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 non-diagonal boundary fields

  boundary field case $\leftrightarrow$ periodic boundary case

- no conservation of magnetization, but 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)
- Separation of variables (Frahm, Seel, Wirth 2008; Nicolli 2012; Faldella, Kitanine, Niccoli 2013)
- Fusion (Frahm, Grelik, Seel, Wirth 2008)
- 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)

Fusion analysis, T-system, Y-system... robust/universal

For arbitrary integrable boundary (historically first for periodic boundary)

Fused transfer matrices T_j with spin $j/2$ in auxiliary space, mutually commuting and with H

$$[T_j(u), T_l(v)] = 0, \qquad \frac{d}{du} \ln T_1(u)\Big|_{u=i} = H$$

(bilinear) functional relations for $j = 1, 2, 3...$ AK, Pearce (1992)

$$T_j(v-\mathrm{i})T_j(v+\mathrm{i}) = \varphi(v-(j+1)\mathrm{i})\varphi(v+(j+1)\mathrm{i}) + T_{j-1}(v)T_{j+1}(v) \qquad \Big(\text{pbc: } \varphi(v) = v^N\Big)$$

so-called T-system according to A. Kuniba, T. Nakanishi, J. Suzuki (1994)

Define

$$Y_j(v) := \frac{T_{j-1}(v)T_{j+1}(v)}{\varphi(v-(j+1)\mathrm{i})\varphi(v+(j+1)\mathrm{i})}, \qquad j = 1, 2, ...$$

immediately we obtain for all $j = 1, 2, 3, \ldots$

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

so-called Y-system according to A. Kuniba, T. Nakanishi, J. Suzuki (1994)

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

Periodic boundary: For $Y_1(v)$ the functional equation reads $(L \equiv N)$

$$Y_1(v-\mathrm{i})Y_1(v+\mathrm{i}) = 1 + Y_2(v),$$

but due to zero of order L at 0 and poles of order L at $\pm 2\mathrm{i}$

$$\ln Y_1(v) = L \log \tanh \frac{\pi}{4} \mathrm{v} + \mathbf{s} * \ln(1 + \mathrm{Y}_2)$$

where $*$ denotes convolution and $\mathbf{s}$ is the function $\mathbf{s}(v) := \dfrac{1}{4 \cosh \pi v/2}$.

Rest of functional equations turn into (simpler) integral equations

$$\ln Y_j(v) = \mathbf{s} * [\ln(1 + Y_{j-1}) + \ln(1 + Y_{j+1})], \quad j \geq 2,$$

Eigenvalue of $T_1(v)$ from

$$T_1(v-\mathrm{i})T_1(v+\mathrm{i}) = \varphi(v-2\mathrm{i})\varphi(v+2\mathrm{i})[1 + Y_1(v)]$$

as

$$\ln T_1(v) = L\phi(v) + \mathbf{s} * \ln(1 + Y_1) \qquad \Rightarrow \qquad E_L = Le_0 + \int_{-\infty}^{\infty} \mathbf{s}'(v+i) \ln(1 + Y_1(v)) dv$$

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

Periodic boundary

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

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

Finite size data from TQ relation I

Periodic boundaries

Bethe ansatz or similar yields TQ relation

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

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

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

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

with kernel $\kappa(v) := \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-|k|}}{\mathrm{e}^{k}+\mathrm{e}^{-k}} \mathrm{e}^{\mathrm{i}kv} dk.$

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

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

Nota bene: $\mathfrak{a}(v) = \varphi(v+\mathrm{i})q(v-2\mathrm{i})/\varphi(v-\mathrm{i})q(v+2\mathrm{i})$, $\overline{\mathfrak{a}}(v) = 1/\mathfrak{a}(v)$

Finite size data from TQ relation II

Off-diagonal boundary

Course of events for calculating eigenvalues of the Hamiltonian

(i) set up the generating family of conserved charges: transfer matrix $T(x)$

(ii) derive functional equation for $T(x)$ with suitable auxiliary function $Q(x)$: TQ-relation

(iii) use the TQ-relation

If analyticity properties of $Q(x)$ are controlled (see periodic bc), the TQ-relation allows to derive Bethe ansatz equations etc.

