On the XXX spin-1/2 quantum chain with non-diagonal boundary fields

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Contents

I learned integrability in a broad scope from Prof. R. J. Baxter well before studying the Bethe ansatz within a condensed matter framework. As a result, I almost always prefer alternative methods like

- inversion / fusion relations, ...
- "Knizhnik-Zamolodchikov" equations for correlation functions

And when I do resort to the Bethe ansatz, I try to avoid working with root density functions.

Outline

- functional equations for transfer matrices: T-, Y-systems $\rightarrow$ non-linear integral equations

  – 2d Ising model, – hard hexagons, – 2d RSOS models

- TQ-relations $\rightarrow$ finite NLIE
- Spin-1/2 Heisenberg chain with non parallel boundary fields

Work in collaboration with H. Frahm, D. Wagner, and with X. Zhang (AvH fellow)
within DFG-Forschergruppe 2316 "Correlations in Integrable Quantum Many-Body Systems"

Historical origin of NLIE: inversion identities

2d Ising model in zero field

Transfer matrix as function of spectral parameter: commuting family, inversion identity

$$T(v-\mathrm{i})T(v+\mathrm{i}) = f(v)\cdot \mathrm{id} \qquad \text{with known function } f(v)$$

For largest eigenvalue $T_{max}(v)$ there are no zeros in “physical strip”, no poles, hence

$$\log T_{max}(v) = \int_{-\infty}^{\infty} s(v-w)\log f(w)dw, \quad \text{in short}: \ \log T_{max} = s*\log f, \qquad s(v) := \frac{1}{4\cosh \pi v/2}$$

Integral *expression* is of convolution type. Excitations come with additional terms.

“Hard hexagon” model

After suitable normalization of transfer matrix we have functional equation

$$T(v-\mathrm{i})T(v+\mathrm{i}) = id + T(v)$$

For largest eigenvalue $T = T_{max}$

$$\log T(v) = L\log\tanh\frac{\pi}{4}v + s*\log(1+T),$$

Integral *equation* of convolution type. Solution by numerical iterations.

"Full story" for $su(2)$ / q-deformation / RSOS models

Fused transfer matrices $T_j(u)$ with spin $j/2$ in auxiliary space, mutually commuting.

So-called T**-system:** (bilinear) functional relations for $j = 1,2,3\ldots$

$$T_j(v-\mathrm{i})T_j(v+\mathrm{i}) = id + T_{j-1}(v)T_{j+1}(v)$$

Y**-system:** for all $j = 1,2,3,\ldots$

$$Y_j(v) := T_{j-1}(v)T_{j+1}(v), \qquad j = 1,2,\ldots$$
$$Y_j(v-\mathrm{i})Y_j(v+\mathrm{i}) = [1+Y_{j-1}(v)][1+Y_{j+1}(v)],$$

AK, Pearce (1992)

higher rank: A. Kuniba, T. Nakanishi, J. Suzuki (1994)

higher rank, discrete Hirota, Bäcklund flow: Krichever, O. Lipan, P. Wiegmann, A. Zabrodin (1997)

Non-linear integral equations... here for ground-state

Non-linear integral equations for Y:

$$\log Y_1(v) = L \log \tanh \frac{\pi}{4} v + s * \log(1+Y_2)$$
$$\log Y_j(v) = s * [\log(1+Y_{j-1}) + \log(1+Y_{j+1})], \quad j \geq 2,$$

Solve the NLIEs, then largest **eigenvalue of** $T_1(v)$ from

$$T_1(v-\mathrm{i})T_1(v+\mathrm{i}) = 1 + Y_1(v) \quad \Rightarrow \quad \log T_1(v) = L\phi(v) + s * \log(1+Y_1)$$

These equations hold for any finite L and numerics are as good for $L = 10^{10}$ as for $L = 2$: integral kernel has exponential asymptotics etc.

