Thermal Transport
in Low-Dimensional Quantum-Spin Systems

Fabian Heidrich-Meisner

University of Tennessse & Oak Ridge National Laboratory

A. Honecker, W. Brenig

Technische Universität Braunschweig, Germany

D.C. Cabra

Université Louis Pasteur Strasbourg, France

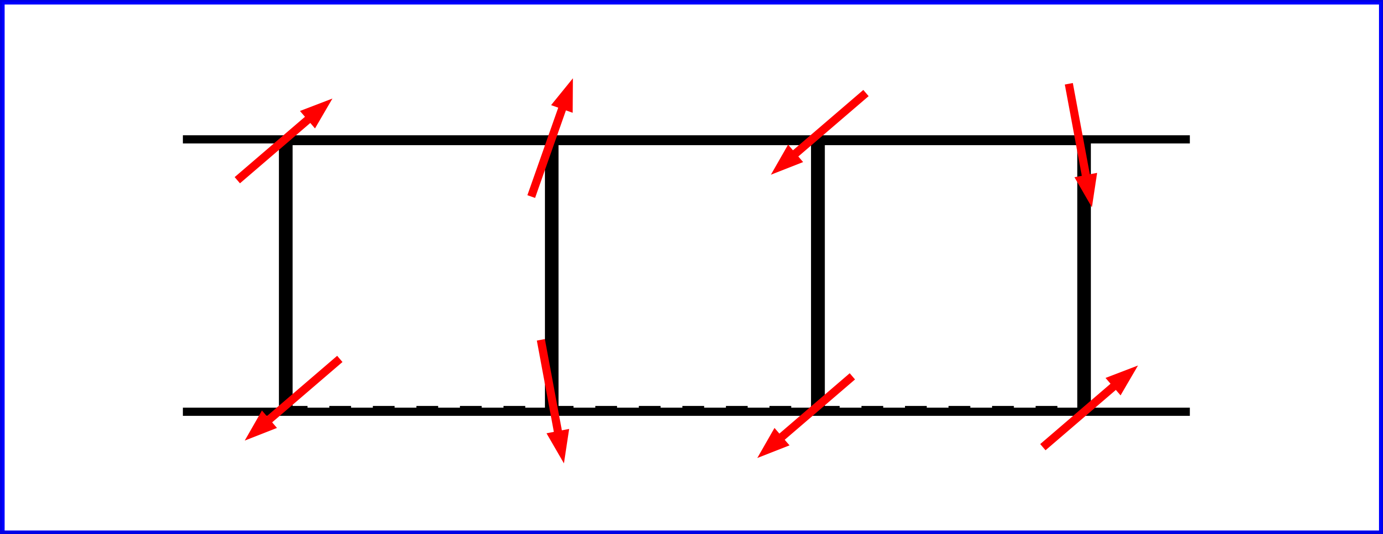
C. Hess and B. Büchner

IFW Dresden, Germany

KITP, UC Santa Barbara, Sept 23, 2005

Thermal Transport

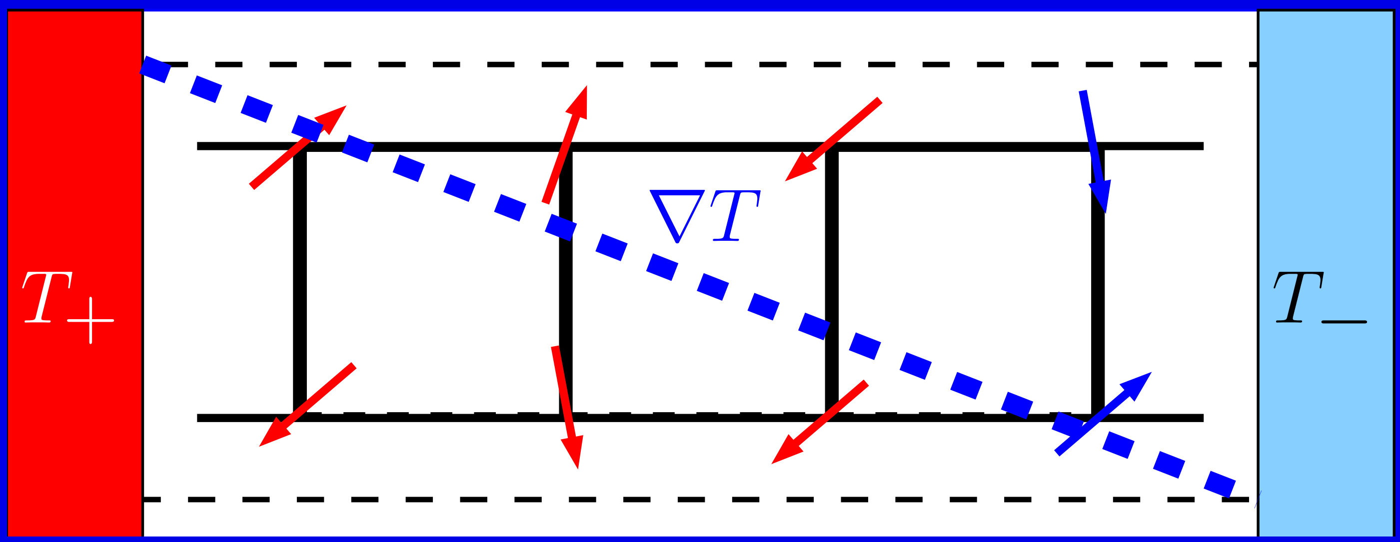
in Low-Dimensional Quantum-Spin Systems



$$H = \sum_{i,j} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

Thermal Transport

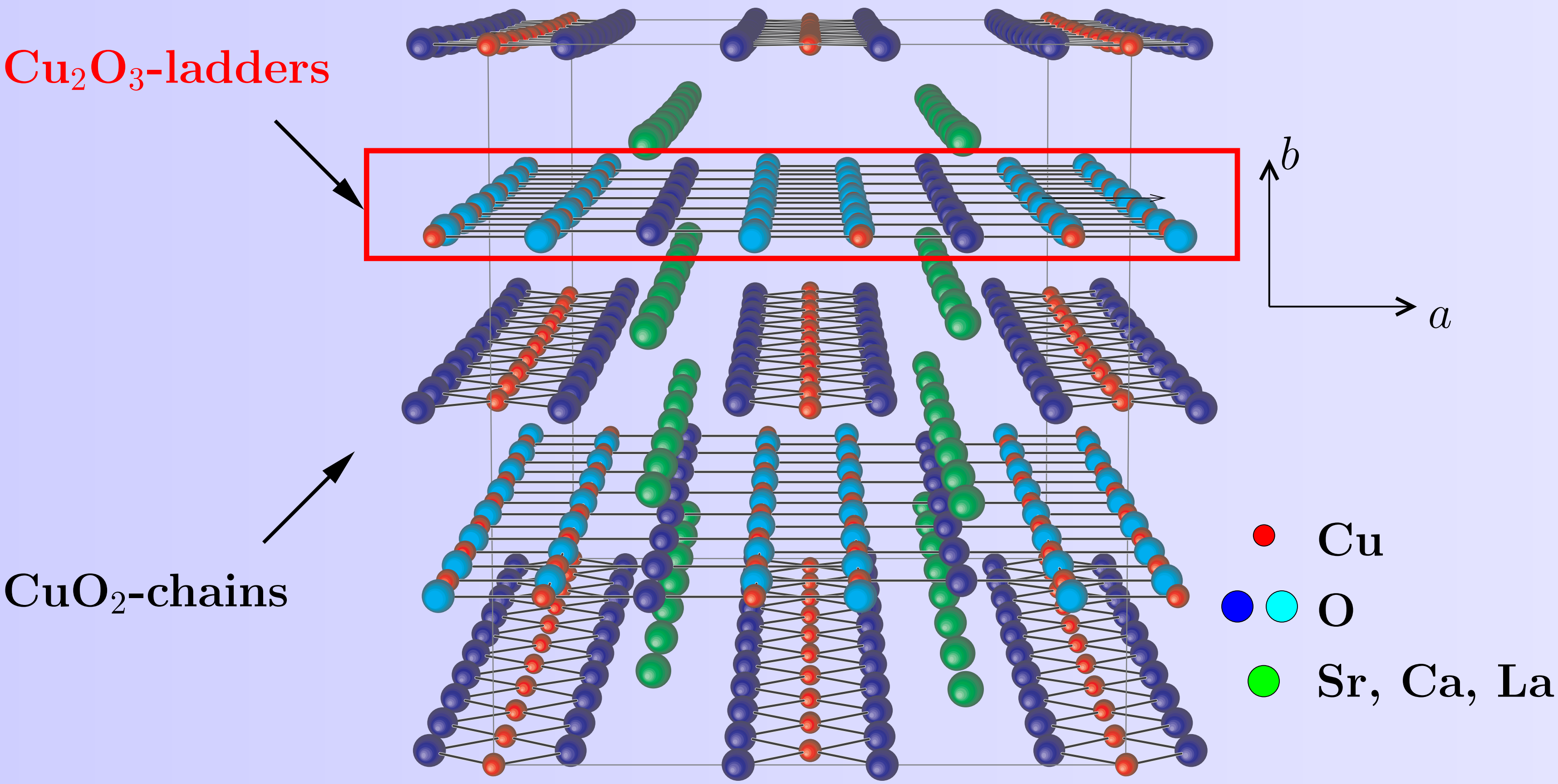
in Low-Dimensional Quantum-Spin Systems



$$H = \sum_{i,j} J_{ij}\, \vec{S}_i \cdot \vec{S}_j$$

Motivation:

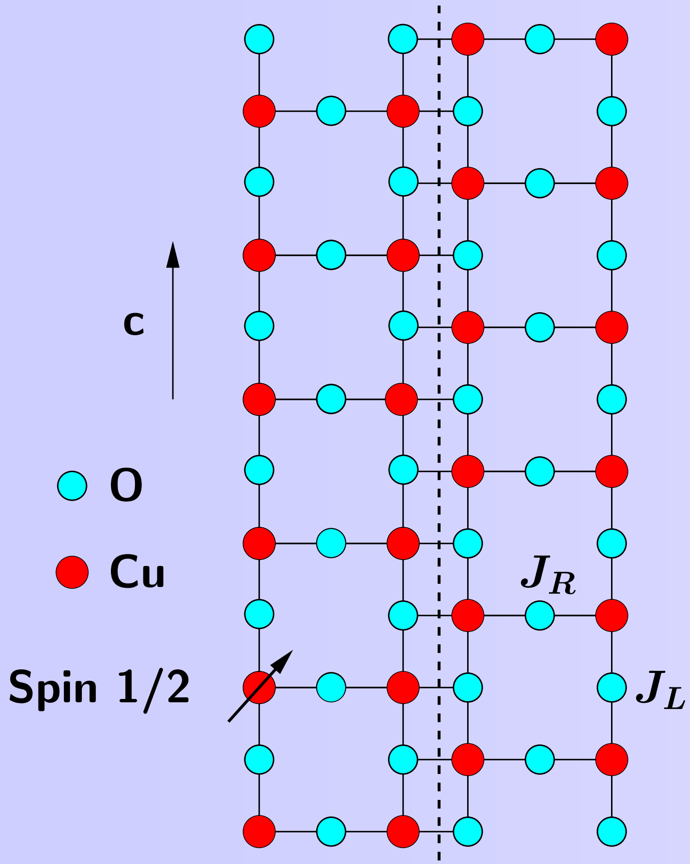
Thermal conductivity of $(Sr,Ca,La)_{14}Cu_{24}O_{41}$

