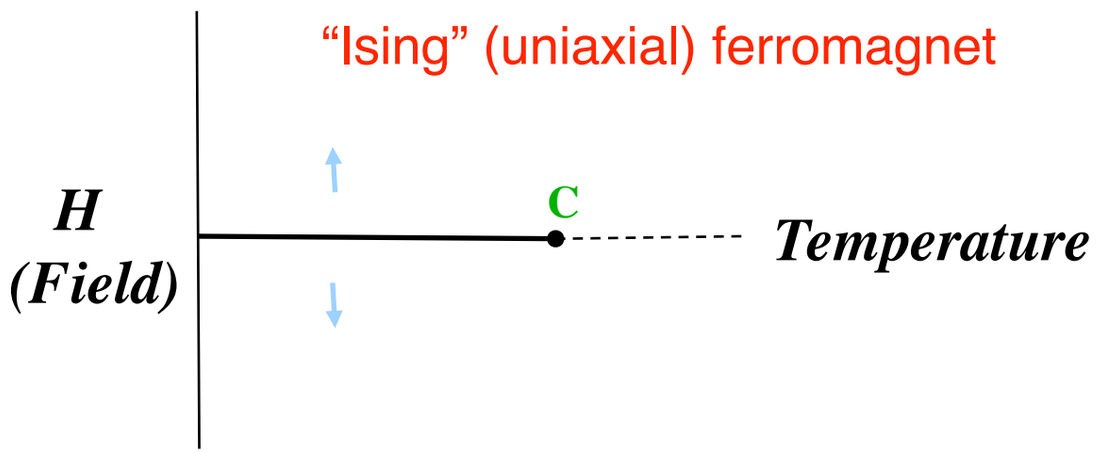
Types of order

At high temperature, entropy dominates and leads to a disordered state.
At low temperature, energy dominates and leads to an ordered state.

In case this sounds too philosophical, there are testable results that come out of the "Landau theory" of symmetry-breaking:



$$\rho_L - \rho_G \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$



$$M_{\uparrow} - M_{\downarrow} \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$

$$\text{Experiment}: \ \beta = 0.322 \pm 0.005$$
$$\text{Theory}: \ \beta = 0.325 \pm 0.002$$

"Universality" at continuous phase transitions (Wilson, Fisher, Kadanoff, ...)

Types of order

In 1980, the first ordered phase beyond symmetry breaking was discovered.

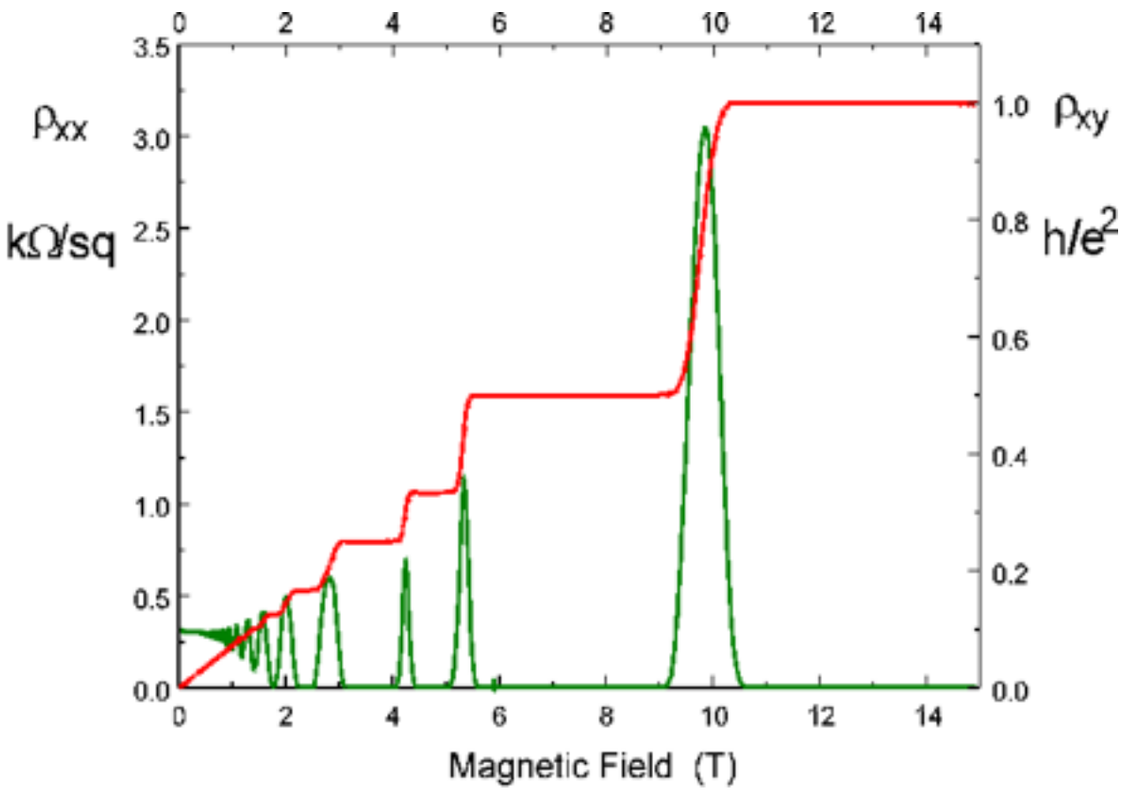
Electrons confined to a plane and in a strong magnetic field show, at low enough temperature, plateaus in the "Hall conductance":

force *I* along *x* and measure *V* along *y*

on a plateau, get

$$\sigma_{xy} = n\frac{e^2}{h}$$

at least within 1 in 10^9 or so.



What type of order causes this precise quantization?

Note I: the AC Josephson effect between superconductors similarly allows determination of *e*/*h*.

Note II: there are also *fractional* plateaus, about which more later.

Topological order

What type of order causes the precise quantization in the Integer Quantum Hall Effect (IQHE)?

Definition I:

In a topologically ordered phase, some physical response function is given by a "topological invariant".

What is a topological invariant? How does this explain the observation?

Definition II:

A topological phase is insulating but always has metallic edges/surfaces when put next to vacuum or an ordinary phase.

What does this have to do with Definition I?

"Topological invariant" = quantity that does not change under continuous deformation

(A third definition: phase is described by a "topological field theory")

Traditional picture: Landau levels

Normally the Hall ratio is (here *n* is a density)

$$R_H = \frac{I_x}{V_y B} = \frac{1}{nec} \Rightarrow \sigma_{xy} = \frac{nec}{B}$$

Then the value (now *n* is an integer)

$$\sigma_{xy} = n\frac{e^2}{h}$$

corresponds to an areal density $\frac{n}{2\pi\ell^2} = neB/hc.$

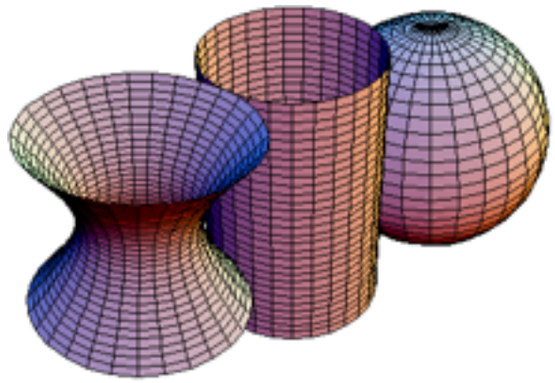
This is exactly the density of "Landau levels", the discrete spectrum of eigenstates of a 2D particle in an orbital magnetic field, spaced by the cyclotron energy. The only "surprise" is how precise the quantization is.

Topological invariants

Most *topological* invariants in physics arise as integrals of some *geometric* quantity.

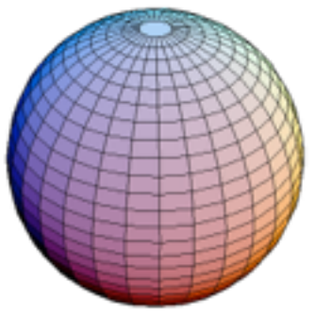
Consider a two-dimensional surface.

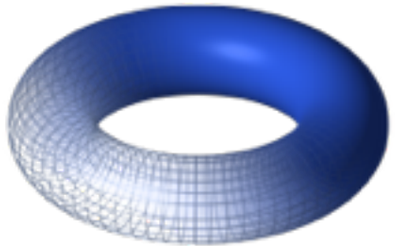
At any point on the surface, there are two radii of curvature.
We define the signed "Gaussian curvature" $\kappa = (r_1 r_2)^{-1}$



from left to right, equators have negative, 0, positive Gaussian curvature

Now consider *closed* surfaces.





The area integral of the curvature over the whole surface is "quantized", and is a topological invariant (Gauss-Bonnet theorem).

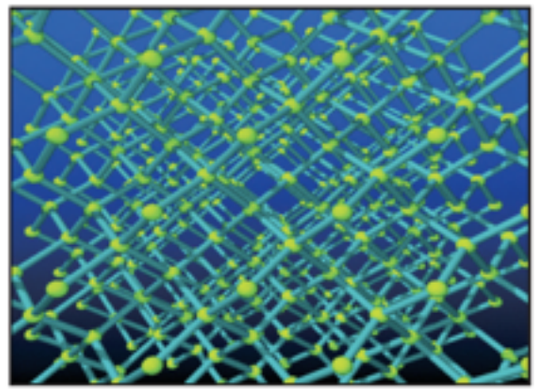
$$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2 - 2g)$$

where the "genus" g = 0 for sphere, 1 for torus, n for "n-holed torus".

Topological invariants

Good news:
for the invariants in the IQHE and topological insulators, we need one fact about solids

Bloch's theorem:
One-electron wavefunctions in a crystal (i.e., periodic potential) can be written



$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

where *k* is "crystal momentum" and *u* is periodic (the same in every unit cell).

Crystal momentum *k* can be restricted to the Brillouin zone, a region of *k*-space with periodic boundaries.
As *k* changes, we map out an "energy band". Set of all bands = "band structure".

The Brillouin zone will play the role of the "surface" as in the previous example,

and one property of quantum mechanics, the Berry phase

which will give us the "curvature".

Berry phase

What kind of "curvature" can exist for electrons in a solid?

Consider a quantum-mechanical system in its (nondegenerate) ground state.

The adiabatic theorem in quantum mechanics implies that, if the Hamiltonian is now changed slowly, the system remains in its time-dependent ground state.

But this is actually very incomplete (Berry).

Michael Berry

When the Hamiltonian goes around a *closed loop k(t)* in parameter space, there can be an irreducible *phase*

$$\phi = \oint \mathcal{A} \cdot d\mathbf{k}, \quad \mathcal{A} = \langle \psi_k | -i\nabla_k | \psi_k \rangle$$

relative to the initial state.

Why do we write the phase in this form?
Does it depend on the choice of reference wavefunctions?

Berry phase

Why do we write the phase in this form?
Does it depend on the choice of reference wavefunctions?

$$\phi = \oint \mathcal{A} \cdot d\mathbf{k}, \quad \mathcal{A} = \langle \psi_k | -i\nabla_k | \psi_k \rangle$$

If the ground state is non-degenerate, then the only freedom in the choice of reference functions is a local phase:

$$\psi_k \rightarrow e^{i\chi(k)}\psi_k$$

Under this change, the "Berry connection" *A* changes by a gradient,

$$\mathcal{A} \rightarrow \mathcal{A} + \nabla_k \chi$$

Michael Berry

just like the vector potential in electrodynamics.

So loop integrals of *A* will be gauge-invariant,
as will the *curl* of *A*, which we call the "Berry curvature".

$$\mathcal{F} = \nabla \times \mathcal{A}$$

Berry phase in solids

In a solid, the natural parameter space is electron momentum.

The change in the electron wavefunction *within the unit cell* leads to a Berry connection and Berry curvature:

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

$$\mathcal{A} = \langle u_{\mathbf{k}} | -i\nabla_k | u_{\mathbf{k}} \rangle \qquad \mathcal{F} = \nabla \times \mathcal{A}$$

We keep finding more physical properties that are determined by these quantum geometric quantities.

S. S. Chern

The first was that the integer quantum Hall effect in a 2D crystal follows from the integral of *F* (like Gauss-Bonnet!). Explicitly,

$$n = \sum_{bands} \frac{i}{2\pi} \int d^2k \left(\left\langle \frac{\partial u}{\partial k_1} \middle| \frac{\partial u}{\partial k_2} \right\rangle - \left\langle \frac{\partial u}{\partial k_2} \middle| \frac{\partial u}{\partial k_1} \right\rangle \right) \qquad \mathcal{F} = \nabla \times \mathcal{A}$$

$$\sigma_{xy} = n\frac{e^2}{h}$$

TKNN, 1982

"first Chern number"

The importance of the edge

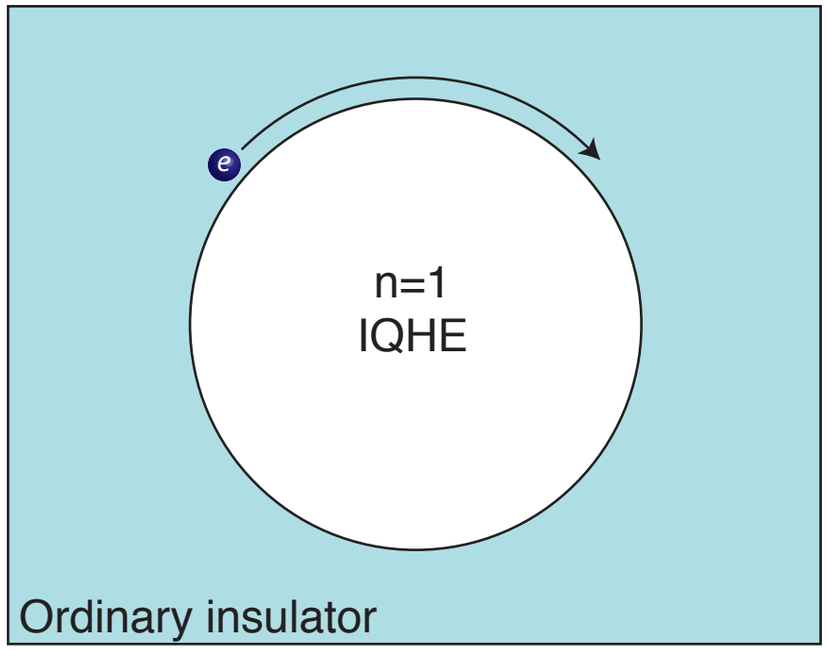
But wait a moment...

This invariant exists if we have energy bands that are either full or empty, i.e., a "band insulator".

How does an *insulator* conduct charge?

Answer: (Laughlin; Halperin)

There are *metallic edges* at the boundaries of our 2D electronic system, where the conduction occurs.



These metallic edges are "chiral" quantum wires (one-way streets). Each wire gives one conductance quantum (e^2/h).

$$\sigma_{xy} = n\frac{e^2}{h}$$

The topological invariant of the *bulk* 2D material just tells how many wires there *have* to be at the boundaries of the system.

How does the bulk topological invariant "force" an edge mode?

