Thermal form factor expansions for the dynamical two-point functions of local operators in integrable quantum chains

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Lyon

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My timeline with Nikita – to be continued

- 1989: 'Calculation of Scalar products of the wave functions and form factors in the framework of the algebraic Bethe ansatz'

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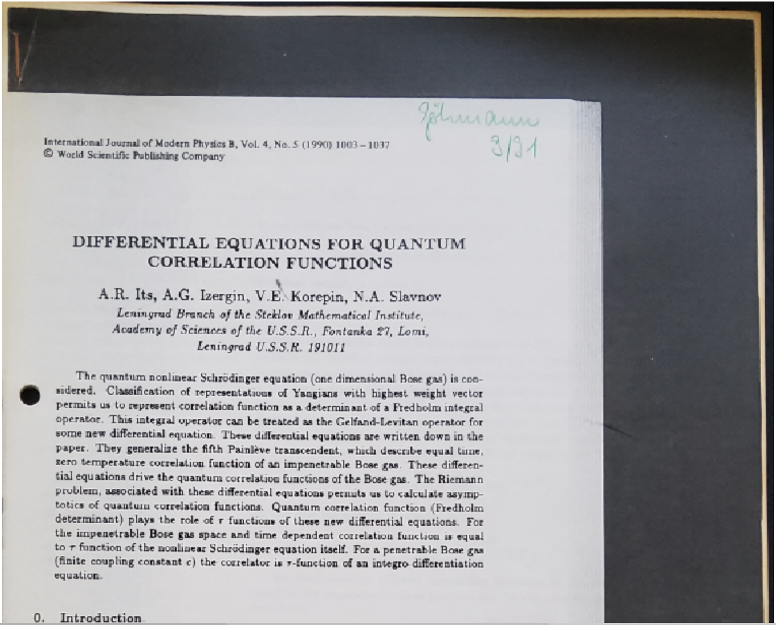

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DIFFERENTIAL EQUATIONS FOR QUANTUM CORRELATION FUNCTIONS

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The quantum nonlinear Schrödinger equation (one dimensional Bose gas) is considered. Classification of representations of Yangians with highest weight vector permits us to represent correlation function as a determinant of a Fredholm integral operator. This integral operator can be treated as the Gelfand-Levitan operator for some new differential equation. These differential equations are written down in the paper. They generalize the fifth Painlève transcendent, which describe equal time, zero temperature correlation function of an impenetrable Bose gas. These differential equations drive the quantum correlation functions of the Bose gas. The Riemann problem, associated with these differential equations permits us to calculate asymptotics of quantum correlation functions. Quantum correlation function (Fredholm determinant) plays the role of τ functions of these new differential equations. For the impenetrable Bose gas space and time dependent correlation function is equal to τ function of the nonlinear Schrödinger equation itself. For a penetrable Bose gas (finite coupling constant c) the correlator is τ-function of an integro-differentiation equation.

0. Introduction

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- 2019: 'Why scalar products in the algebraic Bethe ansatz have determinant representation'

Outline of the talk

- Introduction: Dynamical two-point functions of quantum chains
- Thermal form-factor series (TFFS) for dynamical two-point functions
- Another factorization: thermal form factors and universal amplitude
- On properly normalized thermal form factors
- TFFS for the two-point functions of the local magnetization and spin current operators of the XXZ chain in the massive antiferromagnetic regime – the low-T limit
- Summary and discussion

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- Based on J. Math. Phys. **62** (2021) 041901, Phys. Rev. Lett. **126** (2021) 210602, and SciPost Physics **12** (2022) 158; joint work with C. BABENKO, K. K. KOZLOWSKI, J. SIRKER and J. Suzuki + work in progress with K. K. Kozlowski

StatMech (of quantum chains)

- Quantum chain:

$\mathcal{H}_L = \left(\mathbb{C}^d\right)^{\otimes L}$ finite dimensional Hilbert space

$H_L \in \operatorname{End} \mathcal{H}_L$ Hamiltonian

$x_j = \mathrm{id}^{\otimes (j-1)} \otimes x \otimes \mathrm{id}^{\otimes (L-j)}, \ x \in \operatorname{End}\left(\mathbb{C}^d\right)$ local operator

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- QStatMech:

$x_j \mapsto x_j(t) = \mathrm{e}^{\mathrm{i}H_L t}\, x_j\, \mathrm{e}^{-\mathrm{i}H_L t}$ — Q: Heisenberg time evolution

$\rho_L(T)[X] = \frac{\mathrm{tr}\left\{\mathrm{e}^{-H_L/T} X\right\}}{\mathrm{tr}\left\{\mathrm{e}^{-H_L/T}\right\}}$ — StatMech: canonical density matrix

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- Linear response theory ('Kubo theory') connects the response of a large quantum system to time-($= t$)-dependent perturbations (= experiments) with dynamical correlation functions at finite temperature T

$$\langle x_1(t) y_{m+1} \rangle_T = \lim_{L\to\infty} \rho_L(T)[x_1(t) y_{m+1}]$$

Interpretation of two point functions

Meaning of dynamical correlation functions (example $x = y^\dagger$)

$$\langle y_1^\dagger(t) y_{m+1} \rangle_T = \sum_n p_n \langle y_1 \, \mathrm{e}^{-\mathrm{i}Ht} \varphi^{(n)}, \mathrm{e}^{-\mathrm{i}Ht} y_{m+1} \varphi^{(n)} \rangle$$

where (e.g.) $p_n = \mathrm{e}^{-\frac{E_n}{T}} / Z$

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- **rhs:** Create local perturbation at site $m+1$ by means of y, then time evolve it for some time t
- **lhs:** Wait for some time t, then create a local perturbation at site 1 by means of y

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- **rhs:** Create local perturbation at site $m+1$ by means of y, then time evolve it for some time t
- **lhs:** Wait for some time t, then create a local perturbation at site 1 by means of y
- $\langle \cdot, \cdot \rangle$: probability amplitude for observing a local perturbation y at site 1 and at time t, provided it was created at site $m+1$ time t ago — probability amplitude for the propagation of a perturbation

Prime example of an integrable spin chain Hamiltonian

- The XXZ model

$$H_L(\Delta) = J \sum_{j=1}^{L} \big\{ \sigma^x_{j-1}\sigma^x_j + \sigma^y_{j-1}\sigma^y_j + \Delta \sigma^z_{j-1}\sigma^z_j \big\} - \frac{h}{2} \sum_{j=1}^{L} \sigma^z_j$$

$J > 0$, $h \in \mathbb{R}$, $\Delta = \mathrm{ch}(\gamma) \in \mathbb{R}$, $q = \mathrm{e}^{-\gamma}$

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- Main goal of my research: Calculate

$$\langle \sigma_1^z(t) \sigma_{m+1}^z \rangle_T, \quad \langle \sigma_1^-(t) \sigma_{m+1}^+ \rangle_T, \quad \dots$$

explicitly for all values of m, t, T and Δ, h!