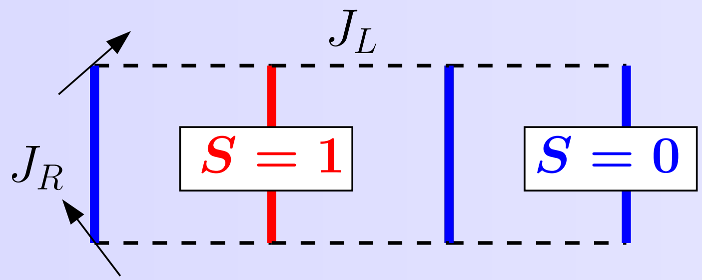


McCarron et al. Mater. Res. Bull. 1998

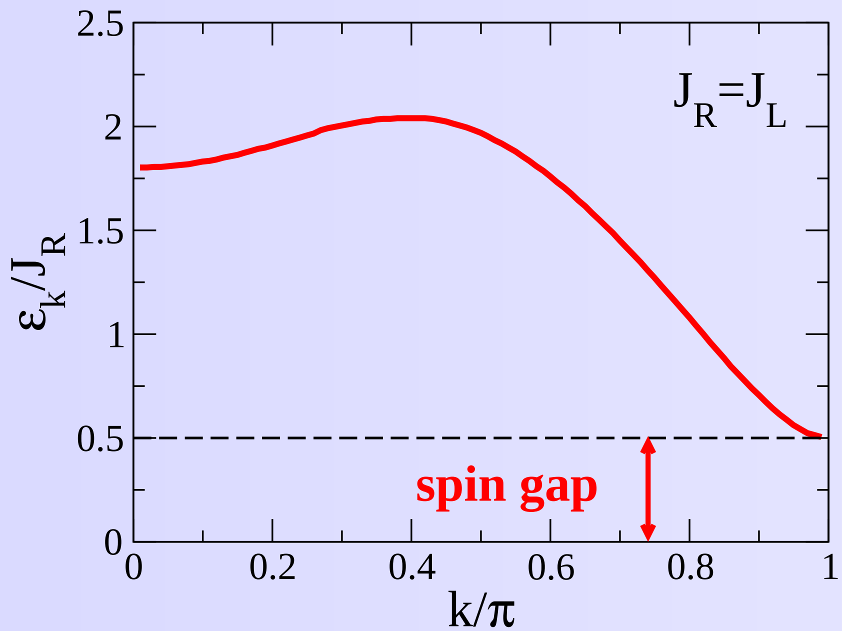
Spin ladders: Elementary excitations and spin gap

Cu_2O_3-layer:





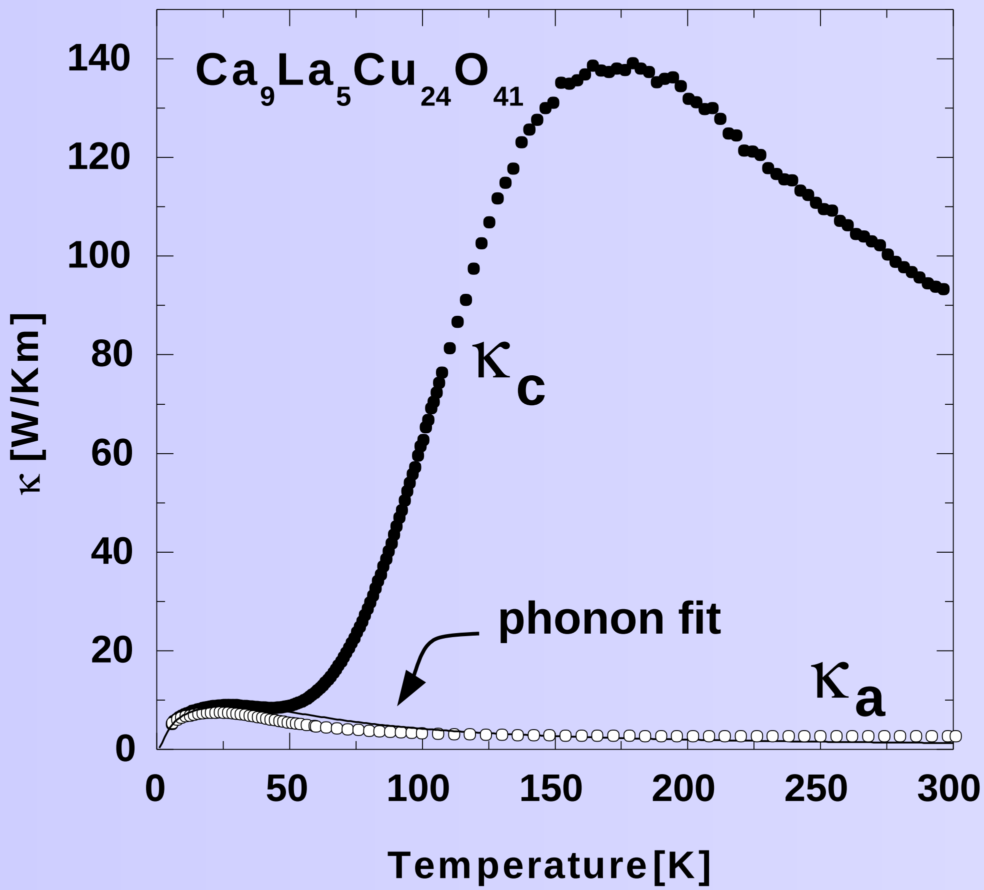
Triplet dispersion:



$$H = \sum_{i,j} J_{ij}\, \vec{S}_i \cdot \vec{S}_j \quad J \sim 1000\,\mathrm{K}$$

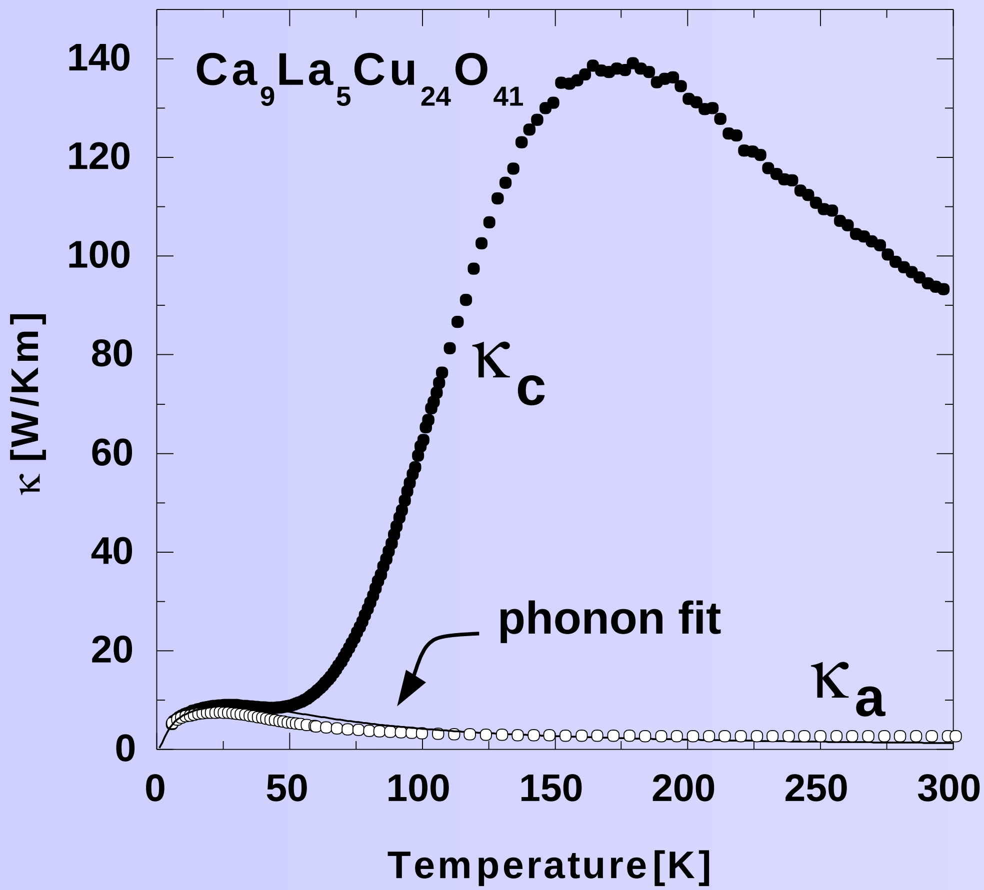
Knetter et al. PRL 2001

Thermal conductivity of $Ca_9La_5Cu_{24}O_{41}$



Hess et al. PRB 2001

Thermal conductivity of $Ca_9La_5Cu_{24}O_{41}$



Hess et al. PRB 2001

Separation: $\kappa_{\rm mag} = \kappa_c - \kappa_{\rm ph}$

Low temperatures $T \lesssim 100K$:

$$\kappa_{\rm mag} \propto \exp(-G/T)$$

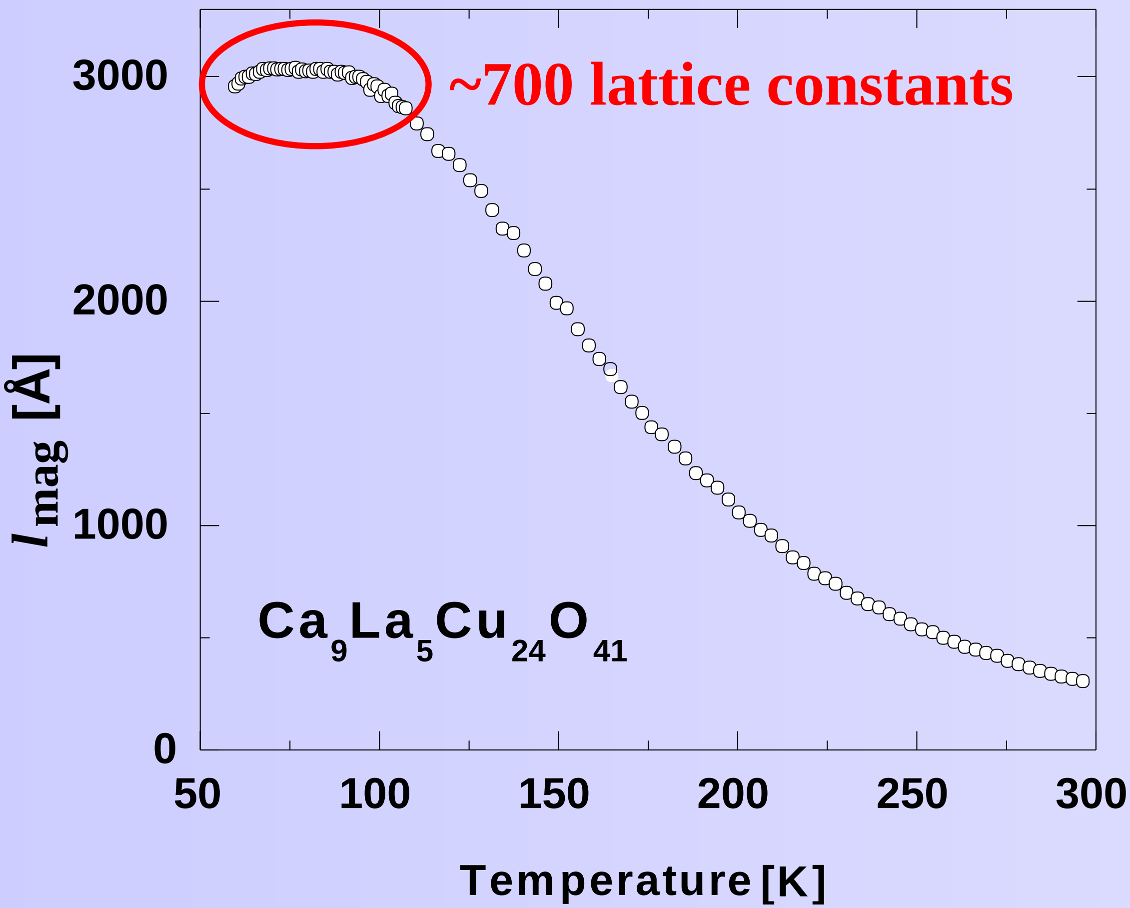
G: spin gap of ladder!

"Magnon" contribution to the thermal conductivity

(Sr,Ca,La)$_{14}$Cu$_{24}$O$_{41}$: Sologubenko et al. PRL 2000; Kudo et al. JPSJ 2001

2D: La$_2$CuO$_4$: Nakamura et al. Physica C 1991; Hess, HM et al. PRL 2003

$Ca_9La_5Cu_{24}O_{41}$: Mean free path



Hess et al. PRB 2001

Kinetic theory:

$$\kappa_{mag} = \boxed{l_{mag}} \sum_k C_{V,k}\ v_k$$

$\rightarrow$ **mean free path**

$$l_{mag} = l_{mag}(T)$$

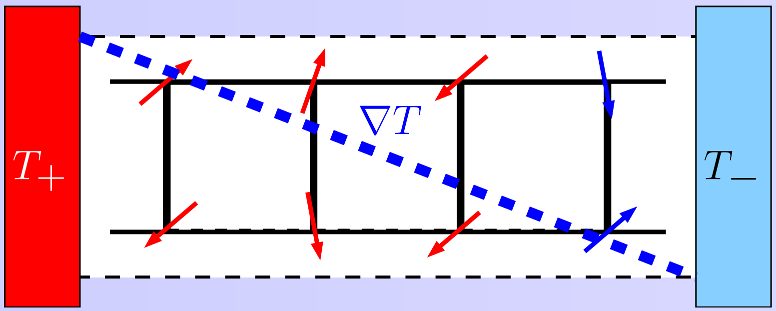
Ballistic thermal transport?

Outline

Intrinsic scattering — ballistic heat transport? — $\kappa = \kappa(T)$?

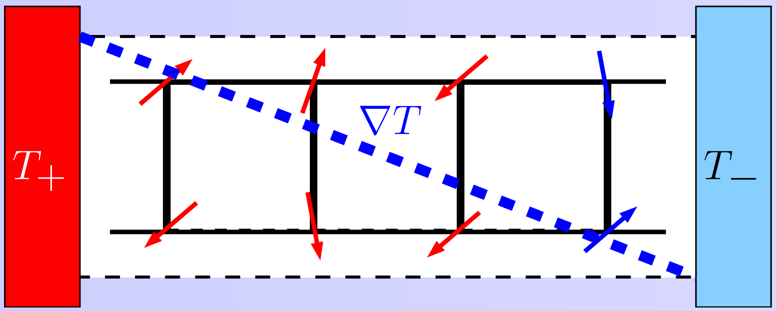
Outline

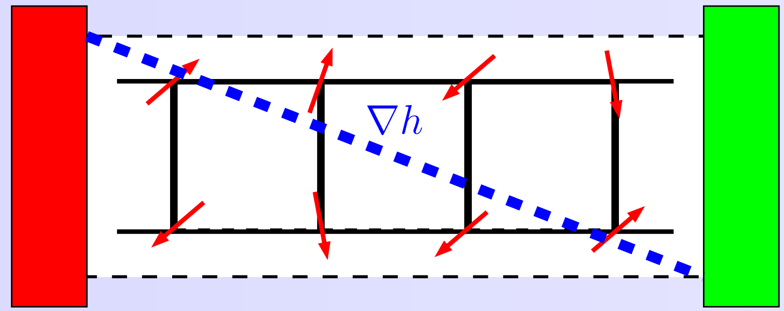
Intrinsic scattering — ballistic heat transport? — $\kappa = \kappa(T)$?



Outline

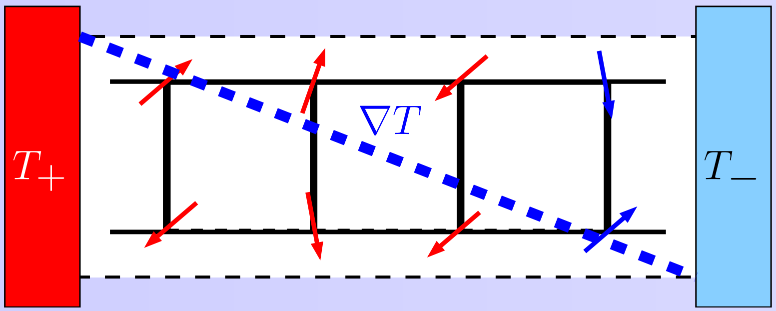
Intrinsic scattering — ballistic heat transport? — $\kappa = \kappa(T)$?

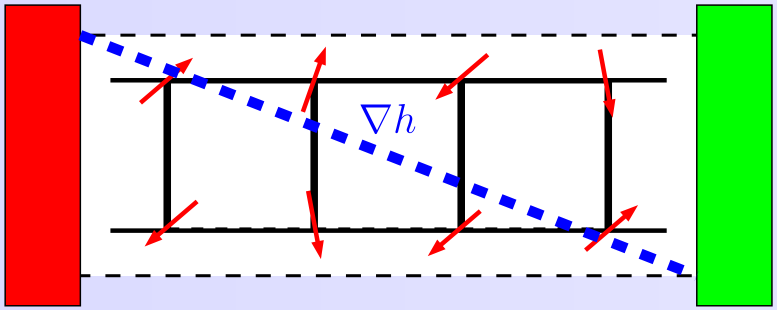




Outline

Intrinsic scattering — ballistic heat transport? — $\kappa = \kappa(T)$?





0. **Motivation: Experiments**
1. **Transport coefficients: Drude weights & conversation laws**
2. **The thermal Drude weight of the spin-1/2 Heisenberg chain**
3. **Thermal conductivity of spin ladders**
4. **Summary**

1. Transport coefficients

Thermal conductivity κ:

$$\mathcal{J}_{\rm th} = -\kappa \, \nabla T$$

Linear response theory:

$$\kappa(\omega) \sim \int_0^{\infty} dt \, e^{-i\omega t} \int_0^{1/T} d\tau \langle j_{\rm th} j_{\rm th}(t + i\tau) \rangle$$

1. Transport coefficients

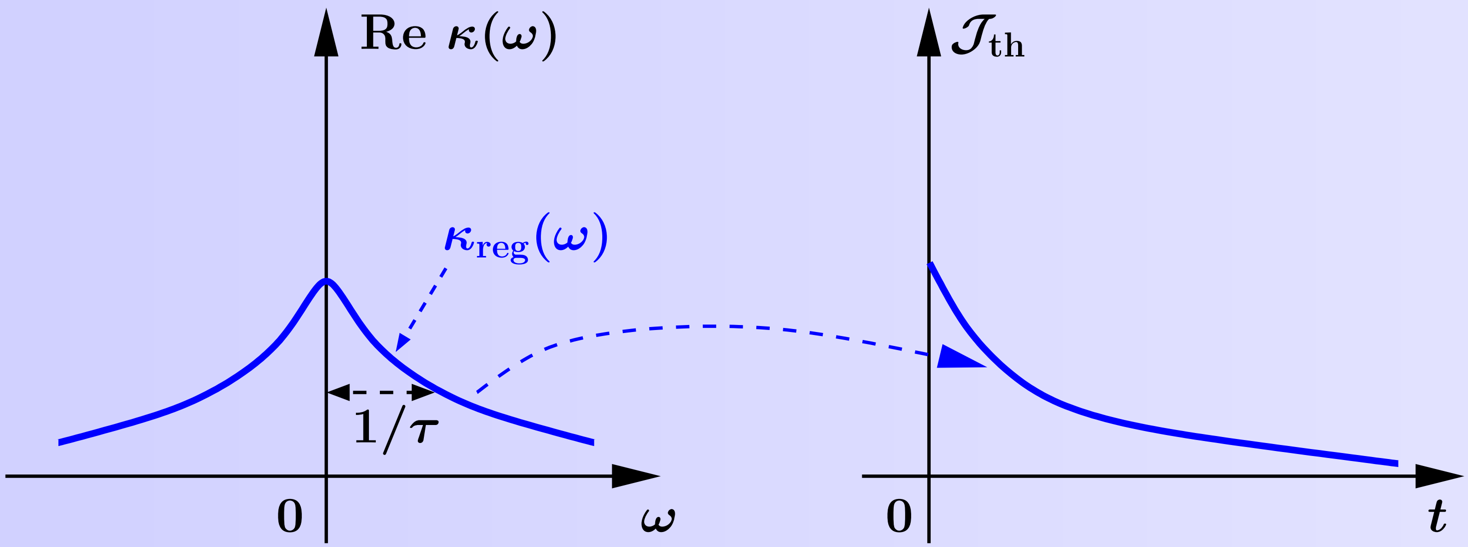
Thermal conductivity κ:

$$\mathcal{J}_{\rm th} = -\kappa \, \nabla T$$

Linear response theory:

$$\kappa(\omega) \sim \int_0^\infty dt \, e^{-i\omega t} \int_0^{1/T} d\tau \langle j_{\rm th} j_{\rm th}(t + i\tau) \rangle$$

