Thermal form factor expansions for the correlation functions of the XXZ chain

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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
- 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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- Summary and discussion

- Based on J. Math. Phys. **62** (2021) 041901, Phys. Rev. Lett. **126** (2021) 210602, and arXiv:2202.05304; joint work with C. BABENKO, K. K. KOZLOWSKI, J. SIRKER and J. Suzuki

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

$\rho_L(T)[X] = \dfrac{\mathrm{tr}\left\{\mathrm{e}^{-H_L/T} X\right\}}{\mathrm{tr}\left\{\mathrm{e}^{-H_L/T}\right\}}$ 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 $x = y^\dagger$)

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

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

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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 perturabtion

Prime example of an integrable spin chain Hamiltonian

- The XXZ model

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

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

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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

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

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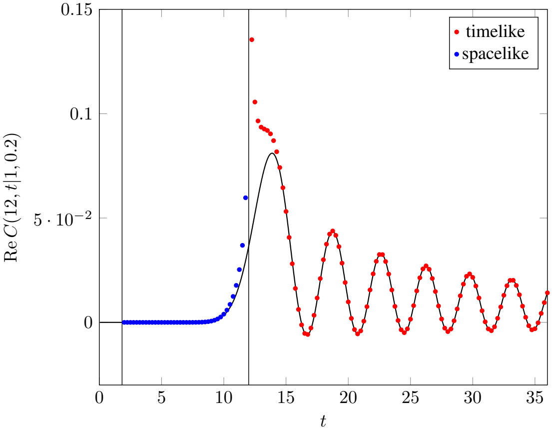
- For the XX model the longitudinal two-point functions are

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

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

Longitudinal correlation functions of XX model

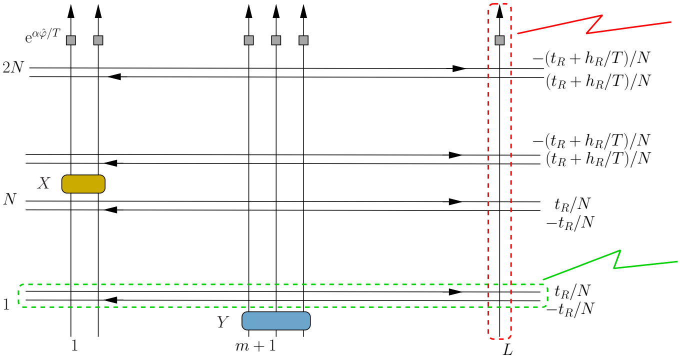
- This simple expression can be analyzed numerically and asymptotically by means of the saddle point method



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', $t_R = -ih_Rt$

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, continously 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: $\varepsilon(\lambda) = (2n-1)\mathrm{i}\pi T + \text{scattering}$
- $t(0)$ non-hermitian, $\rho_n(0) = e^{-\frac{1}{\xi_n} + \mathrm{i}\varphi_n}$, correlation length and phase
- $\{\lambda_j\}$ Bethe roots, continously distributed 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

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

Explicit form factor series for $T = 0$, $\Delta > 1$, $|h| < h_\ell$

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. 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 two magnetic current densities (with K. K. Kozlowski, J. Sirker, and J. Suzuki, Preprint) $\rightarrow \mathcal{A}_{\mathcal{J}\mathcal{J}}^{(2\ell)}$ spin conductivity

Dispersion relation

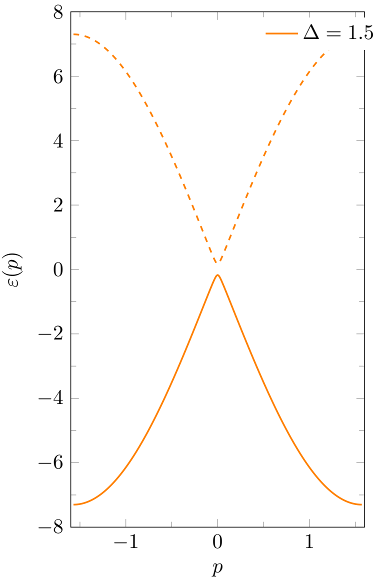
In the antiferromagnetic massive regime the dispersion relation of the elementary excitation can be expressed explicitly in terms of theta functions

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

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

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

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

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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

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

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

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

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

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

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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

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

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where

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

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

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

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

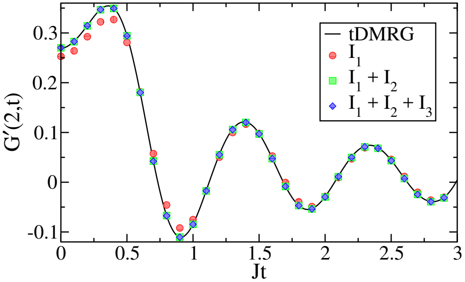
By $\hat{\mathcal{M}}$ we denote the matrix obtained from $\mathcal{M}$ upon replacing $x_j \leftrightharpoons -y_j$. Finally

