

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 Profs. R. J. Baxter and C. N. Yang 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 (former 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

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

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

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

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

“Hard hexagon” model

After suitable normalization of transfer matrix we have functional equation

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

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 $j = 1, 2, 3, \dots$

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

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

$$Y_j(v) := T_{j-1}(v)T_{j+1}(v), \quad j = 1, 2, \dots$$

$$Y_j(v - i)Y_j(v + i) = [1 + Y_{j-1}(v)][1 + Y_{j+1}(v)],$$

AK, Pearce (1992)

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

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

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

Non-linear integral equations for Y :

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

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

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

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,..., Bazhanov, Rhesetikhin 1988,..., AK, Pearce 1992

Spin-1/2 XXX chain: periodic boundary

Periodic boundary success story

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

- 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 .

$$\log Y_1(v) = N \log \tanh \frac{\pi}{4} v + s * \log(1 + Y_2)$$

$$\log Y_2(v) = 0 \quad + s * [\log(1 + Y_1) + \log(1 + Y_3)],$$

$$\log Y_3(v) = 0 \quad + s * [\log(1 + Y_2) + \log(1 + Y_4)],$$

...

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

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

parameters of later use: $p := 1/h_1^z$, $q := 1/h_N^z$ and $\xi := \textcolor{red}{h_N^x}/h_N^z$. 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** .

$$\log Y_1(v) = d_1(v) + s * \log(1 + Y_2)$$

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

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

...

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; Niccoli 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

$$T_1(v)q(v) = \varphi(v - i)q(v + 2i) + \varphi(v + i)q(v - 2i) \quad (\varphi(v) = v^L)$$

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

Functional equations may be rewritten as NLIE for two auxiliary functions $a, \bar{a}$

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

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

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

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

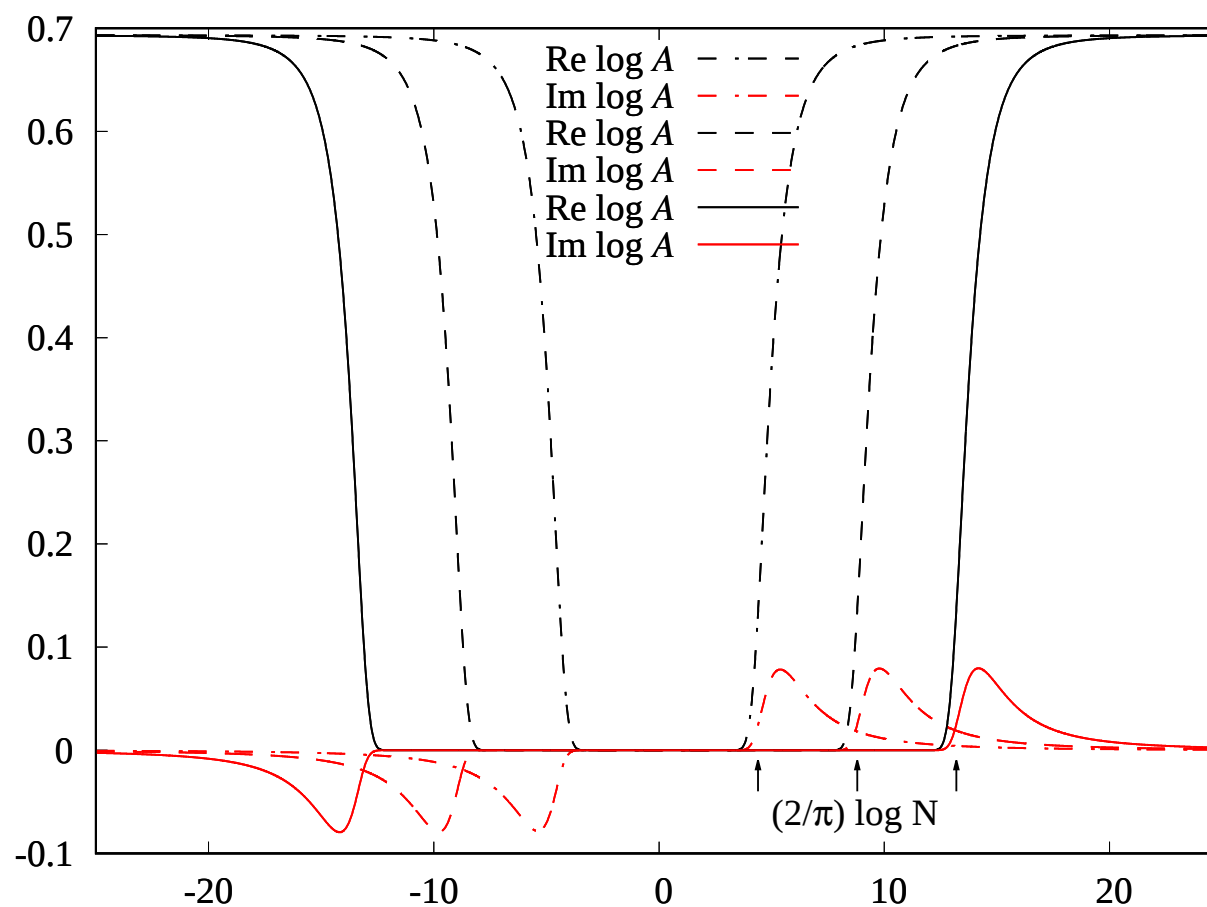
Nota bene:

$$a(v) = \frac{\varphi(v)q(v - 3i)}{\varphi(v - 2i)q(v + i)}, \quad \bar{a}(v) = 1/a(v)$$

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

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: $\frac{2}{\pi} \log N$ ($\rightarrow$ 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)

$$q_1(x) := Q_1 \left(\frac{i}{2} x - \frac{1}{2} \right) \quad q_2(x) := Q_2 \left(\frac{i}{2} x - \frac{1}{2} \right)$$
$$t(x) = T \left(\frac{i}{2} x - \frac{1}{2} \right) = \underbrace{\Phi_1(x) \frac{q_1(x+2i)}{q_2(x)}}_{\lambda_1(x)} + \underbrace{\Phi_2(x) \frac{1}{q_1(x)q_2(x)}}_{\lambda_2(x)} + \underbrace{\Phi_3(x) \frac{q_2(x-2i)}{q_1(x)}}_{\lambda_3(x)}$$

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

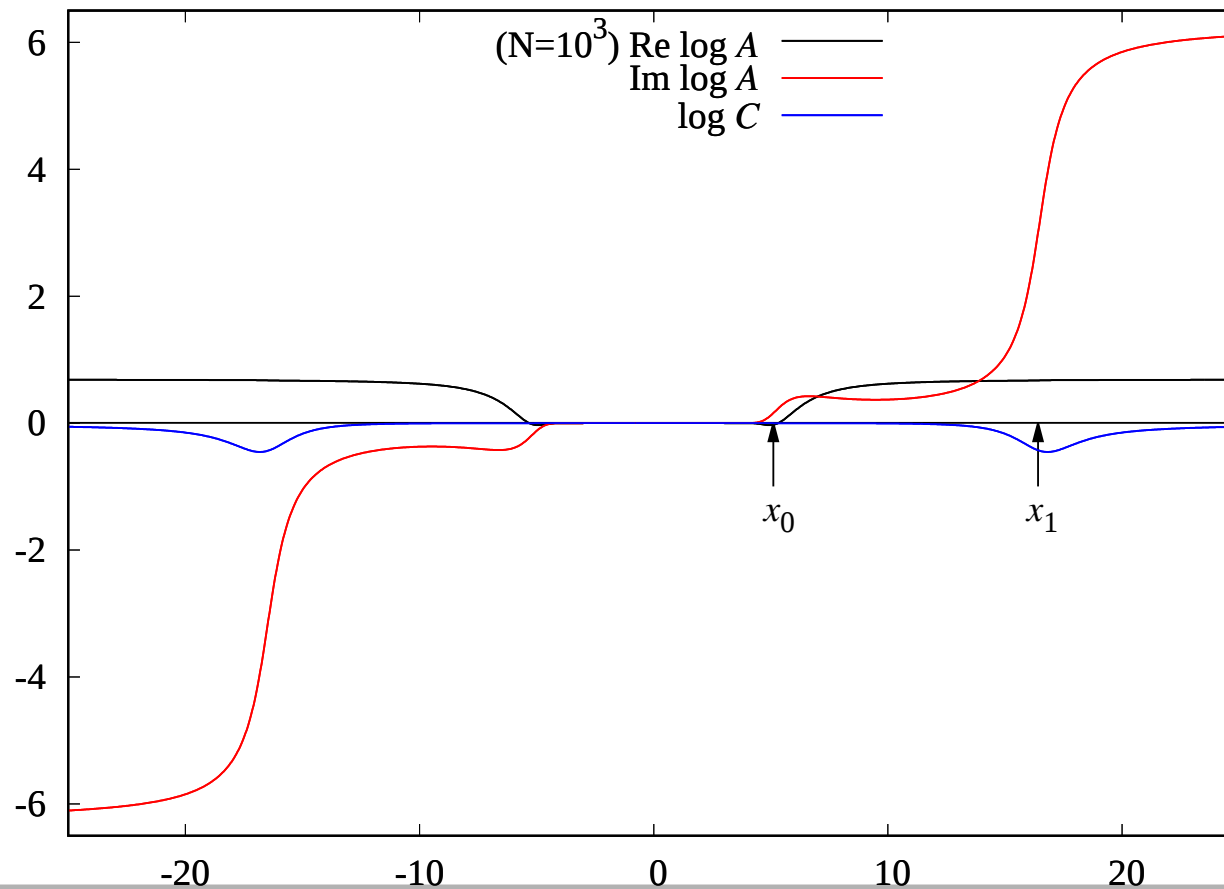
$$a := \frac{\lambda_2(x) + \lambda_3(x)}{\lambda_1(x)}, \quad A := 1 + a = \frac{\lambda_1(x) + \lambda_2(x) + \lambda_3(x)}{\lambda_1(x)},$$
$$\bar{a} := \frac{\lambda_1(x) + \lambda_2(x)}{\lambda_3(x)}, \quad \bar{A} := 1 + \bar{a} = \frac{\lambda_1(x) + \lambda_2(x) + \lambda_3(x)}{\lambda_3(x)},$$
$$c := \frac{\lambda_2(x) [\lambda_1(x) + \lambda_2(x) + \lambda_3(x)]}{\lambda_1(x)\lambda_3(x)}, \quad C := 1 + c = \frac{[\lambda_1(x) + \lambda_2(x)] [\lambda_2(x) + \lambda_3(x)]}{\lambda_1(x)\lambda_3(x)},$$

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