Dissipation:



1. Transport coefficients

Thermal conductivity κ:

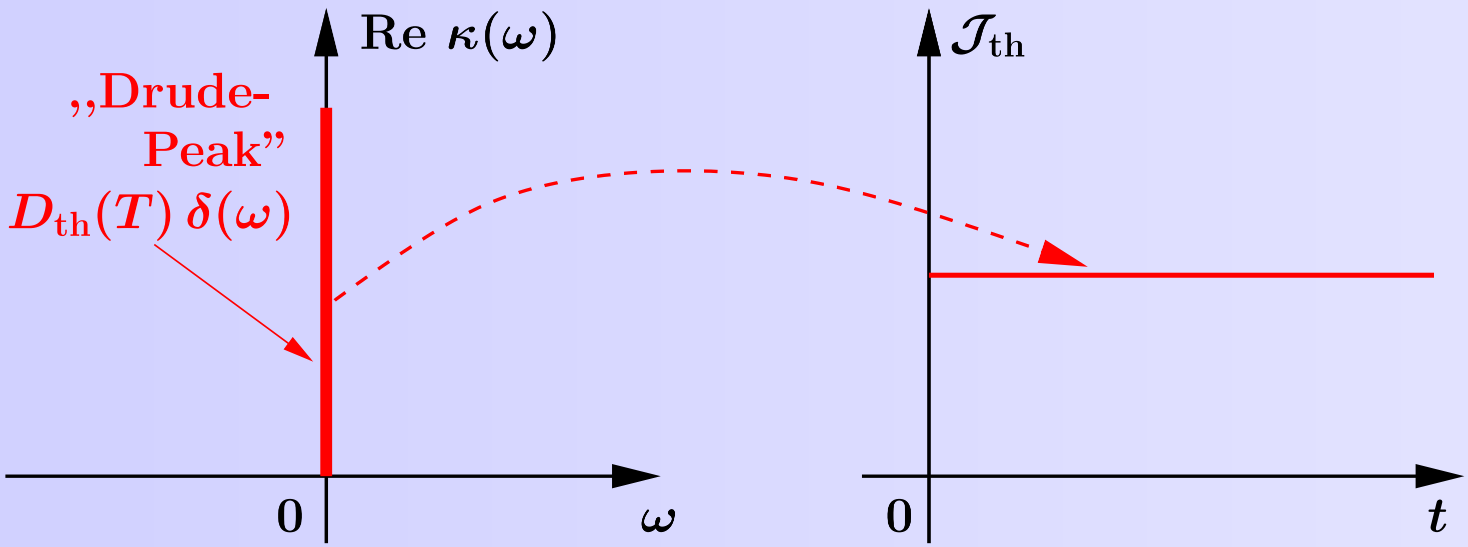
Kohn PRB 1964; Scalapino et al PRB 1993; Shastry cond-mat/0508711

$$\mathcal{J}_{\rm th} = -\kappa \nabla T$$

Linear response theory:

$$\kappa(\omega) \sim \int_0^\infty dt\, e^{-i\omega t} \int_0^{1/T} d\tau \langle j_{\rm th} j_{\rm th}(t + i\tau)\rangle$$

Conservation law $[H, j_{\rm th}] = 0 \Rightarrow$ **ballistic**



1. Transport coefficients

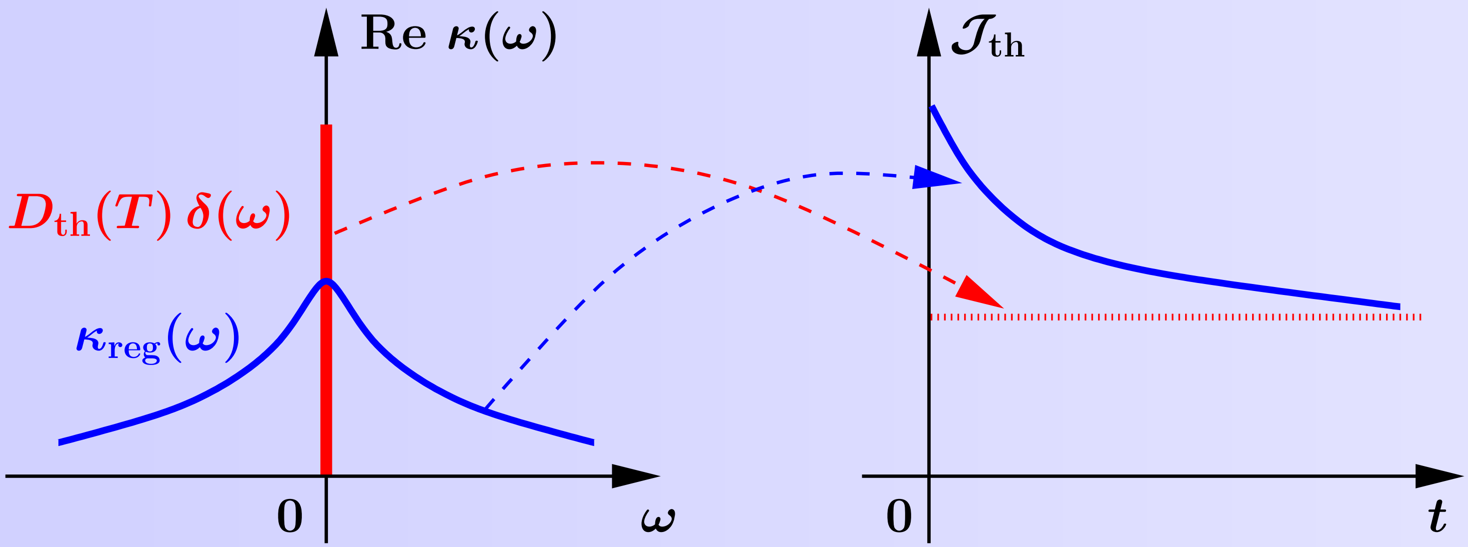
Thermal conductivity κ:

$$\mathcal{J}_{\mathrm{th}} = -\kappa \nabla T$$

Linear response theory:

$$\kappa(\omega) \sim \int_0^\infty dt\, e^{-i\omega t} \int_0^{1/T} d\tau \langle j_{\mathrm{th}} j_{\mathrm{th}}(t + i\tau)\rangle$$

Drude weight D_{th} and regular part $\Rightarrow$ ballistic



2. The spin-1/2 Heisenberg chain

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

Continuity equation:

$$\partial_t h_l + \textbf{div}\, j_{\mathrm{th},l} = 0$$

Ballistic transport:

Zotos et al. PRB 1997

$$j_{\mathrm{th}} \propto \sum_l \vec{S}_l \cdot (\vec{S}_{l+1} \times \vec{S}_{l+2})$$

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

Divergent thermal conductivity!

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

Spectral representation:

$$D_{\mathrm{th}} \propto \sum_{E_n = E_m} e^{-E_n/T} \, |\langle m | j_{\mathrm{th}} | n \rangle|^2$$

$$\Rightarrow \quad D_{\mathrm{th}} \propto \langle j_{\mathrm{th}}^2 \rangle$$

2. The spin-1/2 Heisenberg chain

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

Continuity equation:

$$\partial_t h_l + \text{div}\, j_{\text{th},l} = 0$$

Ballistic transport:

Zotos et al. PRB 1997

$$j_{\text{th}} \propto \sum_l \vec{S}_l \cdot (\vec{S}_{l+1} \times \vec{S}_{l+2})$$

$$[H, j_{\text{th}}] = 0$$

Divergent thermal conductivity!

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

Spectral representation:

$$D_{\text{th}} \propto \sum_{E_n = E_m} e^{-E_n/T} \, |\langle m | j_{\text{th}} | n \rangle|^2$$

$$\Rightarrow \quad D_{\text{th}} \propto \langle j_{\text{th}}^2 \rangle$$

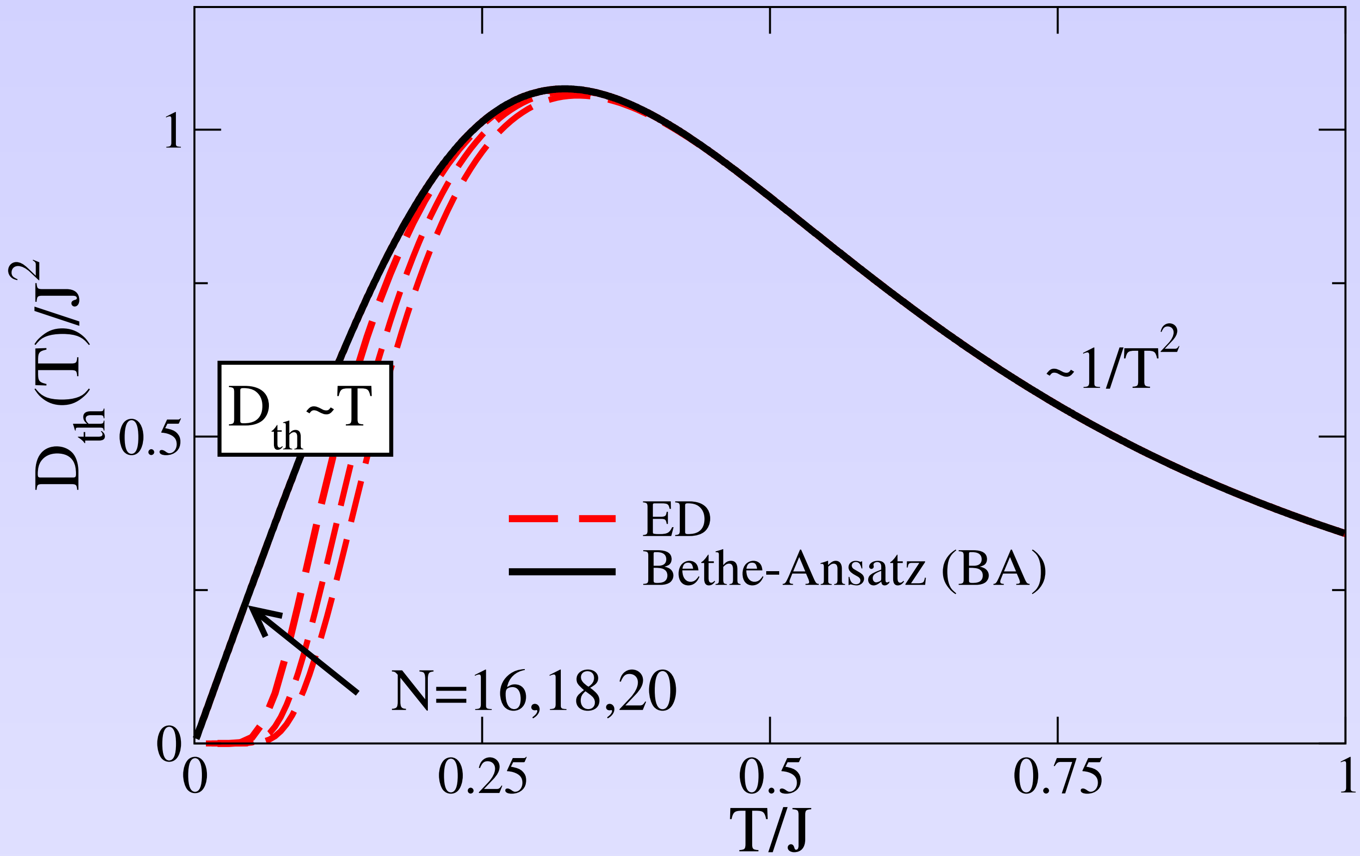
→ **Thermal transport: anisotropy**

→ **Spin transport: Ballistic?**
Wiedemann-Franz law

→ **Magnetic field:**
„Seebeck" effect,...