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- State of the art: Dynamical correlation functions at finite temperature not known for any Yang-Baxter integrable lattice model, except for the XX model

$$H_{XX} = H_L(0)$$

Prime example of an integrable spin chain Hamiltonian

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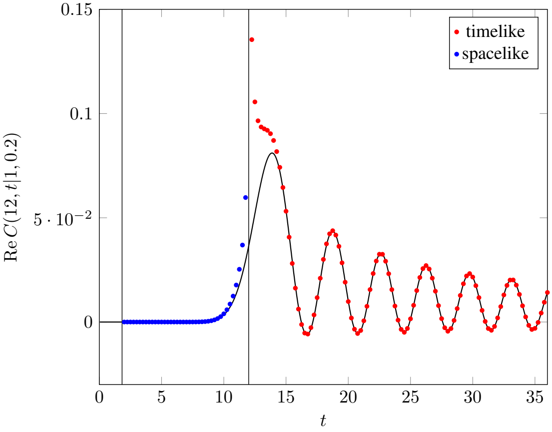
- For the XX model the longitudinal two-point functions are

$$\langle \sigma_1^z(t) \sigma_{m+1}^z \rangle_T - \langle \sigma_1^z \rangle_T^2 = \left[\int_{-\pi}^{\pi} \frac{\mathrm{d}p}{\pi} \frac{\mathrm{e}^{\mathrm{i}(mp - t\varepsilon(p))}}{1 + \mathrm{e}^{-\varepsilon(p)/T}} \right] \left[\int_{-\pi}^{\pi} \frac{\mathrm{d}p}{\pi} \frac{\mathrm{e}^{-\mathrm{i}(mp - t\varepsilon(p))}}{1 + \mathrm{e}^{\varepsilon(p)/T}} \right]$$

where $\varepsilon(p) = h - 4J\cos(p)$

Longitudinal correlation functions of XX model

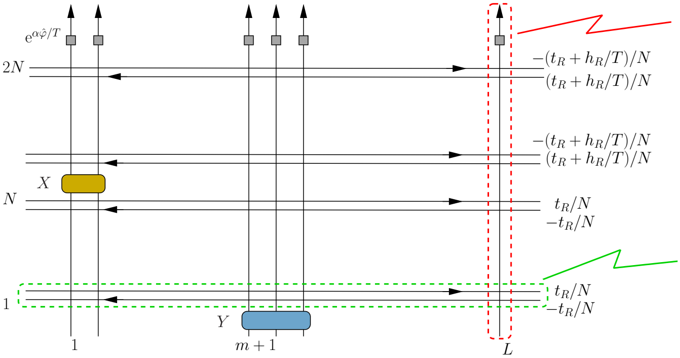
- This simple expression can be analyzed numerically and asymptotically by means of the saddle point method



Real part of the connected longitudinal two-point function of the XX chain at $m = 12$, $T = 1$, $h = 0.2$ and $J = 1/4$ as a function of time

Dynamical two-point functions as a lattice path integral

Vertex model representation at finite Trotter number N



Quantum transfer matrix

$$t(\lambda)|\Psi_n\rangle = \Lambda_n(\lambda)|\Psi_n\rangle$$

$$\rho_n(\lambda) = \frac{\Lambda_n(\lambda)}{\Lambda_0(\lambda)}$$

Double row transfer matrix

$\sim e^{-2iHt/N+\dots}$

A graphical representation of the unnormalized finite Trotter number approximant to the dynamical two-point function [SAKAI 07], h_R 'energy scale', $t_R = -ih_R t$

Double row transfer matrix versus quantum transfer matrix

DRTM

- $\overline{t_\perp}(-\lambda)t_\perp(\lambda) = e^{2\lambda H/h_R + \mathcal{O}(\lambda^2)}$ time translation
- PBCs in space direction $\rightarrow$ BAEs: $p(\lambda) = \frac{2\pi n}{L} +$ scattering
- H hermitian, real spectrum, gapped or gapless
- $\{\lambda_j\}$ Bethe roots, continuously distributed for $L \rightarrow \infty$
- For $L \rightarrow \infty$ described by linear integral equations

QTM

- $t(0)$ 'space translation'
- PBCs in time direction $\rightarrow$ BAEs: $\varepsilon(\lambda) = (2n-1)\mathrm{i}\pi T +$ scattering
- $t(0)$ non-hermitian, $\rho_n(0) = e^{-\frac{1}{\xi_n} + \mathrm{i}\varphi_n}$, correlation length and phase
- $\{\lambda_j\}$ Bethe roots, continuously distributed only for $T \rightarrow 0$, at every finite T, a set with a single accumulation point
- Described by non-linear integral equations

Form factor series expansion in the thermodynamic limit

- Sets of consecutive integers are denoted $[\![j,k]\!]$, where $j,k \in \mathbb{Z}$, $j \le k$. We consider dynamical correlation functions of two local operators

$$X_{[\![1,\ell]\!]} = x_1^{(1)} \cdots x_\ell^{(\ell)} , \quad Y_{[\![1,r]\!]} = y_1^{(1)} \cdots y_r^{(r)}$$

where $x^{(j)}, y^{(k)} \in \operatorname{End} \mathbb{C}^d$. ℓ and r are lengths of X and Y. We shall assume that these operators have fixed $U(1)$ charge (or 'spin') $s \in \mathbb{C}$,

$$[\hat{\Phi}, X_{[\![1,\ell]\!]}] = s(X) X_{[\![1,\ell]\!]} , \quad [\hat{\Phi}, Y_{[\![1,r]\!]}] = s(Y) Y_{[\![1,r]\!]}$$

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Theorem (GK)

$$\big\langle X_{[\![1,\ell]\!]}(t) Y_{[\![1+m,r+m]\!]} \big\rangle_T = \mathrm{e}^{-\mathrm{i}ht\,s(X)}$$

$$\times \lim_{N\to\infty} \sum_n \frac{\langle \Psi_0 | \prod^{\curvearrowright}_{k\in[\![1,\ell]\!]} \mathrm{tr}\{x^{(k)} T(0)\} | \Psi_n \rangle}{\langle \Psi_0 | \Psi_0 \rangle \Lambda_n^\ell(0)} \frac{\langle \Psi_n | \prod^{\curvearrowright}_{k\in[\![1,r]\!]} \mathrm{tr}\{y^{(k)} T(0)\} | \Psi_0 \rangle}{\langle \Psi_n | \Psi_n \rangle \Lambda_0^r(0)}$$

$$\times \rho_n(0)^m \left(\frac{\rho_n\big(\frac{t_R}{N}\big)}{\rho_n\big(-\frac{t_R}{N}\big)} \right)^{\frac{N}{2}}$$

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proper normalization?

$$\times \rho_n(0)^m \left(\frac{\rho_n\left(\frac{t_R}{N}\right)}{\rho_n\left(-\frac{t_R}{N}\right)} \right)^{\frac{N}{2}}$$

