UNIVERSITY OF AMSTERDAM

Dynamical correlation functions of higher spin chains

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Contents

- Dynamical correlations for spin-$\frac{1}{2}$ Heisenberg (review)

$$H = J \sum_{j=1}^{N} \hat{S}_j \hat{S}_{j+1}$$

- Higher spin chains

- Babujian-Takhtajan spin-1 chain
  - Structure of deviated string solutions
  - Dynamical correlations (results)

- Conclusions

Dynamical Structure Factor

Connecting theory and experiment

- Inelastic Neutron Scattering
- Fourier Transform of connected spin-spin correlation

$$S^{a\bar{a}}(q,\omega) = \frac{1}{N}\sum_{j,j'}^{N} e^{iq(j-j')} \int_{-\infty}^{\infty} \mathrm{d}t \; e^{i\omega t} \langle S_j^a(t) S_{j'}^{\bar{a}}(0)\rangle_c$$

- Resolution of identity: $\mathbb{1} = \sum_\alpha |\alpha\rangle\langle\alpha|$

$$\boxed{S^{a\bar{a}}(q,\omega) = 2\pi \sum_\alpha |\langle \mathrm{GS}|S_q^a|\alpha\rangle|^2 \delta(\omega - \omega_\alpha)}$$

Coordinate Bethe Ansatz

1931

- Reference state $|0\rangle = \bigotimes_{m=1}^{N} |\uparrow\rangle_m$
- Basis states $|n_1 ... n_M\rangle = \prod_m^M S^-_{n_m} |0\rangle$
- Impose plane wave solutions
- Periodic boundary conditions $\rightarrow$ Bethe Equations

$$\left(\frac{\lambda_j + \frac{i}{2}}{\lambda_j - \frac{i}{2}} \right)^N = \prod_{k \neq j}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}$$

Coordinate Bethe Ansatz

1931

- String hypothesis
  - $\alpha_j^{n,a} = \alpha_j^n + \frac{i}{2}(n + 1 - 2a)$
  - Bound states

Coordinate Bethe Ansatz

1931

- String hypothesis
  - $\alpha_j^{n,a} = \alpha_j^n + \frac{i}{2}(n+1-2a)$
  - Bound states
- Bethe-Takahashi equations for n-strings

$$\boxed{\theta_n(\alpha_j^n) - \frac{1}{N}\sum_m \sum_{k\neq j}^{M_n} \Theta_{nm}(\alpha_j^n - \alpha_k^m) = \frac{2\pi}{N} I_j^n}$$

where

$$\theta_n(\lambda) = 2\arctan\frac{2\lambda}{n}$$

$$\Theta_{nm}(\lambda) = (1-\delta_{nm})\theta_{|n-m|}(\lambda) + 2\theta_{|n-m|+2}(\lambda) + \ldots + \theta_{n+m}(\lambda)$$

Algebraic Bethe Ansatz

1980's-now

- Overlap between Bethe states
  - 1989 - Slavnov's formula - determinants
- Quantum inverse problem
  - 1999 - Spin operators in terms of ABA operators
- Form factors
  - 1999 - Matrix elements of spin operators
  - N. Kitanine, J. M. Maillet, and V. Terras, *Nucl. Phys. B* **554**, 647 (1999).

Dynamical Structure Factor

from Algebraic Bethe Ansatz

$$S^{a\bar{a}}(q,\omega) = 2\pi \sum_{\alpha} |\langle \mathsf{GS}|S^a_q|\alpha\rangle|^2 \delta(\omega - \omega_\alpha)$$

- $\langle\{\mu\}|S^a_j|\{\lambda\}\rangle \rightarrow$ determinant expression from ABA
- $|\{\lambda\}\rangle \rightarrow$ Which states?