The thermal Drude weight of the Heisenberg chain

Comparison: Exact diagonalization (ED) vs Bethe Ansatz (BA)



agreement **Klümper, Sakai JPA 2002; HM et al. PRB 2002**

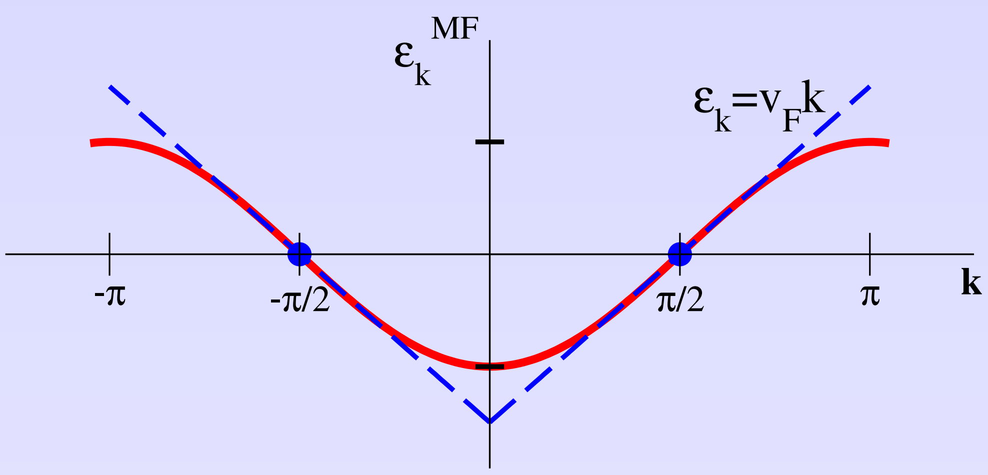
Thermal Drude weight: Low temperatures

Jordan-Wigner transformation: Spinless fermions $c_l^\dagger$ Jordan, Wigner 1928

$$H = J \sum_l \vec{S}_l \cdot \vec{S}_{l+1} = J \sum_l \{ \frac{1}{2}(c_l^\dagger c_{l+1} + h.c.) + n_l n_{l+1} \}$$

Mean field theory:

$$H = \sum_k \epsilon_k^{MF} c_k^\dagger c_k$$



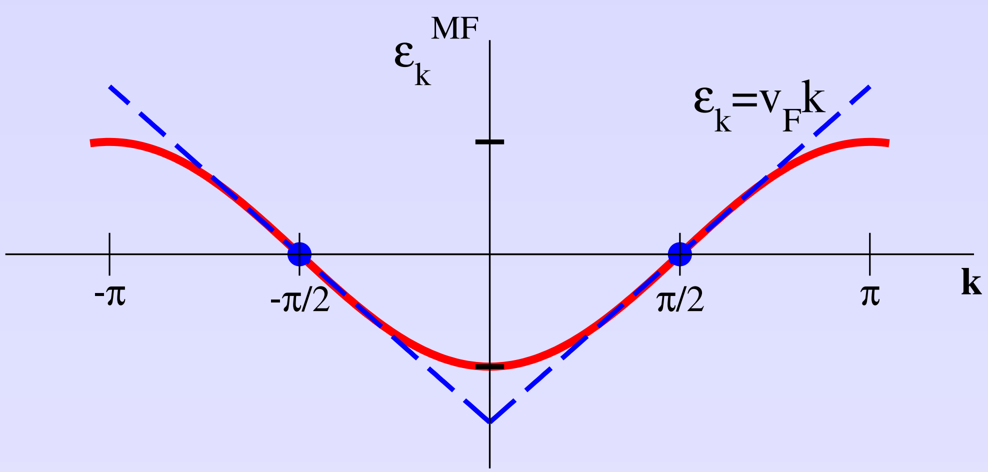
Thermal Drude weight: Low temperatures

Jordan-Wigner transformation: **Spinless fermions** $c_l^\dagger$ **Jordan, Wigner 1928**

$$H = J \sum_l \vec{S}_l \cdot \vec{S}_{l+1} = J \sum_l \{ \frac{1}{2}(c_l^\dagger c_{l+1} + h.c.) + n_l n_{l+1} \}$$

Mean field theory:

$$H = \sum_k \epsilon_k^{MF} c_k^\dagger c_k$$



Conformal field theory

$$H = \frac{v}{2} \int dx \left(K (\partial_x \theta)^2 + \frac{1}{K} (\partial_x \phi)^2 \right)$$

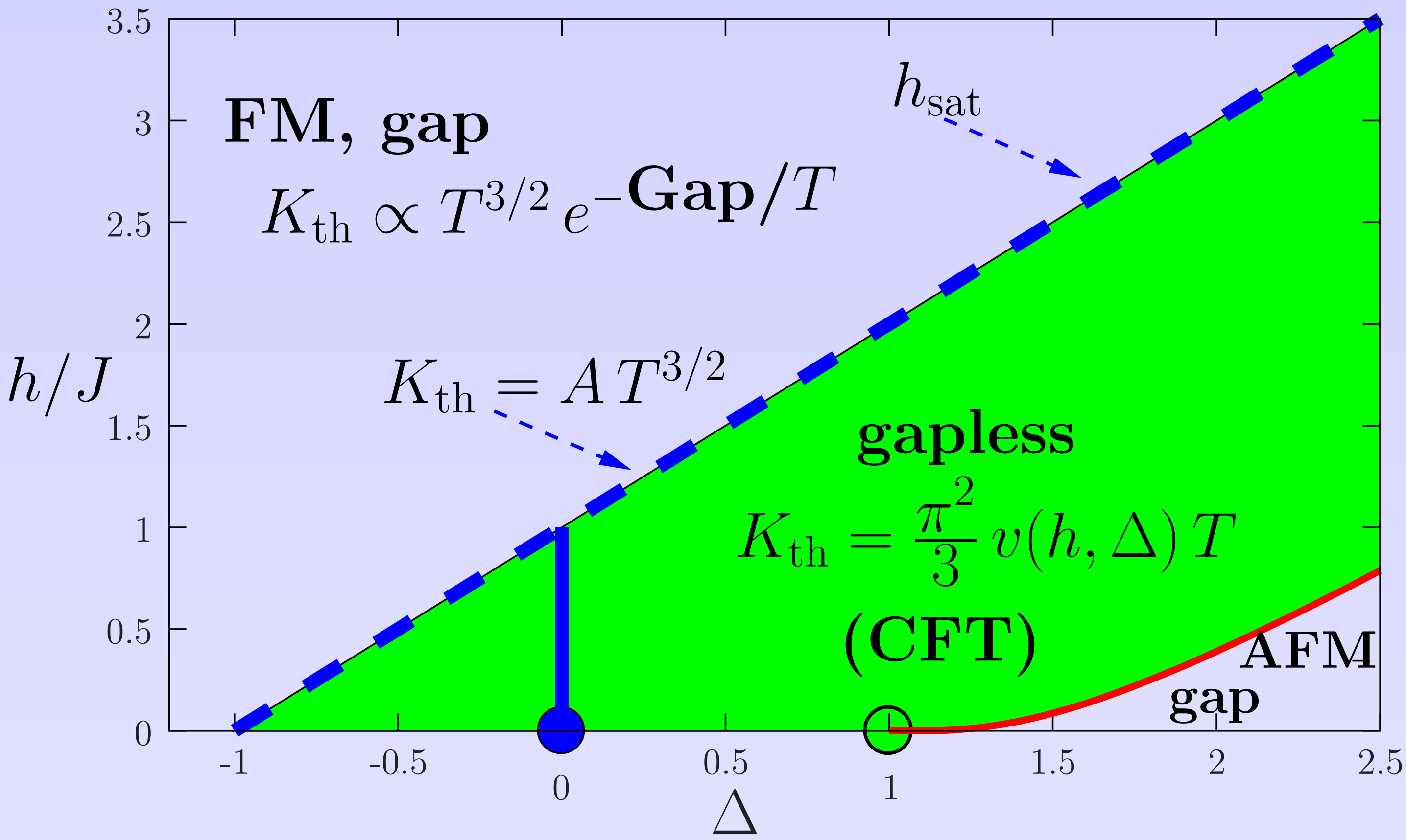
$$j_{\rm th} \propto \int dx \, \partial_x \phi \partial_x \theta$$

$$D_{\rm th} = \frac{\pi^2}{3} v \, T$$

Klümper, Sakai JPA 2002; HM et al. PRB 2002

Thermal Drude weight: Low temperatures

$$H = H^{h=0} - hS^z_{\rm tot} \;\Rightarrow\; j_{\rm th}(h) = j_{\rm th}(0) - h j_{\rm s} \quad \boxed{K_{\rm th}(h,T)} = D_{\rm th} - \frac{D^2_{\rm th,s}}{T\,D_{\rm s}}$$



