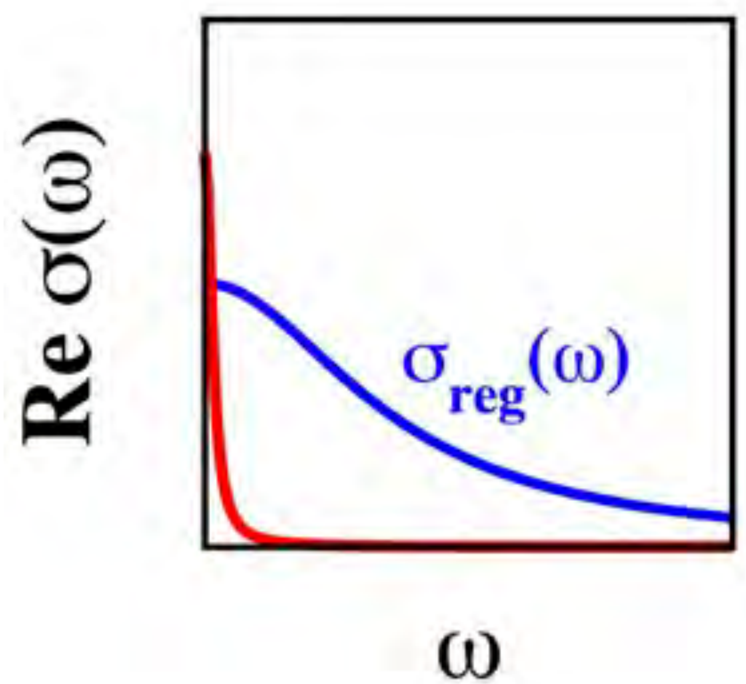
Spin (& heat) transport in low-dimensional quantum magnets



Fabian Heidrich-Meisner
Ludwig-Maximilians-University Munich
Mainz, Sept. 22, 2016

In collaboration with:





Christoph Karrasch, Joel Moore
UC Berkeley → FU Berlin

Dante Kennes
RWTH Aachen

Stephan Langer
LMU → U Pittsburgh

Johannes Hauschild
LMU → MPI PKS

Optical-lattice experiments (LMU & MPQ):
P. Ronzheimer, S. Hodgman, M. Schreiber, S. Braun, I. Bloch, U. Schneider

Q-mag transport experiments (IFW Dresden):
C. Hess, B. Buechner

Other related theory work with:
R. Steinigeweg, J. Gemmer (Osnabrück), K. Michielsen (FZ Jülich), H. de Raedt (Groningen)
W. Brenig (Braunschweig), A. Honecker (Cergy), C. Cabra (La Plata)

Deutsche Forschungsgemeinschaft DFG
DFG-FG 912
DFG-Forschergruppe 801

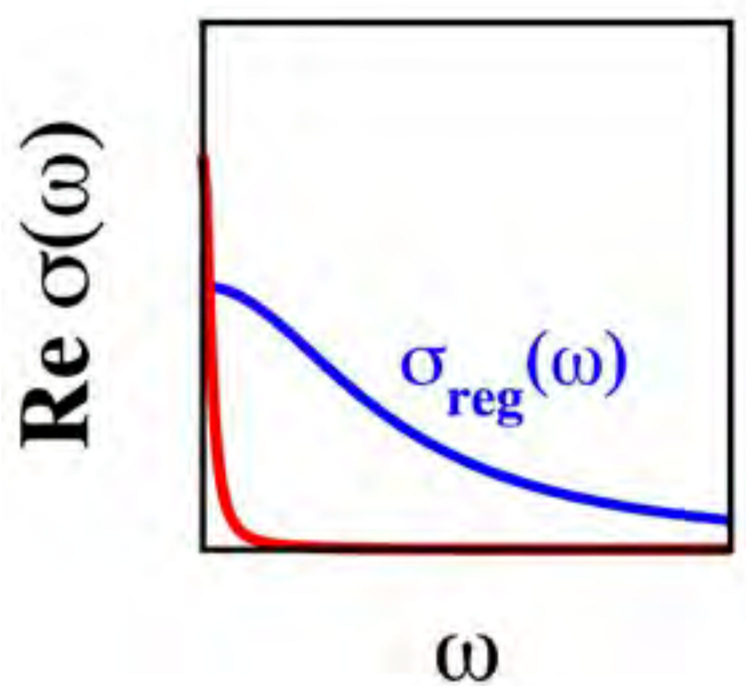
1D Heisenberg model and relatives

Antiferromagnetic
Heisenberg chain

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Bethe ansatz solution, bosonization
numerics (DMRG, ...):

ground-state properties ✓
thermodynamics ✓
spectral functions ✓



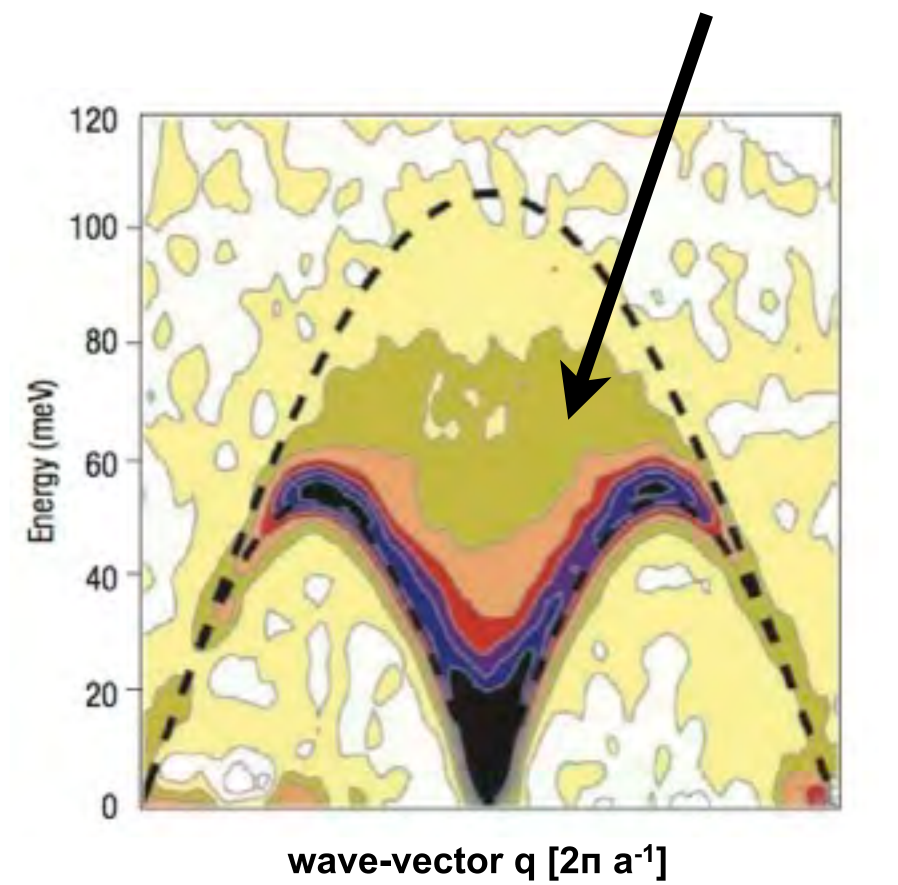
(some) Key open questions:

Non-equilibrium dynamics

Disorder: MBL

Finite-temperature transport !

2-spinon
continuum

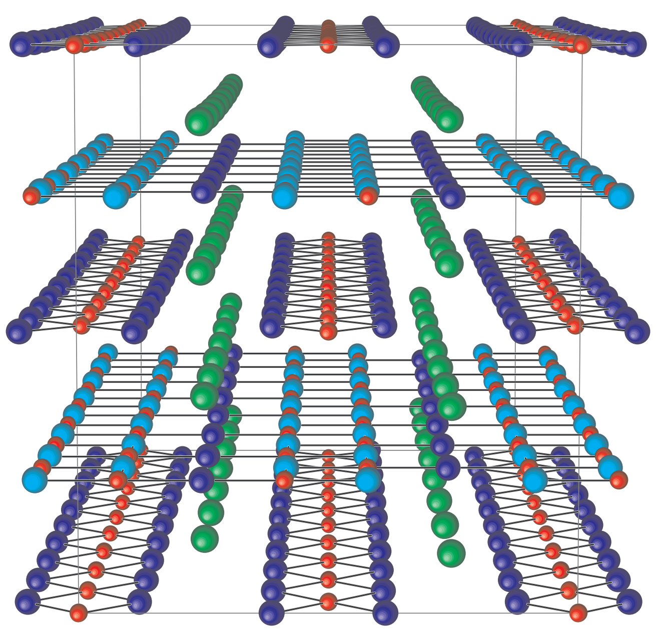


Lake et al. Nature Mat. 4, 329 (2005)
Theory: Caux, Maillet Phys. Rev. Lett. 95, 077201 (2005)

Quantum spin systems in experiments

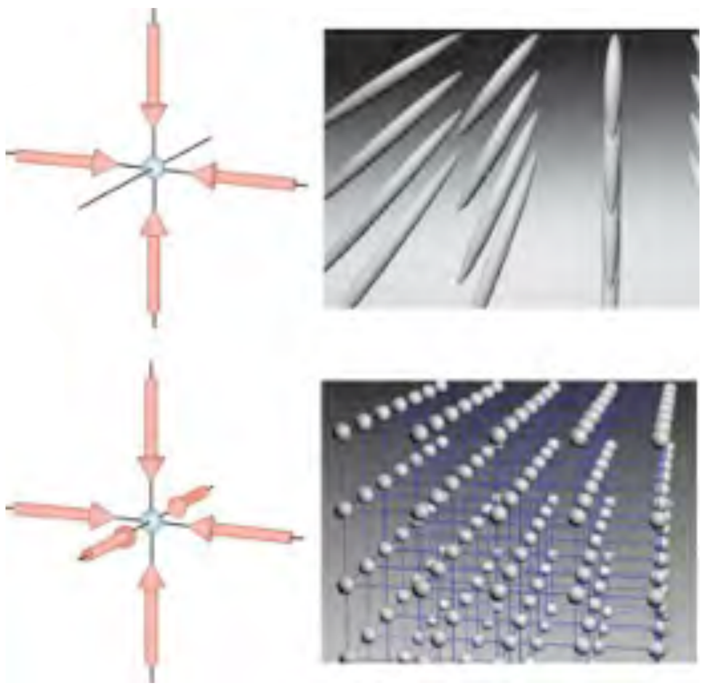
$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

Quantum magnets



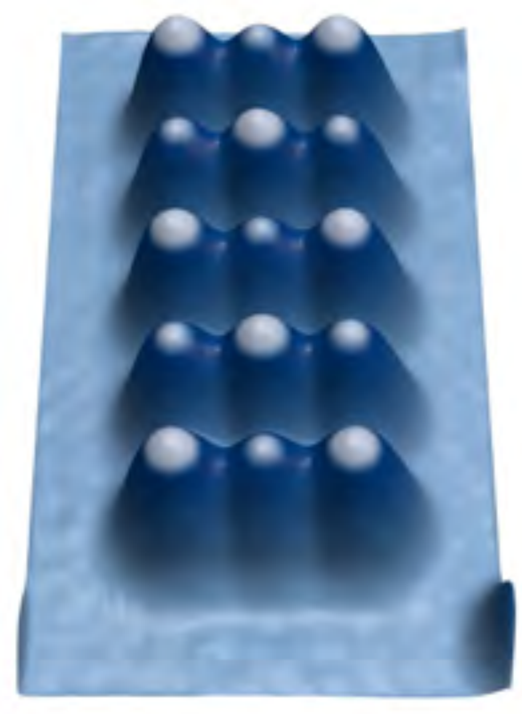
Dagotto Rep. Prog. Phys. 62, 1525 (1999)

Optical lattices



Bloch, Dalibard, Zwerger RMP (2008)

Adatoms



15 atoms AFM cluster

From Otte Lab @ Delft
See also Loth et al. Science 335, 196, (2012)
Toskovic et al. Nature Phys. (2016)

Outline

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$$

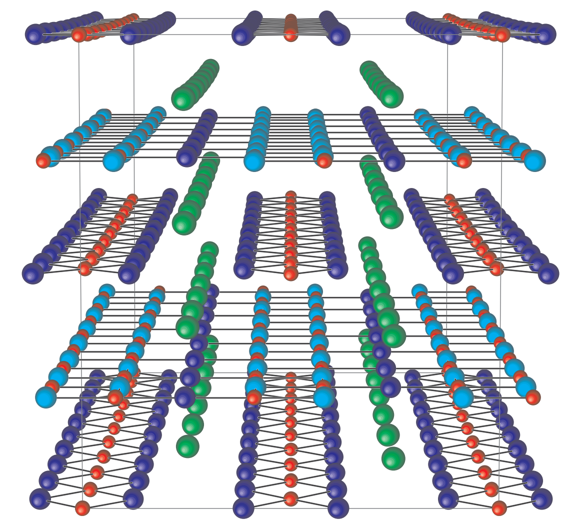
Strongly correlated systems

Anomalous conductivities in 1D integrable models
Reason: Non-trivial conservation laws in 1D

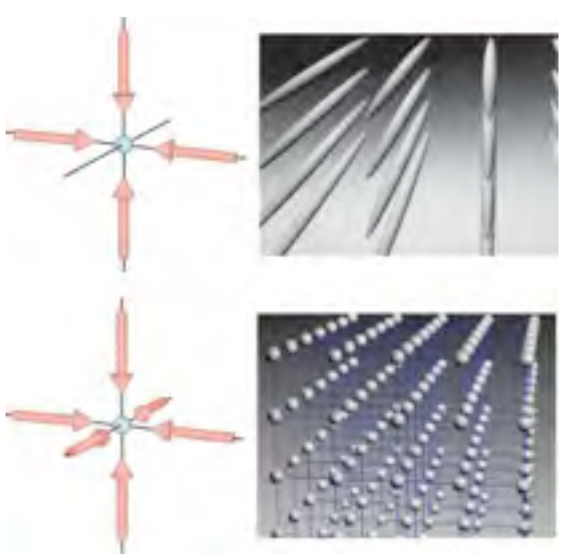
$$[H, Q] = 0 \rightarrow \sigma_{dc} = \infty$$

