

The density matrix of a finite segment of the Heisenberg spin chain

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 $H_{XXZ} = J \sum_{j=1}^{L} \left(\sigma_{j-1}^{x} \sigma_{j}^{x} + \sigma_{j-1}^{y} \sigma_{j}^{y} + \Delta(\sigma_{j-1}^{z} \sigma_{j}^{z} - 1) \right)$

Contents and context



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- Introduction
- Multiple integral formula for the density matrix of a chain segment
- Reduction of the multiple integrals
- Exponential formula for the density matrix
- Summary and outlook

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With Michael Bortz, Herman E. Boos, Jens Damerau, Nils P. Hasenclever, Andreas Klümper, Alexander Seel and Junji Suzuki from 2003

Our contribution: finite temperature T and magnetic field h; arbitrary finite size

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Related work for T, h, 1/L = 0:

- Jimbo et al. 1992, Jimbo & Miwa 1996
- Kitanine, Maillet, Slavnov & Terras 2000, 2002, 2004 ('Lyon group')
- Boos, Korepin, Smirnov 2001, 2002, 2003
- Kato, Nishiyama, Sakai, Sato, Shiroishi, Takahashi, Tsuboi from 2003 ('ISSP group')
- Boos, Jimbo, Miwa, Smirnov & Takeyama from 2004

Introduction



• Ground state correlations for L = 4, $\Delta = 1$. $U|gs\rangle = |gs\rangle$, $S^{\alpha}|gs\rangle = 0$, $\alpha = x, y, z$.

 $|gs\rangle = 2|\downarrow\uparrow\downarrow\uparrow\rangle + 2|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle$

 $\Rightarrow \langle gs | gs \rangle = 12$, $\langle \sigma_j^{\alpha} \rangle = 0$ perfectly homogeneous, no structure

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 $\Rightarrow \langle gs | gs \rangle = 12$, $\langle \sigma_i^{\alpha} \rangle = 0$ perfectly homogeneous, no structure



For translationally invariant systems structure reveals itself in the two-point functions

The thermodynamic limit



- One is often interested in $L \rightarrow \infty$, thermodynamic limit
- Above method can be carried out by hand up to L = 10 lattice sites ($2^{10} \sim 10^3$, $S^z = 0$: $\binom{10}{5} = 252$) (Hulthén 1938)
- Using a computer we gain a further factor of 3 or 4 in the system size ($2^{30} = (2^{10})^3 \sim 10^9$).

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- Using a computer we gain a further factor of 3 or 4 in the system size ($2^{30} = (2^{10})^3 \sim 10^9$).
- Analytical solution: $\langle S_1^z S_{n+1}^z \rangle = \frac{1}{4} \langle \sigma_1^z \sigma_{n+1}^z \rangle$ from multiple integral formula and functional equations

	L = 4	L = 6	$L ightarrow \infty$
n = 1	$-\frac{1}{6}$	$-\frac{1}{4(\sqrt{13}-2)}$	$\frac{1}{12} - \frac{\ln 2}{3} \simeq -0.148$
n = 2	$\frac{1}{12}$	$\frac{1}{4\sqrt{13}}$	$\frac{1}{12} - \frac{4\ln 2}{3} + \frac{3\zeta(3)}{4} \simeq 0,061$
<i>n</i> = 3	—	$-rac{29}{4(65+8\sqrt{13})}$	$\frac{1}{12} - 3\ln 2 + \frac{37\zeta(3)}{6} - \frac{14\zeta(3)\ln 2}{3} - \frac{3\zeta^2(3)}{2} - \frac{125\zeta(5)}{24} + \frac{25\zeta(5)\ln 2}{3} \simeq -0.050$
<i>n</i> = 4	—	—	$\simeq 0.034652776982$
<i>n</i> = 5	—	—	$\simeq -0.030890366647$
<i>n</i> = 6	_	—	$\simeq 0.024446738328$
<i>n</i> = 7	_	_	$\simeq -0.022498222763$

