Exact solution of the spin-1/2 XXX chain with off-diagonal boundary fields

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Contents

Outline

- Spin-1/2 Heisenberg chain with off-diagonal (non parallel) boundary fields

  boundary field case $\leftrightarrow$ periodic boundary case

- parallel field case: Alcaraz et al. 1987

- no conservation of magnetization, but still infinitely many conserved charges

  integrability, various eigenvalue equations

  – fusion, T-system, Y-system

  – TQ relations

- derivation of finite set of non-linear integral equations

  3 versus 2 equations

- numerics: ground-state with "kinks"

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

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

Periodic boundary

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

- 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.

Off-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 $\xi := h_N^x / h_N^z$.

Curious situation: 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.

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

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)
- Off-diagonal Bethe ansatz: Commuting transfer matrices + inversion identities (J. Cao, W.-L. Yang, K. Shi, Y. Wang 2013, R.I. Nepomechie 2013)
- Modified Bethe ansatz (Belliard 2015; Belliard, Pimenta 2015; Crampé N; Avan, Belliard, Grosjean, Pimenta 2015)

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

Fusion: TBA-like non-linear integral equations - Comparison

Periodic boundary

$$\begin{aligned}
\ln Y_1(v) &= N \log \tanh \frac{\pi}{4} \mathrm{v} + \mathbf{s} * \ln(1+\mathrm{Y}_2) \\
\ln Y_2(v) &= 0 \qquad\qquad\qquad + \mathbf{s} * [\ln(1+Y_1) + \ln(1+Y_3)], \\
\ln Y_3(v) &= 0 \qquad\qquad\qquad + \mathbf{s} * [\ln(1+Y_2) + \ln(1+Y_4)], \\
&\dots
\end{aligned}$$

Off-diagonal boundary

$$\begin{aligned}
\ln Y_1(v) &= d_1(v) + \mathbf{s} * \ln(1+Y_2) \\
\ln Y_2(v) &= d_2(v) + \mathbf{s} * [\ln(1+Y_1) + \ln(1+Y_3)], \\
\ln Y_3(v) &= d_3(v) + \mathbf{s} * [\ln(1+Y_2) + \ln(1+Y_4)], \\
&\dots
\end{aligned}$$

with non-trivial driving terms in each line: not so useful.

Large deal of the work by Frahm et al. 2008 spent on coping with this situation:

- infinitely many non-linear integral equations (for non-hermitian field, i.e. imaginary ξ)
- truncation, numerics for relatively short chains (with applications to stochastic systems)

(Alternative) Inhomogeneous TQ-relation I

J. Cao, W.-L. Yang, K. Shi, Y. Wang derived the following ansatz for a polynomial $T(u)$ that satisfies a couple of discrete functional equations:

$$
\begin{aligned}
T(u) = & \frac{2(u+1)^{2N+1}}{2u+1}(u+p)[(1+\xi^2)^{\frac{1}{2}}u+q]\frac{Q_1(u-1)}{Q_2(u)} \\
& + \frac{2u^{2N+1}}{2u+1}(u-p+1)[(1+\xi^2)^{\frac{1}{2}}(u+1)-q]\frac{Q_2(u+1)}{Q_1(u)} \\
& + 2[(-1)^N-(1+\xi^2)^{\frac{1}{2}}]\frac{[u(u+1)]^{2N+1}}{Q_1(u)Q_2(u)}
\end{aligned}
$$

where Q_1 and Q_2 are polynomials

$$
Q_1(u) = \prod_{l=1}^{N}(u-\mu_l) \qquad\qquad Q_2(u) = (-1)^N\prod_{l=1}^{N}(u+\mu_l+1)
$$

with zeros μ_j to be determined by analyticity conditions. There are N of them, they are complex valued...

(Alternative) Inhomogeneous TQ-relation II

Characteristic properties of ansatz: eigenvalue $T(u)$ is analytic and satisfies at $u = 0$ the inversion identities

$$T(u-1)T(u) = \frac{(u^2-1)^{2N+1}}{u^2-1/4}(u^2-p^2)\left[(1+\xi^2)u^2-q^2\right] + O\left(u^{2N+1}\right),$$

This property can be established on the lattice (standard initial condition, crossing).

Also:

- eigenvalue $T(u)$ is polynomial of degree $2N+2$ with highest coefficient 2
- $T(-1) = T(0) = 2pq$
- symmetry $T(-u-1) = T(u)$

(To my mind this derivation is as exact/rigorous as Takahashi's thermodynamics in 2000/2001.)