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

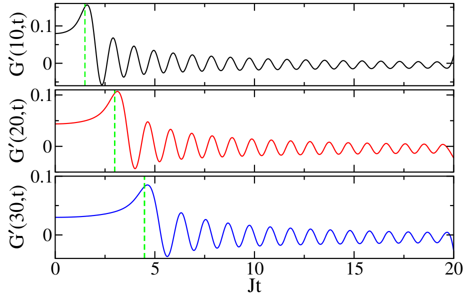
Then the universal weight of the form factor amplitudes is

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

Numerical efficiency

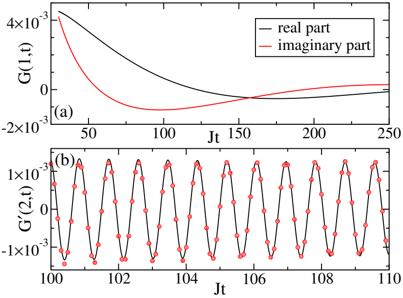


Real part of $\langle \sigma_1^z(t)\sigma_3^z \rangle - (\vartheta_1'/\vartheta_2)^2$ for $\Delta = 1.2$. Increasing number of terms of the series taken into account



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

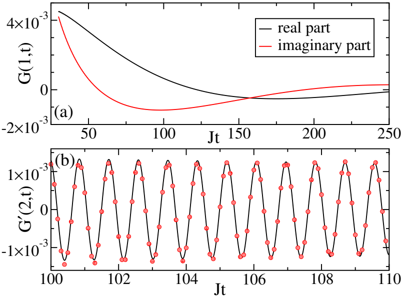
Numerical efficiency



(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 $\Delta = 1.4$.

Numerical efficiency



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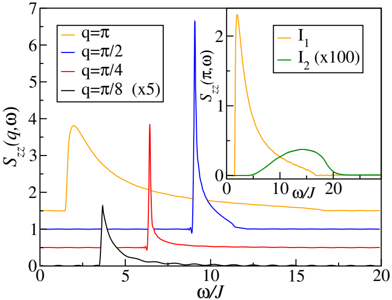
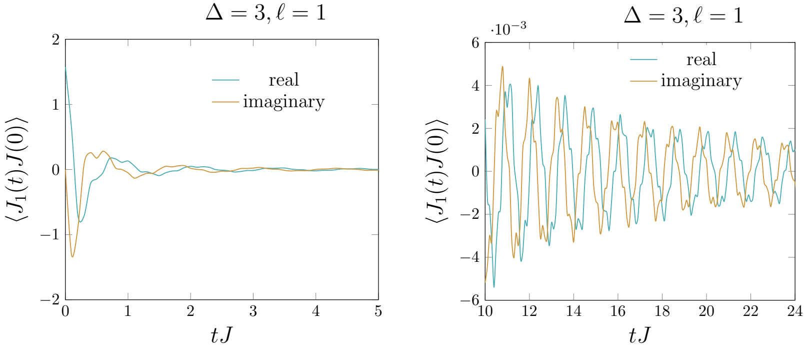


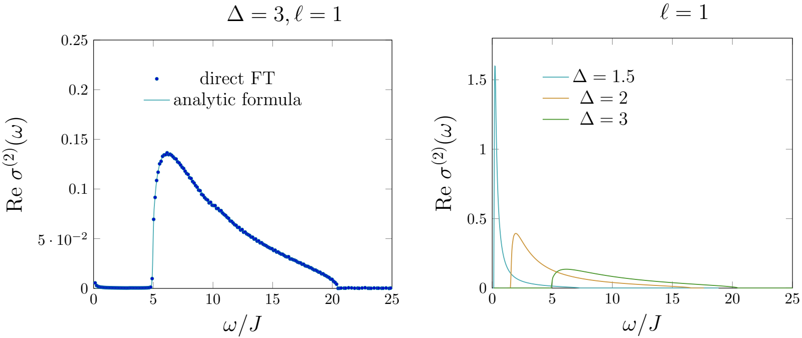
$S^{zz}(q,\omega)$ for $\Delta = 2$ and various wave numbers q

Spin transport



$\langle \mathcal{J}_1(t)\mathcal{J}\rangle$ for $\Delta = 3$, $0 < tJ < 5$ (left) $10 < tJ < 24$ (right). We sum up to $\mathcal{J}_{350}$

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

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

where arcsn is the inverse of the Jacobi elliptic sn function

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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

Summary and outlook

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2. For $T \to 0$ we have obtained explicit expressions for the form factor amplitudes that contain only finite determinants
3. The resulting TFFSs for the two-point functions are numerically highly efficient

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Future work:

1. Series for all spin-zero operators and relation with Fermionic basis of Boos et al., higher-spin operators
2. Extend this work to the massless regime of XXZ
3. Show convergence of the series and estimate the truncation error
4. Obtain the isotropic limit and perform the long-time large-distance analysis of two-point functions of the XXX chain
5. Perform a high-T analysis (for XX case cf. [GKS 20A])