Theme for today: different kinds of "transport" in topological systems

Normal metallic transport: *states* are fixed but *occupancy* changes

Topological edge/surface transport: same idea, but set of available states is unusual (e.g., IQHE edge is "one-way street")

Pumping transport: adiabatic evolution of ground state
(Laughlin picture of IQHE; Thouless picture of polarization)
No dissipation so possibility of precise quantization

Are there transport effects of wave function geometry in *bulk* metals?

What about nonzero frequency (AC transport, optics, …)?

Will not cover superconductors, Majorana fermions, FQHE, …

The importance of the edge

The topological invariant of the *bulk* 2D material just tells how many wires there *have* to be at the boundaries of the system.

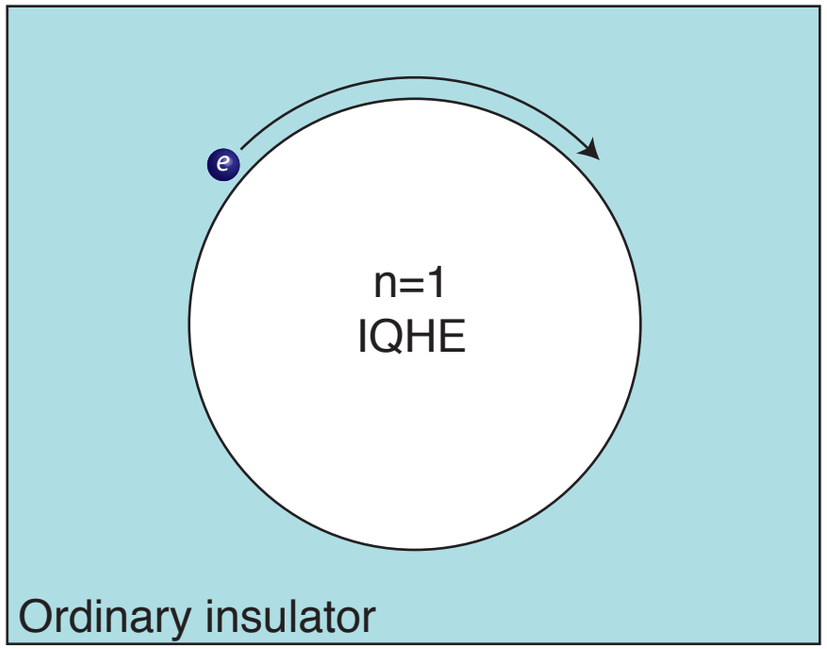
How does the bulk topological invariant "force" an edge mode?

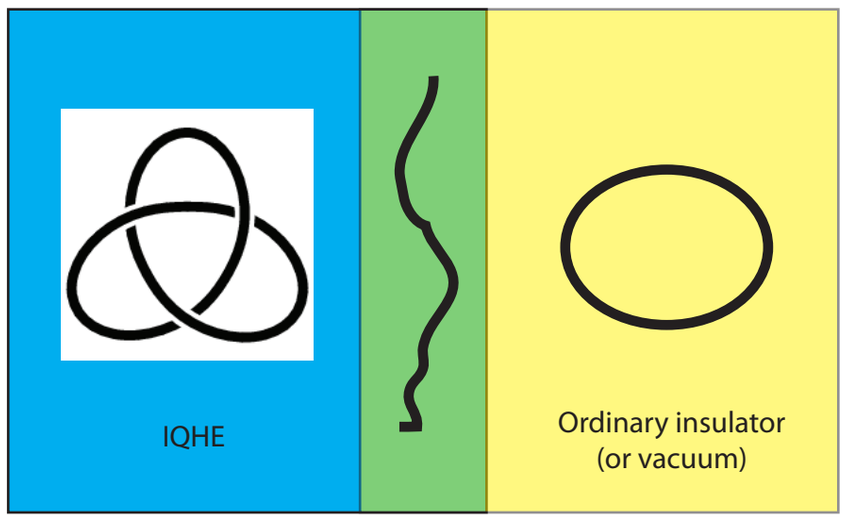
Answer:

Imagine a "smooth" edge where the system gradually evolves from IQHE to ordinary insulator. The topological invariant must change.

But the definition of our "topological invariant" means that, *if the system remains insulating* so that every band is either full or empty, the invariant cannot change.

$\therefore$ the system must not remain insulating.





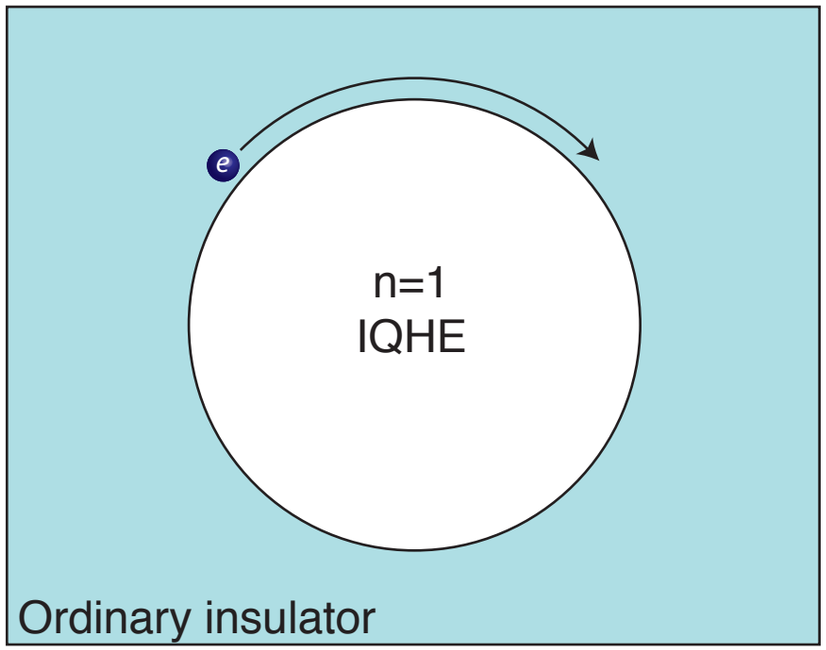
(What is "knotted" are the electron wavefunctions)

2005-present and "topological insulators"

The same idea will apply in the new topological phases discovered recently:

a "topological invariant", based on the Berry phase, leads to a nontrivial edge or surface state at any boundary to an ordinary insulator or vacuum.

However, the physical origin, dimensionality, and experiments are all different.



We discussed the IQHE so far in an unusual way. The magnetic field entered only through its effect on the Bloch wavefunctions (no Landau levels!).

This is not very natural for a magnetic field.
It is ideal for spin-orbit coupling in a crystal.

The "quantum spin Hall effect"

Spin-orbit coupling appears in nearly every atom and solid. Consider the standard atomic expression

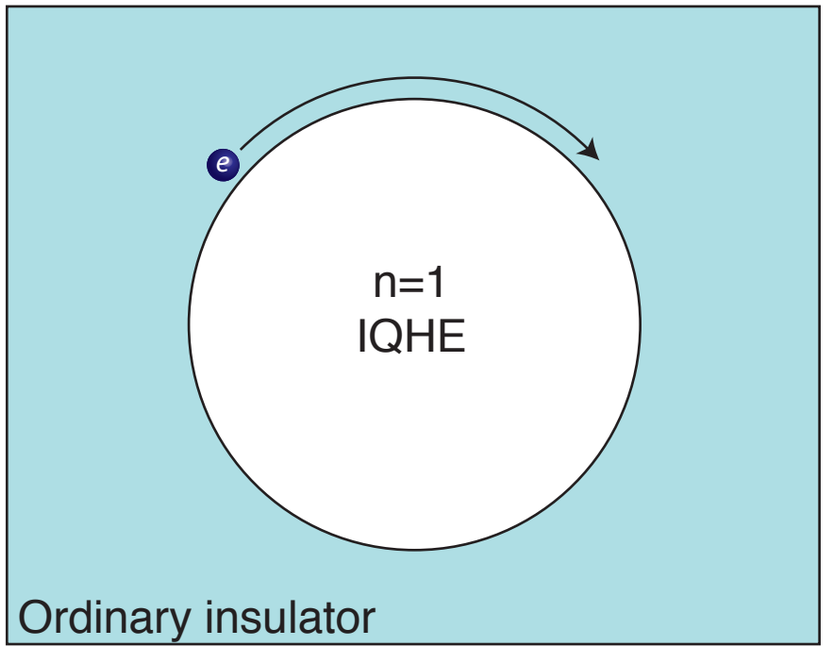
$$H_{SO} = \lambda \mathbf{L} \cdot \mathbf{S}$$

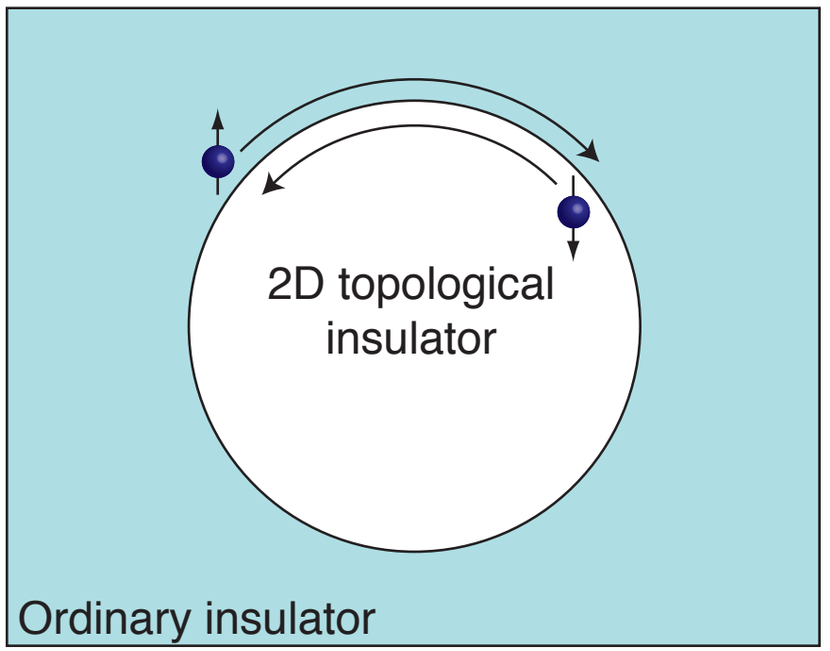
For a given spin, this term leads to a momentum-dependent force on the electron, somewhat like a magnetic field.

The spin-dependence means that the *time-reversal symmetry* of SO coupling (even) is different from a real magnetic field (odd).

It is possible to design lattice models where spin-orbit coupling has a remarkable effect: (Murakami, Nagaosa, Zhang 04; Kane, Mele 05)

spin-up and spin-down electrons are in IQHE states, with opposite "effective magnetic fields".



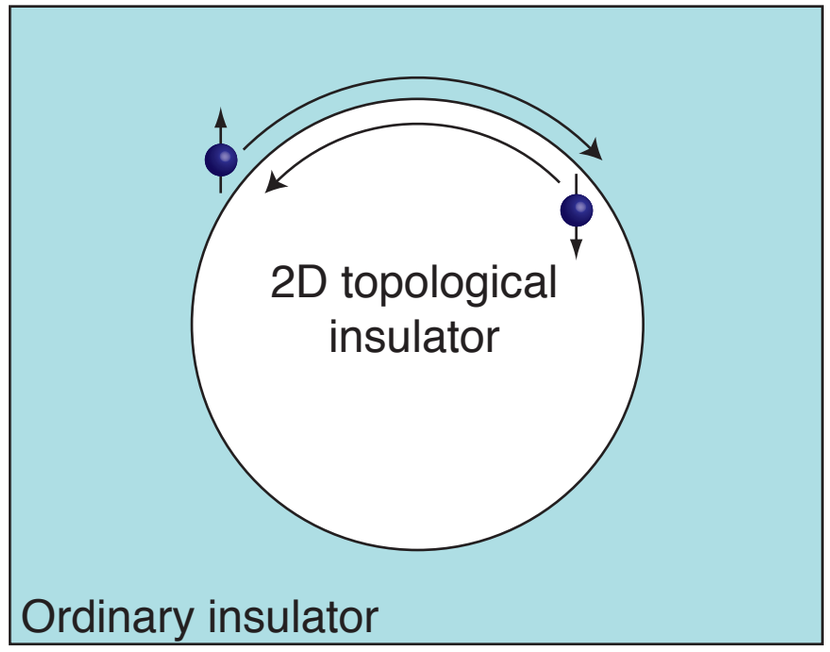


The "quantum spin Hall effect"

In this type of model, electron spin is conserved, and there can be a "spin current".

An applied electrical field causes oppositely directed Hall currents of up and down spins.

The charge current is zero, but the "spin current" is nonzero, and even quantized!



$$\mathcal{J}_j^i = \sigma_H^s \epsilon_{ijk} E_k$$

However...

1. In real solids there is no conserved direction of spin.

2. So in real solids, it was expected that "up" and "down" would always mix and the edge to disappear.

3. The theory of the above model state is just two copies of the IQHE.

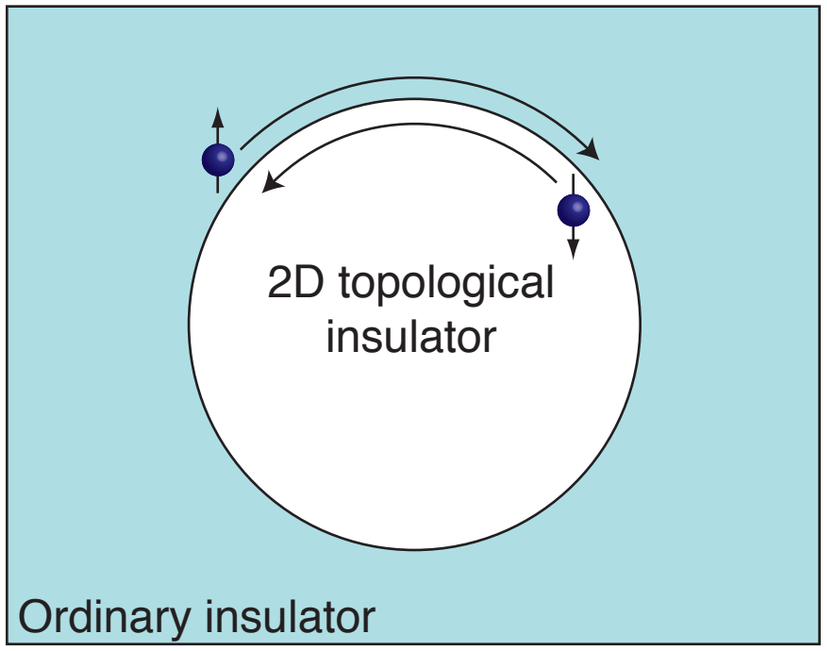
The 2D topological insulator

It was shown in 2005 (Kane and Mele) that, in real solids with all spins mixed and no "spin current", something of this physics does survive.

In a material with only spin-orbit, the "Chern number" mentioned before always vanishes.

Kane and Mele found a new topological invariant in time-reversal-invariant systems of fermions.

But it isn't an integer! It is a Chern *parity* ("odd" or "even"), or a "Z2 invariant".