Functional equations: Definition of auxiliary functions

We shift the arguments of the functions

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

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

and find that the following auxiliary functions have useful properties:

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

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

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

tJ model like ansatz of suitable auxiliary functions (Jüttner, AK 97)

Factorization into “elementary factors” yields integral equations for logs.

Non-linear integral equations I

3 non-linear integral equations take the compact form

$$\begin{pmatrix} \log \mathfrak{a} \\ \log \bar{\mathfrak{a}} \\ \log \mathfrak{c} \end{pmatrix} = d + K * \begin{pmatrix} \log(1+\mathfrak{a}) \\ \log(1+\bar{\mathfrak{a}}) \\ \log(1+\mathfrak{c}) \end{pmatrix}, \qquad K = \begin{pmatrix} \kappa & -\kappa & k \\ -\kappa & \kappa & k^* \\ k^* & k & 0 \end{pmatrix}, \qquad k(x) := -\frac{\mathrm{i}}{x - \mathrm{i}0+}$$

where $\kappa(x)$ was introduced before and

$$d := \begin{pmatrix} (2N+1)\log \mathrm{th}(x+\mathrm{i}) + \gamma(x-x_0,1) + \gamma(x+x_0,1) + \ldots \\ (2N+1)\log \mathrm{th}(x-\mathrm{i}) + \tilde{\gamma}(x-x_0,1) + \tilde{\gamma}(x+x_0,1) + \ldots \\ \log[x^2(x^2-x_0^2)] + \log c_\infty + \ldots \end{pmatrix},$$

where $\gamma(x,a)$ and ... denote terms containing $O(1)$ expressions of type

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

Warning: function $c(x)$ may diverge like $O(x^4)$ instead of approaching c_∞!

(Subsidiary condition $a(x_0+\mathrm{i}) = \bar{a}(x_0-\mathrm{i}) = -1$)

Non-linear integral equations II

Once solutions to NLIEs are found, the eigenvalue function $\Lambda(x)$ and (ground-state) energy are given by

$$\begin{aligned}\log\Lambda(x) =&(2N+1)L(x,2)-L(x,1)+L(x,p_1)+L(x,p_2)\\&+\log(x^2-x_0^2)-L(x-x_0,1)-L(x+x_0,1)\\&+e*(\log A+\log\overline{A})\end{aligned}$$

