Unusual transport properties of quasi one-dimensional magnets

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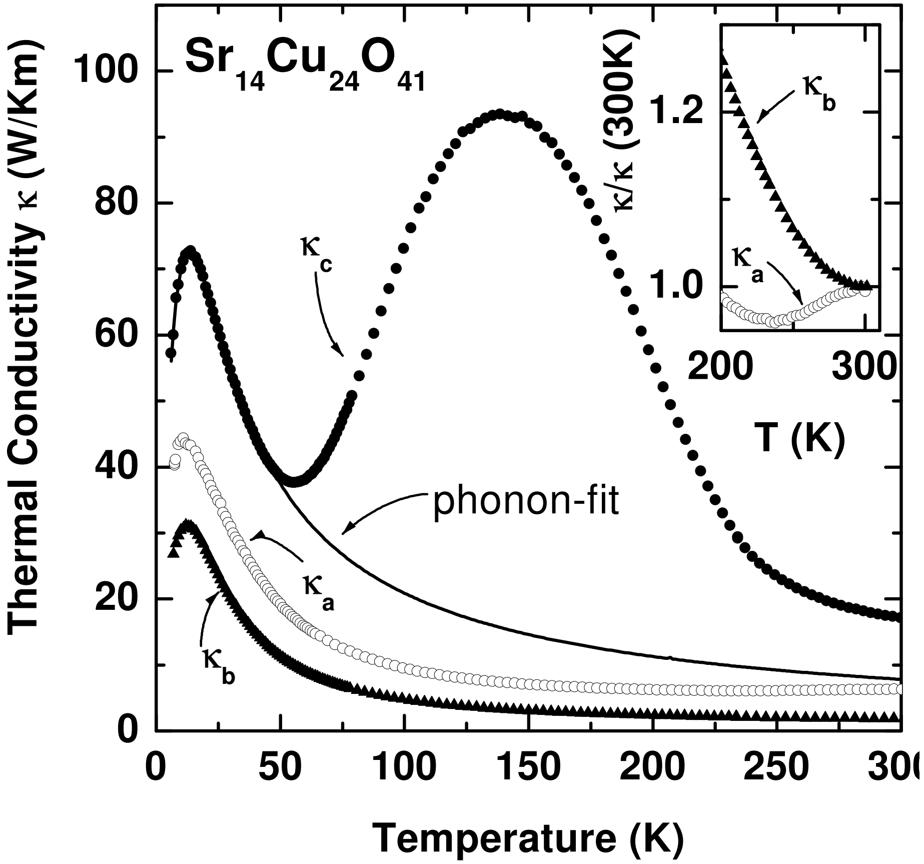
- anomalous transport in integrable systems
- quantum Monte-Carlo and transport
- magnetic Drude weight
- thermal conductivity

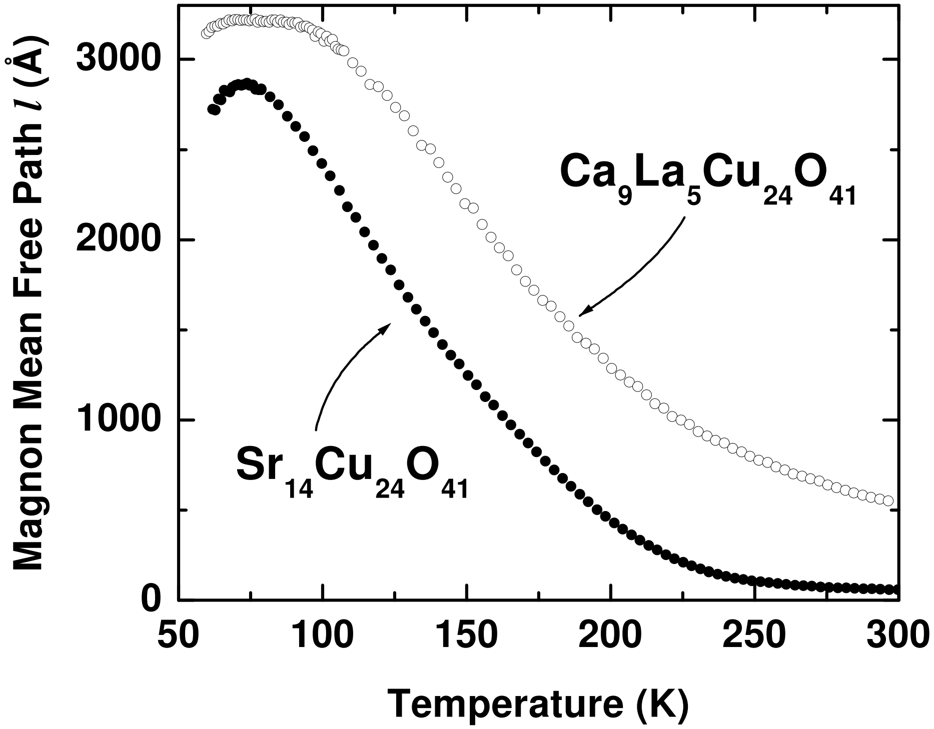
Anomalous big transport coefficients in ladders

thermal conductivity

magnetic mean free path



[Hess *et al.* '01]

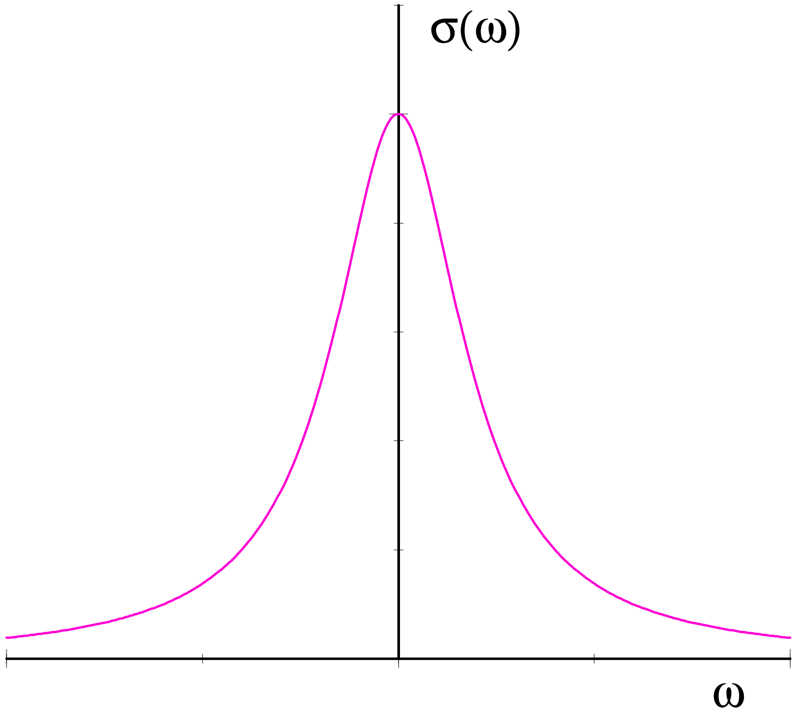


- normal magnets: magnetic contributions negligible

Drude transport

[finite lifetime]