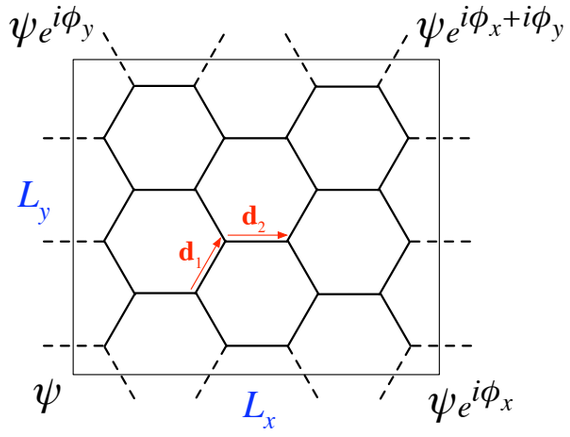


Systems in the "odd" class are "2D topological insulators"

1. Where does this "odd-even" effect come from?
2. What is the Berry phase expression of the invariant?
3. How can this edge be seen?

Example: Kane-Mele-Haldane model for graphene

The spin-independent part consists of a tight-binding term on the honeycomb lattice, plus possibly a sublattice staggering



$$H_0 = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + \lambda_v \sum_i \xi_i c^\dagger_{i\sigma} c_{i\sigma}$$

$$\xi_i = \begin{cases} 1 & \text{if i in } A \text{ sublattice} \\ -1 & \text{if i in } B \text{ sublattice} \end{cases}$$

The first term gives a semimetal with Dirac nodes (as in graphene).

The second term, which appears if the sublattices are inequivalent (e.g., BN), opens up a (spin-independent) gap.

When the Fermi level is in this gap, we have an ordinary band insulator.

Example: Kane-Mele-Haldane model for graphene

The spin-independent part consists of a tight-binding term on the honeycomb lattice, plus possibly a sublattice staggering

$$H_0 = -t \sum_{\langle ij \rangle} c_{i\sigma}^\dagger c_{j\sigma} + \lambda_v \sum_i \xi_i c_{i\sigma}^\dagger c_{i\sigma}$$

The spin-dependent part contains two SO couplings

$$H' = i\lambda_{SO} \sum_{\langle\langle ij \rangle\rangle} v_{ij} c_i^\dagger s^z c_j + i\lambda_R \sum_{\langle ij \rangle} c_i^\dagger (\mathbf{s} \times \hat{\mathbf{d}}_{ij})_z c_j$$

The first spin-orbit term is the key: it involves second-neighbor hopping (v_{ij} is ±1 depending on the sites) and Sz. It opens a gap in the bulk and acts as the desired "pseudofield" if large enough. $v_{ij} \propto (\mathbf{d_1} \times \mathbf{d_2})_z$

Claim: the system with an SO-induced gap is fundamentally different from the system with a sublattice gap: it is in a different phase.
It has gapless edge states for *any* edge (not just zigzag).

Example: Kane-Mele-Haldane model for graphene

$$H_0 = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + \lambda_v \sum_i \xi_i c^\dagger_{i\sigma} c_{i\sigma}$$

$$H' = i\lambda_{SO} \sum_{\langle\langle ij \rangle\rangle} v_{ij} c^\dagger_i s^z c_j + i\lambda_R \sum_{\langle ij \rangle} c^\dagger_i (\mathbf{s} \times \hat{\mathbf{d}}_{ij})_z c_j$$

Without Rashba term (second SO coupling), have two copies of Haldane's IQHE model. All physics is the same as IQHE physics.

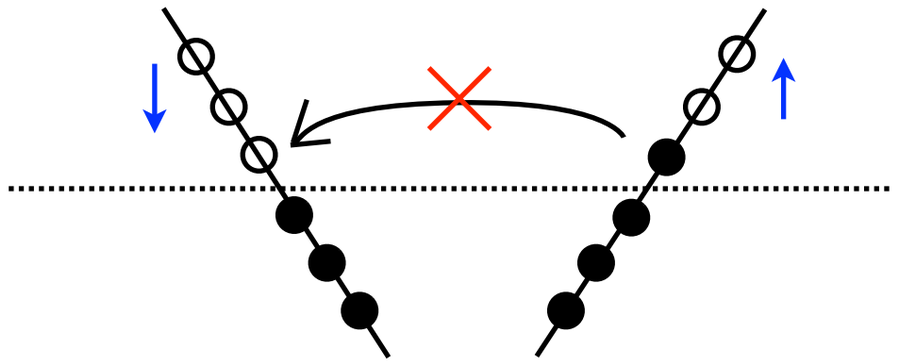
The Rashba term violates conservation of Sz--how does this change the phase? Why should it be stable once up and down spins mix?

The 2D topological insulator

1. Where does this "odd-even" effect come from?

In a time-reversal-invariant system of electrons, all energy eigenstates come in degenerate pairs.

The two states in a pair cannot be mixed by any T-invariant perturbation. (disorder)



So an edge with a single Kramers pair of modes is perturbatively stable (C. Xu-JEM, C. Wu et al., 2006).

The 2D topological insulator

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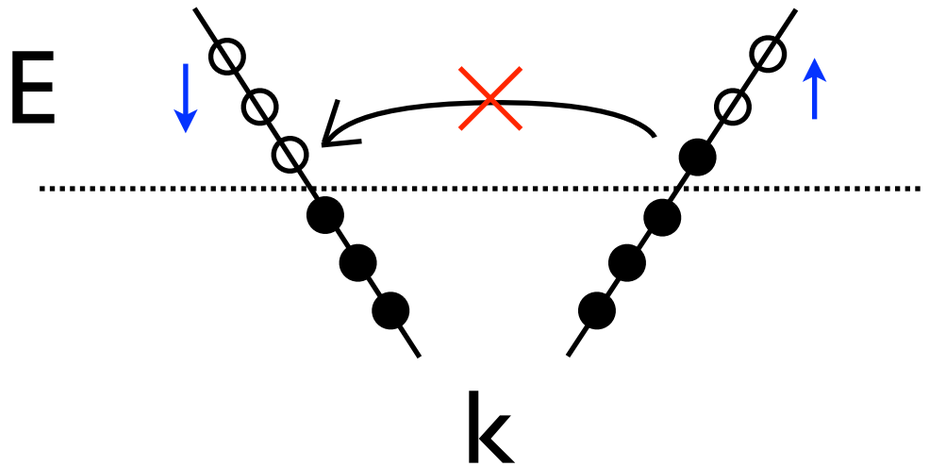
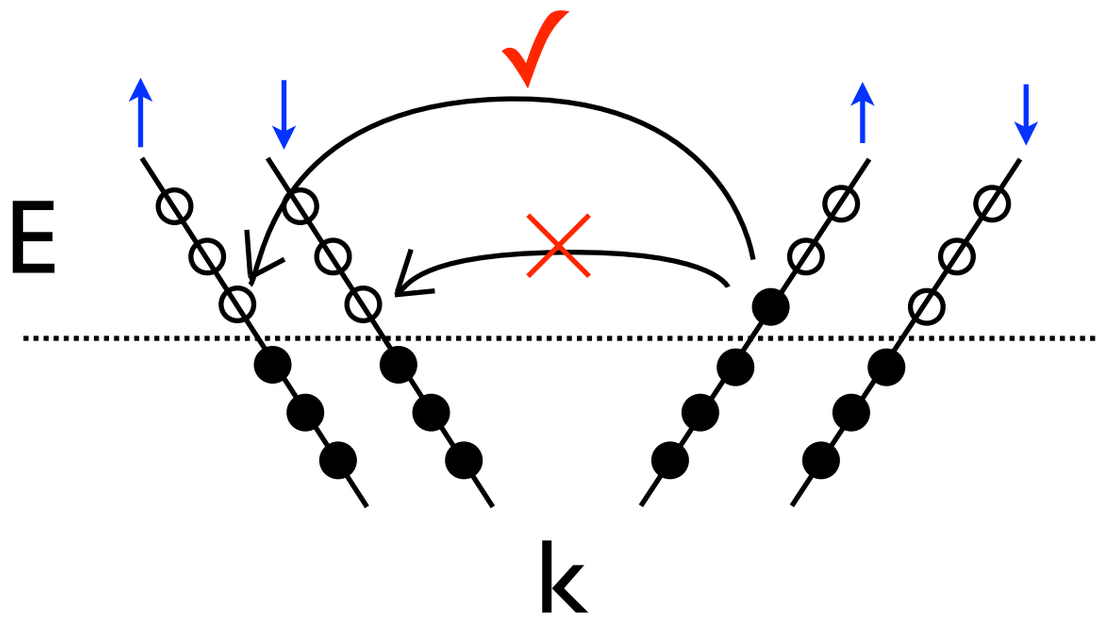


But this rule does not protect an ordinary quantum wire with 2 Kramers pairs:



The topological vs. ordinary distinction depends on time-reversal symmetry.

Experimental signatures

Key physics of the edges: robust to disorder and hence good *charge* conductors .

The topological insulator is therefore detectable by measuring the two-terminal conductance of a finite sample: should see maximal 1D conductance. $G = \frac{2e^2}{h}$

In other words, *spin transport does not have to be measured* to observe the phase.

Materials recently proposed: Bi, InSb, strained Sn (3d), HgTe (2d) (Bernevig, Hughes, and Zhang, *Science* (2006); *experiments by Molenkamp et al. (2007) see an edge, but G ~ 0.3 G_0)*

The 2D topological insulator

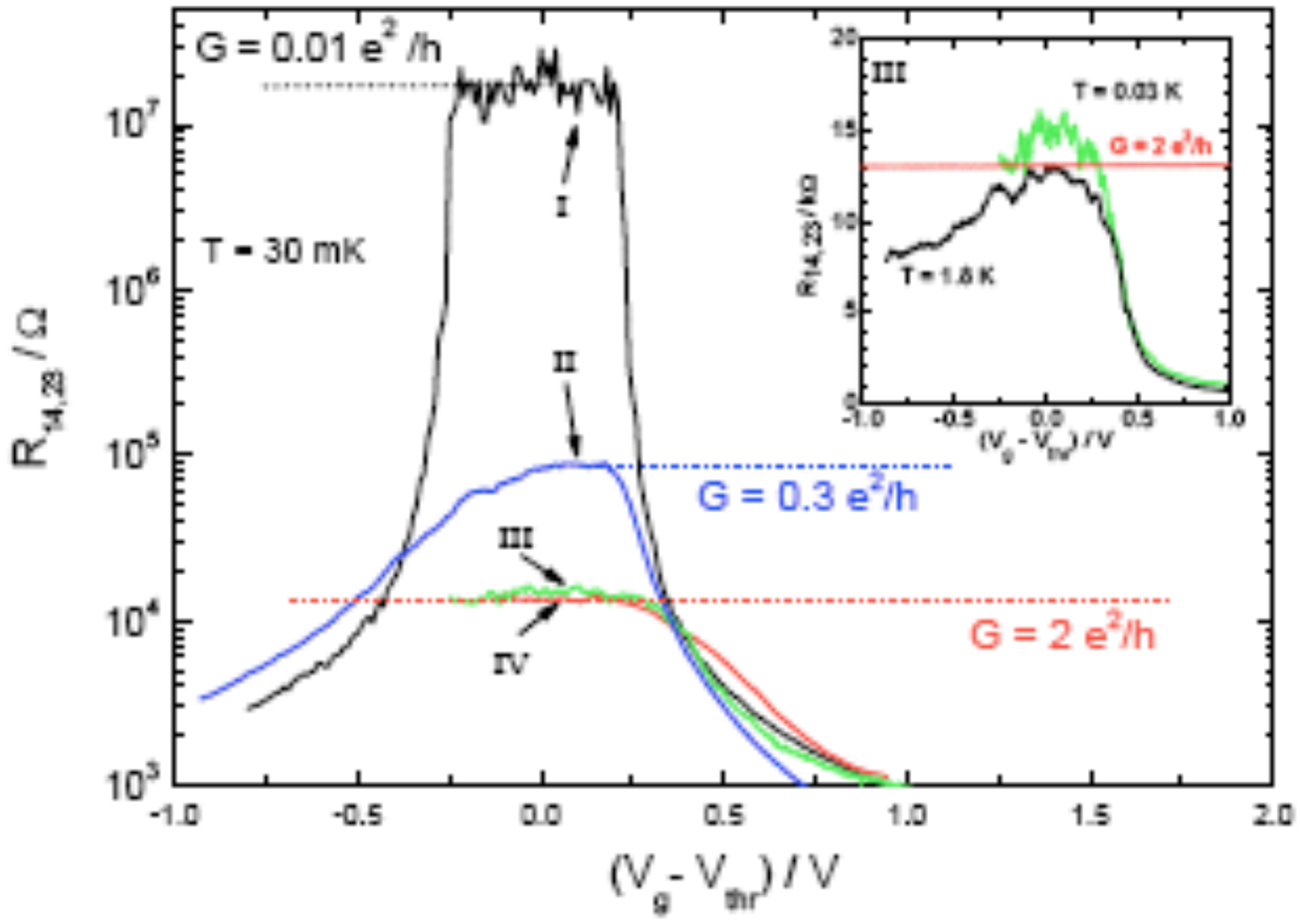
Key: the topological invariant predicts the "number of quantum wires".

While the wires are not one-way, so the Hall conductance is zero, they still contribute to the *ordinary* (two-terminal) conductance.

