Correlation functions of the integrable isotropic spin-1 chain at finite temperature

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Annecy
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Outline

(Static) correlation functions of the spin-$\frac{1}{2}$ XXZ chain

q-vertex operator approach and representation theory of $U_q(\widehat{sl_2})$ (JMMN 92)

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multiple integral representation for $D^{\alpha_1 \ldots \alpha_m}_{\beta_1 \ldots \beta_m}$

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$\langle S_1^z S_3^z \rangle = \frac{1}{12} - \frac{4\ln 2}{3} + \frac{3\zeta(3)}{4}$
U-Tokyo 03-08, U-Wuppertal 06-

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$\Omega = \int \int \omega\, bc$, factorization at $h = T = 0$ (BJMST 07-09)

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$\mathrm{tr}\{e^{-\frac{H}{T} + \frac{hS^z}{T}} \cdot\} \to Z^{\kappa}(\cdot)$
$Z^{\kappa}(t^* \dots t^* c^* \dots c^* b^* \dots b^*)$
$= \det \omega_{jk} \prod 2\rho_j$

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large distance asymptotics at $T = 0$ (KKMST 09)

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One possible direction of generalization: The integrable isotropic spin-1 Heisenberg model

$$\boxed{H = \frac{J}{4} \sum_{n=-L+1}^{L} \left(S_{n-1}^{\alpha} S_n^{\alpha} - \left(S_{n-1}^{\alpha} S_n^{\alpha} \right)^2 \right)}$$

- Critical quantum spin chain, integrable generalization of the Heisenberg model to spin 1

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- Here extention to finite T and h
- Joint work with A. Seel and J. Suzuki

Correlation functions and density matrix

- Correlation functions are (thermal) expectation values of products of (local) operators
- The partition function

$$Z_L(T,h) = \mathrm{tr}_{-L+1,\dots,L}\, \mathrm{e}^{-H/T + hS^z/T}$$

  with

$$S^z = \sum_{j=-L+1}^{L} S_j^z$$

  conserved z-component of the total spin, T temperature and h longitudinal magnetic field
- The statistical operator (density matrix)

$$\rho_L(T,h) = \frac{\mathrm{e}^{-H/T + hS^z/T}}{Z_L(T,h)}$$

  defines mean values of operator $\mathcal{O}$

$$\langle \mathcal{O} \rangle_{T,h} = \mathrm{tr}_{-L+1,\dots,L}\big(\rho_L(T,h)\mathcal{O}\big)$$

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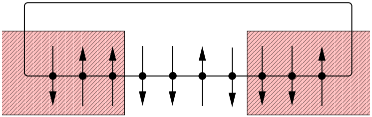
- The (reduced) density matrix describes a sub-system of a larger system in thermodynamic equilibrium in terms of the degrees of freedom of the sub-system.



- Density matrix of a chain segment of length m

$$D_m(T,h|L) = \mathrm{tr}_{-L+1,\dots,-1,0,m+1,m+2,\dots,L}\, \rho_L(T,h)$$

- Thermal average of an operator $\mathcal{O}$ of length $\le m$

$$\langle \mathcal{O} \rangle_{T,h} = \mathrm{tr}_{1,\dots,m}\big(D_m(T,h|L)\mathcal{O}\big)$$

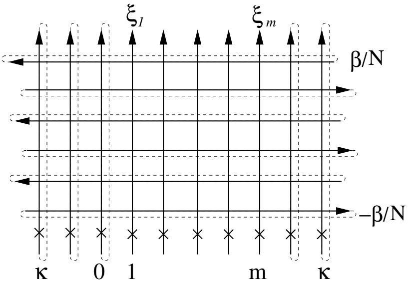
- The limit

$$D_m(T,h) = \lim_{L\to\infty} D_m(T,h|L)$$

exists (and only this limit can be calculated). Naive limit $\lim_{L\to\infty} \rho_L(T,h)$ does not exist

Density matrix and quantum transfer matrix

- The density matrix of any integrable quantum chain with fundamental unitary *R*-matrix can be approximated by a set of special partition functions of the related vertex model ($\beta \sim 1/T$, $\kappa \sim h/T$)