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

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
 $\text{Im log } A$ shows a steep increase ($\log A$ on $\mathbb{R} - i$ and $\log \bar{A}$ on $\mathbb{R} + i$)



Non-periodic case: non-linear integral equations 0

The defined functions have nice graphs, but why are they actually good for anything?

The rational functions $a, \bar{a}, c, A, \bar{A}, C$ allow for the following factorizations in terms of polynomials

$$a(x) = \text{cst.} \frac{(x+i)^{2N+1}}{\varphi(x)(x-i)^{2N+1}} \frac{D(x)}{q_1(x+2i)},$$

$$\bar{a}(x) = \text{cst.} \frac{(x-i)^{2N+1}}{\bar{\varphi}(x)(x+i)^{2N+1}} \frac{\bar{D}(x)}{q_2(x-2i)},$$

$$c(x) = \text{cst.} \frac{x^2}{\varphi(x)\bar{\varphi}(x)} \frac{\Lambda(x)}{q_1(x+2i)q_2(x-2i)},$$

$$A(x) = \text{cst.} \frac{x}{\varphi(x)(x-i)^{2N+1}} \frac{q_2(x)}{q_1(x+2i)} \Lambda(x),$$

$$\bar{A}(x) = \text{cst.} \frac{x}{\bar{\varphi}(x)(x+i)^{2N+1}} \frac{q_1(x)}{q_2(x-2i)} \Lambda(x),$$

$$C(x) = \text{cst.} \frac{1}{\varphi(x)\bar{\varphi}(x)} \frac{D(x)\bar{D}(x)}{q_1(x+2i)q_2(x-2i)},$$

Strategy:

Compute from the three functions $A(x), \bar{A}(x), C(x)$ the five functions $q_1(x), q_2(x), D(x), \bar{D}(x)$ and $\Lambda(x)$. This works by use of the Fourier transforms of the logarithms, and: $q_1(x), q_2(x), D(x), \bar{D}(x)$ “count only half”.