There should be a low-temperature *edge* conductance from one spin channel at each edge:

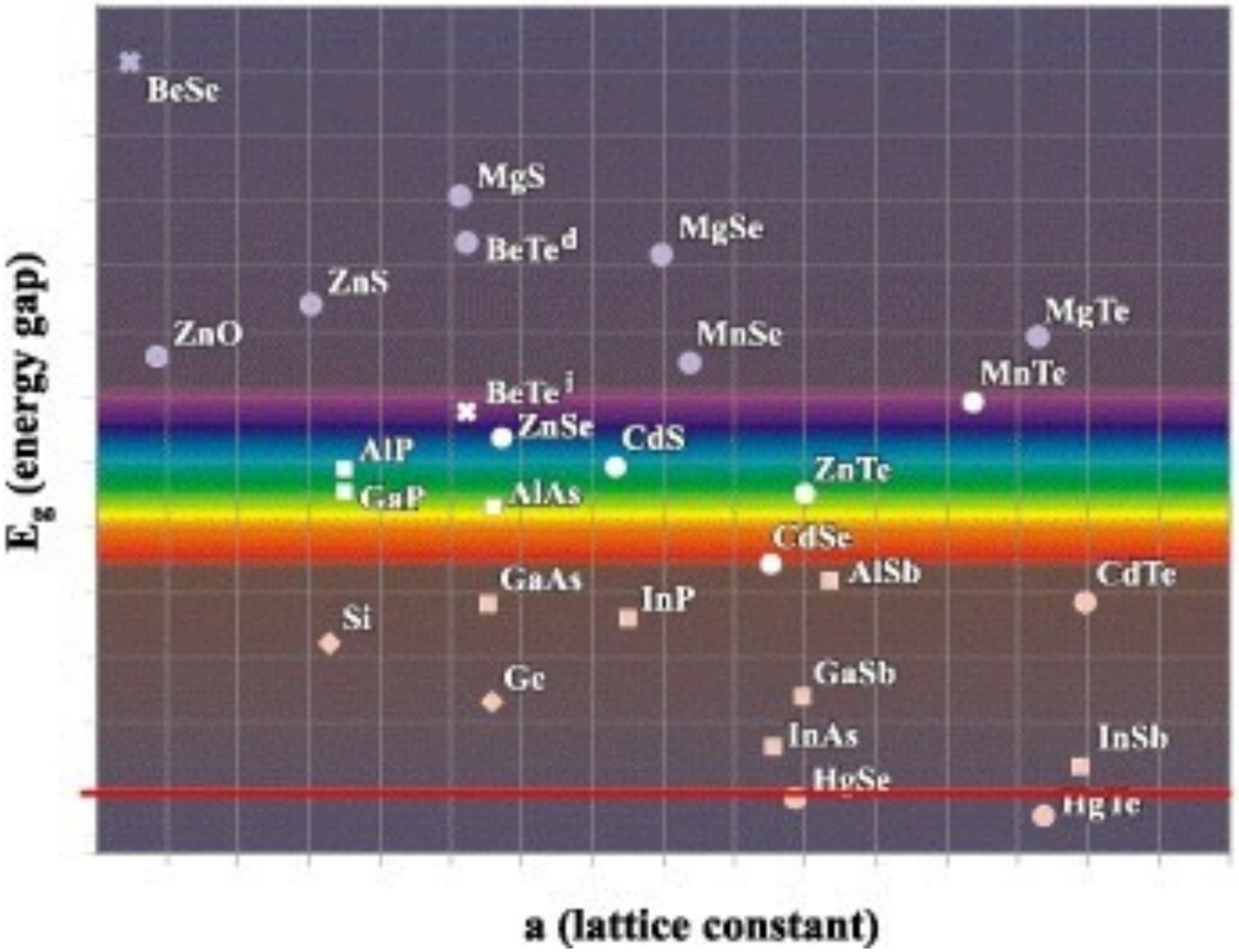
$$G = \frac{2e^2}{h}$$

König et al., *Science* (2007)



Laurens Molenkamp

This appears in (Hg,Cd)Te quantum wells as a quantum Hall-like plateau *in zero magnetic field.*



“Negative” bandgap of
HgTe = inverted band

Review of 3D facts

The 2D conclusion is that band insulators come in two classes:
ordinary insulators (with an even number of edge modes, generally 0)
"topological insulators" (with an odd number of Kramers pairs of edge modes, generally 1).

What about 3D? The only 3D IQHE states are essentially layered versions of 2D states:
Mathematically, there are three Chern integers:

Cxy (for *xy* planes in the 3D Brillouin torus), *Cyz*, *Cxz*

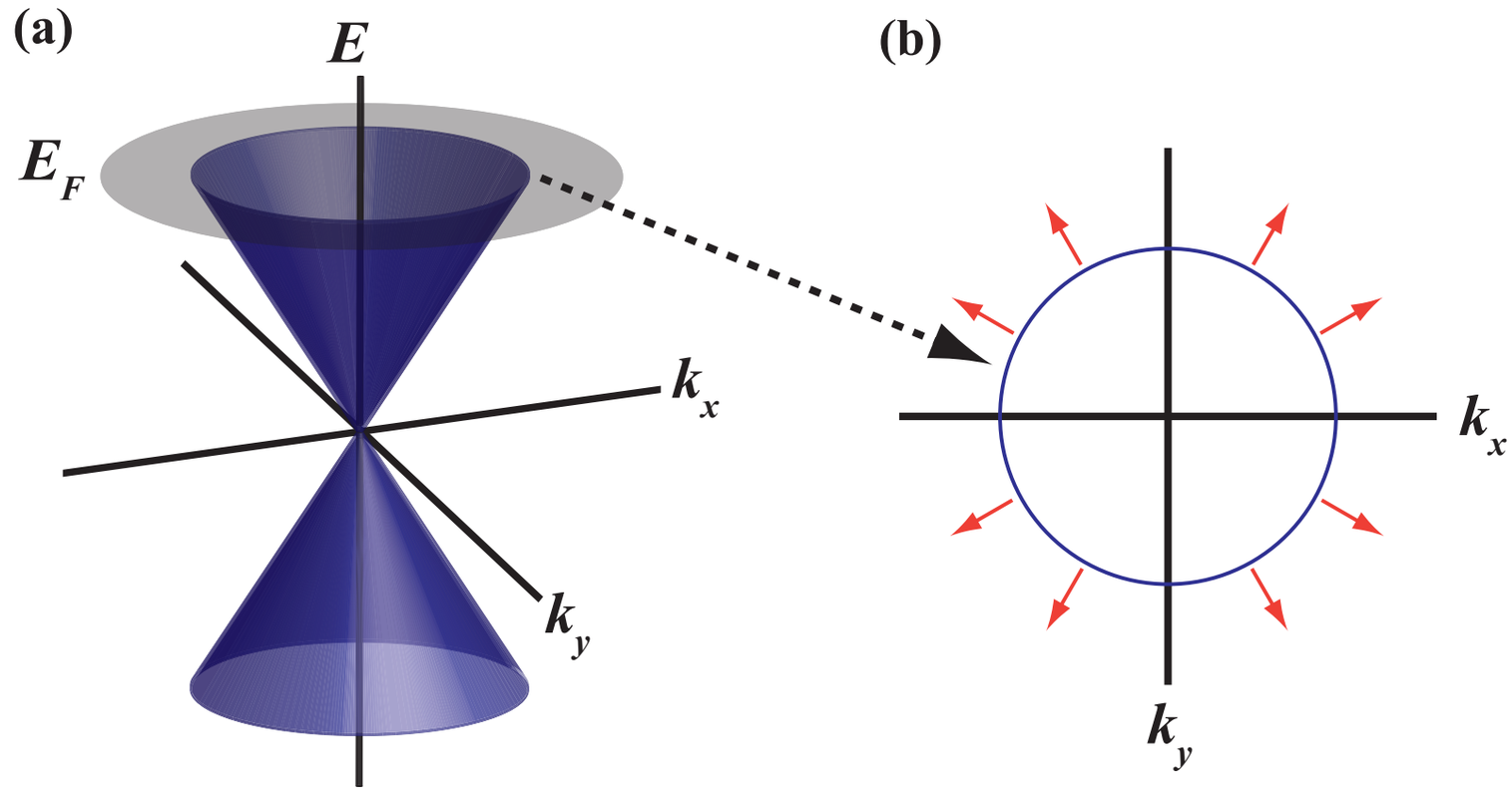
There are similar layered versions of the topological insulator, but these are not very stable; intuitively, adding parities from different layers is not as stable as adding integers.

However, there is an unexpected 3D topological insulator state that does not have any simple quantum Hall analogue. For example, it cannot be realized in any model where up and down spins do not mix!

General description of invariant from JEM and L. Balents, PRB RC 2007.
The connection to physical consequences in inversion-symmetric case (proposal of BiSb, Dirac surface state): Fu, Kane, Mele, PRL 2007. See also R. Roy, arXiv.

Topological insulators in 3D

1. This fourth invariant gives a robust 3D "strong topological insulator" whose metallic surface state in the simplest case is a single "Dirac fermion" (Fu-Kane-Mele, 2007)



2. Some fairly common 3D materials might be topological insulators! (Fu-Kane, 2007)

Claim:
Certain insulators will *always* have metallic surfaces with strongly spin-dependent structure

How can we look at the metallic surface state of a 3D material to test this prediction?

What is quantized in a 3D TI? Electrodynamics in insulators…

We know that the constants ε and μ in Maxwell's equations can be modified inside an ordinary insulator.

Particle physicists in the 1980s considered what happens if a 3D insulator creates a new term ("axion electrodynamics", Wilczek 1987)

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

This term is a total derivative, unlike other magnetoelectric couplings.
It is also "topological" by power-counting.

The angle θ is periodic and odd under T.

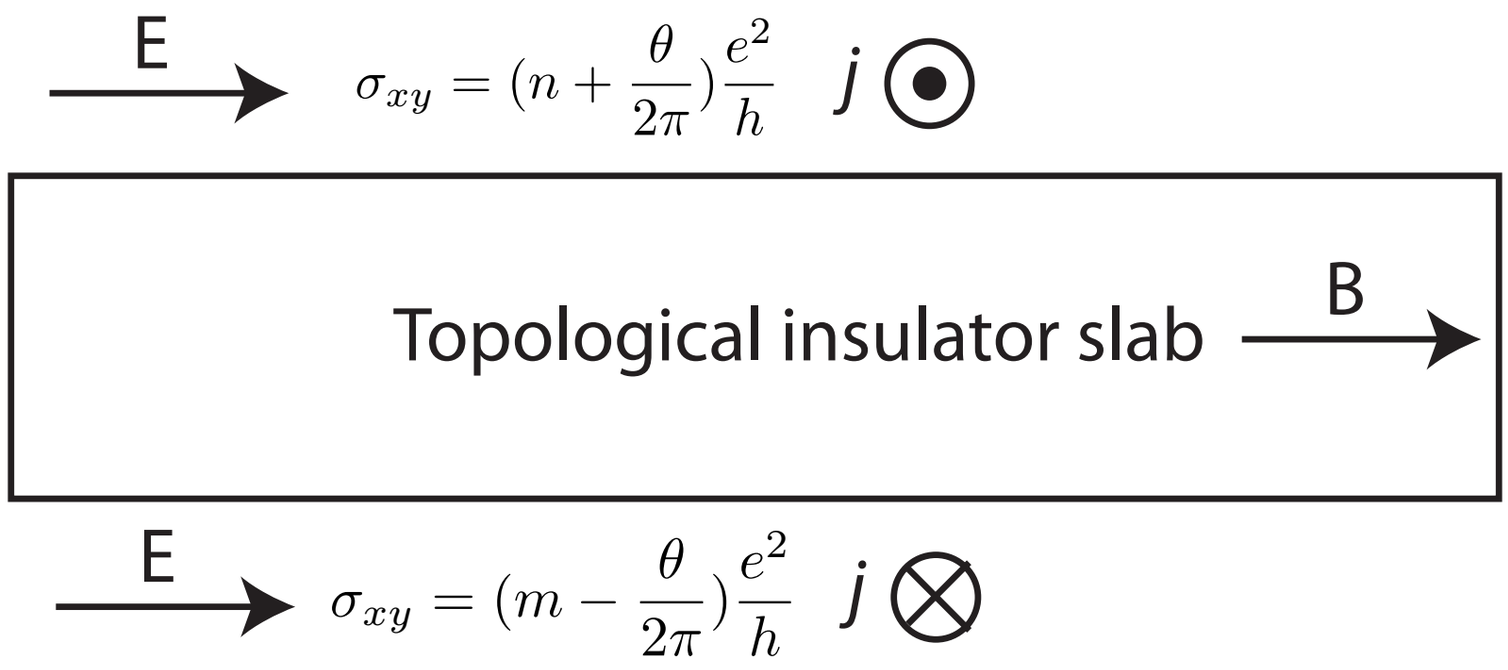
A T-invariant insulator can have *two* possible values: 0 or π.

Axion E&M

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

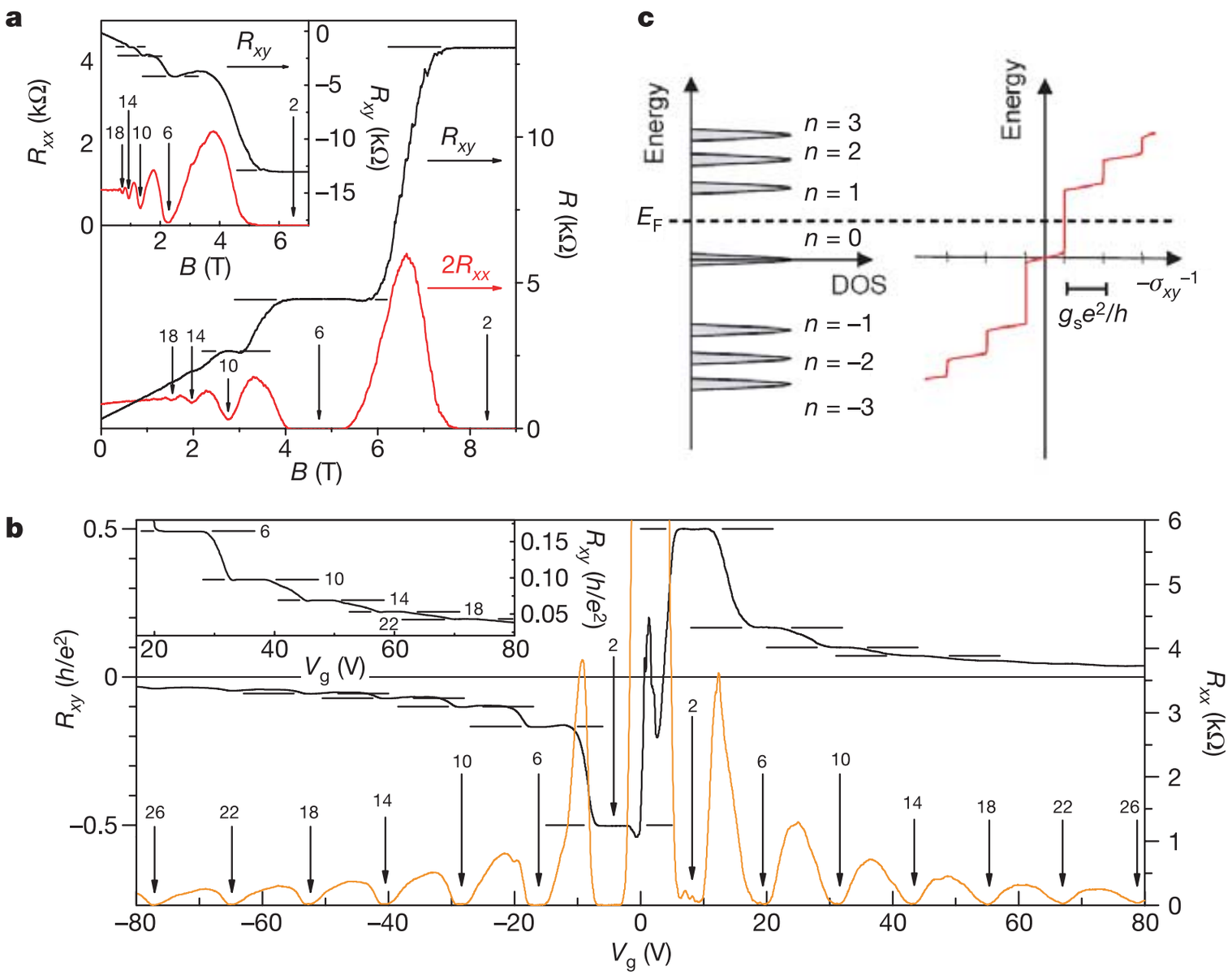
This explains a number of properties of the 3D topological insulator when its surfaces become gapped by breaking T-invariance:

Magnetoelectric effect:
applying B generates polarization P, applying E generates magnetization M)



Graphene QHE

The connection is that a single Dirac fermion contributes a *half-integer QHE*: this is seen directly in graphene if we recall the extra fourfold degeneracy.
Data shown below from Y. Zhang et al. (Kim group, Columbia)



Berry phase

Why do we write the phase in this form?
Does it depend on the choice of reference wavefunctions?

$$\phi = \oint \mathcal{A} \cdot d\mathbf{k}, \quad \mathcal{A} = \langle \psi_k | -i\nabla_k | \psi_k \rangle$$

If the ground state is non-degenerate, then the only freedom in the choice of reference functions is a local phase:

$$\psi_k \rightarrow e^{i\chi(k)} \psi_k$$

Under this change, the "Berry connection" *A* changes by a gradient,

$$\mathcal{A} \rightarrow \mathcal{A} + \nabla_k \chi$$

just like the vector potential in electrodynamics.