Properly normalized thermal form factors for spin-zero operators in XXZ

- In order to have good properties of the thermal form factors, we rather would like to divide by $\langle\Psi_0(h)|\Psi_n(h)\rangle\langle\Psi_n(h)|\Psi_0(h)\rangle$. But $\langle\Psi_0(h)|\Psi_n(h)\rangle = \langle\Psi_n(h)|\Psi_0(h)\rangle = 0$ for $n \neq 0$

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- Way out: different magnetic fields,

$$\langle \Psi_0(h)|\Psi_n(h)\rangle\langle \Psi_n(h)|\Psi_0(h)\rangle \to \langle \Psi_0(h)|\Psi_n(h')\rangle\langle \Psi_n(h')|\Psi_0(h)\rangle$$

  which is generally non-zero if $|\Psi_n(h')\rangle$ has pseudo-spin zero

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- This leads us to define the amplitude and twisted eigenvalue ratio

$$A_n(h,h') = \frac{\langle\Psi_0(h)|\Psi_n(h')\rangle\langle\Psi_n(h')|\Psi_0(h)\rangle}{\langle\Psi_0(h)|\Psi_0(h)\rangle\langle\Psi_n(h')|\Psi_n(h')\rangle}, \qquad \rho_n(\lambda|h,h') = \frac{\Lambda_n(\lambda|h')}{\Lambda_0(\lambda|h)}$$

  as well as the properly normalized form factors

$$\mathcal{F}^{(-)}_{n;\ell}(\xi_1,\dots,\xi_\ell|h,h') = \frac{\langle\Psi_0(h)|T(\xi_1|h')\otimes\cdots\otimes T(\xi_\ell|h')|\Psi_n(h')\rangle}{\langle\Psi_0(h)|\Psi_n(h')\rangle\prod_{j=1}^{\ell}\Lambda_n(\xi_j|h')}$$

$$\mathcal{F}^{(+)}_{n;r}(\zeta_1,\dots,\zeta_r|h,h') = \frac{\langle\Psi_n(h')|T(\zeta_1|h)\otimes\cdots\otimes T(\zeta_r|h)|\Psi_0(h)\rangle}{\langle\Psi_n(h')|\Psi_0(h)\rangle\prod_{j=1}^{r}\Lambda_0(\zeta_j|h)}$$

Dynamical correlation functions of elementary blocks of spin-zero operators

Corollary

Using these functions the two-point functions of spin-zero elementary blocks can be written as

$$
\begin{aligned}
&\Big\langle \big(e_1{}^{\alpha_1}_{\beta_1} \dots e_\ell{}^{\alpha_\ell}_{\beta_\ell} \big)(t)\, e_{1+m}{}^{\gamma_1}_{\delta_1} \dots e_{r+m}{}^{\gamma_r}_{\delta_r} \Big\rangle_T = \\
&\qquad \lim_{N\to\infty} \lim_{\xi_j, \zeta_k \to 0} \lim_{h' \to h} \sum_n A_n(h,h') \rho_n(0|h,h')^m \left(\frac{\rho_n\big(-\frac{\mathrm{i}t}{\kappa N}\big|h,h'\big)}{\rho_n\big(\frac{\mathrm{i}t}{\kappa N}\big|h,h'\big)} \right)^{\frac{N}{2}} \\
&\qquad\qquad \times \mathcal{F}^{(-)}_{n;\ell}{}^{\alpha_1 \dots \alpha_\ell}_{\beta_1 \dots \beta_\ell}(\xi_1, \dots, \xi_\ell|h,h')\, \mathcal{F}^{(+)}_{n;r}{}^{\gamma_1 \dots \gamma_r}_{\delta_1 \dots \delta_r}(\zeta_1, \dots, \zeta_r|h,h')
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$$\lim_{N \to \infty} \lim_{\xi_j, \zeta_k \to 0} \lim_{h' \to h} \sum_n A_n(h,h') \rho_n(0|h,h')^m \left(\frac{\rho_n\big(-\frac{\mathrm{i}t}{\kappa N}\big|h,h'\big)}{\rho_n\big(\frac{\mathrm{i}t}{\kappa N}\big|h,h'\big)} \right)^{\frac{N}{2}}$$

$$\times \mathcal{F}^{(-)}_{n;\ell}{}^{\alpha_1 \dots \alpha_\ell}_{\beta_1 \dots \beta_\ell}(\xi_1, \dots, \xi_\ell|h,h')\, \mathcal{F}^{(+)}_{n;r}{}^{\gamma_1 \dots \gamma_r}_{\delta_1 \dots \delta_r}(\zeta_1, \dots, \zeta_r|h,h')$$

For $n = 0$ the thermal form factors reduce to the generalized reduced density matrix

$$\mathcal{D}_m(\xi_1, \dots, \xi_m|h,h') = \mathcal{F}^{(-)}_{0;m}(\xi_1, \dots, \xi_m|h,h') = \mathcal{F}^{(+)}_{0;m}(\xi_1, \dots, \xi_m|h',h)$$

studied intensively in the literature by means of the algebraic Bethe ansatz [BG09] and by 'the Fermionic basis approach' [BJMST05,BJMST07,BJMST09,BJMS09,JMS09]

General σ-staggered inhomogeneous monodromy matrix

- The σ-staggered monodromy matrix: Fix $M \in \mathbb{N}$. For $j \in [\![0, M]\!]$ let $V_j = \mathbb{C}^d$. For $j \in [\![1, M]\!]$ fix $\sigma_j \in \{-1, 1\}$, $\nu_j \in \mathbb{C}$. Let $\sigma = (\sigma_1, \dots, \sigma_M)$, $\nu = (\nu_1, \dots, \nu_M)$ and

$$R_{0,j}^{(\sigma_j)}(\lambda, \nu_j) = \begin{cases} R_{0,j}(\lambda, \nu_j) & \text{if } \sigma_j = 1 \\ R_{j,0}^{t_1}(\nu_j, \lambda) & \text{if } \sigma_j = -1, \end{cases}$$

where t_1 denotes the transposition with respect to the first space R is acting on. By definition the σ-staggered monodromy matrix $T_0(\lambda|\sigma, \nu, h) \in \mathrm{End}\left(\bigotimes_{j=0}^M V_j\right)$ is

$$T_0(\lambda|\sigma, \nu, h) = \theta_0(h/T) \overset{\curvearrowleft}{\prod_{j \in [\![1, M]\!]}} R_{0,j}^{(\sigma_j)}(\lambda, \nu_j)$$

Here $\theta(\kappa) = \mathrm{e}^{\kappa \sigma^z/2}$, and the arrow above the product indicates descending order

