Conformal data of integrable Hamiltonians from non-linear integral equations

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- integrability: commuting families of transfer matrices, hamiltonians
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- finite size L and $T = 0$, or finite temperature T and $L = \infty$
- 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”

CFT and finite size-scaling

Why are finite size data interesting?

Central charge c and conformal weights $\Delta, \bar{\Delta}$ of the underlying CFT from ground state and low lying excitations

$$E_0 = Le_0 - \frac{\pi v}{6L} c + o(1/L)$$

$$E_x - E_0 = \frac{2\pi}{L} v(\Delta + \bar{\Delta}) + o(1/L), \quad P_x - P_0 = \frac{2\pi}{L}(\Delta - \bar{\Delta}) + o(1/L)$$

Spectral data for integrable quantum spin chains

from commuting family of transfer matrices for 2d classical models satisfying Yang-Baxter

$$T(u)T(v) = T(v)T(u), \qquad \text{for arbitrary } u, v$$

Hamiltonian as derivative

$$H = \partial_u \log T(u)$$

From now on focus on $T(v)$.

Note: Thermodynamics from Trotterization and quantum transfer matrix $T^{QTM}(v)$ vs. Yang-Yang.

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 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 $T = T_{max}$

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

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

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

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

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

$$[T_j(u), T_l(v)] = 0,$$

So-called T**-system:** (bilinear) functional relations for $j = 1, 2, 3\ldots$ AK, Pearce (1992)

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

Define

$$Y_j(v) := T_{j-1}(v) T_{j+1}(v), \qquad j = 1, 2, \ldots.$$

Y**-system:** for all $j = 1, 2, 3, \ldots$ AK, Pearce (1992)

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

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: For $Y_1(v)$ the functional equation reads

$$Y_1(v-\mathrm{i})Y_1(v+\mathrm{i}) = 1+Y_2(v) \quad \Rightarrow \quad \log Y_1(v) = L\log\tanh\frac{\pi}{4}\mathrm{v} + \mathrm{s} * \log(1+\mathrm{Y}_2)$$

where we assumed spin-1/2 in the quantum space.

Rest of functional equations turn into (simpler) integral equations

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

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

Explicit finite size corrections in terms of dilogarithm integrals

Eigenvalue of T_1 in scaling limit by use of symmetry of the kernel leads to explicit dilogarithms

$$
\begin{aligned}
2\int_{-\infty}^{\infty} dx\, \mathrm{e}^{-x}\log(1+Y_1(x)) &= \sum_{q=1}^{r-3} L\left(\frac{\sin^2\left(\frac{\pi}{r-1}\right)}{\sin^2\left(\frac{\pi}{r-1}q\right)}\right) - \sum_{q=1}^{r-3} L\left(\frac{\sin^2\left(\frac{\pi}{r}\right)}{\sin^2\left(\frac{\pi}{r}(q+1)\right)}\right) \\
&= \left(1-\frac{6}{r(r-1)}\right)\frac{\pi^2}{6}
\end{aligned}
$$

Arguments of dilogarithms are asymptotics of Y-functions. That generalizes! (Morin-Duchesne, AK, Pearce 2017)

Excited states

(1) similar equations with additional driving terms

(2) dilogarithms with non standard contours, towers from circling the singularities of the integrand.