Note: If more than 1 degenerate state, the connection is *non-Abelian*:

$$\mathcal{A}^{\alpha\beta} = \langle \psi_k^\alpha | -i\nabla_k | \psi_k^\beta \rangle$$

So loop integrals of *A* will be gauge-invariant,
as will the *curl* of *A*, which we call the "Berry curvature".

$$\mathcal{F} = \nabla \times \mathcal{A}$$

Topological response

Idea of "axion electrodynamics in insulators"

there is a "topological" part of the magnetoelectric term

$$\Delta\mathcal{L}_{EM} = \frac{\theta e^2}{2\pi h}\mathbf{E}\cdot\mathbf{B} = \frac{\theta e^2}{16\pi h}\epsilon^{\alpha\beta\gamma\delta}F_{\alpha\beta}F_{\gamma\delta}.$$

that is measured by the orbital magnetoelectric polarizability

$$\theta\frac{e^2}{2\pi h} = \frac{\partial M}{\partial E} = \frac{\partial}{\partial E}\frac{\partial}{\partial B}H = \frac{\partial P}{\partial B}$$

and computed by integrating the "Chern-Simons form" of the Berry phase

$$\theta = -\frac{1}{4\pi}\int_{\mathrm{BZ}} d^3k\ \epsilon_{ijk}\,\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k] \qquad (2)$$

(Qi, Hughes, Zhang, 2008; Essin, JEM, Vanderbilt 2009)

This integral is quantized only in T-invariant insulators, but contributes in all insulators.
Has just the right gauge ambiguity under "large gauge transformations".

Warmup for metals: polarization in insulators

Electrical polarization: "simple" Berry phase effect in solids (took about 50 years to understand how to calculate polarization of a solid from its unit cell)

Sum the integral of *A* over bands: in one spatial dimension,

$$P = \sum_v e \int \frac{dq}{2\pi} \langle u_v(q)| - i\partial_q |u_v(q)\rangle$$

Intuitive idea: think about the momentum-position commutation relation

$$A = \langle u_k| - i\nabla_k |u_k\rangle \approx \langle r \rangle$$

More seriously: relate changes in *P* to currents moving through the unit cell.

Polarization isn't quantized in general; it is just a simple physical observable determined by the Berry phase. Note that there is an ambiguity *ne*.

Broader reason, in hindsight: E(k), the band structure, is k-symmetric with time-reversal, even with broken inversion. Anything related to inversion-breaking has to come from the wavefunction, and at low energy, *usually* from the Berry phase.

What about metals?

Claim: the biggest omission in Ashcroft and Mermin (standard solids text) is a term in the semiclassical equations of motion, the (Karplus-Luttinger) ***anomalous velocity***.

$$\frac{dx^a}{dt} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial k_a} + \mathcal{F}_n^{ab}(\mathbf{k})\frac{dk_b}{dt}.$$

a "magnetic field" in momentum space.

The anomalous velocity results from changes in the electron distribution *within the unit cell*: the Berry phase is connected to *the electron spatial location.*

Example I: the intrinsic anomalous Hall effect in itinerant magnets (Fe, e.g.)

Example II: helicity-dependent photocurrents in optically active materials

Example III: optical rotation in gyrotropic/chiral materials with T symmetry

Can we get anything quantized/interesting in a metal?

Anomalous Hall effect (100+ years)

From Nagaosa et al., RMP 2011

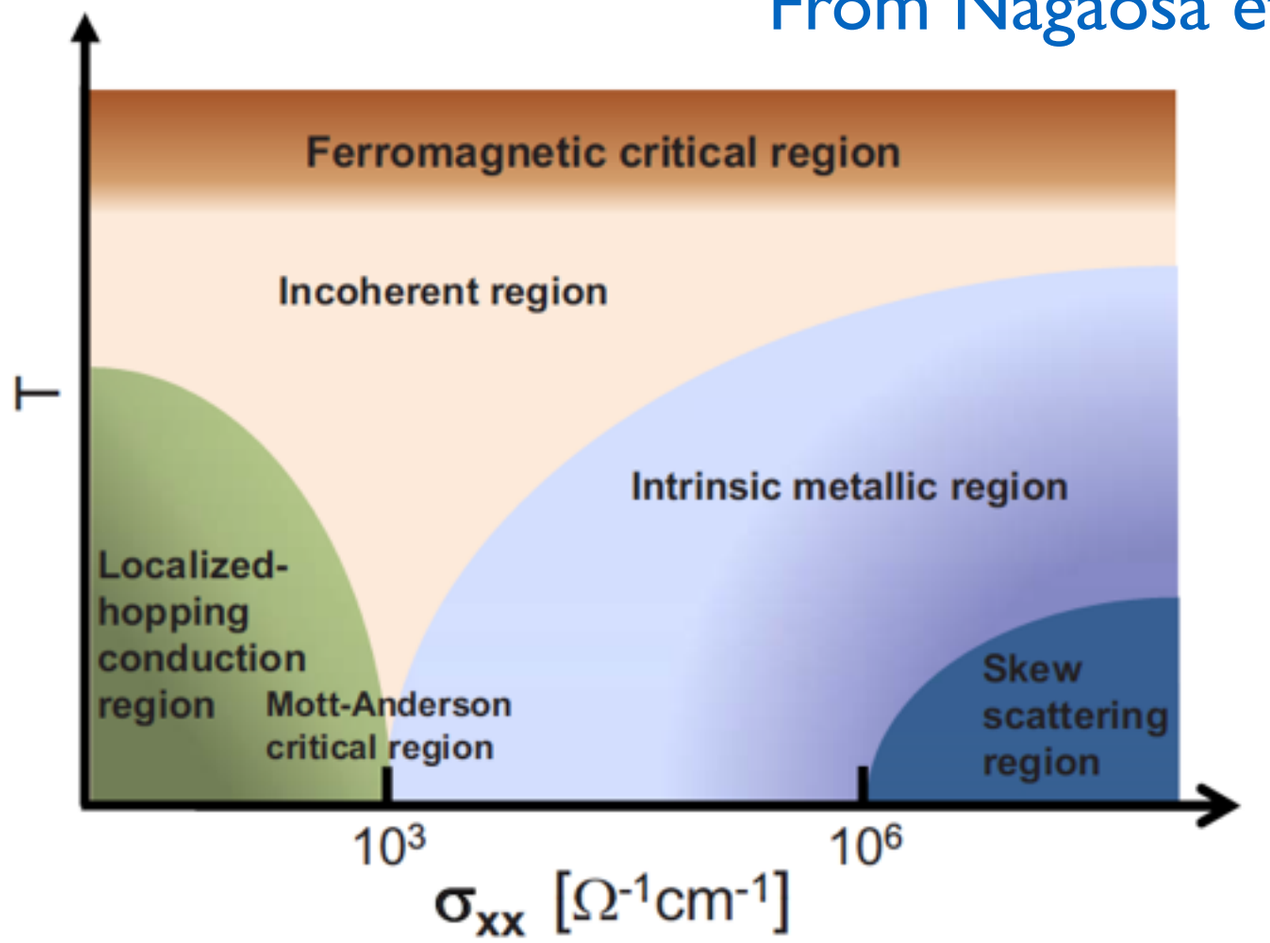


FIG. 47. (Color online) A speculative and schematic phase diagram for the anomalous Hall effect in the plane of the diagonal conductivity σ_{xx} and the temperature T.

Sundaram and Niu, 1999

$$\sigma_{xy} = \frac{e^2}{h} \int_{\mathrm{FS}} d^2k \, \frac{F}{2\pi} + \text{extrinsic}$$

Remark on metallic piezoelectric and piezoelectromagnetic effects

D. Varjas, A. G. Grushin, R. Ilan, JEM, PRL 2016

The polarization integral is not well-defined in a metal, and we know that static polarization is not observable.

Changes in polarization introduce currents, and it turns out that these currents still exist in a metal: this dynamical piezoelectricity involves Berry curvature in a mixed parameter and momentum space.

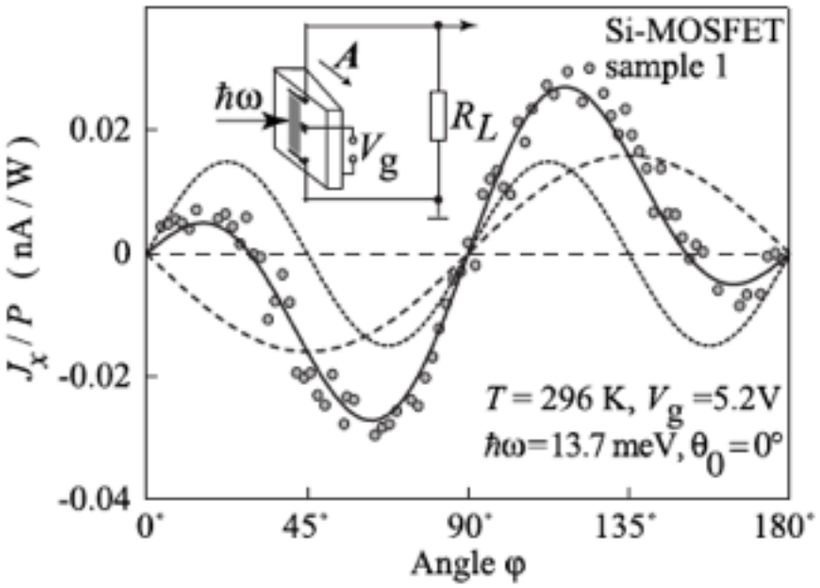
Also works for magnetoelectric effect: like P, the Chern-Simons integral

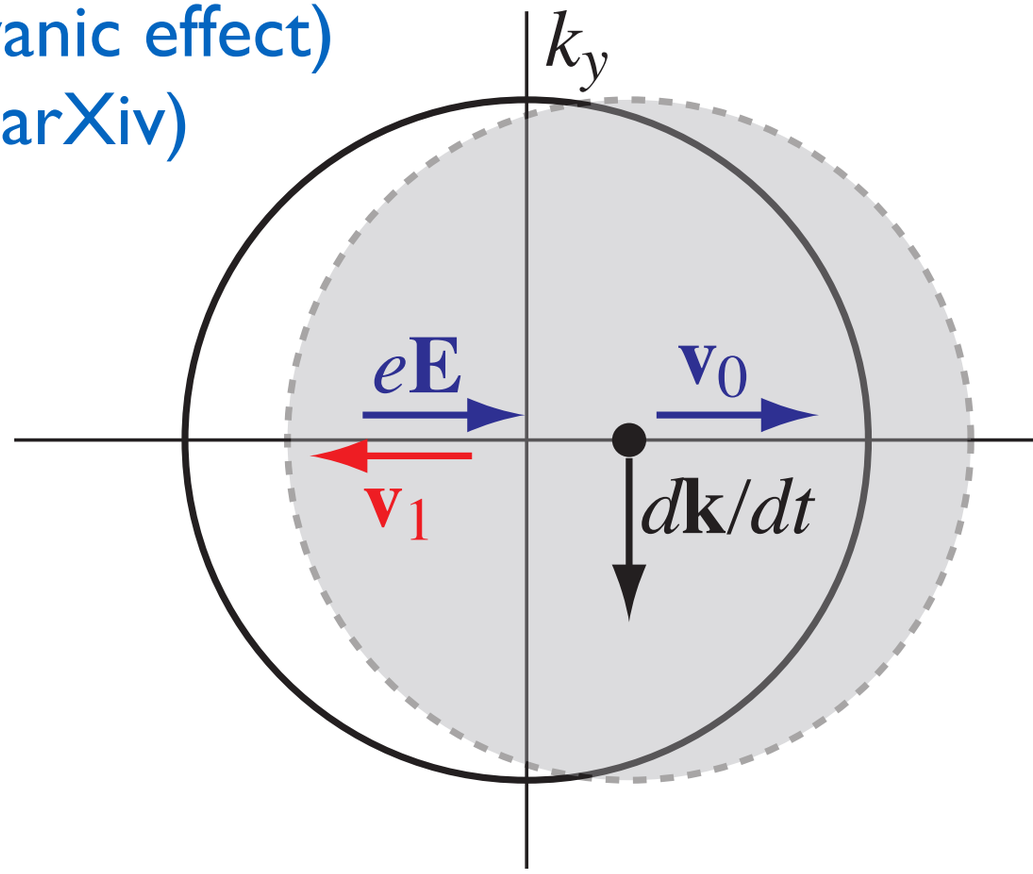
$$\theta = -\frac{1}{4\pi}\int_{\mathrm{BZ}} d^3k\ \epsilon_{ijk}\,\mathrm{Tr}[\mathcal{A}_i\partial_j\mathcal{A}_k - i\frac{2}{3}\mathcal{A}_i\mathcal{A}_j\mathcal{A}_k]$$

is related to (*second)* Chern form F ^ F in 4D (3 momenta + 1 parameter). What if we don't change the material in time?

Two other "mystery" effects in metals:

I. Nonlinear optics: CPGE (circular photogalvanic effect)
(JEM and J. Orenstein, PRL 2010; Deyo et al., arXiv)





Currents are switched by the sense of circular polarization, as previously observed in a series of experiments by S.D. Ganichev et al. We believe this is entirely or almost entirely a Berry-phase effect.

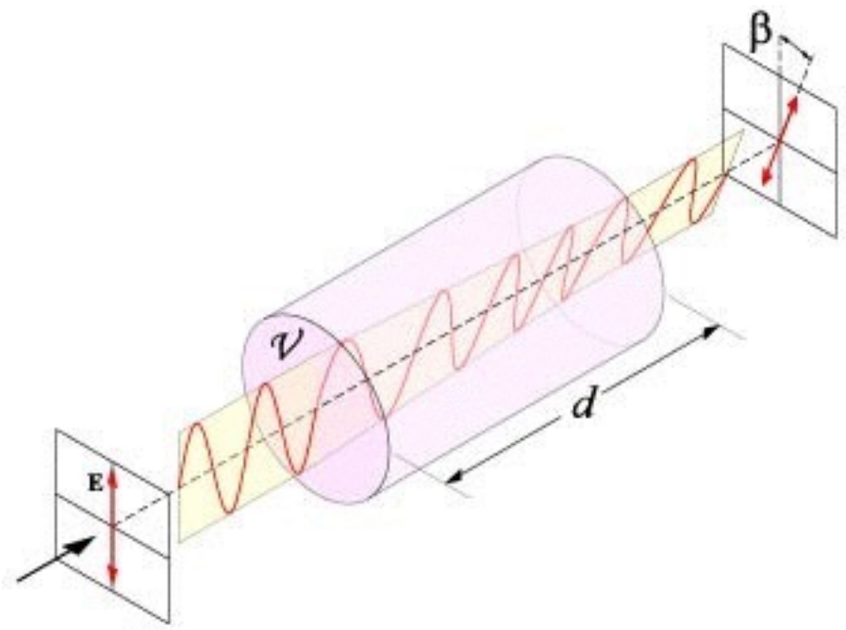
Can we understand this effect beyond semiclassics?