General σ-staggered inhomogeneous monodromy matrix

- The σ-staggered monodromy matrix: Fix $M \in \mathbb{N}$. For $j \in [\![0, M]\!]$ let $V_j = \mathbb{C}^d$. For $j \in [\![1, M]\!]$ fix $\sigma_j \in \{-1, 1\}$, $\nu_j \in \mathbb{C}$. Let $\sigma = (\sigma_1, \dots, \sigma_M)$, $\nu = (\nu_1, \dots, \nu_M)$ and

$$R_{0,j}^{(\sigma_j)}(\lambda, \nu_j) = \begin{cases} R_{0,j}(\lambda, \nu_j) & \text{if } \sigma_j = 1 \\ R_{j,0}^{t_1}(\nu_j, \lambda) & \text{if } \sigma_j = -1, \end{cases}$$

where t_1 denotes the transposition with respect to the first space R is acting on. By definition the σ-staggered monodromy matrix $T_0(\lambda|\sigma, \nu, h) \in \mathrm{End}\left(\bigotimes_{j=0}^{M} V_j\right)$ is

$$T_0(\lambda|\sigma, \nu, h) = \theta_0(h/T) \overset{\curvearrowleft}{\prod_{j \in [\![1, M]\!]}} R_{0,j}^{(\sigma_j)}(\lambda, \nu_j)$$

Here $\theta(\kappa) = \mathrm{e}^{\kappa \sigma^z/2}$, and the arrow above the product indicates descending order

- Corresponding form factors (this is now what we love)

$$\mathcal{F}_{n;m}^{(-)}(\xi|\sigma, \nu, h, h') = \frac{\langle \Psi_0(\sigma, \nu, h)| T(\xi_1|\sigma, \nu, h') \otimes \cdots \otimes T(\xi_m|\sigma, \nu, h') |\Psi_n(\sigma, \nu, h')\rangle}{\langle \Psi_0(\sigma, \nu, h)|\Psi_n(\sigma, \nu, h')\rangle \prod_{j=1}^{m} \Lambda_n(\xi_j|\sigma, \nu, h')}$$

$$\mathcal{F}_{n;m}^{(+)}(\xi|\sigma, \nu, h, h') = \frac{\langle \Psi_n(\sigma, \nu, h')| T(\xi_1|\sigma, \nu, h) \otimes \cdots \otimes T(\xi_m|\sigma, \nu, h) |\Psi_0(\sigma, \nu, h)\rangle}{\langle \Psi_n(\sigma, \nu, h')|\Psi_0(\sigma, \nu, h)\rangle \prod_{j=1}^{m} \Lambda_0(\xi_j|\sigma, \nu, h)}$$

Properties of the thermal form factors of spin-zero operators

Define $\rho_n(\lambda|\sigma,\nu,h,h') = \Lambda_n(\lambda|\sigma,\nu,h')/\Lambda_0(\lambda|\sigma,\nu,h)$, $\alpha = (h-h')/2\gamma T$

Lemma

1. *Normalization condition*

$$\mathrm{tr}_{1,\dots,m}\{\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h')\} = 1$$

2. *Reduction relations*

$$\mathrm{tr}_m\{\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h')\} = \mathcal{F}^{(\pm)}_{n;m-1}((\xi_1,\dots,\xi_{m-1})|\sigma,\nu,h,h'),$$

$$\mathrm{tr}_1\{q^{\pm\alpha\sigma_1^z}\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h')\} = \rho_n^{\pm 1}(\xi_1|\sigma,\nu,h,h')\,\mathcal{F}^{(\pm)}_{n;m-1}((\xi_2,\dots,\xi_m)|\sigma,\nu,h,h')$$

3. *Exchange relation. Let $\check{R} = PR$. Then*

$$\check{R}_{j,j+1}(\xi_j,\xi_{j+1})\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h') = \mathcal{F}^{(\pm)}_{n;m}(\xi\Pi_{j,j+1}|\sigma,\nu,h,h')\check{R}_{j,j+1}(\xi_j,\xi_{j+1})$$

for $j \in [\![1, m-1]\!]$

4. *$U(1)$ symmetry. For any $\kappa \in \mathbb{C}$*

$$\big[\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h'),\, (\theta(\kappa))^{\otimes m}\big] = 0$$

Properly normalized thermal form factors for spin-zero operators in XXZ

Lemma

5. *Row reflection ('crossing')*

$$\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h') = \mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma\iota_j,\nu S_j,h,h')$$

for all $j \in [\![1,M]\!]$

6. *Commutativity of rows*

$$\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h') = \mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma P,\nu P,h,h')$$

for all $P \in \mathfrak{S}^M$

7. *Transposition property*

$$\mathcal{F}^{(-)}_{n;m}{}^{\alpha_1,\dots,\alpha_m}_{\beta_1,\dots,\beta_m}(\xi|\sigma,\nu,h,h') = \Big[\prod_{j=1}^m \rho_n^{-1}(\xi_j|\sigma,\nu,h,h')\Big] \times \big((q^{\alpha\sigma_z})^{\otimes m}\mathcal{F}^{(+)}_{n;m}\big)^{\beta_m,\dots,\beta_1}_{\alpha_m,\dots,\alpha_1}((\xi_m,\dots,\xi_1)|\sigma,\nu,h,h')$$

Properly normalized thermal form factors for spin-zero operators in XXZ

Lemma

8. *The functions* $\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma,\nu,h,h')$ *are meromorphic in all* ξ_j, $j \in [\![1,m]\!]$
9. *Asymptotic behaviour*

$$\lim_{\mathrm{Im}\,\xi_m \to \pm\infty} \mathcal{F}^{(+)}_{n;m}(\xi|\sigma,\nu,h,h') = \mathcal{F}^{(+)}_{n;m-1}((\xi_1,\dots,\xi_{m-1})|\sigma,\nu,h,h') \frac{\theta_m\big(\frac{h}{T}\big)}{\mathrm{tr}\big\{\theta\big(\frac{h}{T}\big)\big\}}$$

$$\lim_{\mathrm{Im}\,\xi_m \to \pm\infty} \mathcal{F}^{(-)}_{n;m}(\xi|\sigma,\nu,h,h') = \mathcal{F}^{(-)}_{n;m-1}((\xi_1,\dots,\xi_{m-1})|\sigma,\nu,h,h') \frac{\theta_m\big(\frac{h'}{T}\big)}{\mathrm{tr}\big\{\theta\big(\frac{h'}{T}\big)\big\}}$$

10. *Discrete form of the reduced q-Knizhnik-Zamolodchikov equation [AK12]. The functions* $\mathcal{F}^{(\pm)}_{n;m}$ *satisfy the 'discrete functional equations'*

$$\mathcal{F}^{(\pm)}_{n;m}\big((\xi_1,\dots,\xi_{m-1},\xi_m - \mathrm{i}\gamma)\big|\sigma_-,\nu,h,h'\big) = \rho_n^{\mp 1}(\xi_m|\sigma_-,\nu,h,h')$$

$$\times\, \mathrm{tr}_0\Big\{ T^{-1}_{\perp,0;m}(\xi_m|\xi,h)\mathcal{F}^{(\pm)}_{n;m}(\xi|\sigma_-,\nu,h,h')\sigma_0^y P_{0,m}\sigma_0^y T_{\perp,0;m}(\xi_m|\xi,h')\Big\}$$

if $\xi_m = \nu_1$

Calculating the form factors

- The thermal form factors can be calculated from their properties or by the algebraic Bethe Ansatz (using Nikita's scalar product formula)