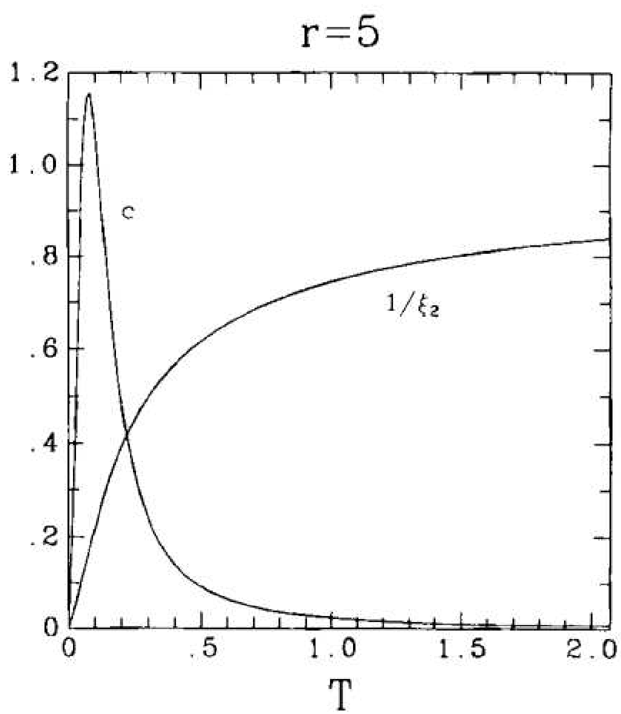
Thermodynamics of RSOS quantum chains

(1) structure of **TBA equations** known from Yang-Yang thermodynamics + Takahashi-Suzuki

(2) **algebraic approach to thermodynamics** via Trotter+QTM

(M. Suzuki 85; M. Suzuki, M. Inoue 87; T. Koma 87; J. Suzuki, Akutsu, Wadati 90; Takahashi 91; J. Suzuki, Nagao, Wadati 92; AK 92; Destri, de Vega 92...)

Specific heat ($\times 5$) and (inverse) length of the leading magnetic correlation corresponding to the conformal weight $\Delta_{2,2} = 3/80$ resp. $\Delta_{2,2} = 1/40$ and $\Delta_{3,3} = 1/15$ (AK 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.

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

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.

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

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

Finite size data from TQ relation and alternative NLIE

Periodic boundaries: Getting rid of ∞ many NLIEs

Bethe ansatz or similar yields TQ relation

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

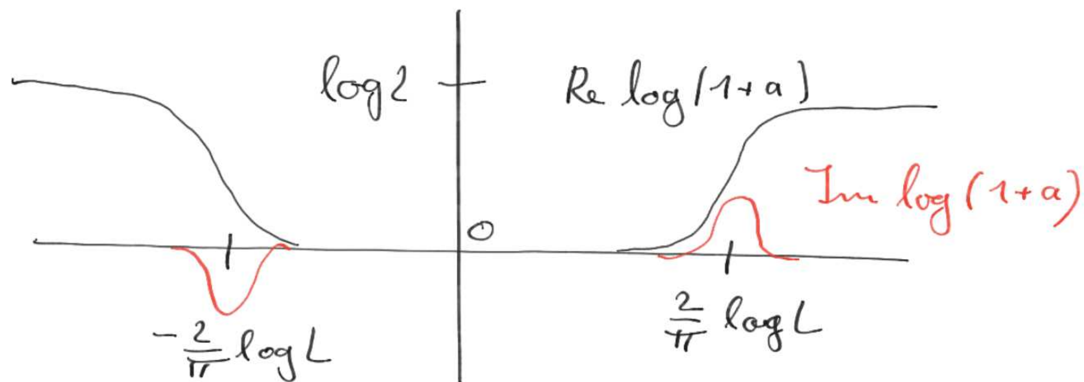
with polynomial $q(v)$ with zeros satisfying the Bethe ansatz equations.

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

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

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

$$E_L = L e_0 + \int_{-\infty}^{\infty} s' \log[(1+\mathfrak{a})(1+\overline{\mathfrak{a}})] dv$$



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

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

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

(Alternative) Inhomogeneous TQ-relation

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:

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

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...

Almost any established method yields the correct bulk $O(N)$ and boundary $O(N^0)$ terms of the ground state. **The $O(N^{-1})$ terms are unknown.**