Off-diagonal case: the function $Q(x)$ has unpleasant properties. No non-linear integral equations for two functions!

Alternatively, a modified TQ-relation can be derived with polynomial $Q(x)$, but with ill-posed Bethe ansatz equations.

Even the ground-state is described by intrinsically complex-valued rapidities, iterative procedure for roots is unstable. However, ...

(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

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

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

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

and dots denote terms containing $O(1)$ expressions of type

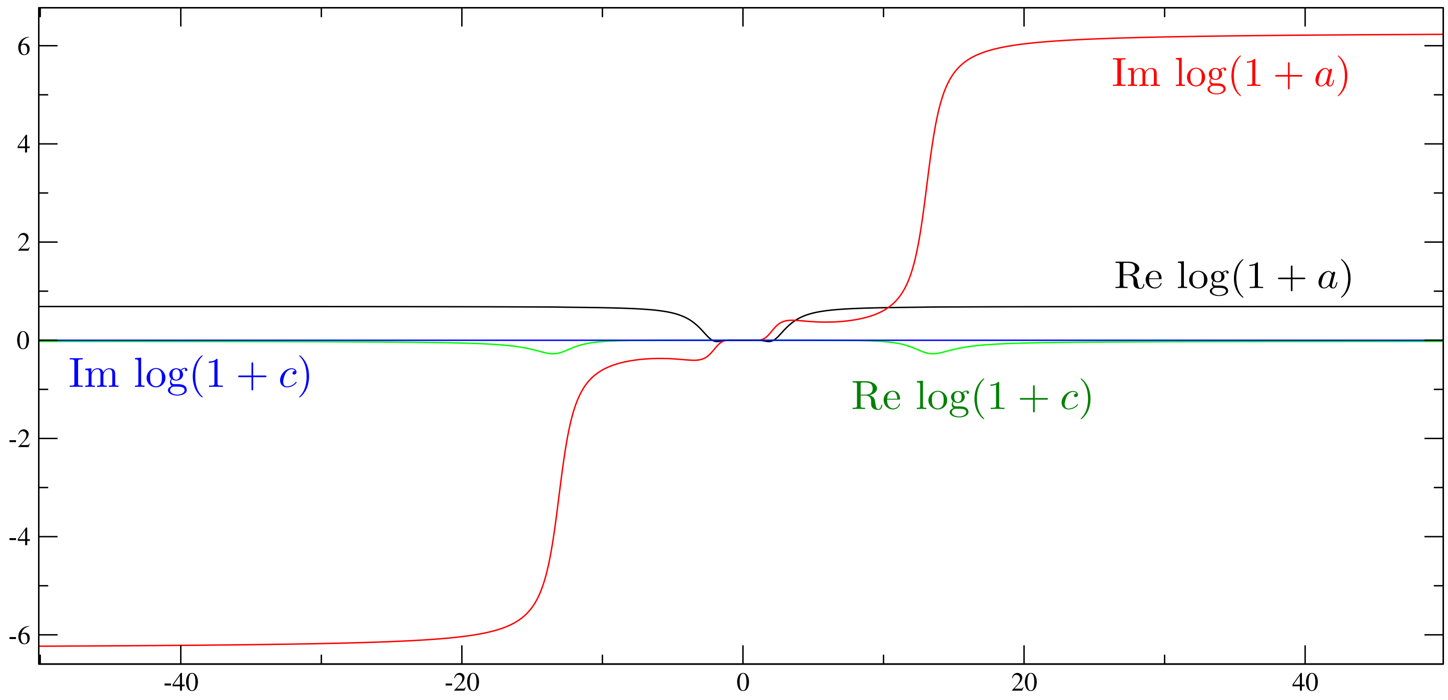
$$\log \frac{\Gamma(\mathrm{cst.} - \mathrm{i}x/4)}{\Gamma(\mathrm{cst.} + \mathrm{i}x/4)}$$

with “cst.” like p, q etc.