Then insert the results into expressions for $a(x), \bar{a}(x), c(x)$.

Non-periodic case: non-linear integral equations I

The three functions satisfy a closed system of NLIEs

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

with kernel matrix

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

with concrete/explicit driving terms containing the parameters

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

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

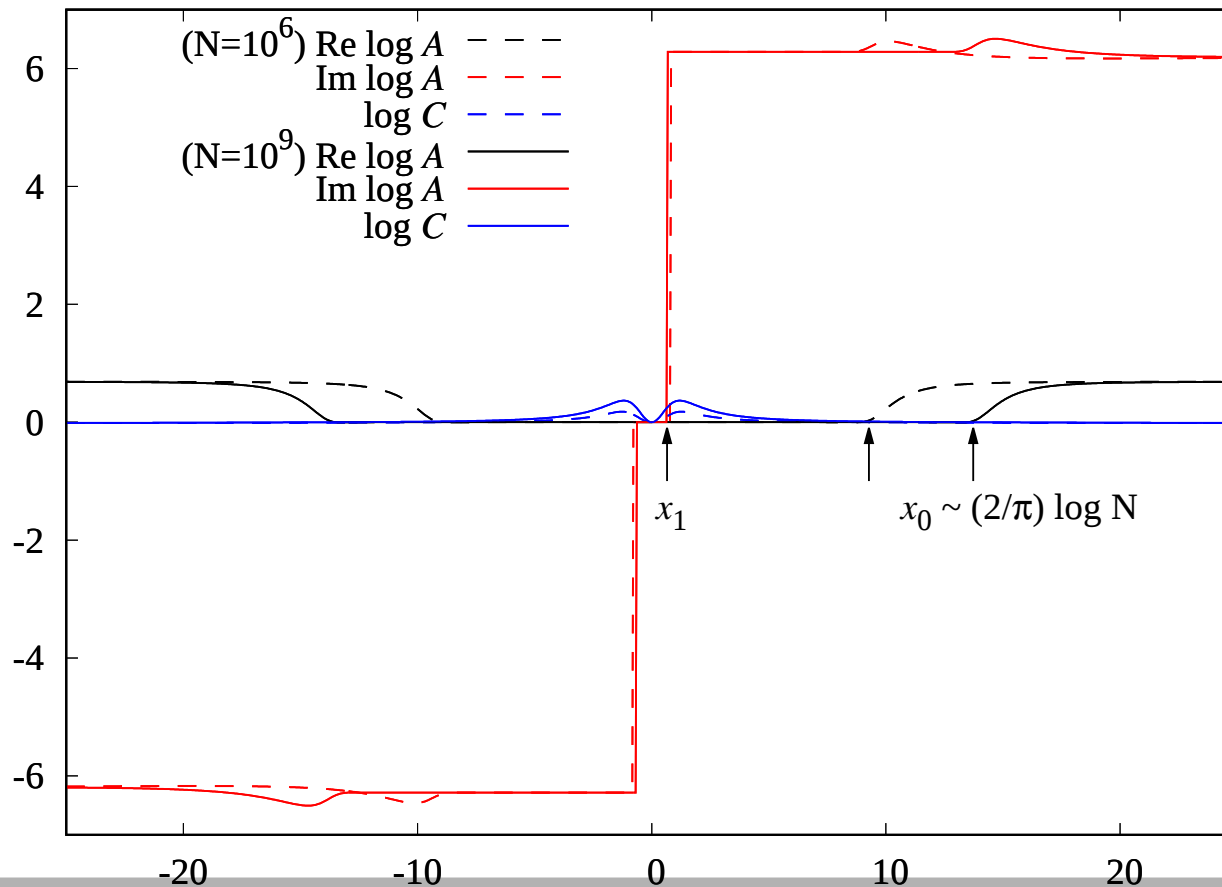
$$\begin{aligned}
 d_1(x) &= (2N+1) \log \operatorname{th} \left(\frac{\pi}{4} x \right) + \frac{\pi}{2} i - i\alpha(x-i, 1) \\
 &\quad + i\alpha(x-i, p_1) + i\alpha(x-i, p_2) - i\alpha(x-x_0-i, 1) - i\alpha(x+x_0-i, 1) \\
 &\quad + \log \left(a(\infty) \cdot \frac{x-x_{r+}-2i}{x-x_{r-}} \cdot \frac{x-x_{l+}-2i}{x-x_{l-}}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

