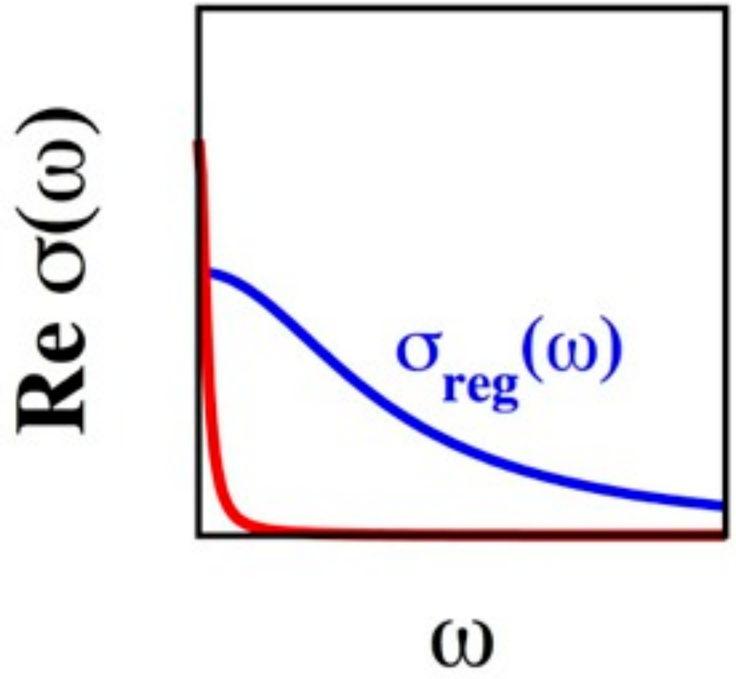
Transport in spin ladders and the 1D Hubbard model



Fabian Heidrich-Meisner
Ludwig-Maximilians-University Munich
Kolymbari, Sept. 17, 2015

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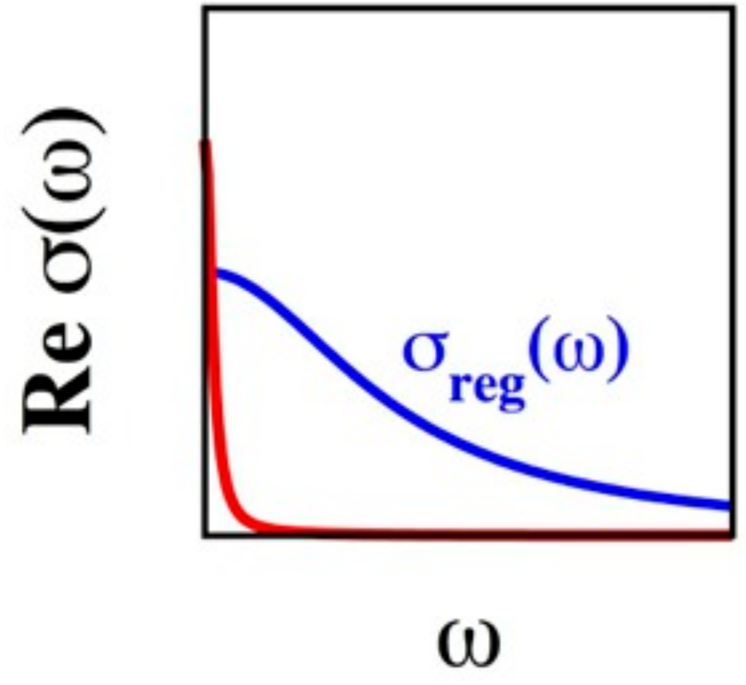
Transport in spin ladders (& chains) and the 1D Hubbard model



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DFG-FG 912

Outline

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

Non-trivial conservation laws in 1D

Divergent conductivities in 1D integrable models

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

Ballistic, ..., diffusive dynamics

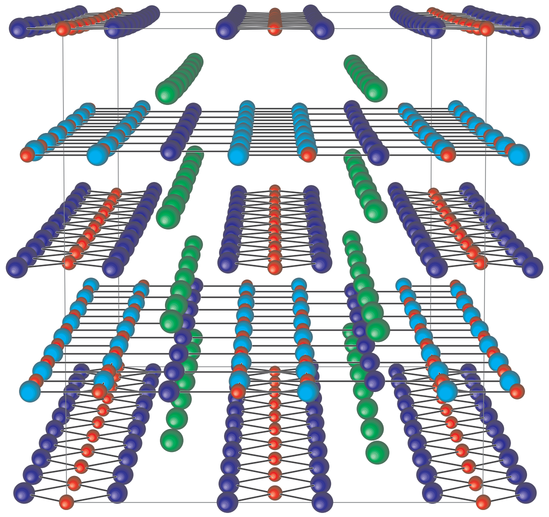
1) Experimental context

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

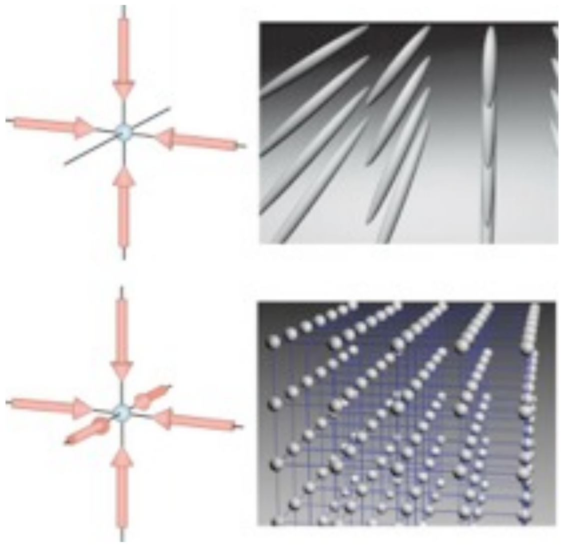
3) Spin-1/2 ladders

4) Hubbard chains

Quantum magnets



Optical lattices



In collaboration with:





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UC Berkeley

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RWTH Aachen

Stephan Langer
LMU → U Pittsburgh

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Deutsche Forschungsgemeinschaft DFG

DFG-FG 912

DFG-Forschergruppe 801

Finite-temperature Drude weights

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

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 finite temperatures

Same reasoning for
charge, particle, spin, thermal transport

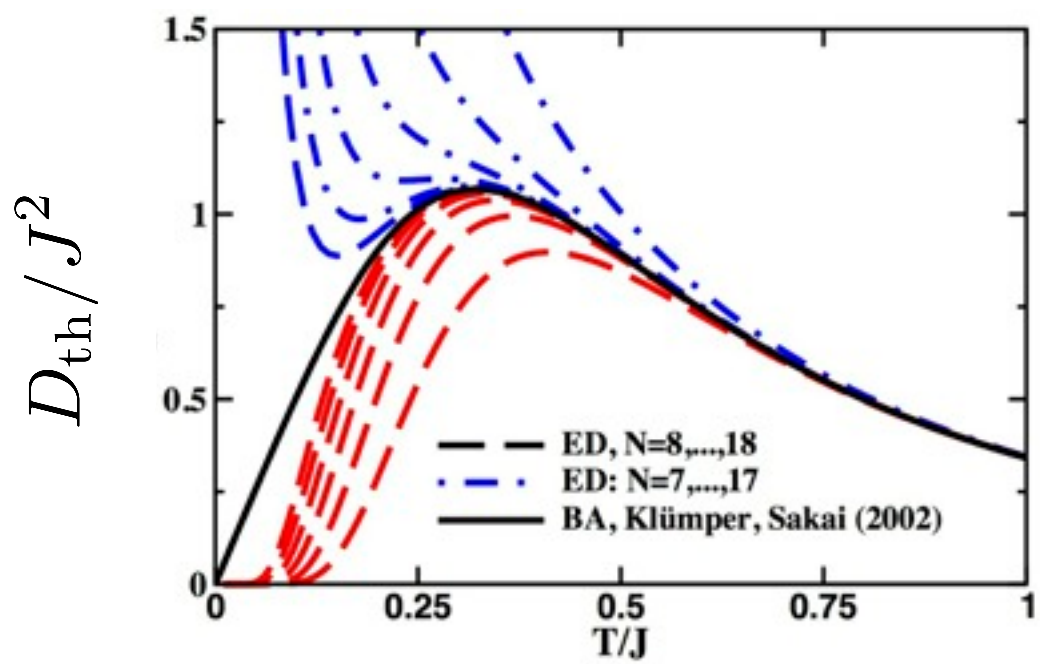
Best-known (non-trivial) example
S=1/2 Heisenberg chain

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

$$j_{\mathrm{th},l} \sim \vec{S}_l \cdot (\vec{S}_{l+1} \times \vec{S}_{l+3}) \;\; [H, j_{\mathrm{th}}] = 0$$

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

Zotos, Naef, Prelovsek, Phys. Rev. B 55, 11029 (1997)



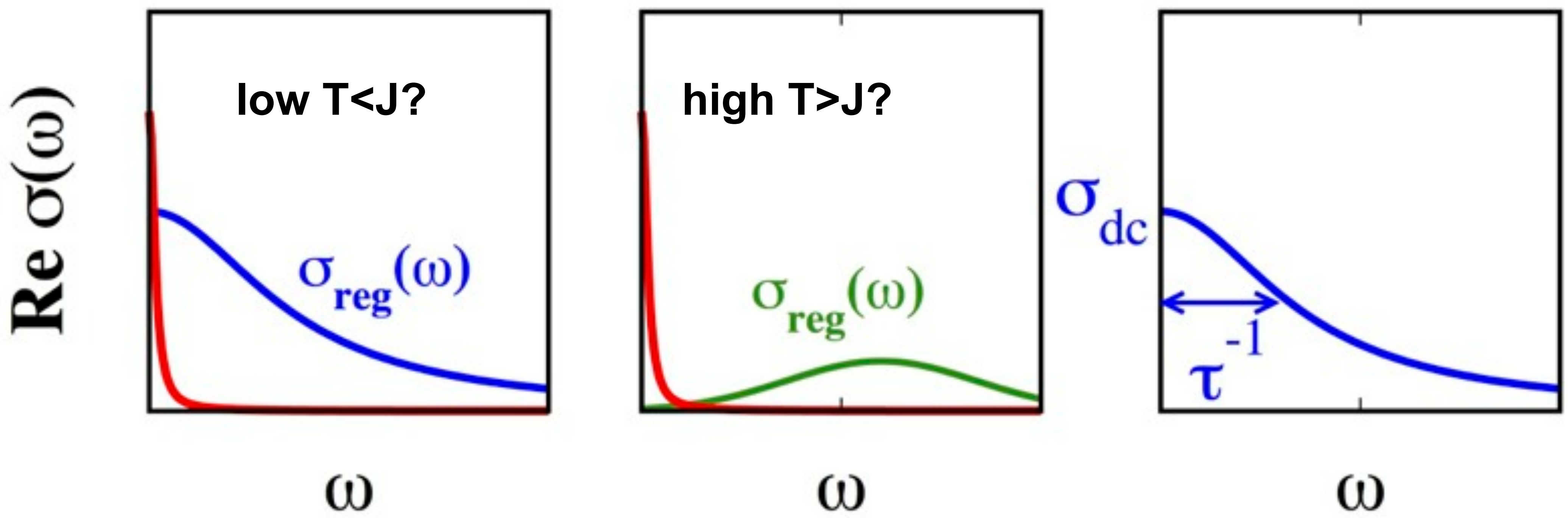
Klümper, Sakai J. Phys. A 35, 2173 (2002)
FHM, Honecker, Cabra, Brenig, Phys. Rev. B 66, 140406(R) (2002)

Open questions, possible scenerios

In general:
(spin transport, Hubbard)

$$[H, j] \neq 0$$

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



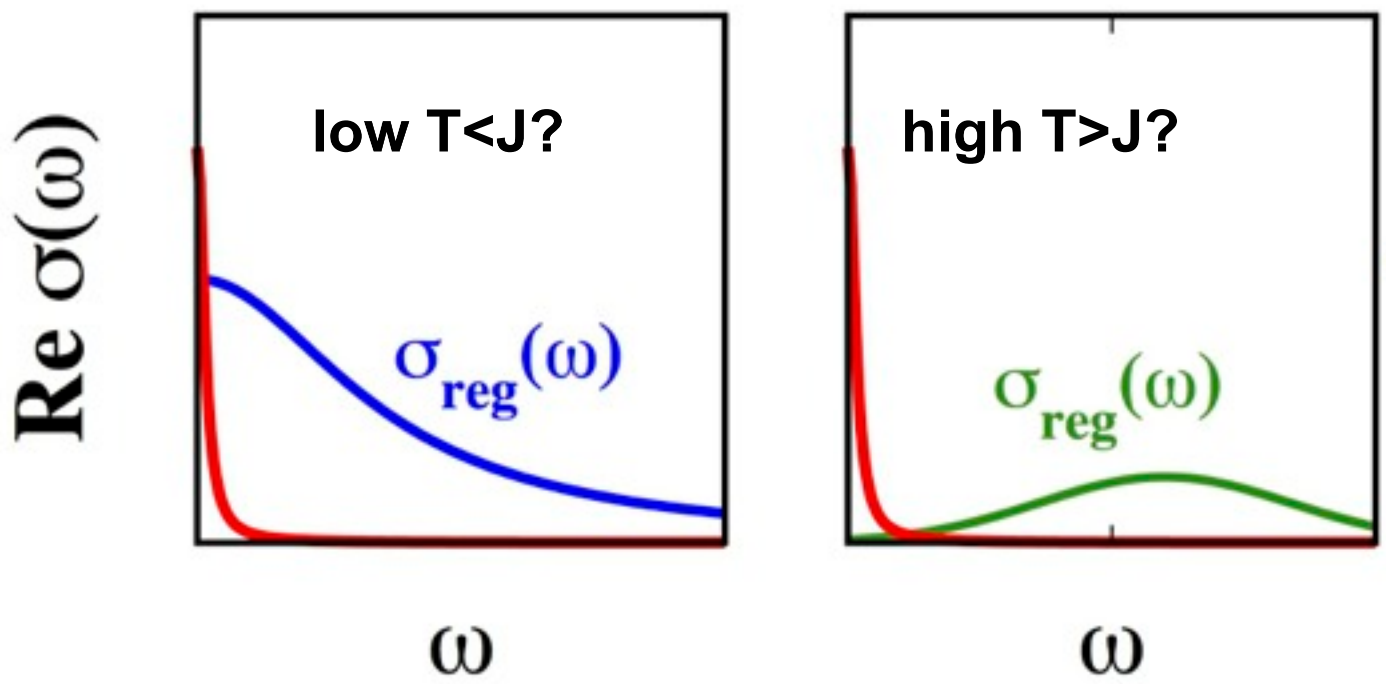
Low-frequency dependence
Finite Drude weights at T>0 - dissipationless transport?
Standard diffusion in 1d? Diffusion constants?
Role of integrability?