Warning: not all convolution integrals well-defined, logarithmic divergencies! “kinks” in $\log a(x)$

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, but show tendency to numerical instability in iterative treatment.

Non-linear integral equations II

Proper formulation containing counter terms

$$\begin{pmatrix} \log \mathfrak{a} \\ \log \bar{\mathfrak{a}} \\ \log \mathfrak{c} \end{pmatrix} = d + K * \begin{pmatrix} \log(1+\mathfrak{a}) - \log\left(\frac{x-x_{r+}}{x-x_{r-}} \cdot \frac{x-x_{l+}}{x-x_{l-}}\right) \\ \log(1+\bar{\mathfrak{a}}) - \log\left(\frac{x-x_{r-}}{x-x_{r+}} \cdot \frac{x-x_{l-}}{x-x_{l+}}\right) \\ \log(1+\mathfrak{c}) \end{pmatrix},$$

where x_{r+} and x_{r-} are some complex numbers at “the right axis” with positive and negative imaginary parts; x_{l+} and x_{l-} on the “left”.

$$d := \begin{pmatrix} (2N+1)\log \mathrm{th}(x+\mathrm{i}) + \log\left(\frac{x-x_{r+}-2\mathrm{i}}{x-x_{r-}} \cdot \frac{x-x_{l+}-2\mathrm{i}}{x-x_{l-}}\right) + \dots \\ (2N+1)\log \mathrm{th}(x-\mathrm{i}) + \log\left(\frac{x-x_{r-}+2\mathrm{i}}{x-x_{r+}} \cdot \frac{x-x_{l-}+2\mathrm{i}}{x-x_{l+}}\right) + \dots \\ \log \frac{x^2(x^2-x_0^2)}{(x-x_{r-}+\mathrm{i})(x-x_{r+}-\mathrm{i})(x-x_{l-}+\mathrm{i})(x-x_{l+}-\mathrm{i})} + \dots \end{pmatrix},$$

Now all convolution integrals well-defined. Curious: the $x_{r\pm}$, $x_{l\pm}$ drop out, they may be arbitrary.

Spin offs: non-trivial solutions to NLIE of periodic chain with $L = 0$

Take $L = 0$ in

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

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

No driving term! Ansatz for solution: constants, integral equation turns into algebraic equation.

Result: $\mathfrak{a}(v) = \overline{\mathfrak{a}}(v) \equiv 1$. Simple!

Question: Is the solution unique?

No! There are solutions of the above counter-term type!

$$\mathfrak{a}(x) = \frac{x - x_c - 2\mathrm{i}}{x - x_c + 2\mathrm{i}}, \qquad \overline{\mathfrak{a}}(x) = \frac{x - x_c + 2\mathrm{i}}{x - x_c - 2\mathrm{i}}$$

with arbitrary constant x_c.

Back to the off-diagonal case

Observations:

- For small ξ the "kinks" in $\log \mathfrak{a}(x)$ are far from the origin.
- They disappear for $\xi \to 0$ (parallel boundary fields) which also enforces $\mathfrak{c} \to 0$. Then only two NLIE for two functions are left.
- 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.

  Question: Is this responsible for numerical instabilities?