Conformal data can be obtained without numerics: **dilog trick**

Fateev, Wiegmann 1981,..., AK, Pearce 1992

Spin-1/2 XXX chain: periodic boundary

Periodic boundary success story

$$H = \sum_{j=1}^{N} \vec{\sigma}_j \vec{\sigma}_{j+1}, \qquad (\sigma_{N+1}^{x,y,z} = \sigma_1^{x,y,z})$$

- Yang-Baxter: infinite number of conserved charges $Q_n = \frac{d^n}{dx^n} \log T(x)$, $H = Q_1$
- magnetization $\sum_j \sigma_j^z$ commutes with H and Q_n.

$$\begin{aligned}
\log Y_1(v) &= N \log \tanh \frac{\pi}{4} v + s * \log(1 + Y_2) \\
\log Y_2(v) &= 0 \qquad\qquad\quad + s * [\log(1 + Y_1) + \log(1 + Y_3)], \\
\log Y_3(v) &= 0 \qquad\qquad\quad + s * [\log(1 + Y_2) + \log(1 + Y_4)], \\
&\ldots
\end{aligned}$$

Spin-1/2 XXX chain: general integrable boundary condition

Non-diagonal boundary System with arbitrary boundary fields $\mathbf{h}_1$, $\mathbf{h}_N$ can be written as

$$H = \sum_{j=1}^{N-1} \vec{\sigma}_j \vec{\sigma}_{j+1} + h_1^z \cdot \sigma_1^z + h_N^z \cdot \sigma_N^z + h_N^x \cdot \sigma_N^x$$

parameters of later use: $p := 1/h_1^z$, $q := 1/h_N^z$ and $\xi := h_N^x/h_N^z$. We have Yang-Baxter, reflection matrix/equation

- infinite number of conserved charges for any p, q, ξ: $Q_n = \frac{d^n}{dx^n} \log T(x)$, $H = Q_1$
- for $\xi \neq 0$ the **magnetization** $\sum_j \sigma_j^z$ **does not commute with** H **and** Q_n.

$$\log Y_1(v) = d_1(v) + s * \log(1 + Y_2)$$
$$\log Y_2(v) = d_2(v) + s * [\log(1 + Y_1) + \log(1 + Y_3)],$$
$$\log Y_3(v) = d_3(v) + s * [\log(1 + Y_2) + \log(1 + Y_4)],$$
$$\ldots$$

with non-trivial driving terms in each line: **not so useful** (Frahm et al. 2008)

Spin-1/2 XXX chain: general integrable boundary conditions

Integrability is proven by the Yang-Baxter equation and Sklyanin's reflection algebra

Several methods of solution have been applied

- TQ relations in case of roots of unity, special boundary terms (Nepomechie 2002/04)
- Fusion (Frahm, Grelik, Seel, Wirth 2008)
- Separation of variables (Frahm, Seel, Wirth 2008; Nicolli 2012; Faldella, Kitanine, Niccoli 2013; Kitanine, Maillet, Niccoli, Terras 2018)
- Off-diagonal Bethe ansatz: Commuting transfer matrices + inversion identities (J. Cao, W.-L. Yang, K. Shi, Y. Wang 2013, R.I. Nepomechie 2013, Li, Cao, Yang, Shi, Wang 2014)
- Modified Bethe ansatz (Belliard 2015; Belliard, Pimenta 2015; Crampé N; Avan, Belliard, Grosjean, Pimenta 2015; Belliard, Rodrigo A Pimenta, Slavnov 2021)

- parallel field case: Alcaraz, Barber, Batchelor, Baxter, Quispel 1987

Finite size data from TQ relation and alternative NLIE

Periodic boundaries: Getting rid of ∞ many NLIEs

Bethe ansatz or similar yields TQ relation

$$T_1(v)q(v) = \varphi(v-\mathrm{i})q(v+2\mathrm{i}) + \varphi(v+\mathrm{i})q(v-2\mathrm{i}) \qquad \left(\varphi(v) = v^L\right)$$

with polynomial $q(v)$ with zeros satisfying the Bethe ansatz equations.