Adapted from Cabra et al. PRB 1998; **HM et al PRB 2005**

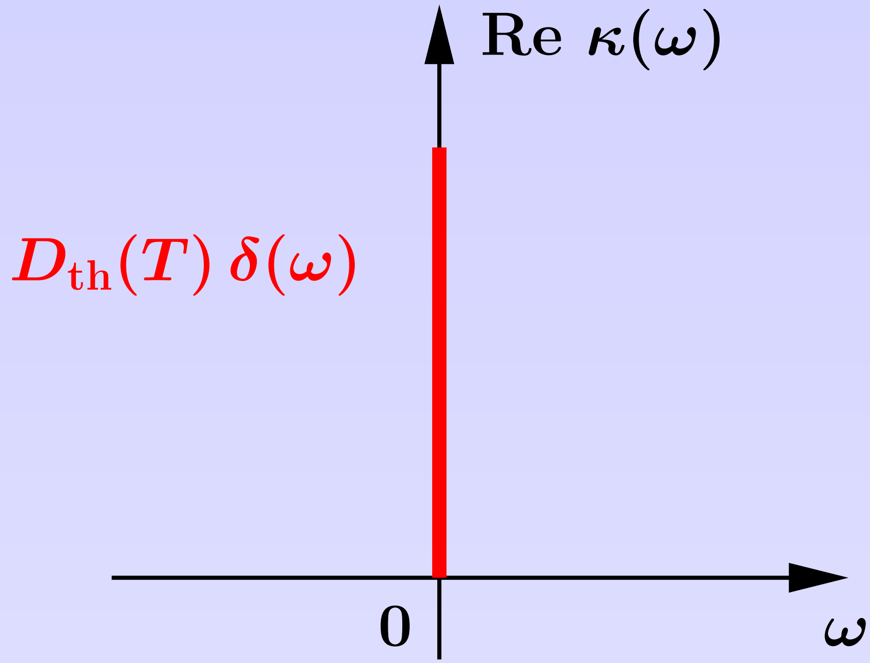
The spin-1/2 Heisenberg chain

- **Interacting quantum model:**
  Ballistic transport $D_{\mathrm{th}}(T) > 0$

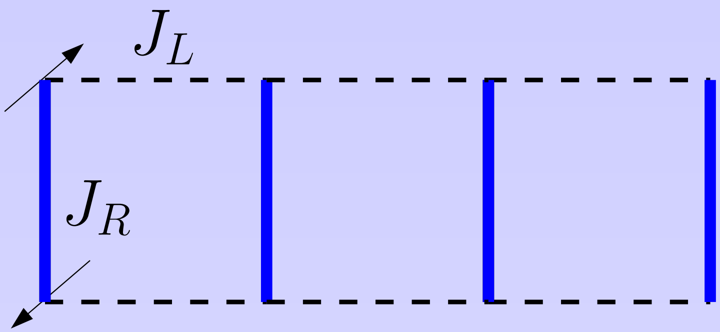
- **ED: temperatures** $T/J \gtrsim 0.2$

- **Low temperatures:** $D_{\mathrm{th}} \propto T$

- **Finite magnetic fields**



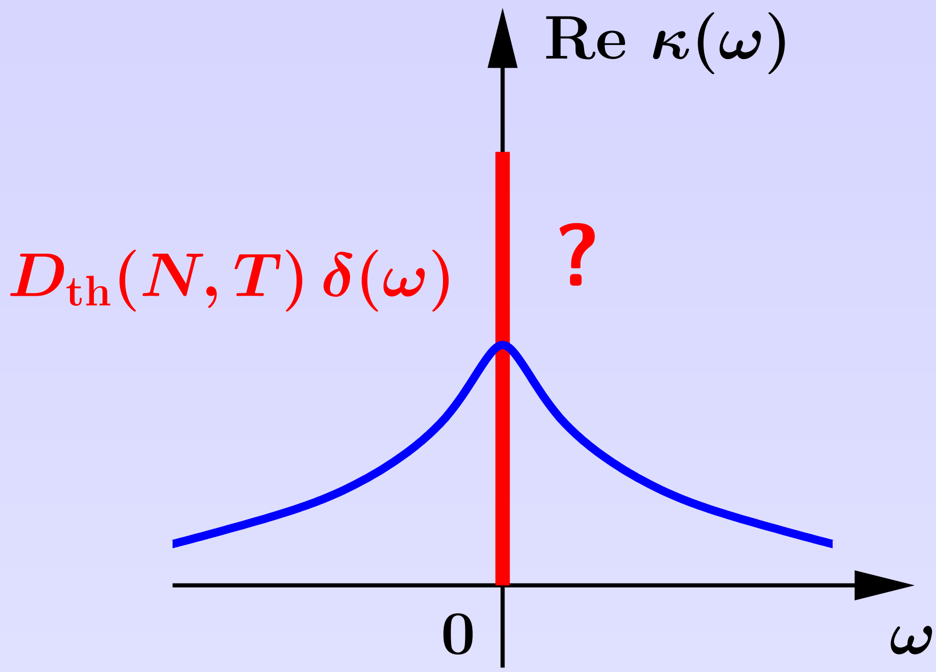
3. Thermal conductivity of spin ladders



No conserved currents (umklapp):

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

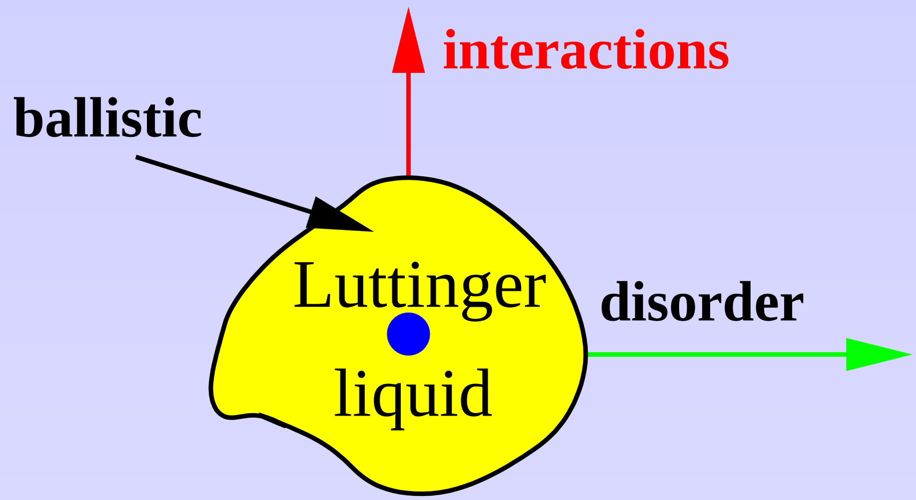
Rosch, Andrei PRL 2000; Shimshoni et al. PRB 2003; HM et al. PRB 2003



$D_{\rm th}(T>0) > 0$**?** **Alvarez, Gros PRL 2002 & 2004; Saito PRB 2003; Orignac et al. PRB 2003**

Umklapp scattering: Bosonization

Continuum-limit for lattice models



Fixed point: Luttinger liquid

$$H_{\mathrm{LL}} = \int dx \left(vK(\partial_x \Theta)^2 + \frac{v}{K}(\partial_x \phi)^2 \right)$$

$$j_{\mathrm{th}} = v^2 \int dx\, \partial_x \phi \partial_x \Theta \quad [H_{\mathrm{LL}}, j_{\mathrm{th}}] = 0$$

Relevant perturbations:

$$H_{\rm LL} \rightarrow H_{\rm LL} + H_{\rm rel} \quad H_{\rm rel} = g(\dots) \int dx \cos(c\,\phi) \quad [H_{\rm LL} + H_{\rm rel}, j_{\rm th}] = 0$$

Irrelevant/ incommensurate operators: $H_{\rm LL} \rightarrow H_{\rm LL} + H_{\rm rel} + 1 \times H_{\rm irr}$

$$H_{\rm irr} \sim \sum_{n,m} \int dx\, \mathcal{O}_{n,m}(x) = \int dx\, g_{nm} \cos(\sqrt{2\pi} n\,\phi + k_{nm} x) \quad [H_{\rm irr}, j_{\rm th}] \neq 0$$

But: conserved currents still exist:

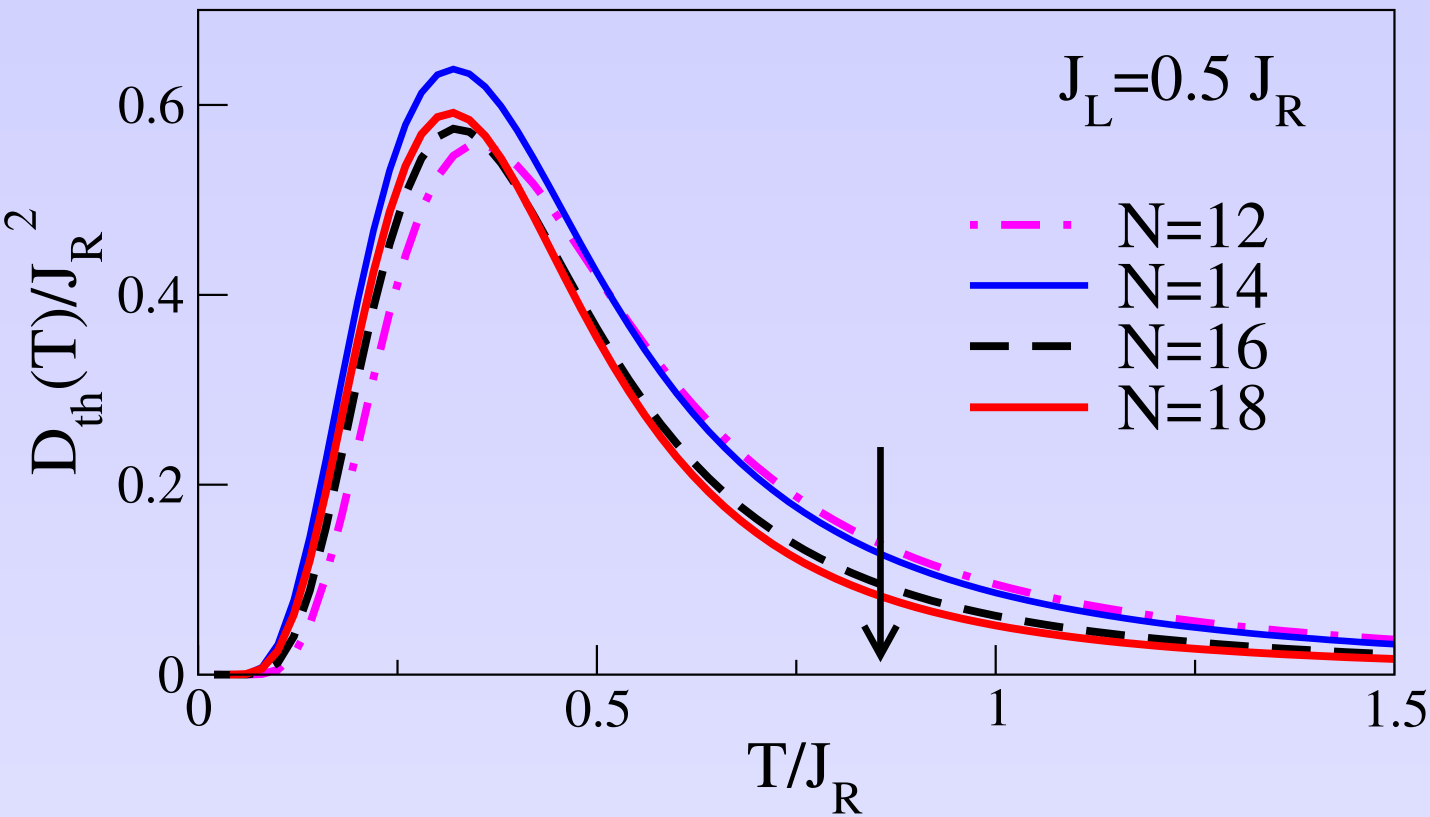
$$j_{\rm erhalten} = k_{nm} j_{\rm s} + 2n j_{\rm th}$$