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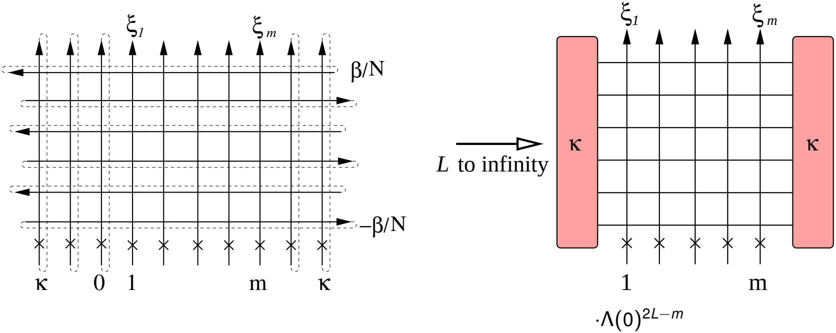

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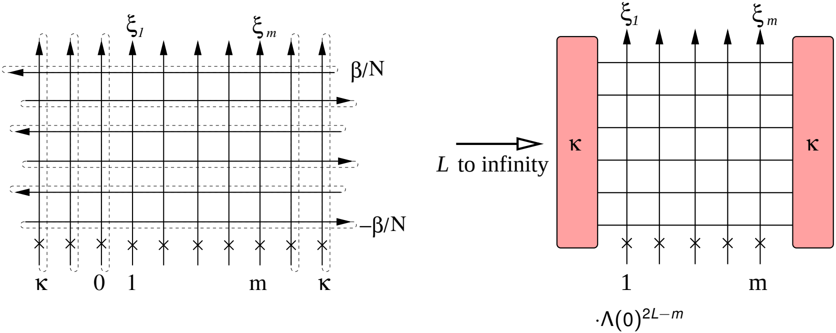


- Inhomogeneous density matrix

$$D^{[2]}(\xi) = \frac{\langle \Psi_0 | T^{[2]}(\xi_1) \otimes \cdots \otimes T^{[2]}(\xi_m) | \Psi_0 \rangle}{\langle \Psi_0 | \Psi_0 \rangle \Lambda^{[2]}(\xi_1) \ldots \Lambda^{[2]}(\xi_m)}$$

Physical correlation function $D_m(T, h)$ in the Trotter limit $N \to 0$ for $\xi_j \to \infty$

Multiple integral

Here is the result for the density matrix elements for spin 1

$$D^{[2]}{}^{\alpha_1,\dots,\alpha_m}_{\beta_1,\dots,\beta_m}(\xi) = \frac{2^{-m-n_+(\alpha)-n_-(\beta)}\,\mathrm{i}^m}{\prod_{1\le j<k\le m}(\xi_k-\xi_j)^2[(\xi_k-\xi_j)^2+4]}$$

$$\left[\prod_{j=1}^{p}\int_{\mathcal{C}}\frac{d\omega_j}{2\pi\mathrm{i}}F_{z_j}(\omega_j)\right]\left[\prod_{j=p+1}^{2m}\int_{\mathcal{C}}\frac{d\omega_j}{2\pi\mathrm{i}}\overline{F}_{z_j}(\omega_j)\right]\frac{\det_{2m}\Theta^{(p)}_{j,k}}{\prod_{1\le j<k\le 2m}(\omega_j-\omega_k-2\mathrm{i})}$$

where

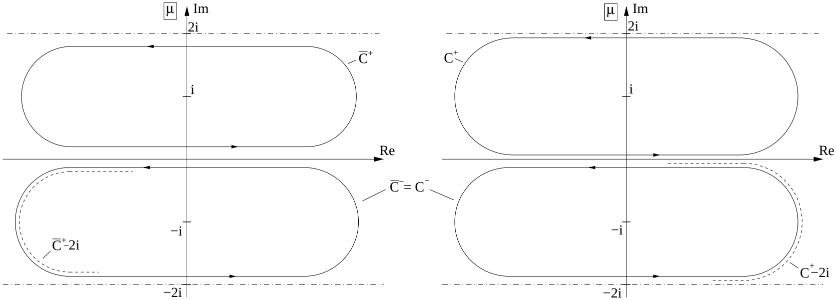
$$\Theta^{(p)}_{j,2k-1} = \begin{cases} G^-(\omega_j,\xi_k) & j=1,\dots,p \\ G^+(\omega_j,\xi_k) & j=p+1,\dots,2m \end{cases}$$

