Transport properties of quantum chains at finite temperature: the elusive Drude weight

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Contents

- Heisenberg spin chain
- thermal and spin transport

  Drude weight at zero frequency in dynamical conductivity
- thermodynamics of Heisenberg spin chain: 3 different, but equivalent sets of NLIEs

  quantum chain $\leftrightarrow$ 2d vertex model

  Y-system ('magnons'), A-system ('spinons')
- finite temperature spin Drude weight, different works:

  numerical: Density matrix RG (DMRG), exact diagonalization

  rigorous: Mazur inequality, symmetries, matrix product operators

  analytical: Bethe ansatz, TBA, bosonization, conformal perturbation theory

collaborators: K. Sakai

Support by Volkswagen Foundation, DFG, JSPS

Heisenberg Chain

Spin-1/2 Hamiltonian

$$H = \sum_{k=1}^{L} \left(S_k^x S_{k+1}^x + S_k^y S_{k+1}^y + \Delta S_k^z S_{k+1}^z \right)$$

$-1 < \Delta < 1$	critical phase (parameterization $\Delta = \cos\gamma$)
$\Delta < -1$	gapped ferromagnetic phase
$1 < \Delta$	gapped antiferromagnetic phase

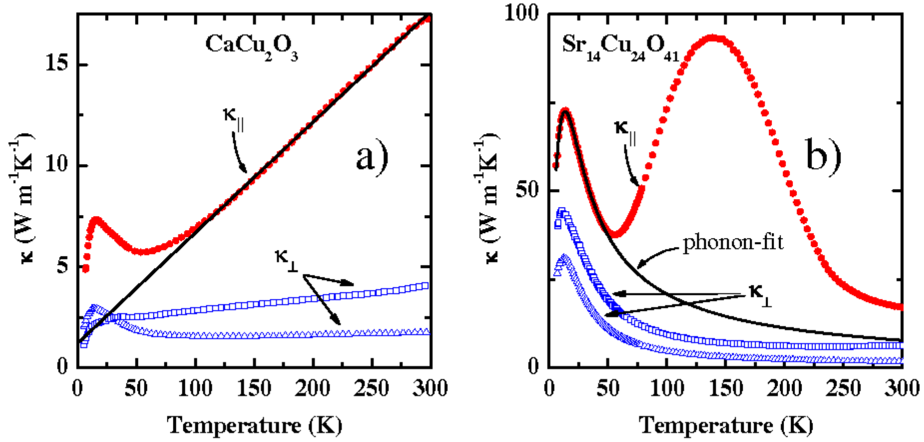
Formulation as lattice gas of spinless fermions

$$H = \sum_{k=1}^{L} \left(c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k \right) + 2\Delta \sum_{k=1}^{L} n_k n_{k+1}$$

Heisenberg Chain: Thermal Conductivities I

Thermal conductivity κ relates thermal current $\mathcal{J}_{\mathrm{E}}$ to gradient ∇T: $\quad \mathcal{J}_{\mathrm{E}} = \kappa \nabla T$

Chain and ladder compounds



Kubo Theory Calculation from 2-pt-fcts $\kappa(\omega) = \frac{\beta}{L}\int_0^{\infty} dt\, e^{-i\omega t}\int_0^{\beta} d\tau \langle \mathcal{J}_{\mathrm{E}}(-t - i\tau)\mathcal{J}_{\mathrm{E}}\rangle$

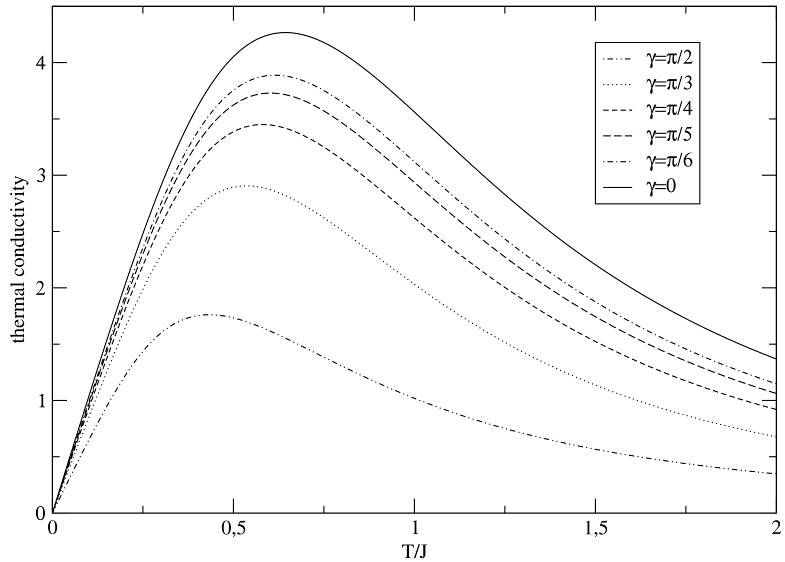
Simplification for Heisenberg chain: current is conserved $[H, \mathcal{J}_{\mathrm{E}}] = 0$:

$$\kappa(\omega) = \frac{1}{i(\omega - i\varepsilon)}\frac{\beta^2}{L}\langle \mathcal{J}_{\mathrm{E}}^2\rangle, \quad (\varepsilon \to 0+) \qquad \Rightarrow \mathrm{Re}\,\kappa(\omega) = \pi D_{\mathrm{th}}\delta(\omega) \qquad D_{\mathrm{th}} = \frac{\beta^2}{L}\langle \mathcal{J}_{\mathrm{E}}^2\rangle$$

Thermal conductivity of XXZ chain at zero frequency is infinite!

Heisenberg Chain: Thermal Conductivities II

Thermal Drude weight D_{th} (in units of J^2)



(critical) $\Delta = \cos\gamma = 0,\ 0.5,\ 0.707,\ 0.809,\ 0.866,\ 1$ (AK, K. Sakai 2002)

Wiedemann-Franz law $D_{\text{th}}/D_{\text{s}} \simeq \frac{2}{3}\pi(\pi-\gamma)T$

Thermal/energy current

defining expression for j^{E} from continuity equation $\frac{\partial}{\partial t} h = -\mathrm{div}\, j^{\mathrm{E}}$

on lattice: $$\frac{\partial}{\partial t} h_{k,k+1} = -\left(j^{\mathrm{E}}_{k+1} - j^{\mathrm{E}}_{k}\right)$$

difference equation for spin-1/2 Heisenberg is satisfied by

$$j^{\mathrm{E}}_{k} = \mathrm{i}[h_{k-1k}, h_{kk+1}]$$

Lüscher 76, Tsvelik 90, Frahm 92, Grabowski et al. 94/95, Zotos et al. 97, Rácz 00

Heisenberg chain: total energy current $\mathcal{J}_{\mathrm{E}} = \sum_k j^{\mathrm{E}}_{k}$ conserved ($[\mathcal{J}_{\mathrm{E}}, H] = 0$)

Proof:

– direct, or

– $\mathcal{J}_{\mathrm{E}}$ equals 2nd logarithmic derivative of transfer matrix of six-vertex model.