- Drude: $$\boxed{\sigma(\omega) \;=\; \frac{\sigma_0}{1+(\omega\tau)^2}}$$
- relaxation time τ



ballistic transport

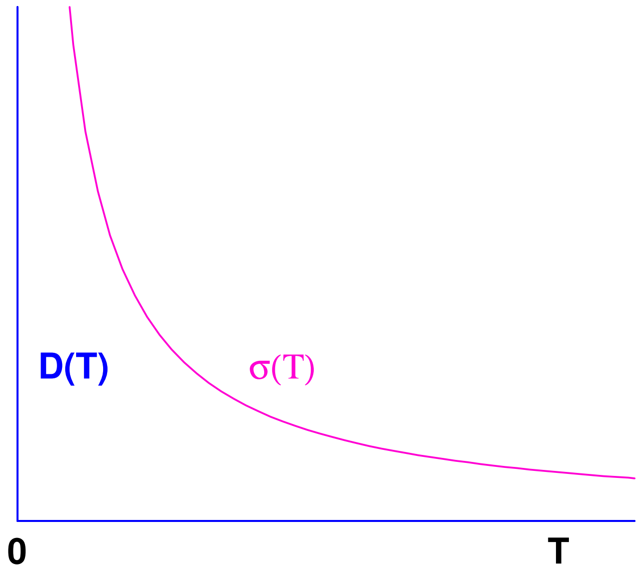
$[\tau \to \infty]$

$$\boxed{\sigma(\omega) \;\to\; \pi\, D\, \delta(\omega)}$$

Drude weight $D \;=\; \dfrac{\sigma_0}{\tau} \;=\; \dfrac{e^2 n_p}{m_e}$

conductivity of a normal metal

[3D, no disorder]



- $T = 0$: translational invariance

  – $\boxed{\text{ballistic transport}}$

- $T > 0$: quasiparticle scattering

  – $\boxed{\text{diffusive transport}}$

ballistic transport in integrable quantum system

[1D]

- current j_A does not decay – ballistic transport
- Drude weight $\boxed{D(T) > 0}$ even for $\boxed{T > 0}$

[Castella *et al.* '95]

conservation laws

- conserved quantities Q_n $\boxed{[H, Q_n] = 0}$
- Mazur inequality $$\boxed{\lim_{T\to\infty} \frac{1}{T} \int_0^T dt \, \langle A(t) A(0) \rangle \geq \sum_n \frac{\langle A\, Q_n \rangle^2}{\langle Q_n^2 \rangle^2}}$$

- A $\rightarrow$ current operator J: no decay $\rightarrow$ ballistic transport
- Drude weight $$\boxed{D(T) \geq \frac{\beta}{2L} \sum_n \frac{\langle J\, Q_n \rangle^2}{\langle Q_n^2 \rangle^2}}$$

[Zotos *et al.* '97]

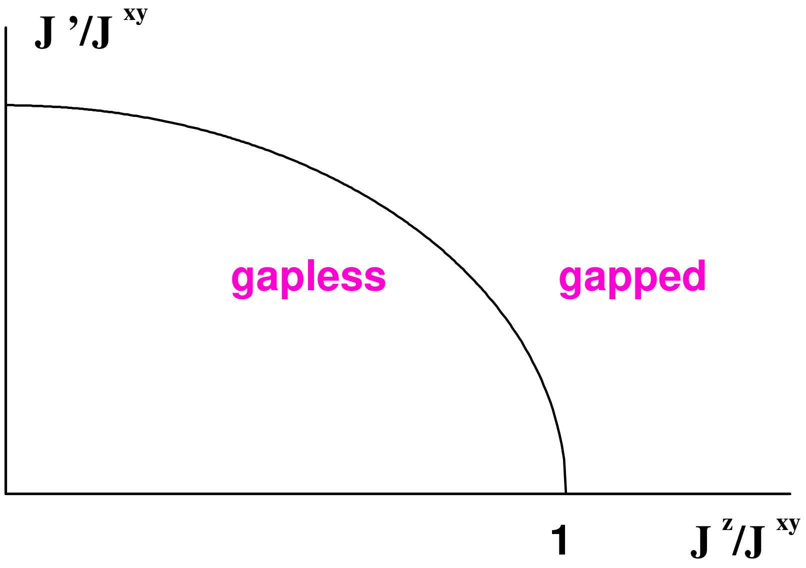
- integrable systems: many Q_n

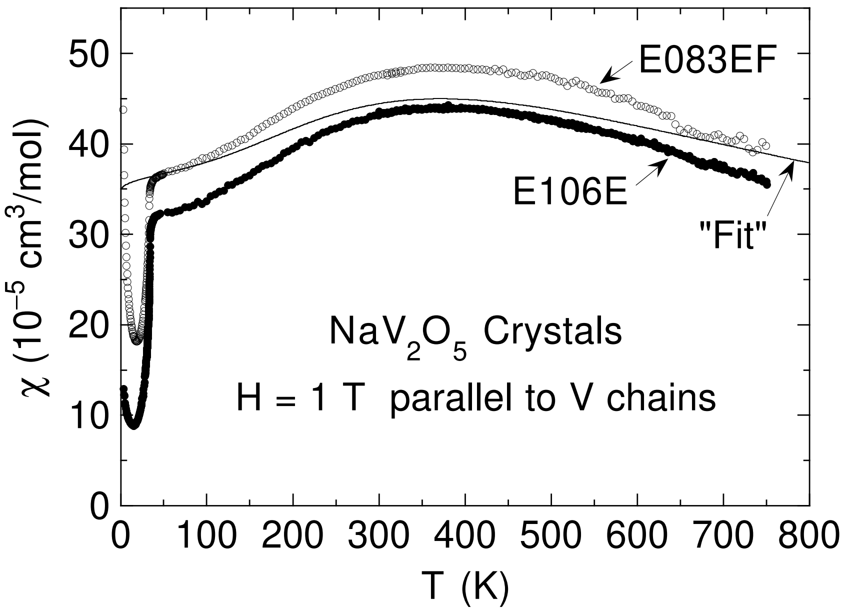
Heisenberg model

[1D]

$$H = J_{xx} \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y \right) + J_z \sum_i S_i^z S_{i+1}^z + J_z' \sum_i S_i^z S_{i+3}^z$$

Bethe-Ansatz solvable for $J' = 0$ quantum-critical for $J_z / J_{xx} < 1$

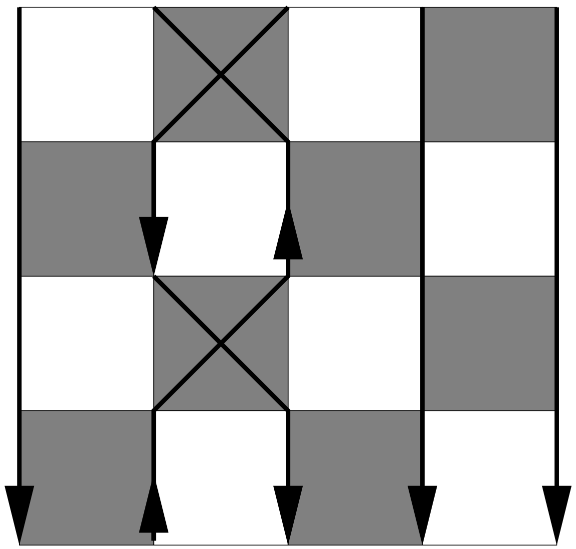




[Hemberger *et al.*, '98]