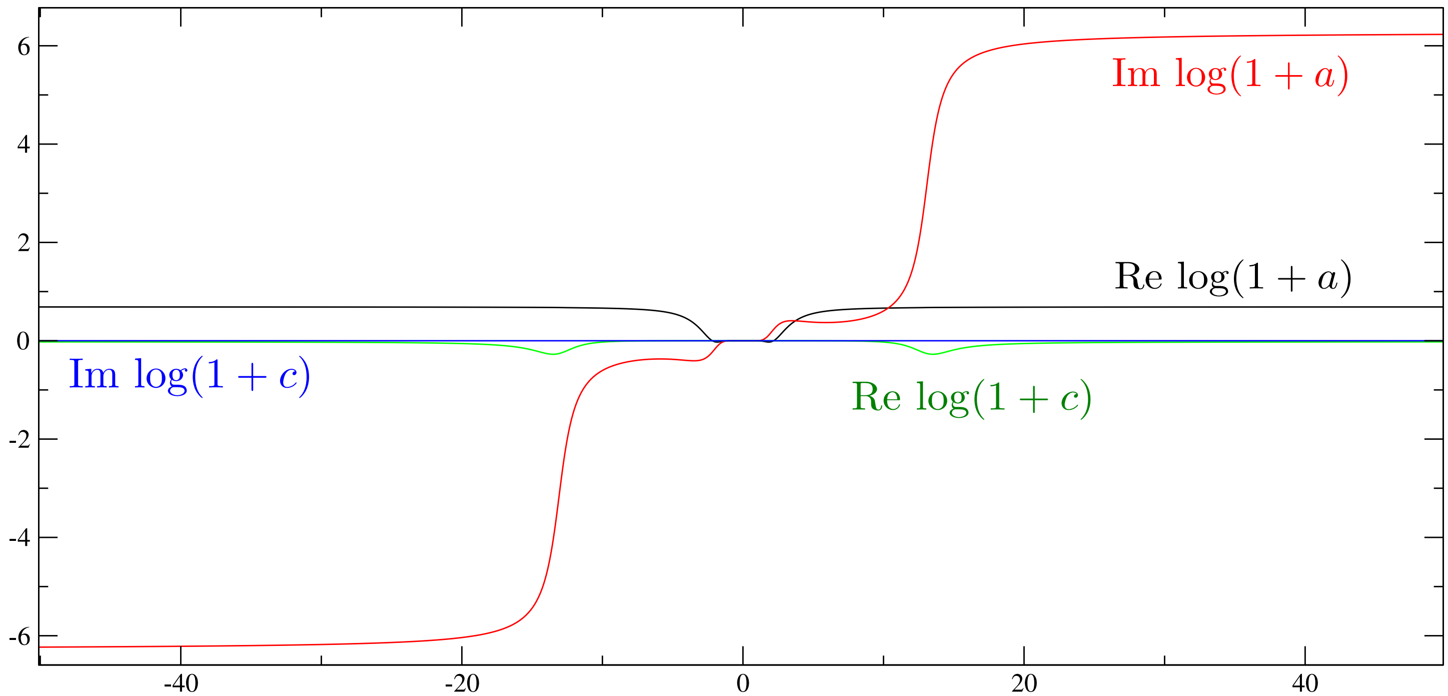
where

$$L(x,a):=\log\frac{\Gamma\left(\frac{1}{4}(a+3+\mathrm{i}x)\right)\Gamma\left(\frac{1}{4}(a+3-\mathrm{i}x)\right)}{\Gamma\left(\frac{1}{4}(a+1+\mathrm{i}x)\right)\Gamma\left(\frac{1}{4}(a+1-\mathrm{i}x)\right)}+\log 4\,,\qquad e(x):=\frac{\frac{\pi}{2}}{\cosh\frac{\pi}{2}x},$$

cp. Yi Qiao, Junpeng Cao, Wen-Li Yang, et al. 2021

Numerical solution to NLIE: ground-state I

Solution for $p = -0.6, q = -0.3, \xi = 0.1$ and $N = 10$



(Functions are rather boring.)

Limit of parallel fields: $\xi \to 0$

Observations:

- For small ξ the "kinks" in $\log \mathfrak{a}(x)$ are far from the origin.
- The position of the kinks is difficult to understand "intuitively". For large arguments all driving terms take "flat values". And somewhere the functions $\mathfrak{a}$ and $\overline{\mathfrak{a}}$ encircle -1.
- For flat driving terms the following functions with suitable constants solve the NLIEs

$$a(x) = a_\infty \frac{x - y_+}{x - x_-}, \quad \bar{a}(x) = a_\infty \frac{x - y_-}{x - x_+}, \quad c(x) = \frac{d}{(x - x_- + \mathrm{i})(x - x_+ - \mathrm{i})}$$

- The kinks disappear to infinity for $\xi \to 0$ (parallel boundary fields) which also enforces $\mathfrak{c} \to 0$. Then only two NLIEs for two functions are left.

CFT data for $\xi = 0$:

The finite size data for the ground-state energy can be obtained by the dilog-trick.

Two cases to distinguish:

(i) The left or right boundary field is zero (or both): parameter $x_0 = \infty$

(ii) generic case: parameter x_0 finite, but scales like $\frac{2}{\pi} \log N$

CFT from scaling limit and dilog trick I

Parallel boundary fields

$$\log \mathfrak{a}(v) = (2N+1)\log\tanh\frac{\pi}{4}(v+\mathrm{i}) + \ldots + \kappa * [\log(1+\mathfrak{a}) - \log(1+\overline{\mathfrak{a}})],$$

$$\log \overline{\mathfrak{a}}(v) = (2N+1)\log\tanh\frac{\pi}{4}(v-\mathrm{i}) + \ldots + \kappa * [\log(1+\overline{\mathfrak{a}}) - \log(1+\mathfrak{a})]$$

Consider functions in the scaling limit

$$a(x) := \lim_{L\to\infty} \mathfrak{a}\left(x - \mathrm{i} + \frac{2}{\pi}\log 4N\right), \qquad \bar{a}(x) := \lim_{L\to\infty} \overline{\mathfrak{a}}\left(x + \mathrm{i} + \frac{2}{\pi}\log 4N\right)$$