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

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

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

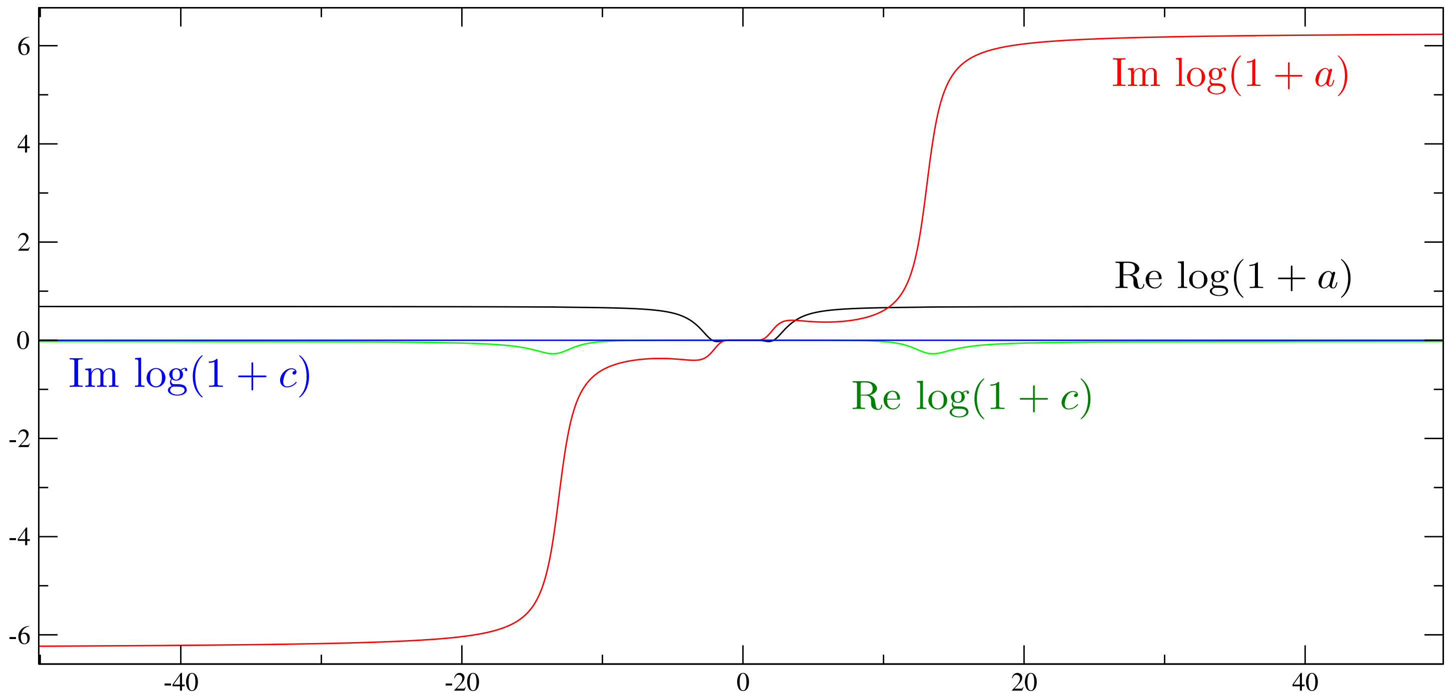
where $\gamma(.)$, $\tilde{\gamma}(.)$ and ... denote terms containing $O(1)$ expressions of type

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

Warning: auxiliary functions show windings

Numerical solution to NLIE: ground-state

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



Notice the kinks, otherwise functions are rather boring.

Small and large ξ, short and long chains

Observations:

- 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 small ξ the "kinks" in $\log \mathfrak{a}(x)$ are far from the origin.
- 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 $\frac{2}{\pi} \log N$