Thermodynamics I: TBA *or* Y-system ('magnons')

Thermodynamical Bethe Ansatz (Yang+Yang 69, Gaudin 71, Takahashi 71):

combinatorial, free energy functional, ∞-many auxiliary functions $Y_j,\ j=1,2,3\ldots$

$$\begin{aligned}
\ln Y_1(v) &= -\beta \frac{\frac{\pi}{2}}{\cosh \frac{\pi}{2} v} + \mathbf{s} * \ln(1+Y_2) \\
\ln Y_j(v) &= \mathbf{s} * [\ln(1+Y_{j-1}) + \ln(1+Y_{j+1})], \quad j \geq 2
\end{aligned}$$

where $*$ denotes convolutions and **s** is the function

$$\mathbf{s}(v) := \frac{1}{4\cosh \pi v/2}.$$

asymptotical behaviour $\lim_{j\to\infty} \ln Y_j(v)/j = \beta h$ free energy per lattice site

$$\beta f = \beta e - \int_{-\infty}^{\infty} \mathbf{s}(v) \ln(1+Y_1(v)) dv.$$

From TBA to Y-system: Zamolodchikov 90

from T-system to Y-system and TBA: AK, Pearce 92 two auxiliary functions $\mathfrak{a}$, $\overline{\mathfrak{a}}$

$$\begin{aligned}
\log \mathfrak{a}(v) &= +\frac{\beta h}{2} - \beta e(v+\mathrm{i}) + \kappa * [\log(1+\mathfrak{a}) - \log(1+\overline{\mathfrak{a}})], \\
\log \overline{\mathfrak{a}}(v) &= -\frac{\beta h}{2} - \beta e(v-\mathrm{i}) + \kappa * [\log(1+\overline{\mathfrak{a}}) - \log(1+\mathfrak{a})].
\end{aligned}$$

where $e(v)$ and the kernel $\kappa(v)$ take the form

$$e(v) := \frac{\frac{\pi}{2}}{\cosh \frac{\pi}{2} v}, \qquad \kappa(v) := \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{e}^{-|k|}}{\mathrm{e}^{k} + \mathrm{e}^{-k}} \mathrm{e}^{\mathrm{i}kv} dk$$

free energy $$\beta f = \beta e_0 - \frac{1}{2\pi} \int_{-\infty}^{\infty} e(v) \log[(1+\mathfrak{a}(v-\mathrm{i}))(1+\overline{\mathfrak{a}}(v+\mathrm{i}))] dv,$$

AK, Batchelor 90; AK, Batchelor, Pearce 91; AK 92,93; Destri, de Vega 92,95; J. Suzuki 98, Hegedűs 05

general $sl(N)$ etc./Bäcklund transformations: ...; Zabrodin 07; Arutyunov, Frolov 09; Tsuboi 11; Kazakov, Leurent, Tsuboi 12; Balog, Hegedűs 12

Spin current

The spin current density

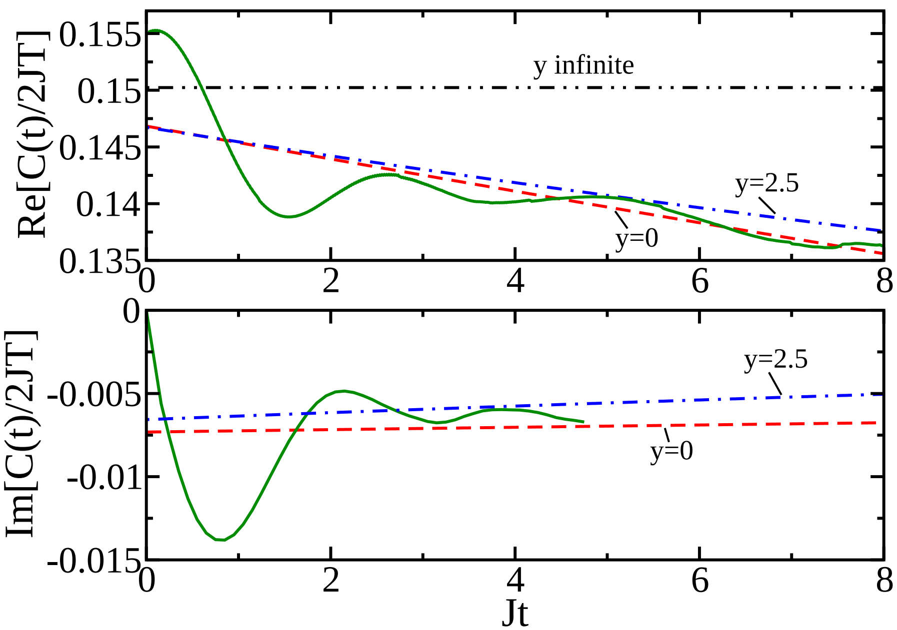
$$j_k = \mathrm{i}\left(S_k^+ S_{k+1}^- - S_k^- S_{k+1}^+\right)$$

and its continuity equation

$$\frac{\partial}{\partial t} S_k^z = -\left(j_k - j_{k-1}\right)$$

Total spin current $\mathcal{J} = \sum_k j_k$ is not conserved (except for $\Delta = 0$, free fermions)

$$[H, \mathcal{J}] \neq 0, \qquad D(T) \neq \beta \langle \mathcal{J}^2 \rangle.$$



$$C(t) := \frac{1}{L} \langle \mathcal{J}(t) \mathcal{J} \rangle$$

$$\Delta = 0.6, T/J = 0.2$$

Sirker, Pereira, Affleck PRL09, PRB11

bosonization + memory matrix ($\rightarrow y$)

(keeping umklapp + band curvature)

TMRG (DMRG for transfer matrix)

Spin current (rigorous results)

1) Mazur inequality for general current $\mathcal{J}$ and conserved Q $\quad([Q,H]=0)$

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\langle\mathcal{J}(t)\mathcal{J}\rangle \geq \frac{\langle\mathcal{J}Q\rangle^2}{\langle Q^2\rangle}$$

If current $\mathcal{J}$ is not conserved, but conserved Q exists with nonvanishing overlap

$\langle\mathcal{J}Q\rangle \neq 0 \longrightarrow$ finite Drude weight

For Heisenberg chain at zero field: all known conserved currents Q are spin-reversal symmetric, hence: $\langle\mathcal{J}Q\rangle = \langle R\mathcal{J}R^{-1}RQR^{-1}\rangle = -\langle\mathcal{J}Q\rangle = 0$.