n = 1 Hulthén 1938, n = 2 Takahashi 1977, n = 3, ..., 7 ISSP group 2003-05

Finite size



L	$\langle \sigma_1^z \sigma_2^z \rangle$	$\langle \sigma_1^z \sigma_3^z \rangle$
2	-1.000000000000000000000000000000000000	_
4	-0.666666666666666	0.3333333333333333
6	-0.62283903060711	0.27735009811261
8	-0.60851556815620	0.26103720534839
16	-0.59519136338473	0.24696584167998
32	-0.59193864328956	0.24374937989865
64	-0.59113127886152	0.24297329183505
128	-0.59092994011745	0.24278223127753
256	-0.59087965782193	0.24273481483257
512	-0.59086709385781	0.24272300601642
1024	-0.59086395383499	0.24272006021644
∞	-0.59086290741326	0.24271907982574

zz-correlators as functions of the system size

Finite size n = 1



• Finite size data from integral formula (with J. Damerau, N. P. Hasenclever, A. Klümper)



Finite size n = 2



• Finite size data from integral formula (with J. Damerau, N. P. Hasenclever, A. Klümper)





• All properties of the XXZ chain can be derived from the well-known trigonometric solution

$$R(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

of the Yang-Baxter equation, where

$$b(\lambda) = rac{\operatorname{sh}(\lambda)}{\operatorname{sh}(\lambda + \eta)}, \ c(\lambda) = rac{\operatorname{sh}(\eta)}{\operatorname{sh}(\lambda + \eta)}$$



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• This *R*-matrix generates the XXZ Hamiltonian

$$H_{XXZ} = 2J \operatorname{sh}(\eta) \sum_{j=1}^{L} \partial_{\lambda} (PR)_{j-1,j}(\lambda) \Big|_{\lambda=0}$$

P transposition in $\mathbb{C}^2 \otimes \mathbb{C}^2$, $\Delta = ch(\eta)$.



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• Setting $\Theta = diag(e^{i\Phi}, e^{-i\Phi}), \Phi \in [0, 2\pi]$, we fix twisted boundary conditions requiring that

$$\begin{pmatrix} e_{0}{}_{1}^{1} & e_{0}{}_{2}^{1} \\ e_{0}{}_{1}^{2} & e_{0}{}_{2}^{2} \end{pmatrix} = \Theta \begin{pmatrix} e_{L}{}_{1}^{1} & e_{L}{}_{2}^{1} \\ e_{L}{}_{1}^{2} & e_{L}{}_{2}^{2} \end{pmatrix} \Theta^{-1}$$



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• Setting $\Theta = diag(e^{i\Phi}, e^{-i\Phi}), \Phi \in [0, 2\pi]$, we fix twisted boundary conditions requiring that

$$\begin{pmatrix} e_0 & 1 & e_0 & 1 \\ e_0 & 1 & e_0 & 2 \\ e_0 & 1 & e_0 & 2 \end{pmatrix} = \Theta \begin{pmatrix} e_L & 1 & e_L & 1 \\ e_L & 1 & e_L & 2 \\ e_L & 1 & e_L & 2 \end{pmatrix} \Theta^{-1}$$

L-matrix

$$L_{j\beta}^{\alpha}(\lambda) = R^{\alpha\gamma}_{\beta\delta}(\lambda) e_{j\gamma}^{\delta}$$

Monodromy matrix

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix} = \Theta L_L(\lambda) \dots L_1(\lambda)$$

Yang-Baxter algebra

$$\check{R}(\lambda-\mu)(T(\lambda)\otimes T(\mu)) = (T(\mu)\otimes T(\lambda))\check{R}(\lambda-\mu)$$

where $\check{R} = PR$. Twisted transfer matrix $t(\lambda) = tr T(\lambda)$.