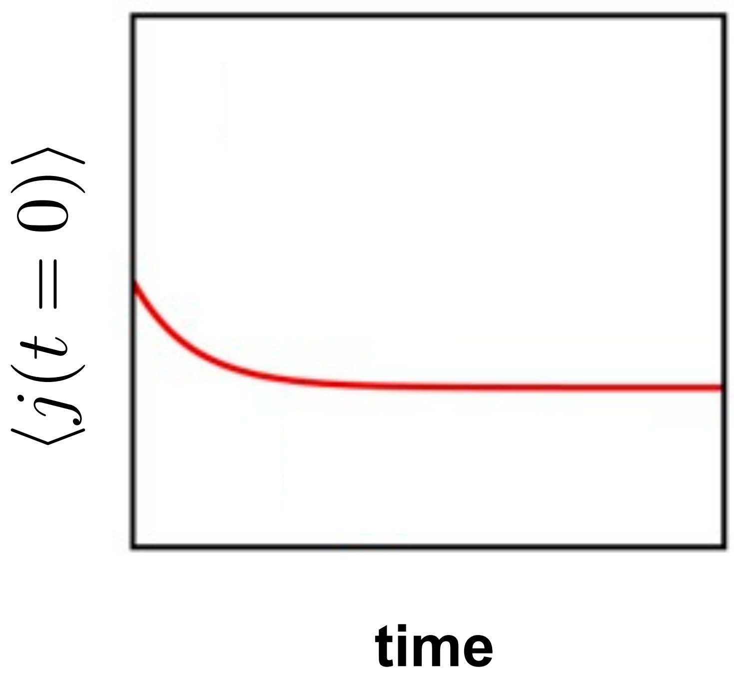
Bethe ansatz: Zotos, Klümper, Prosen, ...
ED: Herbrych, Steinigeweg, Prelovsek, Zotos, ...
Field theory: Sirker, Perreira, Affleck, Rosch, Andrei, Fujimoto, Kawakami, Giamarchi, Damle, Sachdev....
QMC: Grossjohann, Brenig, Sorella, Alvarez, Gros, ...
DMRG: Karrasch, Moore, ...
Open quantum systems: Znidaric,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

HERE:
ED & DMRG

Open questions, possible scenerios

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





$$[H, j] \neq 0 \qquad [H, Q_\alpha] = 0$$

$$\langle j Q_\alpha \rangle \neq 0$$

$$\langle j(t) j \rangle \to \mathrm{const}$$

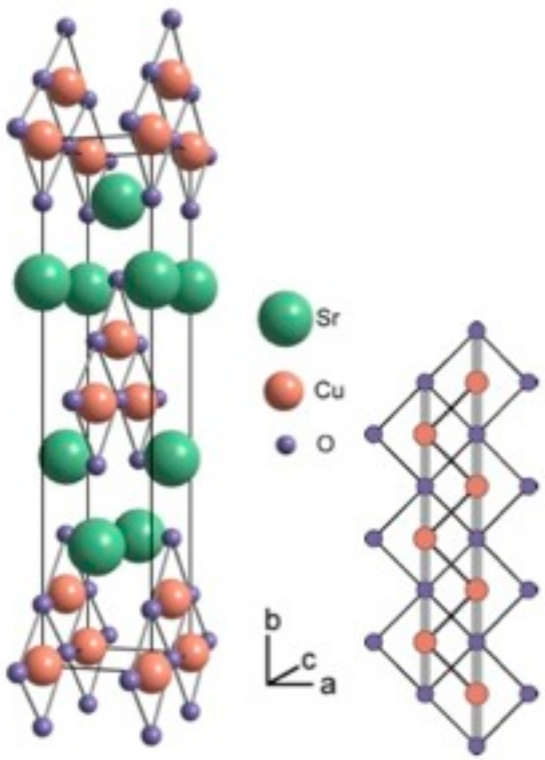
Decay of currents protected by conservation law

Generalized Gibbs ensemble!

See Caux' talk

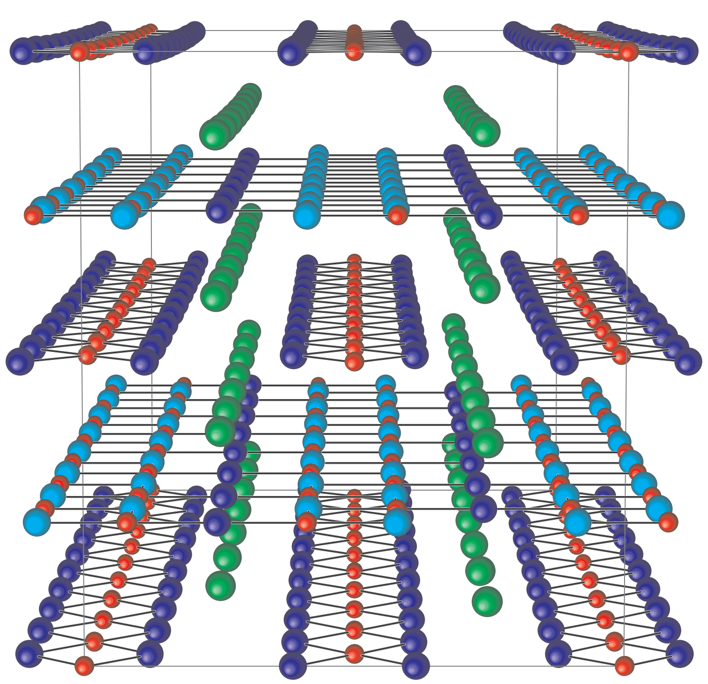
Thermal transport in quantum magnets

1D



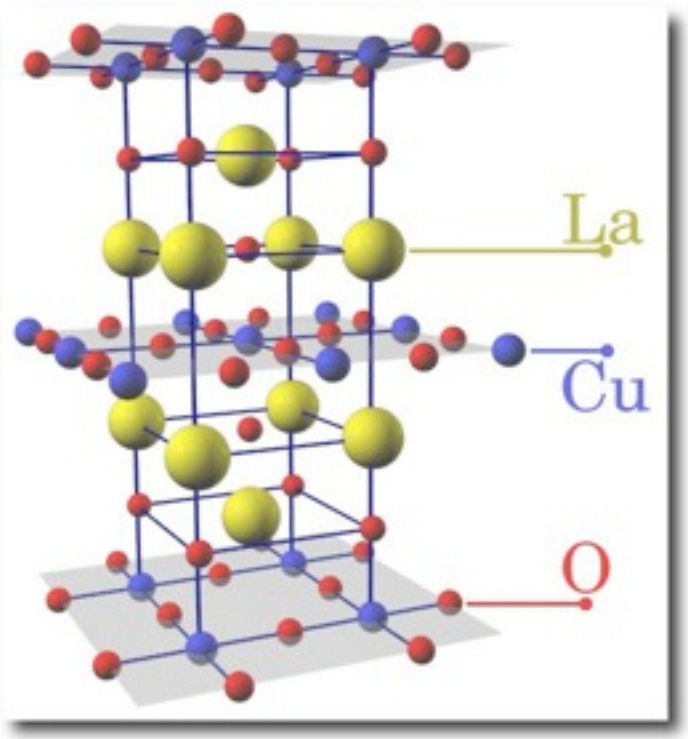
$SrCuO_2$

Ladders



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

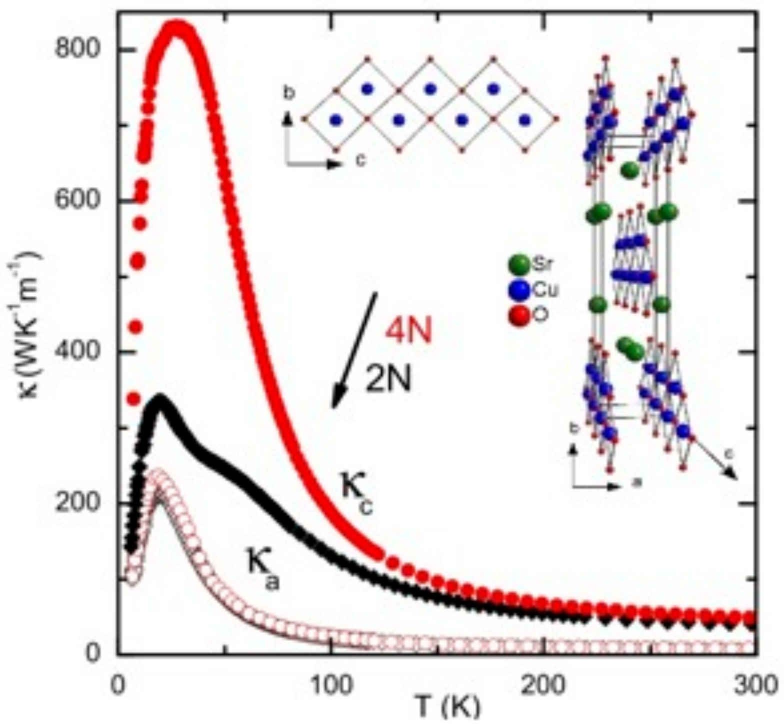
2D



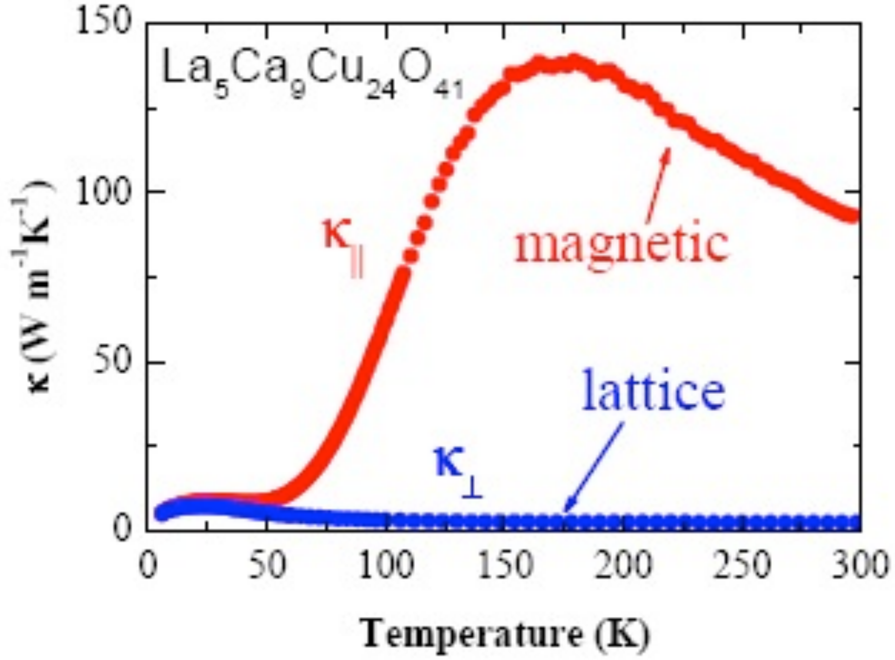
La_2CuO_4

Thermal transport in quantum magnets

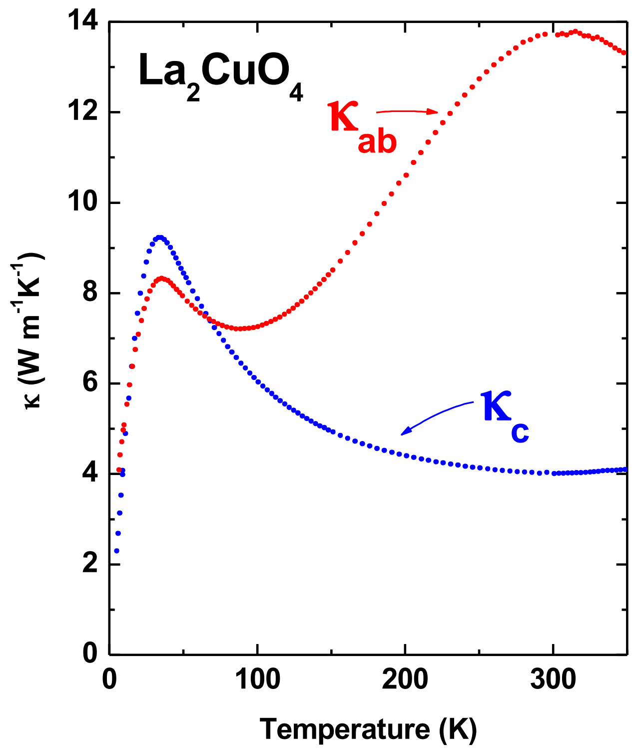
1D - Spinons | **Ladders - Triplett excitations** | **2D - Magnons**



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



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



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

Magnetic excitations contribute significantly to thermal conductivity κ

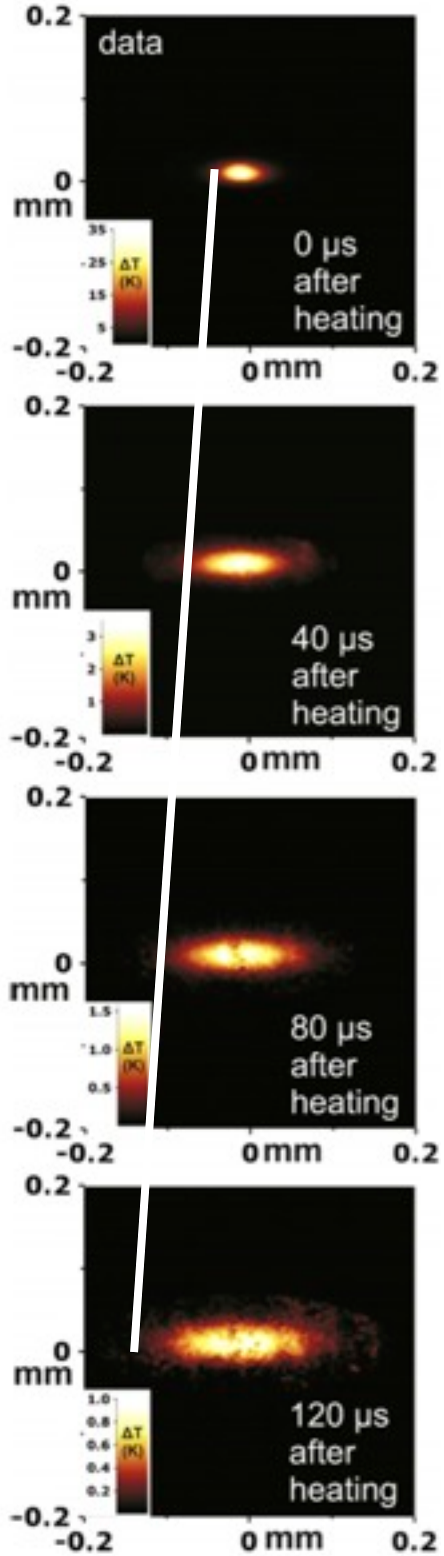
Many other thermal transport experiments: Lorenz, Sun, Sales, Mandrus, ...

Spin transport only probed indirectly via NMR, μsr

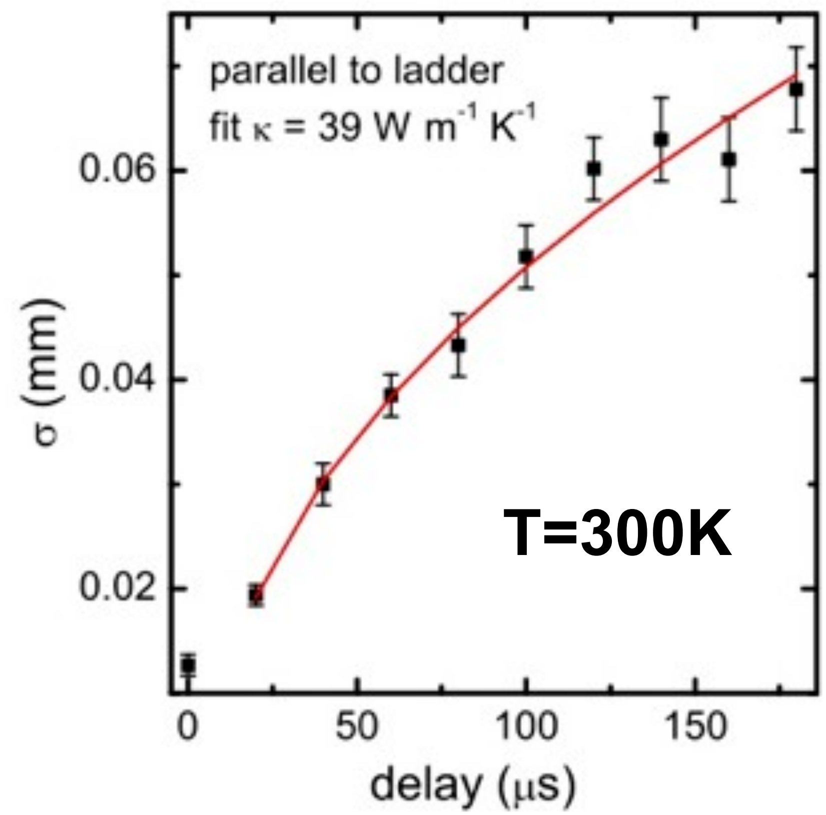
Thurber et al. PRL 2001, Maeter et al. 2013, Xiao et al. 2014

New experiments: Time-resolved measurements

Ladders



See
Montagnese's talk



Width of Gaussian fits:

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

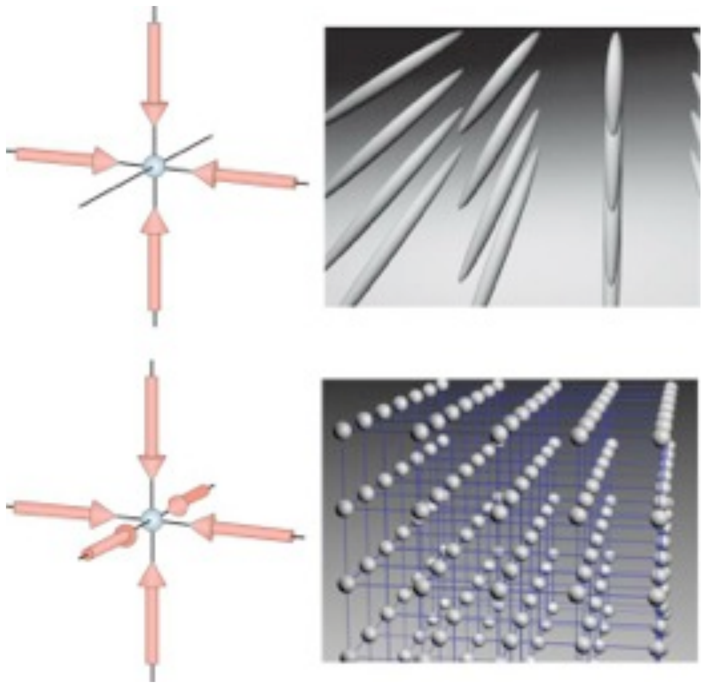
Experiments:
Phonons are important

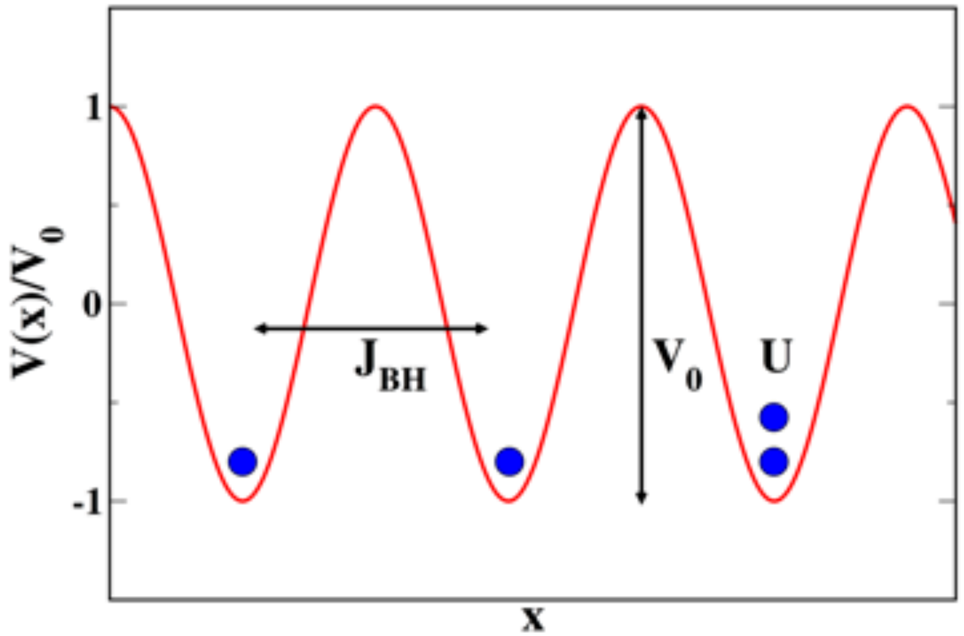
Montagnese, van Loosdrecht, Hess, et al., Phys. Rev. Lett., 110, 147206 (2013)
Otter et al. Int. J. of Heat and Mass Transfer 55, 2531 (2012)

Wave-packet spreading in spin systems

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

Mass transport in optical lattices





$$U/J_{BH} = f(V_0)$$

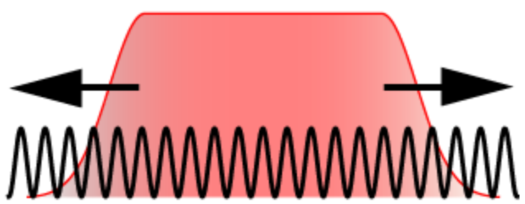
$$H = -J_{BH} \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i(n_i - 1)$$

Greiner, et al. Nature 2002; Bloch, Dalibard, Zwerger, Rev. Mod. Phys. 2008

Sudden expansion: Experimental sequence

^{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:

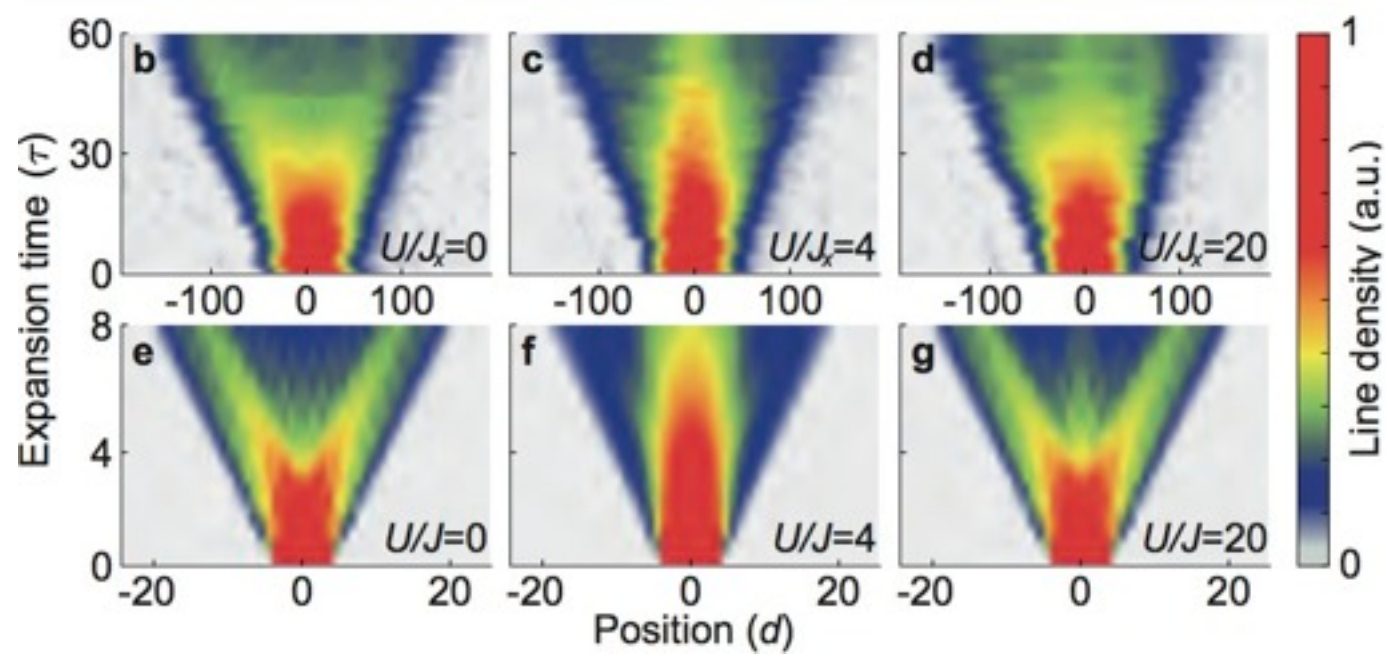
$$|\psi_{\text{initial}}\rangle = \prod_i a_i^\dagger |0\rangle$$

Spin-down - up - down

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

Exp. data

DMRG

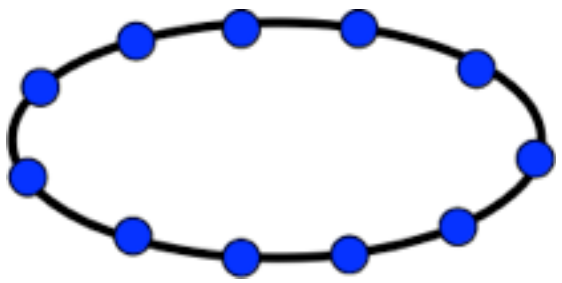


Profiles for non-interacting and *strongly* interacting bosons are identical!

Ronzheimer, Schreiber, Braun, Hodgman, Langer, McCulloch, FHM, Bloch, Schneider Phys. Rev. Lett. 110, 205301 (2013)

Optical-lattice experiment on spin diffusion in 1D Heisenberg: Hild et al. Phys. Rev. Lett. 113, 147205 (2014)

Strongly interacting bosons in 1D



$$H = -J_{BH}\sum_i (a^\dagger_{i+1}a_i + h.c.) + \frac{U}{2}\sum_i n_i(n_i - 1)$$

$$a_i^{\dagger\,2} = 0$$

U=∞: Hard-core bosons = XY models = spinless non-interacting fermions!

$$\rightarrow H_{HCB} = -J_{BH}\sum_i (f^\dagger_{i+1}f_i + h.c.) = \sum_k \epsilon_k n_k^f$$

Integrable quantum model

Cazalilla et al. Rev. Mod. Phys. 2011
Paredes et al. Nature 2004, Wenger et al. Science 2004

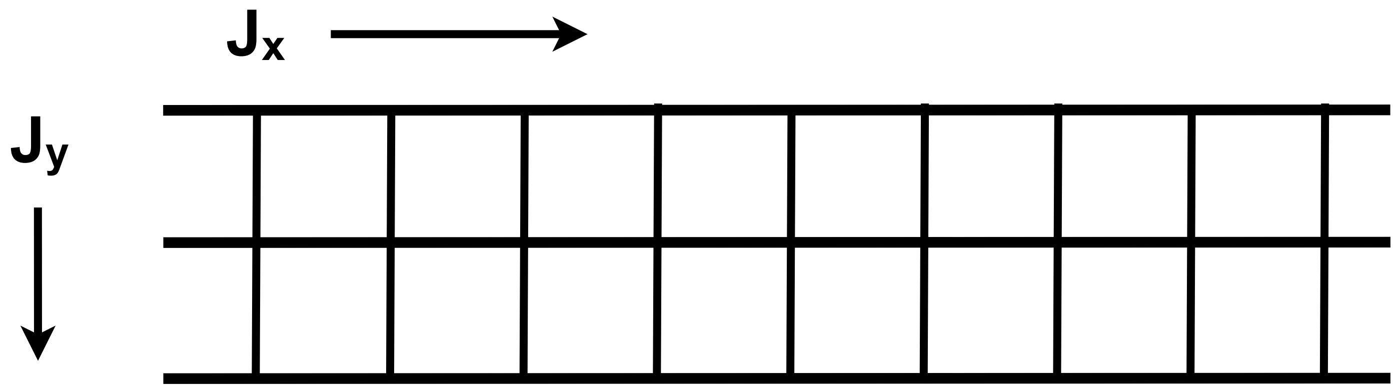
Conserved charges

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

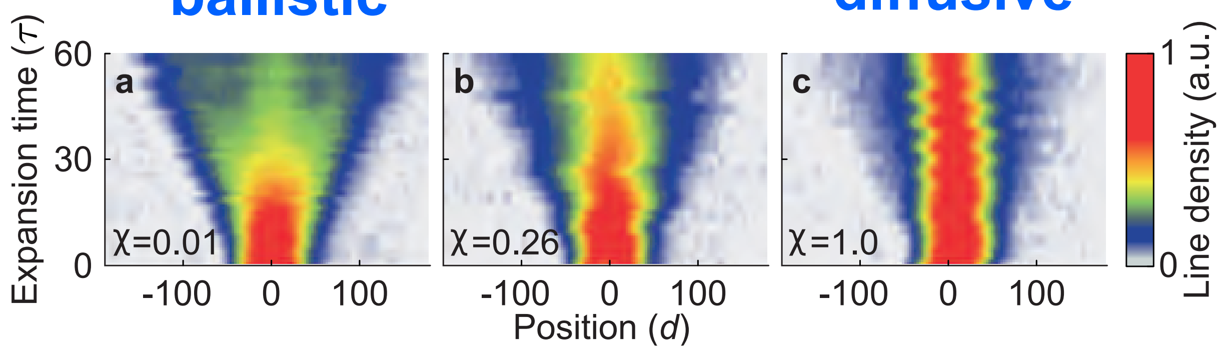
$$H_{HCB} = H_{XX} = \frac{J}{2}\sum_{\langle i,j\rangle}(S_i^+ S_j^- + h.c.)$$

S=1/2 XX model: Dimensional crossover, ladders

$$\chi = \frac{J_y}{J_x}$$



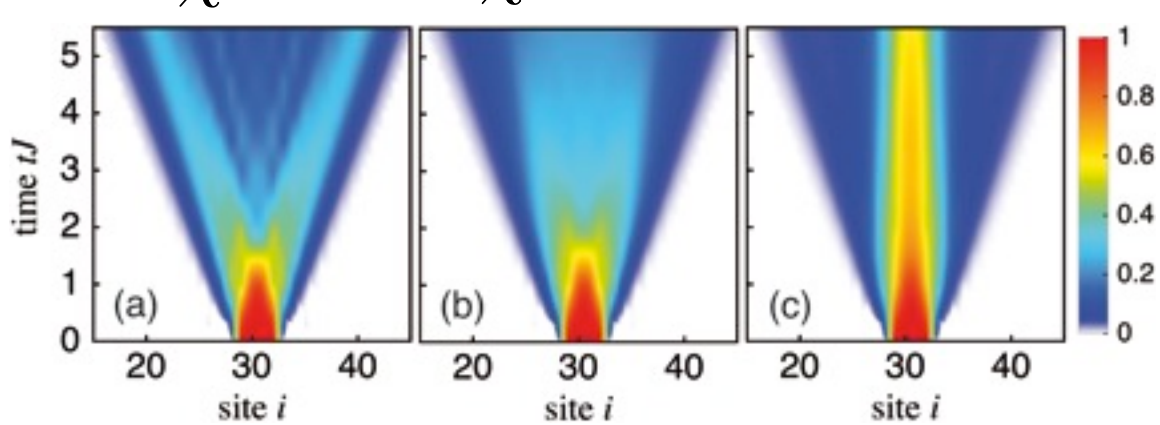
ballistic **diffusive**



1D **2D**

Ronzheimer et al. Phys. Rev. Lett. 2013

$\chi = 0$ $\chi = 0.5$ $\chi = 1$



XX ladders

Vidmar, Langer, McCulloch, Schneider, Schollwöck, FHM PRB 88, 235117(2013)

Hard-core bosons = Spin-1/2 XX model: Study integrability breaking !

Ladders:
“Textbook” diffusive conductor

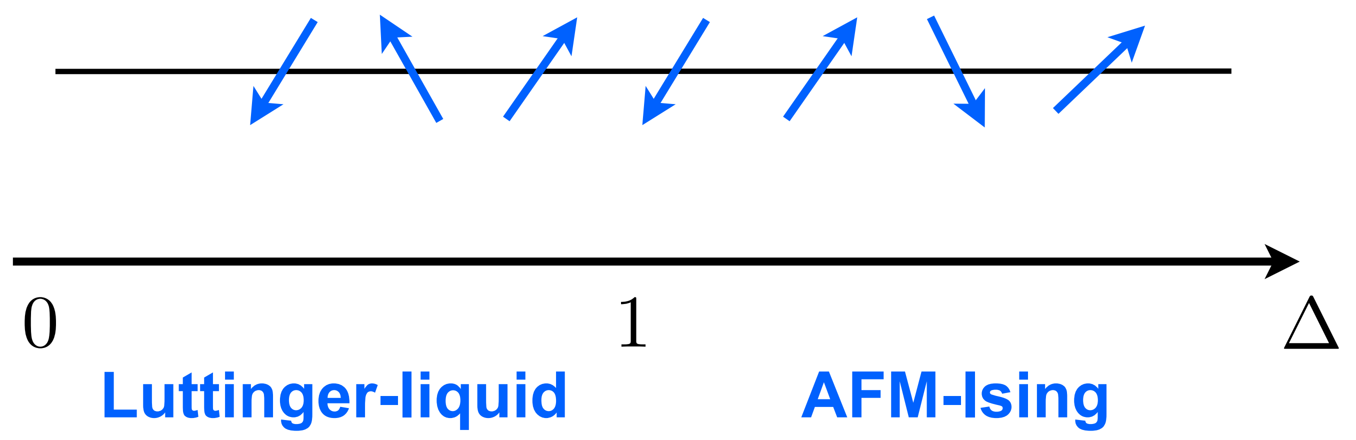
$$\mathrm{Re}\,\sigma(\omega) \propto \frac{D}{\omega^2 + {\tau^{-1}}^2}$$

Steinigeweg, FHM, Gemmer, Michielsen, de Raedt
Phys. Rev. B 90, 094417 (2014)
Karrasch, Kennes, FHM
Phys. Rev. B 91, 115130 (2015)

Spin transport in the spin-1/2 XXZ model

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

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



The role of extra non-trivial conservation laws

In general:

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

Integrable 1D systems:
Many local conservation laws Q_α

Ballistic transport -
protected by (local) conservation laws
- if:

$$D(T) \geq \text{const} \frac{|\langle j_s Q_\alpha \rangle|^2}{\langle Q_\alpha^2 \rangle} > 0$$

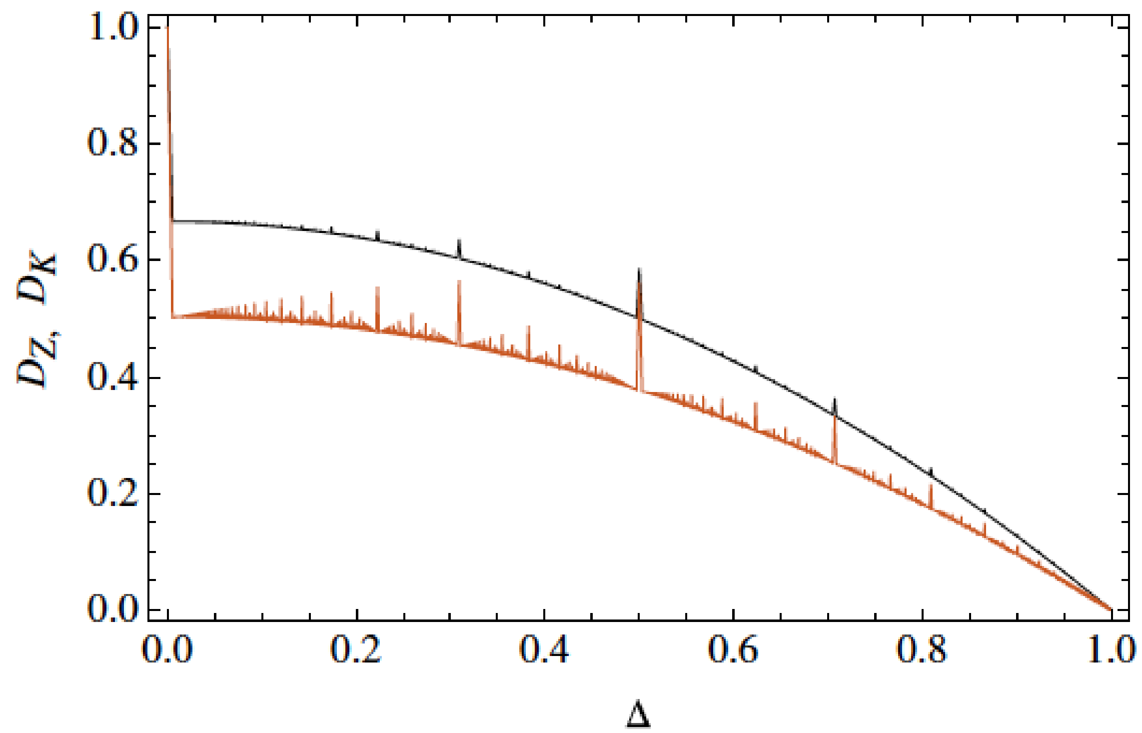
Mazur inequality
Zotos, Naef, Prelovsek, Phys. Rev. B 55, 11029 (1997)

Zero magnetization, XXZ:

$$\langle j_s Q_\alpha^{BA} \rangle = 0$$

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
Prosen Nucl. Phys, B 886, 1177 (2014), Pereira et al. J. Stat. Mech. (2014) P09037
Related ED: Jung, Rosch PRB 2007
Mierzierjewski, Prelovsek, Prosen PRL 2014

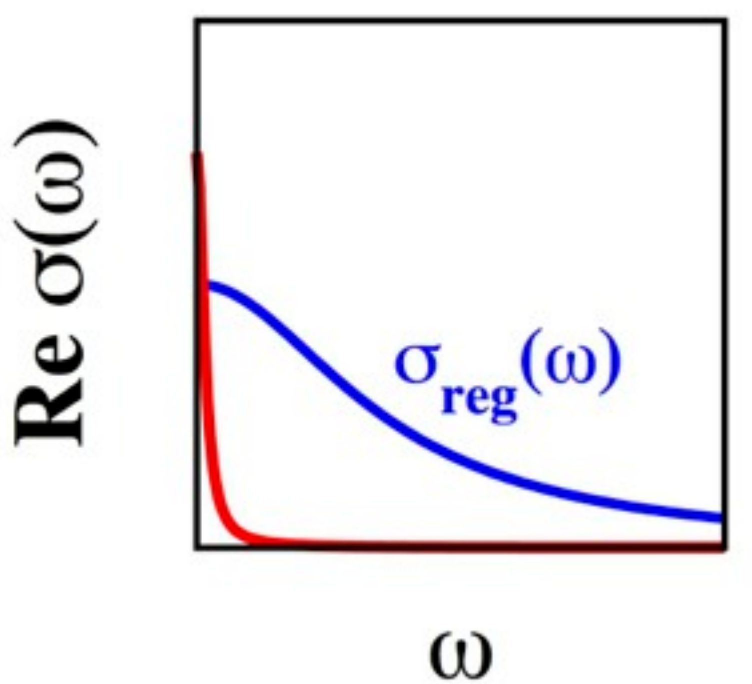
See A. Klümper's talk

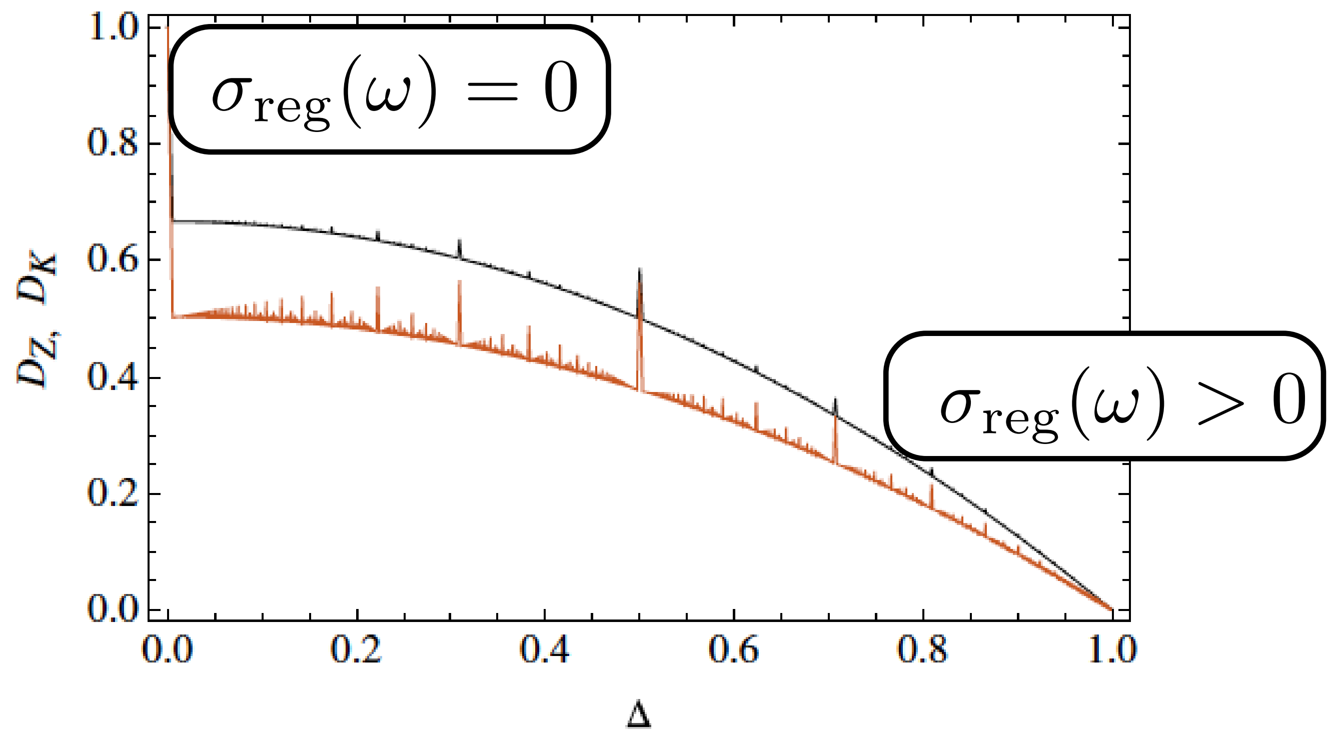
Ballistic channel & finite frequency coexist

Lower bound - quasi-local conserved charge:

Coexistence of ballistic & finite-frequency contributions

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





Sirker, Pereira, Affleck PRL 103, 216602 (2009), Naef, Zotos JPCM 10, 138 (1998)
Grossjohann, Brenig PRB 81, 012404 (2010) (low T)
Karrasch, Kennes, FHM PRB 91, 115130 (2015) (high T)

Prosen PRL 2011; Prosen, Ilievski PRL 2013
Prosen Nucl. Phys, B 886, 1177 (2014), Pereira et al. J. Stat. Mech. (2014) P09037
Related ED: Jung, Rosch PRB 2007
Mierzierjewski, Prelovsek, Prosen PRL 2014

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

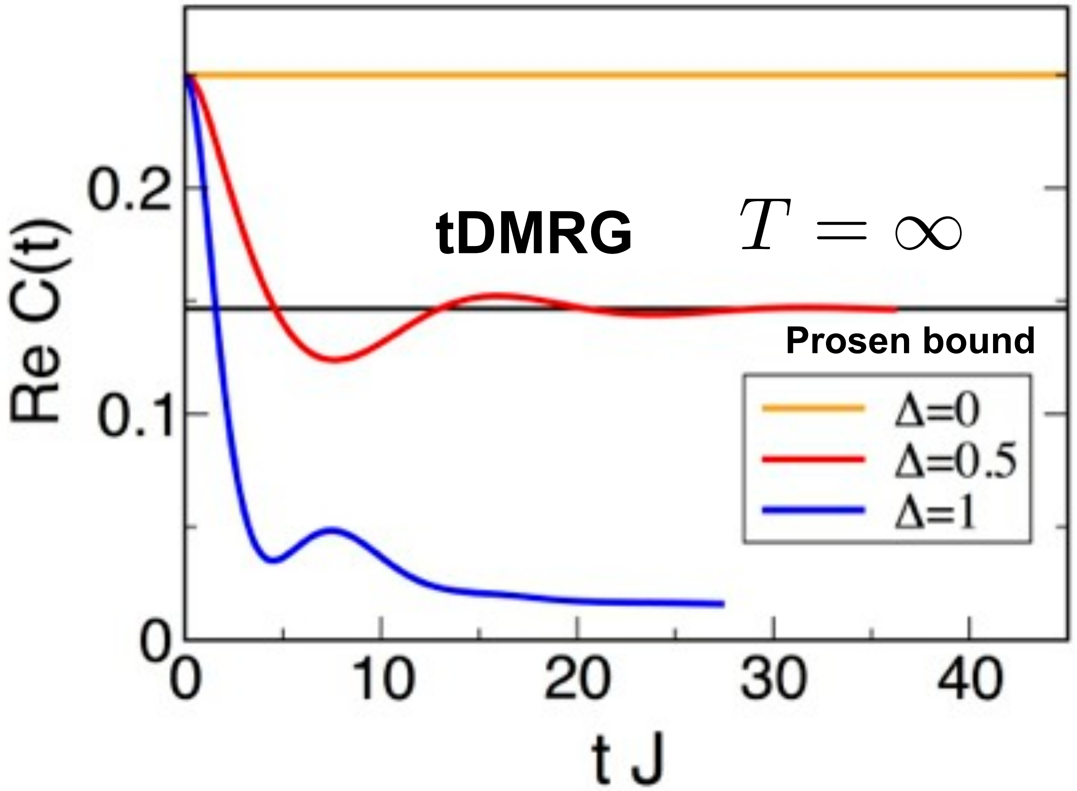
Many-body, 1D

L ~ 100 possible

Infinite times not accessible

Real-time:
Spin-current autocorrelations

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

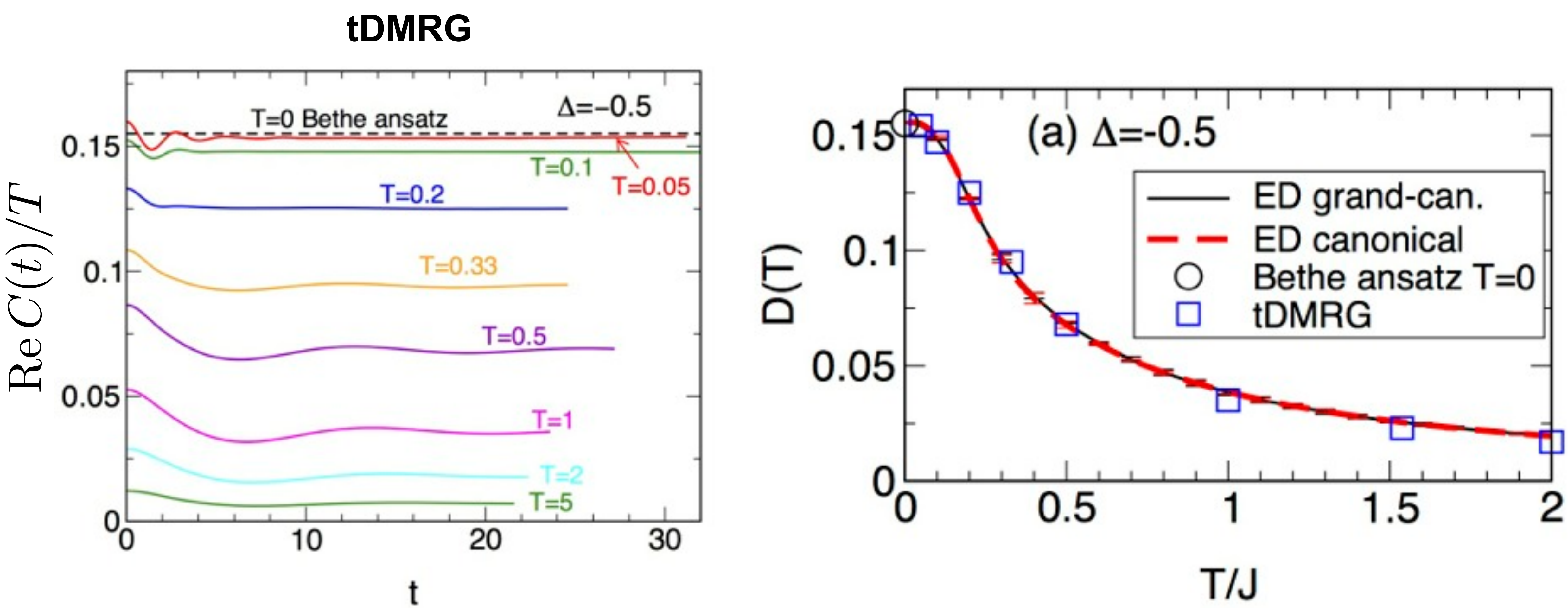


no finite-size effects!