where $\alpha(x, r)$

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

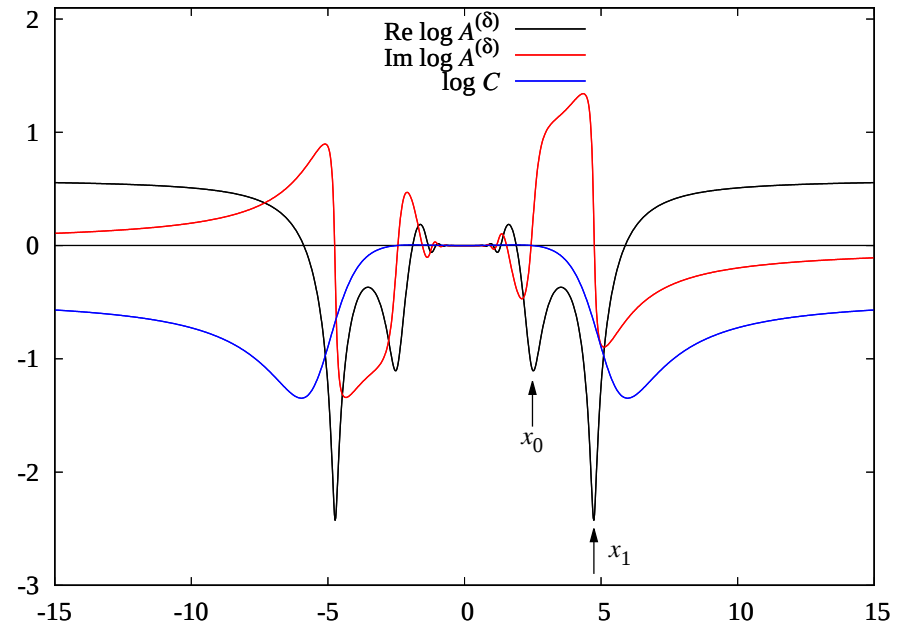
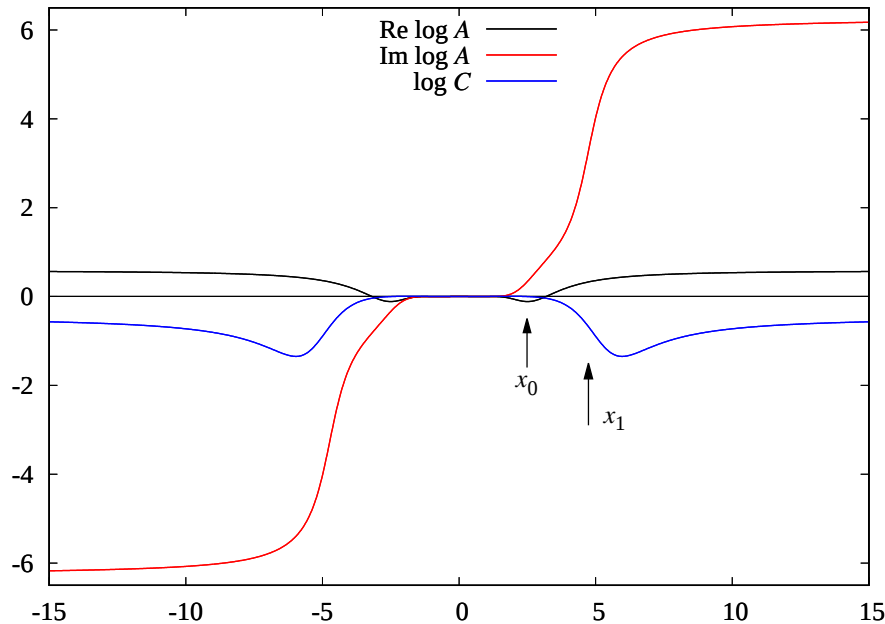
Towards the thermodynamical limit