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- The thermal form factor of the magnetization operator follow from the reduction relations

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$$\mathrm{tr}\left\{\tfrac{1}{2}\sigma^z \mathcal{F}_{n;1}^{(-)}(\xi|h,h')\right\} = \frac{\frac{1}{2}(q^\alpha + q^{-\alpha}) - 1/\rho_n(\xi|h,h')}{q^\alpha - q^{-\alpha}}$$

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- This allows us to conclude that

$$\lim_{\xi,\zeta\to 0}\lim_{h'\to h} A_n(h,h')\,\mathrm{tr}\left\{\sigma^z\,\mathcal{F}^{(-)}_{n;1}(\xi|h,h')\right\}\mathrm{tr}\left\{\sigma^z\,\mathcal{F}^{(+)}_{n;1}(\zeta|h,h')\right\}$$

$$= 2T^2\left(\partial^2_{h'}A_n(h,h')\right)\Big|_{h'=h}\Big(\rho_n(0|h,h) - 2 + 1/\rho_n(0|h,h)\Big)$$

Calculating the form factors

- The form factors of the magnetic current operator

$$\mathcal{J} = -2\mathrm{i}J\big(\sigma^- \otimes \sigma^+ - \sigma^+ \otimes \sigma^-\big)$$

follow by means of the reduction relation and the exchange relation

$$\lim_{\zeta_2 \to \zeta_1} \mathrm{tr}\big\{\mathrm{i}(\sigma_1^- \sigma_2^+ - \sigma_1^+ \sigma_2^-)\mathcal{F}^{(+)}_{n;2}(\zeta_1, \zeta_2 | h, h')\big\} \sim -\frac{\mathrm{sh}(\gamma)\rho_n'(\zeta_1|h,h)}{q^\alpha - q^{-\alpha}}$$

$$\lim_{\xi_2 \to \xi_1} \mathrm{tr}\big\{\mathrm{i}(\sigma_1^- \sigma_2^+ - \sigma_1^+ \sigma_2^-)\mathcal{F}^{(-)}_{n;2}(\xi_1, \xi_2 | h, h')\big\} \sim \frac{\mathrm{sh}(\gamma)\partial_{\xi_1} 1/\rho_n(\xi_1|h,h)}{q^\alpha - q^{-\alpha}}$$

- Leading (for $n \neq 0$) to

$$\lim_{h' \to h} \lim_{\xi_j, \zeta_k \to 0} A_n(h, h')$$

$$\times\, \mathrm{tr}\big\{\mathrm{i}(\sigma_1^- \sigma_2^+ - \sigma_1^+ \sigma_2^-)\mathcal{F}^{(-)}_{n;2}(\xi_1, \xi_2 | h, h')\big\}\, \mathrm{tr}\big\{\mathrm{i}(\sigma_1^- \sigma_2^+ - \sigma_1^+ \sigma_2^-)\mathcal{F}^{(+)}_{n;2}(\zeta_1, \zeta_2 | h, h')\big\}$$

$$= \frac{\mathrm{sh}^2(\gamma) T^2}{2} \big(\partial^2_{h'} A_n(h, h')\big)\big|_{h'=h} \left(\frac{\rho_n'(0|h,h)}{\rho_n(0|h,h)}\right)^2$$

Calculating the form factors – nonlinear integral equations

Two functions, the bare energy

$$\varepsilon_0(\lambda) = h - \frac{4J(\Delta^2 - 1)}{\Delta - \cos(2\lambda)}$$

and the kernel function

$$K(\lambda) = \mathrm{ctg}\,(\lambda - \mathrm{i}\gamma) - \mathrm{ctg}\,(\lambda + \mathrm{i}\gamma)$$

are needed in the definition of the non-linear integral equation

$$\ln \mathfrak{a}_n(\lambda|h) = -\frac{\varepsilon_0(\lambda - \mathrm{i}\gamma/2)}{T} + \int_{\mathcal{C}_n} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} K(\lambda - \mu) \ln_{\mathcal{C}_n}(1 + \mathfrak{a}_n)(\mu|h)$$

The simple closed contours $\mathcal{C}_n$ are such that $0 \in \mathrm{Int}\,\mathcal{C}_n$, $\lambda \pm \mathrm{i}\gamma \in \mathrm{Ext}\,\mathcal{C}_n$ if $\lambda \in \mathrm{Int}\,\mathcal{C}_n$ and

$$\int_{\mathcal{C}_n} \mathrm{d}\lambda\, \frac{\mathfrak{a}_n'(\lambda|h)}{1 + \mathfrak{a}_n(\lambda|h)} = 0$$

The function $\ln_{\mathcal{C}_n}(1 + \mathfrak{a}_n)$ is the logarithm along the contour $\mathcal{C}_n$

Calculating the form factors – linear integral equations

Functions $G_n^{(\pm)}$ are defined as the solutions of the linear integral equations

$$G_n^{(\pm)}(\lambda,\xi) = q^{\mp\alpha}\,\mathrm{ctg}\,(\lambda-\xi+\mathrm{i}\gamma) - \rho_n^{\pm 1}(\xi|h,h')\,\mathrm{ctg}\,(\lambda-\xi) \\ - \int_{\mathcal{C}_n^{(\pm)}} \mathrm{d}m_n^{(\pm)}(\mu)\, K_{\mp\alpha}(\lambda-\mu) G_n^{(\pm)}(\mu,\xi)$$

Here $\xi \in \mathrm{Int}\,\mathcal{C}_n^{(\pm)}$,

$$K_\alpha(\lambda) = q^{-\alpha}\,\mathrm{ctg}\,(\lambda-\mathrm{i}\gamma) - q^{\alpha}\,\mathrm{ctg}\,(\lambda+\mathrm{i}\gamma)$$

is a deformed version of the kernel function, and the integration 'measures' are

$$\mathrm{d}m_n^{(+)}(\lambda) = \frac{\mathrm{d}\lambda}{2\pi\mathrm{i}\rho_n(\lambda|h,h')\big(1+\mathfrak{a}_0(\lambda|h)\big)}\,, \quad \mathrm{d}m_n^{(-)}(\lambda) = \frac{\mathrm{d}\lambda\,\rho_n(\lambda|h,h')}{2\pi\mathrm{i}\big(1+\mathfrak{a}_n(\lambda|h')\big)}$$

The contours $\mathcal{C}_n^{(\pm)}$ are deformations of the contour $\mathcal{C}_n$ in such a way that the zeros of $\rho_n(\cdot|h,h')$ are excluded from $\mathcal{C}_n$ for $\mathcal{C}_n^{(+)}$, while the poles of $\rho_n(\cdot|h,h')$ are excluded from $\mathcal{C}_n$ for $\mathcal{C}_n^{(-)}$.