Functional equations may be rewitten as NLIE for two auxiliary functions $\mathfrak{a}$, $\overline{\mathfrak{a}}$

$$\log \mathfrak{a}(v) = L \log \tanh \frac{\pi}{4} v + \kappa * \log(1+\mathfrak{a}) - \kappa_- * \log(1+\overline{\mathfrak{a}}), \quad \kappa(v) := \frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-|k|}}{\mathrm{e}^k + \mathrm{e}^{-k}} \mathrm{e}^{\mathrm{i}kv} dk$$

$$\log \overline{\mathfrak{a}}(v) = L \log \tanh \frac{\pi}{4} v - \kappa_+ * \log(1+\mathfrak{a}) + \kappa * \log(1+\overline{\mathfrak{a}})$$

$$E_L = Le_0 + \int_{-\infty}^{\infty} s' \log[(1+\mathfrak{a})(1+\overline{\mathfrak{a}})] dv$$

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

Nota bene:

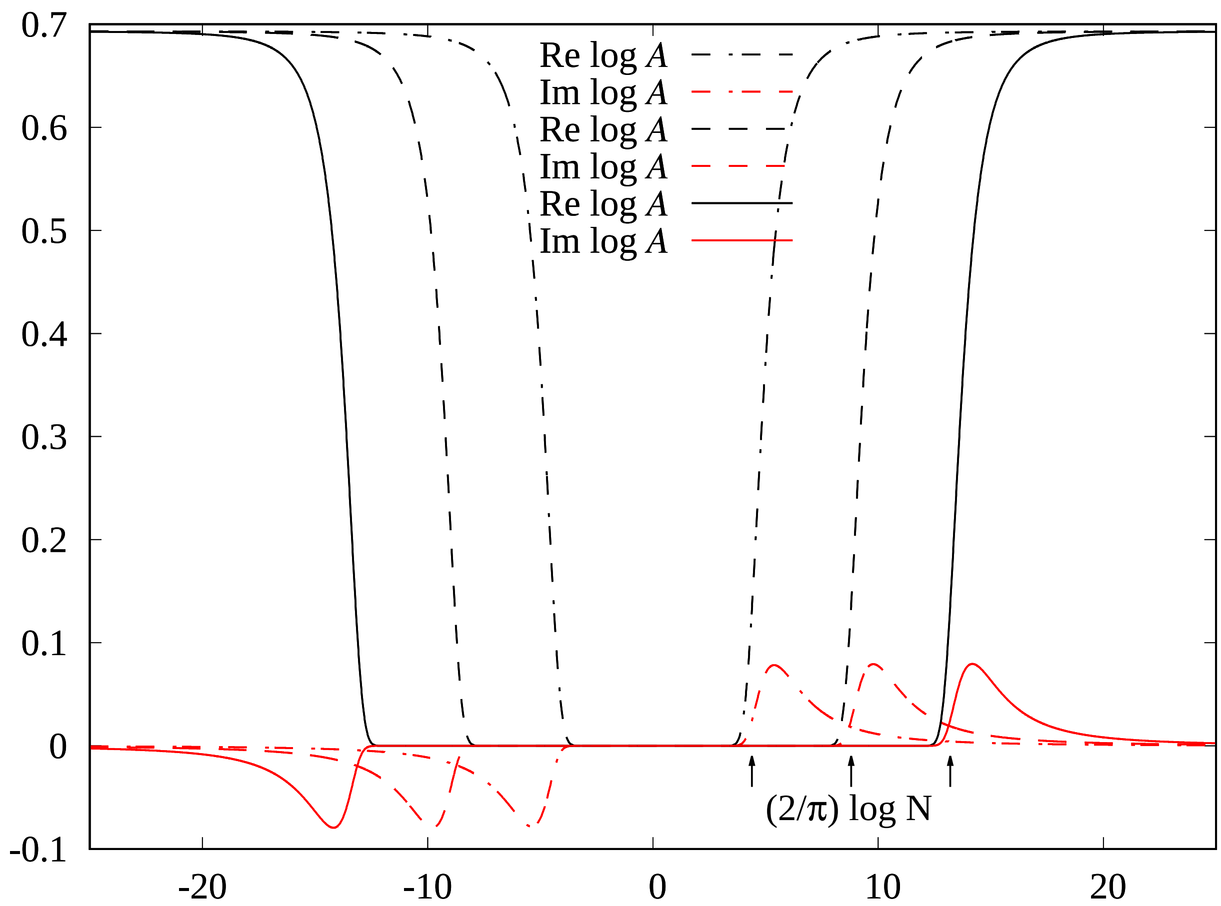
$$\mathfrak{a}(v) = \frac{\varphi(v)q(v-3\mathrm{i})}{\varphi(v-2\mathrm{i})q(v+\mathrm{i})}, \qquad \overline{\mathfrak{a}}(v) = 1/\mathfrak{a}(v)$$