Monte-Carlo approach

[Heisenberg-model]



- Trotter-Suzuki $\beta = N_t \Delta\tau$

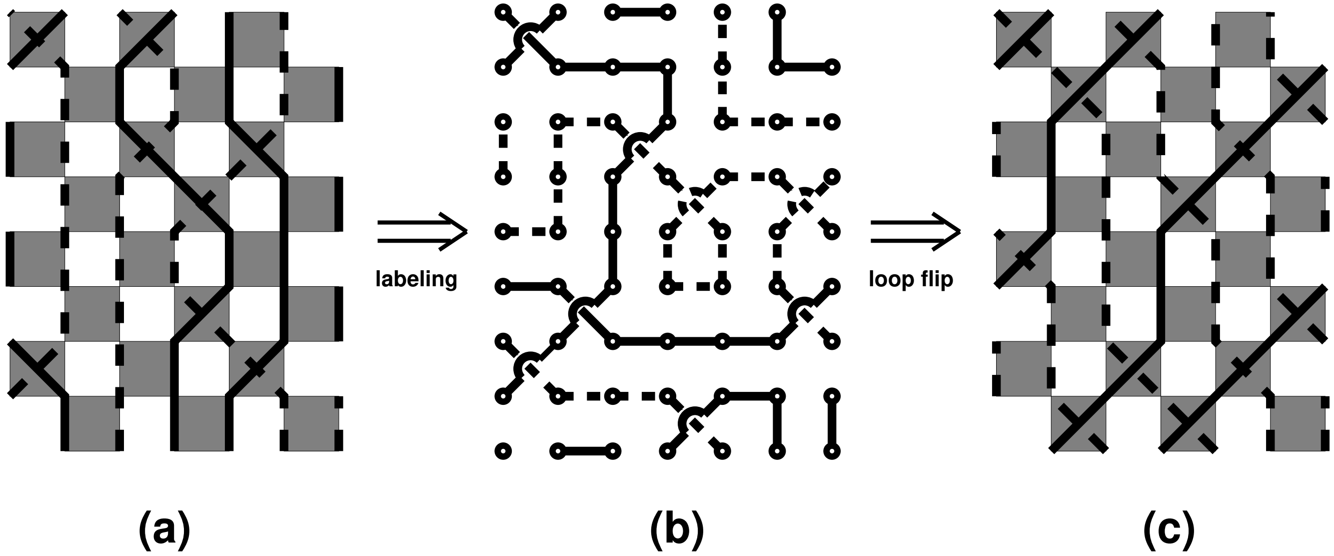
$$e^{-\beta H} = \prod e^{-\Delta\tau H}$$

- $\boxed{\text{1D spin-1/2} \;\hat{=}\; \text{2D classical}}$
- worldlines $\hat{=}$ spin-$\uparrow$
- Monte-Carlo: stochastic evaluation

loop-algorithm

[Amon *et al.*, '97]

- loop-breakups $\hat{=}$ cluster of spin-flips



- efficient: auto-correlation-time ~ 1, continuous Trotter-time
- correlation-functions: n-point, non-diagonal, imaginary-time

transport

- magnetization-density: $\rho_l \;=\; S_l^z - \frac{1}{2}$
- magnetization-current: $j_l \;=\; J_{xx}\left(S_l^y S_{l+1}^x \;-\; S_l^x S_{l+1}^y \right)$

correlation-functions

$$[q \to 0,\; i\omega_n \to \omega + i\delta]$$

$$\boxed{\sigma(q, i\omega_n) \;=\; \frac{\langle K\rangle + \Lambda_{j,j}(q, i\omega_n)}{i\,(i\omega_n)} \;\equiv\; \frac{-\omega_n}{\sin^2(q/2)} S(q, i\omega_n)}$$

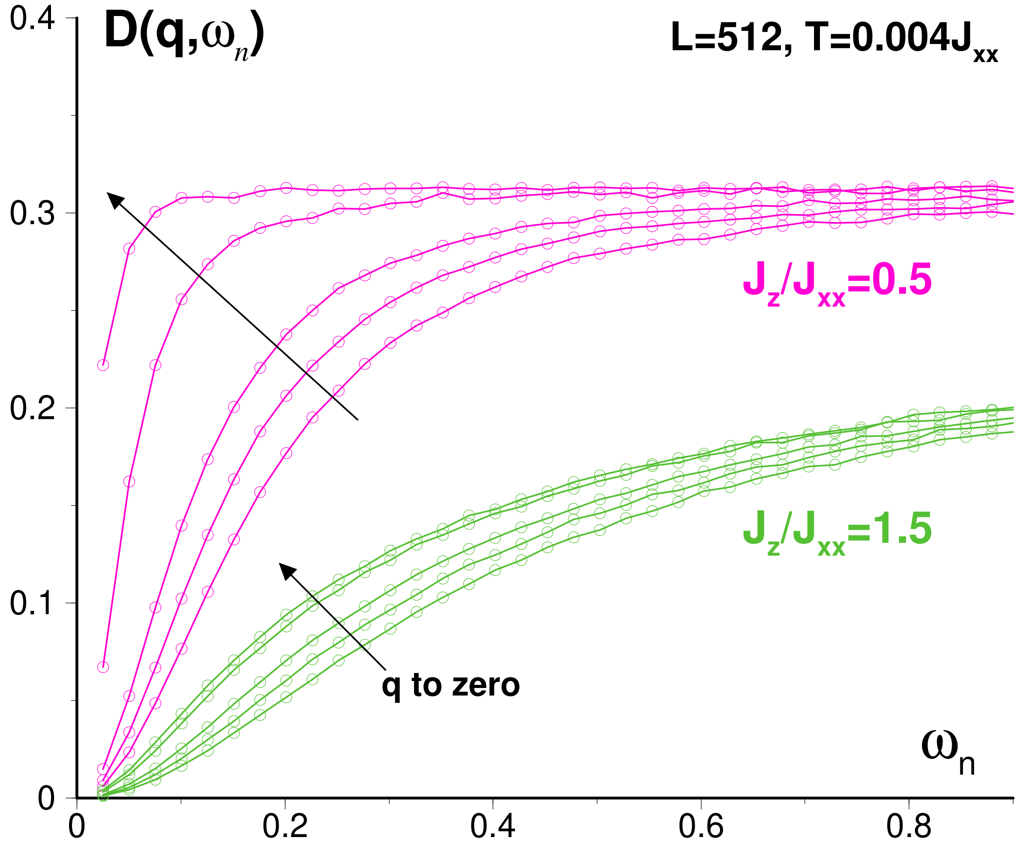
- imaginary axis: $\frac{2\pi}{\beta} n \;=\; 2\pi T n \;=\; \omega_n \;\to\; 0$
- low-T, large systems