In preparation of the following lemma we finally introduce the short-hand notations

$$\mathrm{d}\overline{m}_n^{(+)}(\lambda) = \mathfrak{a}_0(\lambda|h)\mathrm{d}m_n^{(+)}(\lambda)\,, \quad \mathrm{d}\overline{m}_n^{(-)}(\lambda) = \mathfrak{a}_n(\lambda|h')\mathrm{d}m_n^{(-)}$$

Calculating the form factors – multiple integral representation

Lemma

For all $\xi_j \in \operatorname{Int} \mathcal{C}_n^{(\pm)}$, $j = 1, \dots, m$, *the form factors* $\mathcal{F}_{n,m}^{(\pm)}(\xi|h,h')$ *of spin-zero operators have the multiple-integral representations*

$$\mathcal{F}^{(\pm)\,\alpha_1\dots\alpha_m}_{n;m\,\beta_1\dots\beta_m}(\xi|h,h') = \left[\prod_{j=1}^{p} \int_{\mathcal{C}_n^{(\pm)}} \mathrm{d}m_n^{(\pm)}(\lambda_j)\, F_{x_j}^{+}(\lambda_j)\right] \left[\prod_{j=p+1}^{m} \int_{\mathcal{C}_n^{(\pm)}} \mathrm{d}\overline{m}_n^{(\pm)}(\lambda_j)\, F_{x_j}^{-}(\lambda_j)\right] \times \frac{\det_m\{-G_n^{(\pm)}(\lambda_j,\xi_k)\}}{\prod_{1\le j<k\le m} \sin(\lambda_j-\lambda_k+\mathrm{i}\gamma)\sin(\xi_k-\xi_j)}$$

where

$$F_x^{\pm}(\lambda) = \left[\prod_{k=1}^{x-1} \sin(\lambda-\xi_k)\right]\left[\prod_{k=x+1}^{m} \sin(\lambda-\xi_k\pm\mathrm{i}\gamma)\right]$$

and where the sequence $(x_j)_{j=1}^m$ *is defined as*

$$x_j = \begin{cases} \varepsilon_j^+ & j=1,\dots,p \\ \varepsilon_{m-j+1}^- & j=p+1,\dots,m \end{cases}$$

with ε_j^+ *being the position of the* j*th plus in the sequence* $(\beta_j)_{j=1}^m$, ε_j^- *the position of the* j*th minus in the sequence* $(\alpha_j)_{j=1}^m$

Calculating the form factors – factorization

- The double integrals can be factorized and reduce to a linear combination of functions $\omega_n^{(\pm)}(\xi_1, \xi_2|h, h')$ represented by a single integral and the functions $\rho_n^{\pm 1}(\xi|h, h')$. The technique developed for the density matrix [BG09] works in this case as well

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- Conjecture: The thermal form factors $\mathcal{F}^{(\pm)}{}_{n;m}{}^{\alpha_1\dots\alpha_m}_{\beta_1\dots\beta_m}(\xi|h,h')$ factorize in precisely the same way as the corresponding elements of the reduced density matrix: they are polynomials in the derivatives of $\omega_n^{(\pm)}(\xi_1,\xi_2|h,h')$ and $\rho_n^{\pm 1}(\xi|h,h')$ with respect to the spectral parameters at zero, with coefficients that are determined by the Fermionic basis [BJMST09,BJMS09,JMS09]

Explicit form factor series for $T=0$, $\Delta>1$, $|h|<h_\ell=4J\,\mathrm{sh}(\gamma)\vartheta_4^2(0|q)$

The dynamical two-point functions (of spin-zero operators) of the XXZ chain in the antiferromagnetic massive regime at $T=0$ have the form-factor series representation

$$\big\langle X_{[\![1,l]\!]}(t)\,Y_{[\![1+m,r+m]\!]}\big\rangle = \sum_{\substack{\ell\in\mathbb{N}\\ k=0,1}} \frac{(-1)^{km}}{(\ell!)^2}\int_{\mathcal{C}_h^\ell}\frac{\mathrm{d}^\ell u}{(2\pi)^\ell}\int_{\mathcal{C}_p^\ell}\frac{\mathrm{d}^\ell v}{(2\pi)^\ell}\,\mathcal{A}_{XY}^{(2\ell)}(\mathcal{U},\mathcal{V}|k)\,\mathrm{e}^{-\mathrm{i}\sum_{\lambda\in\mathcal{U}\ominus\mathcal{V}}(mp(\lambda)-t\varepsilon(\lambda))}$$

with integration contours $\mathcal{C}_h=[-\frac{\pi}{2},\frac{\pi}{2}]-\frac{\mathrm{i}\gamma}{2}+\mathrm{i}\delta$ and $\mathcal{C}_p=[-\frac{\pi}{2},\frac{\pi}{2}]+\frac{\mathrm{i}\gamma}{2}+\mathrm{i}\delta'$, where $\delta,\delta'>0$ are small

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with integration contours $\mathcal{C}_h = [-\frac{\pi}{2},\frac{\pi}{2}] - \frac{\mathrm{i}\gamma}{2} + \mathrm{i}\delta$ and $\mathcal{C}_p = [-\frac{\pi}{2},\frac{\pi}{2}] + \frac{\mathrm{i}\gamma}{2} + \mathrm{i}\delta'$, where $\delta,\delta'>0$ are small

Two cases worked out so far

1. $X=Y=\sigma^z$, two-point function of local magnetization (C. Babenko, F. Göhmann, K. Kozlowski, J. Sirker, and J. Suzuki, Phys. Rev. Lett. **126**, 210602 (2021))
   $\to \mathcal{A}_{zz}^{(2\ell)}$ spectral function
2. $X=Y=\mathcal{J}=-2\mathrm{i}J(\sigma^-\otimes\sigma^+ - \sigma^+\otimes\sigma^-)$, correlation function of magnetic current densities (with K. Kozlowski, J. Sirker, and J. Suzuki, SciPost Phys. **12**, 158 (2022))
   $\to \mathcal{A}_{\mathcal{J}\mathcal{J}}^{(2\ell)}$ spin conductivity