Finite size data: Graphs of $\mathrm{Re}\log A$ and $\mathrm{Im}\log A$

For ground-state eigenvalue of the spin-$1/2$ XXX chain with periodic boundary conditions

chain lengths $N = 10^3, 10^6, 10^9$ (dash-dotted, dashed, solid lines)

(only) one important length scale in the system: $\frac{2}{\pi}\log N$ (→ additive scaling limit)



Non-periodic case: inhomogeneous TQ-relation / auxiliary functions

J. Cao, W.-L. Yang, K. Shi, Y. Wang (2013) derived the following ansatz for the eigenvalue function (here we shift the arguments of the functions)

$$q_1(x) := Q_1\left(\frac{\mathrm{i}}{2}\,x - \frac{1}{2}\right) \qquad q_2(x) := Q_2\left(\frac{\mathrm{i}}{2}\,x - \frac{1}{2}\right)$$

$$t(x) = T\left(\frac{\mathrm{i}}{2}\,x - \frac{1}{2}\right) = \underbrace{\Phi_1(x)\frac{q_1(x+2\mathrm{i})}{q_2(x)}}_{\lambda_1(x)} + \underbrace{\Phi_2(x)\frac{1}{q_1(x)q_2(x)}}_{\lambda_2(x)} + \underbrace{\Phi_3(x)\frac{q_2(x-2\mathrm{i})}{q_1(x)}}_{\lambda_3(x)}$$

We – H. Frahm, AK, D. Wagner and X. Zhang (2025) – find that the following auxiliary functions have useful properties:

$$\mathfrak{a} := \frac{\lambda_2(x)+\lambda_3(x)}{\lambda_1(x)}, \qquad 1+\mathfrak{a} = \frac{\lambda_1(x)+\lambda_2(x)+\lambda_3(x)}{\lambda_1(x)},$$

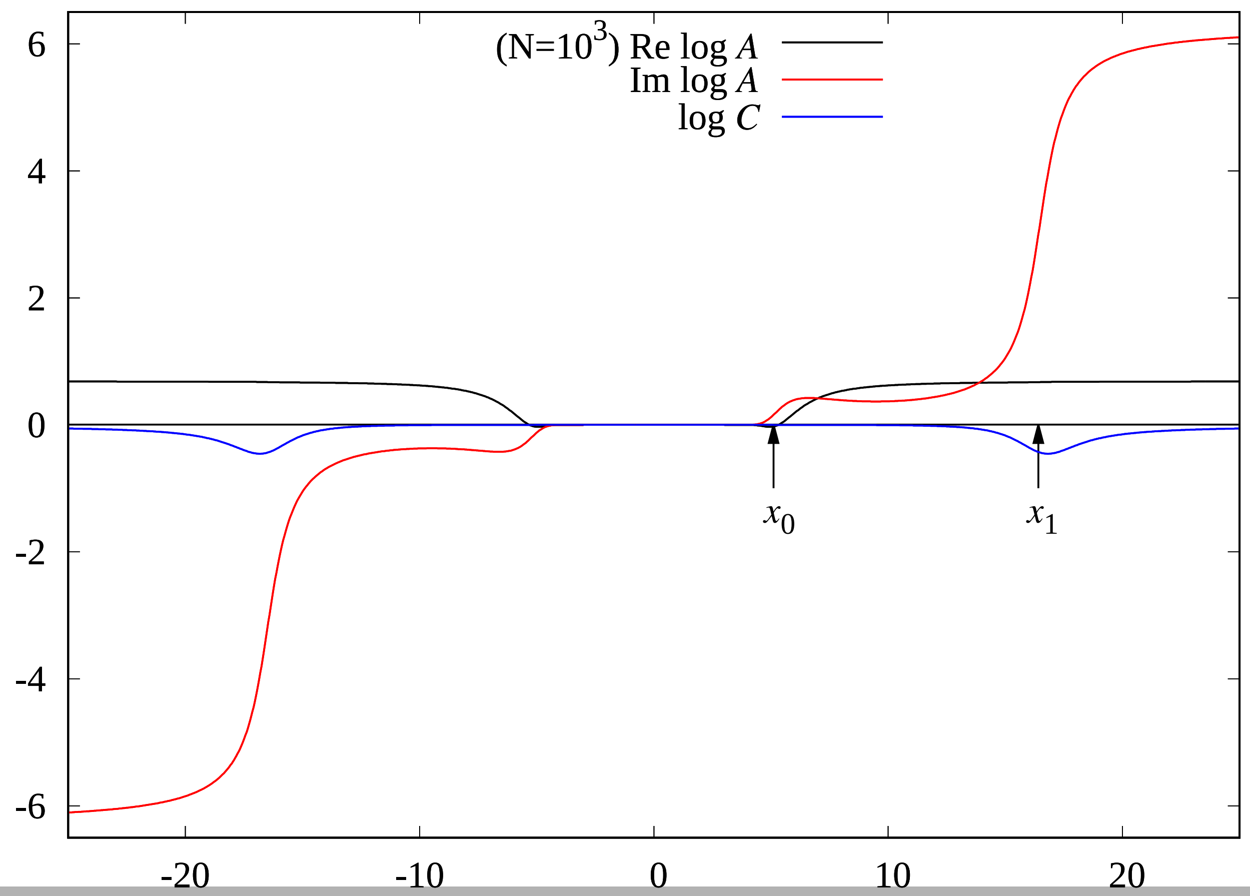
$$\overline{\mathfrak{a}} := \frac{\lambda_1(x)+\lambda_2(x)}{\lambda_3(x)}, \qquad 1+\overline{\mathfrak{a}} = \frac{\lambda_1(x)+\lambda_2(x)+\lambda_3(x)}{\lambda_3(x)},$$