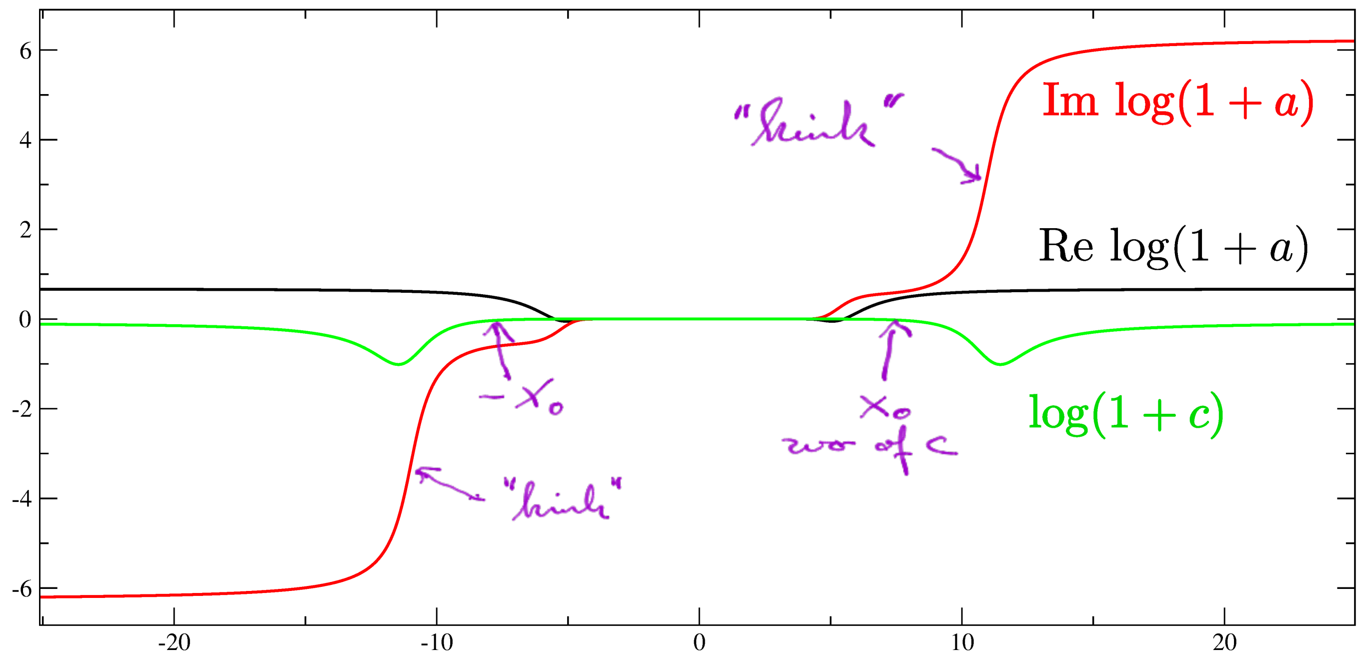
$$E_N - Ne_0 - f_s = -\frac{\pi v}{24N} \cdot \begin{cases} 1, & \text{vanishing boundary field(s)} \\ 1-6=-5, & \text{non-vanishing boundary fileds} \end{cases}$$