Finally: $H_{\rm LL} \rightarrow H_{\rm LL} + H_{\rm rel} + \text{MANY} \times H_{\rm irr}$

No current survives

Rosch, Andrei, PRL 2000; Saito PRB 2003, Shimshoni et al., PRB 2003, HM et al., PRB 2003

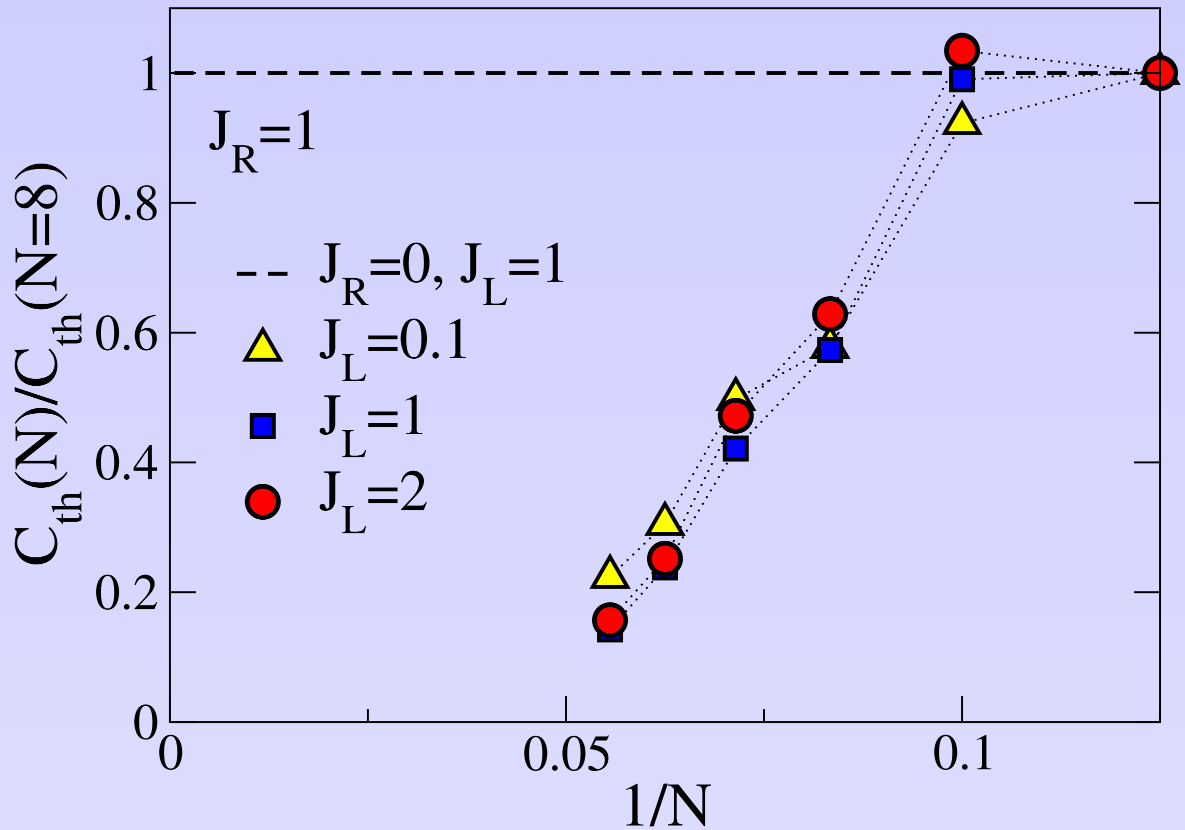
The thermal Drude weight of spin ladders



HM et al. PRB 2003

No convergence!

