Thermal form factors and form factor series for correlation functions of the XXZ chain

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Why care about correlation functions of integrable systems?

- The QM interacting many-body problem – or how to deal with complexity (most interesting and most challenging problem in physics)
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- Includes: From micro- to macro-physics (hierarchy problem)
  1. Derive thermodynamics
  2. Derive long-time large distance asymptotic behaviour of correlation functions
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- Includes: From micro- to macro-physics (hierarchy problem)
  1. Derive thermodynamics
  2. Derive long-time large distance asymptotic behaviour of correlation functions

- Approaches
  1. from no interaction to little interaction (perturbation theory)
  2. from one particle to few particles (numerical approaches)
  3. from simple observables to correlation functions (1d integrability)
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- No general theory for calculation of correlation functions of integrable models
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- Rather XXZ as an example

\[ H = J \sum_{j=-L+1}^{L} \left( \sigma_{j-1}^x \sigma_j^x + \sigma_{j-1}^y \sigma_j^y + \Delta \left( \sigma_{j-1}^z \sigma_j^z - 1 \right) \right) - \frac{\hbar}{2} \sum_{j=-L+1}^{L} \sigma_j^z \]
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Methods

1. Representation theory of quantum groups [JMMN 92]
2. Functional equations of qKZ-type [JM 96, BJMST 04, AK 12]
3. Algebraic Bethe ansatz based approach [S 89, KMT 99, 00, GKS 04]
4. Fermionic basis [BJMST 06, 08, JMS 09, BJMS 10]
5. Algebraic Bethe ansatz based form factor approach [S 89, KMT 99, IKMT 99, KKMST 09, 11A, 11B, 12, DGK 13]
6. SoV
Main goals of my research

1. Explicit results for finite temperature correlation functions
2. In particular, dynamical correlation functions at finite $T$
3. Go beyond XXZ
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Invaluable benefit and inspiration

0: Drinfel’d twists and algebraic Bethe ansatz, 1996
1: Form factors of the XXZ Heisenberg spin-$\frac{1}{2}$ finite chain, 1999
2: Correlation functions of the XXZ Heisenberg spin-$\frac{1}{2}$ chain in a magnetic field, 2000
3: Spin-spin correlation functions of the XXZ-$\frac{1}{2}$ Heisenberg chain in a magnetic field, 2002
4: Spontaneous magnetization of the XXZ Heisenberg spin-$\frac{1}{2}$ chain, 1999
5: A form factor approach to the asymptotic behavior of correlation functions in critical models, 2011
Generalized reduced density matrix

- Integrability of XXZ chain based on the underlying quantum group $U_q(\hat{sl}_2)$
- From this: $R$-matrix, transfer matrix, quantum transfer matrix, reduced density matrix (rather than $H(L), e^{-H(L)/T}$)
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\[
\begin{align*}
D_{[1,n]}(\xi_1, \ldots, \xi_n| T, h, \alpha, N) &= \frac{\langle h + \alpha | T(\xi_1 | h) \otimes \cdots \otimes T(\xi_n | h)| h \rangle}{\langle h + \alpha | \prod_{j=1}^n t(\xi_j | h)| h \rangle} \\
&= \Lambda(0, h + \alpha)^{L/2} \Lambda(0, h)^{L/2-n}
\end{align*}
\]
Here

$$T(\xi|\hbar) = e^{\frac{\hbar \sigma^2}{2T}} T(\xi) = \begin{pmatrix} A(\xi|h) & B(\xi|h) \\ C(\xi|h) & D(\xi|h) \end{pmatrix}$$

is the monodromy matrix corresponding to the staggered column-to-column transfer matrix in the picture.
Reduced density matrix and QTM form factor expansion

- Here

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- Using the generalized density matrix we obtain e.g. the transverse two-point functions of the XXZ chain as

\[
\langle \sigma^-_1 \sigma^+_m \rangle_N = \text{Tr} \left\{ D_{[1,m+1]}(0,\ldots,0|T,h,0,N) \sigma^-_1 \sigma^+_m \right\} = \frac{\langle \Psi_0 | B(0|h) t(0|h)^m C(0|h) | \Psi_0 \rangle}{\langle \Psi_0 |\Psi_0 \rangle \Lambda_0(0)^{m+1}} = \sum_\ell A^-^\ell \rho^m_\ell \quad (*)
\]