They satisfy:

$$\log a(x) = -\mathrm{e}^{-\frac{\pi}{2}x} + \kappa * \log(1+a) - \kappa_- * \log(1+\bar{a}) + \pi\mathrm{i}$$

$$\log \bar{a}(x) = -\mathrm{e}^{-\frac{\pi}{2}x} - \kappa_+ * \log(1+a) + \kappa * \log(1+\bar{a}) - \pi\mathrm{i}$$

The purely exponential form of the driving term and the symmetry of the kernel allow for an analytical calculation of the integral as

$$\frac{\pi}{2}\int_{-\infty}^{\infty} dx\, \mathrm{e}^{-\frac{\pi}{2}x} \log[(1+a(x))(1+\bar{a}(x))] = \int_{-\infty}^{\infty} dx\, (\log a(x))' \log(1+a(x)) + (a \leftrightarrow \bar{a})$$

CFT from scaling limit and dilog trick II

Hence the finite size term in the energy is

$$
\begin{aligned}
E_N - Ne_0 - f_s &= -\frac{1}{2N}\int_{-\infty}^{\infty} dx\,(\log a(x))' \log(1+a(x)) - (a \leftrightarrow \bar{a}) \\
&= -\frac{1}{2N}\int_0^1 da\,\frac{\log(1+a)}{a} - (a \leftrightarrow \bar{a})
\end{aligned}
$$

Final result – for two different integration contours –

$$
E_N - Ne_0 - f_s = -\frac{\pi v}{24N}\cdot 1,
$$

reproducing/extending the results by

Alcaraz, Barber, Batchelor, Baxter, Quispel 1987; Asakawa, Suzuki 1995

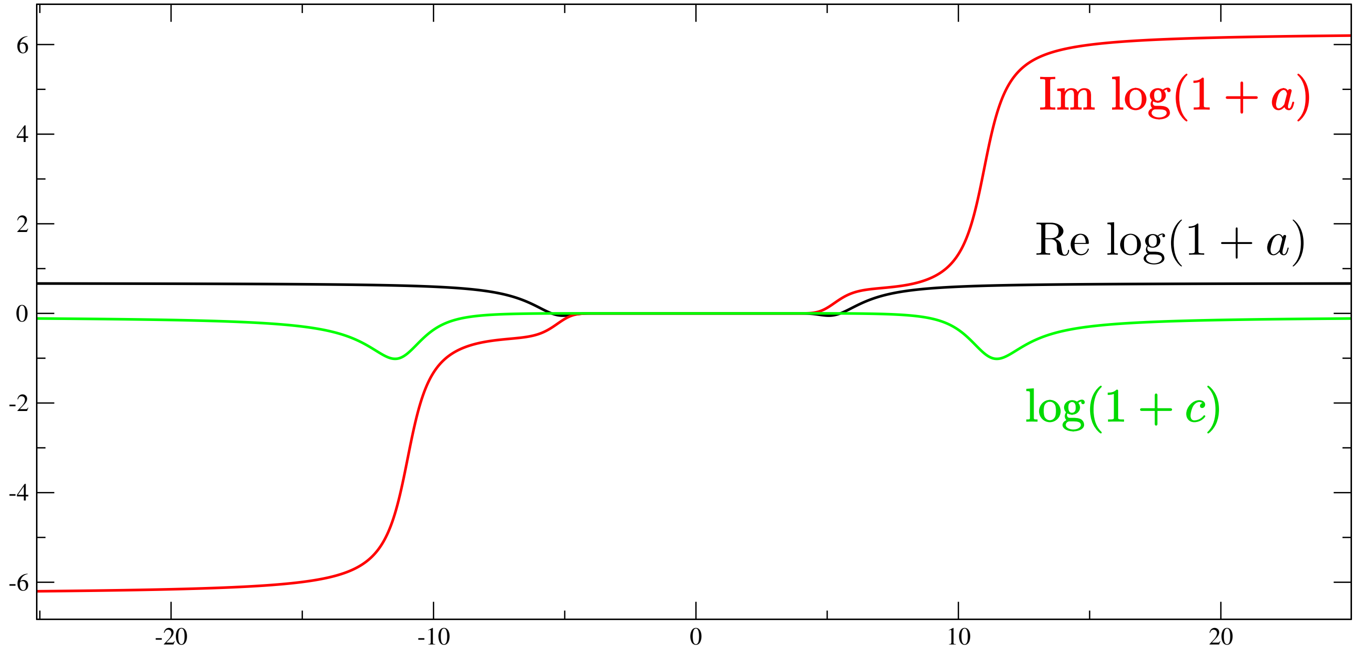
Scaling limit and dilog trick for general off-diagonal case possible

- all three functions enter
- problematic: terminals of scaling functions not known

Numerical solution to NLIE: general case I

Solution for $p = -0.6, q = -0.3, \xi = 0.2$ and $N = 1000$.