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

Numerical solution to NLIE: increasing N

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 $\log(1+\mathfrak{c})$

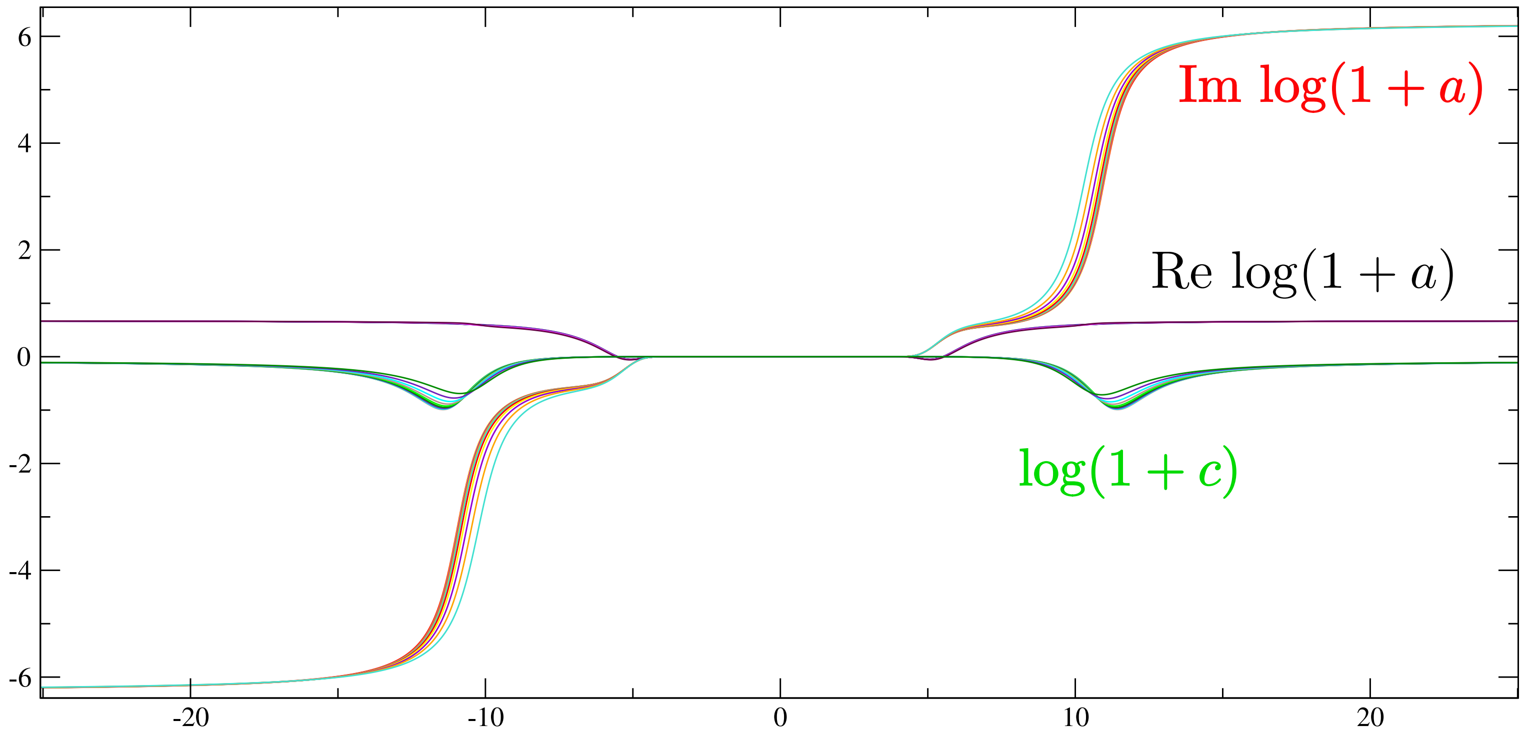


Functions are still boring. However, for increasing N the two characteristics, x_0 and kink, move out to larger arguments and closer to each other $\rightarrow$ instability.

Numerical solution to NLIE: initial transition too low

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

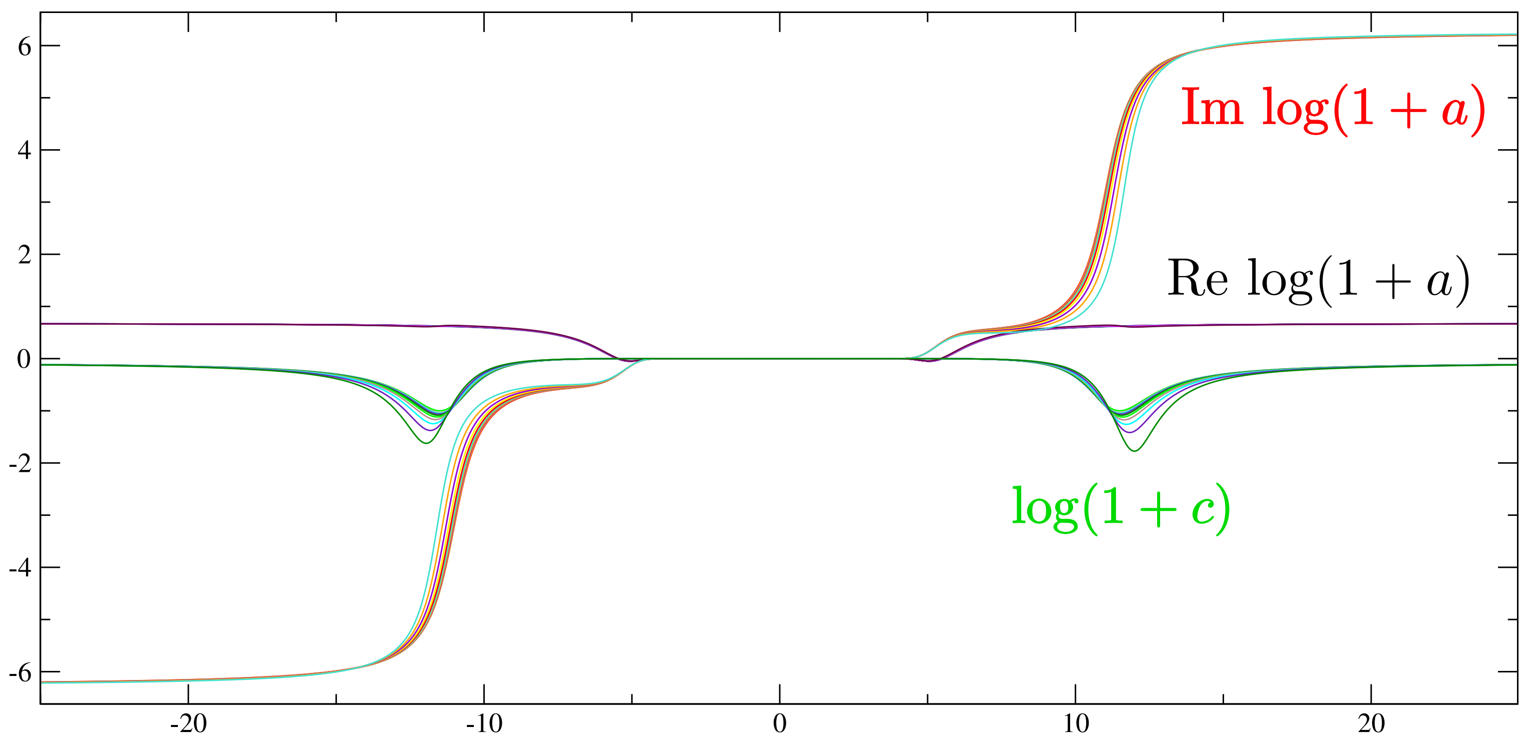
Shown are real and imaginary parts of $\log(1 + \mathfrak{a})$, and the real valued $\log(1 + \mathfrak{c})$ after every 10 steps of in total 100 iterations.