$$\mathfrak{c} := \frac{\lambda_2(x)\left[\lambda_1(x)+\lambda_2(x)+\lambda_3(x)\right]}{\lambda_1(x)\lambda_3(x)}, \qquad 1+\mathfrak{c} = \frac{\left[\lambda_1(x)+\lambda_2(x)\right]\left[\lambda_2(x)+\lambda_3(x)\right]}{\lambda_1(x)\lambda_3(x)},$$

Even for the ground-state the BA roots deviate from the real axis.

Non-periodic case: graphs of Re $\log A$, Im $\log A$ and $\log C$

For ground-state eigenvalue of the spin-$1/2$ XXX chain with non-periodic boundary conditions chain length $N = 10^3$, boundary parameters $p = -0.6$, $q = -0.3$, $\xi = 0.1$
two important length scales in the system: $x_0 \simeq \frac{2}{\pi} \log N \approx 5.1$ and some $x_1 \sim 16.5$ where Im $\log A$ shows a steep increase



Non-periodic case: non-linear integral equations I

The three functions satisfy a closed system of NLIEs

$$\begin{pmatrix} \log a \\ \log \overline{a} \\ \log c \end{pmatrix} = d + K * \begin{pmatrix} \log(A/A(\infty)) - \log\left(\dfrac{x-x_{r+}}{x-x_{r-}} \cdot \dfrac{x-x_{l+}}{x-x_{l-}}\right) \\ \log(\overline{A}/\overline{A}(\infty)) - \log\left(\dfrac{x-x_{r-}}{x-x_{r+}} \cdot \dfrac{x-x_{l-}}{x-x_{l+}}\right) \\ \log(C/C(\infty)) \end{pmatrix},$$

with kernel matrix

$$K(x) = \begin{bmatrix} \kappa(x) & -\kappa_-(x) & -\mathrm{i}/(x-\mathrm{i}) \\ -\kappa_+(x) & \kappa(x) & \mathrm{i}/(x+\mathrm{i}) \\ \mathrm{i}/(x+\mathrm{i}) & -\mathrm{i}/(x-\mathrm{i}) & 0 \end{bmatrix},$$

with concrete/explicit driving terms containing the parameters

$$x_{r\pm} = \tilde{x}_1 \pm \mathrm{i}\,\delta, \qquad x_{l\pm} = -\tilde{x}_1 \pm \mathrm{i}\,\delta,$$

which drop out of the calculations. For practical purposes we choose $\tilde{x}_1$ as an estimate of the location of the transition of the imaginary part of $\log A$.

