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

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Les Diablerets

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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
- On the universal amplitude
- 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 (discrete space, continuous time)

- 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

$\rho_L(T)[X] = \frac{\mathrm{tr}\{\mathrm{e}^{-H_L/T} X\}}{\mathrm{tr}\{\mathrm{e}^{-H_L/T}\}}$ — 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

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

Prime example of an integrable spin chain Hamiltonian

- The XXZ model

$$H_L(\Delta) = J \sum_{j=1}^{L} \{\sigma_{j-1}^x \sigma_j^x + \sigma_{j-1}^y \sigma_j^y + \Delta \sigma_{j-1}^z \sigma_j^z\} - \frac{h}{2} \sum_{j=1}^{L} \sigma_j^z$$

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

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

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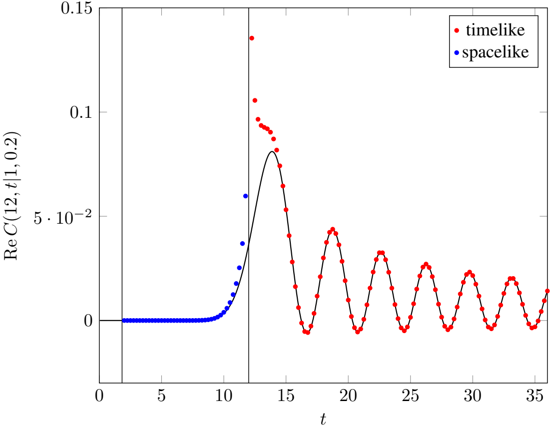
- For the XX model the longitudinal two-point functions are

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

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

Longitudinal correlation functions of XX model

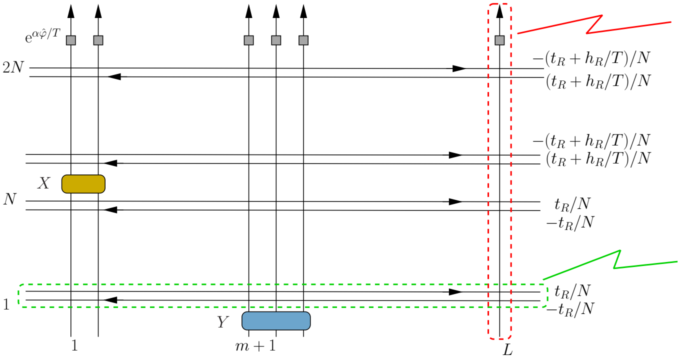
- This simple expression can be analyzed numerically and asymptotically by means of the saddle point method



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: $p(\lambda) = \frac{2\pi n}{L} + \text{scattering}$
- 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: $\varepsilon(\lambda) = (2n-1)i\pi T + \text{scattering}$
- $t(0)$ non-hermitian, $\rho_n(0) = e^{-\frac{1}{\xi_n} + i\varphi_n}$, 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

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

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 (GKKKS17 + GK)

$$\begin{aligned}\big\langle X_{[\![1,\ell]\!]}(t) Y_{[\![1+m,r+m]\!]}\big\rangle_T = {} & \mathrm{e}^{-\mathrm{i}ht\,s(X)} \\ & \times \lim_{N\to\infty} \sum_n \frac{\langle \Psi_0 | \prod^{\curvearrowright}_{k\in[\![1,\ell]\!]} \mathrm{tr}\{x^{(k)} T(0)\} | \Psi_n\rangle}{\langle \Psi_0 | \Psi_0 \rangle \Lambda_n^\ell(0)} \frac{\langle \Psi_n | \prod^{\curvearrowright}_{k\in[\![1,r]\!]} \mathrm{tr}\{y^{(k)} T(0)\} | \Psi_0\rangle}{\langle \Psi_n | \Psi_n \rangle \Lambda_0^r(0)} \\ & \times \rho_n(0)^m \left(\frac{\rho_n\big(\frac{t_R}{N}\big)}{\rho_n\big(-\frac{t_R}{N}\big)} \right)^{\frac{N}{2}}\end{aligned}$$

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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,

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

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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

$$\Big\langle \big(e_1{}^{\alpha_1}_{\beta_1} \dots e_\ell{}^{\alpha_\ell}_{\beta_\ell}\big)(t)\, e_{1+m}{}^{\gamma_1}_{\delta_1} \dots e_{r+m}{}^{\gamma_r}_{\delta_r} \Big\rangle_T =$$

$$\lim_{N\to\infty} \lim_{h'\to h} \lim_{\xi_j,\zeta_k\to 0} \sum_n A_n(h,h')\rho_n(0|h,h')^m \left(\frac{\rho_n\big(-\frac{\mathrm{i}t}{\kappa N}\big|h,h'\big)}{\rho_n\big(\frac{\mathrm{i}t}{\kappa N}\big|h,h'\big)}\right)^{\frac{N}{2}}$$