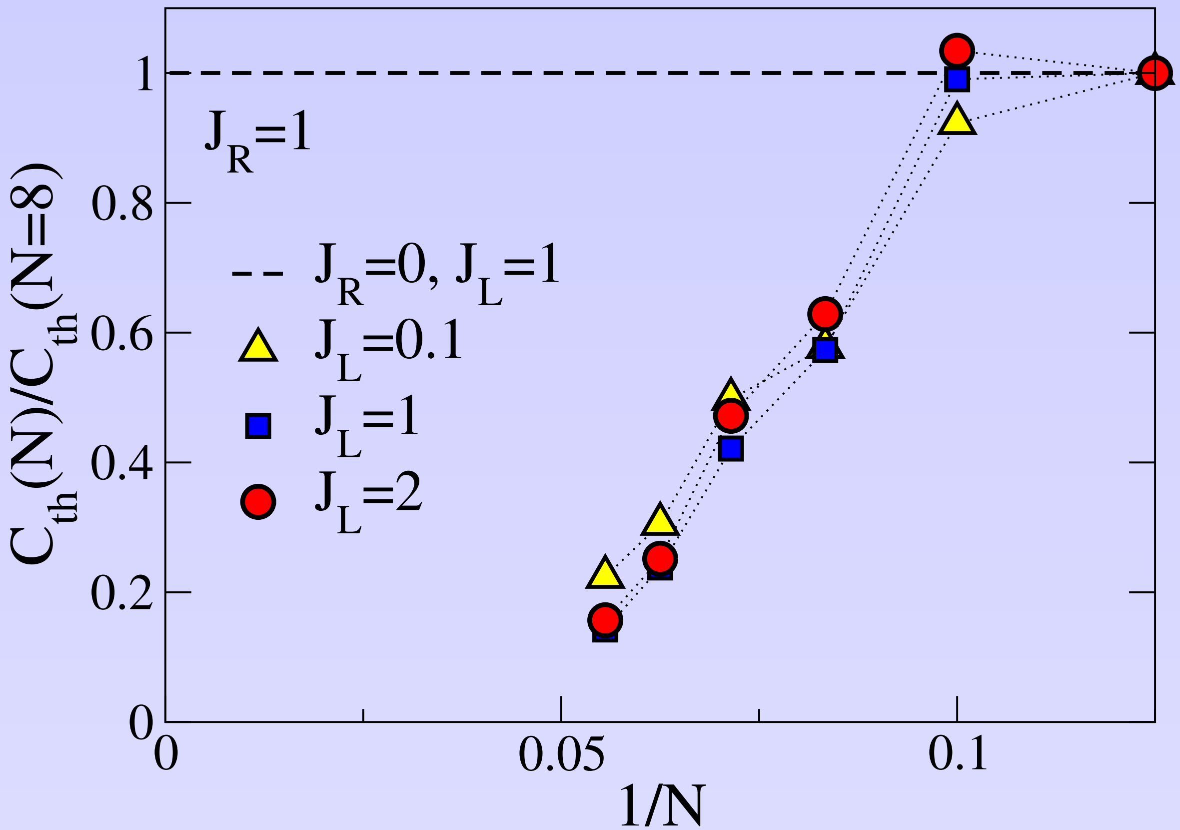
High-temperature limit



$$D_{\rm th}(N,T) = \frac{C_{\rm th}(N)}{T^2} + \frac{C_2(N)}{T^3} + \ldots$$

$$D_{\rm th}(N,T) \to 0$$

High-temperature limit



$$D_{\rm th}(N,T) = \frac{C_{\rm th}(N)}{T^2} + \frac{C_2(N)}{T^3} + \ldots$$

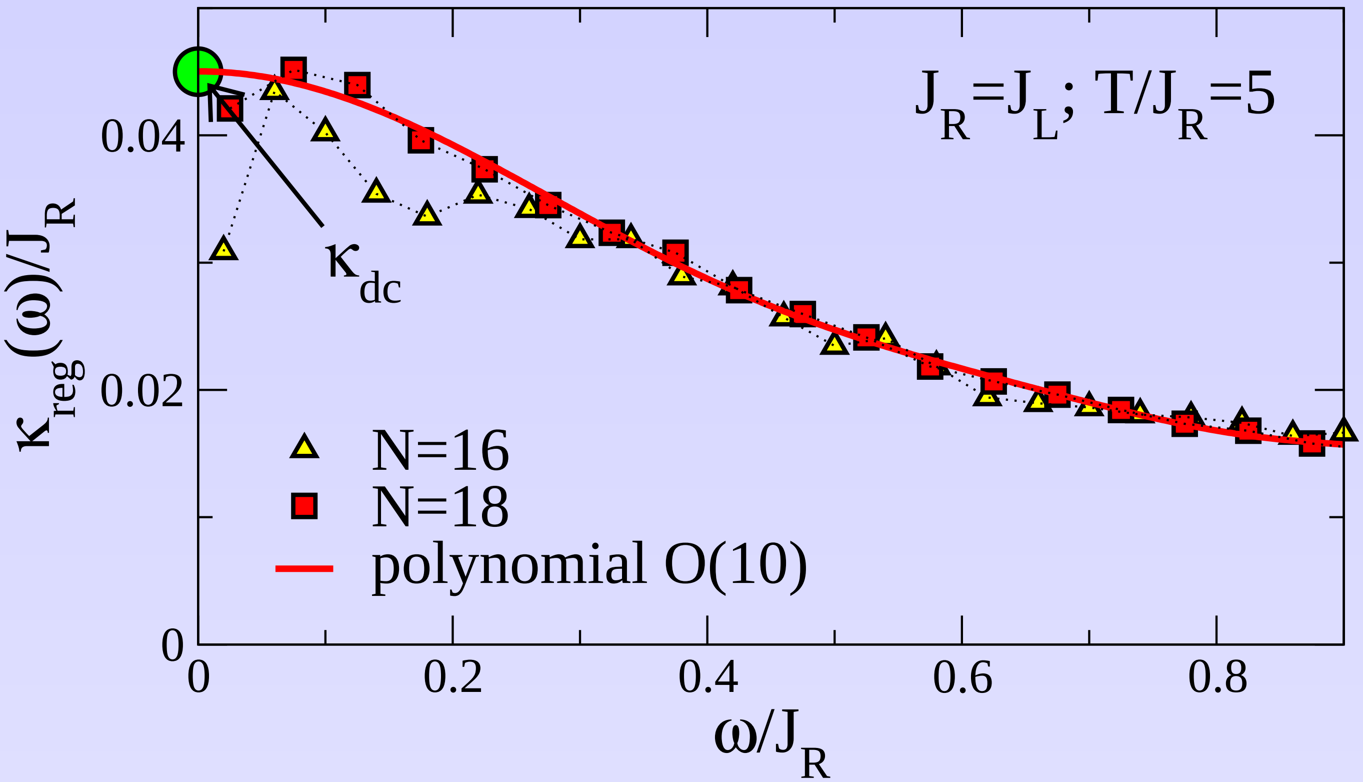
$$D_{\rm th}(N,T) \rightarrow 0$$

$\surd$ **Frustrated and dimerized chain; spin transport**

HM et al. PRB 2002, 2003, PRL 2004, JMMM 2004, Physica B 2005; Zotos PRL 2004

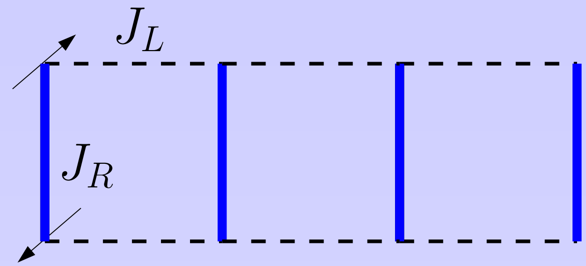
Spin ladder: $\kappa(\omega)$

$$\kappa_{\rm reg}(\omega) \propto \sum_{E_n \neq E_m} e^{-E_n/T} \, |\langle m | j_{\rm th} | n \rangle|^2 \, \delta(\omega - (E_m - E_n))$$

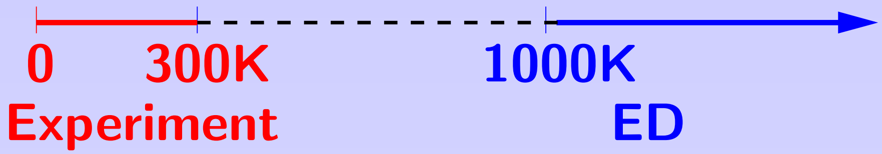


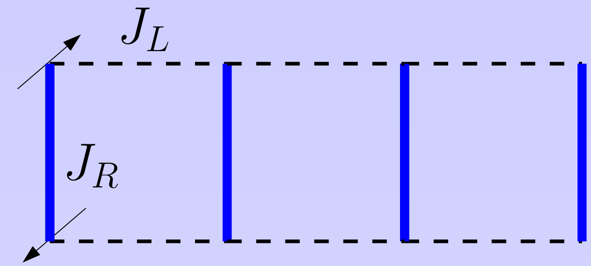
$\longrightarrow$ $\kappa_{\rm dc}$ can be extracted

Spin ladder: Comparison with experiment?

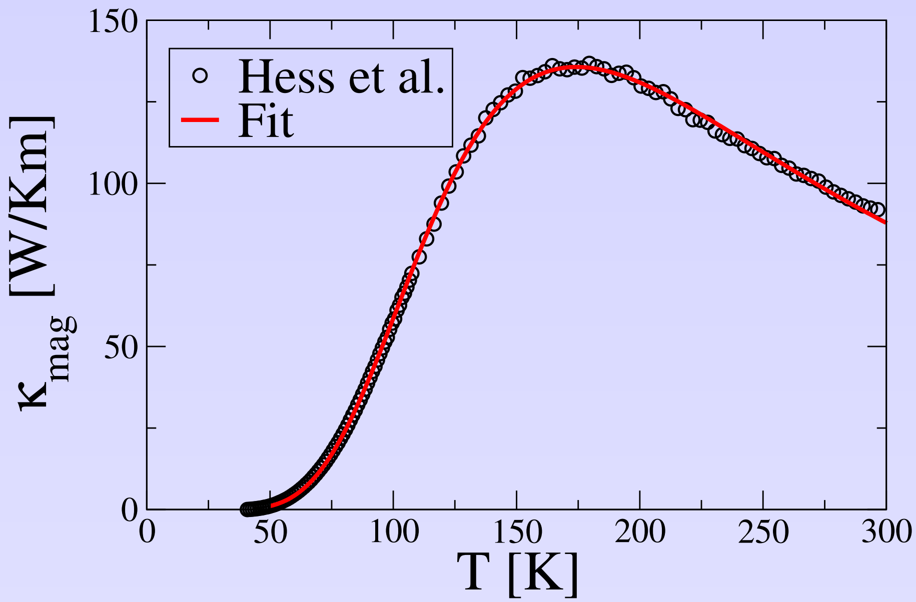


Spin ladder: Comparison with experiment?





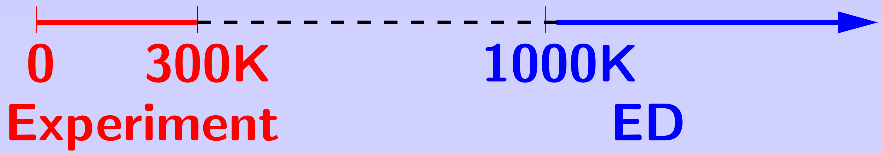
Experiment $Ca_9La_5Cu_{24}O_{41}$:

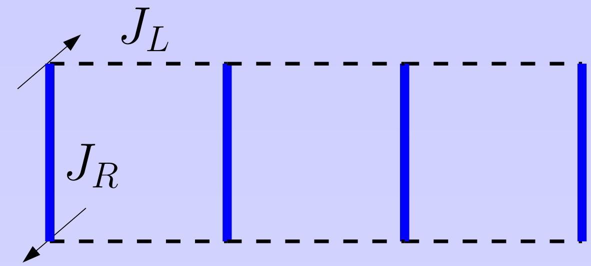


Extrapolation to high T using fit:

$\kappa_{mag} \approx$ const T^{-2} **Alvarez, Gros PRL 2002**

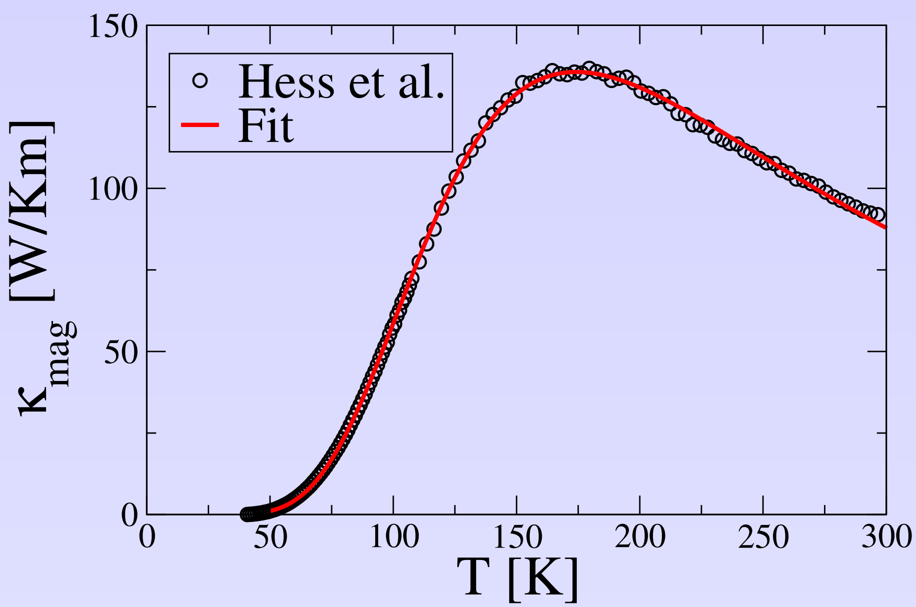
Spin ladder: Comparison with experiment?

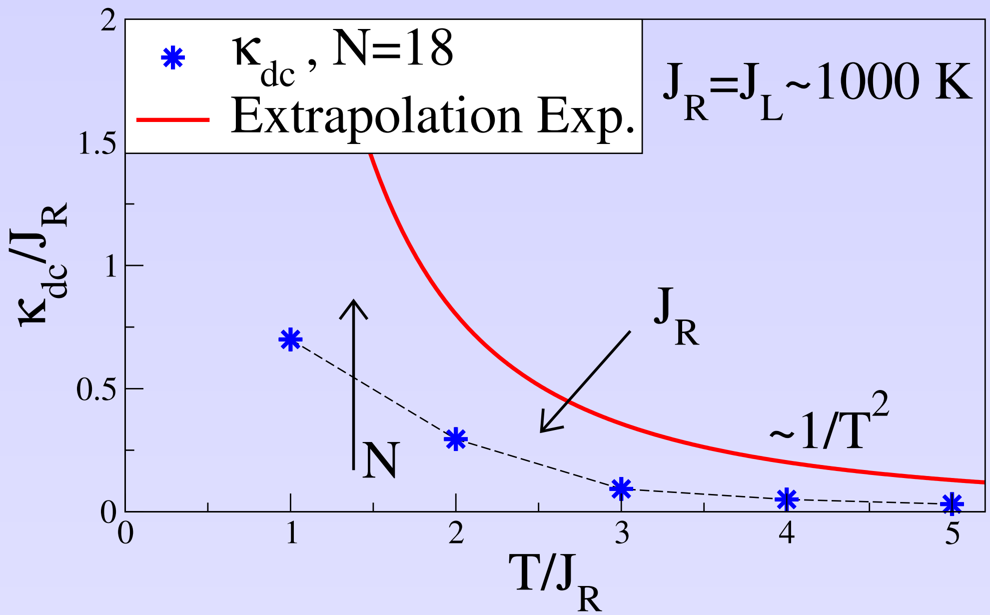




Experiment $Ca_9La_5Cu_{24}O_{41}$:

Exact diagonalization:





Extrapolation to high T using fit:

$\kappa_{\mathrm{mag}} \approx$ **const** T^{-2}

Alvarez, Gros PRL 2002

Order of magnitude o.k.

Summary

→ **Experimental motivation**

– **Significant ”magnon” heat conduction**

→ **Spin-1/2 Heisenberg chain**

– **Conservation laws: Ballistic transport**
– **Thermal Drude weight:** $D_{\mathrm{th}}(h, \Delta, T)$

→ **Thermal conductivity of spin ladders**

– **ED: normal transport**
– **Frequency dependence and DC-limit**