Non-periodic case: non-linear integral equations II

Driving/source terms

$$d_1(x) = (2N+1)\log \mathrm{th}\left(\frac{\pi}{4}x\right) + \frac{\pi}{2}\mathrm{i} - \mathrm{i}\alpha(x-\mathrm{i},1)$$
$$+\mathrm{i}\alpha(x-\mathrm{i},p_1) + \mathrm{i}\alpha(x-\mathrm{i},p_2) - \mathrm{i}\alpha(x-x_0-\mathrm{i},1) - \mathrm{i}\alpha(x+x_0-\mathrm{i},1)$$
$$+\log\left(a(\infty)\cdot\frac{x-x_{r+}-2\mathrm{i}}{x-x_{r-}}\cdot\frac{x-x_{l+}-2\mathrm{i}}{x-x_{l-}}\right),$$
$$d_2(x) = (2N+1)\log \mathrm{th}\left(\frac{\pi}{4}x\right) - \frac{\pi}{2}\mathrm{i} + \mathrm{i}\alpha(x+\mathrm{i},1)$$
$$-\mathrm{i}\alpha(x+\mathrm{i},p_1) - \mathrm{i}\alpha(x+\mathrm{i},p_2) + \mathrm{i}\alpha(x-x_0+\mathrm{i},1) + \mathrm{i}\alpha(x+x_0+\mathrm{i},1)$$
$$+\log\left(\overline{a}(\infty)\cdot\frac{x-x_{r-}+2\mathrm{i}}{x-x_{r+}}\cdot\frac{x-x_{l-}+2\mathrm{i}}{x-x_{l+}}\right),$$
$$d_3(x) = \log\left(c(\infty)\cdot\frac{x^2(x^2-x_0^2)}{(x-x_{r-}+\mathrm{i})(x-x_{r+}-\mathrm{i})(x-x_{l-}+\mathrm{i})(x-x_{l+}-\mathrm{i})}\right).$$

where $\alpha(x,r)$

$$\alpha(x,r) := \mathrm{i}\log\frac{\Gamma\left(\frac{1}{4}(r+3-\mathrm{i}x)\right)\Gamma\left(\frac{1}{4}(r+1+\mathrm{i}x)\right)}{\Gamma\left(\frac{1}{4}(r+3+\mathrm{i}x)\right)\Gamma\left(\frac{1}{4}(r+1-\mathrm{i}x)\right)}.$$