correlation functions on imaginary axis

$$\boxed{\sigma(q, i\omega_n) \equiv \frac{D(q,\omega_n)}{\omega_n}}$$

need

$$\lim_{\omega_n \to 0} \lim_{q \to 0} D(q,\omega_n)$$

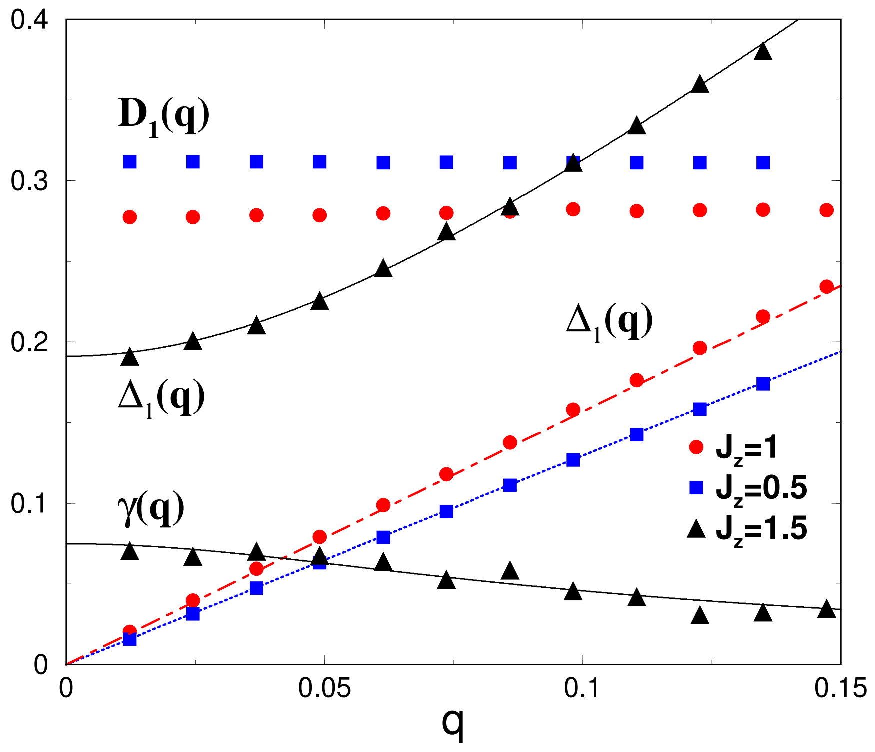


[Alvarez & Gros '01]

data analysis

[QMC]

$$\boxed{D(q,\omega_n) = \frac{D_1(q)\omega_n^2}{\Delta_1^2(q)+2\gamma_1(q)\omega_n+\omega_n^2} + \frac{D_2(q)\omega_n^2}{\Delta_2^2(q)+\omega_n^2}}$$



2-magnon energy $\boxed{\Delta_1(q)}$

Bethe-Ansatz $J_z < J_{xx}$

$$\lim_{q\to 0} \Delta_1(q) = \frac{\pi q}{2} \frac{\sqrt{J_{xx}^2 - J_z^2}}{arcos(J_z/J_{xx})}$$

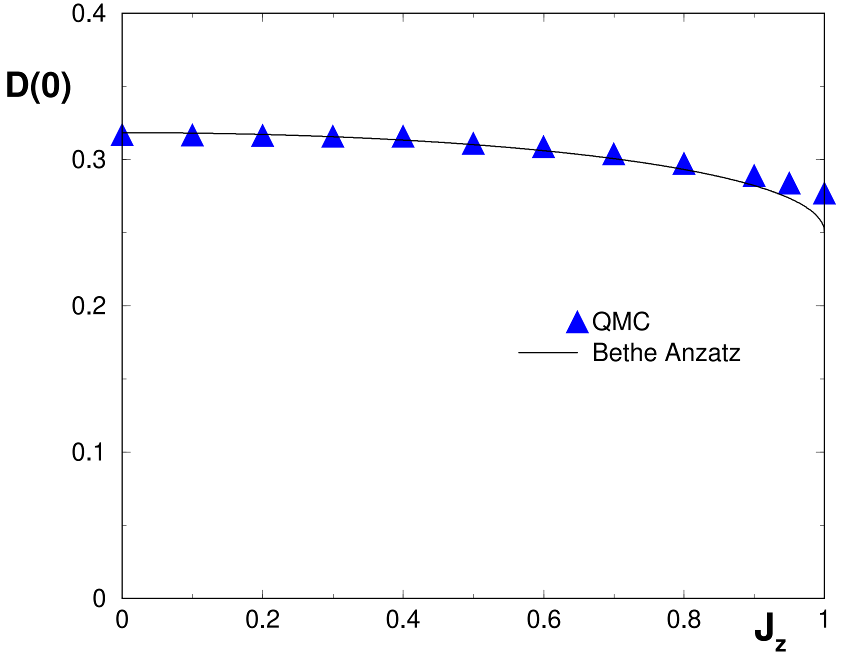
Drude weight

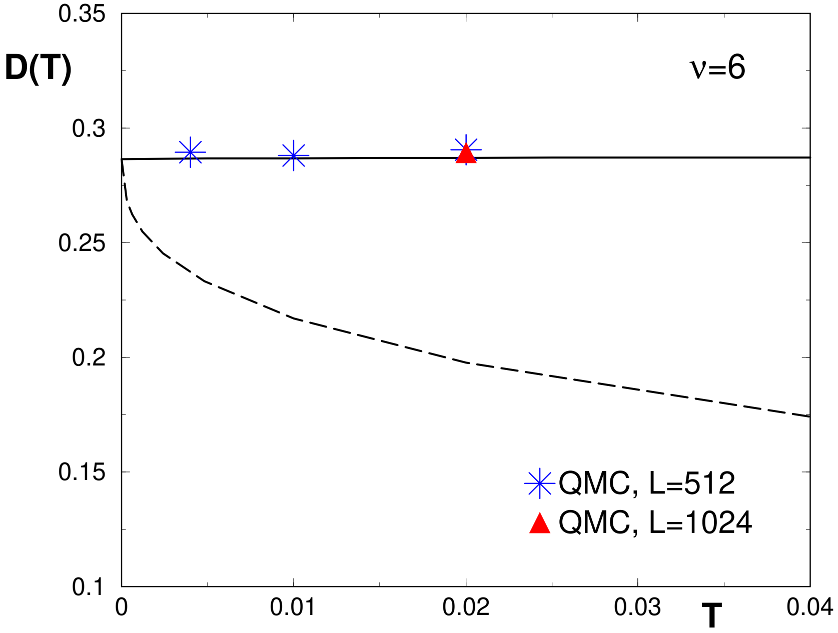
$$\boxed{\lim_{q\to 0} D_1(q) = D(T)}$$

Drude weight

$$\sigma(\omega) = \pi D(T)\delta(\omega) + \sigma_{reg}(\omega)$$

[Alvarez & Gros '01]