$$\Theta^{(p)}_{j,2k} = \begin{cases} S^-(\omega_j,\xi_k) & j=1,\dots,p \\ S^+(\omega_j,\xi_k) & j=p+1,\dots,2m \end{cases}$$

$$F_\ell(\lambda) = \prod_{k=1}^{m}(\lambda-\xi_k-\mathrm{i})\prod_{k=1}^{\ell-1}(\lambda-\xi_k-3\mathrm{i})\prod_{k=\ell+1}^{m}(\lambda-\xi_k+\mathrm{i}),$$

$$\overline{F}_\ell(\lambda) = \prod_{k=1}^{m}(\lambda-\xi_k+\mathrm{i})\prod_{k=1}^{\ell-1}(\lambda-\xi_k+3\mathrm{i})\prod_{k=\ell+1}^{m}(\lambda-\xi_k-\mathrm{i})$$

Regularization and integration contours



For the regularization in the multiple integral representation the dashed lines show the relative positions of the contours $\mathcal{C}^\pm$, $\overline{\mathcal{C}}^\pm$. We define

$$\mathcal{C} = \mathcal{C}^+ \cup \mathcal{C}^- \quad \overline{\mathcal{C}} = \overline{\mathcal{C}}^+ \cup \overline{\mathcal{C}}^-$$

Regularization necessary to avoid relative singularities stemming from terms of the form

$$\frac{1}{\omega_j - \omega_k - 2i}$$

Corresponds to familiar ‘iε-regularization’ for open contours

Counting the indices

For any two sequences $(\alpha) = (\alpha_n)_{n=1}^m$ and $(\beta) = (\beta_n)_{n=1}^m$ of upper and lower matrix indices we shall obtain a different multiple integral. Let us introduce the notation $n_\sigma(x)$, $\sigma = -, 0, +$, $(x) = (\alpha), (\beta)$, for the number of σs in the sequence (x), e.g. $n_0(\beta)$ is the number of zeros in (β). Then

$$\begin{aligned} n_+(\alpha) + n_0(\alpha) + n_-(\alpha) &= m \\ n_+(\beta) + n_0(\beta) + n_-(\beta) &= m \\ n_+(\beta) - n_-(\beta) - n_+(\alpha) + n_-(\alpha) &= 0 \end{aligned}$$

Here the last equation is equivalent to $2n_+(\alpha) + n_0(\alpha) = 2n_+(\beta) + n_0(\beta)$.
The dependence of the multiple integral on the indices α_j, β_k enters through a sequence $(z) = (z_n)_{n=1}^{2m}$ encoding the positions of $-, 0, +$ in (α) and (β). For the construction of (z) we order the density matrix indices as $\alpha_m, \dots, \alpha_1, \beta_1, \dots, \beta_m$ and inspect them starting from the left. If $\alpha_m = -$ we do nothing, if $\alpha_m = 0$ we define $z_1 = m$, and if $\alpha_m = +$ we define $z_1 = z_2 = m$. We continue this procedure with α_{m-1} and so on. When we have reached α_1 we have defined

$$p = 2n_+(\alpha) + n_0(\alpha)$$

elements of the sequence (z) in this way. If $\beta_1 = -$ we define $z_{p+1} = z_{p+2} = 1$, if $\beta_1 = 0$ we define $z_{p+1} = 1$, and if $\beta_1 = +$ we do nothing. We continue the same way with β_2, β_3 etc. until we end at β_m. The sequence (z) thus constructed has $2n_+(\alpha) + n_0(\alpha) + n_0(\beta) + 2n_-(\beta) = 2m$ elements, and the pair (z), p is in one-to-one correspondence with the sequences (α) and (β). As an example let us consider $(\alpha) = (+, -, 0), \beta = (0, 0, 0)$. Then $z_1 = 3$, $z_2 = z_3 = z_4 = 1$, $z_5 = 2$, $z_6 = 3$, $p = 3$.