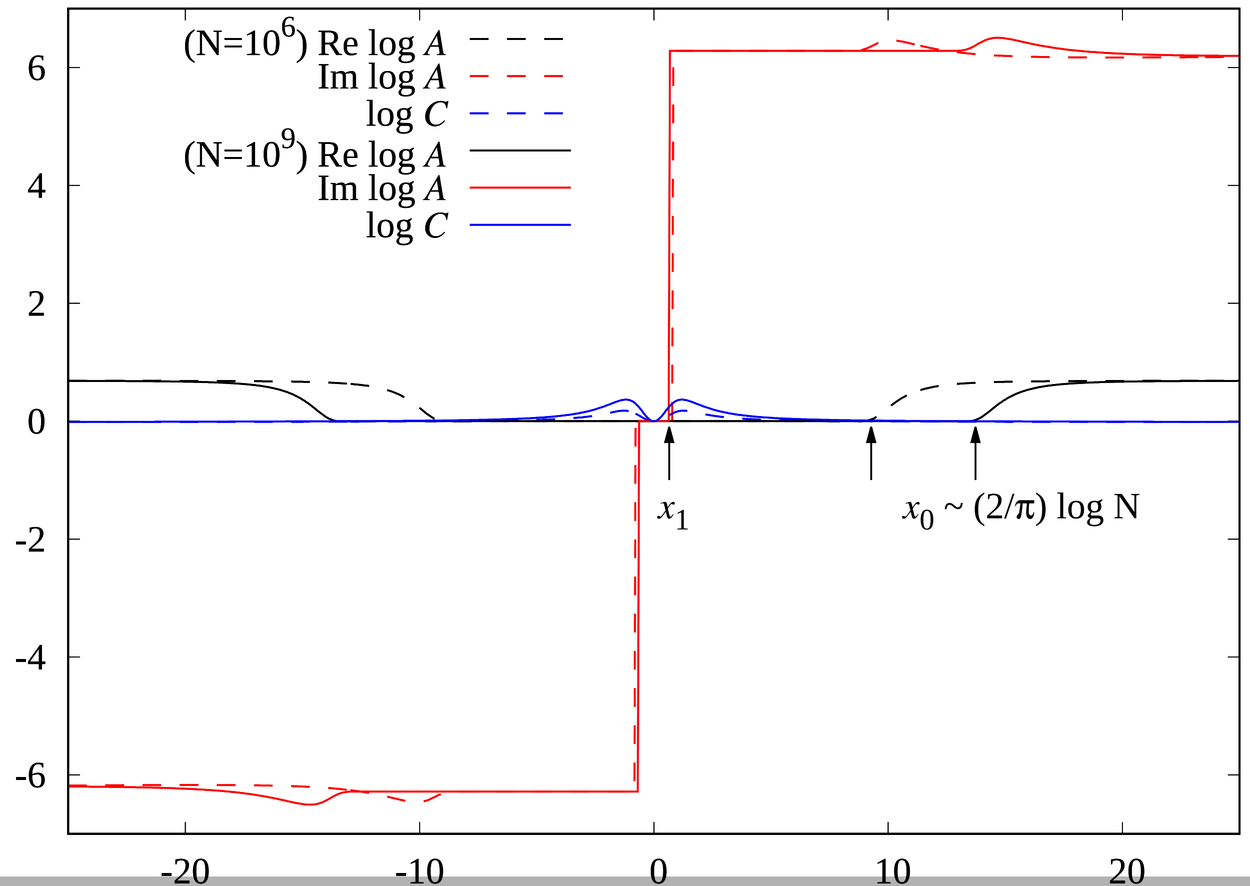
Towards the thermodynamical limit

$\log A$ and $\log C$ for parameters as before, system sizes $N = 10^6$ (dashed) and $N = 10^9$ (solid)

zeros of $\log C$ are at $\pm x_0$, with $x_0 = 9.27..\ (13.72..) \simeq \frac{2}{\pi} \log N$

the transition point of Im $\log A$ is $x_1 = 0.78..\ (0.64..)$ for $N = 10^6\ (10^9)$

unlike before, now $x_1 < x_0$ and the transition appears step-like.



Two step scaling limit

P) For the periodic boundary case *additive scaling limit* of the NLIEs useful

$$a_r(x) := \lim_{N\to\infty} a\left(x + \tfrac{2}{\pi}\log N\right), \quad \text{and} \quad \overline{a}_r(x) := \lim_{N\to\infty} \overline{a}\left(x + \tfrac{2}{\pi}\log N\right),$$

NP) For the non-periodic boundary case we have to first apply a *multiplicative scaling limit* of the NLIEs (AK, X. Zhang 2024)

$$a_m(x) := \lim_{N\to\infty} a\,(x_0\cdot x), \quad \overline{a}_m(x) := \lim_{N\to\infty} \overline{a}\,(x_0\cdot x), \quad c_m(x) := \lim_{N\to\infty} c\,(x_0\cdot x),$$

which leads to a simple, well-defined set of NLIEs for all three functions.

$$\log a_m(x) = \log a(\infty) + \frac{1}{2}\log\frac{A_m(x)}{\overline{A}_m(x)} - \frac{\mathrm{i}}{x-\mathrm{i}\varepsilon} * \log\frac{C_m}{C(\infty)}, \quad \text{for } x \notin [-1,1],$$