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

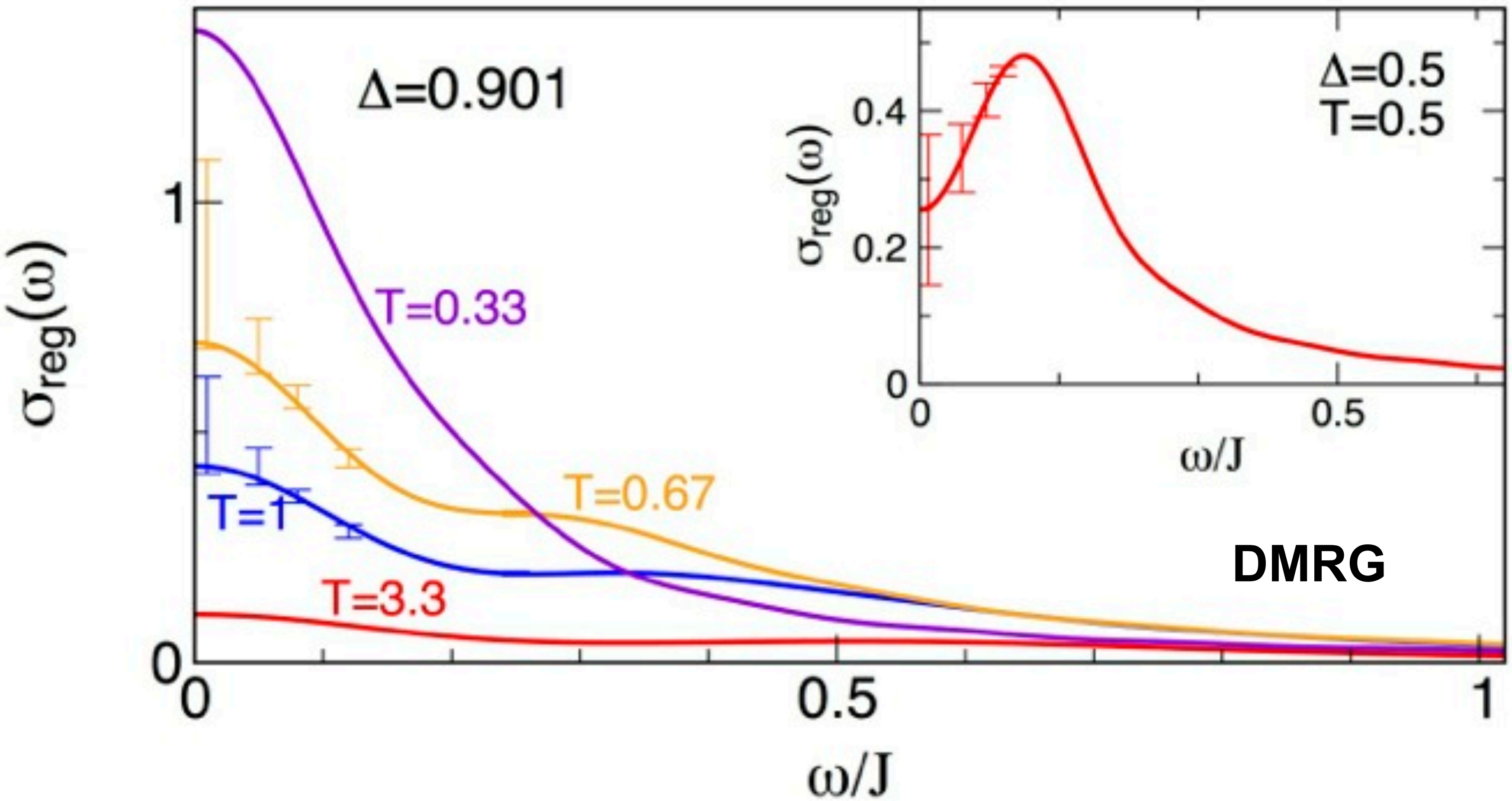
$$-1 < \Delta < 0$$



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)

Spin transport: Optical conductivity



using linear prediction!

Down to T ~ 0.3J: $\sigma_{\mathrm{dc}}(T) > 0$

Inconsistent with Herbrych, Steinigeweg, Prelovsek PRB 86, 115106 (2012)

No simple Lorentzian, suppressed low-frequency weight at special points

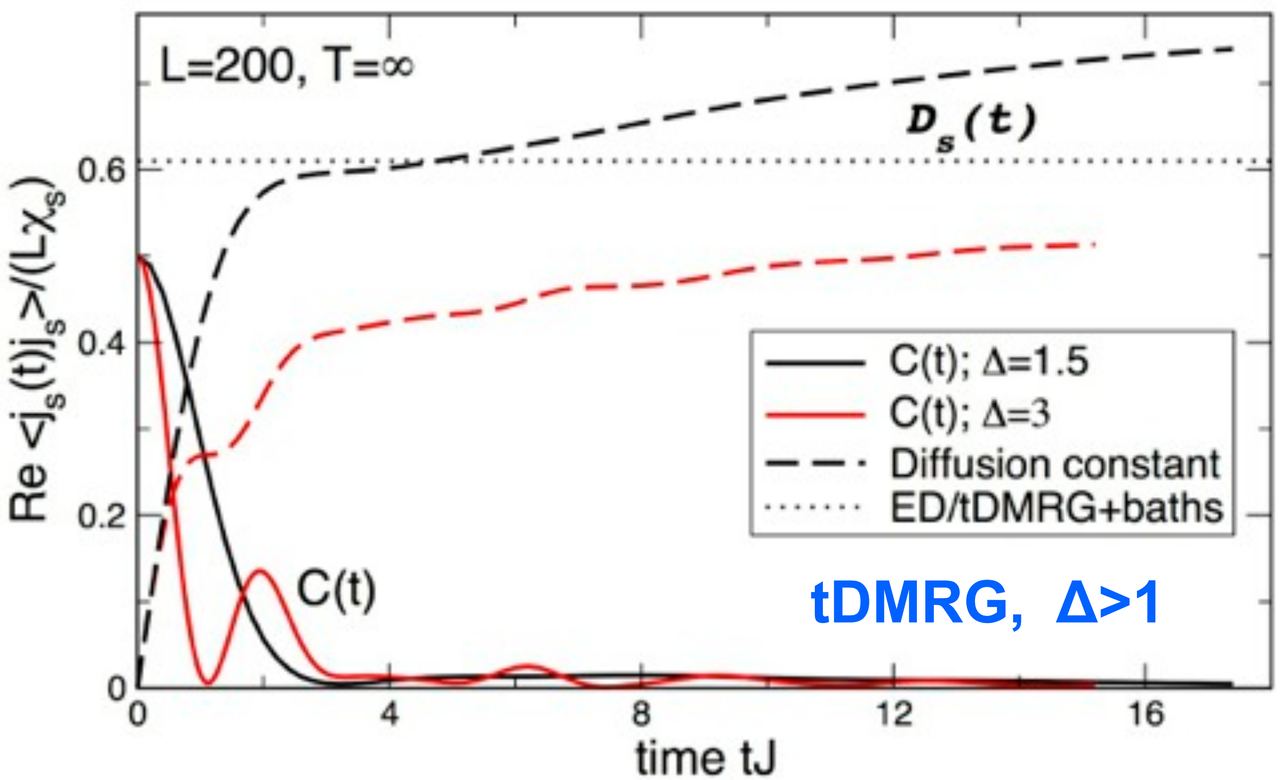
Karrasch, Kennes, FHM; Phys. Rev. B 91, 115130 (2015)

Diffusion in the AFM-Ising phase

$\Delta > 1$

Common belief: spin No Drude weight

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



No ballistic tail

$\mathcal{D}_s(t)$ saturates for large Δ

Diffusion constant - Einstein relation at T= ∞

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

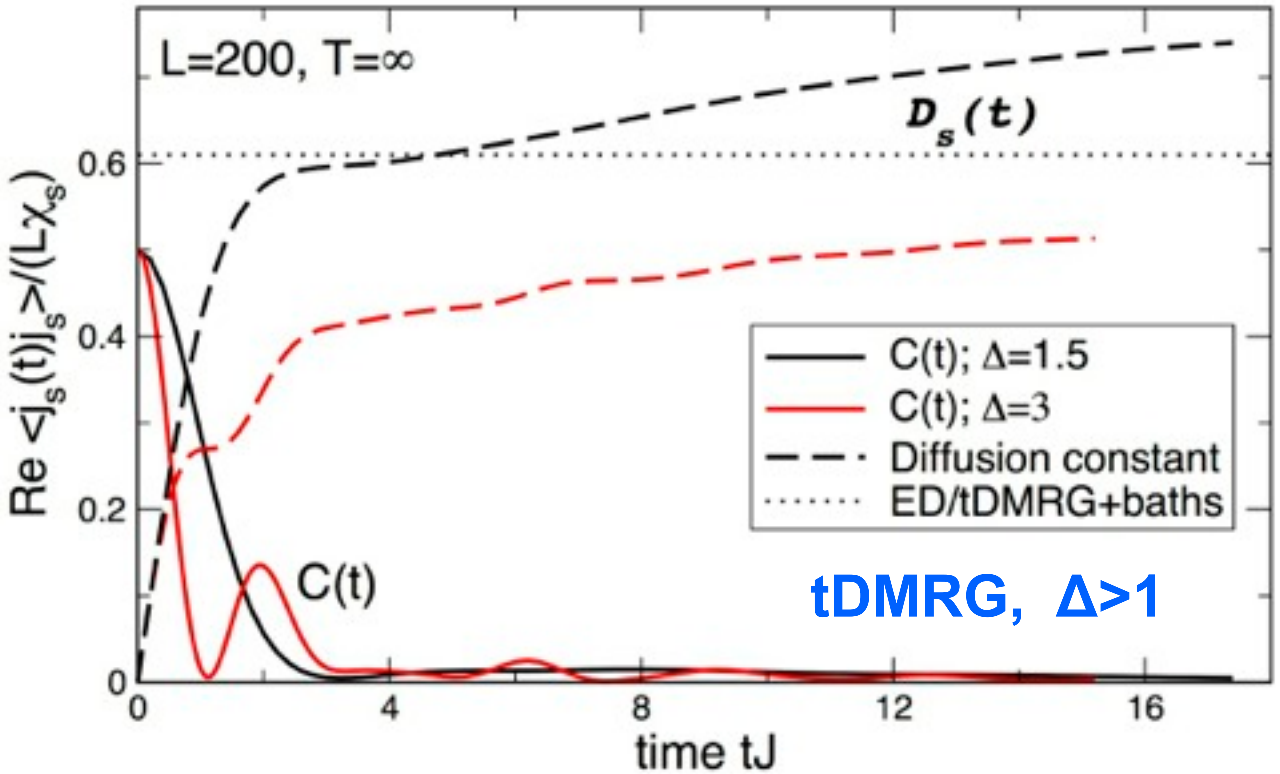
Karrasch, Moore, FHM, Phys. Rev. B 89, 075139 (2014)

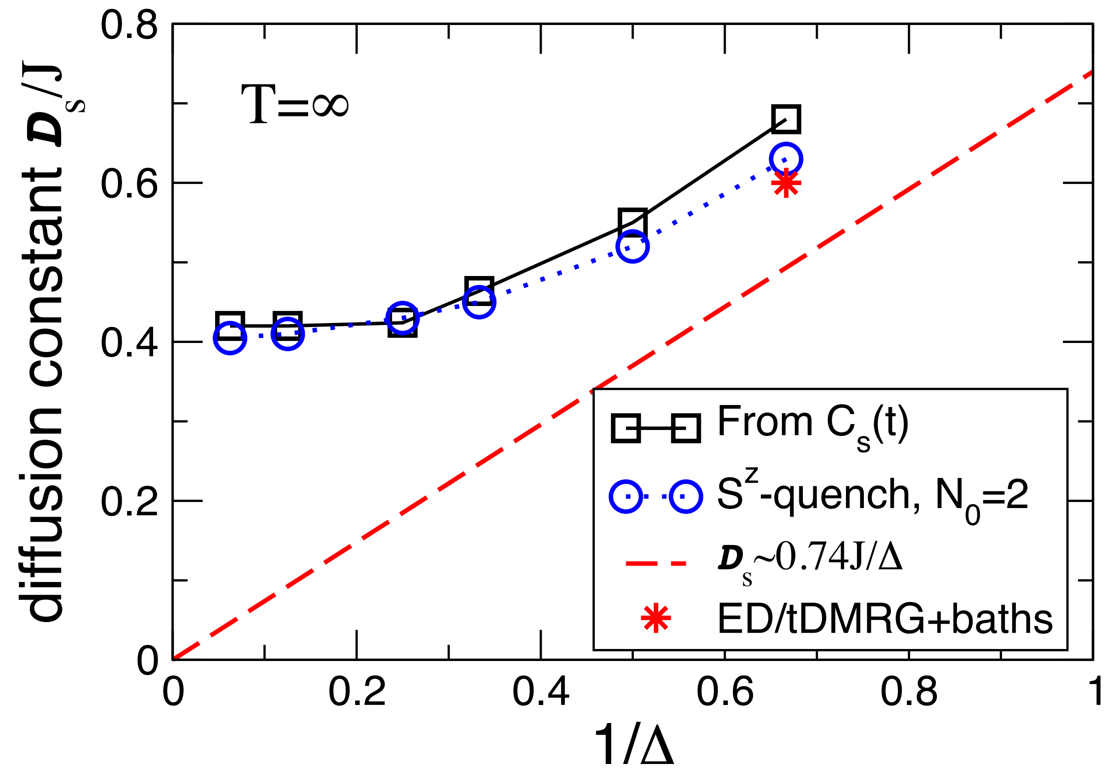
Diffusion in the AFM-Ising phase

$\Delta > 1$

Common belief: spin No Drude weight

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





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)

Intermediate summary

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

Ballistic **Diffusive**

$0 \qquad 1 \qquad \Delta$

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

$D(T) > 0$

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

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

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

$D(T) = 0?$

Results & opinions:

Karrasch, Hauschild, Langer, FHM Phys. Rev. B 87, 245128 (2013)
Karrasch, Moore, FHM, Phys. Rev. B 89, 075139 (2014)
Karrasch, Kennes, FHM; Phys. Rev. B 91, 115130 (2015)

Drude weight small or zero

Sirker, Pereira, Affleck PRL 2009; Karrasch, Bardarson, Moore PRL 2012

Vanishing lower bound at T=∞ Prosen PRL 2011

Latest numerics:

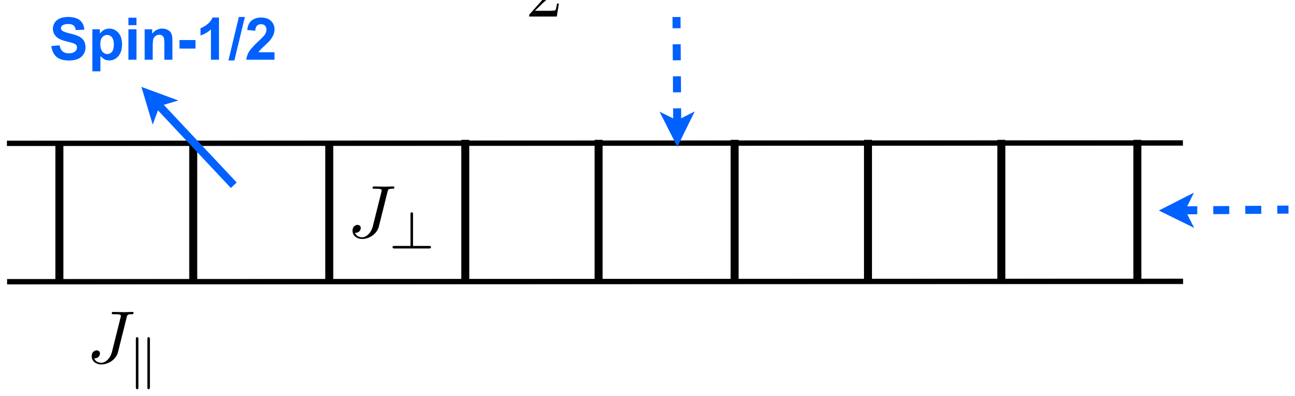
Steinigeweg, Gemmer, Brenig PRL 2014

$$D(T) = \frac{C_\infty}{T} + \frac{C_2}{T^2} + \dots \quad C_\infty = 0 \quad \text{but} \quad D(T>0) > 0$$

ED: Ensembles show very different finite-size dependencies Karrasch, Hauschild, Langer, FHM PRB 2013

Generalized spin-ladder model

$$\frac{J_{\parallel}}{2}(S_i^+ \; S_j^- + h.c.)$$



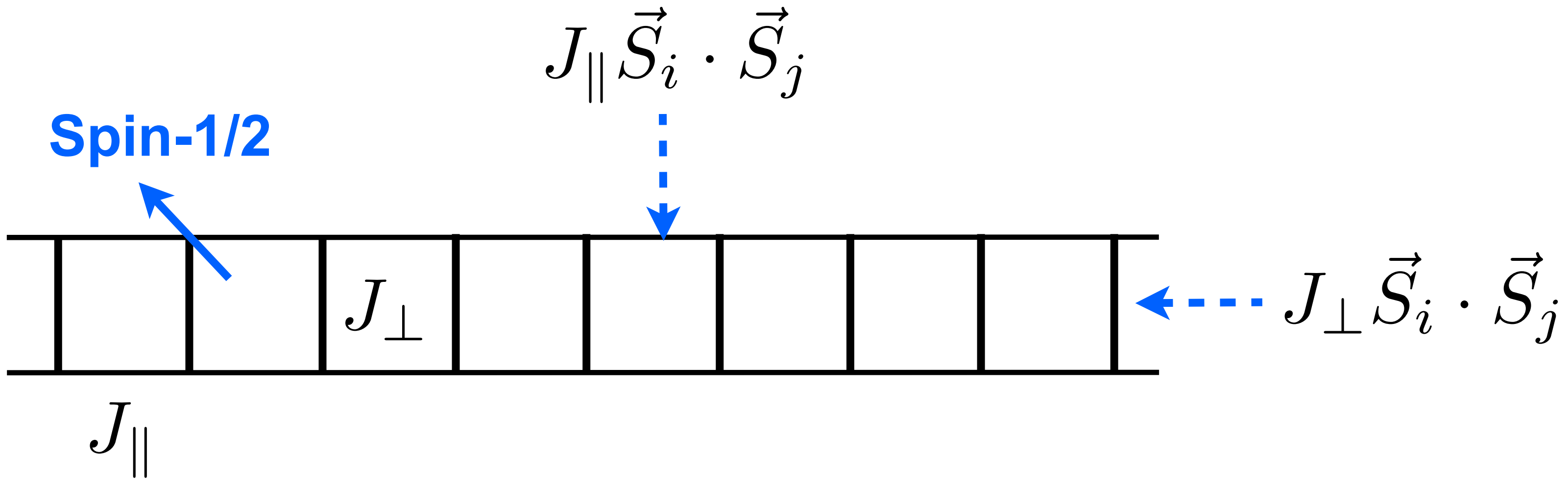
$$\frac{J_{\perp}}{2}(S_i^+ \; S_j^- + h.c.)$$

$$rJ_{\parallel} = J_{\perp}$$

spin-1/2 XX ladder (hard-core bosons, quantum gases)

$$J_{\perp} > 0: \qquad [H, j_s] \neq 0 \quad [H, j_{\text{th}}] \neq 0 \quad [H, Q_\alpha] \neq 0$$