2) However: Drude weight is related to energy level curvature with respect to twist

$$D = \frac{1}{2L}\sum_n p_n \frac{\partial^2\varepsilon_n[\Phi]}{\partial\Phi^2}\Big|_{\Phi=0} \qquad \text{Kohn 1964,...}$$

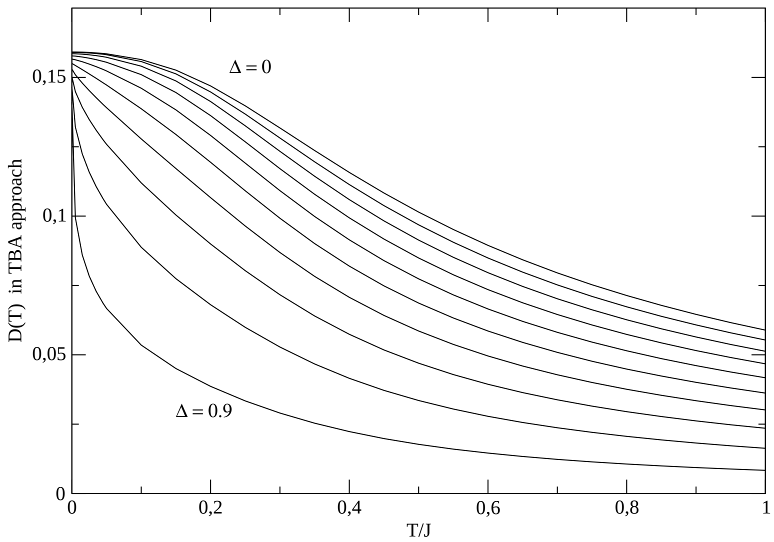
$T=0$: The groundstate value is analytically known (Shastry, Sutherland 90)

$$D_s(T=0) = \frac{v}{2(\pi-\gamma)} \qquad \text{where} \qquad \Delta = \cos\gamma.$$

$T>0$: TBA-like scheme by Fujimoto, Kawakami 98; application to XXZ: Zotos 98

Extended Thermodynamical Bethe ansatz

Thermodynamical Bethe ansatz applied to magnons and their bound states (Zotos 98)



Thermodynamical Bethe ansatz based on:

– magnons and their bound states

– scattering of these ’particles’, construction of scattering states

– minimization of free energy functional

Problems for calculating energy curvatures for large but finite chain length:

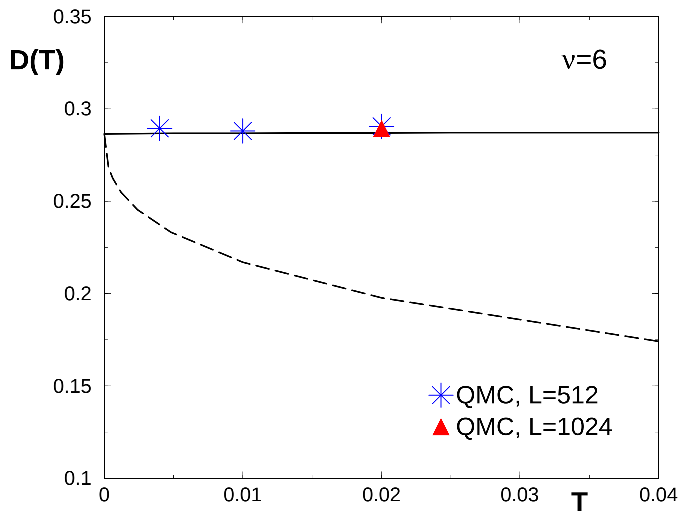
– composition of bound magnon states (assumption in TBA: ’ideal strings’)

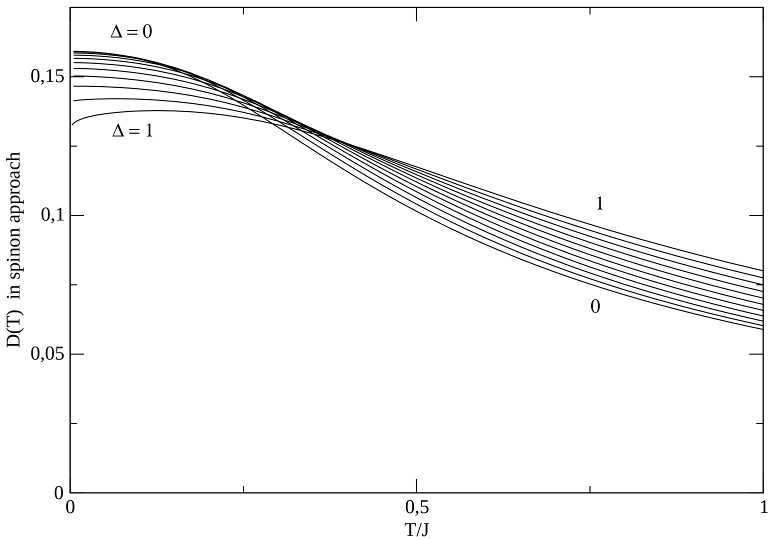
– density distribution not continuous (but assumed in TBA)

QMC and TBA-like approach

Quantum Monte Carlo

TBA on spinon basis





Alvarez, Gros 02

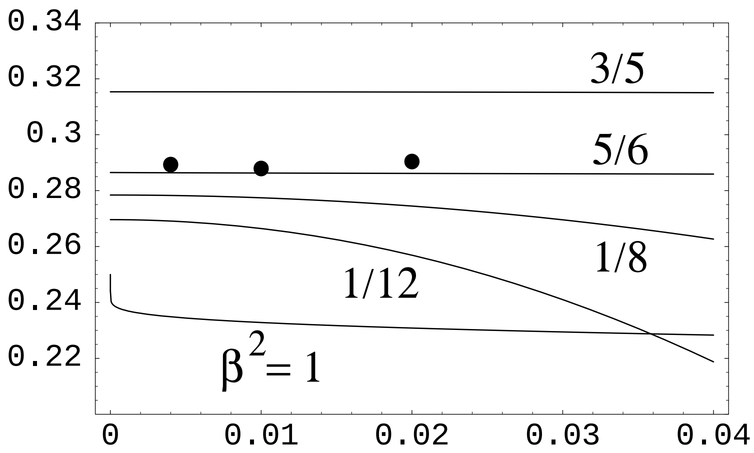
Benz, Fukui, AK, Scheeren (01, 05)