Shown are real and imaginary parts of $\log(1 + \mathfrak{a})$, and the real valued $\log(1 + \mathfrak{c})$

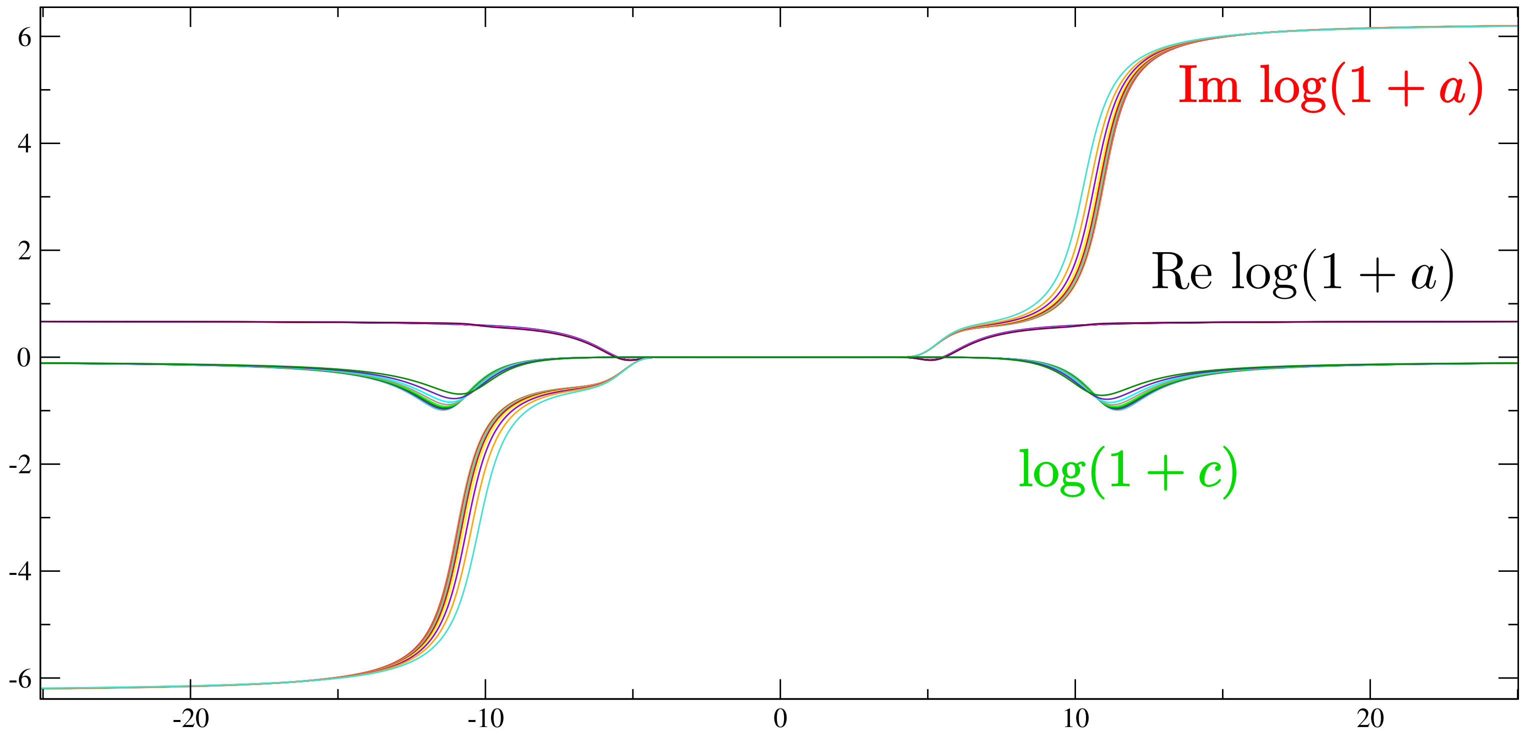


Functions are still boring. However, for increasing N the two transitions move out to larger arguments and closer to each other.