Dispersion relation

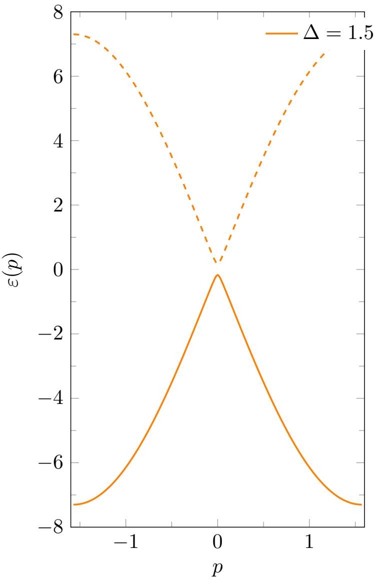
In the antiferromagnetic massive regime the dispersion relation of the elementary excitation can be expressed explicitly in terms of theta functions

$$p(\lambda) = \frac{\pi}{2} + \lambda - \mathrm{i}\ln\left(\frac{\vartheta_4(\lambda + \mathrm{i}\gamma/2|q^2)}{\vartheta_4(\lambda - \mathrm{i}\gamma/2|q^2)}\right)$$

$$\varepsilon(\lambda) = -2J\,\mathrm{sh}(\gamma)\vartheta_3\vartheta_4\frac{\vartheta_3(\lambda)}{\vartheta_4(\lambda)}$$

Here p is the momentum and ε is the dressed energy (for $h = 0$)

Interpretation: dispersion relation of holes



Amplitudes

- The integrands in each term of our form factor series are parameterized in terms of two sets $\mathcal{U} = \{u_j\}_{j=1}^{\ell}$ and $\mathcal{V} = \{v_k\}_{k=1}^{\ell}$ of 'hole and particle type' rapidity variables of equal cardinality ℓ. For sums and products over these variables we shall employ the short-hand notations

$$\sum_{\lambda \in \mathcal{U} \ominus \mathcal{V}} f(\lambda) = \sum_{\lambda \in \mathcal{U}} f(\lambda) - \sum_{\lambda \in \mathcal{V}} f(\lambda), \quad \prod_{\lambda \in \mathcal{U} \ominus \mathcal{V}} f(\lambda) = \frac{\prod_{\lambda \in \mathcal{U}} f(\lambda)}{\prod_{\lambda \in \mathcal{V}} f(\lambda)}$$

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- The amplitudes factorize in a part which depends on the operators X and Y and a universal weight

$$\mathcal{A}_{XY}^{(2\ell)}(\mathcal{U}, \mathcal{V}|k) = \mathcal{F}_{XY}^{(2\ell)}(\mathcal{U}, \mathcal{V}|k) W^{(2\ell)}(\mathcal{U}, \mathcal{V}|k)$$

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- For short operators like σ^z or $\mathcal{J}$ the operator-dependent part is rather simple

$$\mathcal{F}_{zz}^{(2\ell)}(\mathcal{U}, \mathcal{V}|k) = 4 \sin^2 \Big(\tfrac{1}{2} \big(\pi k + \textstyle\sum_{\lambda \in \mathcal{U} \ominus \mathcal{V}} p(\lambda) \big) \Big)$$

$$\mathcal{F}_{\mathcal{J}\mathcal{J}}^{(2\ell)}(\mathcal{U}, \mathcal{V}|k) = \tfrac{1}{4} \Big(\textstyle\sum_{\lambda \in \mathcal{U} \ominus \mathcal{V}} \varepsilon(\lambda) \Big)^2$$

and should be generally related to the theory of factorizing correlation functions (H. Boos, M. Jimbo, T. Miwa, F. Smirnov and Y. Takeyama 2006-10)

Universal weight

We introduce 'multiplicative spectral parameters' $H_j = \mathrm{e}^{2\mathrm{i}x_j}$, $P_k = \mathrm{e}^{2\mathrm{i}y_k}$ and the following special basic hypergeometric series

$$\Phi_1(P_k,\alpha) = {}_{2\ell}\Phi_{2\ell-1}\left(\begin{matrix} q^{-2}, \{q^2 \frac{P_k}{P_m}\}_{m\neq k}^{\ell}, \{\frac{P_k}{H_m}\}_m^{\ell} \\ \{\frac{P_k}{P_m}\}_{m\neq k}^{\ell}, \{q^2 \frac{P_k}{H_m}\}_m^{\ell} \end{matrix} ; q^4, q^{4+2\alpha}\right)$$

$$\Phi_2(P_k,P_j,\alpha) = {}_{2\ell}\Phi_{2\ell-1}\left(\begin{matrix} q^6, q^2 \frac{P_j}{P_k}, \{q^6 \frac{P_j}{P_m}\}_{m\neq k,j}^{\ell}, \{q^4 \frac{P_j}{H_m}\}_m^{\ell} \\ q^8 \frac{P_j}{P_k}, \{q^4 \frac{P_j}{P_m}\}_{m\neq k,j}^{\ell}, \{q^6 \frac{P_j}{H_m}\}_m^{\ell} \end{matrix} ; q^4, q^{4+2\alpha}\right)$$

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We further define

$$\Psi_2(P_k,P_j,\alpha) = q^{2\alpha} r_\ell(P_k,P_j)\Phi_2(P_k,P_j,\alpha)$$

where

$$r_\ell(P_k,P_j) = \frac{q^2(1-q^2)^2 \frac{P_j}{P_k}}{(1-\frac{P_j}{P_k})(1-q^4\frac{P_j}{P_k})}\left[\prod_{\substack{m=1\\ m\neq j,k}}^{\ell} \frac{1-q^2\frac{P_j}{P_m}}{1-\frac{P_j}{P_m}}\right]\left[\prod_{m=1}^{\ell} \frac{1-\frac{P_j}{H_m}}{1-q^2\frac{P_j}{H_m}}\right]$$

and introduce a ‘conjugation’ $\bar{f}(H_j, P_k, q^\alpha) = f(1/H_j, 1/P_k, q^{-\alpha})$

Universal weight

The core part of our form factor densities, is a matrix $\mathcal{M}$

$$\mathcal{M}_{i,j} = \delta_{ij} \left[\overline{\Phi}_1(P_j, 0) - \frac{\phi^{(-)}(y_j)}{\phi^{(+)}(y_j)} \Phi_1(P_j, 0) \right] - (1 - \delta_{ij}) \left[\overline{\Psi}_2(P_j, P_i, 0) - \frac{\phi^{(-)}(y_i)}{\phi^{(+)}(y_i)} \Psi_2(P_j, P_i, 0) \right]$$

where

$$\phi^{(\pm)}(\lambda) = e^{\pm i\Sigma} \prod_{\mu \in \mathcal{U} \ominus \mathcal{V}} \Gamma_{q^4}\left(\tfrac{1}{2} \pm \tfrac{\lambda - \mu}{2i\gamma}\right) \Gamma_{q^4}\left(1 \mp \tfrac{\lambda - \mu}{2i\gamma}\right), \quad \Sigma = -\frac{\pi k}{2} - \frac{1}{2} \sum_{\lambda \in \mathcal{U} \ominus \mathcal{V}} \lambda$$

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By $\hat{\mathcal{M}}$ we denote the matrix obtained from $\mathcal{M}$ upon replacing $x_j \leftrightharpoons -y_j$. Finally