Generalized spin-ladder model



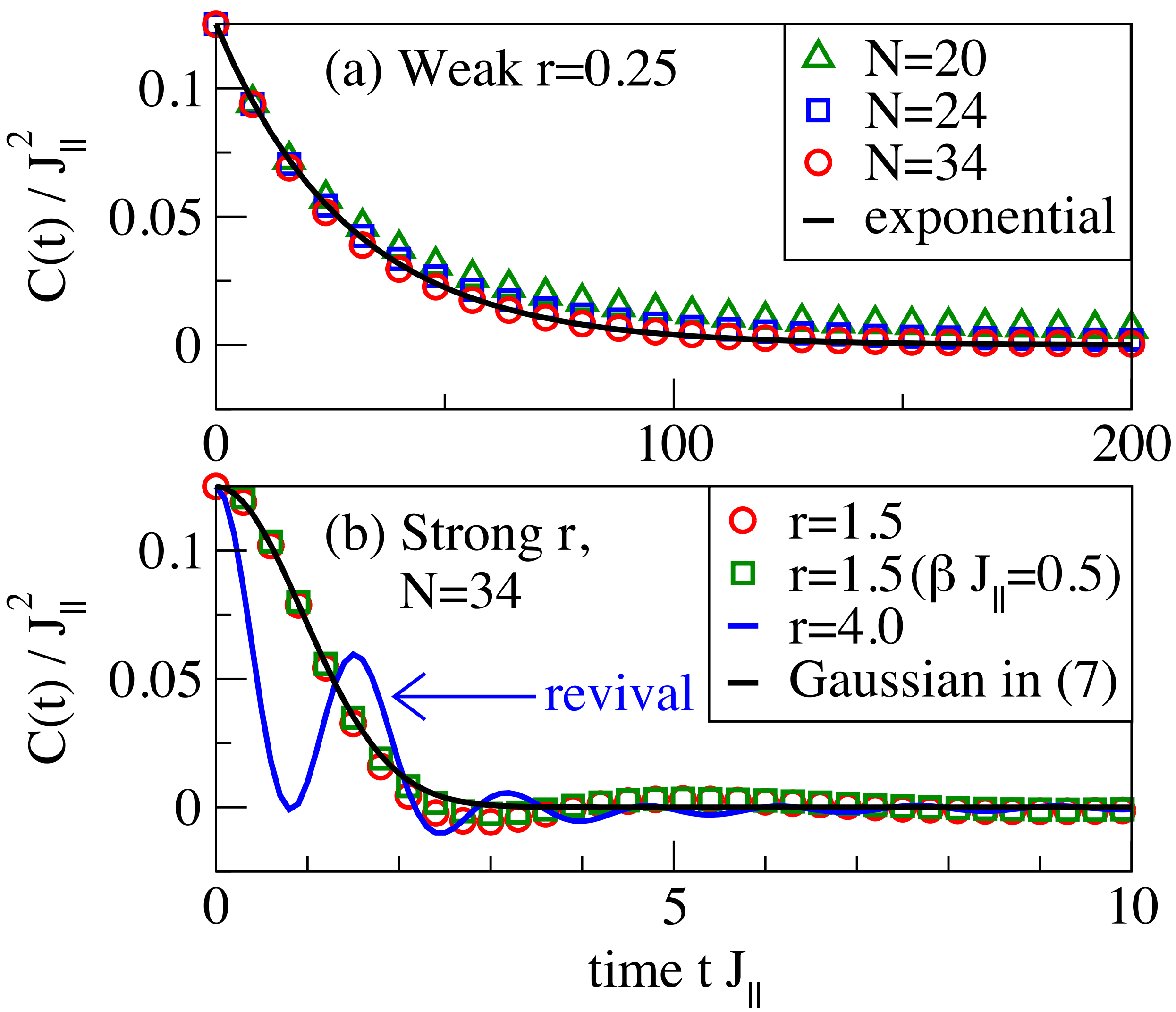
Heisenberg spin ladder (quantum magnets)

$$[H, j_s] \neq 0 \quad [H, j_{\text{th}}] \neq 0 \quad [H, Q_\alpha] \neq 0$$

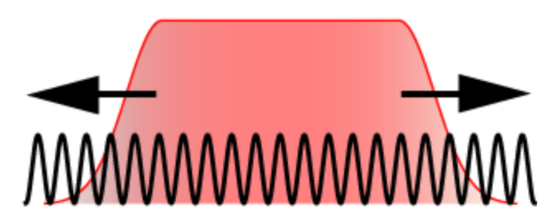
Spin transport in spin-1/2 XX ladders

$$H_{XX} = \frac{J_{\parallel}}{2} \sum_{r=1}^{L} \left[\sum_{l=1,2} (S^+_{l,r} S^-_{l,r+1} + h.c.) + r(S^+_{1,r} S^-_{2,r} + h.c.) \right]$$

Current auto-correlations



Motivated by quantum gas experiments



Method: Dynamical typicality:

Real-time ED method

Initial states that

yield thermal properties

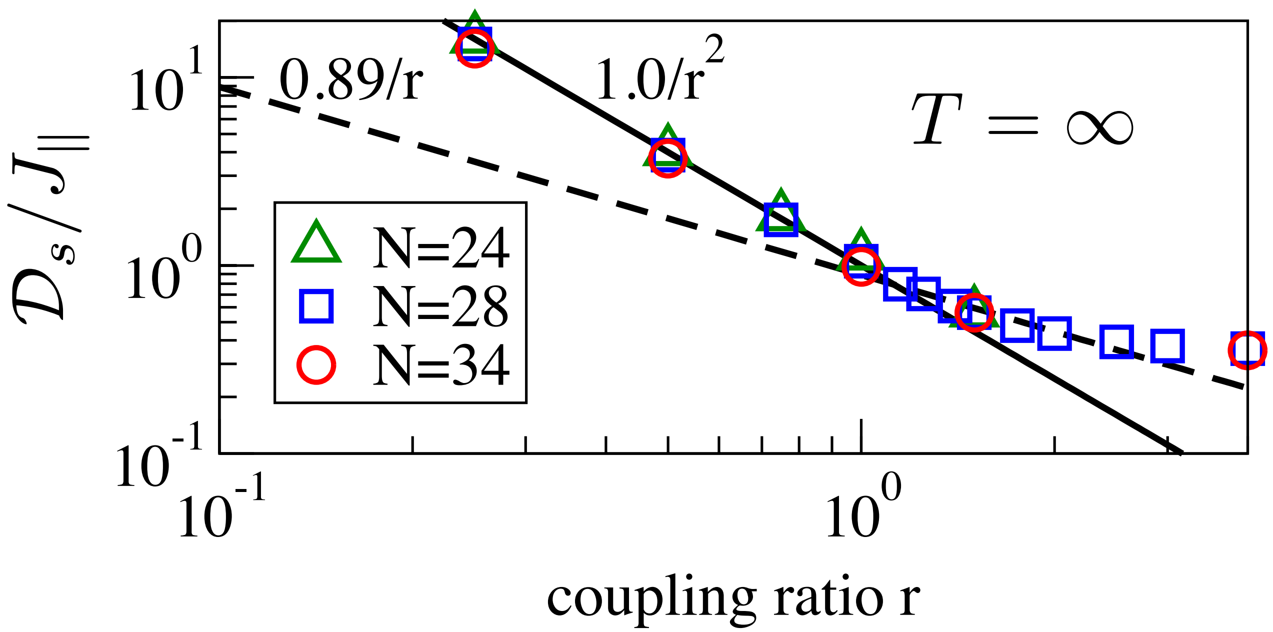
See R. Steinigeweg's talk

Steinigeweg, FHM, Gemmer, Michielsen, de Raedt
Phys. Rev. B 90, 094417 (2014)

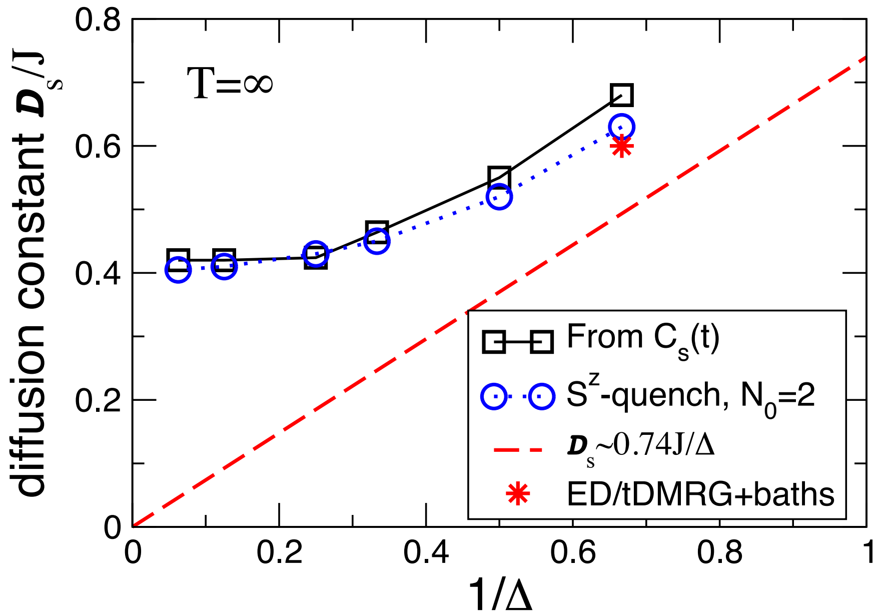
Spin transport in spin-1/2 XX ladders

$$H_{XX} = \frac{J_{\|}}{2} \sum_{r=1}^{L} \left[\sum_{l=1,2} (S^+_{l,r} S^-_{l,r+1} + h.c.) + r(S^+_{1,r} S^-_{2,r} + h.c.) \right]$$

Diffusion constant



Comparison with XXZ chain



→ **Diffusive conductor**

→ **Three scaling regimes**

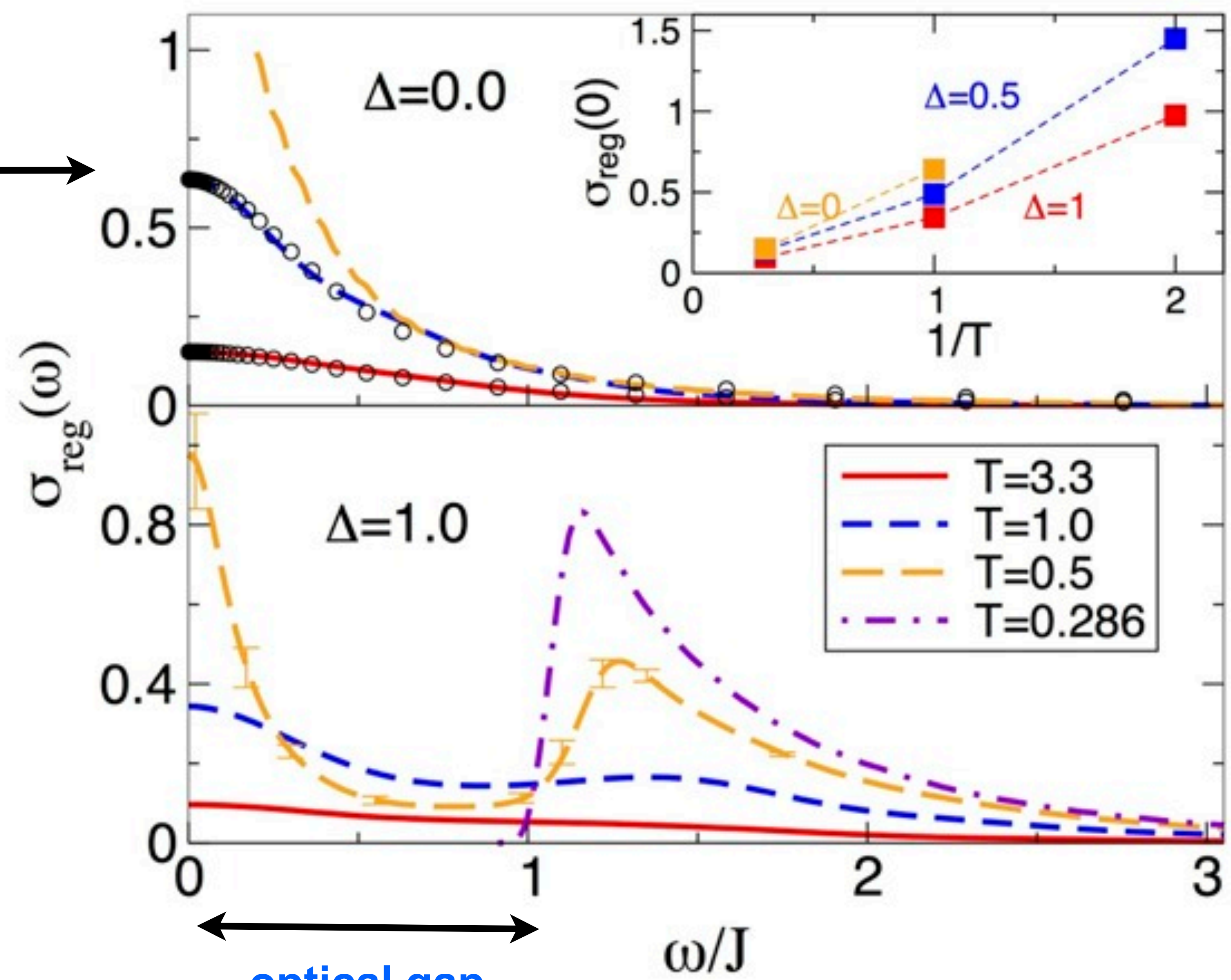
→ **Experimentally realizable in optical lattices**

Steinigeweg, FHM, Gemmer, Michielsen, de Raedt
Phys. Rev. B 90, 094417 (2014)

Spin transport in spin-1/2 XXZ ladders

tDMRG data

Lorentzian →



optical gap

Increasing interactions:

$\Delta S_i^z S_j^z$

$\sigma_{\rm dc}$

decreases

Spin-1/2 XX ladder:

→ **Diffusive conductor:**

$$\mathrm{Re}\,\sigma(\omega) \propto \frac{D}{\omega^2 + {\tau^{-1}}^2}$$

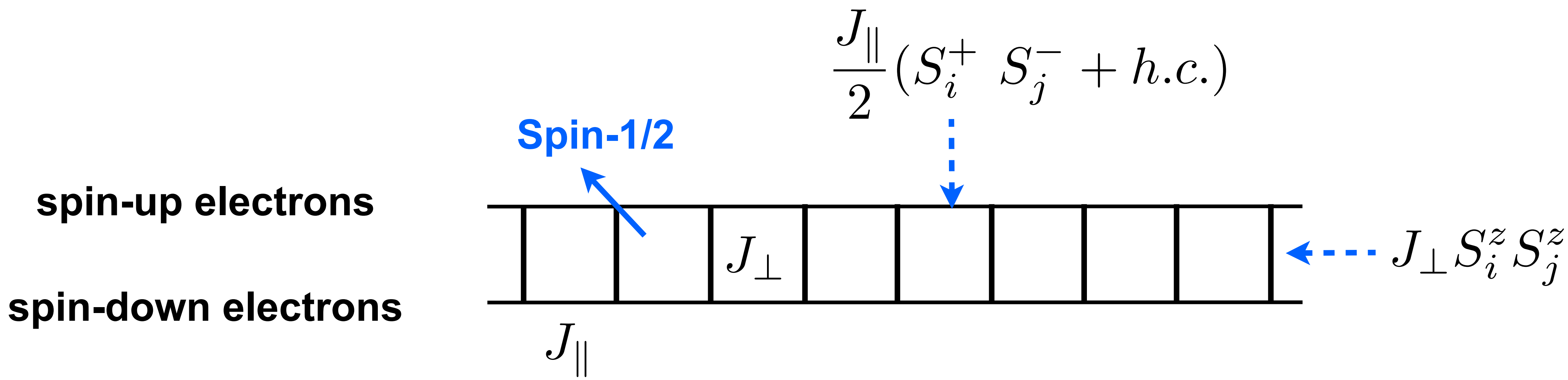
→ **Experimentally realizable in optical lattices = HCBs**

→ Slightly different mean-free paths

$$l_\kappa \approx 4\, l_\sigma$$

Karrasch, Kennes, FHM Phys. Rev. B 91, 115130 (2015)

Generalized spin-ladder model



1D Hubbard model $J_{\parallel}/2 = t_0$ $J_{\perp} = U$

$$H = -t_0 \sum_{i,j} (c_{i\sigma}^{\dagger} c_{i+1\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Thermal conductivity in 1D Hubbard model

Overlap with
local conserved quantity

$$[H, j_{\mathrm{th}}] \neq 0$$

$$D_{\mathrm{th}}(T) \geq \mathrm{const} \frac{|\langle j_{\mathrm{th}} Q_3 \rangle|^2}{\langle Q_3^2 \rangle} > 0$$

Zotos, Naef, Prelovsek PRB 1997

Non-decaying
current auto-correlations

$$\lim_{t \to \infty} \langle j_{\mathrm{th}}(t) j_{\mathrm{th}} \rangle / L \to \mathrm{const}$$

Here: half-filling!

particle-hole symmetry:
vanishing thermopower

$$\langle j_{\mathrm{th}} j_{\mathrm{c}} \rangle = 0$$

Beni ,Coll, Phys. Rev. B 11, 573 (1975)

Thermal conductivity in 1D Hubbard model

Overlap with local conserved quantity

$$[H, j_{\rm th}] \neq 0$$

$$D_{\rm th}(T) \geq {\rm const} \frac{|\langle j_{\rm th} Q_3 \rangle|^2}{\langle Q_3^2 \rangle} > 0$$

Zotos, Naef, Prelovsek PRB 1997

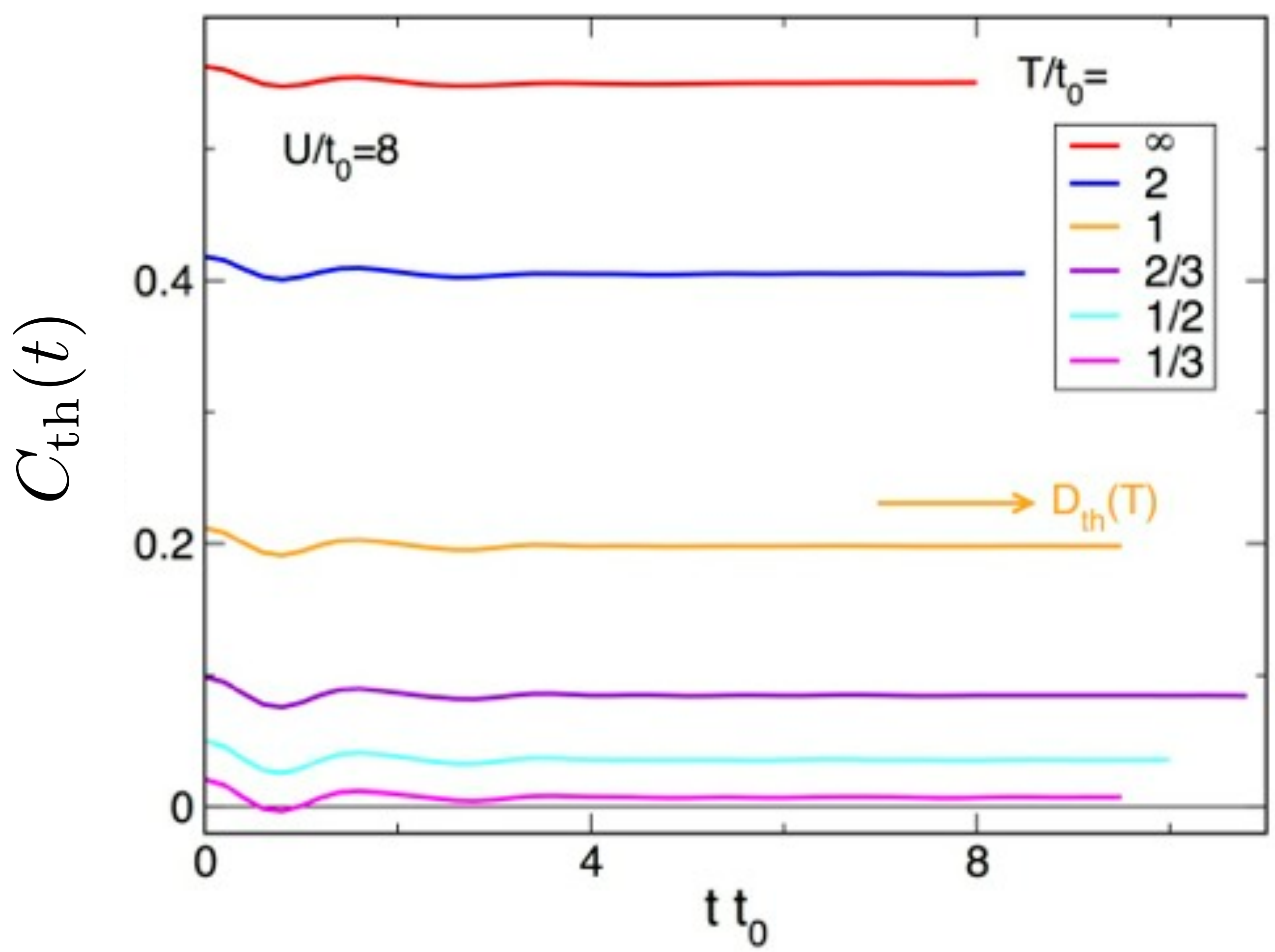
Non-decaying current auto-correlations

$$\lim_{t\to\infty} \langle j_{\rm th}(t) j_{\rm th} \rangle / L \to {\rm const}$$

$$Q_3; j_{\rm th}:$$

identical structure

Finite-T DMRG results



Fast saturation, clearly ballistic

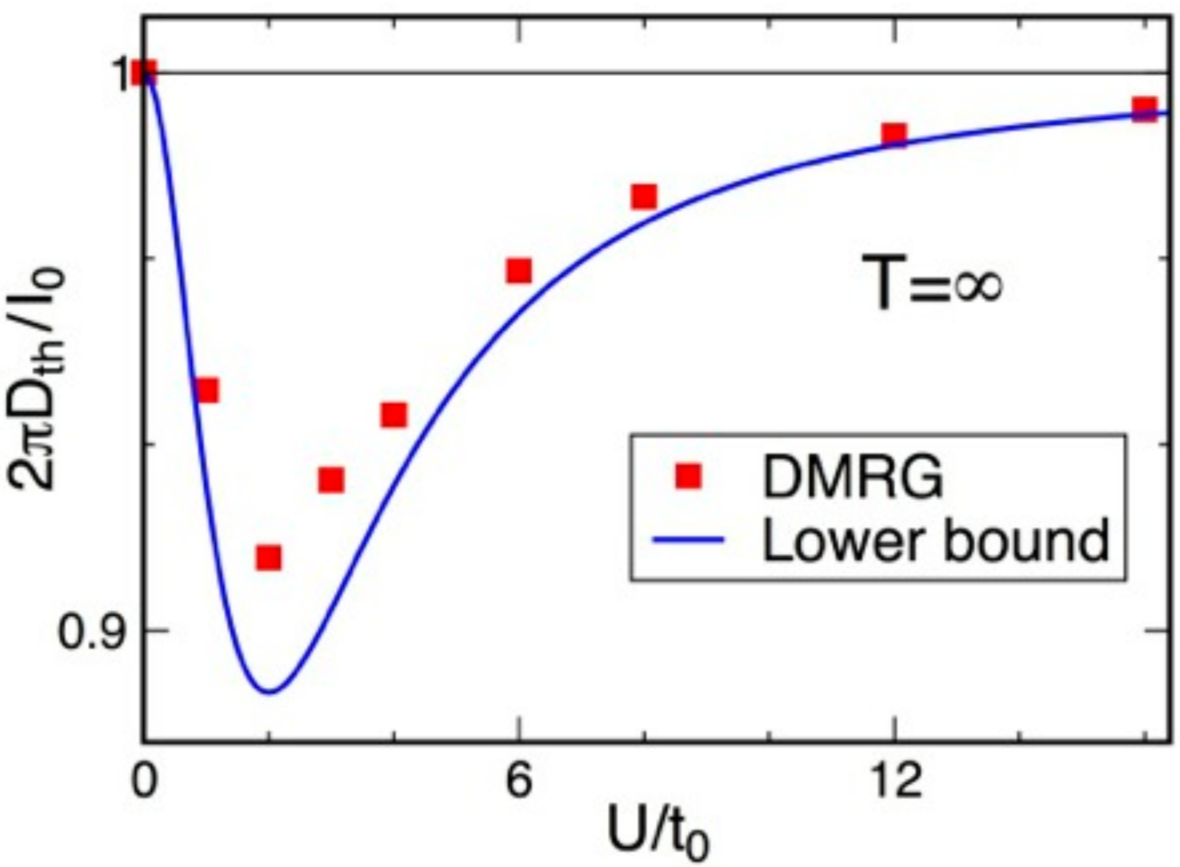
Karrasch, Kennes, FHM arXiv:1506.05788

Thermal conductivity in 1D Hubbard model

Lower bound

$$D_{\text{th}}(T) \geq \text{const} \frac{|\langle j_{\text{th}} Q_3 \rangle|^2}{\langle Q_3^2 \rangle} > 0$$

Zotos, Naef, Prelovsek PRB 1997

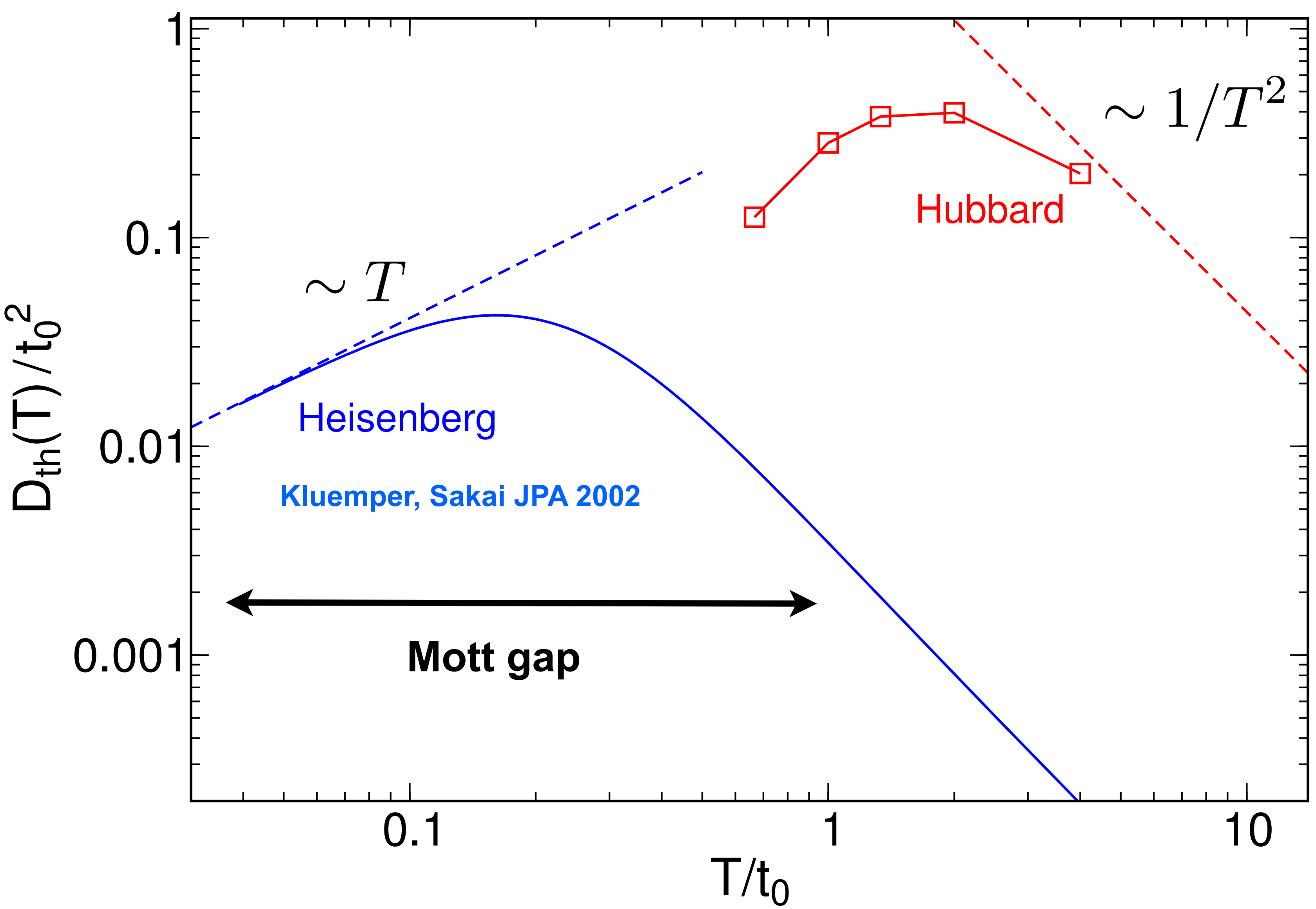


"Strongly" ballistic heat conduction

$$D_{\text{th}} \gg \int d\omega\, \kappa_{\text{reg}}(\omega)$$

Karrasch, Kennes, FHM arXiv:1506.05788

Hubbard versus Heisenberg model



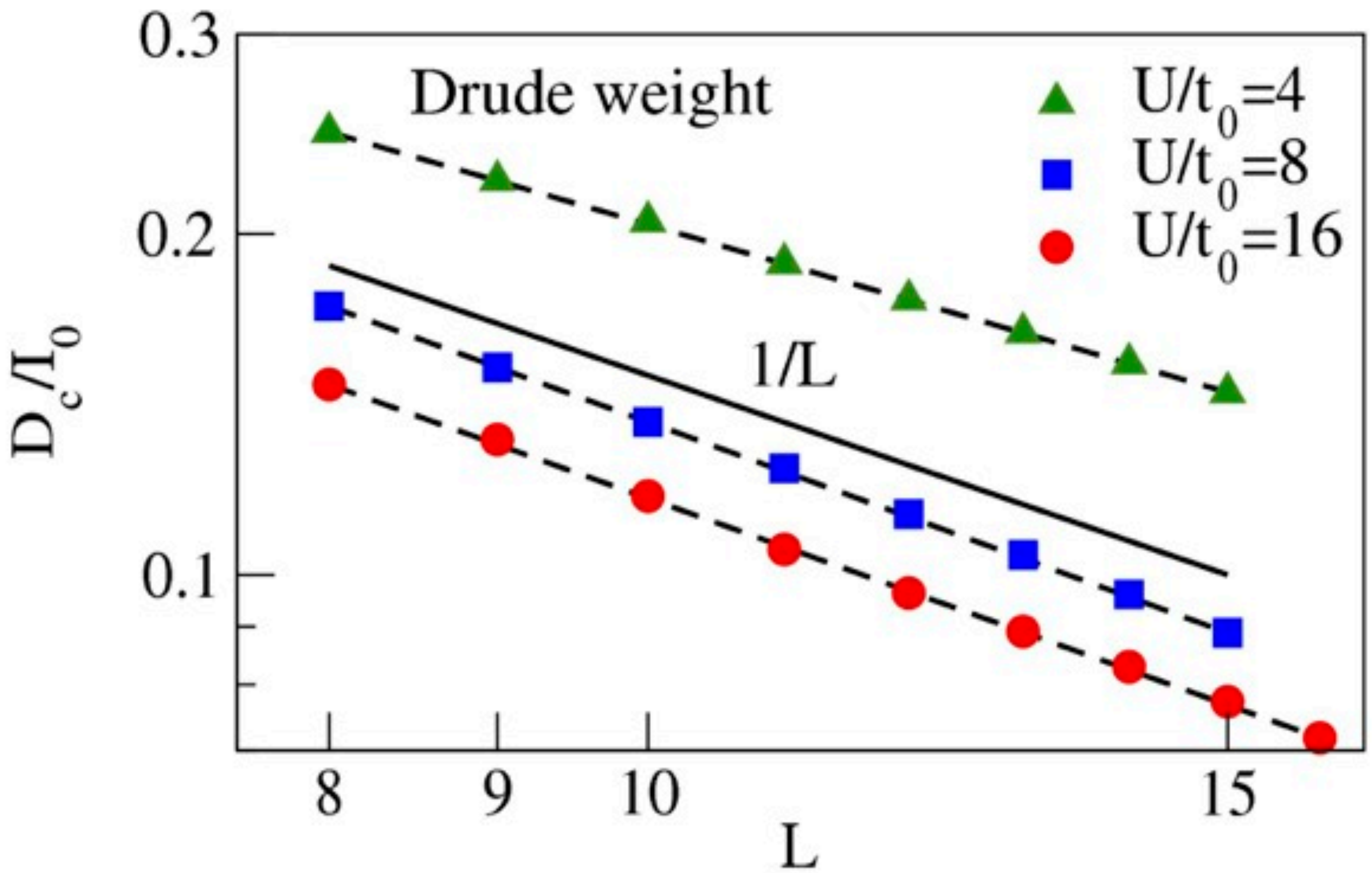
$$T_{\max} \sim \mathcal{O}(t_0^2/U)$$

$$T_{\max} \sim \mathcal{O}(U)$$

Spin-incoherent regime

Karrasch, Kennes, FHM arXiv:1506.05788

Charge transport in 1D Hubbard



Charge Drude weight vanishes algebraically

in agreement with
Carmelo et al. J. Phys. A: Math. Theor. 47 255004 (2014)

Other results:

Optical conductivity
Mass-imbalance
...