Numerical solution to NLIE: initial transition too low

Solution for $p = -0.6, q = -0.3, \xi = 0.2$ and $N = 1000$.

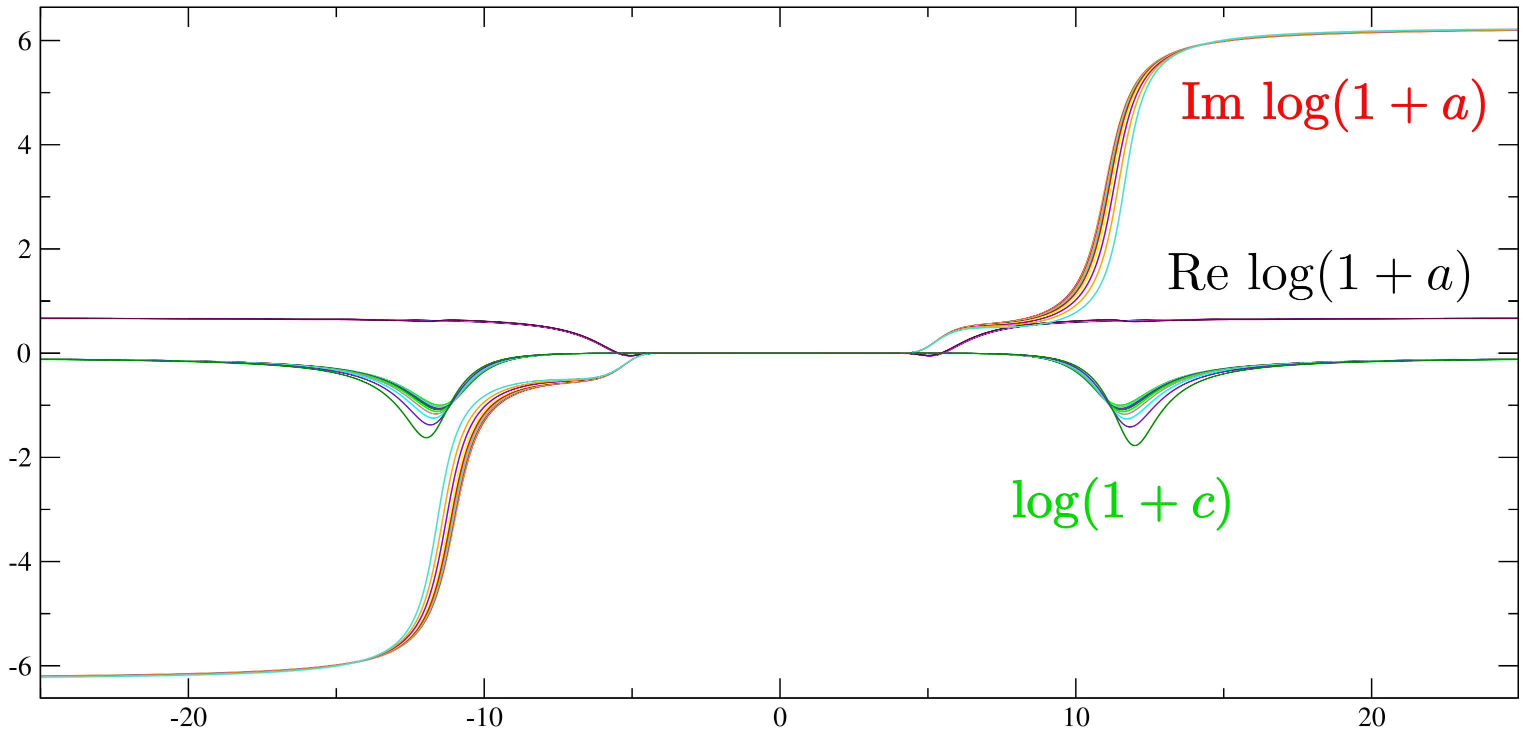
Shown are real and imaginary parts of $\log(1+\mathfrak{a})$, and the real valued $\log(1+\mathfrak{c})$ after every 10 steps of in total 100 iterations.



Numerical solution to NLIE: initial transition too high

Solution for $p = -0.6, q = -0.3, \xi = 0.2$ and $N = 1000$.