where we have used the notation

\[
\rho_\ell = e^{-1/\xi_\ell} = \frac{\Lambda_\ell(0)}{\Lambda_0(0)}, \quad A^-_\ell = \frac{\langle \Psi_0 | B(0|h) |\Psi_\ell \rangle}{\Lambda_\ell(0) \langle \Psi_0 |\Psi_0 \rangle} \frac{\langle \Psi_\ell | C(0|h) |\Psi_0 \rangle}{\Lambda_0(0) \langle \Psi_\ell |\Psi_\ell \rangle}
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\[ \langle \sigma^-_1 \sigma^+_{m+1} \rangle_N = \text{Tr} \left\{ D_{[1,m+1]}(0, \ldots, 0|T, h, 0, N) \sigma^-_1 \sigma^+_{m+1} \right\} 
\]

\[ = \frac{\langle \Psi_0|B(0|h)t(0|h)^{m-1}C(0|h)|\Psi_0 \rangle}{\langle \Psi_0|\Psi_0 \rangle \Lambda_0(0)^{m+1}} = \sum_{\ell} A^{-+}_{\ell} \rho^{m}_{\ell} \quad (*) \]

where we have used the notation

\[ \rho_{\ell} = e^{-1/\xi_{\ell}} = \frac{\Lambda_{\ell}(0)}{\Lambda_0(0)}, \quad A^{-+}_{\ell} = \frac{\langle \Psi_0|B(0|h)|\Psi_{\ell} \rangle}{\Lambda_{\ell}(0) \langle \Psi_0|\Psi_0 \rangle} \frac{\langle \Psi_{\ell}|C(0|h)|\Psi_0 \rangle}{\Lambda_0(0) \langle \Psi_{\ell}|\Psi_{\ell} \rangle} \]

(\ast) is a large-distance asymptotic expansion for static correlation functions at finite temperature. Expressions for \( A^{-+}_{\ell} \) in the Trotter limit \( N \to \infty \) were obtained in [M Dugave, FG, KK Kozlowski 2013]
Calculation of the thermal form factor series consists of three major steps

Step 1: Analyse the spectral problem of the quantum transfer matrix
Step 2: Calculate the amplitudes in the Trotter limit
Step 3: Sum the form factor series
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Step 1: Analyse the spectral problem of the quantum transfer matrix
Step 2: Calculate the amplitudes in the Trotter limit
Step 3: Sum the form factor series

We have been working on these problems jointly with Maxime Dugave, Karol Kozłowski (since 2012), J Suzuki (since 2014), M Karbach and A Klümper (since 2016)

DGK 2014a: SIGMA 10 043
DGKS 2016a: J. Phys. A 49 07LT01
In [DGK 13] we considered \( A_{n}^{\alpha 1} (\xi|\alpha) \) and \( A_{n}^{-+} (\xi|\alpha) \) for finite Trotter number and in the Trotter limit. In both cases the amplitudes consist of three factors

\[
A_{n}^{xy} (\xi|\alpha) = U_{n,s}(\alpha) F_{n}^{xy} (\xi|\alpha) D_{n}^{xy} (\alpha)
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the universal part \( U_{n,s}(\alpha) \), the determinant part \( D_{n}^{xy} (\alpha) \) and the factorizing part \( F_{n}^{xy} (\xi|\alpha) \).
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Conjecture: This structure holds in general, and the factorization of $F_n^{xy}(\xi|\alpha)$ is related to the ‘hidden Fermionic structure’ of [BOOS, JIMBO, MIWA, SMIRNOV AND TAKEYAMA 2006-10]
General structure appropriate for taking Trotter limit

In [DGK 13] we considered $A_{n}^{\alpha 1} (\xi | \alpha)$ and $A_{n}^{\alpha +} (\xi | \alpha)$ for finite Trotter number and in the Trotter limit. In both cases the amplitudes consist of three factors

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Derivation based on

- Scalar product formula [Slavnov 89]
- NLIE techniques [Klümper 92, 93; G, Klümper, Seel 04]
- ‘Cauchy extraction’ [Izergin, Kitanine, Maillet, Terras 99]
- Factorization of multiple integrals [Boos, G, Klümper, Suzuki 06; Boos, G 09]
In general, at finite temperature, a few terms of the form factor series determine the large-distance asymptotics of the correlation functions. Under certain circumstances, however, we have to sum over infinitely many contributions:

- in the low temperature limit of the static correlation functions
- if we want the full correlation functions at all distances
- in the dynamical case
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Recall the ground state phases of the XXZ chain:

- Massless case: 'Restricted sum formula' [KKMST 11]
- Massive case: auxiliary functions and multiple residue calculus [DGKS 15, DGKS 16]

Static correlations for $T \to 0$

- Massless case:
  - infinitely many $\xi_n \to \infty$

- Massive antiferromagnetic case:
  - infinitely many $\xi_n \to \xi_{\text{max}}(h)$