Ballistic, ..., diffusive dynamics

Quantum magnets



Optical lattices



1) Intro & Experimental context

2) Overview: Spin-1/2 XXZ chain
(a numerical DMRG/ED perspective)

3) Ladders, Hubbard, Towards phonons

Theoretical motivation (or obsession): Finite-temperature Drude weights

Linear response regime (Kubo): $C(t) = \langle j(t) j \rangle$

Drude weight & regular part

$$\mathrm{Re}\,\sigma(\omega) = D(T)\delta(\omega) + \sigma_{\mathrm{reg}}(\omega)$$

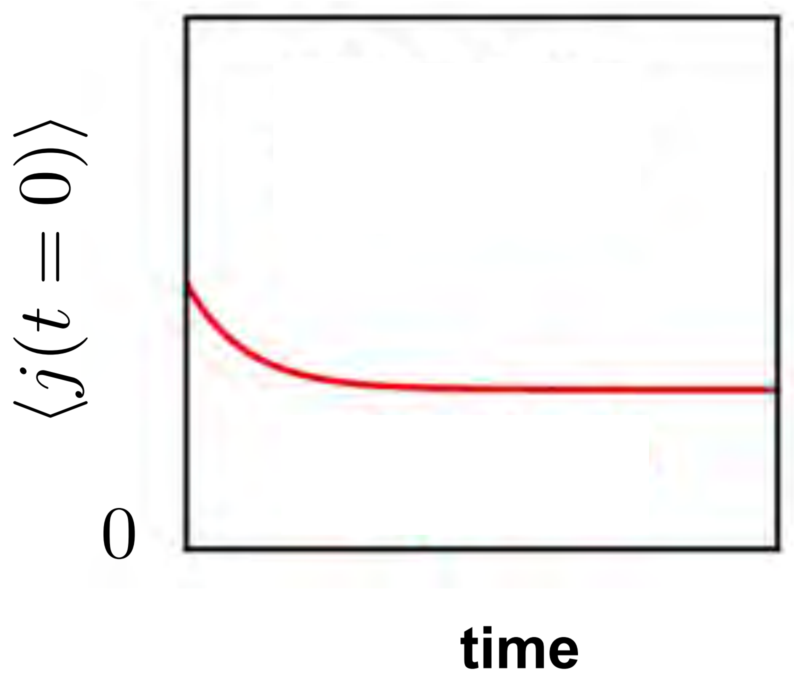
Exactly conserved current

$$[H, j] = 0 \;\; \rightarrow \;\; \mathrm{Re}\;\; \sigma(\omega) = D(T)\delta(\omega)$$

Finite Drude weight:
Divergent dc conductivity
at <u>finite temperatures</u>

Same reasoning for
charge, particle, spin, thermal transport

Decay of currents
protected by conservation law
Non-ergodic dynamics
Dissipationless transport



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Finite Drude weight:
Divergent dc conductivity
at <u>finite temperatures</u>

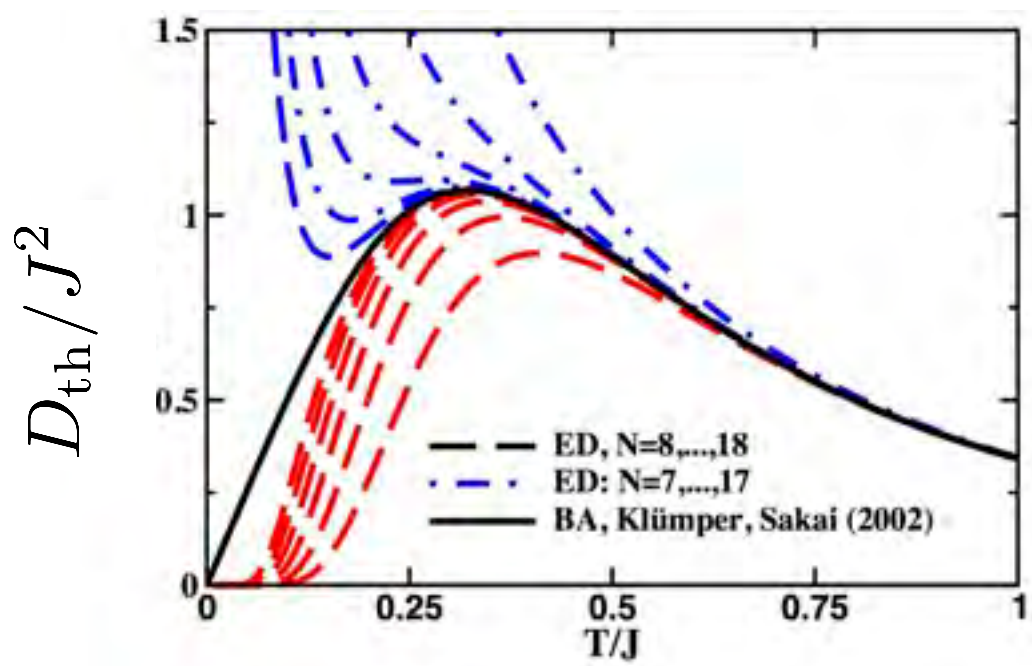
Same reasoning for
charge, particle, spin, thermal transport

Themal conductivity
in S=1/2 Heisenberg chain

$$H = J \sum_i \vec{S}_l \cdot \vec{S}_{l+1}$$

$$j_{\mathrm{th},l} \sim \vec{S}_l \cdot (\vec{S}_{l+1} \times \vec{S}_{l+2}) \;\; [H, j_{\mathrm{th}}] = 0$$

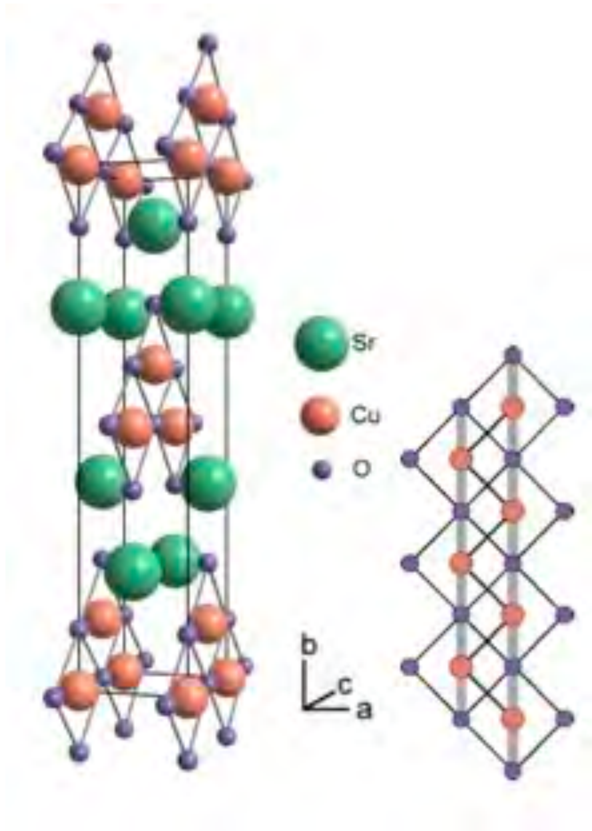
$$\mathrm{Re}\,\kappa(\omega) = D_{\mathrm{th}}(T)\delta(\omega)$$



Klümper, Sakai J. Phys. A 35, 2173 (2002)
Zotos, Naef, Prelovšek, Phys. Rev. B 55, 11029 (1997)
FHM, Honecker, Cabra, Brenig, Phys. Rev. B 66, 140406(R) (2002)

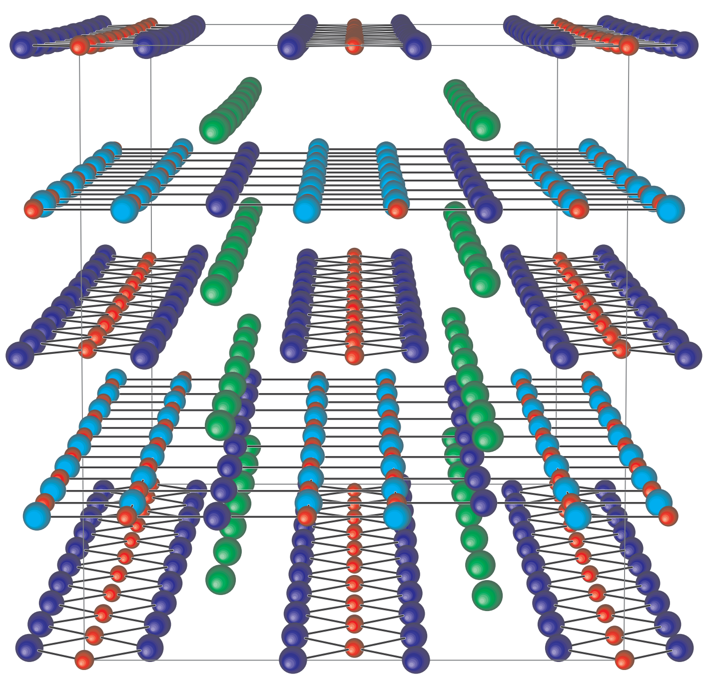
Thermal transport in (AFM) quantum magnets

1D



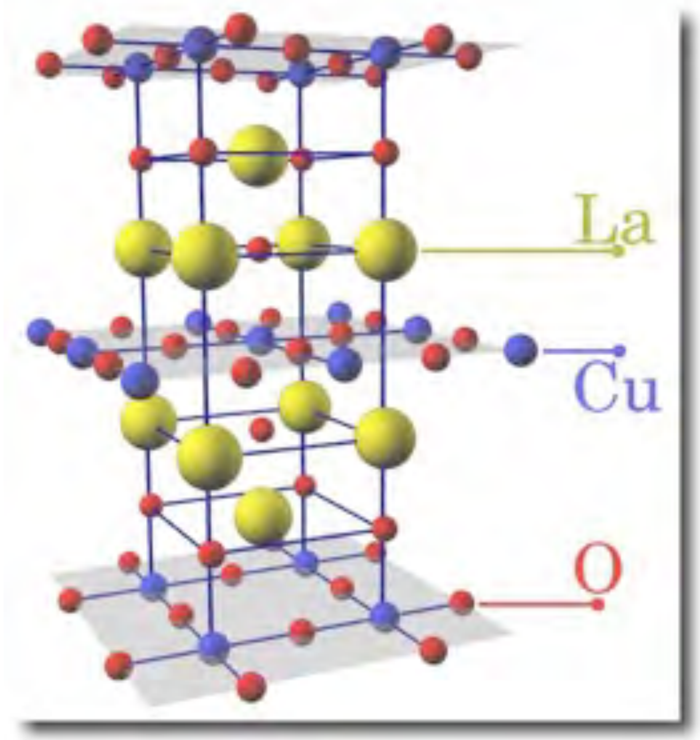
$SrCuO_2$

Ladders



$(Sr,Ca,La)_{14}Cu_{24}O_{41}$

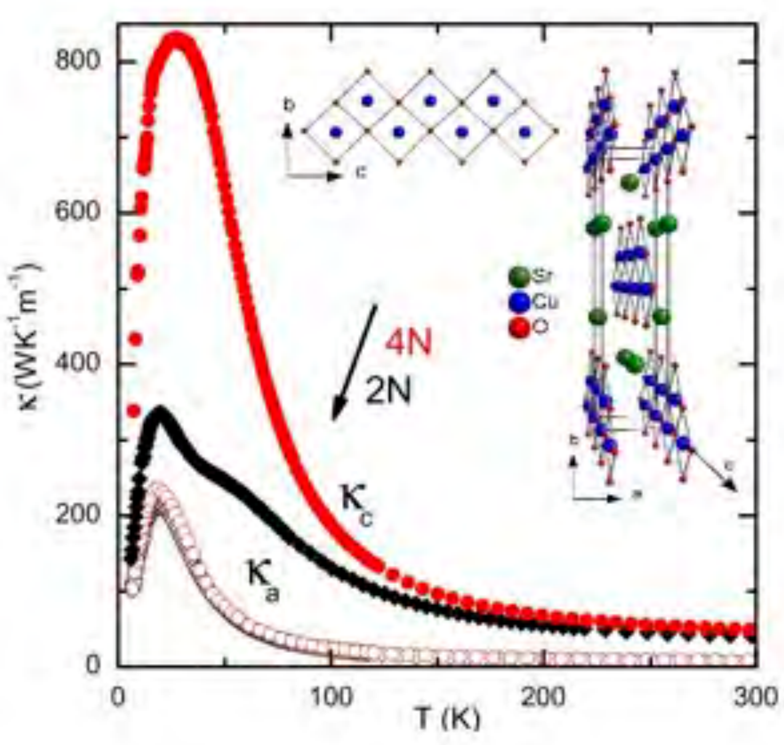
2D



La_2CuO_4

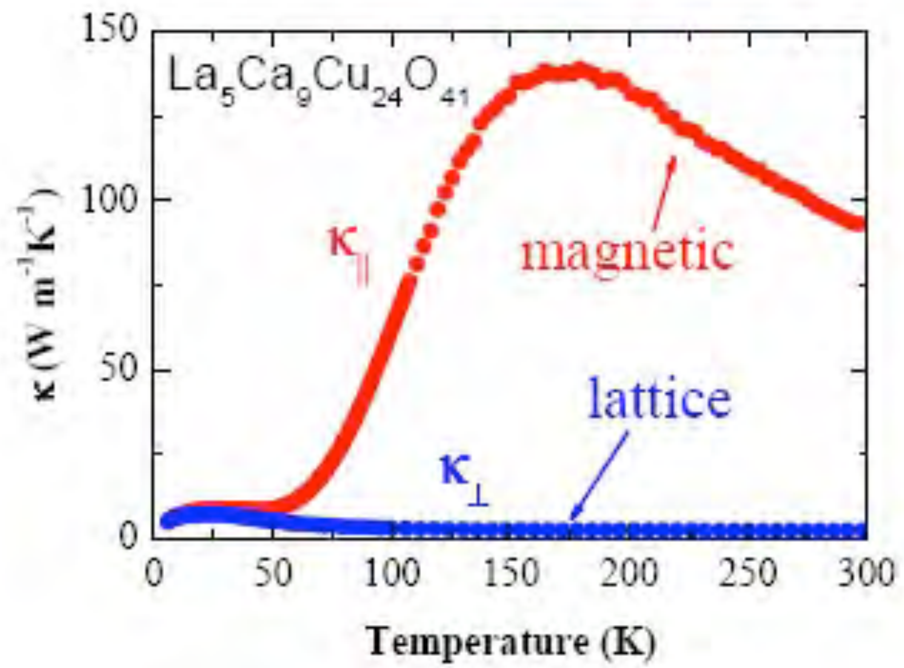
Thermal transport in (AFM) quantum magnets