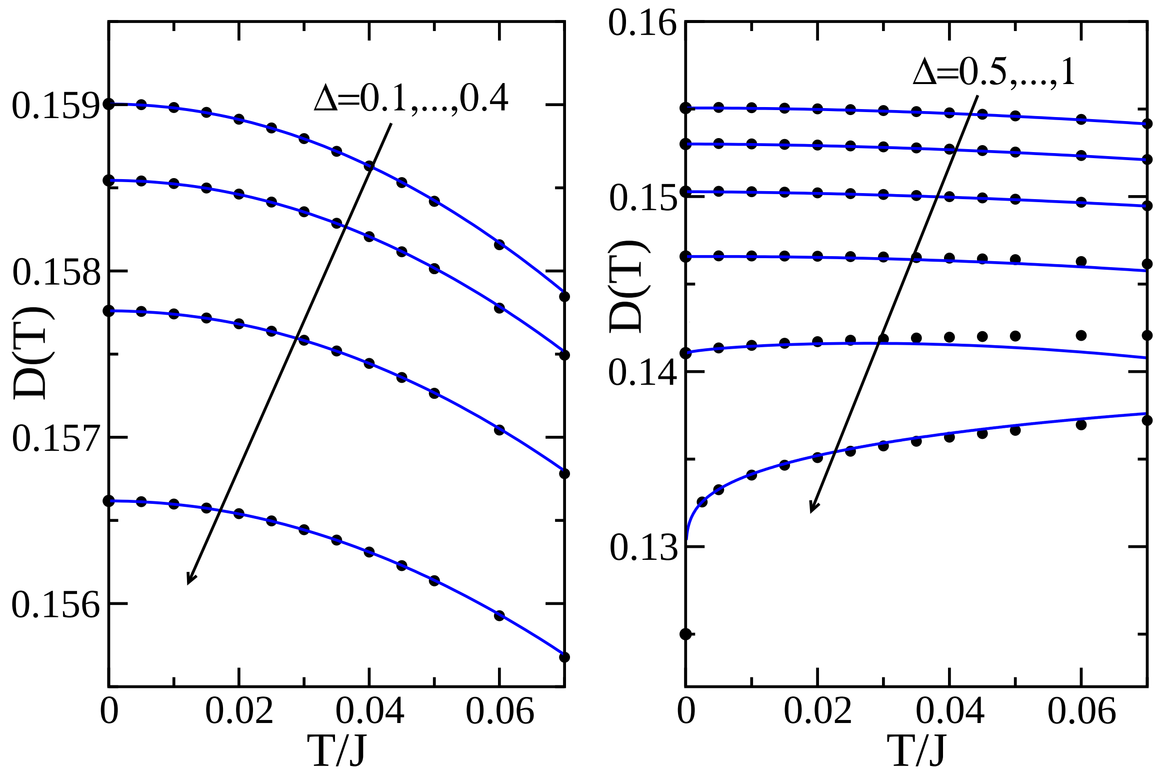
finite chains: Heidrich-Meisner et al. 03; improved QMC Brenig, Grossjohann 10

Extended thermodynamical Bethe ansatz (non-linear integral equation for a and $\overline{a}$):

$$D = \frac{T}{4\pi}\int_{-\infty}^{\infty} dx \frac{\left(\frac{\partial a}{\partial h}\cdot\frac{\partial a}{\partial x}\right)^2}{a^2(1+a)^2\frac{\partial a}{\partial T}} + (a \leftrightarrow \overline{a}), \quad \log a = +\frac{\beta h}{2} - \beta e + \kappa * [\log(1+a) - \log(1+\overline{a})]$$

Conformal perturbation theory





Fujimoto, Kawakami 03

sign change 05

Comparison of spinon-TBA results to CFT
(+band curvature, umklapp) by Sirker (05,09)

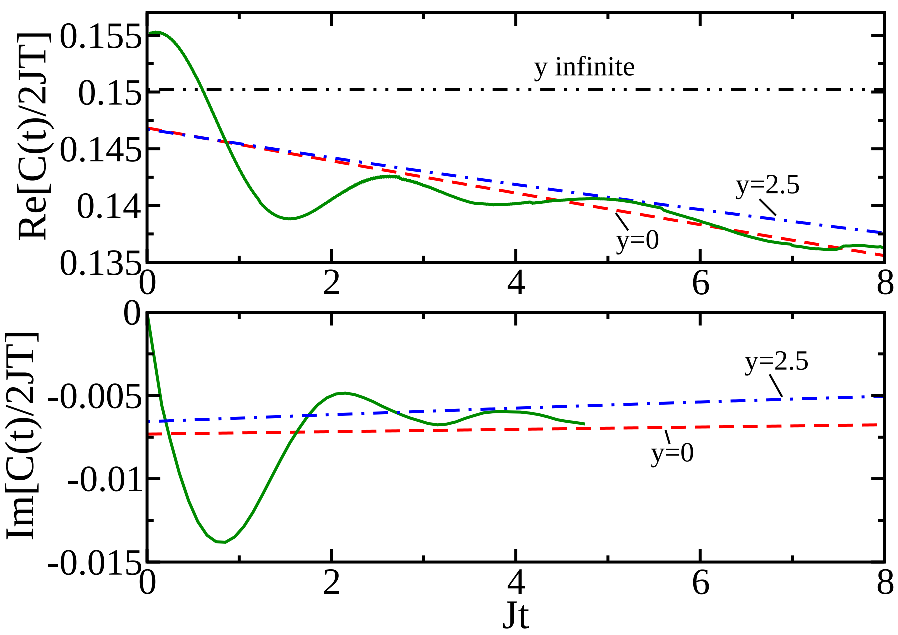
However, real time dynamics by TMRG etc. suggest $D(T) = 0$ or small, for XXZ chain with $h = 0$ (Sirker et al. 09, 11); coexistence of diffusive and ballistic channels