F. Jin, R. Steinigeweg, FHM, H. De Raedt, K. Michielsen, arXiv:1508.01304
See also Karrasch, Kennes, Moore Phys. Rev. B 90, 155104 (2014)

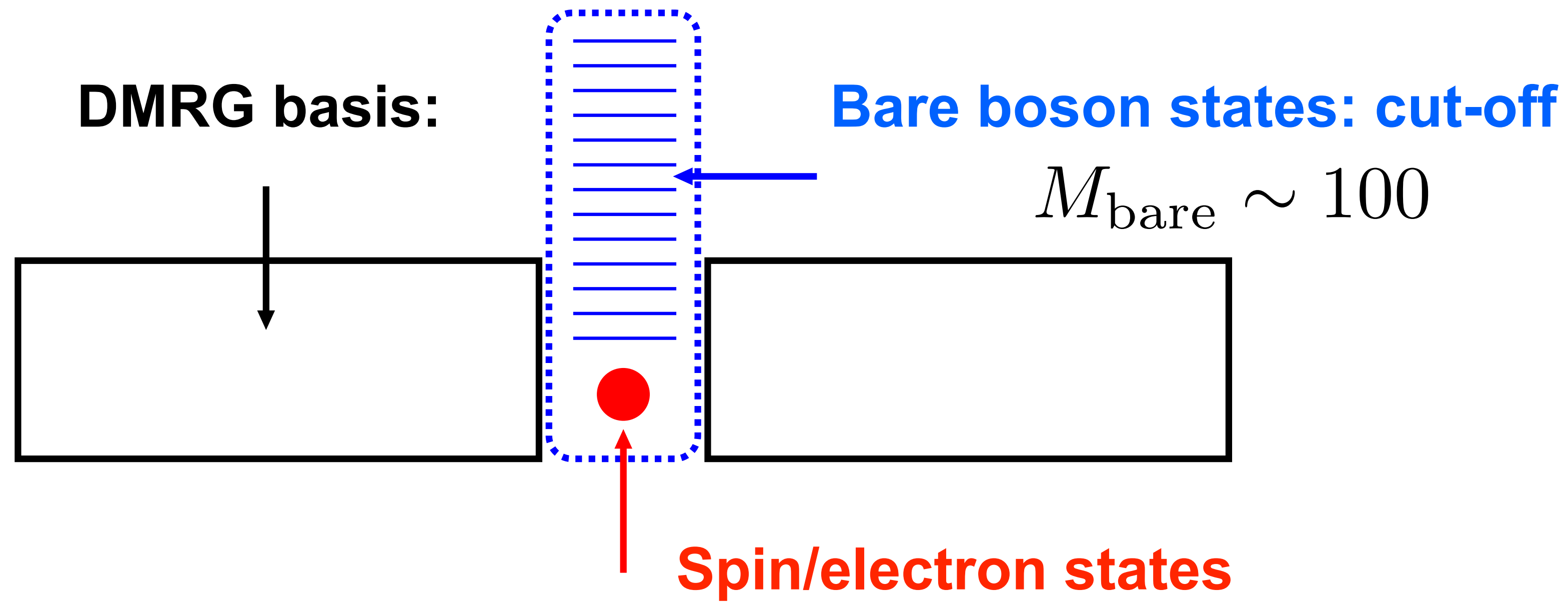
Finally ... towards phonons !

Novel DMRG/TEBD algorithm

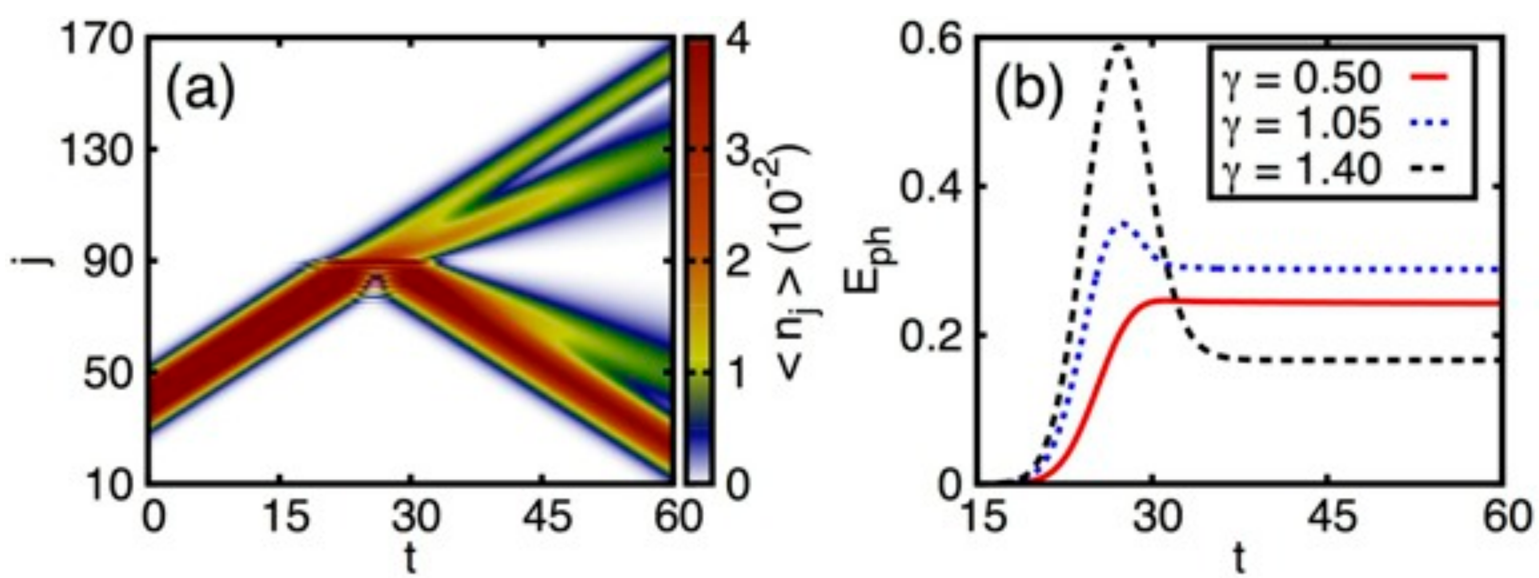
Adaptive update & truncation
DMRG & local state space
Diagonalize reduced
single-site density matrix

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

Zhang, Jeckelmann, White PRL 1998



First applications: Polaron formation & wave packets in Holstein chains



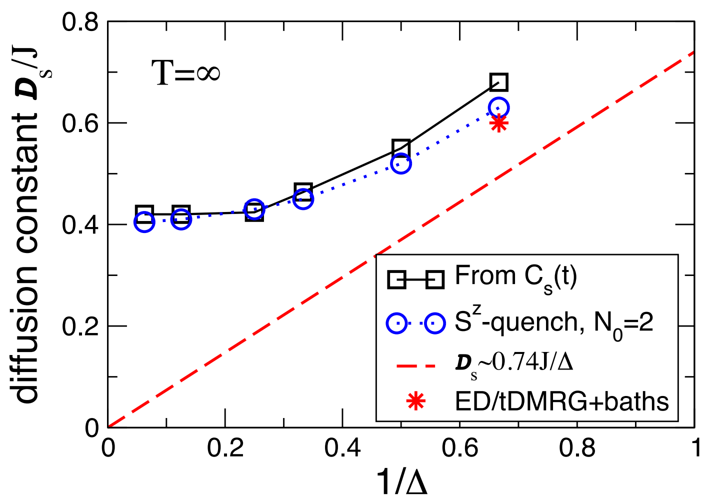
Brockt, Dorfner, Vidmar, FHM, Jeckelmann, arXiv:1508.01304

Summary

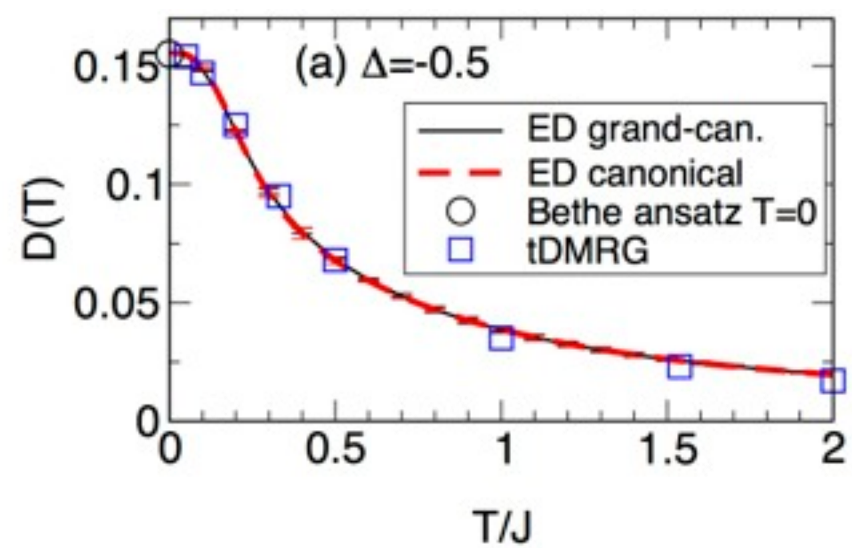
Spin-1/2 chains: Ballistic and diffusive dynamics

Diffusion constant $\Delta > 1$

Drude weight $|\Delta| < 1$



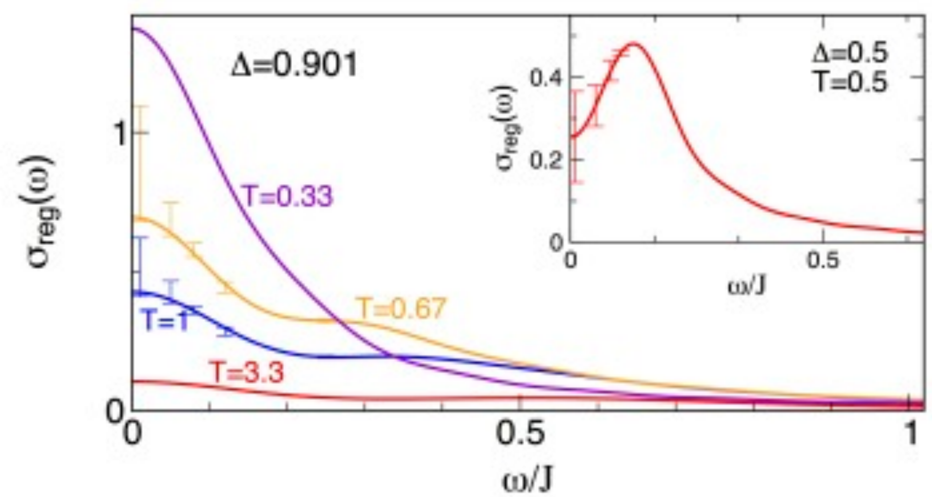
Karrasch, Moore, FHM
Phys. Rev. B 89, 075139 (2014)



Karrasch, Hauschild, Langer, FHM
Phys. Rev. B 87, 245128 (2013)

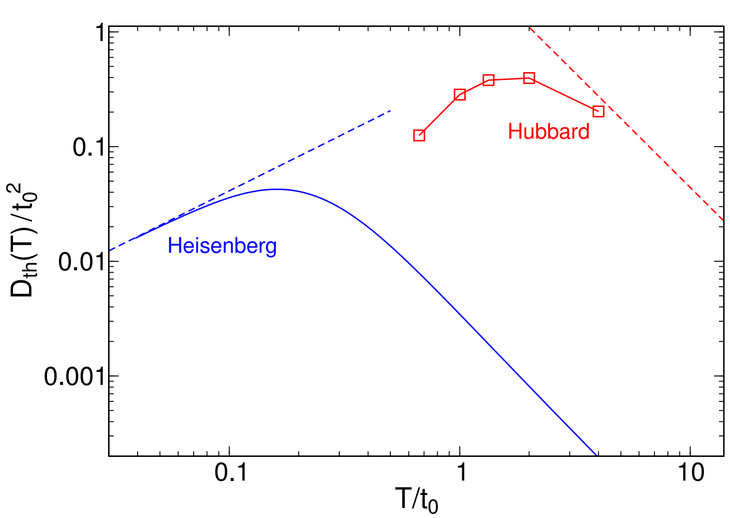
Optical spin conductivity

"Diffusive" conductors



Karrasch, Kennes, FHM Phys. Rev. B 91, 115130 (2015)
Steinigeweg, FHM, Gemmer, Michielsen, de Raedt
Phys. Rev. B 90, 094417 (2014)

Hubbard, thermal conductivity

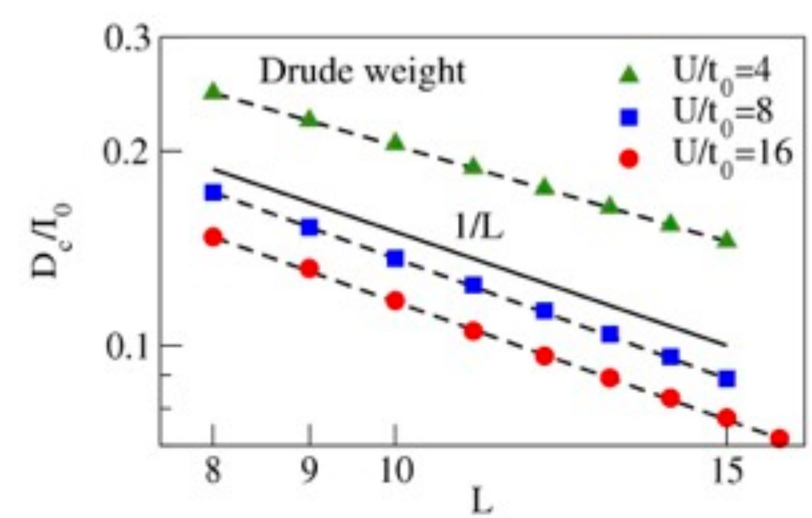


Karrasch, Kennes, FHM arXiv:1506.05788

1D & integrable:
Ballistic transport possible

tDMRG & ED/typicality:
Diffusion constants, $\sigma(\omega)$

Hubbard, charge transport



F. Jin, R. Steinigeweg, FHM, H. De Raedt, K. Michielsen
arXiv:1508.01304