1D - Spinons



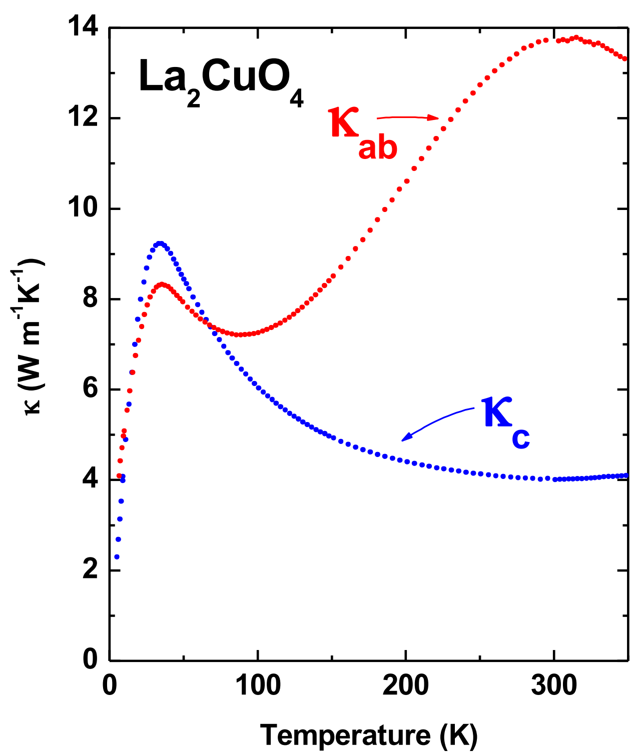
Hlubek, Büchner, Hess, et al., PRB 2010
Sologubenko et al. PRB 2001

Ladders - Triplett excitations



Hess, FHM, Brenig, Büchner, et al., PRB 2001
Solugubenko et al. PRL 2000

2D - Magnons



Hess, FHM, Brenig, Büchner et al., PRL 2003

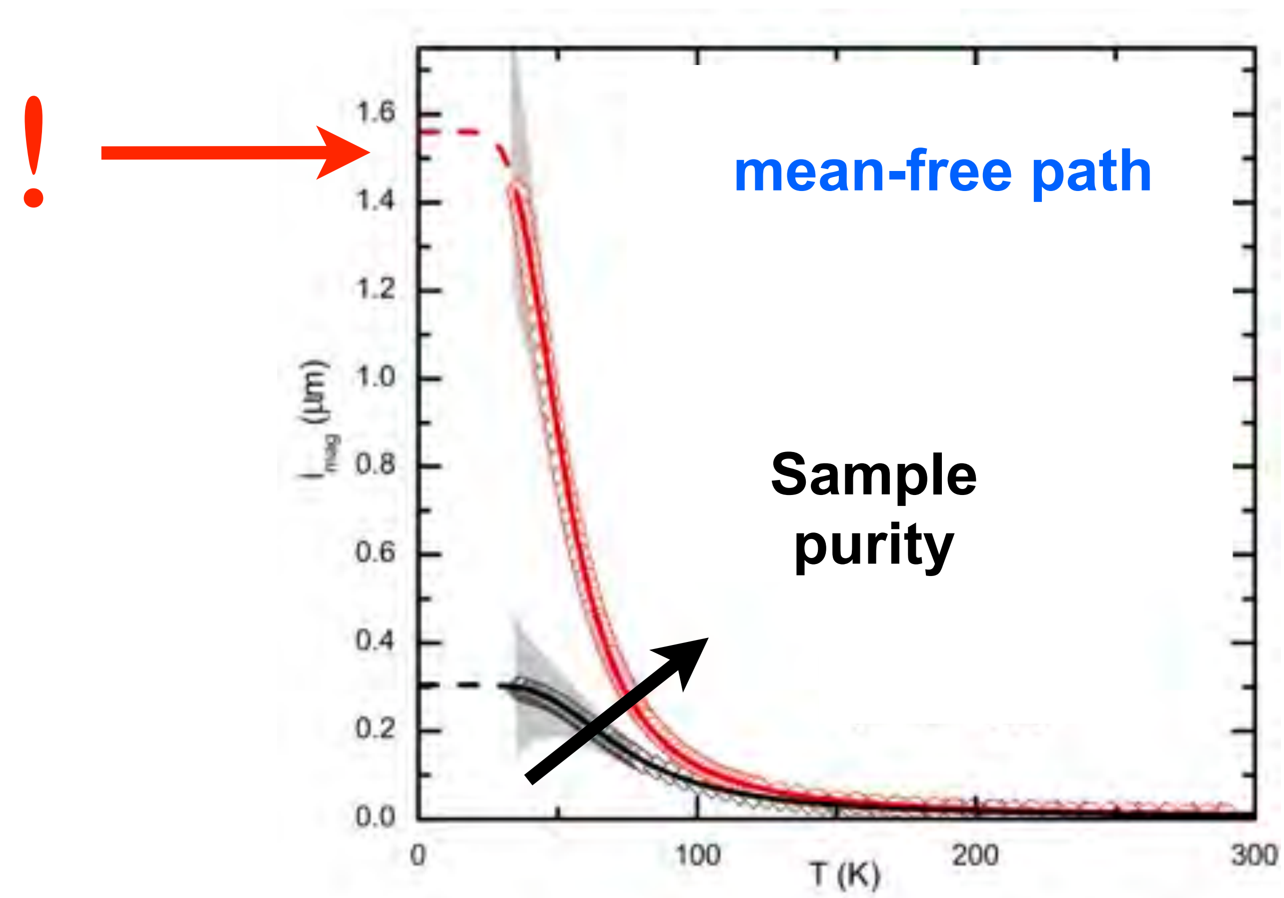
Magnetic excitations contribute significantly to thermal conductivity κ
mean-free paths ~ 1µm

Many other thermal transport experiments: Lorenz, Sun, Sales, Mandrus, ...

Spin transport only probed indirectly via NMR, µsr

Thurber et al. PRL 2001, Maeter et al. 2013, Xiao et al. 2014

Thermal transport in experiments: Spin chains



$$\kappa_{\text{mag}} \propto C_V \, v \, l_{\text{mag}}$$

Hlubek, Buechner, Hess, et al., Phys. Rev. B 81, 020405(R) (2010)

Time-resolved experiments

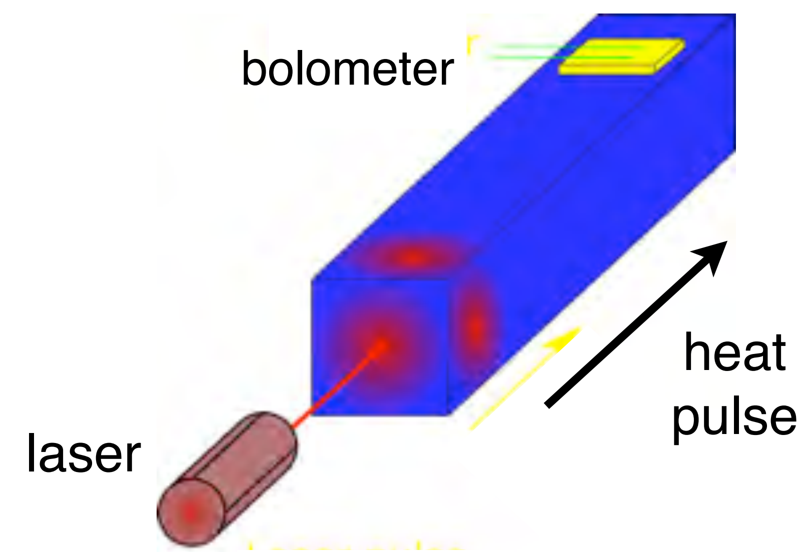


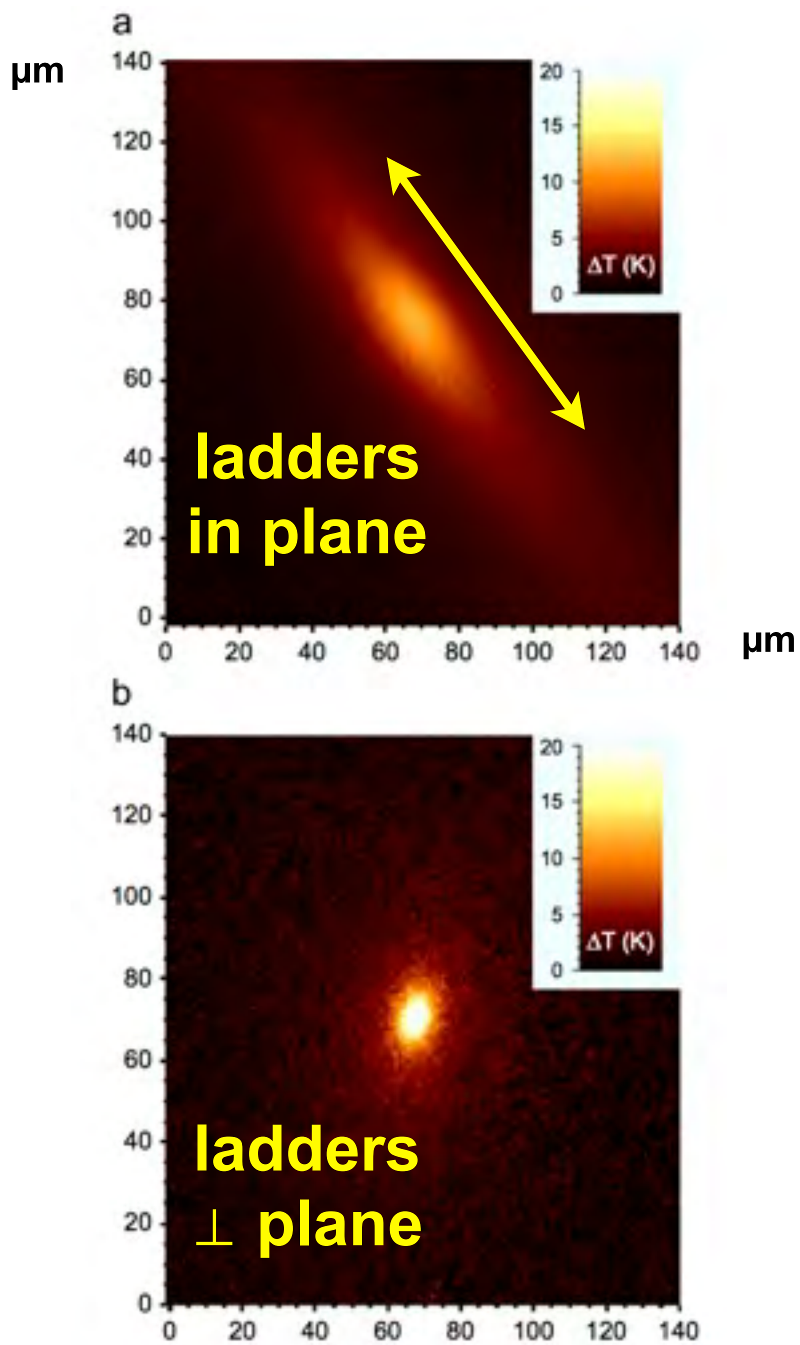
Figure courtesy of C. Hess

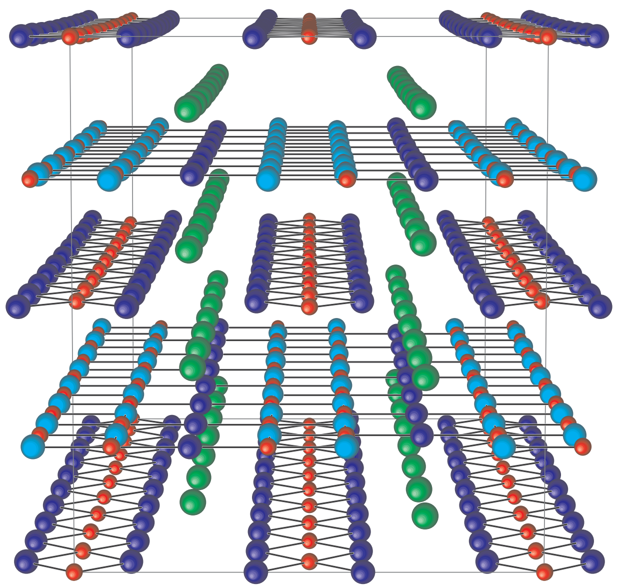
"Heat"-management in electronics

High-purity samples: Macroscopically large mean free path l_{mag} ≈1μm

New experiments: Time-resolved measurements

Temperature profiles





$(Sr,Ca,La)_{14}Cu_{24}O_{41}$

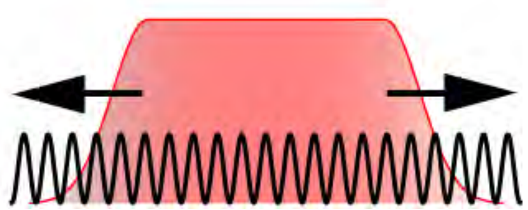
Anisotropic dynamics similar to thermal conductivity!
"Magnon" thermal transport

Montagnese, van Loosdrecht, et al., Phys. Rev. Lett., 110, 147206 (2013)
Otter et al. Int. J. of Heat and Mass Transfer 55, 2531 (2012)
Also: Hohensee, Wilson, Feser, Cahill, Phys. Rev. B 89, 024422 (2014)

Nonequilibrium transport in optical lattice

^{39}K atoms

$$H = -J_{BH} \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i (n_i - 1) + V(t) \sum_i n_i \vec{r}_i^{\,2}$$



Remove trap V → 0,
Go to desired U/J_{BH}

Initial state:

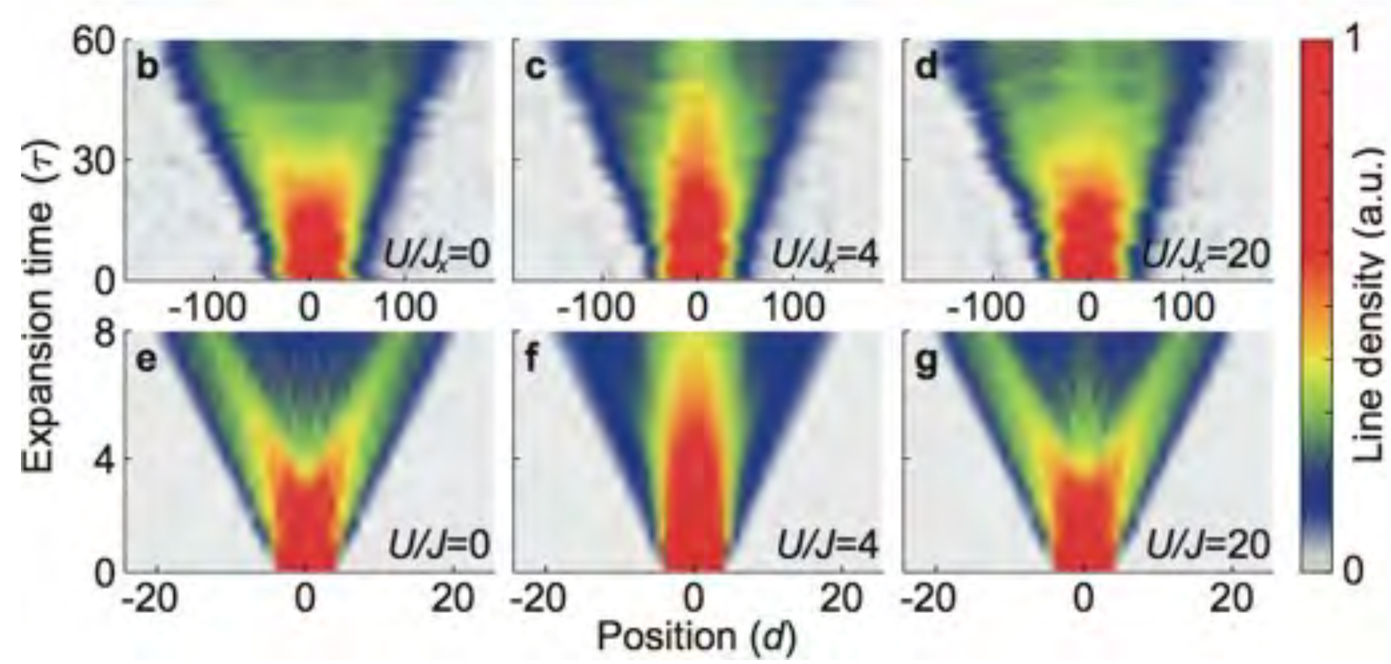
$$|\psi_{\text{initial}}\rangle = \prod_i a_i^\dagger |0\rangle$$

Spin-down - up - down

ballistic **diffusive?** **ballistic**

Exp. data

DMRG

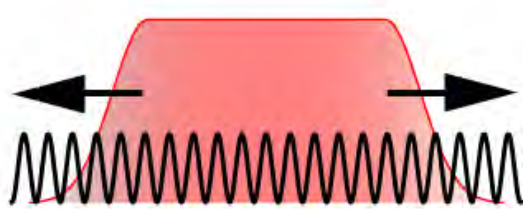


Identical Density Profiles for non-interacting & *strongly* interacting bosons: Ballistic nonequilibrium dynamics in integrable 1D model

Ronzheimer, Schreiber, Braun, Hodgman, Langer, McCulloch, FHM, Bloch, Schneider Phys. Rev. Lett. 110, 205301 (2013)
Nonequilibrium quasi-condensation: Vidmar, Ronzheimer, FHM, Bloch Schneider et al. PRL 115, 175301 (2015)

Nonequilibrium transport in optical lattice

$$U/J = \infty, n = 1: \quad H = -J_{\mathrm{BH}} \sum_i (S_i^+ S_{i+1}^- + h.c.)$$



Remove trap V → 0,
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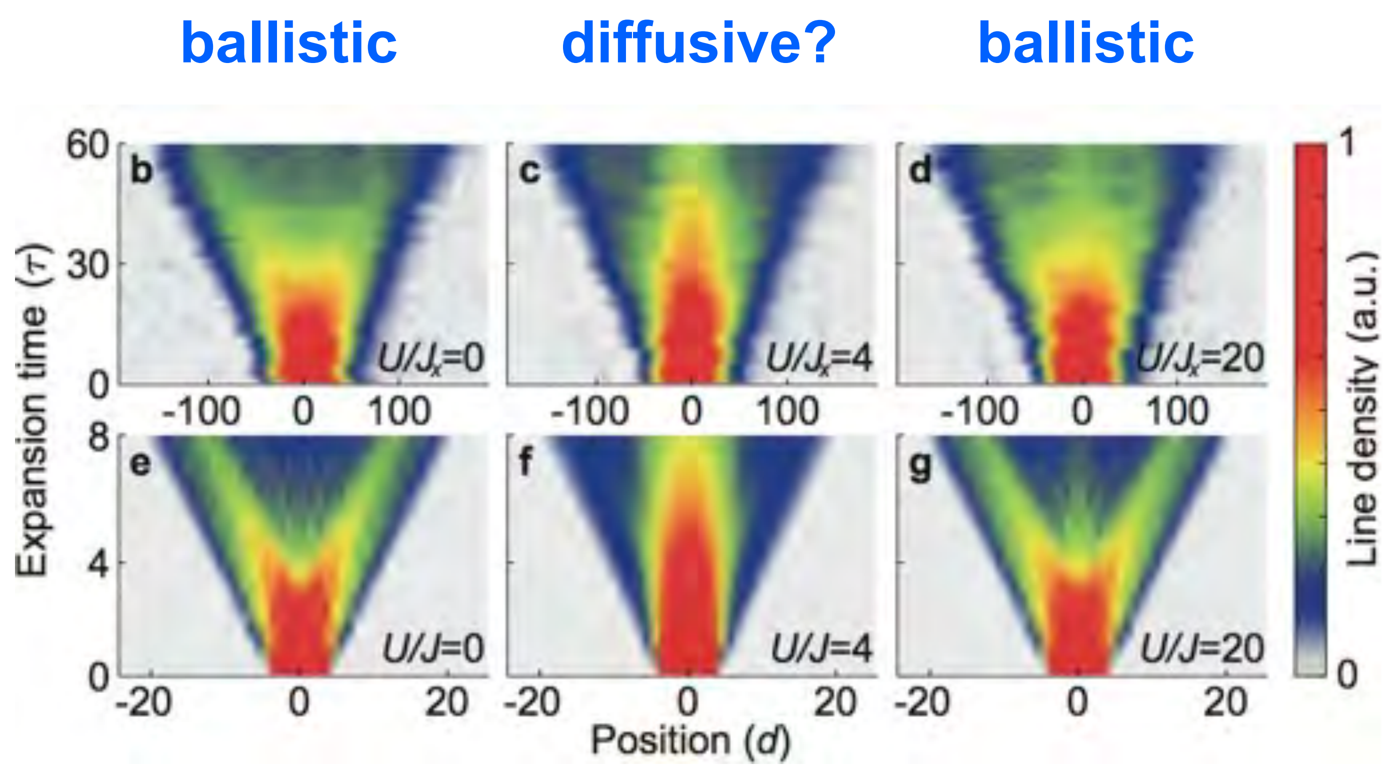
$$|\psi_{\mathrm{initial}}\rangle = \prod_i a_i^\dagger |0\rangle$$

Spin-down - up - down

Exp. data

DMRG



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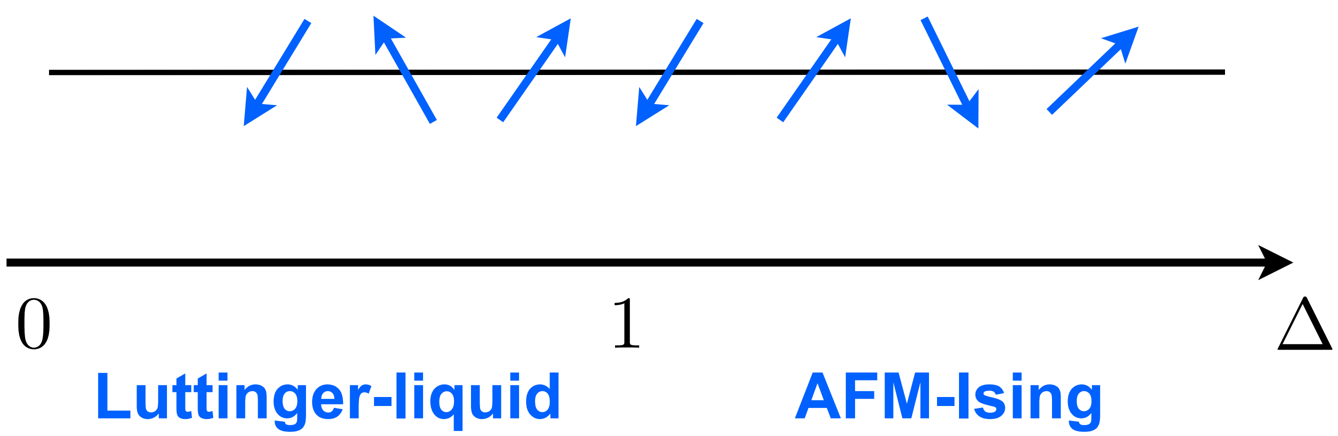
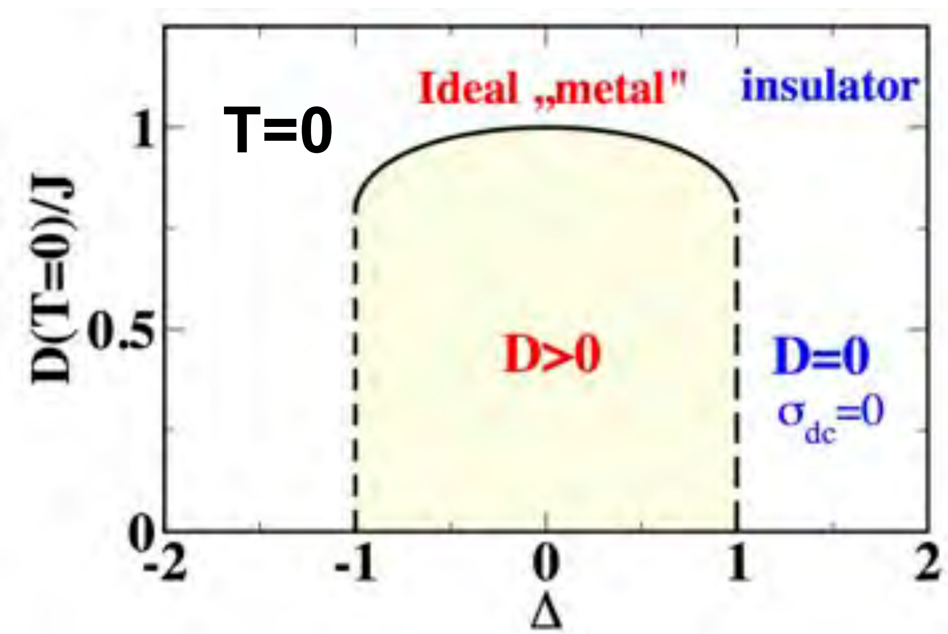
Spin transport in the spin-1/2 XXZ model

$$H = J\sum_{i=1}^{L}\left[\frac{1}{2}(S_i^+S_{i+1}^- + h.c.) + \Delta S_i^z S_{i+1}^z\right]$$

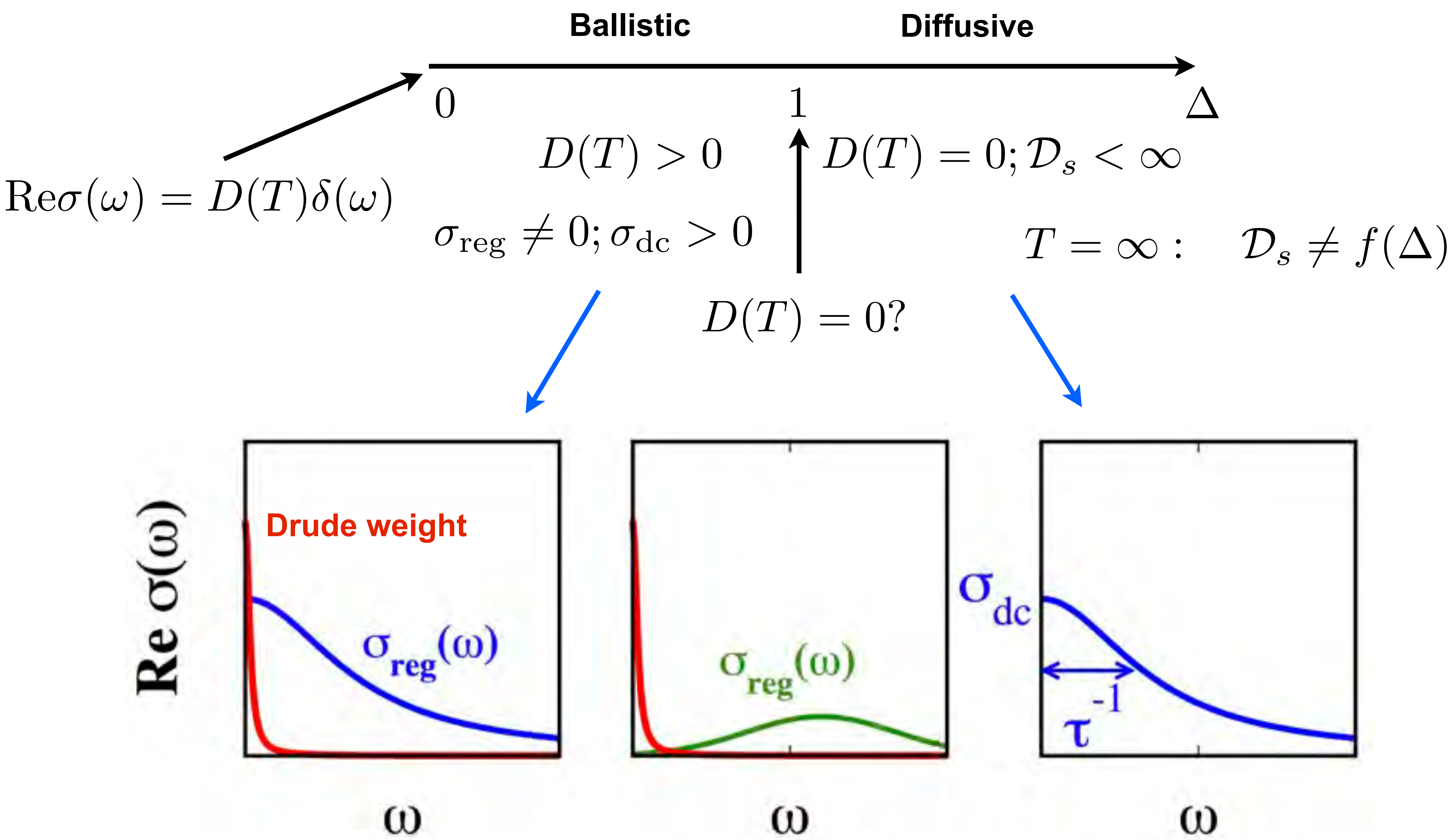
$$\Delta \neq 0: \quad [H, j_s] \neq 0; \quad j_{s,l} \sim S_l^+ S_{l+1}^- - h.c.$$





Shastry, Sutherland Phys. Rev. Lett. 65, 243 (1990)

Spin-1/2 XXZ chains: Finite T spin transport



Bethe ansatz: Zotos, Klümper, Prosen, ... ED: Herbrych, Steinigeweg, Prelovsek, Zotos, ...
Field theory: Sirker, Perreira, Affleck, Rosch, Andrei, Fujimoto, Kawakami, Giamarchi, Damle, Sachdev....
QMC: Grossjohann, Brenig, Sorella, Alvarez, Gros, ...
DMRG: Karrasch, Moore, ...Open quantum systems: Znidaric, Gemmer. Prosen, ...