![Graph of ground state phases of the XXZ chain]

- Ferromagnetic
- Massive
- Antiferromagnetic
- Critical
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Means of summation:

1. Massless case: ‘Restricted sum formula’ [KKMST 11]
2. Massive case: auxiliary functions and multiple residue calculus [DGKS 15A, DGKS 16B]
Example large-distance asymptotics for equal times and $T \to 0$

- In [DGKS15A] (using a result of Lashkevich 03) we obtained an explicit formula for the next-to-leading term in the asymptotics of the static longitudinal two-point function

$$\langle \sigma_1^z \sigma_{m+1}^z \rangle = \frac{(q^2; q^2)^4}{(-q^2; q^2)^4} \left( -1 \right)^m$$

$$+ A \cdot \frac{k(q^2)^m}{m^2} \left( (-1)^m - \text{th}^2(\gamma/2) \frac{(q; q^2)^4}{(-q; q^2)^4} \right) \left( 1 + O(m^{-1}) \right)$$

where

$$k(q^2) = \frac{\vartheta_2^2(0|q^2)}{\vartheta_3^2(0|q^2)}, \quad A = \frac{1}{\pi \text{sh}^2(\gamma/2)} \frac{(-q; q^2)^4}{(q^2; q^2)^2} \frac{(q^4; q^4)^8_{\infty}}{(q^2; q^4, q^4)^8_{\infty}}$$

generalizing the result of the correlation length of Johnson, Krinsky and McCoy 73 (recall that $\Delta = (q + q^{-1})/2, \ q = e^{-\gamma}$)

- Time dependent case can be analyzed in a similar way [DGKS16A]
Above asymptotic result holds in the whole antiferromagnetic massive regime $\Delta > 1$, $|h| < h_\ell$, in particular, also if the phase boundary $h = h_\ell$ is approached from below. Hence, to leading order, on the phase boundary

$$\langle \sigma_1^z \sigma_{m+1}^z \rangle \sim (-1)^m \frac{(q^2; q^2)^4}{(-q^2; q^2)^4} \quad (*)$$
Asymptotics on phase boundary

- Above asymptotic result holds in the whole antiferromagnetic massive regime $\Delta > 1$, $|h| < h_\ell$, in particular, also if the phase boundary $h = h_\ell$ is approached from below. Hence, to leading order, on the phase boundary

$$\langle \sigma^z_1 \sigma^z_{m+1} \rangle \sim (-1)^m \frac{(q^2; q^2)^4}{(-q^2; q^2)^4} \quad (\star)$$

- Remarkably this can be reproduced if we approach the phase boundary from above and introduce an appropriate scaling function. Using the techniques developed in [DGK 13a] it can be shown [Dugave 15] that, asymptotically for large $m$ and small positive $h - h_\ell$,

$$\langle \sigma^z_1 \sigma^z_{m+1} \rangle \sim (-1)^m \frac{(q^2; q^2)^4}{(-q^2; q^2)^4} g(m, h)$$

where

$$g(m, h) = \frac{\sqrt{e} 2^{1/6}}{A^6} \left( \frac{2k}{1 - k^2} \right)^{1/4} \left( \frac{h}{h_\ell - 1} \right)^{-1/4} \frac{1}{\sqrt{m}}$$

and $A$ is the Glaisher-Kinkelin constant. Approaching the phase boundary from above in such a way that $g(m, h) = 1$ we reproduce $(\star)$
As a result of summing over all excited states and partially turning sums into integrals we obtain the full form factor series e.g. for the longitudinal correlation functions

\[ \langle \sigma_z^1 \sigma_z^{m+1} \rangle = (-1)^m \frac{(q^2; q^2)^4}{(-q^2; q^2)^4} \]

\[ + \sum_{n \in \mathbb{N}, k=0,1} \frac{(-1)^{km}}{(n!)^2} \int_{-\pi/2 - i\gamma/2}^{\pi/2 - i\gamma/2} \frac{d^n u}{(2\pi)^n} \int_{-\pi/2 + i\gamma/2}^{\pi/2 + i\gamma/2} \frac{d^n v}{(2\pi)^n} e^{-2\pi i m \sum_{j=1}^{n} (p(u_j) - p(v_j))} \]

\[ \times \mathcal{A}^{zz}(\{u_i\}_{i=1}^{n}, \{v_j\}_{j=1}^{n} | k) \]

valid up to multiplicative temperature corrections of the form \( (1 + \mathcal{O}(T^\infty)) \)