Bethe-Ansatz $J_z = J_{xx}\cos(\pi/\nu)$

$$\boxed{D(0) = \frac{\nu^2}{4\pi}\frac{\sin(\pi/\nu)}{\nu-1}}$$

[Shastry & Sutherland '90]

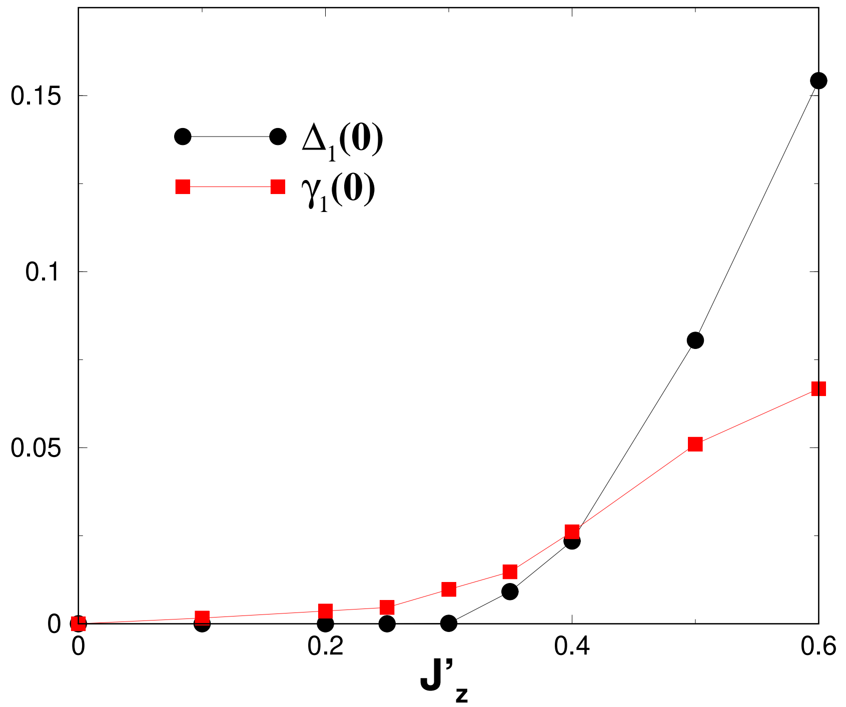
ballistic transport $T > 0$

compare:

two analytic theories

diffusive transport

[non-integrable system]

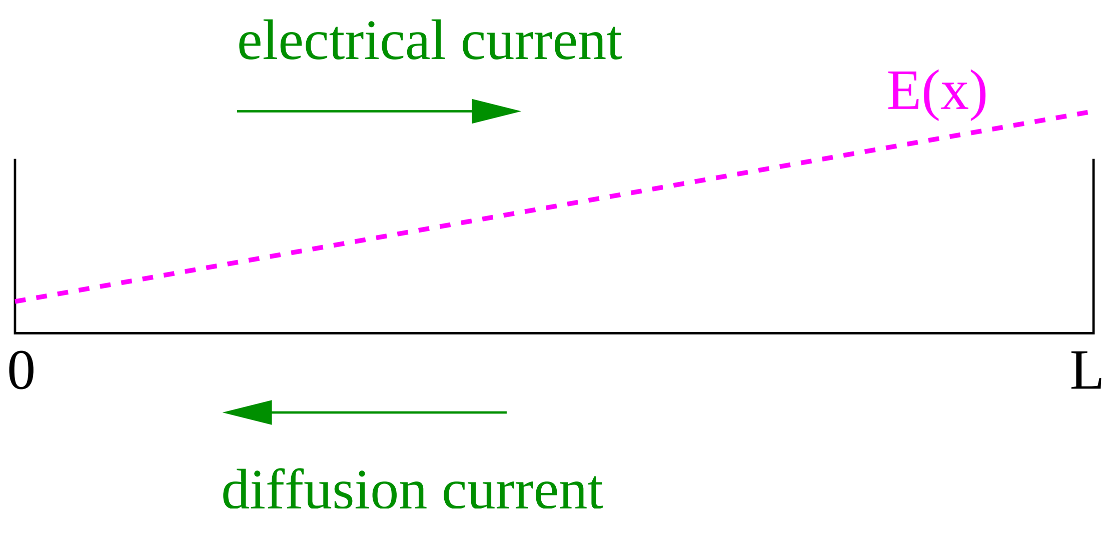


- term $J'_z \sum_i S^z_i S^z_{i+3}$
- $\gamma_1(0)$ finite
- $$\boxed{\sigma(0) = \frac{D_1(0)}{2\gamma_1(0)}}$$ finite
- $D \equiv D_1(0),\ D_1(q) \simeq cq,$
  $\gamma \equiv \gamma_1(0)$

$$Re\,\sigma(q,\omega) = \frac{2\gamma D\,\omega^2}{(\omega^2 - (cq)^2)^2 + 4\gamma^2\omega^2} = \begin{cases} \dfrac{2\gamma D}{\omega^2 + 4\gamma^2} & \text{Drude} \quad (q=0) \\[2ex] \dfrac{2\gamma D\omega^2}{(cq)^2 + 4\gamma^2\omega^2} & \text{diffusive} \quad (\omega < cq) \end{cases}$$

phenonenolgical transport formula

- finite system $\rightarrow$ equilibrium $\boxed{j_E + j_D = 0}$
  - ◇ electrical current $j_E = \sigma E$
  - ◇ difiussion current $j_D = -D \nabla n = -D \chi E$
- generalized Einstein relation: $\boxed{\sigma = D \chi}$



ballistic transport formula

$[\sigma = D\,\chi]$

- diffusion constant: D, Drude weight: D_1
  - $*$ $\sigma = D_1\,\tau$ and $D = v_s^2\,\tau$
  - $*$ 'external' lifetime: τ, single-particle velocity: v_s

- phenomenolgical relation $\boxed{\dfrac{D_1}{\chi} = v_s^2}$
  - ◇ fullfilled by Bethe-Ansatz $T \to 0$
  - ◇ fullfilled by Luttinger-liquid

- v_s non-singular for $T \to 0$

  $\to$ $D_1(T)$ and $\chi(T)$ have same low-T behaviour
  (for $J_z > J_{xx}/2$; exponent crossover)

thermal conductivity

- continuity-equation $$\frac{dh_{\mathbf{x}}}{dt} + \nabla \cdot \mathbf{j}^{E}_{\mathbf{x}} \;=\; 0$$
  - $h_{\mathbf{x}}$ energy-density
  - $\mathbf{j}^{E}_{\mathbf{x}}$ energy-current density
- $\mathbf{j}^{E}_{\mathbf{x}} \;=\; \kappa \nabla T$ units: $[\kappa] \;=\; \frac{\mathrm{W}}{\mathrm{K\,m^{d-2}}}$
  - κ thermal conductivity
  - d dimension