Auxiliary functions satisfying linear integral equations

$$
\begin{aligned}
G^+(\lambda,\xi) &= K(\lambda-\xi+\mathrm{i}) - K(\lambda-\xi+3\mathrm{i}) \\
&+ \int_{\mathcal{C}^-} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\overline{\mathfrak{F}}(\mu)}{\mathfrak{B}(\mu)} G^+(\mu,\xi) K(\lambda-\mu) - \int_{\overline{\mathcal{C}}^+} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\mathfrak{F}(\mu)}{\overline{\mathfrak{B}}(\mu)} G^-(\mu,\xi) K(\lambda-\mu+4\mathrm{i}), \qquad \lambda \in \mathcal{C}^- \\
G^-(\lambda,\xi) &= K(\lambda-\xi-3\mathrm{i}) - K(\lambda-\xi-\mathrm{i}) \\
&+ \int_{\overline{\mathcal{C}}^-} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\overline{\mathfrak{F}}(\mu)}{\mathfrak{B}(\mu)} G^+(\mu,\xi) K(\lambda-\mu-4\mathrm{i}) - \int_{\mathcal{C}^+} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\mathfrak{F}(\mu)}{\overline{\mathfrak{B}}(\mu)} G^-(\mu,\xi) K(\lambda-\mu), \qquad \lambda \in \mathcal{C}^+
\end{aligned}
$$

$$
\begin{aligned}
S^+(\lambda,\xi) &= -\mathrm{e}(\lambda-\xi-\mathrm{i}) - \mathrm{e}(\lambda-\xi+3\mathrm{i}) - \frac{1}{Y(\xi)}\big(K(\lambda-\xi+\mathrm{i}) + K(\lambda-\xi+3\mathrm{i})\big) \\
&+ \int_{\mathcal{C}^-} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\overline{\mathfrak{F}}(\mu)}{\mathfrak{B}(\mu)} S^+(\mu,\xi) K(\lambda-\mu) - \int_{\overline{\mathcal{C}}^+} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\mathfrak{F}(\mu)}{\overline{\mathfrak{B}}(\mu)} S^-(\mu,\xi) K(\lambda-\mu+4\mathrm{i}), \qquad \lambda \in \mathcal{C}^- \\
S^-(\lambda,\xi) &= -\mathrm{e}(\lambda-\xi-5\mathrm{i}) - \mathrm{e}(\lambda-\xi-\mathrm{i}) - \frac{1}{Y(\xi)}\big(K(\lambda-\xi-3\mathrm{i}) + K(\lambda-\xi-\mathrm{i})\big) \\
&+ \int_{\overline{\mathcal{C}}^-} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\overline{\mathfrak{F}}(\mu)}{\mathfrak{B}(\mu)} S^+(\mu,\xi) K(\lambda-\mu-4\mathrm{i}) - \int_{\mathcal{C}^+} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{\mathfrak{F}(\mu)}{\overline{\mathfrak{B}}(\mu)} S^-(\mu,\xi) K(\lambda-\mu), \qquad \lambda \in \mathcal{C}^+
\end{aligned}
$$

where

$$
K(\lambda) = \frac{1}{\lambda-2\mathrm{i}} - \frac{1}{\lambda+2\mathrm{i}}, \qquad \mathrm{e}(\lambda) = \frac{1}{\lambda} - \frac{1}{\lambda+2\mathrm{i}}
$$

Auxiliary functions for thermodynamics

The functions $\mathfrak{b}$, $\overline{\mathfrak{b}}$, $\mathfrak{B} = 1 + \mathfrak{b}$, $\overline{\mathfrak{B}} = 1 + \overline{\mathfrak{b}}$ as well as y and $Y = 1 + y$ are familiar from J. Suzuki's 1999 description of the thermodynamics ot the higher spin XXX chains. In addition we need here

$$\mathfrak{f}(\lambda) = \frac{1}{\mathfrak{b}(\lambda - 2i)}, \qquad \overline{\mathfrak{f}}(\lambda) = \frac{1}{\overline{\mathfrak{b}}(\lambda + 2i)}$$

and similar capital functions.