- Antiferromagnetic ground state at zero field
  - Néel ordering
  - $M = \frac{N}{2}$ real rapidities

Spinons and strings in the spin-$\frac{1}{2}$ chain

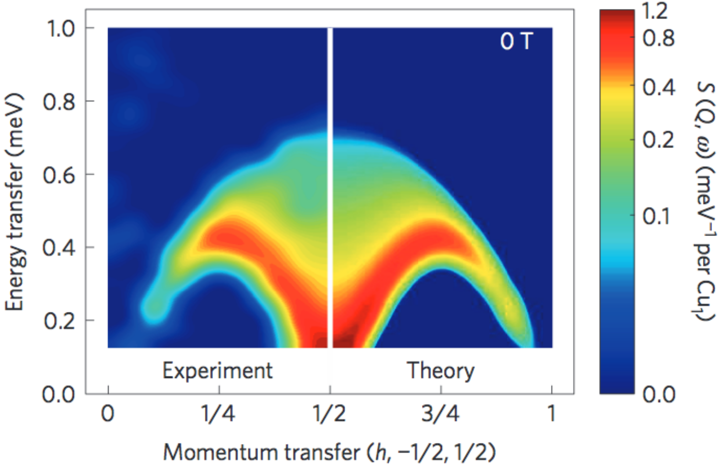
Transverse dynamical structure factor

- One flipped spin with respect to GS
- $M = \frac{N}{2} - 1$ rapidities

- Two-spinons
  - Remaining real rapidities
  - Two domain walls propagating through chain
  - Fractional excitation
- Four-spinons
  - One two-string together with real rapidities
  - Two-string deviations: $\delta \sim \mathcal{O}\left(e^{-N}\right)$

Dynamical structure factor

Inelastic Neutron Scattering versus Algebraic Bethe Ansatz



- M. Mourigal et al. *Nature Physics*, **9** 435-441 (2013).

Integrable higher spin chains

- Fusion of R-matrices
- Hamiltonian for higher spin chains

$$H_s = \sum_{m=1}^{N} Q_{2s}\left(\hat{S}_m \hat{S}_{m+1}\right)$$

$$Q_{2s}(x) = \sum_{j=1}^{2s}\left(\sum_{k=1}^{j}\frac{1}{k}\right)\prod_{l\neq j}^{2s}\frac{x-x_l}{x_j-x_l}$$

where $x_l = \frac{1}{2}[l(l+1) - 2s(s+1)]$.

Integrable higher spin chains

- Bethe equations

$$\left(\frac{\lambda_j + is}{\lambda_j - is}\right)^N = \prod_{k\neq j}^{M} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i}$$

- Form factors for higher spin chains
  - O. A. Castro-Alvaredo and J. M. Maillet. *J. Phys. A: Math. Theor.* **40** 7451-7471 (2007)
- Spin-1 chain
  - Repeat spin-$\frac{1}{2}$ roadmap to dynamical correlations
  - What are the states?
  - String deviations?

Babujan-Takhtajan Spin-1 Chain

$$H = \frac{J}{4} \sum_{j=1}^{N} \left[\hat{S}_j \hat{S}_{j+1} - (\hat{S}_j \hat{S}_{j+1})^2 \right]$$

- Antiferromagnetic ground state
  - $M = N$ rapidities
  - Two-strings
- GS and excitations dominated by string solutions
- Bethe-Takahashi equations

$$\boxed{(1-\delta_{n,1})\theta_{n-1}(\alpha_j^n) + \theta_{n+1}(\alpha_j^n) - \frac{1}{N}\sum_{m,k}\Theta_{nm}(\alpha_j^n - \alpha_k^m) = \frac{2\pi}{N} I_j^n}$$

Well behaving (Pauli principle) string quantum numbers I_j^n

Deviated string solutions

- Two-string deviations not exponentially vanishing

- Start with well behaving string quantum numbers
- Solve BAE for deviations

- Parametrisation

$$\lambda_j^{2,\pm} = \lambda_j^2 \pm i \left(\frac{1}{2} + \delta_j^2 \right)$$

- R. Hagemans and J.-S. Caux *J. Phys. A: Math. Theor.* **40** 14605 (2007)