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

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

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 $T_0(\lambda|\sigma, \nu, h) \in \mathrm{End}\big(\bigotimes_{j=0}^{M} V_j\big)$ 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

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

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

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

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 $\kappa \in \mathbb{C}$*

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

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. *TP property*

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

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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*

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

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

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

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

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

if $\xi_m = \nu_1$

Calculating the form factors

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

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- This allows us to conclude that

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

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

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

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

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

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

$$\lim_{h' \to h} \lim_{\xi_j, \zeta_k \to 0} A_n(h,h') \operatorname{tr}\big\{\mathcal{J}_{1,2}\mathcal{F}^{(-)}_{n;2}(\xi_1, \xi_2|h, h')\big\} \operatorname{tr}\big\{\mathcal{J}_{1,2}\mathcal{F}^{(+)}_{n;2}(\zeta_1, \zeta_2|h, h')\big\}$$

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

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 $0 \in \operatorname{Int} \mathcal{C}_n$, $\lambda \pm \mathrm{i}\gamma \in \operatorname{Ext} \mathcal{C}_n$ if $\lambda \in \operatorname{Int} \mathcal{C}_n$ 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

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

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

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

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

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

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

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

Calculating the form factors – multiple integral representation

Lemma (following BG09)

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

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

where

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

p is the number of plusses in $(\beta_j)_{j=1}^m$ and the sequence $(x_j)_{j=1}^m$ is defined as

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

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

Calculating the form factors – factorization

- The double integrals can be factorized and reduce to a linear combination of just two functions

$$\Phi_n^{(\pm)}(\xi) = \int_{\mathcal{C}_n^{(\pm)}} \mathrm{d}m_n^{(\pm)}(\lambda)\, G_n^{(\pm)}(\lambda,\xi) = \frac{q^{\mp\alpha} - \rho_n^{\pm 1}(\xi|h,h')}{q^{\pm\alpha} - q^{\mp\alpha}}$$

$$\Psi_n^{(\pm)}(\xi_1,\xi_2) = -\mathrm{i} \int_{\mathcal{C}_n^{(\pm)}} \mathrm{d}m_n^{(\pm)}(\lambda)\, \big(q^{\pm\alpha} \operatorname{ctg}(\lambda - \xi_1 + \mathrm{i}\gamma) \\ - \rho_n^{\pm 1}(\xi_1|h,h') \operatorname{ctg}(\lambda - \xi_1)\big)\, G_n^{(\pm)}(\lambda,\xi_2)$$

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- The thermal form factors $\mathcal{F}^{(\pm)\,\alpha_1\dots\alpha_m}_{n;m\,\beta_1\dots\beta_m}(\xi|h,h')$ are compatible with the Fermionic basis of BJMST. Within the Fermionic basis approach all form factors become polynomials in just two functions, the function $\rho_n^{(\pm)}$ and a function $\omega_n^{(\pm)}$ that can be obtained as

$$\omega_n^{(\pm)}(\xi_1,\xi_2|h,h') = -\operatorname{tr}\{\mathcal{F}^{(\pm)}_{n;2}(\xi_1,\xi_2|h,h')\mathbf{c}^*_{[1,2]}(\zeta_2,\mp\alpha)\mathbf{b}^*_{[1,2]}(\zeta_1,\mp\alpha-1)(1)\}$$

Calculating the form factors – factorization

- Using the latter formula we obtain the representation

$$\omega_n^{(\pm)}(\xi_1, \xi_2 | h, h') =$$
$$2\zeta^{-\alpha}\psi_n^{(\pm)}(\xi_1, \xi_2) + \Delta\psi(\zeta, -\alpha) + 2\big(\rho_n^{\pm 1}(\xi_1|h, h') - \rho_n^{\pm 1}(\xi_2|h, h')\big)\psi(\zeta, -\alpha)$$

Here $\zeta = e^{i(\xi_1 - \xi_2)}$, $\psi(\zeta, \alpha) = \frac{\zeta^\alpha(\zeta^2+1)}{2(\zeta^2-1)}$ and Δ is the difference operator whose action on a function f is defined by $\Delta f(\zeta) = f(q\zeta) - f(q^{-1}\zeta)$