\[ p(x) = \frac{1}{4} + \frac{x}{2\pi} + \frac{1}{2\pi i} \ln \left( \frac{\vartheta_4(x + i\gamma/2, q^2)}{\vartheta_4(x - i\gamma/2, q^2)} \right) \]

is the momentum function
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\]

\[
+ \sum_{n \in \mathbb{N}} \frac{(-1)^{km}}{(n!)^2} \int_{-\frac{\pi}{2} - i\frac{\gamma}{2}}^{\frac{\pi}{2} - i\frac{\gamma}{2}} \frac{d^n u}{(2\pi)^n} \int_{-\frac{\pi}{2} + i\frac{\gamma}{2}}^{\frac{\pi}{2} + i\frac{\gamma}{2}} \frac{d^n v}{(2\pi)^n} e^{-2\pi i m \sum_{j=1}^{n} (p(u_j) - p(v_j))}
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\]

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Series is different from the previously known form factor series which were obtained by the \(q\)-vertex operator approach [Jimbo, Miwa 95] or by applying the algebraic Bethe Ansatz approach to the usual transfer matrix [DGKS 15a]
In the massive parameter regime the amplitudes in the above form factor series were obtained explicitly in [DGKS 16b]

\[ A_{zz}^{zz}(\{x_i\}_{i=1}^{n_p}, \{y_j\}_{j=1}^{n_p}|k) \]

\[ = \left[ \frac{2}{(1 - q^4)\Gamma_q(\frac{1}{2})G_q(\frac{1}{2})} \right]^{2n_p} \left[ \prod_{j=1}^{n_p} \left( 1 - e^{-2\pi i F(x_j)} \right) \left( 1 - e^{-2\pi i F(y_j)} \right) \right] \]

\[ \times \left[ \prod_{j,k=1}^{n_p} e^{\phi(x_j,y_k) - \phi(y_k,x_j)} \right] \prod_{1 \leq j < k \leq n_p} \psi(x_j - x_k)\psi(y_j - y_k) \]

\[ \prod_{j,k=1}^{n_p} \psi(x_j - y_k) \]

\[ \times \frac{\sin^2\left( \frac{\pi k}{2} + \pi \sum_{j=1}^{n_p} (p(y_j) - p(x_j)) \right)}{(-q^2; q^2)^4 \sin^2(\pi F(\theta))} \]

\[ \det_{dx,[-\pi/2,\pi/2]} (1 + \hat{V}^-) \det_{dx,[-\pi/2,\pi/2]} (1 + \hat{V}^+) \]

\[ \times \det_{m,n=1,...,n_p} \left\{ \delta_{m,n} + v^- (x_m, x_n) - \int_{-\pi/2}^{\pi/2} dy \, v^- (x_m, y) R^- (y, x_n) \right\} \]

\[ \times \det_{m,n=1,...,n_p} \left\{ \delta_{m,n} + v^+ (y_m, y_n) - \int_{-\pi/2}^{\pi/2} dy \, R^+ (y_m, y) v^+ (y, y_n) \right\} \]
Convergence of the form factor expansion to exact exact value of $g^{zz}(1)$ for various values of $\Delta$. By definition

$$g^{zz}(m) = (-1)^m \langle \sigma_1^z \sigma_{m+1}^z \rangle - \frac{(q^2; q^2)^4}{(-q^2; q^2)^4}$$

which vanishes asymptotically for large $m$. 
Comparison of $g^{zz}(m)$ estimated by the Lanczos method (squares) and by DMRG (triangles) against $g^{zz}(m)_{ph}$. The spin distance $m$ is 3 (left panel) or 8 (right panel). The red circles in the left panel denote the exact values.
Plots of $g^{zz}(m)$ vs. $m$ for $\Delta = 2$ obtained by three different methods. The curves are almost indistinguishable.
Comparison of $g^{zz}(m)$ with its asymptotic form derived in [DGKS 15A]. For $\Delta = 1.5$ (left), due to large $\xi$, $g^{zz}(m)$ still deviates considerably from its asymptotic form. For $\Delta = 2$ (right) $g^{zz}(m)$ exhibits already a good agreement with the asymptotic form as $\xi \sim 5.29$
For the dynamical case we consider the following auxiliary vertex model, normalize by the partition function and take the Trotter limit $N \rightarrow \infty$ [K SAKAI 2007]
**Theorem:** The dynamical transverse two-point functions of the XXZ chain have the form-factor series expansion

