On the finite temperature Drude weight of the spin-1/2 XXZ Heisenberg chain

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Contents

- Heisenberg spin chain
- spin transport

  Drude weight at zero frequency in dynamical conductivity
- thermodynamics of Heisenberg spin chain (TBA, NLIE)
- 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
- coupled NLIE for finite T and L

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

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

Thermodynamics I: TBA ('bound magnons')

Thermodynamical Bethe Ansatz (Yang+Yang 69, Gaudin 71, Takahashi 71):
combinatorial, free energy functional, ∞-many auxiliary functions η_j, $j = 1, 2, 3\ldots$

$$\begin{aligned} \ln \eta_1(v) &= -\beta \frac{\frac{\pi}{2}}{\cosh \frac{\pi}{2} v} + \mathbf{s} * \ln(1+\eta_2) \qquad (XXX \text{ case}) \\ \ln \eta_j(v) &= \mathbf{s} * [\ln(1+\eta_{j-1}) + \ln(1+\eta_{j+1})], \quad j \geq 2 \end{aligned}$$

where $*$ denotes convolutions and $\mathbf{s}$ is the function

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

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

$$\beta f = \beta e - \int_{-\infty}^{\infty} \mathbf{s}(v) \ln(1+\eta_1(v)) dv.$$

From TBA to Y-system: Zamolodchikov 90

from T-system to Y-system and TBA: AK, Pearce 92

Spin current, rigorous results (I)

Dynamical spin conductivity

$$\sigma(\omega) = 2\pi D_s \delta(\omega) + \sigma_{reg}(\omega).$$

Drude weight of the zero frequency delta-function peak is related to energy level curvature with respect to twist (spin stiffness)

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

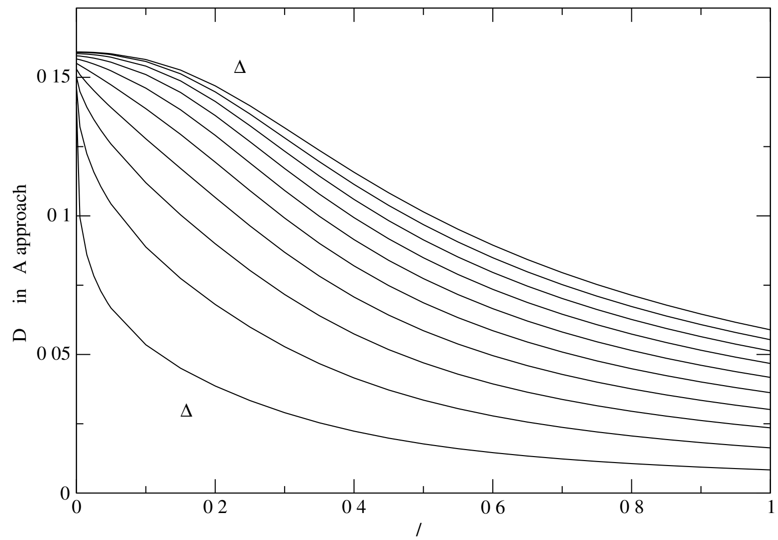
$T = 0$: The groundstate value is analytically known (Shastry, Sutherland 90)

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

$T > 0$: 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

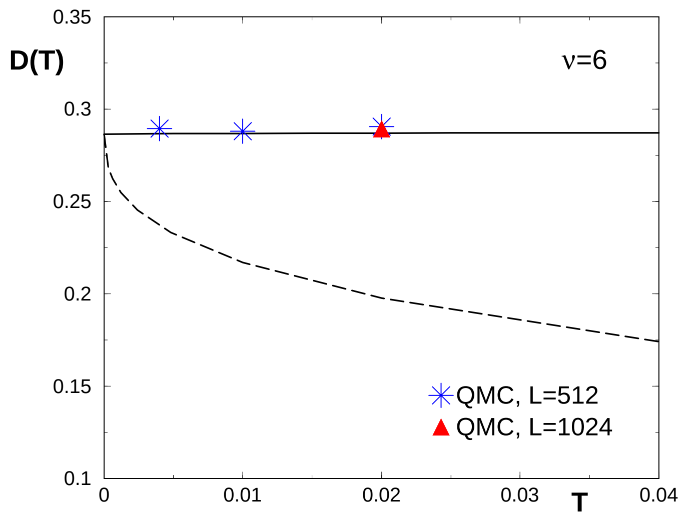
Problems for calculating energy curvatures for large but finite chain length:

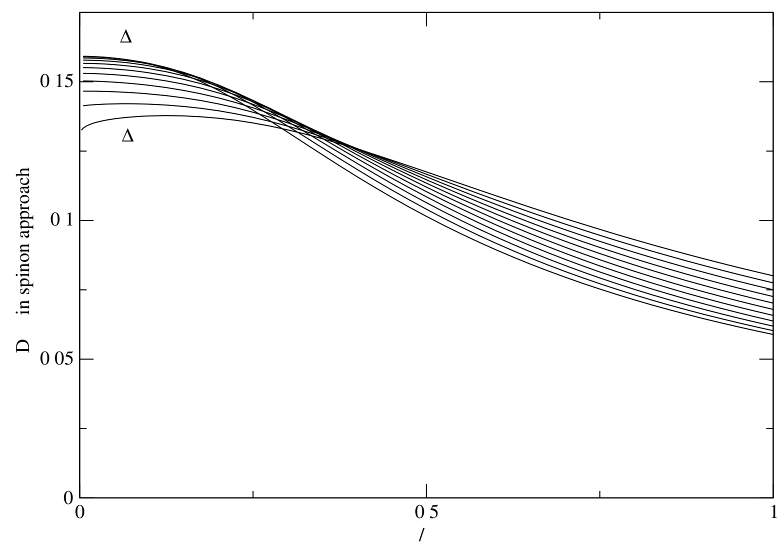
– composition of bound magnon states (assumption in TBA: ‘ideal strings’)

– density distribution not continuous (but assumed in TBA)

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 $\bar{a}$):

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

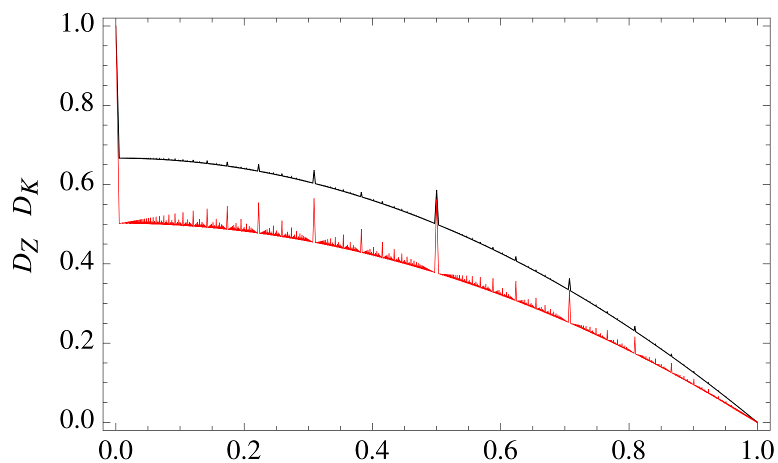
Spin current, rigorous results (II)