Deviated string solutions

- Bethe equations for conjugate roots inside a two-string

$$\theta_2(\lambda_j^+) = \frac{2\pi}{N} J_j^+ + \frac{1}{N} \sum_k \left[\theta_2(\lambda_j^+ - \lambda_k^+) + \theta_2(\lambda_j^+ - \lambda_k^-) \right]$$

$$\theta_2(\lambda_j^-) = \frac{2\pi}{N} J_j^- + \frac{1}{N} \sum_k \left[\theta_2(\lambda_j^- - \lambda_k^+) + \theta_2(\lambda_j^- - \lambda_k^-) \right]$$

- Sum: root center λ_j
- Difference: deviation δ_j

- How:

$$\arctan(a + ib) + \arctan(a - ib) = \xi(a, 1 + b) + \xi(a, 1 - b)$$

$$\xi(\epsilon, \delta) = \arctan\left(\frac{\epsilon}{\delta}\right) + \pi\ \Theta(-\delta)\ \mathsf{sign}(\epsilon)$$

Deviated string solutions

Parametrisation

- Sum: root center λ_j

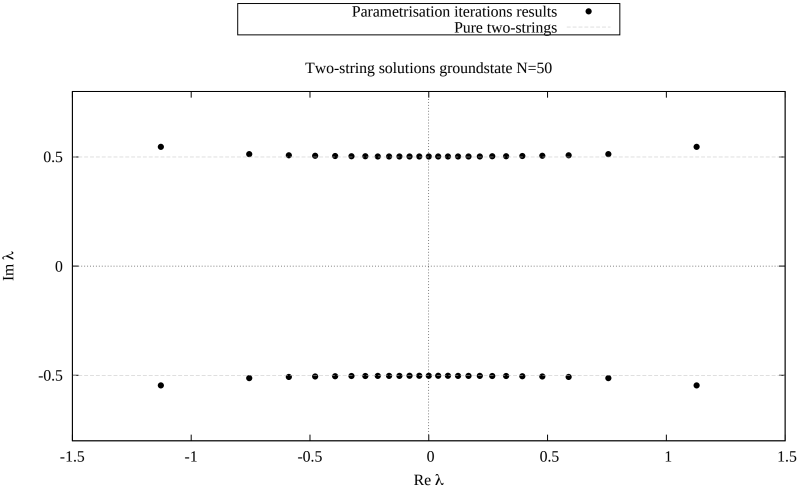
$$\xi\left(\lambda_j^2, \frac{3}{2}+\delta_j^2\right) + \xi\left(\lambda_j^2, \frac{1}{2}-\delta_j^2\right) = \frac{\pi}{N}(J^+ + J^-)$$
$$+\frac{1}{N}\sum_k^{(n=1)}\left[\xi\left(\lambda_j^2-\lambda_k^1, \frac{3}{2}+\delta_j^2\right) + \xi\left(\lambda_j^2-\lambda_k^1, \frac{1}{2}-\delta_j^2\right)\right]$$
$$+\frac{1}{N}\sum_{k\neq j}^{(n=2)}\Big[\xi\left(\lambda_j^2-\lambda_k^2, \delta_j^2+\delta_k^2+2\right) + \xi\left(\lambda_j^2-\lambda_k^2, -\delta_j^2-\delta_k^2\right)$$
$$+\,\xi\left(\lambda_j^2-\lambda_k^2, \delta_j^2-\delta_k^2+1\right) + \xi\left(\lambda_j^2-\lambda_k^2, -\delta_j^2+\delta_k^2+1\right)\Big]$$

- Difference: deviation δ_j

$$\left[\frac{1+\delta_j^2}{\delta_j^2}\right]^2 = \left[\frac{(\lambda_j^2)^2+(\delta_j^2+2)(\delta_j^2+1)+\frac{1}{4}}{(\lambda_j^2)^2+\delta_j^2(\delta_j^2-1)+\frac{1}{4}}\right]^N \prod_k^{(n=1)} \frac{\left(\delta_j^2-\frac{1}{2}\right)^2+\left(\lambda_j^2-\lambda_k^1\right)^2}{\left(\delta_j^2+\frac{3}{2}\right)^2+\left(\lambda_j^2-\lambda_k^1\right)^2}$$
$$\cdot\prod_{k\neq j}^{(n=2)} \frac{(\delta_j^2+\delta_k^2)^2+(\lambda_j^2-\lambda_k^2)^2}{(\delta_j^2+\delta_k^2+2)^2+(\lambda_j^2-\lambda_k^2)^2}\,\frac{(1-\delta_j^2+\delta_k^2)^2+(\lambda_j^2-\lambda_k^2)^2}{(1+\delta_j^2-\delta_k^2)^2+(\lambda_j^2-\lambda_k^2)^2}$$