\[
\langle \sigma_m^- \sigma_{m+1}^+ (t) \rangle_T = \lim_{N \to \infty} \lim_{\epsilon \to 0} e^{i\alpha_s(\sigma^-)} \sum_n \frac{\langle \psi_0 | B(\epsilon | \kappa) | \psi_n \rangle \langle \psi_n | C(\epsilon | \kappa) | \psi_0 \rangle}{\Lambda_n(\epsilon | \kappa) \langle \psi_0 | \psi_0 \rangle \Lambda_0(\epsilon | \kappa) \langle \psi_n | \psi_n \rangle} \times \left( \frac{\Lambda_n(0 | \kappa)}{\Lambda_0(0 | \kappa)} \right)^m \frac{\Lambda_n \left( \frac{t_R}{N} | \kappa \right) \Lambda_0 \left( -\frac{t_R}{N} | \kappa \right)}{\Lambda_0 \left( \frac{t_R}{N} | \kappa \right) \Lambda_n \left( -\frac{t_R}{N} | \kappa \right)} \right)^{\frac{N}{2}}
\]

\[
= \lim_{N \to \infty} \lim_{\epsilon \to 0} e^{-iht} \sum_n A_n^- (\epsilon | \kappa, \kappa) \rho_n^m (0 | \kappa, \kappa) \rho_n^{\frac{N}{2}} (t_R / N | \kappa, \kappa) \rho_n^{\frac{N}{2}} (-t_R / N | \kappa, \kappa)
\]
**Theorem:** The dynamical transverse two-point functions of the XXZ chain have the form-factor series expansion

\[
\langle \sigma_1^- \sigma_{m+1}^+ (t) \rangle_T = \lim_{N \to \infty} \lim_{\varepsilon \to 0} \sum_n \langle \Psi_0 | B(\varepsilon | \kappa) | \Psi_n \rangle \langle \Psi_n | C(\varepsilon | \kappa) | \Psi_0 \rangle \Lambda_n(\varepsilon | \kappa) \Lambda_0(\varepsilon | \kappa) \langle \Psi_n | \Psi_0 \rangle \Lambda_0(0 | \kappa) \Lambda_n(0 | \kappa) \rho_n^{-N^2} \left( t_R / N | \kappa, \kappa \rangle \langle t_R / N | \kappa, \kappa \right)
\]

Here the amplitudes are of the same form as in the static case [Dugave, G, Kozlowski 2013]. All time dependence disappears from the amplitudes in the Trotter limit.

- The sum over \( n \) is a sum over all solutions of the Bethe ansatz equations. How to deal with such sums?
- Usual transfer matrix and low-\( T \) limit in [Dugave, G, Kozlowski, Suzuki 15, 16]
Suggestion: Summation by means of multiple residue calculus and of shell solutions of the non-linear integral equations:

\[
\langle \sigma^- \sigma^+_{m+1} (t) \rangle_T = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!(n-1)!} \int_{C_{0,1}} \frac{du^n}{(2\pi i)^n} \int_{C_{0,1}} \frac{dv^{n-1}}{(2\pi i)^{n-1}} \times \left[ \prod_{j=1}^{n} \frac{e^{mE(u_j)} - tRe(u_j)}{1 + \bar{a}(u_j|\{u\}, \{v\}, \kappa)} \right] \left[ \prod_{j=1}^{n-1} \frac{e^{-mE(v_j) + tRe(v_j)}}{1 + a(v_j|\{u\}, \{v\}, \kappa)} \right] \\
\times A^{-+}(0|\{u\}, \{v\}) e^{-iht - \int_{C_{0,1}} d\mu z(\mu|\{u\}, \{v\}, \kappa)(me(\mu) - tRe'(\mu))}
\]

for the transverse correlation functions of the XXZ chain

- A similar form factor series representation can be also derived for the longitudinal correlation functions

- Reproduces known results in XX limit
Conclusions

- Finite temperature correlation functions of the XXZ chain can be treated within a thermal form factor approach.
- At finite temperature a few terms of the series determine the large-distance asymptotics of the static correlation functions [DGK 13].
- The amplitudes are conjectured to be of the form $A = U \times F \times D$ [DGK 13].
- In the massless regime infinitely many low-lying excitations can be summed up in the low-$T$ limit to obtain the large-distance asymptotics of the two-point functions (CFT + non-CFT amplitudes) to leading non-vanishing order in $T$ [DGK 13, DGK 14b].
- In the massive regime the full thermal form factor series can be written as a series over multiple integrals with explicit integrands [DGKS 15b, DGKS 16b].
- The latter allow us to calculate the two-point functions up to the 3-particle, 3-hole contribution [DGKS 16b] and is numerically very efficient.
- Dynamical correlation functions can be treated within the thermal form factor approach. The resulting form-factor series are now being studied.
Congratulations!