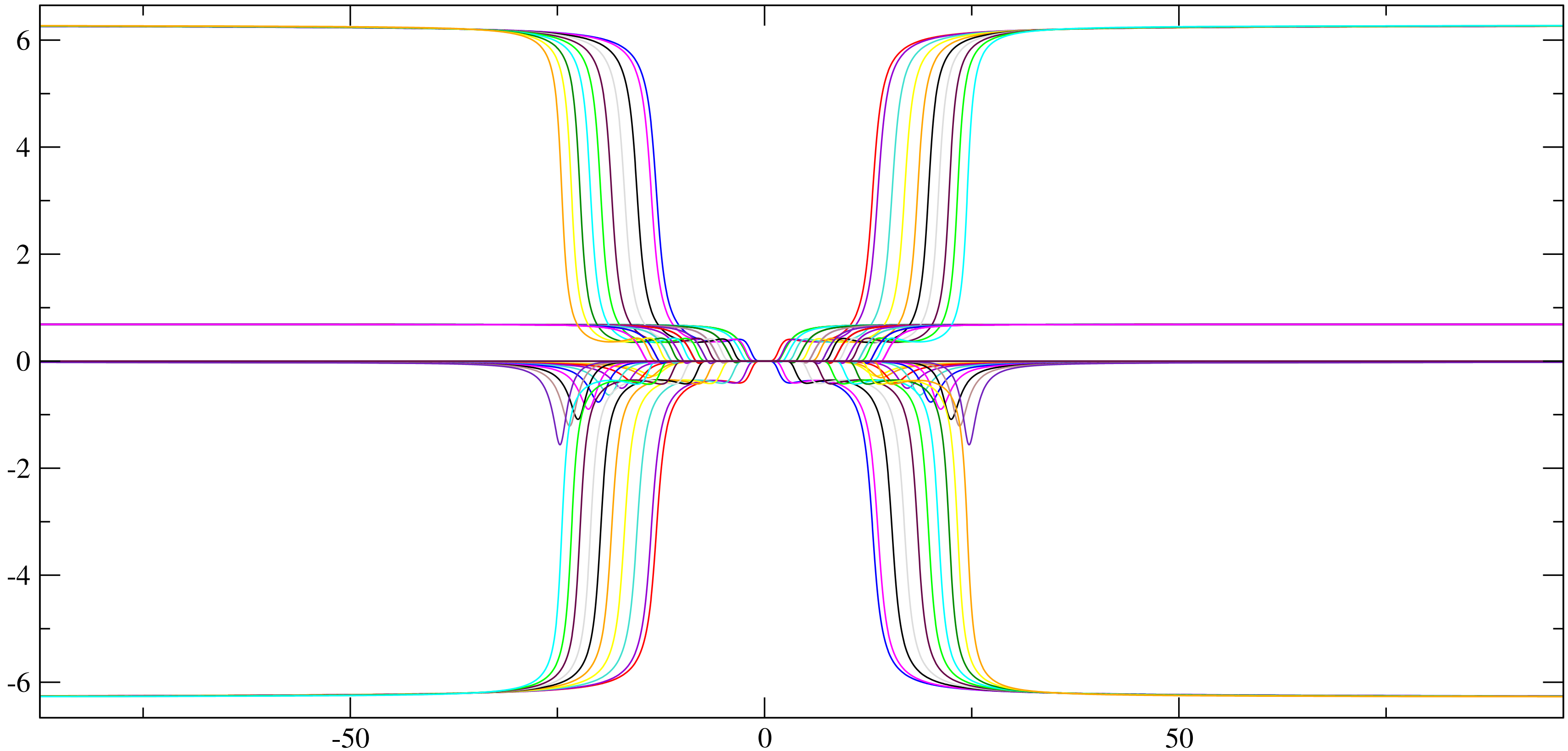
Goal of numerical calculations:

understanding the $L \to \infty$ behaviour of the kinks, of the parameter x_0 for setting up the correct scaling limit for analytical CFT calculations.

Numerical solution to NLIE: ground-state II

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.

CFT from scaling limit

Periodic boundaries

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

Consider functions in the scaling limit

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

They satisfy:

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

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

$$E_L = Le_0 - \frac{\pi}{4L}\int_{-\infty}^{\infty} \mathrm{e}^{-\frac{\pi}{2}x} \log[(1+a(x))(1+\bar{a}(x))]dv$$

How about the ODBA case? There the driving terms have exponential and algebraic behaviour!

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”