Spin-1/2 XXZ chains: Finite T spin transport

Ballistic **Diffusive**

0 1 Δ

$\mathrm{Re}\sigma(\omega) = D(T)\delta(\omega)$

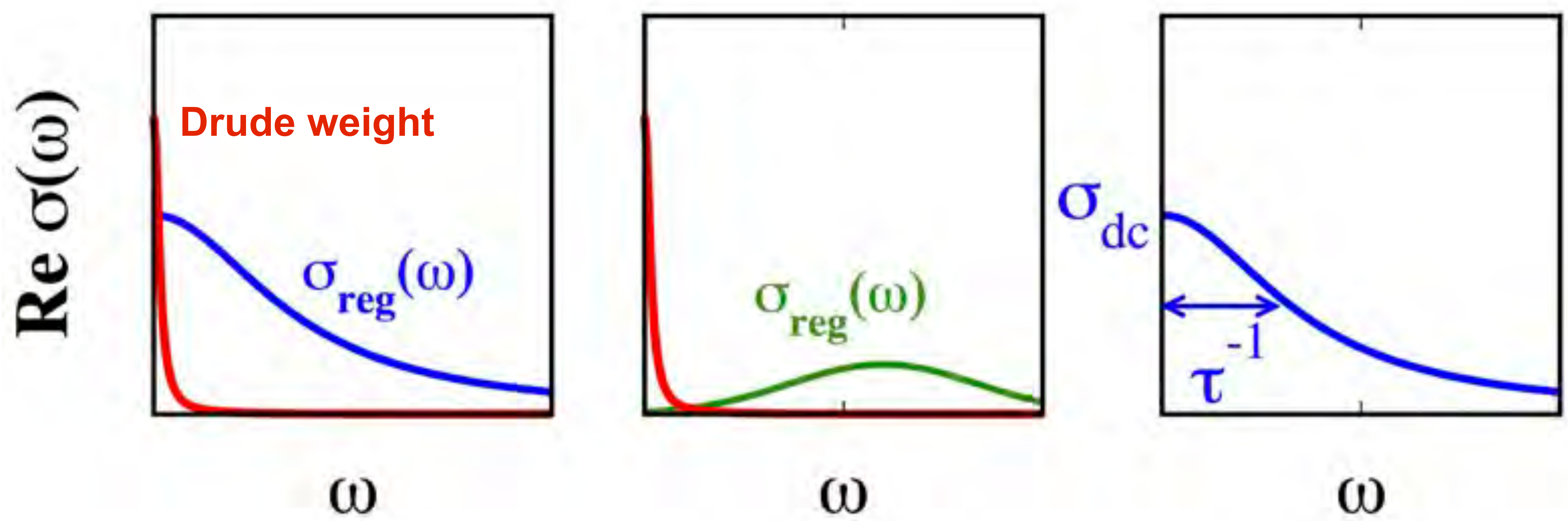
$D(T) > 0$

$\sigma_{\mathrm{reg}} \neq 0; \sigma_{\mathrm{dc}} > 0$

$D(T) = 0?$

$D(T) = 0; \mathcal{D}_s < \infty$

$T = \infty : \quad \mathcal{D}_s \neq f(\Delta)$



dissipationless heat & spin transport

dissipationless heat but diffusive spin transport

Finite-temperature DMRG using purification

Real-time Density-matrix renormalization group simulations

$$|\psi(t)\rangle = e^{-iHt/\hbar}|\psi_0\rangle$$

White Phys. Rev. Lett. 1992, Schollwöck Ann. Phys. 2011
Daley, Kollath, Schollwöck, Vidal, J. Stat. Mech 2004
White, Feiguin PRL 2004, Vidal PRL 2004

Current correlation functions at T>0

$$D(T) \sim \lim_{t\to\infty} \frac{1}{2L}\langle j_s(t) j_s\rangle$$

Verstraete et al. PRL 2004, Feiguin, White PRB 2005
Karrasch, Bardarson, Moore PRL 2012, NJP 2013
Karrasch, Kennes arXiv:1404.2706
Barthel, Schollwöck, Sachdev 2012, Barthel 2013

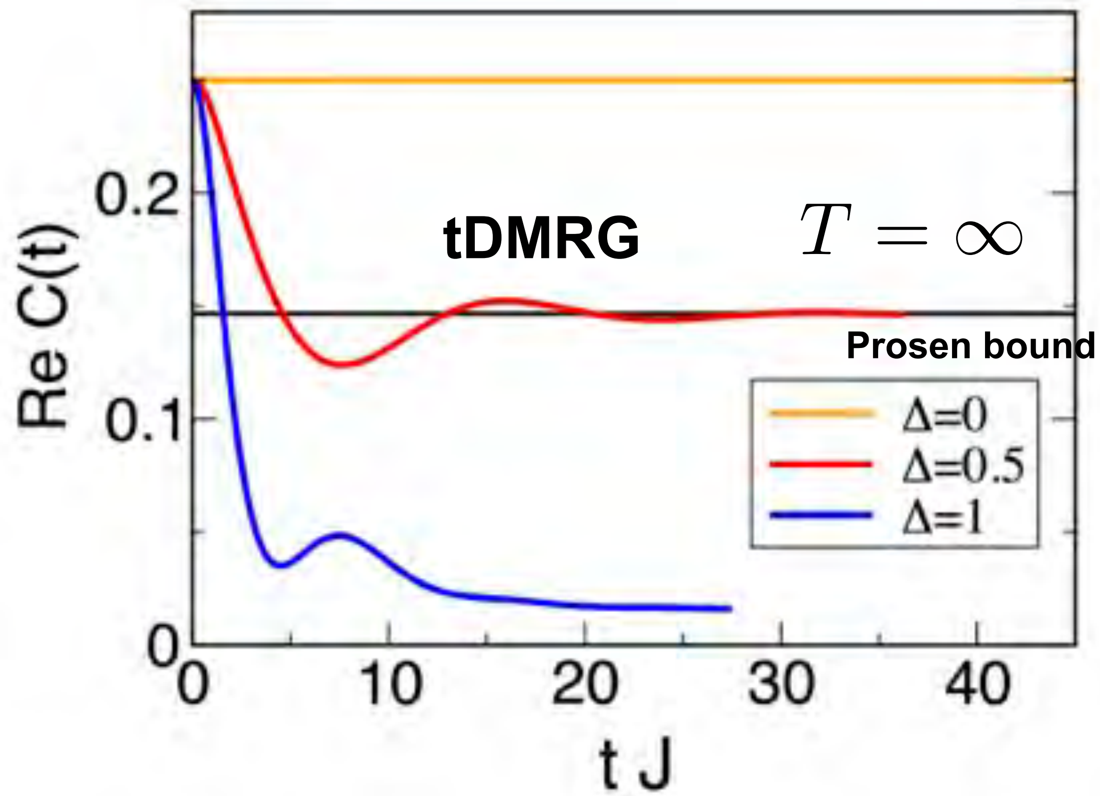
Many-body, 1D

L ~ 100 possible

Infinite times not accessible

Real-time:
Spin-current autocorrelations

$$C(t) = \langle j_s(t) j_s\rangle / L$$



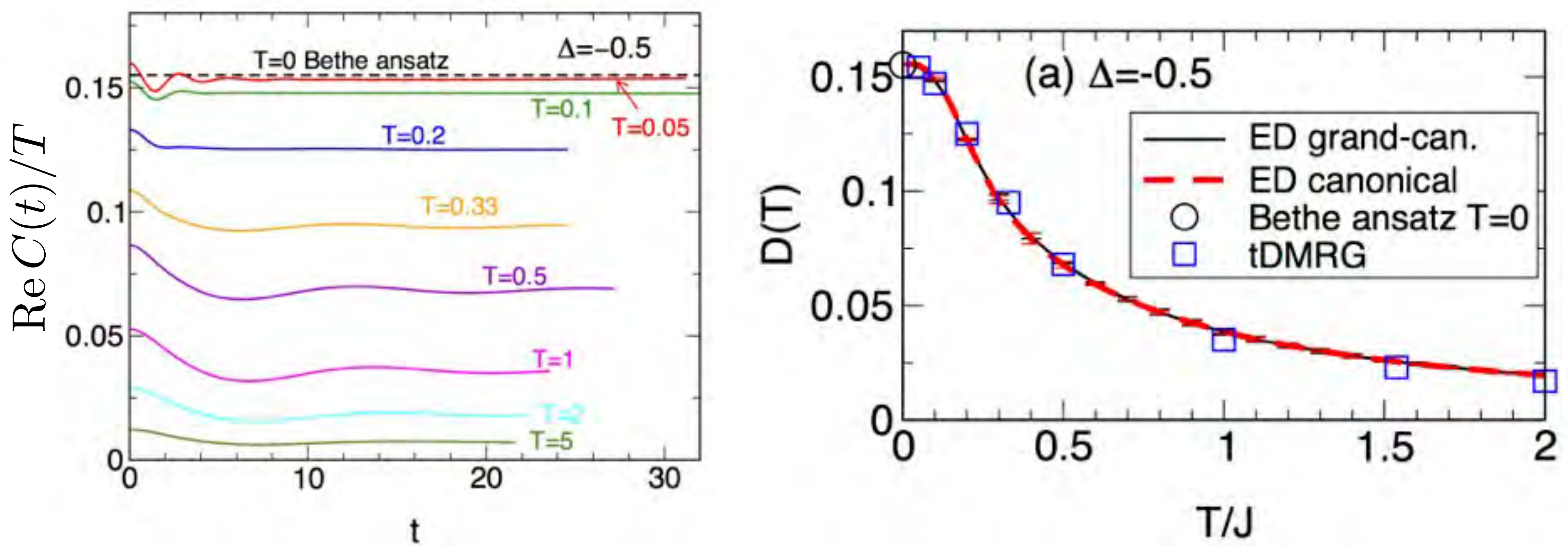
no finite-size effects!

Karrasch, Bardarson, Moore PRL 2012
Karrasch, Kennes, FHM PRB 2015
Karrasch, Moore, FHM PRB 2014
Karrasch, Kennes, Moore PRB 2014

Spin Drude weight: Temperature dependence

$-1 < \Delta < 0$

tDMRG



Negative Δ: Excellent agreement ED = tDMRG
Very short relaxation time

Karrasch, Hauschild, Langer, FHM Phys. Rev. B 87, 245128 (2013)
ED: see also Herbrych, Prelovsek, Zotos PRB 84, 155125 (2011)

Ballistic transport due to integrability

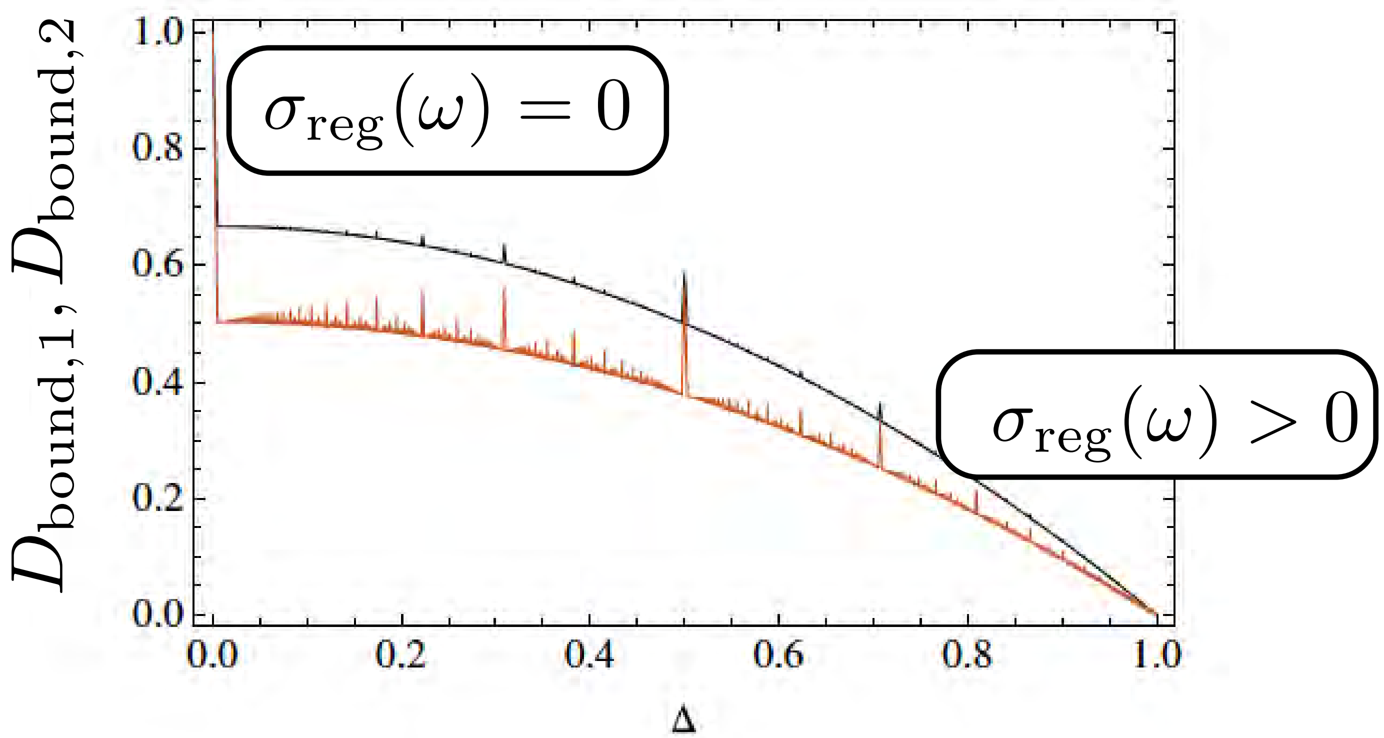
In general:

$$[H, j_s] \neq 0 \quad \text{but} \quad [H, Q_\alpha] = 0$$

Integrable 1D systems:
Many local conservation laws Q_α

Lower bound - quasi-local conserved charge:

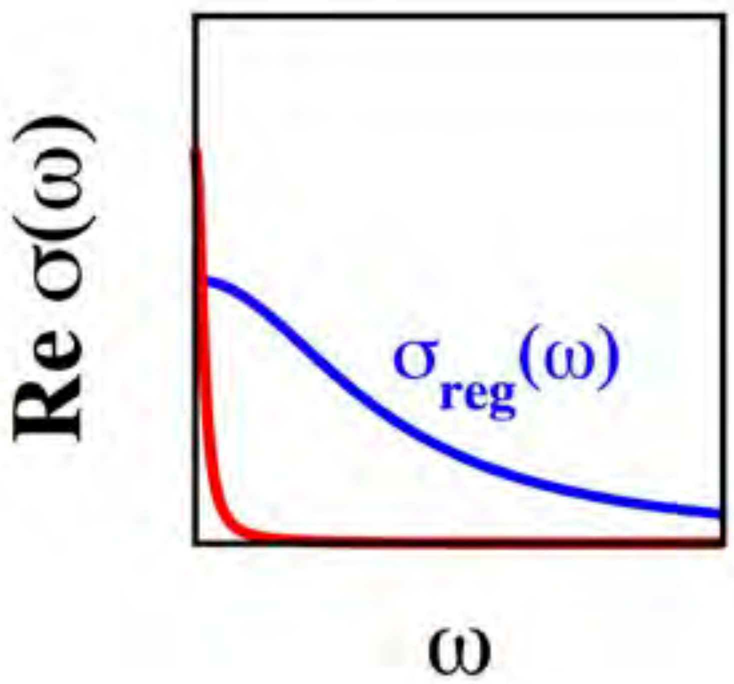
$$\langle j_s \tilde{Q} \rangle \neq 0 \rightarrow D_{\text{bound}}(T) > 0 \ \text{ for } \ |\Delta| < 1$$



Prosen PRL 2011; Prosen, Ilievski PRL 2013

Spin transport for Δ<1:

Coexistence of ballistic & finite-frequency contributions (Δ<1)



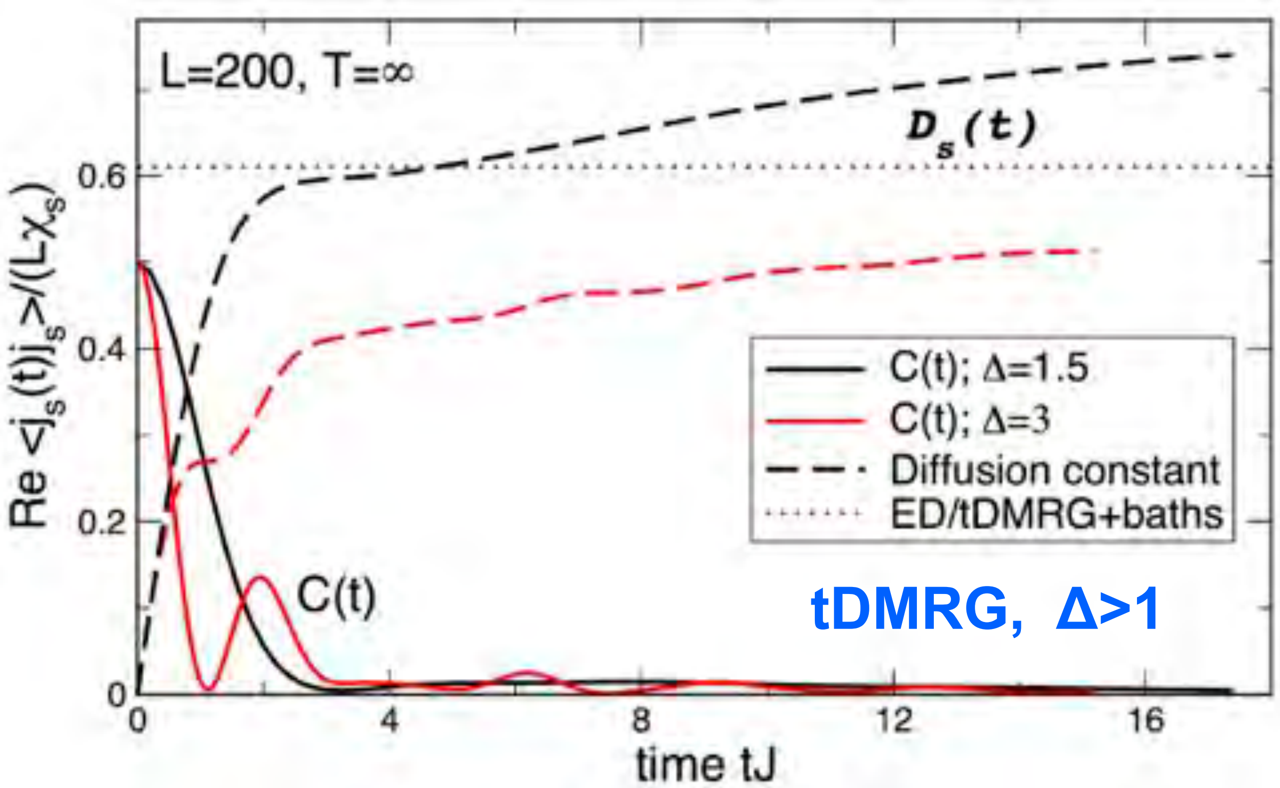
Sirker, Pereira, Affleck PRL 103, 216602 (2009),
Grossjohann, Brenig PRB 81, 012404 (2010) (low T)
Karrasch, Kennes, FHM PRB 91, 115130 (2015) (high T)
Naef, Zotos JPCM 1998

Diffusion in the AFM-Ising phase

$\Delta > 1$

Common belief: spin No Drude weight

$$\mathrm{Re}\,\sigma(\omega) = \sigma_{\mathrm{reg}}(\omega) \qquad 0 < \sigma_{\mathrm{dc}} = \mathcal{D}_s \chi < \infty$$



Current correlations decay to zero

$D_s(t)$ saturates for large Δ

Diffusion constant - Einstein relation at T= ∞

$$\mathcal{D}_s = \frac{\sigma_{dc}}{\chi} \qquad \mathcal{D}_s(t) = \frac{1}{\chi}\int_0^t dt'\, C(t') \qquad C(t) = \frac{1}{L}\mathrm{Re}\langle j_s(t) j_s\rangle$$

Karrasch, Moore, FHM, Phys. Rev. B 89, 075139 (2014)

Diffusion in the AFM-Ising phase

$\Delta > 1$

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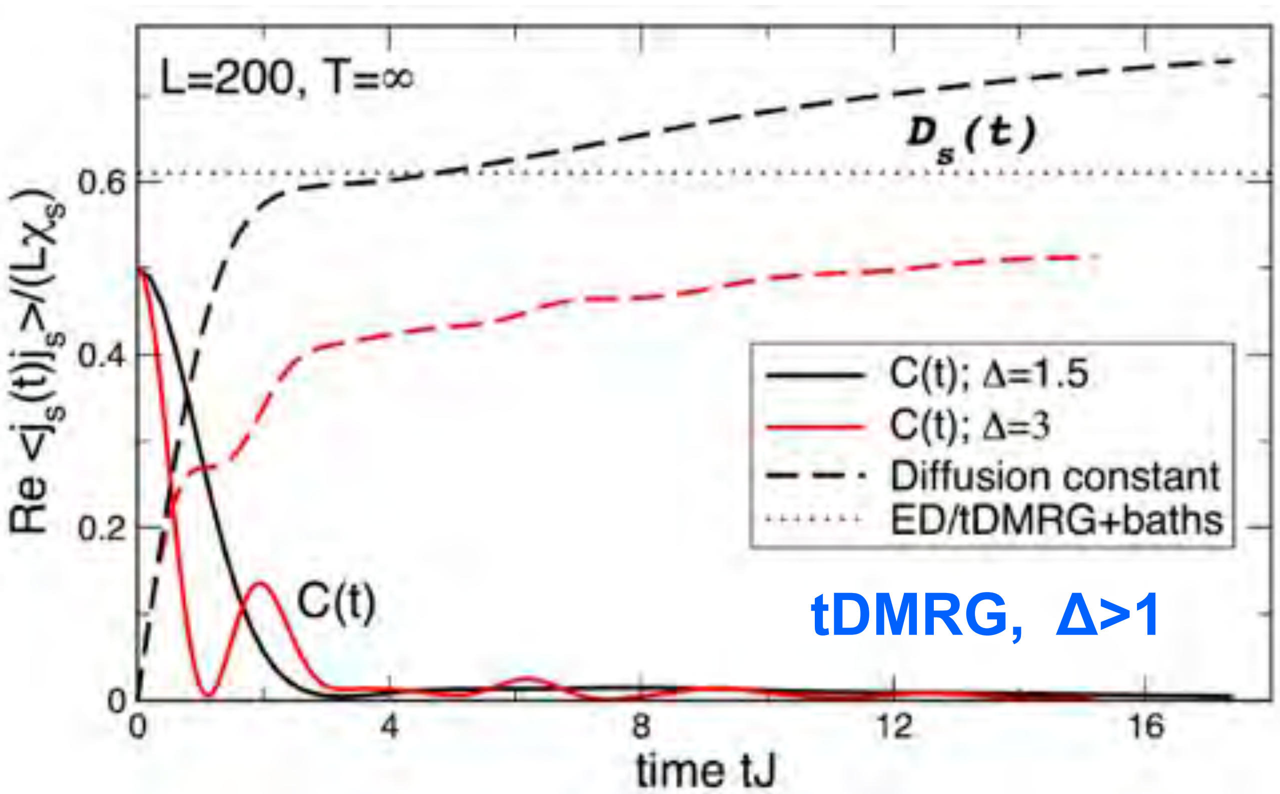
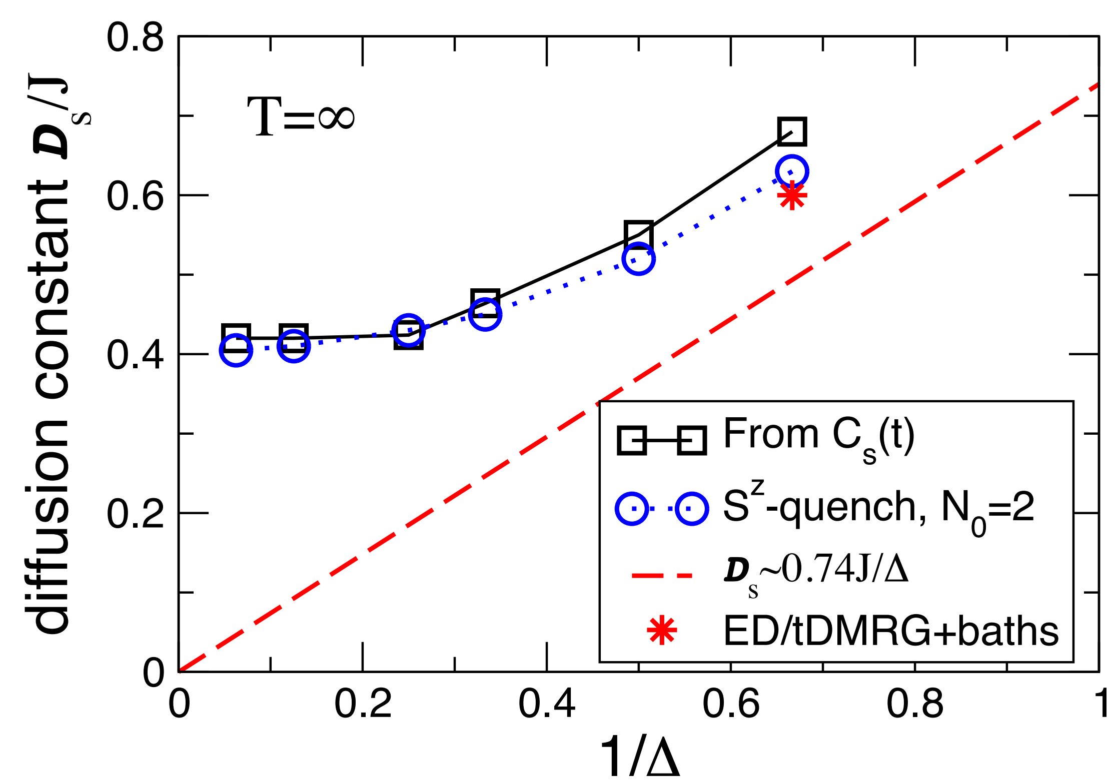