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- The form factors of the energy density operator

$$\mathcal{E}/J = 2\big(\sigma^- \otimes \sigma^+ + \sigma^+ \otimes \sigma^-\big) + \tfrac{1}{2}(q+q^{-1})\sigma^z \otimes \sigma^z$$

are the simplest example of form factors that involve $\omega_n^{(\pm)}$

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- For $n \neq 0$

$$\lim_{h'\to h}\lim_{\xi_j,\zeta_k\to 0} A_n(h,h')\,\mathrm{tr}\big\{\mathcal{E}_{1,2}\mathcal{F}^{(-)}_{n;2}(\xi_1,\xi_2|h,h')\big\}\,\mathrm{tr}\big\{\mathcal{E}_{1,2}\mathcal{F}^{(+)}_{n;2}(\zeta_1,\zeta_2|h,h')\big\}$$
$$= \frac{J^2\,\mathrm{sh}^2(\gamma)}{2}\big(\partial^2_{h'}A_n(h,h')\big)\big|_{h'=h}\,\mathrm{res}_{h'=h}\,\omega_n^{(+)}(0,0|h,h')\,\mathrm{res}_{h'=h}\,\omega_n^{(-)}(0,0|h,h')$$

Calculating the amplitudes, $\Delta > 1$ [BGKS 20]

- Starting point for the study of the universal amplitude is Slavnov's scalar product formula which we use for the four 'scalar products' its definition:

$$A_n(h,h') = \frac{\langle\Psi_0(h)|\Psi_n(h')\rangle\langle\Psi_n(h')|\Psi_0(h)\rangle}{\langle\Psi_0(h)|\Psi_0(h)\rangle\langle\Psi_n(h')|\Psi_n(h')\rangle} = \left[\prod_{j=1}^{M} \frac{\rho_n(\lambda_j|h,h')}{\rho_n(\mu_j|h,h')}\right]$$

$$\times \frac{\det_M\left\{\frac{e(\lambda_j-\mu_k)}{1+\mathfrak{a}(\mu_k|h)} - \frac{e(\mu_k-\lambda_j)}{1+1/\mathfrak{a}(\mu_k|h)}\right\}}{\det_M\left\{\delta^j_k + \frac{K(\lambda_j-\lambda_k)}{\mathfrak{a}'(\lambda_k|h)}\right\}\det_M\left\{\frac{1}{\sin(\lambda_j-\mu_k)}\right\}} \frac{\det_M\left\{\frac{e(\mu_j-\lambda_k)}{1+\mathfrak{a}_n(\lambda_k|h')} - \frac{e(\lambda_k-\mu_j)}{1+1/\mathfrak{a}_n(\lambda_k|h')}\right\}}{\det_M\left\{\delta^j_k + \frac{K(\mu_j-\mu_k)}{\mathfrak{a}'_n(\mu_k|h')}\right\}\det_M\left\{\frac{1}{\sin(\mu_j-\lambda_k)}\right\}}$$

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- This has to be analysed for $N \to \infty$. In general Fredholm determinants are obtained. However, for $\Delta > 1$ and $T \to 0$, thanks to the **no-string hypothesis**,

$$A_n(h,h') = \frac{\vartheta_2^2(\Sigma_0)}{\vartheta_2^2}\left[\prod_{\lambda,\mu\in\mathcal{X}_n\ominus\mathcal{Y}_n} \Psi(\lambda-\mu)\right] \frac{\det_\ell\{\Omega_n(x_j,y_k)\}\det_\ell\{\overline{\Omega}_n(y_j,x_k)\}}{\det_{2\ell}\{\mathcal{J}\}} \times \left(1+\mathcal{O}(T^\infty)\right)$$

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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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)) $\rightarrow \mathcal{A}_{zz}^{(2\ell)}$ 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)) $\rightarrow \mathcal{A}_{\mathcal{J}\mathcal{J}}^{(2\ell)}$ spin conductivity

Dispersion relation

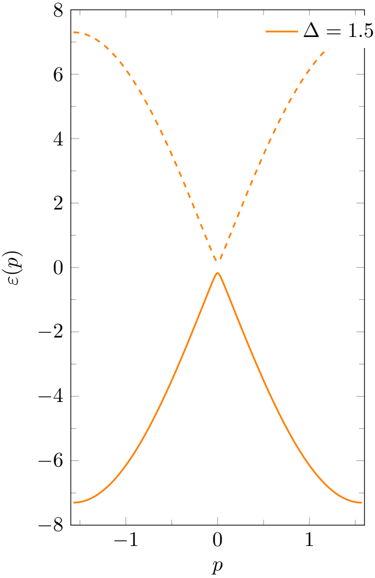
In the antiferromagnetic massive regime the dispersion relation of the elementary excitation can be expressed explicitly in terms of theta functions