Kubo formula

$$\boxed{\kappa \;=\; \frac{\beta^2}{\mathrm{Vol.}} \lim_{\omega\to 0} \int_0^\infty dt\, \mathrm{e}^{t(i\omega - s)} \langle J^E(t) J^E \rangle}$$

◇ $J^E \;=\; \sum_{\mathbf{x}} \mathbf{j}^E_{\mathbf{x}}$ total energy-current

- $\boxed{\kappa \;=\; \pi \kappa^{(th)}\, \delta(\omega)}$ "Drude peak"

◇ $\tau \;=\; s^{-1} = \lambda / v_s$ finite (external) lifetime

◇ λ (external) mean-free path

◇ v_s spin-wave velocity

$$\boxed{\kappa \;=\; \kappa^{(th)} \frac{\lambda}{v_s} \qquad \text{new} \leftrightarrow \text{old} \qquad \kappa \;=\; c_V\, v_s\, \lambda}$$

1D-3D

$$\boxed{\kappa^{3D} \;=\; \frac{k_B J}{\hbar c}\left(\frac{N_c c^3}{abc}\right)\left(\frac{\lambda}{c}\right)\left(\frac{Jc}{\hbar v_s}\right)\kappa^{th}}$$

◇ $N_c/(abc)$ # of chains per unit-cell

◇ $\kappa^{(th)}$ dimensionless 'Drude-weight' of the 1D thermal conductance

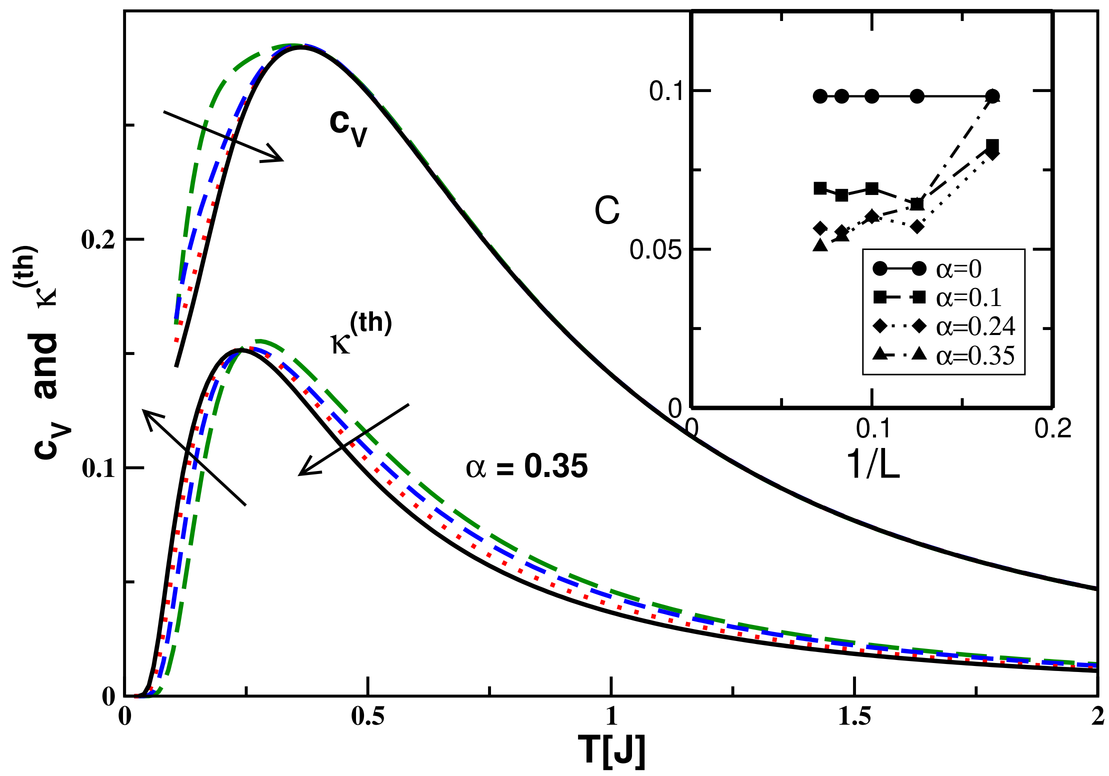
$$\boxed{\kappa^{th} \;=\; \left(\frac{J}{k_B T}\right)^2 \frac{1}{L}\langle \tilde{J}^E \tilde{J}^E \rangle_{\omega=0}}$$

◇ $[\tilde{J}^E, H] = 0$ $\rightarrow$ static expectation value

$\rightarrow$ 1D-Heisenberg: Bethe-Ansatz (Klümper)

exact diagonalization

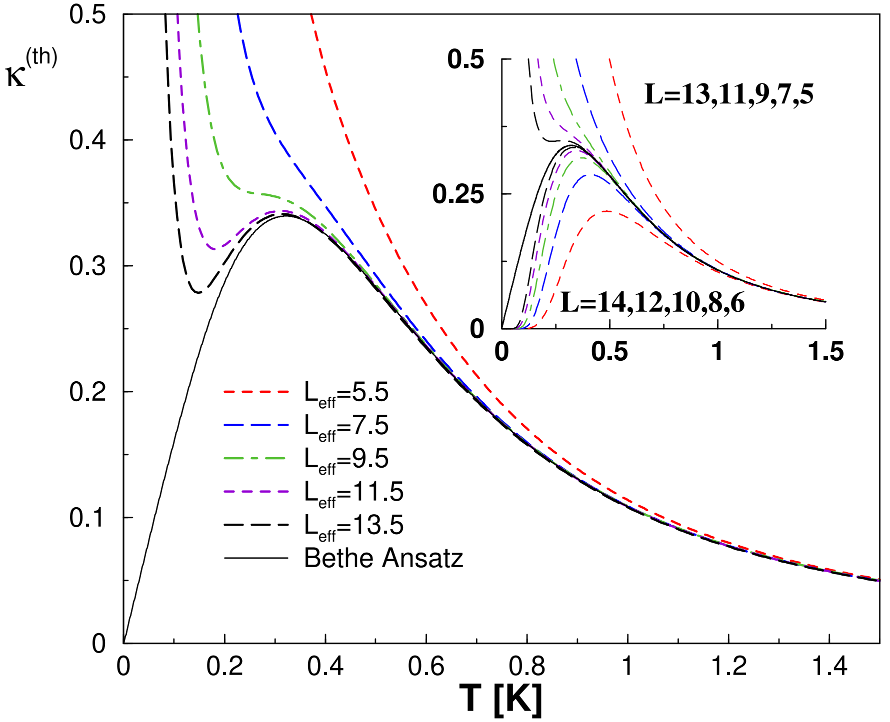
$$H \;=\; J \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \;+\; \alpha\, \mathbf{S}_i \cdot \mathbf{S}_{i+2} \right)$$