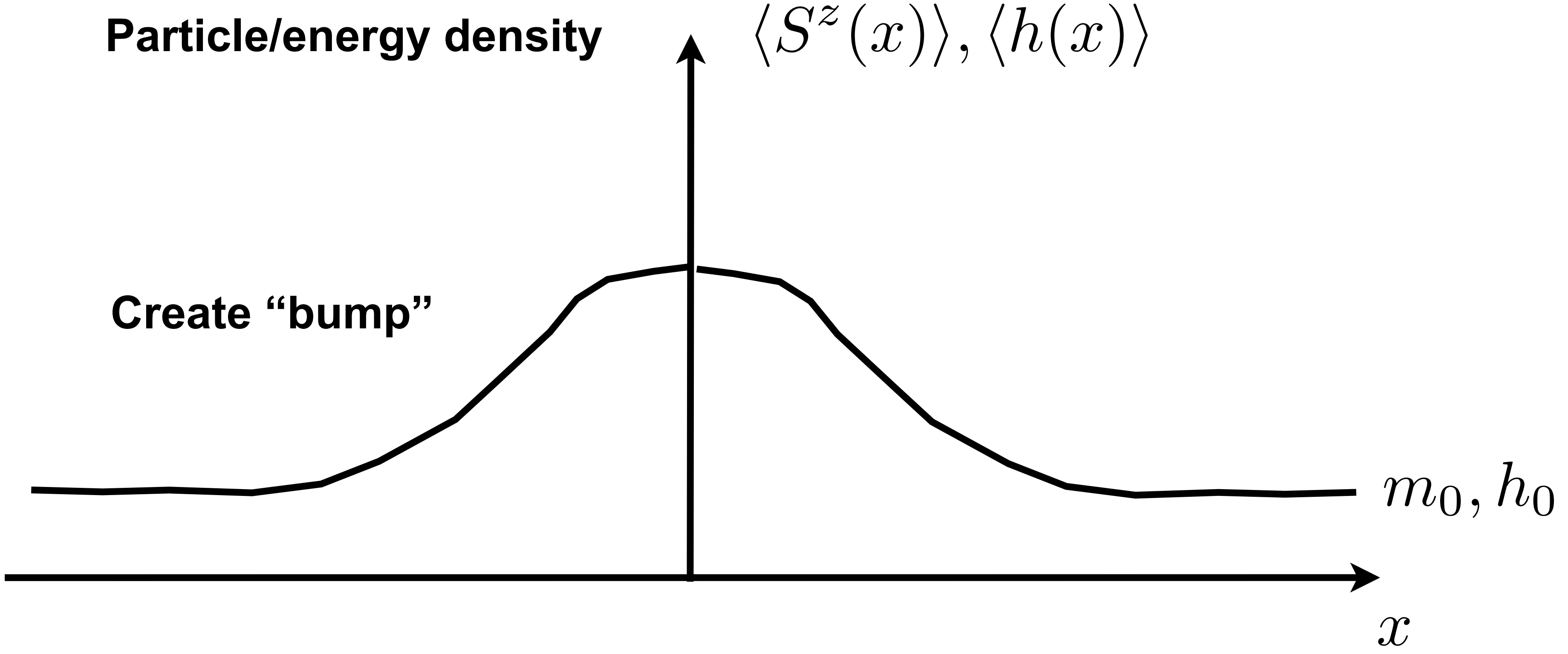
Diffusion constant - Einstein relation at T= ∞

disagrees with Znidaric PRL 2011

$$\mathcal{D}_s = \frac{\sigma_{dc}}{\chi} \qquad \mathcal{D}_s(t) = \frac{1}{\chi}\int_0^t dt'\, C(t') \qquad C(t) = \frac{1}{L}\mathrm{Re}\langle j_s(t) j_s \rangle$$

Karrasch, Moore, FHM, Phys. Rev. B 89, 075139 (2014)

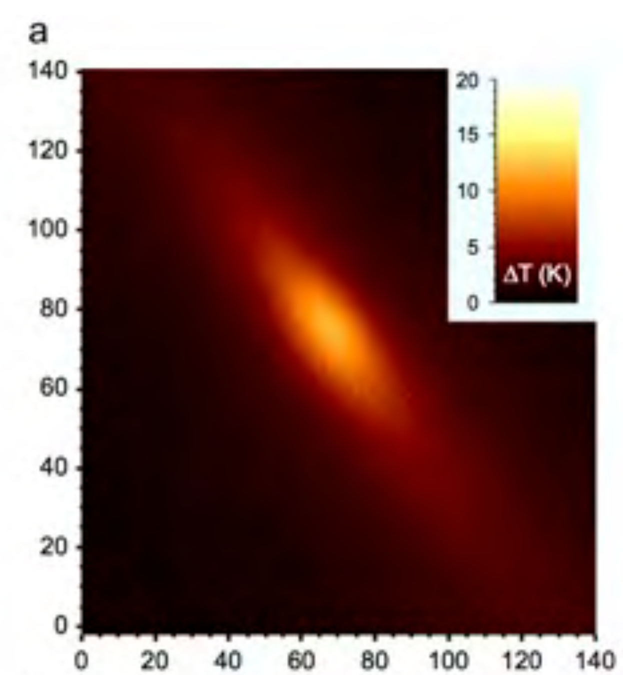
Signatures in local quenches



Study width:

$\sigma(t) \propto t^{\alpha}$

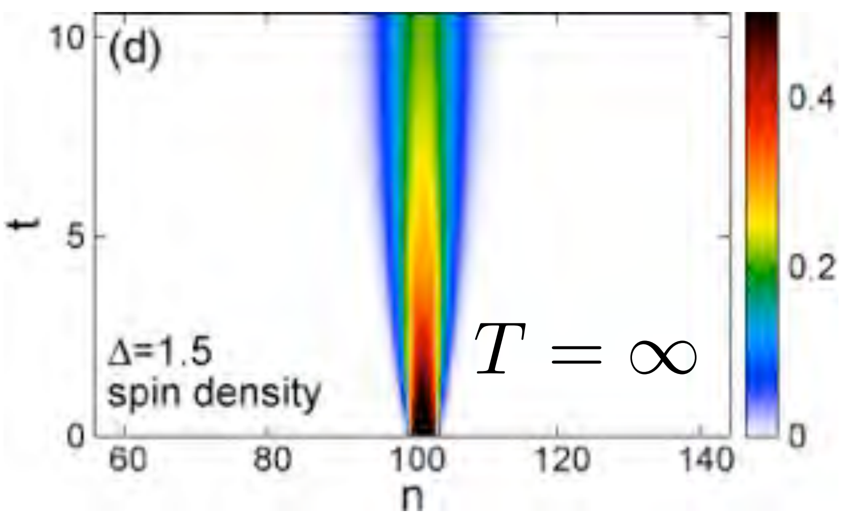
$$\sigma^2(t) \sim \frac{1}{S^z}\sum_i (i-i_0)^2 \langle S_i^z(t)\rangle$$



For 1D spin systems:
Langer, FHM, Gemmer, McCulloch, Schollwöck PRB 2009
Langer, Heyl, McCulloch, FHM, PRB 2011
Karrasch, Moore, FHM, Phys. Rev. B 89, 075139 (2014)

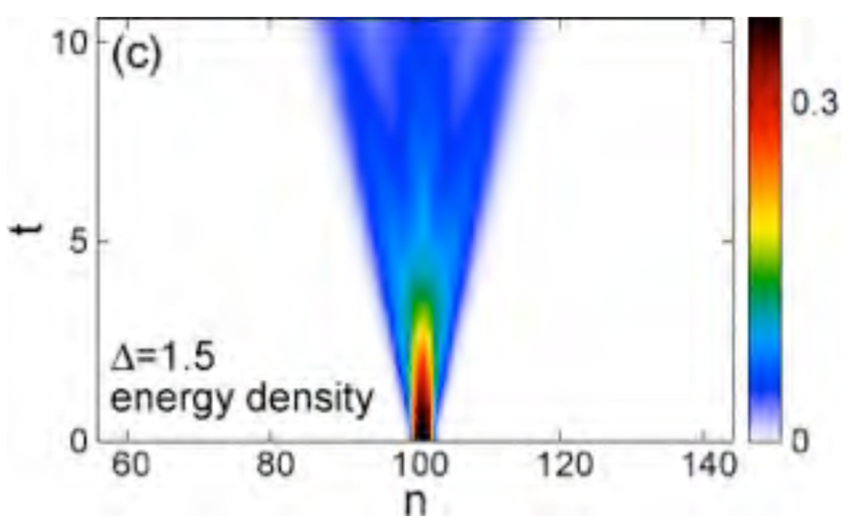
Diffusive spin dynamics in local quenches at finite T

Spin density: Diffusive

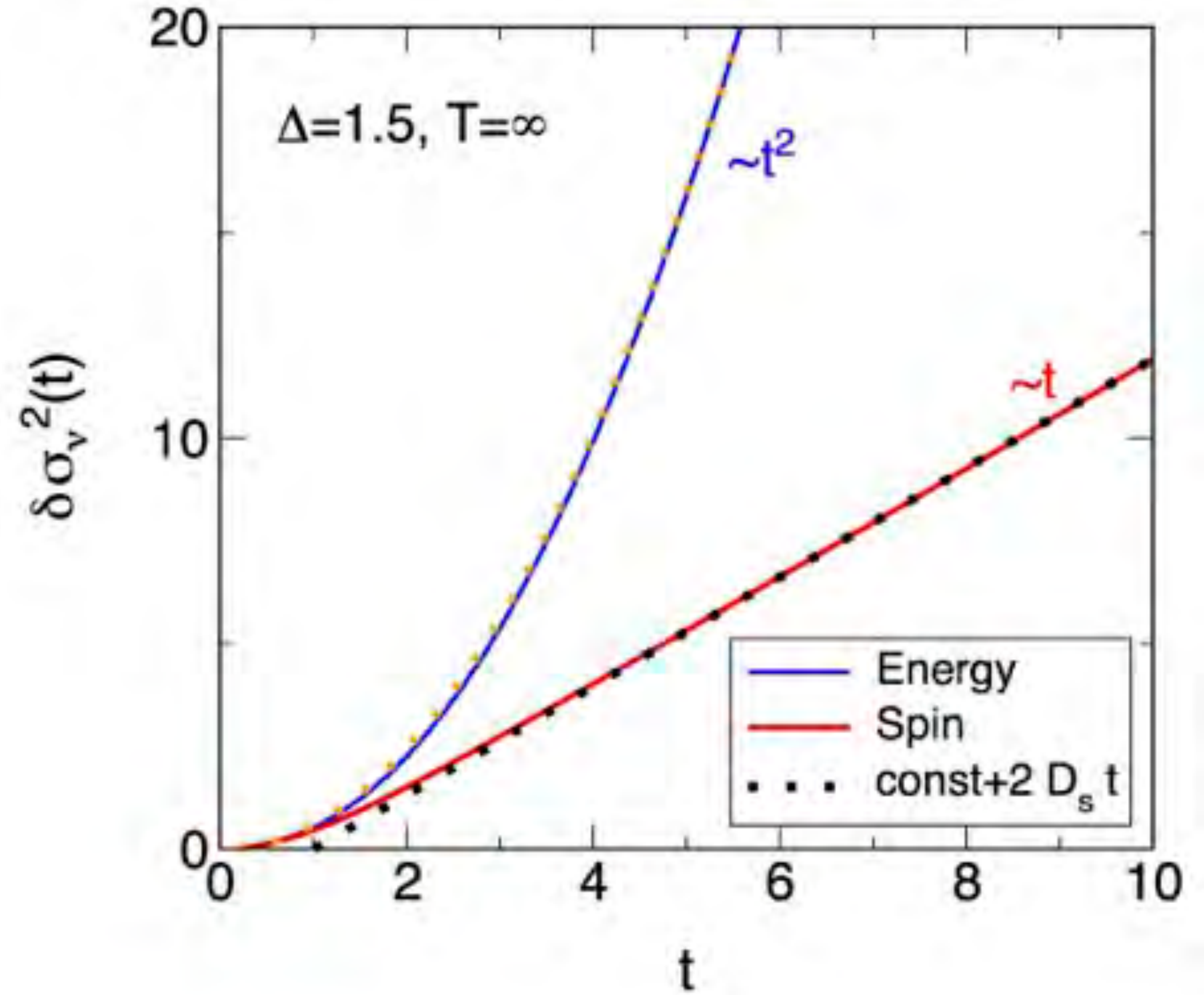


$$\sigma(t) \sim \sqrt{t}$$

Energy density: Ballistic



$$\sigma_e(t) \sim t$$



spin diffusion constant

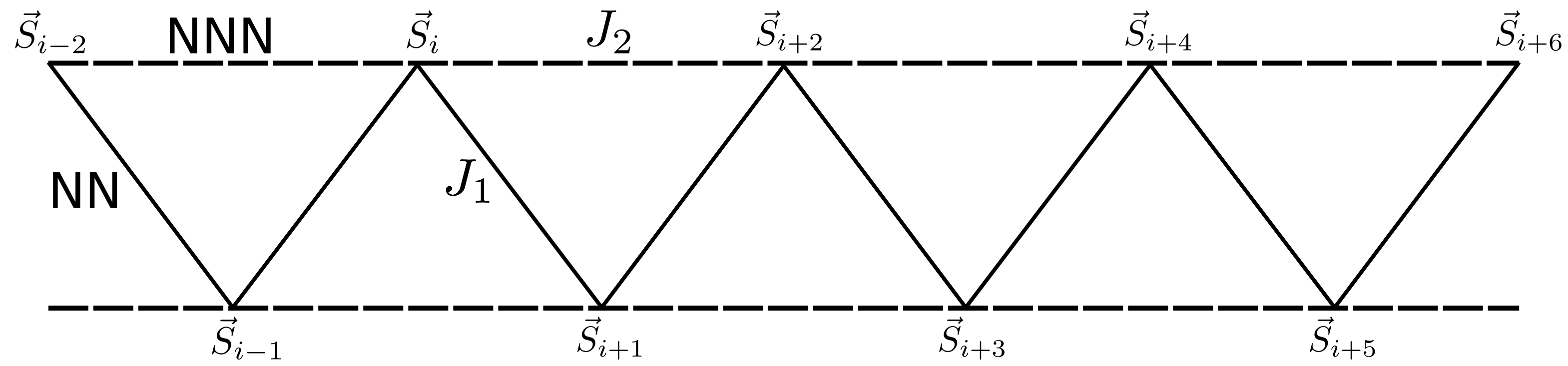
$$\sigma(t) \sim \sqrt{\mathcal{D}_s t}$$

(agrees with Kubo!)