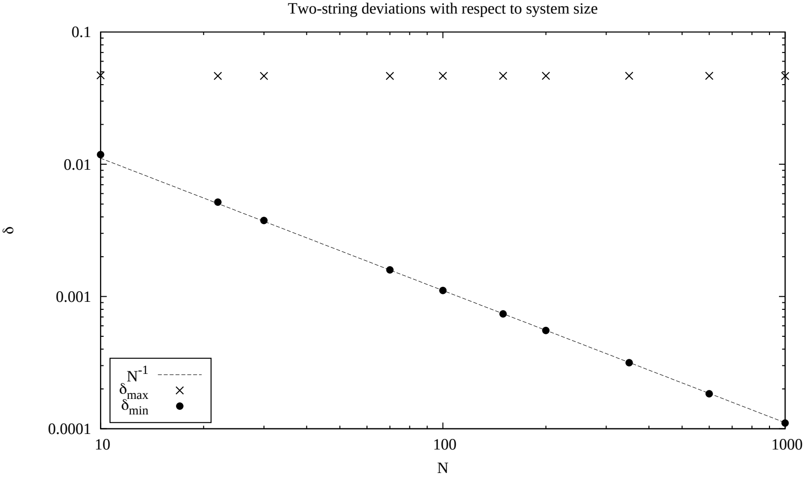
Deviated string solutions - Ground state

Results - iterative procedure



Deviated string solutions - Ground state

Results - N dependence of two-string deviations



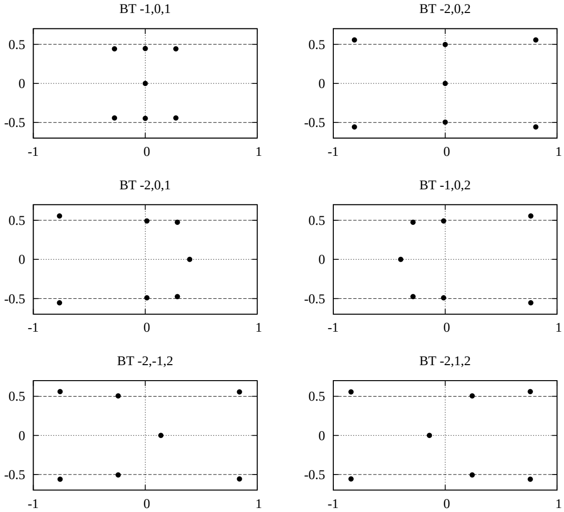
Spinons in the Babujan-Takhtajan chain

- One flipped spin with respect to GS
- $M = N - 1$ rapidities

- Two-spinons
  - Remove one of the two-strings
  - One real rapidity
  - Dimensionality of subspace same as spin-$\frac{1}{2}$ two-spinons
  - Solve using earlier introduced parametrisation

Spinons in the Babujan-Takhtajan chain

- $N = 8$ Two-spinon rapidities (Transverse direction)



E=-7.72386 (l)

E=-5.70696 (r)

E=-6.70341

E=-5.33523

Form factors

- Ready to use in computations:

$$|\langle\{\mu\}|S_q^-|\{\lambda\}\rangle|^2 = N\delta_{q,q_\lambda - q_\mu} \prod_{j=1}^{M} |\phi_{-2}(\mu_j)|^2 \prod_{j=1}^{M-1} |\phi_{-2}(\lambda_j)|^{-2}$$

$$\cdot \prod_{j,k}^{j\neq k} |\phi_2(\mu_j - \mu_k)|^{-1} \prod_{j,k}^{j\neq k} |\phi_2(\lambda_j - \lambda_k)|^{-1} \frac{|\det H^-(\{\mu\},\{\lambda\})|^2}{||\{\mu\}||\ ||\{\lambda\}||}$$