$$\text{else } a_m(x) = 0,$$

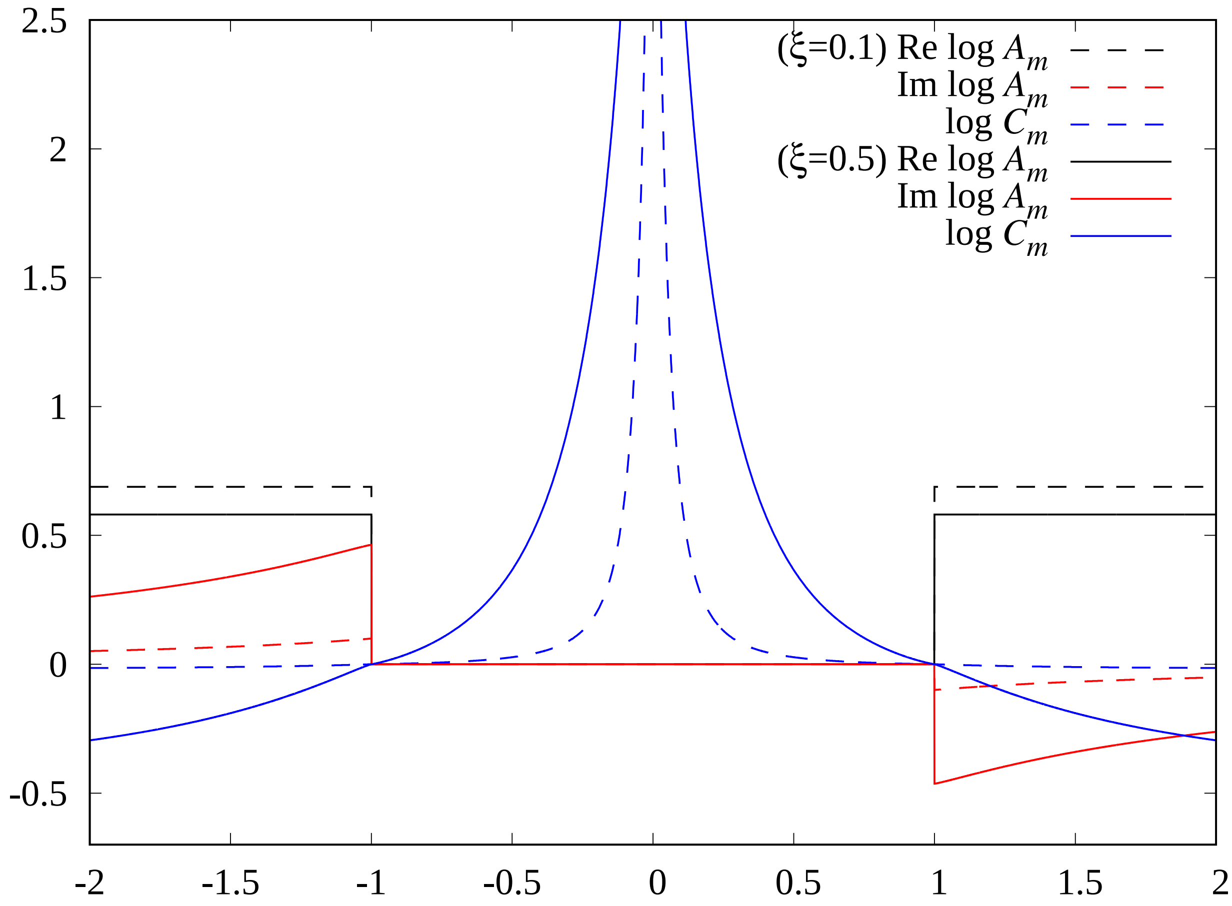
$$\log c_m(x) = \log\left(c(\infty)\cdot\frac{x^2-1}{x^2}\right) + \frac{\mathrm{i}}{x+\mathrm{i}\varepsilon} * \log\frac{A_m}{A(\infty)} - \frac{\mathrm{i}}{x-\mathrm{i}\varepsilon} * \log\frac{\overline{A}_m}{\overline{A}(\infty)},$$

which is easy to solve numerically. After that the *additive scaling limit* is applied.

Thermodynamic limit

Plot of the functions $\log A_m$ and $\log C_m$ defined in the multiplicative scaling limit.

The functions depend only on ξ. Here we show results for two cases, $\xi = 0.1$ and $\xi = 0.5$.



Finite size data

The dilog-trick is applicable. The finite size data are given by dilogarithms evaluated at the asymptotics of the auxiliary functions.

The numerical results for finite boundary fields indicate

$$E_N - Ne_0 - f_s = -\frac{\pi v}{24N}\left(1 - 6\left(1 - \frac{\phi}{\pi}\right)^2\right)$$

where ϕ is the angle between the boundary fields, i.e. $\xi = \tan\phi$ and v is the velocity of elementary excitations.

Summary

Results:

- presentation of three (!) non-linear integral equations for the Heisenberg chain with broken conservation of magnetization
- potentially much more powerful than usual numerics (direct Bethe ansatz, Lanczos)
- direct iterative treatment of NLIE suffers from instabilities, especially for medium sizes
- calculations in conjectured scaling limit work very well
- finite size data depend on orientation of boundary fields

To do:

- check of conjectured scaling limit
- ...