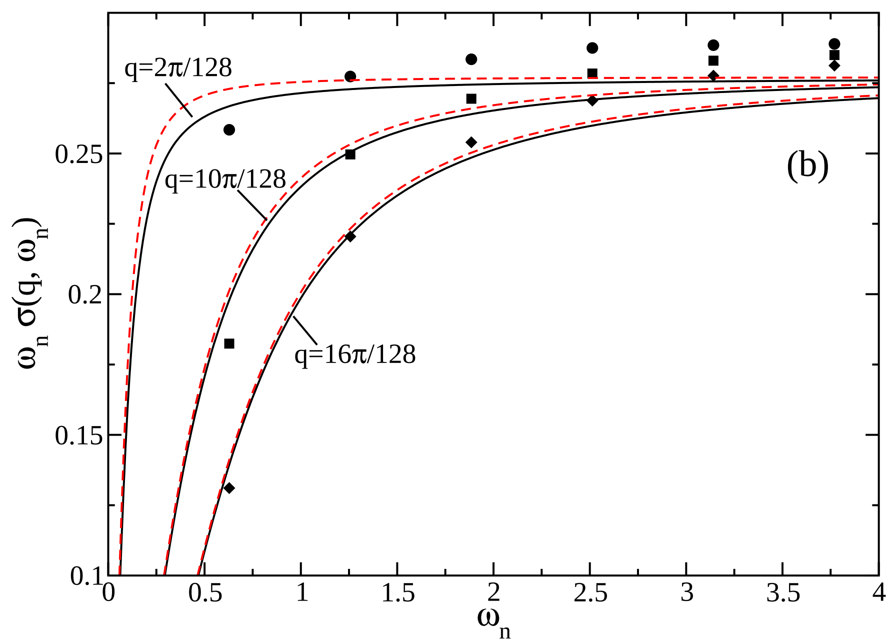
Field theory and TMRG

free boson Hamiltonian+umklapp+band curvature (Sirker, Pereira, Affleck 09, 11)

– correlations generically decay to zero, “protection” built in by hand (memory matrix)

TMRG (transfer matrix/temperature DMRG)





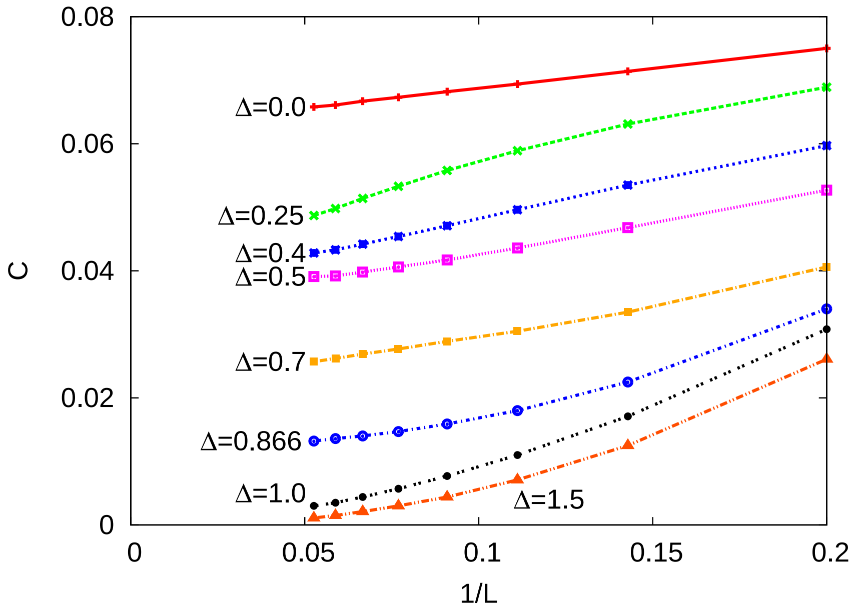
optical sum rule imposes constraint on weight in ballistic and diffusive channels

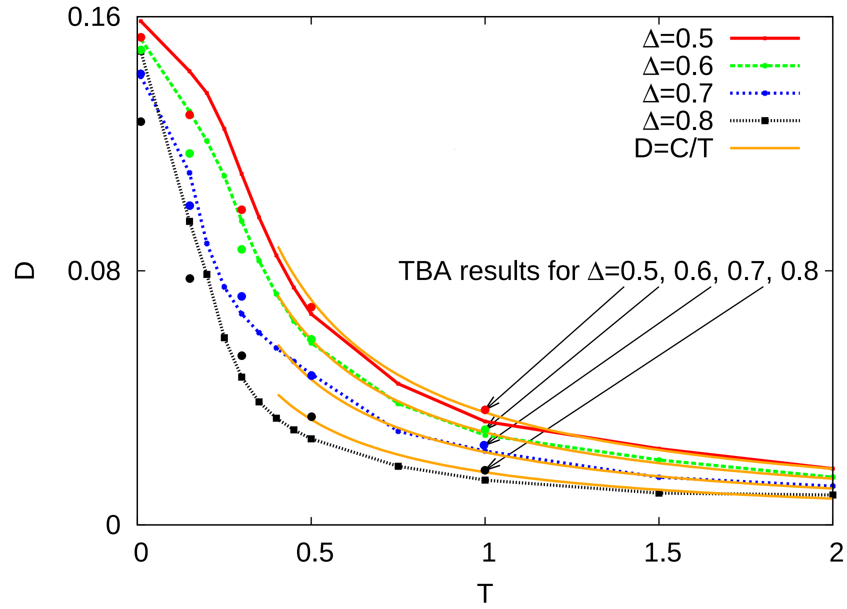
QMC results by Alvarez + Gros consistent with zero/small Drude weight... if singular scaling at small frequencies is allowed... as suggested by field theoretical results

Exact diagonalization for finite chains

ED for odd chains $L = 5..19$, canonical ensemble (Herbrych, Prelovšek, Zotos PRB 11)

$\leftrightarrow$ (Karrasch, Hauschild, Langer, Heidrich-Meisner 13)





finite size scaling for high temperature

extrapolated results for arbitrary T

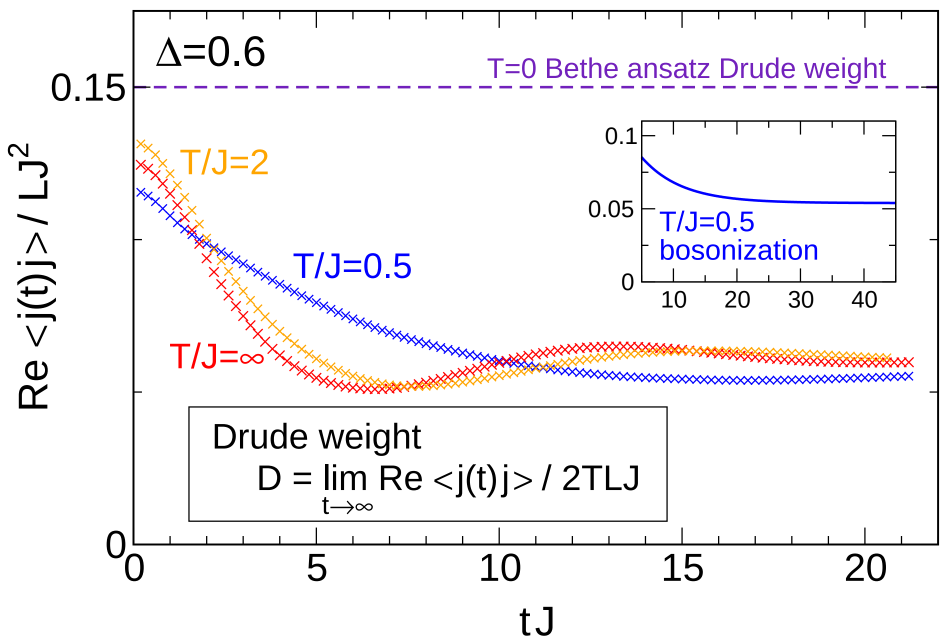
Results agree well with high-T asymptotics of TBA (Zotos 98, Benz et al. 05)