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

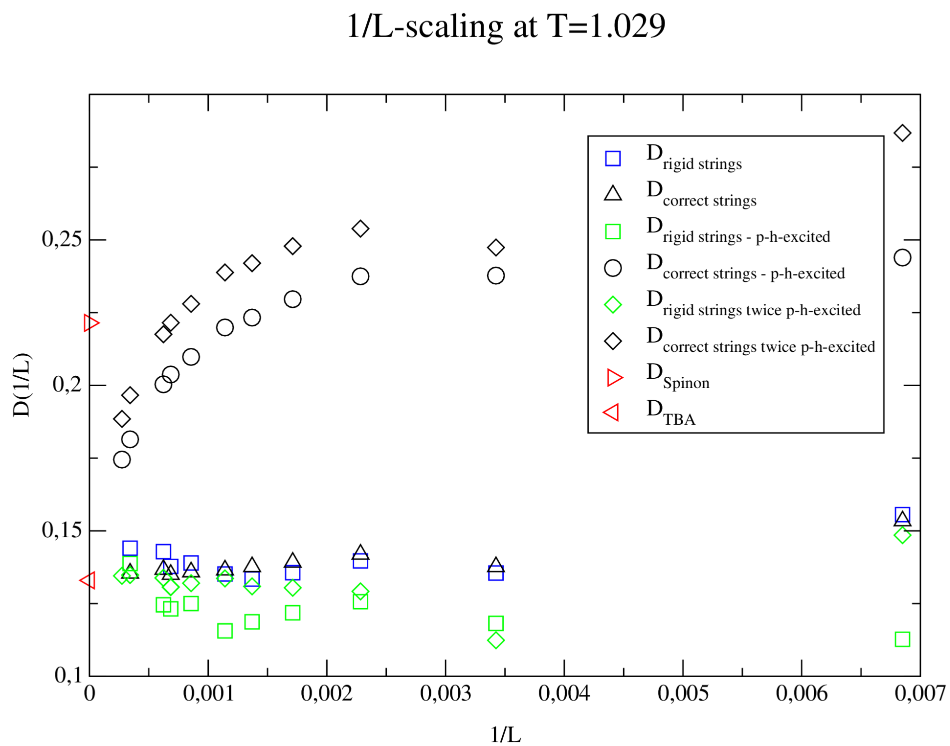
$$2LTD_s = \lim_{t_0\to\infty} \frac{1}{t_0}\int_0^{t_0} dt \langle \mathcal{J}(t)\mathcal{J}\rangle \geq \frac{\langle \mathcal{J}Q\rangle^2}{\langle Q^2\rangle}$$

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

New conserved charges from commuting transfer matrices $T(u,s)$ by first and arbitrary derivatives w.r.t. s and u (Prosen et al. 13, 14), evaluated in high T limit



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



Glocke, AK 02 unpublished

Curvature depends on state/size! Just in 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):

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

Proper calculation of curvatures by use of integrability

Problem in calculations 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 $\Delta = \cos\frac{\pi}{\nu}$)

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

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

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

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

(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 (ideal) string centers

The sums are over rapidities $\zeta_j \in M_j$ ($j = 1, \ldots, \nu$) with densities ρ_j^h given by TBA

Thermodynamic Bethe Ansatz for $\Delta = \cos(\pi/\nu)$

Bulk distribution functions from TBA equations

$$\log \eta_j(v) \quad = \quad -\beta A s(v) \cdot \delta_{j,1} + \sum_l K_{jl} * \log(1+\eta_l), \qquad A = 4\pi J \frac{\sin\gamma}{\gamma}$$

where

$$s(v) = \frac{1}{4\cosh\frac{\pi}{2}v}, \qquad K_{jl} \text{ kernel functions as on previous page}$$

The density functions ρ_j^h of the (hole) distribution given by

$$\rho_j^h(v) = -\frac{1}{A}\partial_\beta \log(1+\eta_j)$$

$$\frac{D}{D_0 L^2} = \sum_{j=\pm} \left(\int \frac{\rho_j^h(v)}{\partial_v \log Y_j(v+\mathrm{i})} \partial_v \frac{\partial_\psi \log Y_j(v+\mathrm{i})}{\partial_v \log Y_j(v+\mathrm{i})} dv + \frac{1}{2\pi \mathrm{i} L} \int \frac{Y_j(v)}{(1+Y_j(v))^2} \partial_\psi \log Y_j(v) dv \right)$$