The following nonlinear integral equations are well known

$$\begin{pmatrix} \log y(\lambda) \\ \log \mathfrak{b}_\varepsilon(\lambda) \\ \log \overline{\mathfrak{b}}_\varepsilon(\lambda) \end{pmatrix} = \begin{pmatrix} 0 \\ \Delta_b(\lambda) \\ \Delta_{\overline{b}}(\lambda) \end{pmatrix} + \widehat{\mathcal{K}} * \begin{pmatrix} \log Y(\lambda) \\ \log \mathfrak{B}_\varepsilon(\lambda) \\ \log \overline{\mathfrak{B}}_\varepsilon(\lambda) \end{pmatrix}$$

where $(\widehat{\mathcal{K}} * g)_i$ denotes the matrix convolution $\sum_j \int_{-\infty}^{\infty} \mathrm{d}\mu \, \widehat{\mathcal{K}}_{i,j}(\lambda - \mu) g_j(\mu)$, and

$$\Delta_b(\lambda) = -\frac{h}{T} + d(u, \lambda - i\varepsilon), \quad \Delta_{\overline{b}}(\lambda) = \frac{h}{T} + d(u, \lambda + i\varepsilon)$$

$$d(u,\lambda) = \frac{N}{2} \int_{-\infty}^{\infty} \mathrm{d}k \, e^{-ik\lambda} \frac{\sinh uk}{k \cosh k} \overset{N\to\infty}{\longrightarrow} -\frac{J}{T} \frac{\pi}{2\cosh \pi\lambda/2}, \quad u = -\frac{J}{NT}$$

Auxiliary functions for thermodynamics

The kernel matrix is given by

$$\widehat{\mathcal{K}}(\lambda) = \begin{pmatrix} 0 & \mathcal{K}(\lambda + i\varepsilon) & \mathcal{K}(\lambda - i\varepsilon) \\ \mathcal{K}(\lambda - i\varepsilon) & \mathcal{F}(\lambda) & -\mathcal{F}(\lambda + 2i(1-\varepsilon)) \\ \mathcal{K}(\lambda + i\varepsilon) & -\mathcal{F}(\lambda - 2i(1-\varepsilon)) & \mathcal{F}(\lambda) \end{pmatrix}$$

where

$$\mathcal{K}(\lambda) = \frac{1}{4\cosh \pi\lambda/2}, \quad \mathcal{F}(\lambda) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{-ik\lambda}}{1 + e^{2|k|}}$$

The dominant eigenvalue can represented by integration on straight lines as

$$\ln \Lambda^{[2]}(\lambda) = \ln \Lambda_0^{[2]}(\lambda) - \frac{2h}{T} + \int_{-\infty}^{\infty} d\mu\, \mathcal{K}(\lambda - \mu + i\varepsilon) \ln \mathfrak{B}_\varepsilon(\mu) + \int_{-\infty}^{\infty} d\mu\, \mathcal{K}(\lambda - \mu - i\varepsilon) \ln \overline{\mathfrak{B}}_\varepsilon(\mu)$$

Conclusion

- We have derived a multiple integral representation for the density matrix of the integrable isotropic spin1 chain at finite temperature and finite magnetic field

$$D^{[2]}{}^{\alpha_1,\dots,\alpha_m}_{\beta_1,\dots,\beta_m}(\xi) = \frac{2^{-m-n_+(\alpha)-n_-(\beta)}\, \mathrm{i}^m}{\prod_{1\le j<k\le m}(\xi_k-\xi_j)^2[(\xi_k-\xi_j)^2+4]}$$

$$\left[\prod_{j=1}^{p}\int_{\mathcal{C}}\frac{d\omega_j}{2\pi \mathrm{i}}F_{z_j}(\omega_j)\right]\left[\prod_{j=p+1}^{2m}\int_{\overline{\mathcal{C}}}\frac{d\omega_j}{2\pi \mathrm{i}}\overline{F}_{z_j}(\omega_j)\right]\frac{\det_{2m}\Theta^{(p)}_{j,k}}{\prod_{1\le j<k\le 2m}(\omega_j-\omega_k-2\mathrm{i})}$$

- This provides some evidence that results that were obtained for the spin-$\frac{1}{2}$ XXZ chain may hold more generally
- that the general structure of the static correlation functions of integrable models related to the Yang-Baxter equation may be understood
- that we will be able to develop efficient tools for calculating all static correlation functions of integrable models numerically