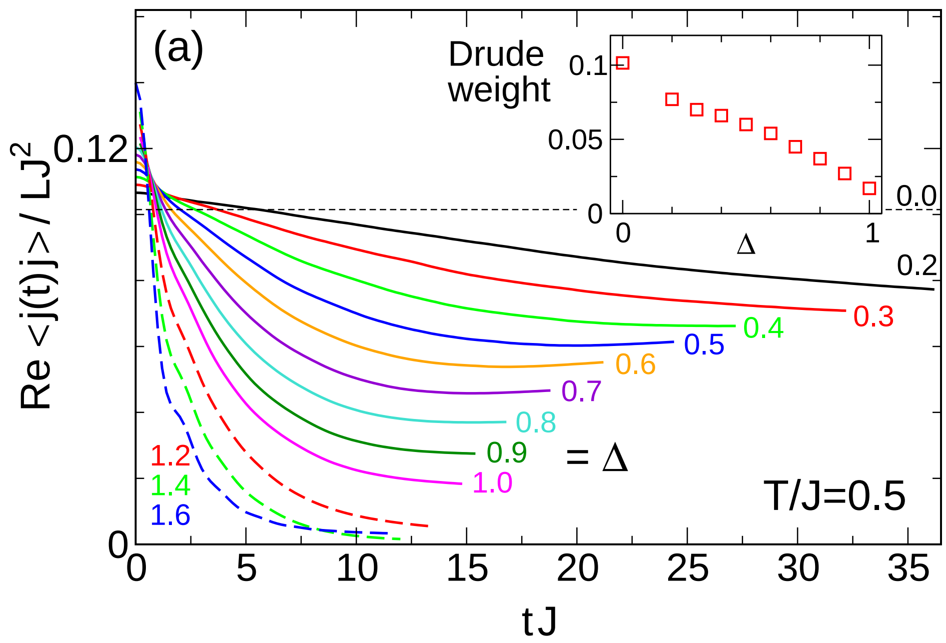
$$D \simeq \frac{D_\infty}{T}, \qquad D_\infty(\Delta) = \frac{\gamma - \frac{1}{2}\sin 2\gamma}{16\gamma}, \quad \Delta = \cos\gamma,$$

Note: Problem with symmetry $D_\infty(\Delta) = D_\infty(-\Delta)$

DMRG for finite temperature

$T > 0$ by purification of thermal ensemble ($\sim$ sum over excited states by doubling the system and use of “open” boundary conditions)





symmetric treatment, larger available times

Karrasch, Bardarson, Moore PRL 12

Non-zero Drude weight for $\Delta = 1$ and $T > 0$!

Application of Mazur's inequality

Goal: Construction of conserved current with non-vanishing overlap with spin current

Problem: the known conserved currents have vanishing overlap with physical current

Idea: (i) Fishing in pool of operators odd w.r.t. spin reversal symmetry

(ii) Start with the physical current operator for $\Delta = 0$ and turn Δ on

Perturbative construction of conserved Q: (AK, Sakai 08, unpublished)

$$
\begin{aligned}
H &= \sum_{k=1}^{L}\left(c_k^\dagger c_{k+1} + c_{k+1}^\dagger c_k\right) + 2\Delta \sum_{k=1}^{L} n_k n_{k+1}, \\
Q &= \mathrm{i}\sum_{k=1}^{L}\left(c_k^\dagger c_{k+1} - c_{k+1}^\dagger c_k\right) + 2\mathrm{i}\Delta \sum_{k=1}^{L}\sum_{l=1}^{L-1} (-1)^l c_k^\dagger c_{k-l} c_{k+1}^\dagger c_{k+1-l}, \\
[H,Q] &= O(\Delta^2) \quad \text{instead of} \quad O(\Delta^1)
\end{aligned}
$$

Mazur inequality applied to Drude weight: $$D \geq \frac{1}{2LT}\frac{\langle \mathcal{J} Q\rangle^2}{\langle Q^2\rangle}.$$

But $\langle Q^2\rangle$ scales like L^2 instead of L, Q is non-local. And $\langle \mathcal{J} Q\rangle$ scales like L.

Mazur inequality and Matrix Product Operators

Construction of conserved currents by "matrix product operators" (Prosen PRL 11): matrices with spin operators as entries

$$\mathbf{A}_j = \mathbf{A}^z \sigma_j^z + \mathbf{A}^+ \sigma_j^+ + \mathbf{A}^- \sigma_j^-$$

and number matrices $\mathbf{A}^z, \mathbf{A}^+, \mathbf{A}^-$ of square shape (finite or infinite).

Let $\mathcal{L}$ and $\mathcal{R}$ be some row and column number vectors of suitable dimension, then $\mathcal{Z} := \mathcal{L} \cdot \mathbf{A}_1 \cdot \mathbf{A}_2 ... \mathbf{A}_L \cdot \mathcal{R}$ is an operator acting on the Heisenberg chain.

If $\mathbf{A}^z, \mathbf{A}^+, \mathbf{A}^-, \mathcal{L}, \mathcal{R}$ satisfy algebra of quadratic and trilinear relations, then

$$[H, \mathcal{Z}] = -\sigma_1^z + \sigma_L^z, \qquad \mathcal{Z} \text{ is "almost conserved"}$$

Take $Q := i(\mathcal{Z} - \mathcal{Z}^+)$ and show $\langle \mathcal{J} Q \rangle_{T=\infty} = (L-1)/2$.