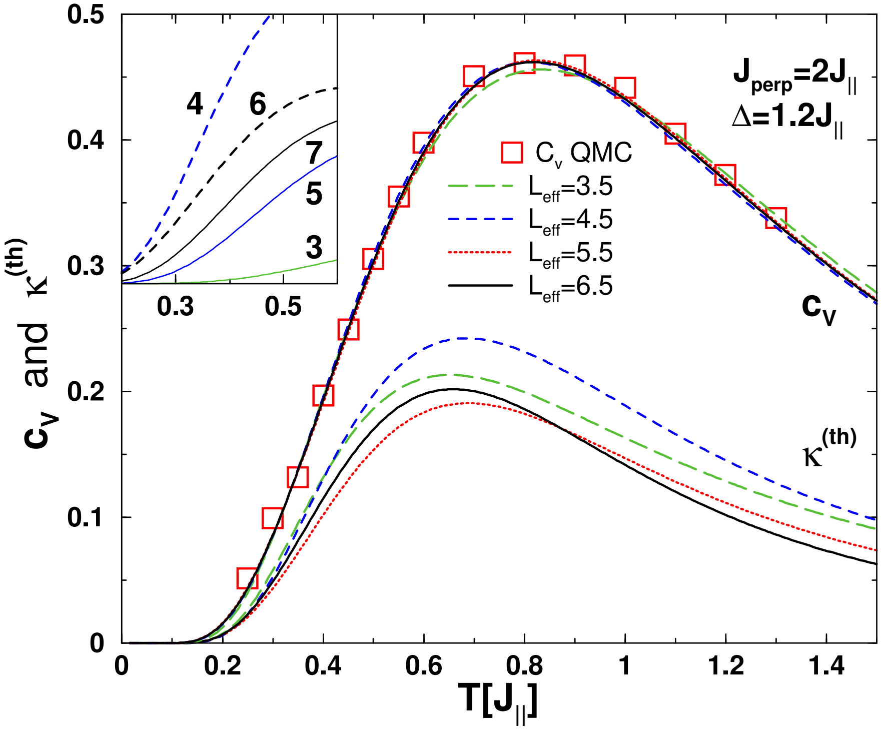
- specific heat c_V
- $\kappa \;=\; \pi \kappa^{(th)}\, \delta(\omega)$

exact diagonalization

Heisenberg chain

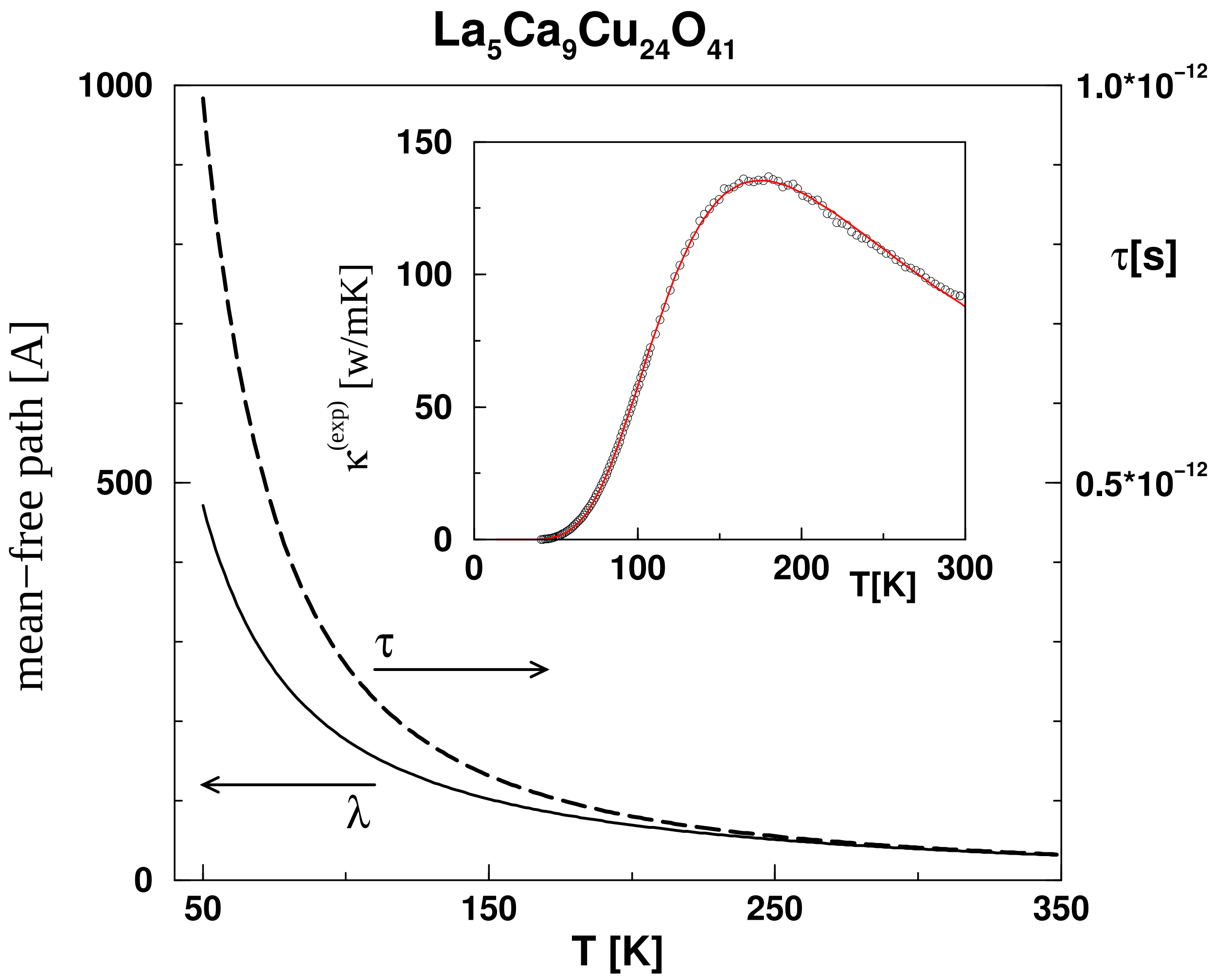


Heisenberg ladder



spin-ladder

[theory $\leftrightarrow$ experiment]



- old formula: $\kappa = c_V \, v_s \, \lambda$

  $\rightarrow \quad \lambda \approx 3000\mathring{A}$

- new: $\kappa = \kappa^{(th)} \, \lambda / v_s$

  $\rightarrow \quad \tau \approx$ pico-seconds

magnetothermal efects

- general response matrix

$$\begin{pmatrix} j_M \\ j_E \end{pmatrix} = \begin{pmatrix} \hat{L}_{MM} & \hat{L}_{ME} \\ \hat{L}_{EM} & \hat{L}_{EE} \end{pmatrix} \begin{pmatrix} \nabla B \\ (-\nabla T) \end{pmatrix}$$