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.



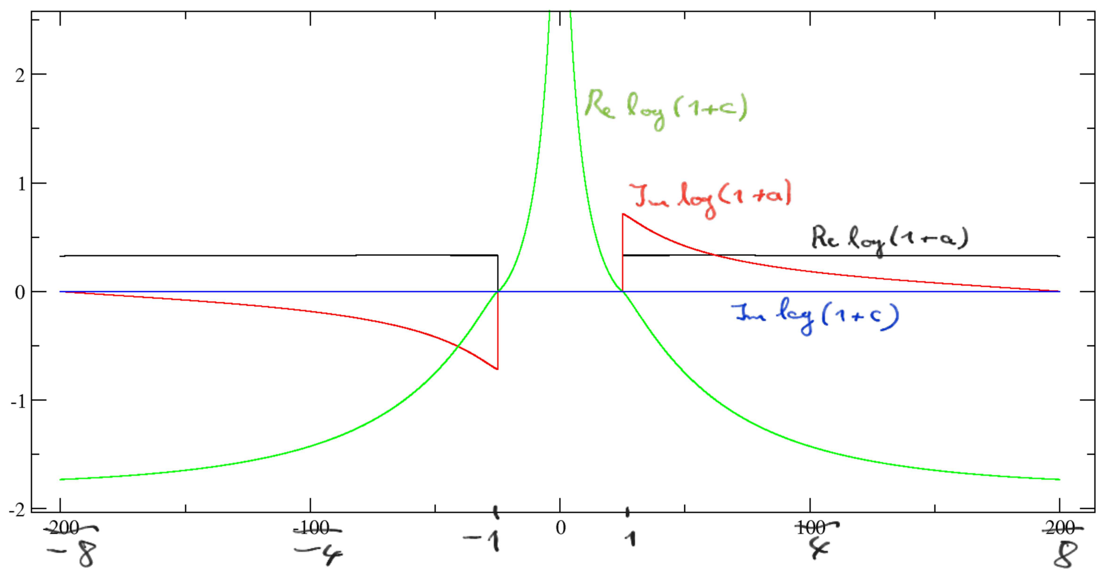
Thermodynamic limit

Positions of kinks $\leftrightarrow$ special roots. The location of the kinks must not be larger than x_0.
Parameter x_0 is of order $\frac{2}{\pi}\log N$. We impose that the kinks do not increase, i.e. are $O(N^0)$.
The scaling limit of the equations is – we rescale x and x_0 by $\frac{2}{\pi}\log N$:

$$\log a(x) = \log\tilde{a}_\infty + \frac{1}{2}\log\frac{1+a(x)}{1+\bar{a}(x)} - \frac{\mathrm{i}}{x-\mathrm{i}\varepsilon} * \log(1+c), \quad \text{for } x \notin [-1,1]; \text{ else } a(x) = 0$$

$$\log c(x) = \log\left(\tilde{c}_\infty\frac{x^2-1}{x^2}\right) + \frac{\mathrm{i}}{x+\mathrm{i}\varepsilon} * \log(1+a) - \frac{\mathrm{i}}{x-\mathrm{i}\varepsilon} * \log(1+\bar{a})$$

Iterations converge



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

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

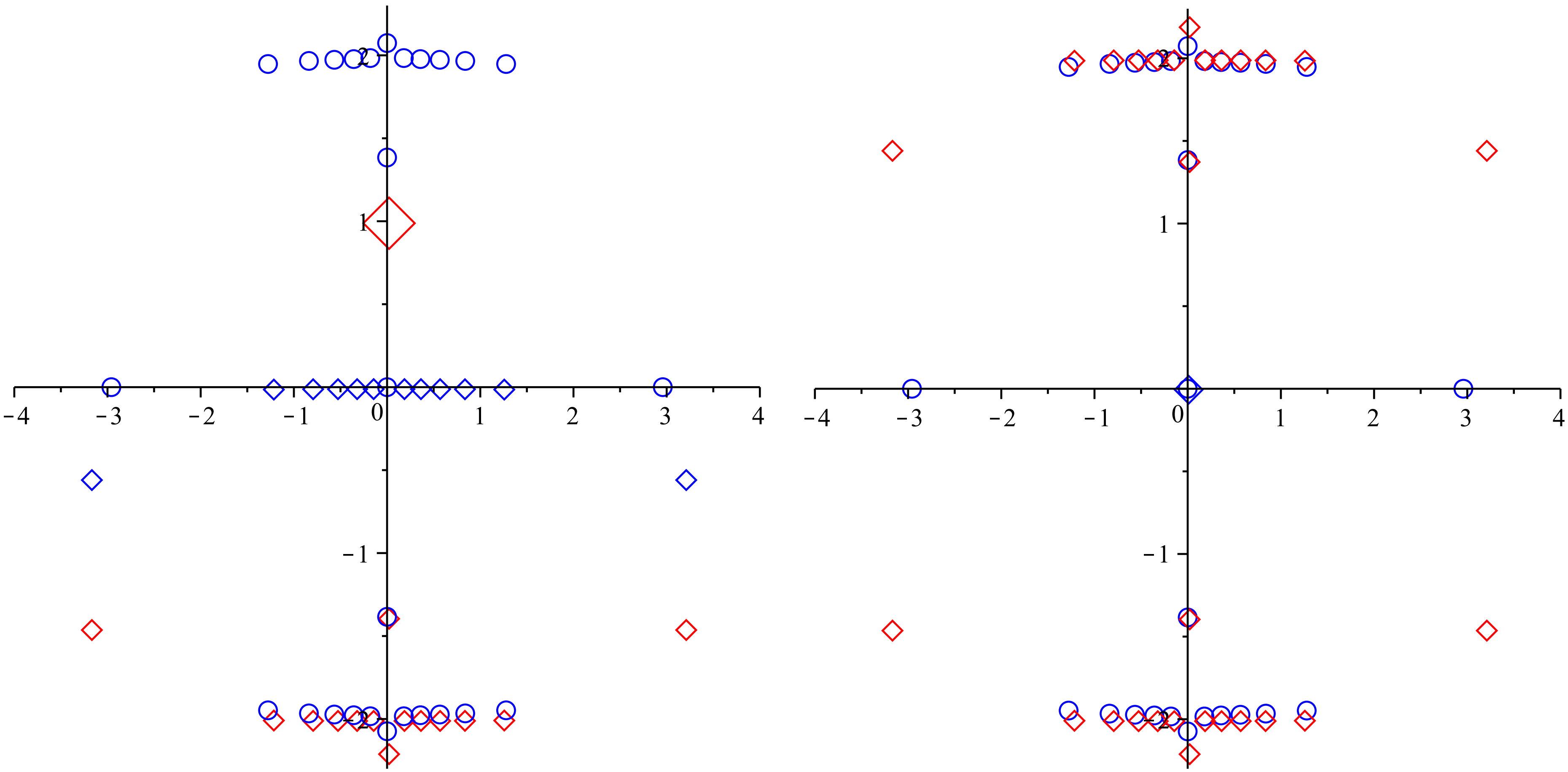
with $\phi = 2\xi$ for small ξ, and possibly for arbitrary values of ξ we have