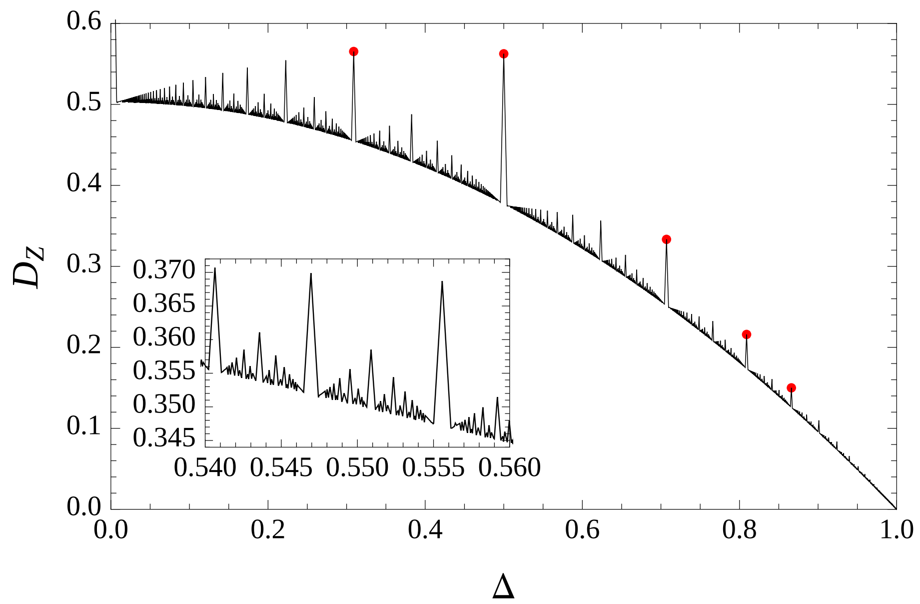
Crucial: keeping $\langle Q^2 \rangle$ "small"

For $\Delta = \cos\gamma$, $\gamma = \pi\frac{l}{m}$ finite representations of matrix algebra $\mathbf{A}^z, \mathbf{A}^+, \mathbf{A}^-$ exist, such that $\langle Q^2 \rangle$ is order L.

quadratic algebra: Karevski, Popkov, Schütz 2013; continuous spin: Prosen et al. 2013

Mazur inequality and Matrix Product Operators

Result: Lower bound for high temperature asymptotics $D \simeq \frac{D_\infty}{T}, \quad D_\infty \geq D_z/4$



T. Prosen 2011

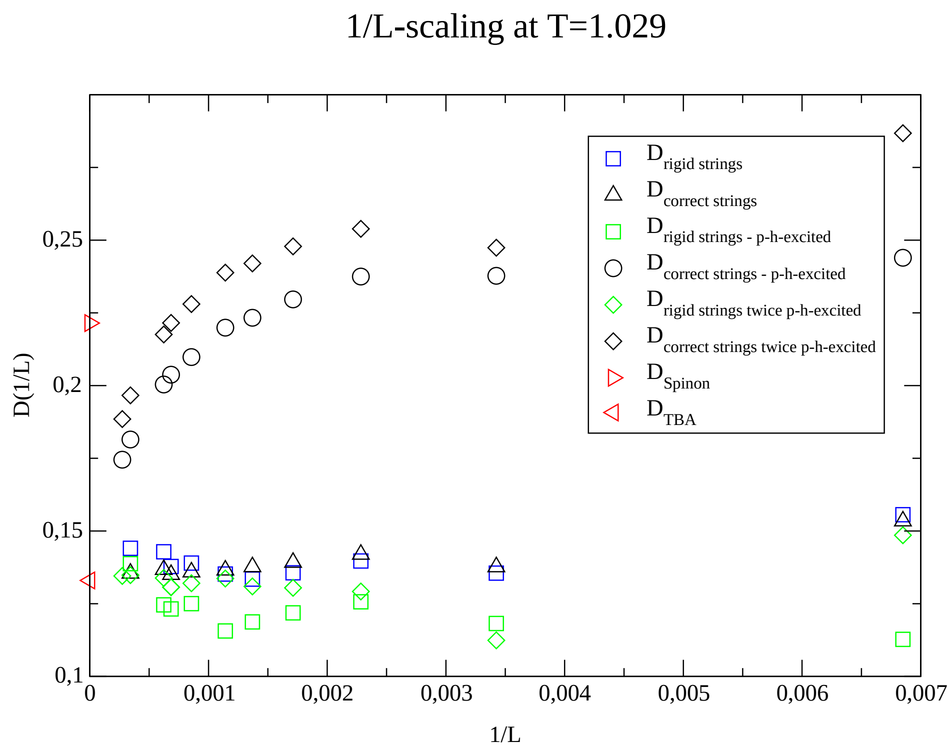
Note:

– high-T asymptotics D_∞ by TBA (Zotos 98, Benz et al. 05) larger than $\Delta_z/4$, but... P13

– lower bound satisfies $D_z(\Delta) = D_z(-\Delta)$

– lower bound fractal ($\longrightarrow$ no perturbative construction of Q, physics fractal?)

Curvatures of energy levels: universal scaling? ($\Delta = 1/2$)



Glocke, AK 02 unpublished

curvature depends on state! just in (wrong) rigid-string picture: all curvatures same

• summation over all states necessary! • case $T > 0$ qualitatively different from $T = 0$!

All microstates for $T = 0$ (low-lying excitations):

$$E_x(\varphi) - E_{g.s.}(0) = \frac{2\pi}{L} v x(\varphi) + o\left(1/L\right), \qquad x(\varphi) = \frac{1-\gamma/\pi}{2} S^2 + \frac{1}{2(1-\gamma/\pi)} \left(m - \frac{\varphi}{\pi}\right)^2$$

Proper calculation of curvatures by use of integrability

Problem of calculation by use of Bethe ansatz equations

–bound states: single magnon rapidities close to poles of scattering phases (singular)

–continuous density distributions not sufficient

Alternative approach to Bethe ansatz: 'fusion algebra' (finite for $\Delta = \cos\frac{\pi}{\nu}$)

$$\log Y_1(v) = L\log\mathrm{th}\tfrac{\pi}{4}v + \sum_{\zeta_2}\log\mathrm{th}\frac{\pi}{4}(v-\zeta_2) + s*\log(1+Y_2)$$

$$\log Y_j(v) = + \sum_{\zeta_{j-1}}\log\mathrm{th}\frac{\pi}{4}(v-\zeta_{j-1}) + \sum_{\zeta_{j+1}}\log\mathrm{th}\frac{\pi}{4}(v-\zeta_{j+1}) + s*\log[(1+Y_{j-1})(1+Y_{j+1})]$$

$$\log Y_{\nu-2}(v) = + \sum_{\zeta_{\nu-3}}\log\mathrm{th}\frac{\pi}{4}(v-\zeta_{\nu-3}) + \sum_{\zeta_\pm}\log\mathrm{th}\frac{\pi}{4}(v-\zeta_\pm) + s*\log[(1+Y_{\nu-3})(1+Y_+)(1+Y_-)]$$

$$\log Y_\pm(v) = \pm i\phi + \sum_{\zeta_{\nu-2}}\log\mathrm{th}\frac{\pi}{4}(v-\zeta_{\nu-2}) + s*\log(1+Y_{\nu-2})$$