where $D_0 = A\nu^2/4$, $j = +/- \equiv \nu - 1/\nu$ and

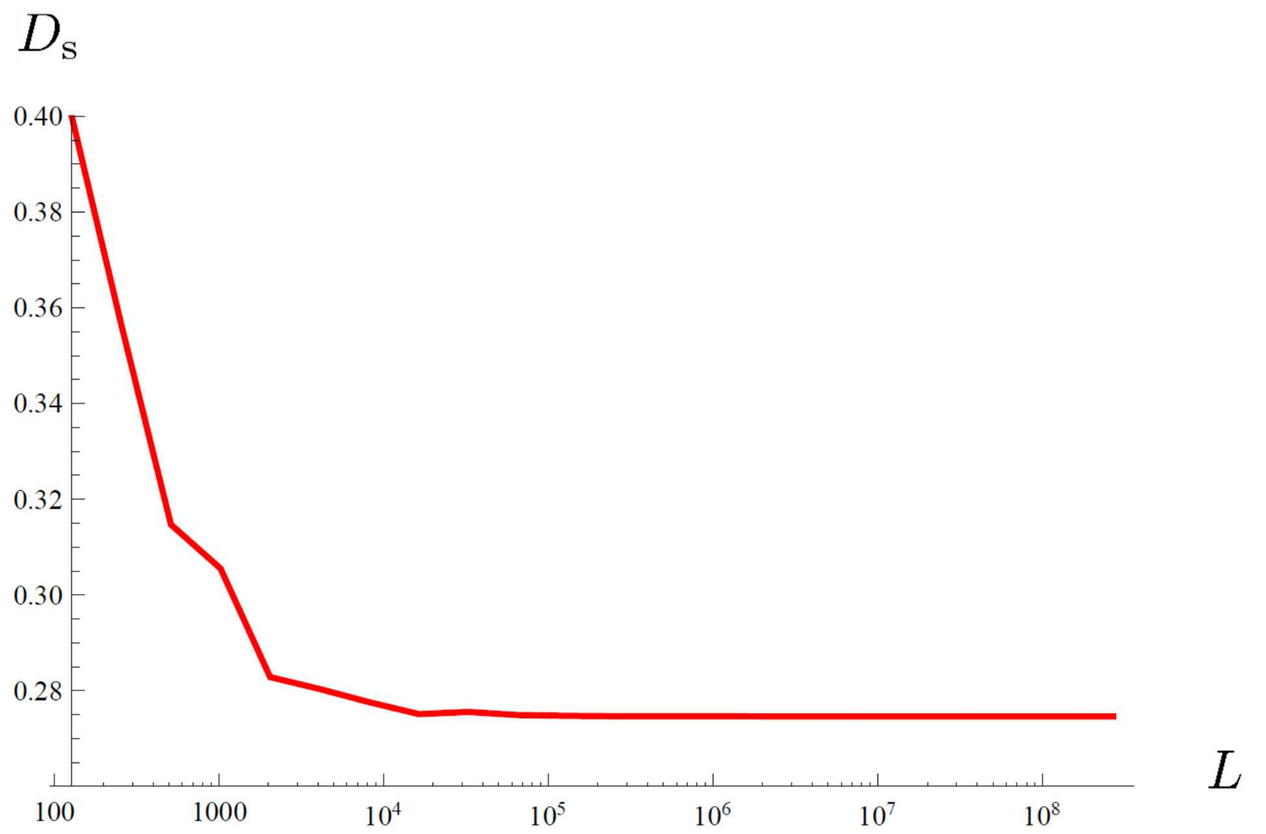
$$\begin{aligned}
\log Y_j(v) &= Lp(v) \cdot \delta_{j,1} + \sum_l A_{jl}\, p * L\rho_l^h(v) + \sum_l K_{jl} * \log(1+Y_l)(v) \\
\partial_v \log Y_j(v) &= L\, 2\pi \mathrm{i}\, s(v+\mathrm{i}) \cdot \delta_{j,1} + 2\pi \mathrm{i} \sum_l K_{jl} * L\rho_l^h + \sum_l K_{jl} * \frac{Y_l}{1+Y_l} \partial_v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

where

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

Numerical solution of coupled NLIEs for finite L

anisotropy $\Delta = 1/2$ ($\nu = 3$), reciprocal temperature $\beta = 1$



explains strong size dependence for L up to 10^4, $D_s(L \to \infty) = 0.274629$, Zotos' result