where

$$H_{ab}^-(\{\mu\},\{\lambda\}) = \begin{cases} H_{ab}(\{\mu\},\{\lambda\}) & \text{for } b < M \\ \dfrac{2}{\phi_2(\mu_a)\phi_{-2}(\mu_a)} & \text{for } b = M \end{cases}$$

$$H_{ab}(\{\mu\},\{\lambda\}) = \frac{1}{\phi_0(\mu_a - \lambda_b)} \left[\prod_{j\neq a} \phi_2(\mu_j - \lambda_b) - \left[\frac{\phi_{-2}(\lambda_b)}{\phi_2(\lambda_b)}\right]^N \prod_{j\neq a} \phi_{-2}(\mu_j - \lambda_b) \right]$$

- Both $\{\mu\}$ and $\{\lambda\}$ might contain deviated strings

Dynamical structure factor

Sumrules

- Integrated density of DSF, sum of all FF contributions

$$t^{a\bar{a}} \equiv \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{1}{N} \sum_q S^{a\bar{a}}(q,\omega)$$

$$t^{-+} = \langle S^- S^+ \rangle_c = \langle S^- S^+ \rangle$$

$$t^{zz} = \langle S^z S^z \rangle_c = \langle S^z S^z \rangle - \langle S^z \rangle^2$$

- Spin-1 representation: $S^- S^+ = 2 - S^z S^z - S^z$

$$t^{-+} = 2 - t^{zz} - \langle S^z \rangle^2 - \langle S^z \rangle$$

Dynamical structure factor

Sumrules

- Zero field ($\langle S^z \rangle = 0$)

$$S^{-+}(q,\omega) = S^{+-}(q,\omega) = 2S^{zz}(q,\omega) \qquad \rightarrow \qquad t^{zz} = \frac{1}{2} t^{-+}$$

- Sumrules for zero field

$$\boxed{t^{-+} = t^{+-} = \frac{4}{3}, \qquad t^{zz} = \frac{2}{3}}$$

- Quantative check on results

- ARPREC: An Arbitrary Precision Computation Package
  - C++/Fortran library

Dynamical structure factor

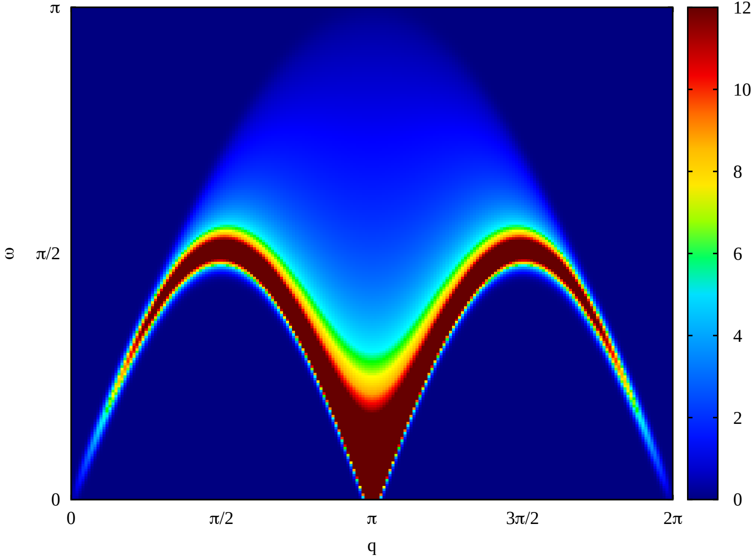
Arbitrary precision sumrule saturation results

- $N = 6, \qquad t^{-+} = \frac{4}{3}$

State	t^{-+}
1 one-string 2 two-strings	1.3255257488748488860163283692758424230579681706120362031941046259
1 two-string 1 three-string	0.0075055971882272731525334425805834021031872300622757573898167819
2 one-strings 1 three-string	0.0002622186877160566127125335739058592402906351705930607556314381
1 one-string 1 four-string	0.0000397543061725485159834550328504808640766215971193428953405972
1 five-string	0.0000000142763685690357755328701511680678106758913089690984398903