$\log A$ 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 $\text{Im } \log A$ 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.



Alternative contours $\mathbb{R} \mp \delta i$ (I)

$\log A$ on $\mathbb{R} - i$ compared to $\log A$ on $\mathbb{R} - \delta i$ with $\delta = 0.25$



Chain length $N = 12$, boundary parameters $p = -0.6$, $q = -0.3$, $\xi = 0.5$

Explanation: A has zeros

$$x_0 = 2.4868..., \quad x_{\text{extr}} = \pm 4.7322... - 0.3365...i$$

Why should we care about $\mathbb{R} \mp \delta i$?

Alternative contours $\mathbb{R} \mp \delta i$ (II)

The integral expressions for the functions $\log a^{(\delta)}(x)$, $\log \bar{a}^{(\delta)}(x)$, $\log c(x)$ are

$$\begin{aligned} \log a^{(\delta)}(x) = & (2N+1) \log \text{th} \left(\frac{\pi}{4} (x + (1-\delta)i) \right) + \frac{\pi}{2} i + \log a_{\infty} - i\alpha(x-i, 1) \\ & + i\alpha(x-\delta i, p_1) + i\alpha(x-\delta i, p_2) - i\alpha(x-x_0-\delta i, 1) - i\alpha(x+x_0-\delta i, 1) \\ & + i\alpha(x-x_{1l}-\delta i, 1) + i\alpha(x-x_{1r}-\delta i, 1) + i\alpha(x-x_{2l}-\delta i, 1) + i\alpha(x-x_{2r}-\delta i, 1) \\ & + K_{11}^{(\delta)} * \log(A^{(\delta)}/A_{\infty}) + K_{12}^{(\delta)} * \log(\bar{A}^{(\delta)}/\bar{A}_{\infty}) + K_{13}^{(\delta)} * \log(C/C_{\infty}), \end{aligned}$$

$$\log \bar{a}^{(\delta)}(x) = \dots$$

$$\log c(x) = \log \left[c_{\infty} \frac{x^2 (x^2 - x_0^2)}{(x-x_{1l})(x-x_{1r})(x-x_{2l})(x-x_{2r})} \right] + K_{31}^{(\delta)} * \log A^{(\delta)}/A_{\infty} + K_{32}^{(\delta)} * \log(\bar{A}^{(\delta)}/\bar{A}_{\infty}).$$

where now no counter-terms are necessary, but explicit **driving terms depending on the extremal roots** show up.

Iterative solution procedure more stable for intermediate sizes. Comparison of ground state energies, errors sort of $O(10^{-4})$:

L	NLIE	Lánczos
12	-23.7997...	-23.8004...
24	-45.2062...	-45.2068...