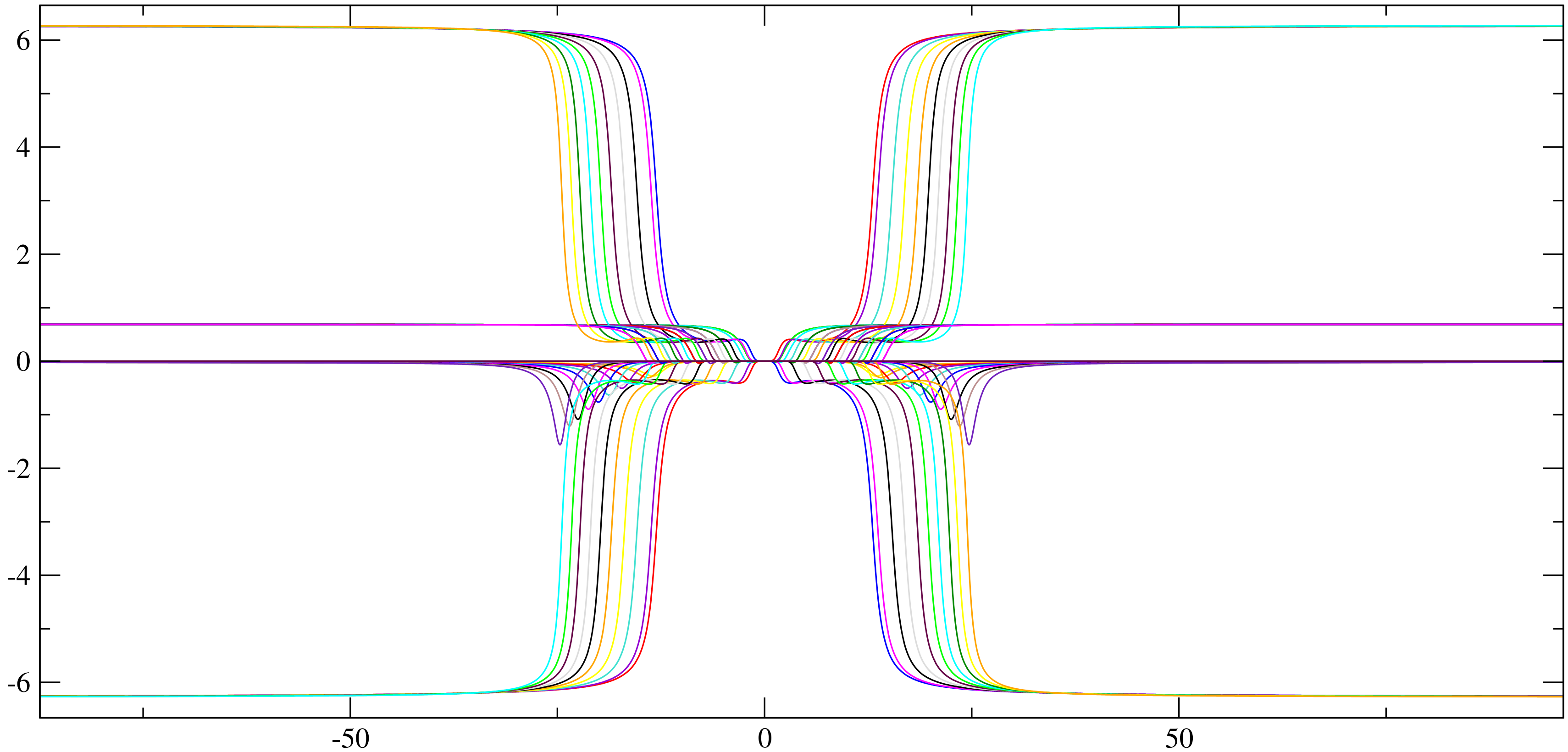
Shown are real and imaginary parts of $\log(1 + \mathfrak{a})$, and the real valued $\log(1 + \mathfrak{c})$ after every 10 steps of in total 100 iterations.



Numerical solution to NLIE: ground-state for large system sizes

Solution for $p = -0.6, q = -0.3, \xi = 0.1$ and $N = 4, 10, 10^2, 10^3, ..., 10^9$.

Shown are real and imaginary parts of $\log(1+\mathfrak{a}), \log(1+\overline{\mathfrak{a}}), \log(1+\mathfrak{c})$



Functions are still boring. However, transitions move out to larger arguments for increasing L.

Also, $\log(1+\mathfrak{c})$ gets more pronounced.

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

To do:

- numerics: modified update rules
- alternative integral equations by fusion + closure
- symmetry of integration kernel for $N \to \infty$ may allow for "dilog-trick"