2. **Linear optics:** Chiral materials (and sugar water!) can show optical rotation in transmission, the Faraday effect, even without time-reversal breaking. (J. Orenstein and JEM, PRB 2012, motivated by cuprates)

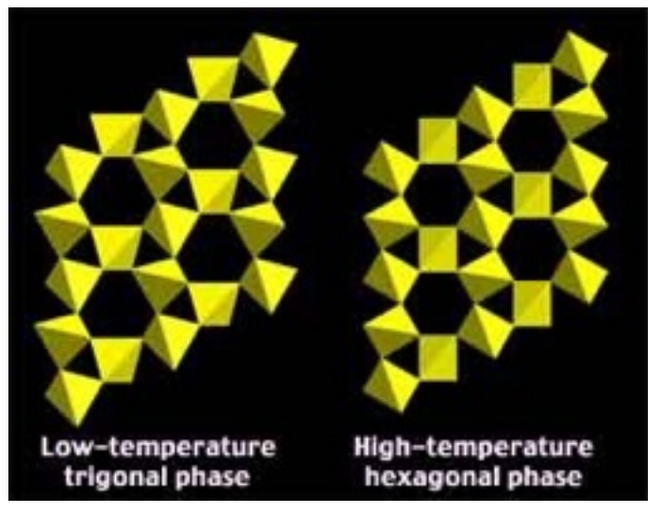
1. Why they do not show Kerr effect (rotation in *reflection*, rather than transmission). (Zhong, Orenstein, Moore, PRL 2015)

2. **Surprise: this problem is intimately connected to the "chiral magnetic effect" proposed in Weyl semimetals,** although as sometimes described that effect is actually *zero* for topological reasons. (Zhong, Moore, Souza, PRL 2016)

Natural optical activity
or optical gyrotropy:
like a Faraday effect in a non-magnetic material



Occurs in materials with low spatial symmetry (intrinsic handedness), such as quartz or selenium



And now for something seemingly different…

3D Dirac and Weyl metals

Can we find 3D materials that are massless semimetals like graphene?

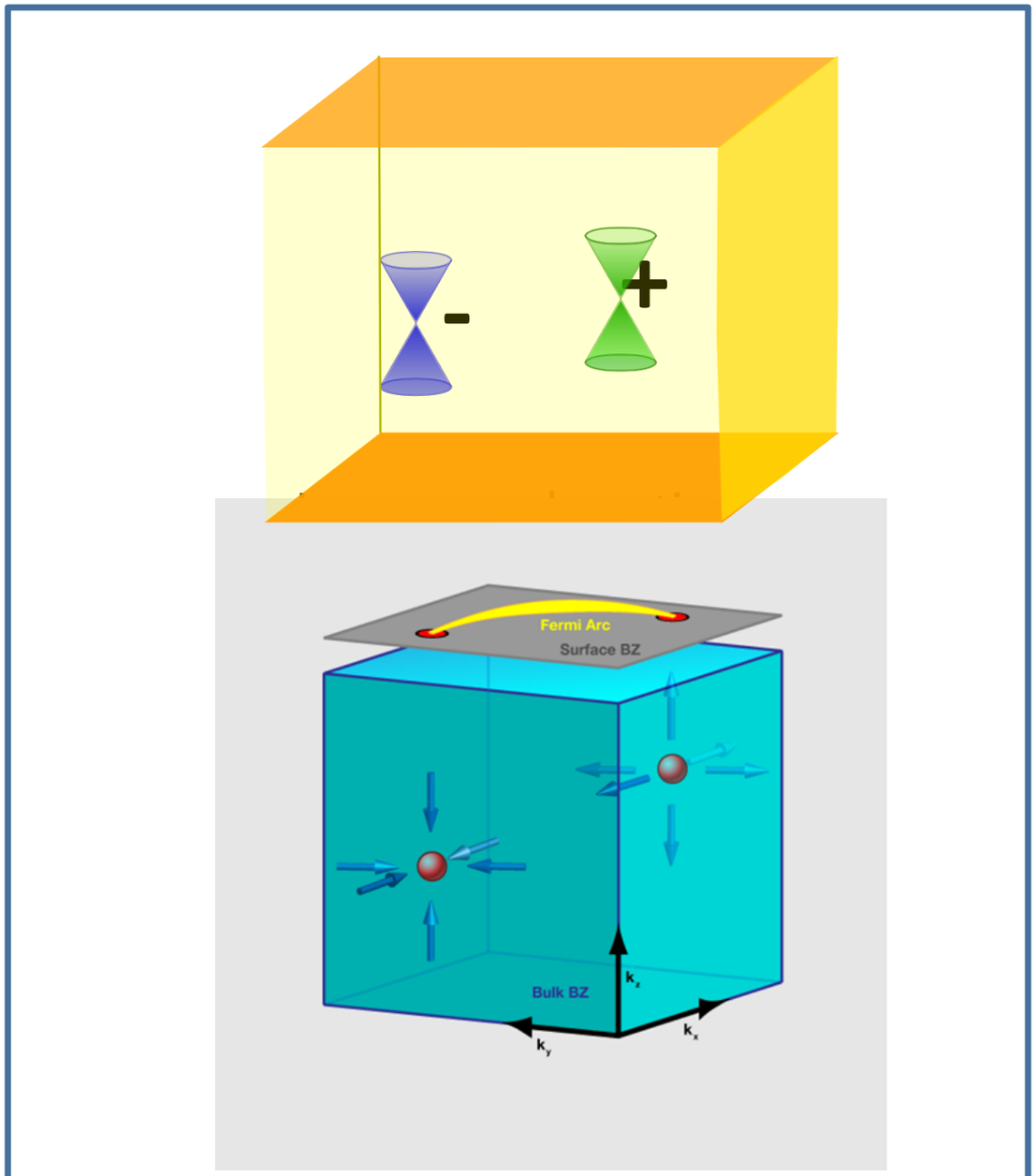
Yes! There are two ways to generalize graphene's massless "Dirac electrons" to 3D.

In the early days of quantum mechanics, two alternatives were put forward that are "half" of Dirac's celebrated equation for the electron. Majorana found one….

Dirac: 4 by 4 matrix equation describes the electron and the positron
4-band semimetals found in Na3Bi, Cd2As3, 2013

Weyl: 2 by 2 matrix equation describes a particle with only one "handedness"
Does not seem to exist in the standard model; neutrinos were a possibility
2-band semimetals found in "inversion-breaking" TaAs, 2014-2015

Weyl semimetal
old theory idea (Herring, …);
trick is finding at Fermi surface



A Weyl point has topological charge: the Chern number from Berry flux through a small sphere around it is an integer. (Volovik; Murakami, 2008)

There are surface Fermi arcs connecting Weyl points (Wan, Turner, Vishwanath, Savrasov, 2010).

What are consequences of this topological property?

Materials and Experiments: Princeton/IOP, Princeton/ Northeastern, Osaka, many others.

Active questions: what is a unique response of Weyl semimetal?
What is “chiral anomaly” in CM?
How is it related to chiral magnetic effect?

Chiral anomaly: current conservation is anomalous for a single Weyl fermion coupled to a U(1) gauge field:

Chiral anomaly: $$\partial^\mu J^W_\mu = \frac{g^2 C}{16\pi^2}\mathbf{E}\cdot\mathbf{B}$$ ***nonlinear; complicated***

CME idea: The total charge of Weyl points in a crystal is 0.

But they can occur at different energies. So *maybe* the (static) energy difference can replace the electric field, giving a **scalar** contribution to

Chiral magnetic effect: $$J_i = -\alpha^{\rm gme}_{ij} B_j$$ ***linear!***

Outline of CME and GME

Many papers have been written on the possibility of a “chiral magnetic effect” in Weyl semimetals and other materials, also of the form

$$J_i = -\alpha_{ij}^{\mathrm{gme}} B_j$$

This would be related to the chiral anomaly in particle physics, and to the Berry curvature around Weyl points.

Consensus now that it is zero at equilibrium (as “Bloch’s other theorem” says).

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This would be related to the chiral anomaly in particle physics, and to the Berry curvature around Weyl points.

Consensus now that it is zero at equilibrium (as "Bloch's other theorem" says). It can be nonzero in transport (non-commutation of q->0 and omega->0 limits) or at nonzero frequency (gyrotropy!), but in its simplest form does not involve the Berry phase but something else: (Zhong, JEM, Souza, PRL 2016; see also Ma-Pesin PRB 2016)

$$\alpha_{ij}^{\mathrm{gme}} = -\frac{1}{(2\pi)^2}\frac{e}{h}\sum_{na}\int_{S_{na}} dS\, \hat{v}_{\mathrm{F},i} m_{n,j}(\mathbf{k}_f)\,.$$

The *only* linear response CME is actually optical rotation! ("gyrotropic magnetic effect") **It comes from orbital moment of Bloch electrons.**

Key identity in a simple, “topological” example: **the uniform chiral magnetic effect**

Apply a constant magnetic field **B** = B **z** to a solid. Solve the Berry-Boltzmann equation.

The currents in the **x** and **y** directions vanish trivially.

The current along **z** has “ordinary” and “anomalous” parts

$$j_z^{(o)} = -(e^2 B/\hbar) \int \frac{f^0 d^3k}{(2\pi)^3} \Omega_z v_z$$

$$j_z^{(a)} = -\frac{e^2 B}{\hbar} \int \frac{f^0 d^3k}{(2\pi)^3} (\Omega_x v_x + \Omega_y v_y).$$

Note for experts: the ordinary part comes from the phase-space volume correction (Xiao et al.). These cancel since

$$\langle \Omega_x(\mathbf{k}) v_x(\mathbf{k}) + \Omega_y(\mathbf{k}) v_y(\mathbf{k}) + \Omega_z(\mathbf{k}) v_z(\mathbf{k}) \rangle = 0$$

In a Weyl semimetal, the trace around one Weyl point is quantized to (Chern number) times (chemical potential), which gives a robust derivation of the “chiral magnetic effect”.

Vanishing of static CME via "tracelessness"

Berry mechanism leads to constraint on gyrotropic tensor

Proof is based on the fact that Ω is a curl of "Berry connection." (Hence div $\Omega = 0$).

$$\int_{occ} d^3k \boldsymbol{\Omega}(\mathbf{k}) \cdot \mathbf{v}(\mathbf{k})$$
$$= \int_{occ} d^3k \boldsymbol{\Omega}(\mathbf{k}) \cdot \nabla\varepsilon(\mathbf{k})$$
$$= \int_{occ} d^3k \nabla \cdot [\varepsilon(\mathbf{k})\boldsymbol{\Omega}(\mathbf{k})]$$
$$= \varepsilon_F \int_{FS} d^2k \hat{\mathbf{n}} \cdot \boldsymbol{\Omega}(\mathbf{k})$$
$$= 0$$

But it was thought that different Weyl points at different energies could make this nonzero. Actually not: for a set of "monopoles" at different energies, the integral is a constant since

$$\frac{d}{dE}\left[\sum_i (E - E_i) m_i\right] = 0$$

by Nielsen-Ninomiya,

and the constant is actually zero by boundary conditions at the bottom of the band.

Supplemental Material for "Gyrotropic magnetic effect and the orbital moment on the Fermi surface"

DERIVATION OF THE EXPRESSION FOR CME AND GME USING KUBO FORMULA

The Kubo formula of the linear current response to a vector potential $\mathbf{A}e^{i\mathbf{q}\cdot\mathbf{r}-i\omega t}$ is[S36]

$$J_i(\omega) = -e^2 \int [d^3k] \sum_{n,m} \frac{f(\epsilon_{n,\mathbf{k}-\mathbf{q}/2}) - f(\epsilon_{m,\mathbf{k}+\mathbf{q}/2})}{\epsilon_{n,\mathbf{k}-\mathbf{q}/2} - \epsilon_{m,\mathbf{k}+\mathbf{q}/2} + \omega} \langle n_{\mathbf{k}-\mathbf{q}/2}|\partial_i H|m_{\mathbf{k}+\mathbf{q}/2}\rangle\langle m_{\mathbf{k}+\mathbf{q}/2}|\partial_j H|n_{\mathbf{k}-\mathbf{q}/2}\rangle A_j(\omega,\mathbf{q}) \tag{24}$$

where we have set $\hbar = 1$ and in the following we would use the expression of the group velocity $\mathbf{v}_n = \nabla_{\mathbf{k}}\epsilon_n$. We are going to expand Eq. (24) and get the term which is zeroth order in ω and first order in q. As been discussed[S12] the result is different whether we set $\omega \to 0$ first or not. The two different results are related to CME and GME respectively.

For CME we set $\omega \to 0$ first and the contribution from interband ($n \neq m$) is

$$\begin{aligned} -e^2 \sum_{n,m\neq n} \int [d^3k] \Big\{ &(\frac{\partial f}{\partial \epsilon_n} v_{nl} + \frac{\partial f}{\partial \epsilon_m} v_{ml}) \langle n|\partial_i m\rangle\langle m|\partial_j n\rangle (\epsilon_n - \epsilon_m) - (f(\epsilon_n) - f(\epsilon_m))\,(v_{nl} + v_{ml}) \langle n|\partial_i m\rangle\langle m|\partial_j n\rangle \\ &+ \frac{(f(\epsilon_n) - f(\epsilon_m))}{\epsilon_n - \epsilon_m} [-\langle \partial_l n|\partial_i H|m\rangle\langle m|\partial_j H|n\rangle + \langle n|\partial_i H|\partial_l m\rangle\langle m|\partial_j H|n\rangle \\ &+ \langle n|\partial_i H|m\rangle\langle \partial_l m|\partial_j H|n\rangle - \langle n|\partial_i H|m\rangle\langle m|\partial_j H|\partial_l n\rangle] \Big\} \frac{q_l}{2} . \end{aligned} \tag{25}$$

The contribution from intraband ($n = m$) is

$$-e^2 \sum_n \int [d^3k] \frac{\partial f}{\partial \epsilon_n} [-\langle \partial_l n|\partial_i H|n\rangle v_{nj} + \langle n|\partial_i H|\partial_l n\rangle v_{nj} + \langle \partial_l n|\partial_j H|n\rangle v_{ni} - \langle n|\partial_j H|\partial_l n\rangle v_{ni}] \frac{q_l}{2} . \tag{26}$$

Combining them together and with some simplification we get

$$-e^2 \sum_{n,m} iq_l \int [d^3k] \,\mathrm{Im} \left[\frac{\partial f}{\partial \epsilon_n} v_{nl} \langle n|\partial_i m\rangle\langle m|\partial_j n\rangle - \frac{\partial f}{\partial \epsilon_n} v_{nj} \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle + \frac{\partial f}{\partial \epsilon_n} v_{ni} \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle \right] (\epsilon_n - \epsilon_m) \tag{27}$$

$$+ - e^2 \sum_{n,m} iq_l \int [d^3k]\, f(\epsilon_n) \{ \mathrm{Im}[-\langle \partial_l n|\partial_i H|m\rangle\langle m|\partial_j n\rangle + \langle n|\partial_i H|\partial_l m\rangle\langle m|\partial_j n\rangle] - (i \leftrightarrow j)\} \tag{28}$$

$$+ - e^2 \sum_{n,m} iq_l \int [d^3k]\, f(\epsilon_n)\, (v_{nl} + v_{ml})\, \mathrm{Im}\langle \partial_i n|m\rangle\langle m|\partial_j n\rangle . \tag{29}$$