- Onsager-relation $T\hat{L}_{ME} = \hat{L}_{EM}$
- ballistic transport for the Heisenberg chain:

$$\boxed{\hat{L}_{ij}(\omega) \equiv L_{ij}\pi\delta(\omega)}$$

$$\boxed{L_{EM} = \langle -T_{EM}\rangle \frac{c}{\hbar} + BL_{MM}}$$

- magnetothermal response $L_{EM} = 0$ if $B = 0$
  since $T_{EM} \sim \mathbf{S}_k\mathbf{S}_l\mathbf{S}_m$

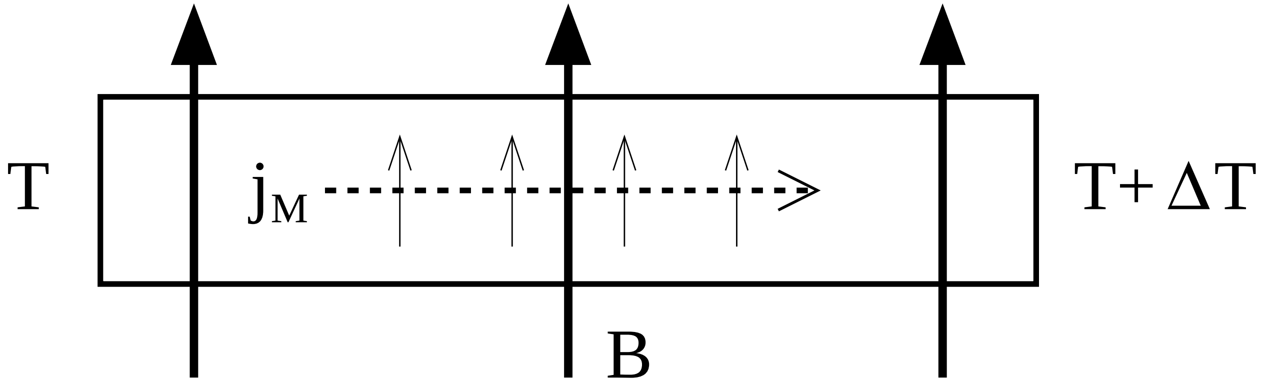
An external magnetic field B induces a magnetic current J_M proportional to the temperature-gradient ΔT

- small magnetic fields:

Louis & Gros '02

$$L_{EM} \;\approx\; B\frac{\partial}{\partial B}L_{EM}\Big|_{B=0} \;=\; B\Big[\langle -T_{EM}(-\beta M)\rangle\frac{c}{\hbar} + L_{MM}\Big]$$

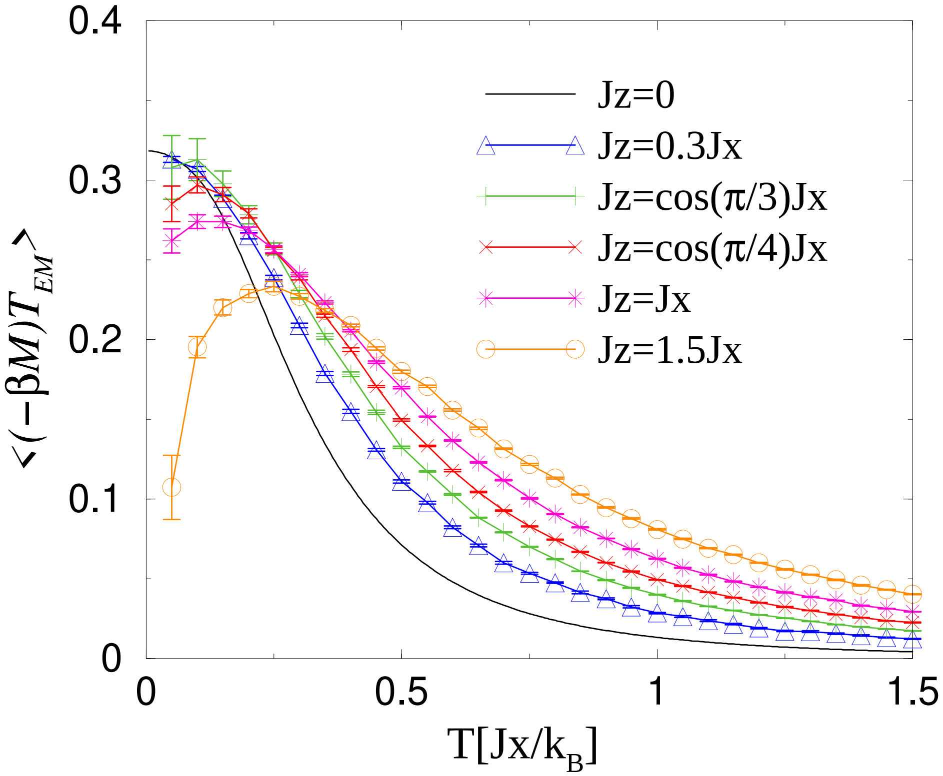
- $L_{MM} \equiv D:$ magnetic Drude weight



results

- explicit form, $\tilde{\mathbf{S}}_n = (J_x S_n^x, J_y S_n^y, J_z S_n^z)$:

$$T_{EM} = \frac{1}{\mathrm{Vol}} \sum_n \left\{ \tilde{\mathbf{S}}_{n+2} \times (\tilde{\mathbf{S}}_n \times \mathbf{S}_{n+1}) - \tilde{\mathbf{S}}_n \times (\mathbf{S}_{n+1} \times \tilde{\mathbf{S}}_{n+2}) \right\}_z$$



- XY-model: exact
- XXZ-model: QMC

order of magnitude

- 1D-Heisenberg compound: Sr_2CuO_3
  - ◇ $J_x \simeq 2200\,\mathrm{K}$
  - ◇ $\tau(200\mathrm{K}) \simeq 0.8 \cdot 10^{-13}\mathrm{s}$

[Sologubenko *et al.* '01]

- XY-model for L_{EM}
  - ◇ cross-section: $1\,\mathrm{mm}^2$

$$J_M \;=\; 1.6 \cdot 10^{15} \left[\frac{\text{magnetic moments}}{\text{seconds}}\right], \qquad \left(\begin{array}{rcl} B & = & 10\,\mathrm{T} \\ \Delta T & = & 10\,\mathrm{K} \end{array}\right)$$

- compare:

$$1\;\text{Ampére} \;\hat{=}\; 1.6 \cdot 10^{19} \left[\frac{\text{electrons}}{\text{seconds}}\right]$$

conclusions

- it is possible to study thermal conductivity with exact diagonalization
- difference between
  - old phenomenological formula $\kappa = c_V \, v_s \, \lambda$
  - new 'exact' formula $\kappa = \kappa^{(th)} \, \lambda / v_s$

  $\rightarrow$ maximum at lower temperature

  $\rightarrow$ realistic mean-free path $\lambda(T)$

- it is possible to study transport with QMC
- difference between
  - gappped system $D = 0$ $\sigma_0 = 0$
  - gapless, integrable $D > 0$ $\sigma_0 = \infty$
  - gapless, non-integrable $D = 0$ $0 < \sigma_0 < \infty$

- collaborators
  - Kim Louis
  - Vicente Alvarez