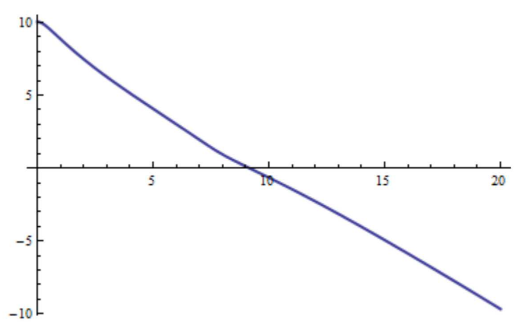
Integral equations: $L \to \infty$ for fixed $T > 0$ (I)

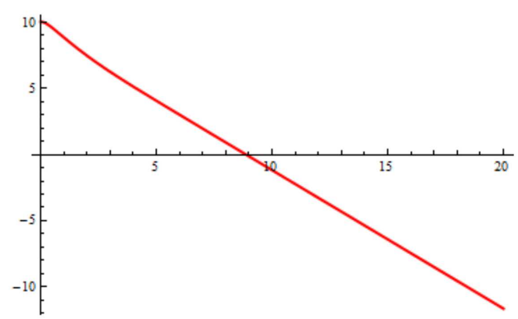
1st integral: $$\int \frac{\rho_j^h(v)}{\partial_v \log Y_j(v+\mathrm{i})} \partial_v \left[\frac{\partial_\psi \log Y_j(v+\mathrm{i})}{\partial_v \log Y_j(v+\mathrm{i})} \right] dv$$

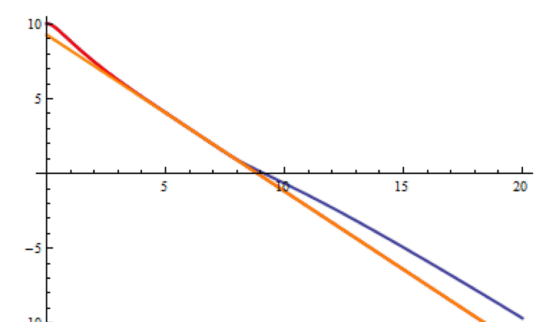
'Too many functions', approximate identities for $|v| < \frac{\nu}{\pi} \log L$:

$$\begin{aligned}
\rho_j^h(v) &= -\frac{1}{A} \partial_\beta \log(1+\eta_j(v)) \\
\partial_v \log Y_j(v) &= -\frac{2\pi \mathrm{i} L}{A} \partial_\beta \log \eta_j(v) \qquad (*) \\
\partial_\psi \log Y_j(v) &= -\frac{1}{\beta A} \partial_v \log \eta_j(v)
\end{aligned}$$

for larger $|v|$ there are deviations: lhs versus rhs of (*)







Integral equations: $L \to \infty$ for fixed $T > 0$ (II)

Surprise: ratios of functions coincide completely for sufficiently large L (numerics, analytical)

$$\frac{\partial_\psi \log Y_j(v+\mathrm{i})}{\partial_v \log Y_j(v+\mathrm{i})} = \frac{1}{2\pi\mathrm{i}\beta L} \frac{\partial_v \log \eta_j(v)}{\partial_\beta \log \eta_j(v)}$$

Not so easy for

$$\begin{aligned} \frac{\rho_j^h(v)}{\partial_v \log Y_j(v+\mathrm{i})} &= \frac{1}{2\pi\mathrm{i}L} \frac{\partial_\beta \log(1+\eta_j(v))}{\partial_\beta \log \eta_j(v)} + \text{corrections} \\ &= \frac{1}{2\pi\mathrm{i}L} \frac{1}{1+1/\eta_j(v)} + \text{corrections} \end{aligned}$$

where ‘corrections’ appear for $|v| > \frac{\nu}{\pi} \log L$.