Integrate by parts for Eq. (27) we have

$$\begin{aligned} -e^2 \sum_{n,m} iq_l \int [d^3k]\, f(\epsilon_n)\, \mathrm{Im}\{\, &[(\epsilon_n - \epsilon_m)(\langle \partial_i n|\partial_l m\rangle\langle m|\partial_j n\rangle + \langle \partial_l n|\partial_j m\rangle\langle m|\partial_i n\rangle + \langle \partial_l n|m\rangle\langle \partial_j m|\partial_i n\rangle) - (i \leftrightarrow j)] \\ &+ \langle \partial_i n|m\rangle\langle m|\partial_j n\rangle (v_{nl} - v_{ml}) + \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle (v_{ni} - v_{mi}) - \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle (v_{nj} - v_{mj})\} \end{aligned} \tag{30}$$

and adding Eq. (28) Eq. (29) together

$$\begin{aligned} -e^2 \sum_{n,m} iq_l \int [d^3k]\, f(\epsilon_n)\, \mathrm{Im}\,\{ &\langle \partial_i n|m\rangle\langle m|\partial_j n\rangle (v_{nl} + v_{ml}) + \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle (v_{ni} + v_{mi}) - \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle (v_{nj} + v_{mj}) \\ &+ [(\epsilon_n - \epsilon_m)(\langle n|\partial_i m\rangle\langle \partial_l m|\partial_j n\rangle + \langle \partial_l n|\partial_i m\rangle\langle m|\partial_j n\rangle + \langle \partial_l n|m\rangle\langle \partial_i m|\partial jn\rangle) - (i \leftrightarrow j)]\} . \end{aligned} \tag{31}$$

Adding Eq. (30) and Eq. (31) together we get

$$-e^2 \sum_{n,m} 2iq_l \int [d^3k]\, f(\epsilon_n)\, \mathrm{Im}[\langle \partial_i n|m\rangle\langle m|\partial_j n\rangle v_{nl} + \langle \partial_l n|m\rangle\langle m|\partial_i n\rangle v_{ni} - \langle \partial_l n|m\rangle\langle m|\partial_j n\rangle v_{nj}] \tag{32}$$

There **is** a nonzero linear effect, though: “transport limit”

Recall that the q->0 and w->0 limits do not commute in an E field:

q->0 first (“uniform”) gives electrical *conductivity*

w->0 first (“static”) gives electrical *compressibility.*

Something similar happens for a magnetic field, and we can calculate in the transport limit.

But a magnetic field at nonzero omega necessarily involves an electrical field as well: the uniform or “transport limit” of the CME is really describing the *low-frequency response to an electromagnetic wave*.

We (e.g., Landau-Lifshitz) know a lot about the symmetry properties of such responses. What is their microscopic origin? Indeed it comes from the B field part of the wave, which couples to the *orbital moment of Bloch electrons.*

Orbital moment of Bloch electrons

Something that is not always taught (at least by me) in solid state courses is that a Bloch electron has an orbital moment

$$m_{n,j} = \frac{e}{2\hbar}\varepsilon_{jln}\mathrm{Im}\ \langle\partial_l n|H-\epsilon_n|\partial_n n\rangle\ .$$

This modifies the group velocity that appears in the semiclassical equations:

$$v_{\mathrm{group}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon_k = \frac{1}{\hbar}\nabla_{\mathbf{k}}(\epsilon_{\mathbf{k}} + \mathbf{m}_{n\mathbf{k}}\cdot\mathbf{B}).$$

In other words, all the previous pieces found by us and other people come together in the full quantum Kubo formula in a very simple Fermi-surface expression that is pretty easy to calculate in actual materials.

The linear response CME is actually optical rotation! ("gyrotropic magnetic effect") Orbital moment should also modify other things.

Summary of CME and GME

Many papers have been written on the possibility of a "chiral magnetic effect" in Weyl semimetals and other materials, also of the form

$$J_i = -\alpha_{ij}^{\mathrm{gme}} B_j$$

The only linear response effect is not a scalar and is properly regarded as a "gyrotropic magnetic effect", easily measured in optical rotation

$$\alpha_{ij}^{\mathrm{gme}} = -\frac{1}{(2\pi)^2}\frac{e}{h}\sum_{na}\int_{S_{na}} dS\, \hat{v}_{\mathrm{F},i} m_{n,j}(\mathbf{k}_f)\,.$$

Beyond linear response there are other effects, including those more like the chiral magnetic effect in particle physics (cf. Son-Spivak). So we would like to compute responses to higher order in EM fields and look for topological pieces.

Additional effects in metals

Now we turn to nonlinear effects in metals.

The point of the preceding section is that the linear response to A(q,omega) is not particularly quantized: for two Weyl nodes split in energy by *E*, the result is

$$\mathbf{j} = \frac{e^2}{3h^2}(\epsilon_R - \epsilon_L)\mathbf{B}.$$

This is scalar, like the proposed CME, but with a different magnitude. More to the point, it depends on the energy difference between nodes, so isn't quantized.

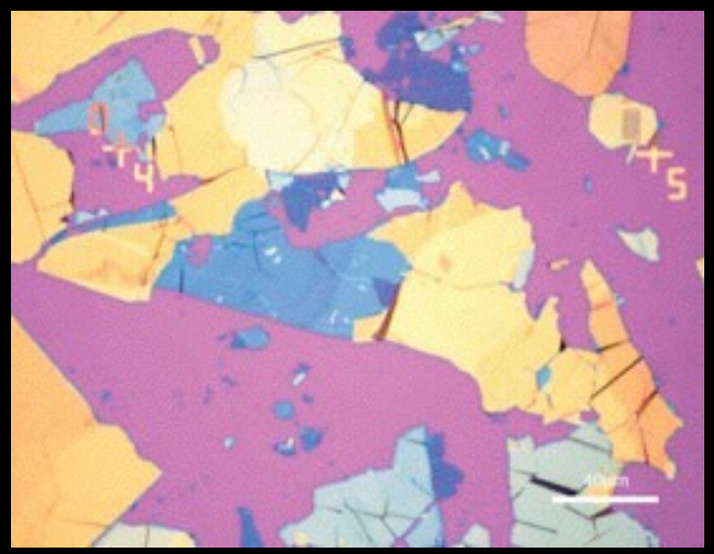
Can we ever see quantized responses in metals? Yes, and even in optics…

Optical quantization in semimetals

Properties of the "semi-metallic" electrons in graphene:
effective mass is *zero*

one layer of graphene attenuates 2.3% of light

(π times the fine structure constant) $\frac{\pi e^2}{hc}$

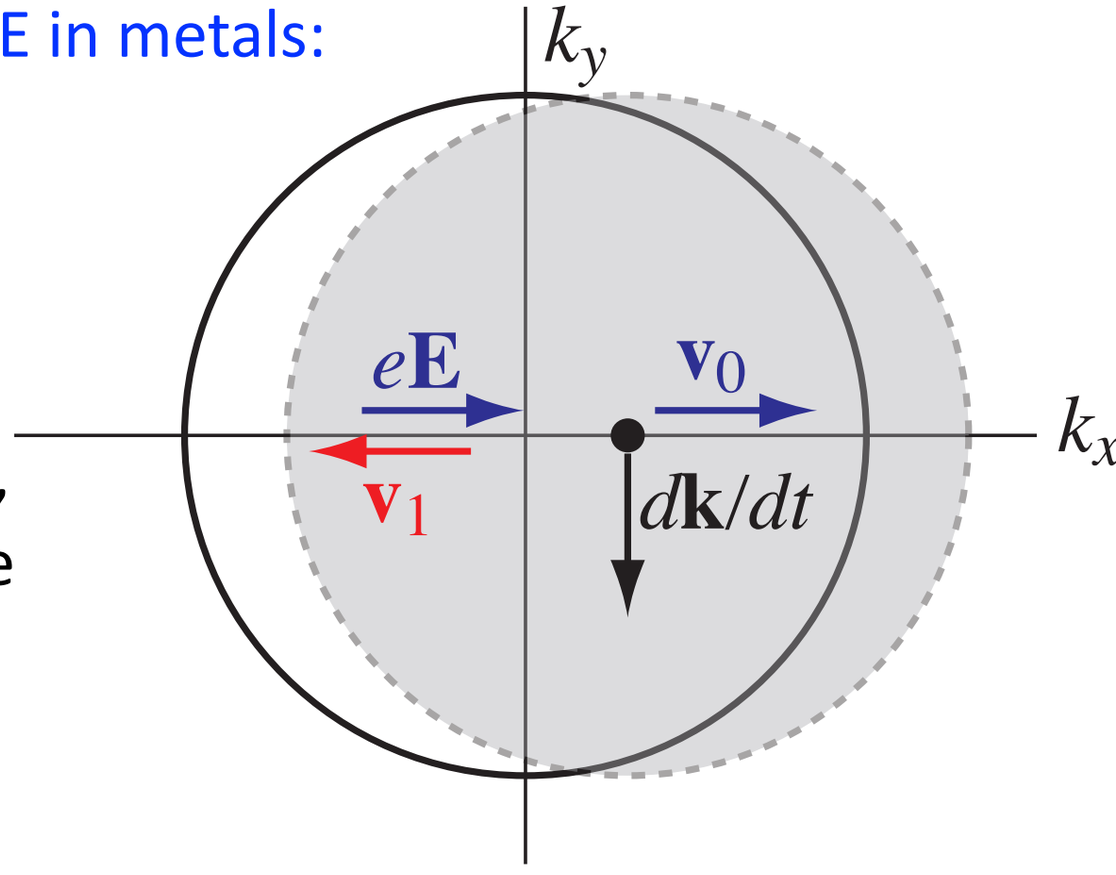


A quantized effect in Weyl semimetals

We believe that the “circular photogalvanic effect”, which made a quick appearance earlier, is effectively quantized in energy-split Weyl semimetals.
(F. de Juan, A. Grushin, T. Morimoto, JEM, Nat. Comm., to appear)

First, recall the semiclassical Berry phase CPGE in metals:

$$\frac{dx^a}{dt} = \frac{1}{\hbar}\frac{\partial \epsilon_n(\mathbf{k})}{\partial k_a} + \mathcal{F}_n^{ab}(\mathbf{k})\frac{dk_b}{dt}.$$

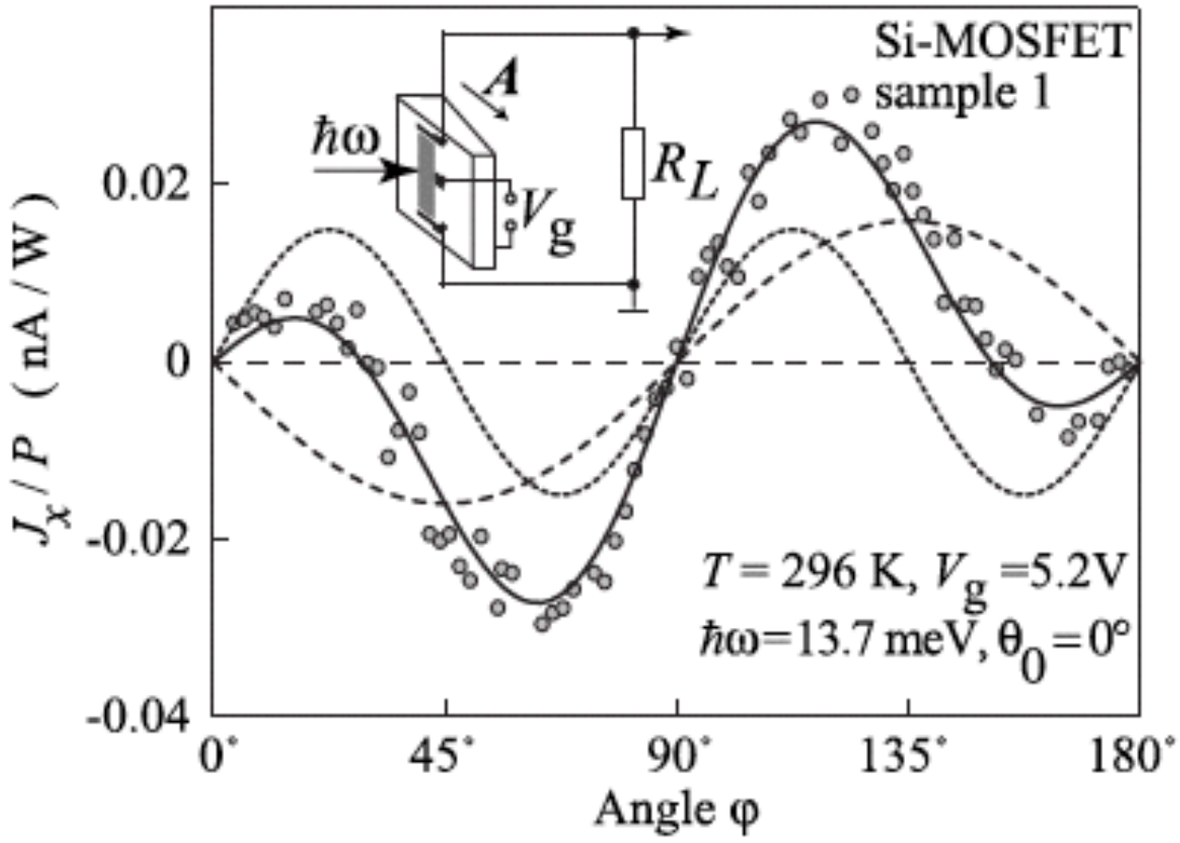


Around a period of the circular incident wave, the ordinary velocity averages to zero, but the anomalous velocity does not, if F is linear in k (requires low symmetry).