$$\cos\phi = \frac{1-\xi^2}{1+\xi^2}$$

Location of zeros and poles for $1+(x)$ and $c(x)$

Solution for $p = -0.6, q = -0.3, \xi = 1.2$ and $N = 12$.

Shown are zeros (blue) and poles (red) of $1 + a(x)$ and $c(x)$

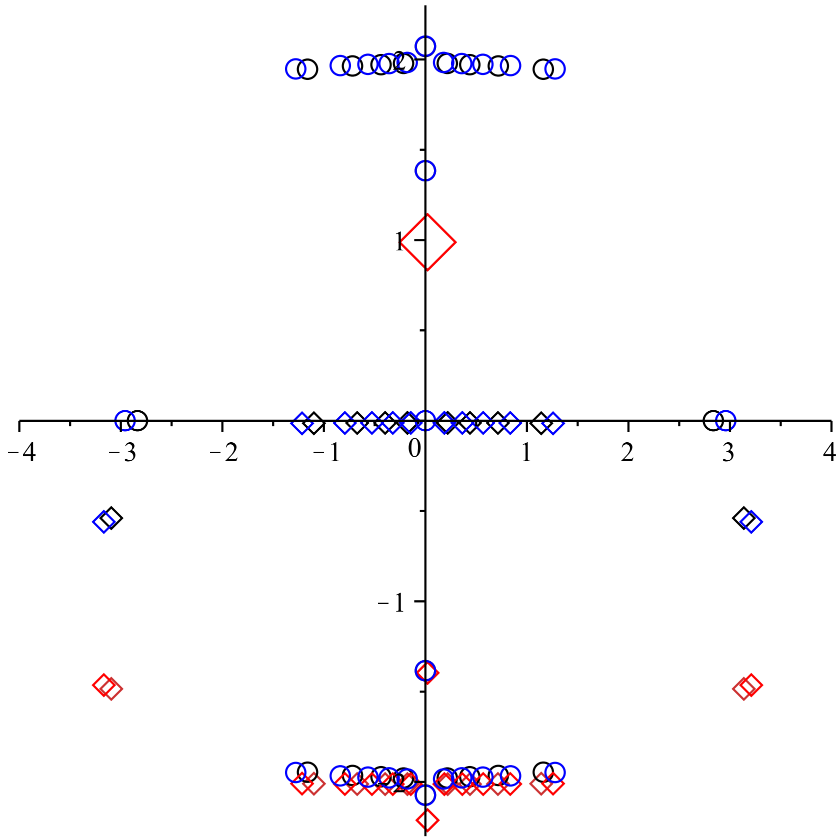


Question about the thermodynamic limit: Where do the poles go?

Location of zeros and poles for $1 + a(x)$ for $N = 10$ and 12

Solution for $p = -0.6, q = -0.3, \xi = 1.2$.

Shown are zeros (blue) and poles (red) of $1 + a(x)$ for $N = 10, 12$



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
- calculations in conjectured scaling limit work
- finite size data depend on orientation of boundary fields

To do:

- check of conjectured scaling limit
- other integrable systems exist with difficult kernels etc.:

  the $3 \times \bar{3}$ network model with $sl(2|1)$ symmetry

  strongly staggered six-vertex model