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

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

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’ $H_j = e^{2ix_j}$, $P_k = e^{2iy_k}$ and the following special basic hypergeometric series

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

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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’ $\bar{f}(H_j,P_k,q^\alpha) = f(1/H_j, 1/P_k, q^{-\alpha})$

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

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

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$$\Xi(\lambda) = \frac{\Gamma_{q^4}\left(\frac{1}{2} + \frac{\lambda}{2\mathrm{i}\gamma}\right) G^2_{q^4}\left(1 + \frac{\lambda}{2\mathrm{i}\gamma}\right)}{\Gamma_{q^4}\left(1 + \frac{\lambda}{2\mathrm{i}\gamma}\right) G^2_{q^4}\left(\frac{1}{2} + \frac{\lambda}{2\mathrm{i}\gamma}\right)}$$

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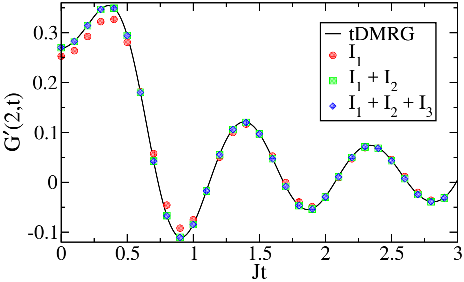
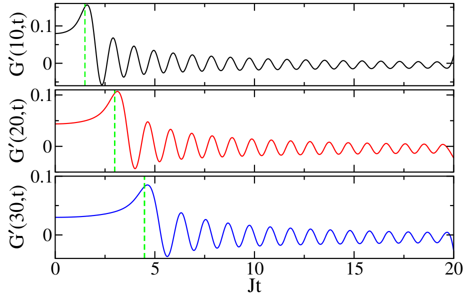
Then the universal weight of the form factor amplitudes is

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

Numerical efficiency

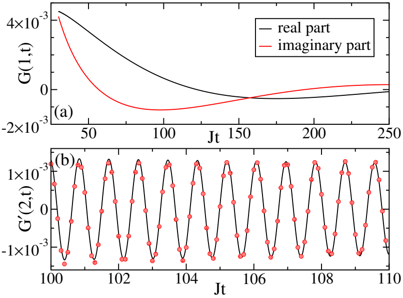


Real part of $\langle \sigma_1^z(t)\sigma_3^z\rangle - (\vartheta_1'/\vartheta_2)^2$ for $\Delta = 1.2$. Increasing number of terms of the series taken into account



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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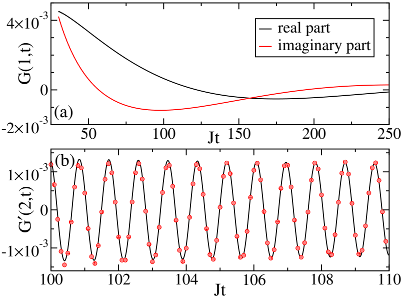

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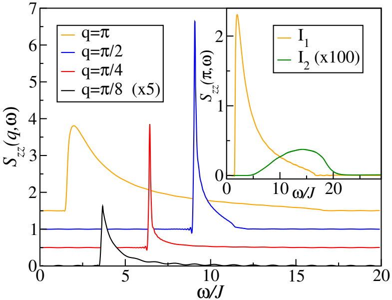
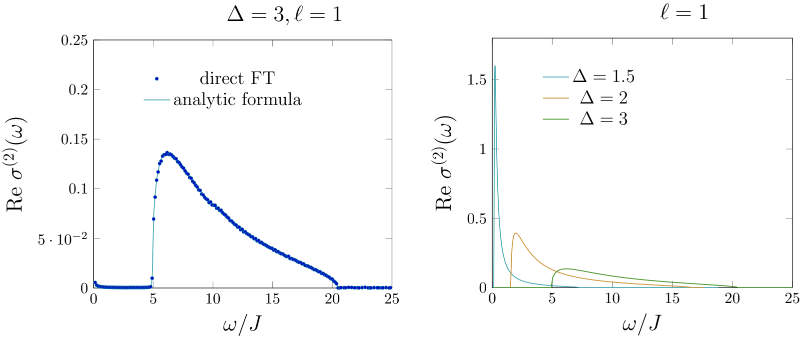


$S^{zz}(q,\omega)$ for $\Delta = 2$ and various wave numbers q

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

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

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Then the two-spinon contribution to the real part of the optical 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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