Karrasch, Moore, FHM, Phys. Rev. B 89, 075139 (2014)

Thermal transport in frustrated spin chains

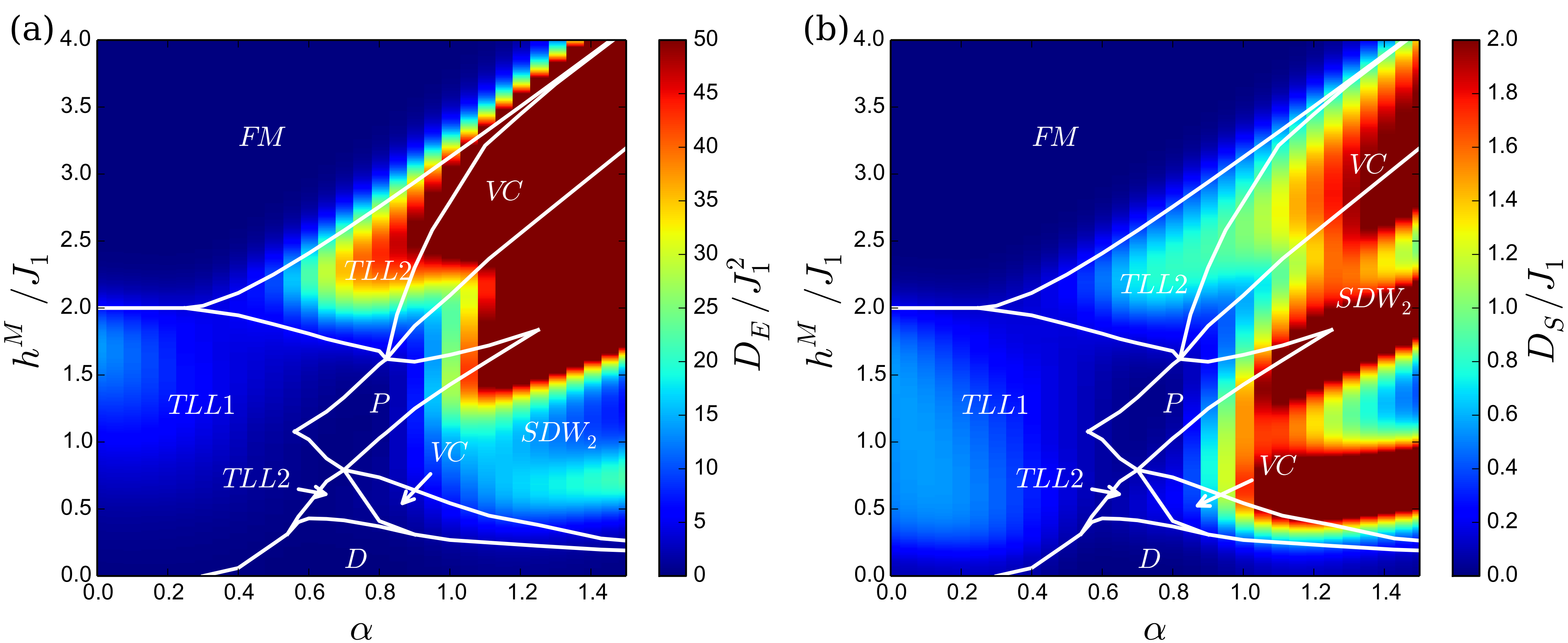
$LiCuVO_4$, $CuGe_2O_3$, ...



Vector chirality

$$\kappa_{ij}^z = (\vec{S}_i \times \vec{S}_j)^z$$

Hikihara et al. Phys. Rev. B 81, 224433 (2010)



Is thermal transport sensitive to vector chiral phase?

Started during a 2015 SPICE workshop !

Stolpp, Karrasch, FHM, Batista, in preparation

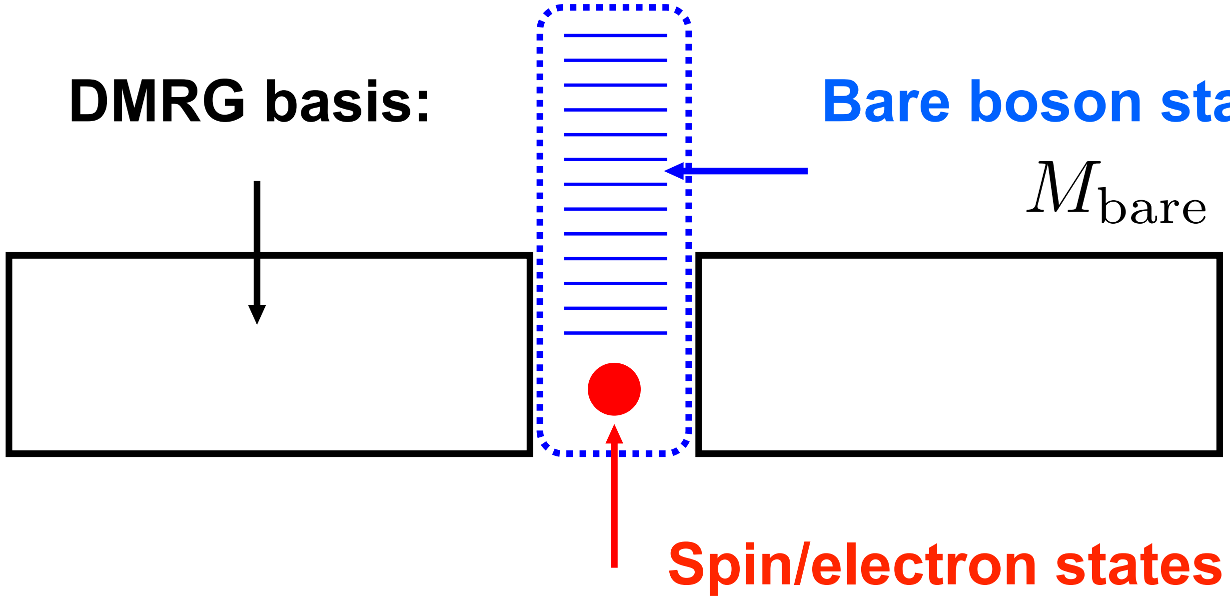
Finally ... towards phonons !

Novel DMRG/TEBD algorithm

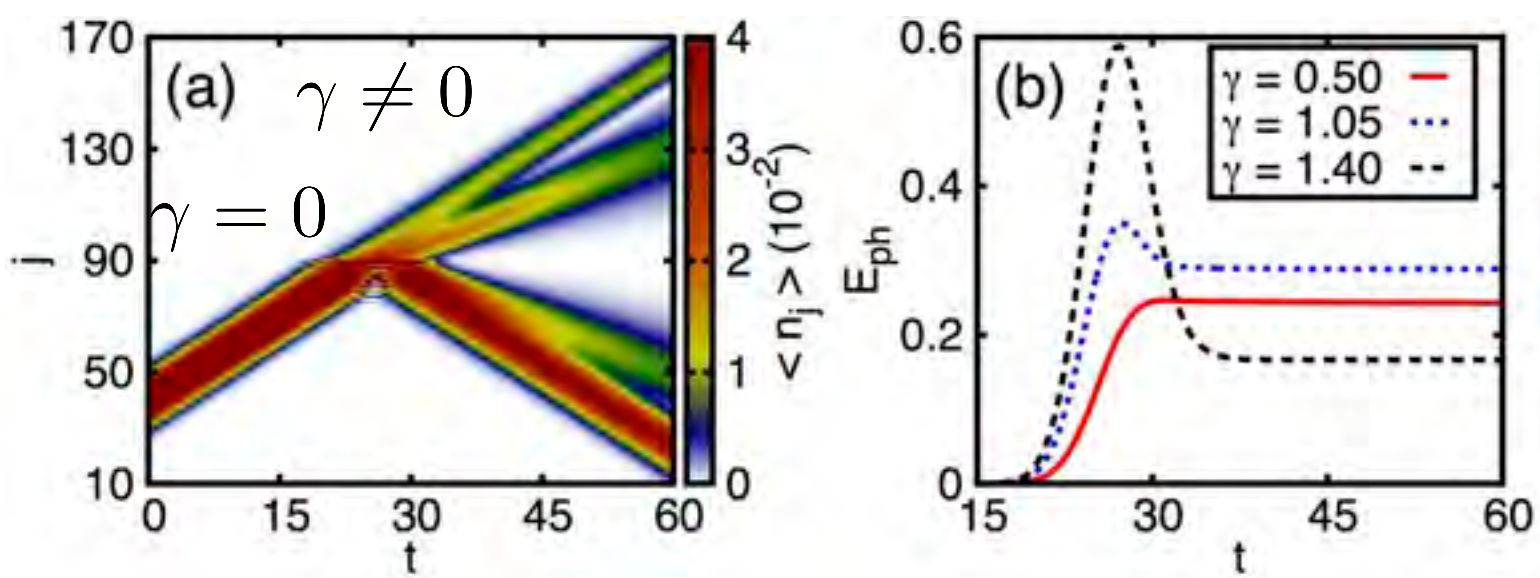
Adaptive update & truncation
DMRG & local state space
Diagonalize reduced
single-site density matrix

$$\rho^{(1)}|\varphi_\alpha\rangle = \omega_\alpha|\varphi_\alpha\rangle$$

Zhang, Jeckelmann, White PRL 1998



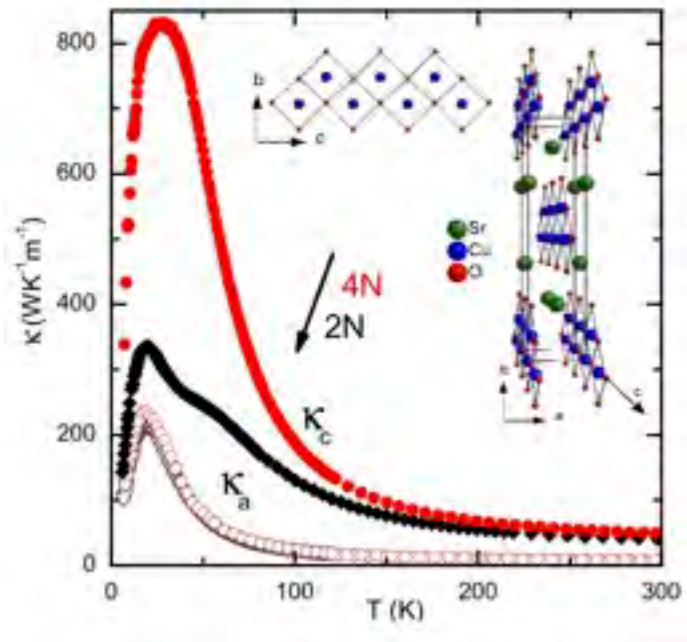
First applications: Polaron formation & wave packets in Holstein chains



Brockt, Dorfner, Vidmar, FHM, Jeckelmann, Phys. Rev. B 92, 241106(R) (2015)

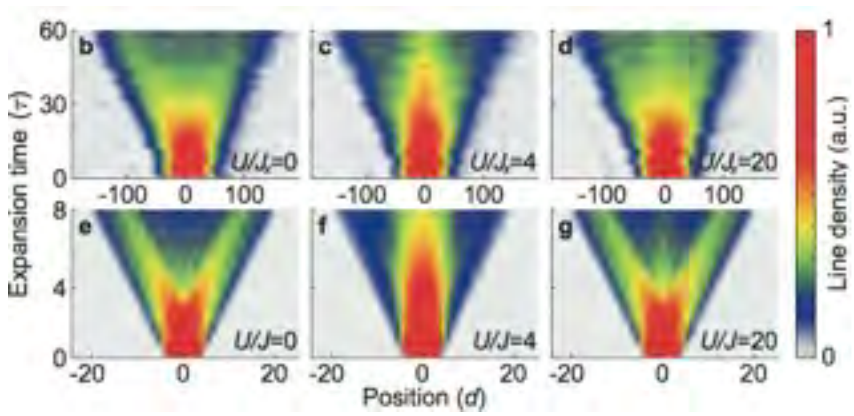
Summary

Large "magnon" heat transport in AFM quantum magnets



Hlubek, Büchner, Hess, et al., PRB 2010
Sologubenko et al. PRB 2001

Ballistic nonequilibrium transport in optical lattice



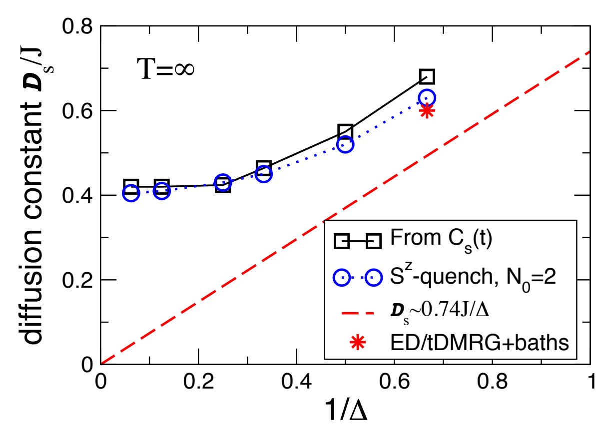
Phys. Rev. Lett. 110, 205301 (2013)

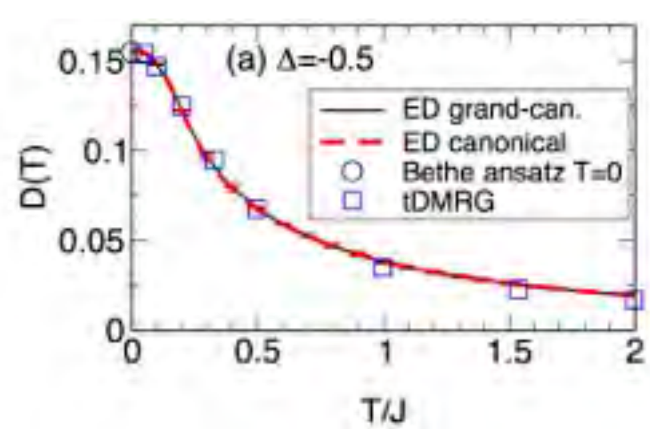
Theory: Spin-1/2 chains

Dissipationless heat & spin transport possible (integrability)

Coexistence of ballistic heat with diffusive spin transport!

Exact numerical calculations





PRB 87, 245128 (2013)
PRB 89, 075139 (2014)

Open questions

Magnetothermal effects?

Spin transport in exp.?

Today: Sr_2Cu0_3
Hirobe et al. arXiv: 1609.06410

Exp. observation of Drude weights?

Heat management?

Thank you!

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