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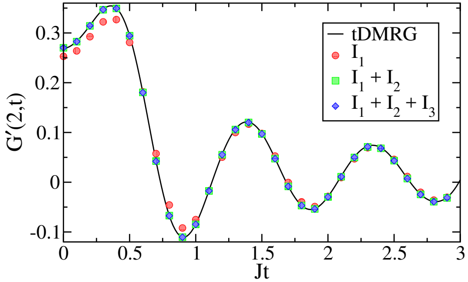
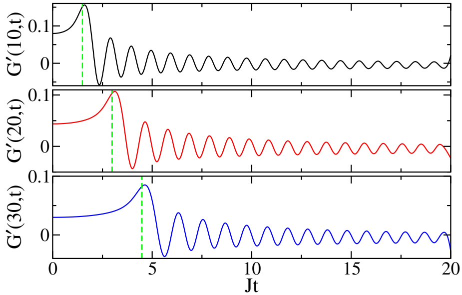
Then the universal weight of the form factor amplitudes is

$$W^{(2\ell)}(\mathcal{U},\mathcal{V}|k) = \left(\frac{\vartheta_1'}{2\vartheta_1(\Sigma)}\right)^2\left[\prod_{\lambda,\mu\in\mathcal{U}\ominus\mathcal{V}}\Xi(\lambda-\mu)\right]\det_\ell\{\mathcal{M}\}\det_\ell\{\hat{\mathcal{M}}\}\det_\ell\left(\frac{1}{\sin(u_j-v_k)}\right)^2$$

Numerical efficiency

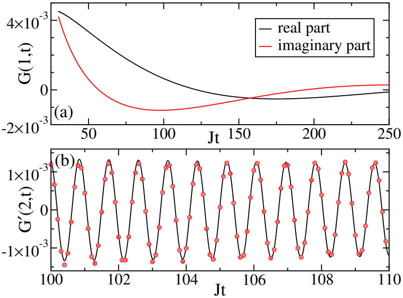


Real part of $\langle\sigma_1^z(t)\sigma_3^z\rangle - (\vartheta_1'/\vartheta_2)^2$ for $\Delta = 1.2$. Increasing number of terms of the series taken into account



Real part of $\langle\sigma_1^z(t)\sigma_{m+1}^z\rangle - (\vartheta_1'/\vartheta_2)^2(-1)^m$ for $\Delta = 1.2$ and different values of m

Numerical efficiency



(a) $\langle \sigma_1^z(t)\sigma_2^z\rangle - (-1)^m \vartheta_1'^2/\vartheta_2^2$ at long times for $\Delta = 1.2$.
(b) Comparison of $\mathrm{Re}\,\langle \sigma_1^z(t)\sigma_3^z\rangle - (-1)^m \vartheta_1'^2/\vartheta_2^2$ obtained by using the form factor expansion (symbols) with the two-spinon asymptotics (line) for $\Delta = 1.4$.

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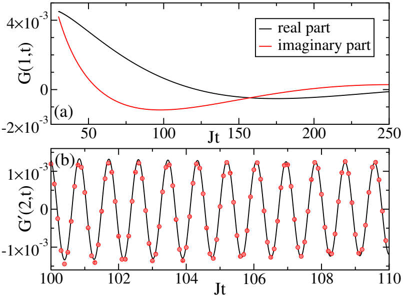

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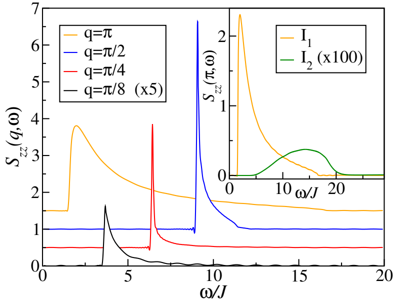
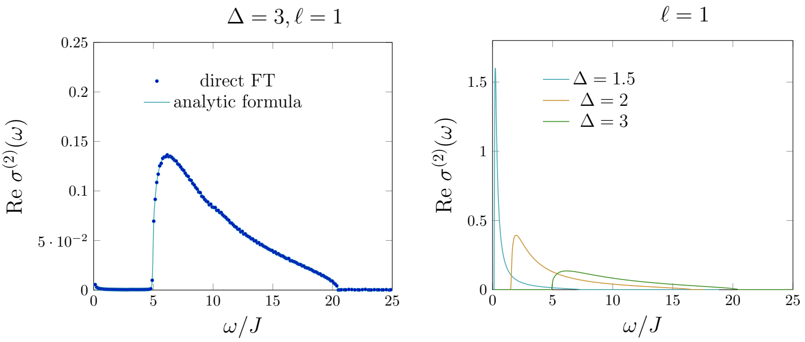


$S^{zz}(q,\omega)$ for $\Delta = 2$ and various wave numbers q

Optical conductivity



Left panel: comparison of the analytic result and the direct Fourier transformation for $\ell = 1$ and $\Delta = 3$. For the latter we used $\langle \mathcal{J}_1(t)\mathcal{J}_{k+1} \rangle$, $0 \le k \le 399$ and $0 \le tJ \le 50$

Right panel: $\mathrm{Re}\, \sigma^{(2)}(\omega)$ for various Δ

Two-spinon optical conductivity

Recall the elliptic module k, the complementary module k' and the complete elliptic integral K

$$k = \vartheta_2^2/\vartheta_3^2, \quad k' = \vartheta_4^2/\vartheta_3^2, \quad K = \pi\vartheta_3^2/2.$$

Further introduce two functions

$$r(\omega) = \frac{\pi}{K}\operatorname{arcsn}\left(\frac{\sqrt{(h_\ell/k')^2 - \omega^2}}{h_\ell k/k'}\middle| k\right), \; B(z) = \frac{1}{G_{q^4}^4\left(\frac{1}{2}\right)} \prod_{\sigma=\pm} \frac{G_{q^4}\left(1+\frac{\sigma z}{2i\gamma}\right)G_{q^4}\left(\frac{\sigma z}{2i\gamma}\right)}{G_{q^4}\left(\frac{3}{2}+\frac{\sigma z}{2i\gamma}\right)G_{q^4}\left(\frac{1}{2}+\frac{\sigma z}{2i\gamma}\right)}$$

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Then the two-spinon contribution to the real part of the dynamical conductivity of the XXZ chain at zero temperature and in the antiferromagnetic massive regime can be represented as

$$\mathrm{Re}\,\sigma^{(2)}(\omega) = \frac{q^{\frac{1}{2}} h_\ell^2 k}{8k'} \frac{B\big(r(\omega)\big)}{\Delta - \cos\big(r(\omega)\big)} \frac{\vartheta_3^2}{\vartheta_3^2\big(r(\omega)/2\big)} \frac{1}{\sqrt{\big((h_\ell/k')^2-\omega^2\big)\big(\omega^2-h_\ell^2\big)}}$$

where $\omega \in [h_\ell, h_\ell/k']$. Outside this interval it vanishes

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