Two step scaling limit towards analytic results

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

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

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

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

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

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

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

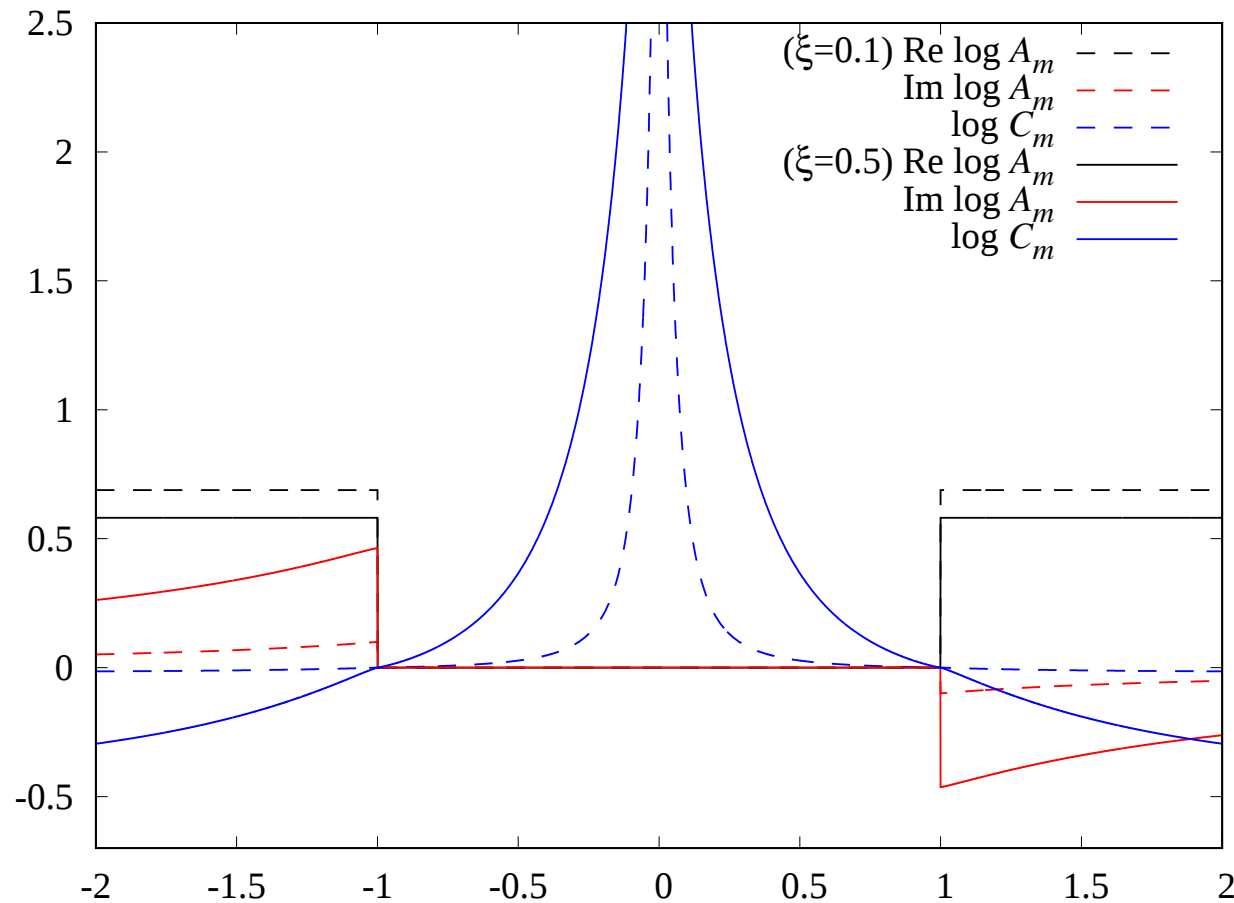
$$\log c_m(x) = \log \left(c(\infty) \cdot \frac{x^2 - 1}{x^2} \right) + \frac{i}{x + i\epsilon} * \log \frac{A_m}{A(\infty)} - \frac{i}{x - i\epsilon} * \log \frac{\bar{A}_m}{\bar{A}(\infty)},$$

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 “some” 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.

The $1/N$ terms only depend on the angle parameter ξ of the boundary fields, not on the absolute values of these.

The $O(1)$ surface terms depend only on the absolute values of the boundary fields separately, not on the angle parameter ξ .

$$E_0 = N - 1 + \frac{2}{p_1} + \frac{2}{p_2} + N\varepsilon_\infty + f_\infty + O\left(\frac{1}{N}\right),$$

$$\varepsilon_\infty = -4\log 2, \quad f_\infty = \pi - 2\log 2 + \sum_{k=1,2} \left(\psi\left(\frac{p_k}{4}\right) - \psi\left(\frac{p_k+2}{4}\right) \right).$$

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, Lánczos)
- 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)
- ...