Simplifications in 1st integral (substitution of 2nd ratio, then 1st ratio)

$$\int \frac{\rho_j^h(v)}{\partial_v \log Y_j(v+\mathrm{i})} \partial_v \left[\frac{\partial_\psi \log Y_j(v+\mathrm{i})}{\partial_v \log Y_j(v+\mathrm{i})} \right] dv = -\frac{1}{4\pi^2 L^2 \beta} \int \frac{1}{1+1/\eta_j(v)} \partial_v \left[\frac{\partial_v \log \eta_j(v)}{\partial_\beta \log \eta_j(v)} \right] dv$$

Integral equations: $L \to \infty$ for fixed $T > 0$ (III)

$$\frac{D}{D_0} = -\frac{1}{4\pi^2\beta}\sum_{j=\pm}\int \frac{1}{1+\eta_j^{-1}(v)}\partial_v \frac{\partial_v \log\eta_j(v)}{\partial_\beta \log\eta_j(v)} dv + \frac{L}{2\pi i}\sum_{j=\pm}\int \frac{Y_j(v)}{(1+Y_j(v))^2}\partial_\psi \log Y_j(v) dv$$

1st integral: integration by parts

$$\int \frac{1}{1+\eta_j^{-1}(v)}\partial_v \frac{\partial_v \log\eta_j(v)}{\partial_\beta \log\eta_j(v)} dv = \frac{1}{1+\eta_j^{-1}(v)} \frac{\partial_v \log\eta_j(v)}{\partial_\beta \log\eta_j(v)}\Bigg|_{-\infty}^{\infty} - \int \partial_v \frac{1}{1+\eta_j^{-1}(v)} \frac{\partial_v \log\eta_j(v)}{\partial_\beta \log\eta_j(v)} dv$$

2nd integral: exact evaluation

$$\begin{aligned}\int \frac{Y_j(v)}{(1+Y_j(v))^2}\partial_\psi \log Y_j(v) dv &= 2\int_0^\infty \frac{Y_j(v)}{(1+Y_j(v))^2}\partial_v \log Y_j(v) \cdot \underbrace{\frac{\partial_\psi \log Y_j(v)}{\partial_v \log Y_j(v)}}_{\to R = \frac{1}{2\pi i\beta L}\frac{\partial_v \log\eta_j}{\partial_\beta \log\eta_j}\big|_\infty} \cdot dv \\ &= 2R\cdot\int_{Y_j(0)}^{Y_j(\infty)} \frac{dY}{(1+Y)^2} = -2R\frac{1}{1+Y}\Bigg|_{Y_j(0)}^{Y_j(\infty)}\end{aligned}$$

Integral equations: $L \to \infty$ for fixed $T > 0$ (IV)

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

$$\frac{D}{D_0} = \frac{1}{4\pi^2\beta}\sum_{j=\pm}\int \frac{1}{[1+\eta_j(v)][1+\eta_j^{-1}(v)]}\,\frac{[\partial_v \log\eta_j(v)]^2}{\partial_\beta \log\eta_j(v)}dv$$

Conditions of validity of Zotos' 1999 result for finite temperature spin stiffness D_s for XXZ spin chain with $\Delta = \cos(\pi/\nu)$

- periodic boundary conditions (energy level curvatures w.r.t. ϕ evaluated at $\phi = 0$)
- robustness with respect to rearrangement of densities ρ_j^h

Open problems:

- general boundary conditions, especially $\phi = \pi$: the $D_s(T,L)$ formula looks different!

  In 'real life' a $\delta(\omega - O(L^{-1}))$ contribution to $\sigma(\omega)$ still qualifies for Drude peak

- What is the status of the 'spinon' approach to the Drude weight?

Summary

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

Exact results obtained for

- spin stiffness for $\Delta = \cos(\pi/\nu)$, finite T, L, periodic b.c.

Open problems

- spin Drude weight
- other anisotropies