Transverse Dynamical Structure Factor

Two spinons ($N = 200$, saturation 89.9%)



Transverse Dynamical Structure Factor

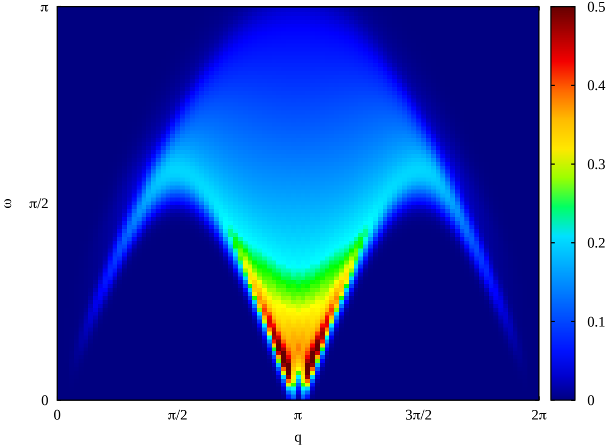
Four spinons

- Three string
- Singular solutions
- Exponentially suppressed three-string deviations
- Regularise determinant expressions by hand for three-strings

Transverse Dynamical Structure Factor

Four spinons I ($N = 100$, saturation 2.1%)

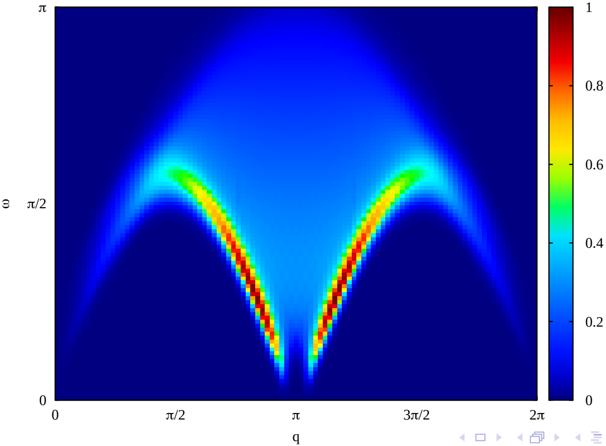
- $\frac{N-4}{2}$ two-strings
- 1 three string



Transverse Dynamical Structure Factor

Four spinons II ($N = 100$, saturation 3.8%)

- 2 one strings
- $\frac{N-6}{2}$ two strings
- 1 three string



Transverse Dynamical Structure Factor

Summary

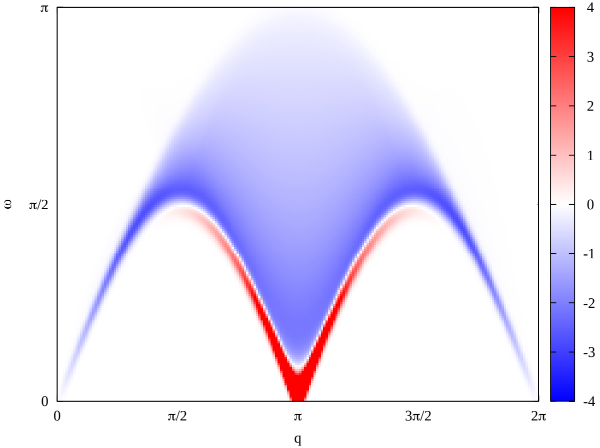
$N = 100$

- Two spinons 92.3%
- Four spinons 2.1% (not all states included yet)
- Four spinons 3.8% (not all states included yet)

- Total saturation result: 98.2%

Transverse Dynamical Structure Factor

Comparison with spin-$\frac{1}{2}$ two-spinons



Conclusion

Dynamical Structure Factor for higher spin chains

- Dynamical structure factor

$$S^{a\bar{a}}(q,\omega) = 2\pi \sum_{\alpha} |\langle \mathsf{GS}|S^a_q|\alpha\rangle|^2 \delta(\omega - \omega_\alpha)$$

- Controlling string deviations

- Possible future directions
  - Finite field
  - XXZ spin-1