Quantum derivation and generalizations:
T. Morimoto, S. Zhong, J. Orenstein, JEM, PRB 2016
(uses Morimoto-Nagaosa Floquet approach)

Non-quantized CPGE

Measure the part of photocurrent that changes sign when the incident polarization changes from right circular to left circular:

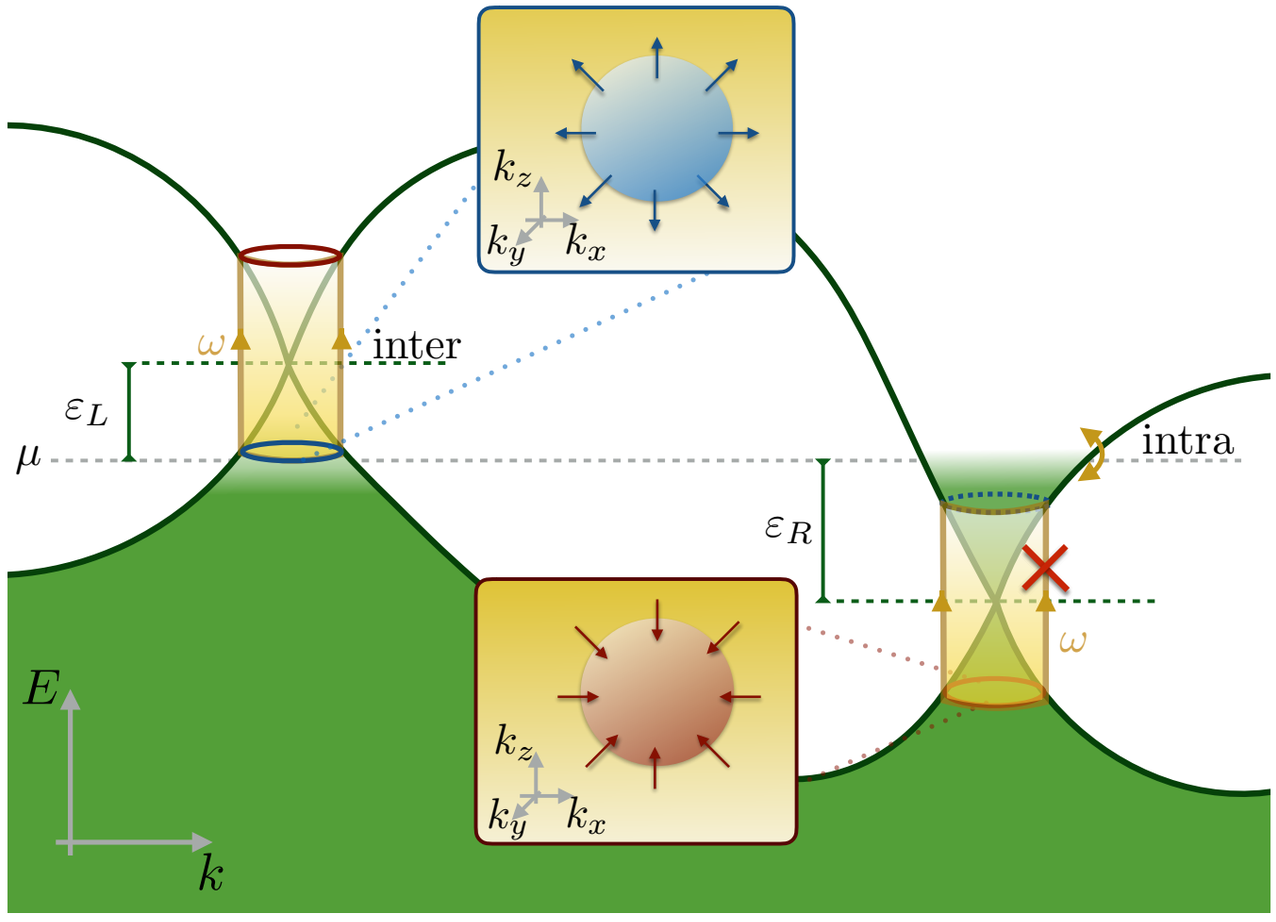


The Berry-phase theory (JEM and Orenstein, PRL 2010; Fu-Sodemann, PRB 2015) may explain many experiments from the group of Ganichev (Regensburg) on a variety of low-symmetry quantum wells.

Strength is determined by degree of inversion breaking. Effect is pretty weak (pA photocurrents for W/cm^2 incident intensity).

Quantized CPGE

The quantum calculation of CPGE from a Weyl node gives a surprising result: there is a large quantized value, over a broad range of frequencies, that will dominate metallic contributions from other parts of the Brillouin zone.



(F. de Juan, A. Grushin, T. Morimoto, JEM, arXiv:1611.05887)

What is the “quantum”?

Because this is a nonlinear effect, the quantum is different from the standard e^2/h. Instead, it is e^3/(h^2 c):

$$\frac{1}{2}\left[\frac{dj_{\circlearrowright}}{dt} - \frac{dj_{\circlearrowleft}}{dt}\right] = \frac{2\pi e^3}{h^2 c\epsilon_0} I C_n,$$

Here I is the incident intensity and C is the Chern number of a Weyl node.

Some quick notes: what’s quantized is the “rate of current injection”. The DC photocurrent will then involve a non-universal relaxation time factor, that would have to be extracted by other means.

Not limited to linearized approx. Stable to disorder if omega tau > 1.

However, not yet understood as an anomaly or something else that would be manifestly stable to interactions.

The circular photogalvanic effect in mirror-free 3D-Weyl semimetals is quantized

$$\frac{dj_i}{dt} = \beta_{ij}(\omega)\left(\mathbf{E}\times\mathbf{E}^*\right)_j$$

$\mathrm{Tr}[\beta]$

Two band model

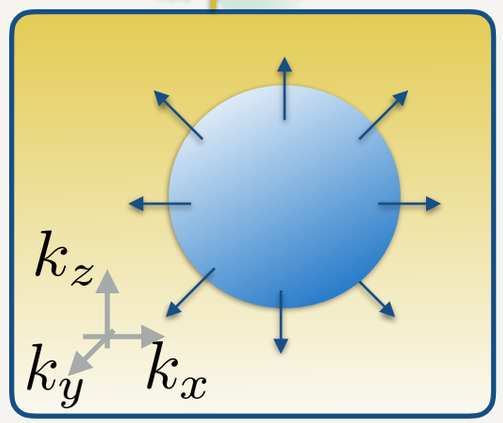
Current is related to excitation rate:

$$\frac{d\Delta j_i}{dt} = e\int \frac{d^3k}{(2\pi)^3}(v_1^i - v_0^i)\Delta\Gamma_{\mathbf{k}}(\omega)$$

Fermi's golden rule

$$\pi\frac{e^2}{2h}|E|^2\Omega^i_{\mathbf{k}}\delta(\varepsilon_1-\varepsilon_0-\hbar\omega)$$

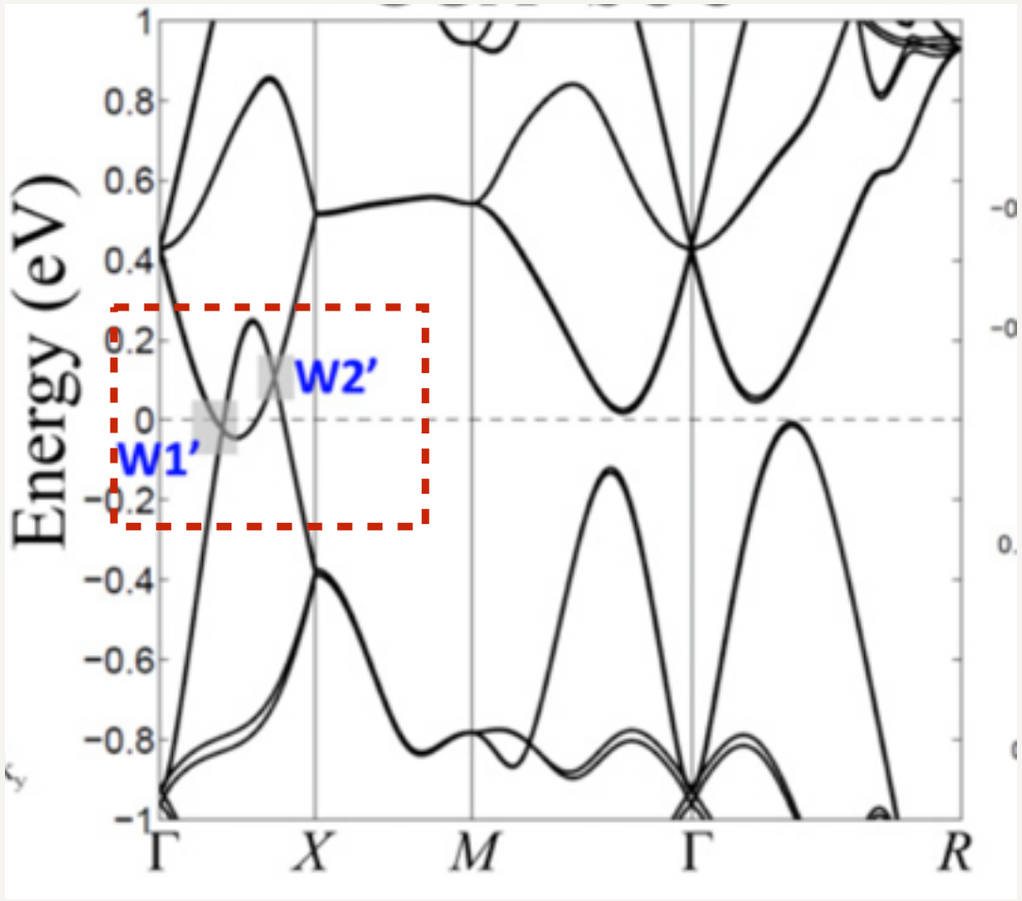
$$\mathrm{Tr}[\beta] = i\frac{e^3}{2h^2}\oint_S d\mathbf{S}\cdot\mathbf{\Omega_1} = i\pi\frac{e^3}{h^2}C$$



from A. Grushin

Mirror free Weyls have nodes at different energies

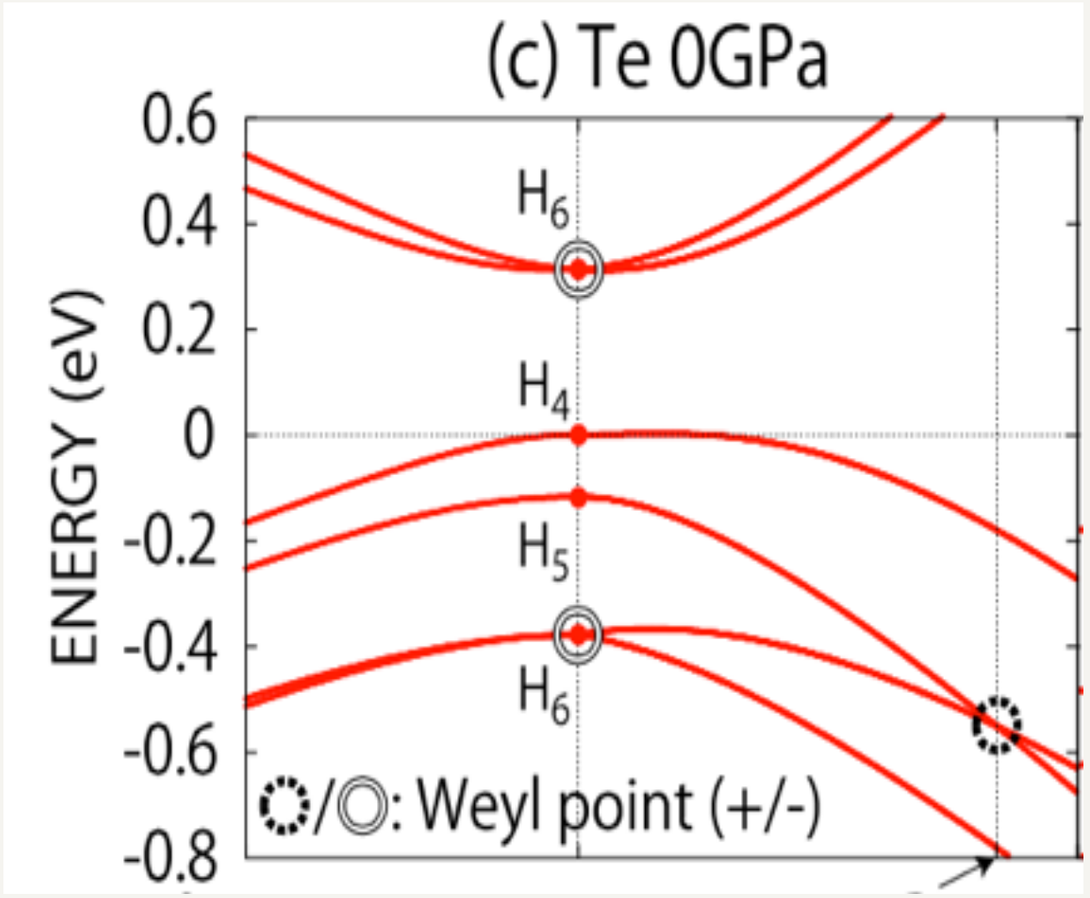
Chiral Weyls



$SrSi_2$

Huang, et al. PNAS **113** 1180 (2015)

Kramers Weyls



(strained) Tellurium

Hirayama, PRL **114**, 206401 (2015)
Chang et. al arXiv: 1611.07925

from A. Grushin

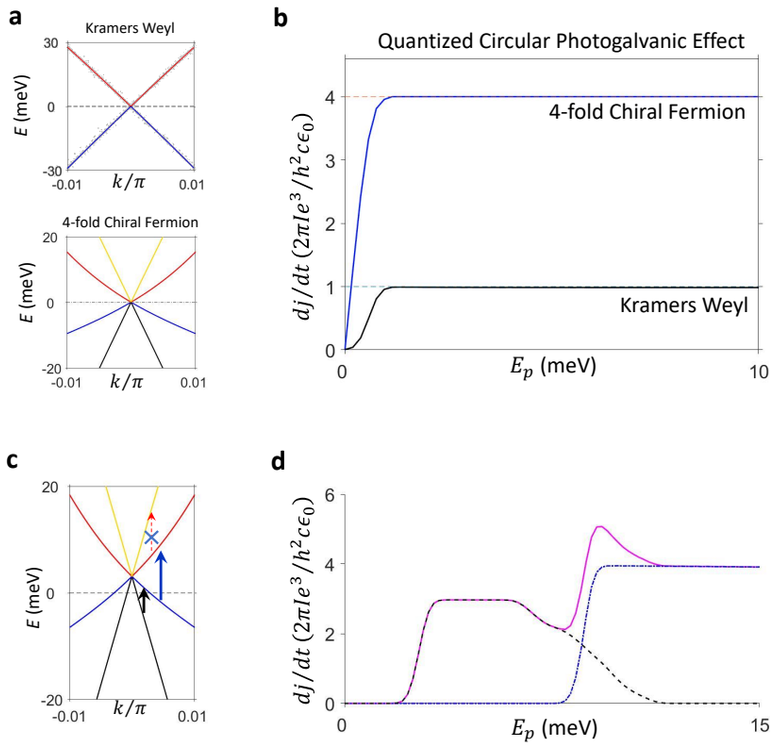


FIG. 4: **Quantized circular photogalvanic effect of the fourfold-degenerate unconventional fermion in RhSi** (a,b) For two bands connected by a single Weyl node that isn't tilted, comparing the injection of left- and right-handed circularly polarized light results in a current density rate quantized by the Chern number of the Weyl point for incident phonon energy E_p on the scale of the finite-q bandgaps of the $k \cdot p$ theory of the Weyl point [44]. For a conventional linear Weyl fermion with, $C = |1|$ and dj/dt is just the product of the incident light intensity I and fundamental constants. For transitions between the $J = 1/2$ bands of a half-occupied fourfold-degenerate unconventional fermion such as the one at Γ in RhSi, dj/dt saturates in incident photon energy E_p at *four times* the value it did for a $C = |1|$ Weyl point.

Predicted CPGE in **RhSi**, from arXiv:1706.04600.

Large Fermi Arcs in Unconventional Weyl Semimetal RhSi

Guoqing Chang,1, 2, Su-Yang Xu,3, Benjamin J. Wieder,4, Daniel S. Sanchez,3, Shin-Ming Huang,5, Ilya Belopolski,3 Tay-Rong Chang,6 Songtian Zhang,3 Arun Bansil,7 Hsin Lin,1, 2, y and M. Zahid Hasan3, y