(A. Kuniba, K. Sakai, J. Suzuki 98)

convolutions with $\mathbf{s}(v) := \frac{1}{4\cosh\pi v/2}$, energy $E = \sum_{\zeta_1}\frac{\pi/2}{\cosh\pi\zeta_1/2} + \int_{-\infty}^{\infty}\frac{\log(1+Y_1)(x)}{\sinh\pi x/2}dx$

dropping of all integrals $\rightarrow$ Bethe ansatz equations for holes in bound magnon states

$$\frac{D}{d} = L^2 \int \frac{\rho^h_\pm(v)}{\partial_v \log Y_\pm(v+i)} \partial_v \left[\frac{\partial_\psi \log Y_\pm(v+i)}{\partial_v \log Y_\pm(v+i)} \right] dv + \frac{L}{2\pi i} \int \frac{Y_\pm(v)}{(1+Y_\pm(v))^2} \partial_\psi \log Y_\pm(v) dv$$

where d is some constant and

$$\begin{aligned}
\log Y_j(v) &= L p(v) \cdot \delta_{j,1} + \sum_l A_{jl}\, p * L\rho^h_l(v) + \sum_l K_{jl} * \log(1+Y_l)(v) \\
\partial_v \log Y_j(v) &= L\, 2\pi \mathrm{i}\, s(v+\mathrm{i}) \cdot \delta_{j,1} + 2\pi\mathrm{i} \sum_l K_{jl} * L\rho^h_l + \sum_l K_{jl} * \frac{Y_l}{1+Y_l} \partial_v \log Y_l \\
\partial_\psi \log Y_j(v) &= -s'(v+\mathrm{i}) \cdot \delta_{j,1} + 2\pi\mathrm{i} \sum_l K_{jl} * L\rho^h_l \frac{\partial_\psi \log Y_l}{\partial_v \log Y_l} + \sum_l K_{jl} * \frac{Y_l}{1+Y_l} \partial_\psi \log Y_l
\end{aligned}$$

where ρ^h_l are the density functions of the hole distribution of the state and

$$p(v) = \log \mathrm{th} \frac{\pi}{4} v, \qquad s(v) = \frac{1}{4 \cosh \frac{\pi}{2} v}.$$

Integral equations: solution for $L \to \infty$

1st integral: integration by parts

$$\int \frac{\rho^h_\pm(v)}{\partial_v \log Y_\pm(v+i)} \partial_v \left[\frac{\partial_\psi \log Y_\pm(v+i)}{\partial_v \log Y_\pm(v+i)} \right] dv$$

$$= \left[\frac{\rho^h_\pm(v)}{\partial_v \log Y_\pm(v+i)} \frac{\partial_\psi \log Y_\pm(v+i)}{\partial_v \log Y_\pm(v+i)} \right] \Bigg|_{-\infty}^{\infty} - \int \partial_v \left[\frac{\rho^h_\pm(v)}{\partial_v \log Y_\pm(v+i)} \right] \frac{\partial_\psi \log Y_\pm(v+i)}{\partial_v \log Y_\pm(v+i)} dv$$

2nd integral: exact evaluation

$$\int \frac{Y_\pm(v)}{(1+Y_\pm(v))^2} \partial_\psi \log Y_\pm(v) dv = 2\int_0^\infty \frac{Y_\pm(v)}{(1+Y_\pm(v))^2} \partial_v \log Y_\pm(v) \underbrace{\frac{\partial_\psi \log Y_\pm(v)}{\partial_v \log Y_\pm(v)}}_{\to R} dv$$

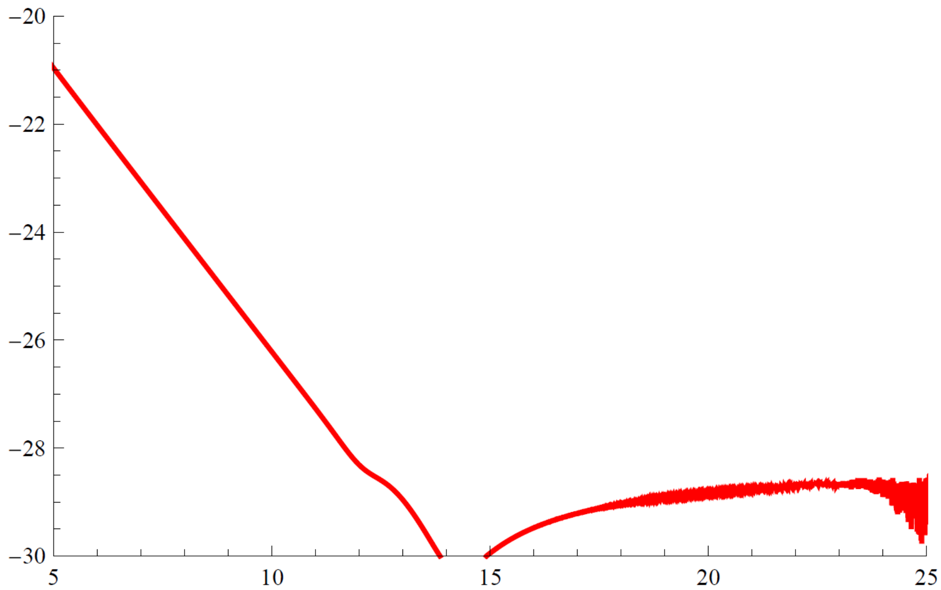
$$= 2R \cdot \int_{Y_\pm(0)}^{Y_\pm(\infty)} \frac{dY}{(1+Y)^2} = -2R \frac{1}{1+Y} \Bigg|_{Y_\pm(0)}^{Y_\pm(\infty)}$$

Surprise: surface term of 1st integral and 2nd integral cancel exactly, remaining term yields exactly Zotos' formula!

Asymptotics?

$$\log\left[\partial_v\left[\frac{\partial_\psi \log Y_\nu^{\rm th}(v+i/2)}{\partial_v \log Y_\nu^{\rm th}(v+i/2)}\right]\right]$$

Real Part



Summary

Spin-1/2 Heisenberg chain for $T > 0$ and arbitrary h

Exact results obtained for

- thermal conductivity ($h = 0$)

Open problems

- spin Drude weight