• Algebraic Bethe ansatz for eigenstates of $t(\lambda)$

$$|\{\lambda\}\rangle = B(\lambda_1 - \frac{\eta}{2}) \dots B(\lambda_N - \frac{\eta}{2})|0\rangle$$

 $\binom{1}{0}^{\otimes L}$ is the ferromagnetic reference state, and the set of Bethe roots $\{\lambda\} = \{\lambda_j\}_{j=1}^N$ must be determined from the Bethe ansatz equations

$$1 + \frac{\mathrm{e}^{-2\mathrm{i}\Phi} \mathrm{sh}^{L}(\lambda_{j} - \frac{\eta}{2})}{\mathrm{sh}^{L}(\lambda_{j} + \frac{\eta}{2})} \prod_{k=1}^{N} \frac{\mathrm{sh}(\lambda_{j} - \lambda_{k} + \eta)}{\mathrm{sh}(\lambda_{j} - \lambda_{k} - \eta)} = 0$$
$$j = 1, \dots, N$$



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 $j = 1, \ldots, N$

• Ground state of the XXZ Hamiltonian is the transfer matrix eigenstate with $\{\lambda_j\}_{j=1}^{L/2}$ the unique real solution of the Bethe ansatz equations for N = L/2. It determines a meromorphic auxiliary function

$$\mathfrak{a}(\lambda) = \frac{\mathrm{e}^{-2\mathrm{i}\Phi} \mathrm{sh}^{L}(\lambda - \frac{\eta}{2})}{\mathrm{sh}^{L}(\lambda + \frac{\eta}{2})} \prod_{k=1}^{L/2} \frac{\mathrm{sh}(\lambda - \lambda_{k} + \eta)}{\mathrm{sh}(\lambda - \lambda_{k} - \eta)}$$



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• In terms of this function the ground state eigenvalue $\Lambda_0(\lambda)$ becomes

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• Bethe ansatz equations imply that $\Lambda_0(\lambda)$ is regular at the points $\lambda_j - \frac{\eta}{2}$, $j = 1, \ldots, L/2$. Extensive numerical studies support the conjecture that $\Lambda_0(\lambda)$ is non-zero inside a strip $-|\eta| \leq \mathrm{Im}\,\lambda \leq 0$. Then $1 + \mathfrak{a}(\lambda)$ is analytic inside the strip $-\frac{|\eta|}{2} < \mathrm{Im}\,\lambda \leq \frac{|\eta|}{2}$ and its only zeros in this strip are the Bethe roots. This together with the obvious analytic and asymptotic properties of $\mathfrak{a}(\lambda)$ is enough to set up a set of functional equations for the second logarithmic derivatives of $\mathfrak{a}(\lambda)$ and $1 + \mathfrak{a}(\lambda)$ which together with their known asymptotics determine $\mathfrak{a}(\lambda)$ uniquely.

Auxiliary function



• Non-linear integral equation

$$\ln \mathfrak{a}(\lambda) = -2i\Phi + L\eta + L\ln\left(\frac{\mathrm{sh}(\lambda - \frac{\eta}{2})}{\mathrm{sh}(\lambda + \frac{\eta}{2})}\right) - \int_{\mathfrak{C}} \frac{\mathrm{d}\omega}{2\pi} K_{\eta}(\lambda - \omega)\ln(1 + \mathfrak{a}(\omega))$$



The canonical contour (for the critical regime) ${\mathcal C}$ surrounds the real axis in counterclockwise manner inside the strip $-\frac{|\eta|}{2} < {\rm Im}\,\lambda < \frac{|\eta|}{2}$

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• The kernel $K_{\eta}(\lambda)$ is defined as

$$K_{\eta}(\lambda) = \frac{\operatorname{sh}(2\eta)}{\operatorname{i}\operatorname{sh}(\lambda - \eta)\operatorname{sh}(\lambda + \eta)}$$

The ground state eigenvalue $\Lambda_0(\lambda)$ can be expressed as an integral over $\mathfrak{a}(\lambda)$,

$$\ln \Lambda_0(\lambda) = i\Phi + \frac{L(i\pi - \eta)}{2} + \int_{\mathcal{C}} \frac{d\omega}{2\pi} K_{\frac{\eta}{2}}(\lambda - \omega) \ln(1 + \mathfrak{a}(\omega))$$

This determines the ground state energy and the eigenvalues of the higher conserved quantities as a function of L.



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Density matrix of a finite segment

• The density matrix is a means to describe a sub-system as part of a larger system in thermodynamic equilibrium in terms of the degrees of freedom of the sub-system.

$$\rho_L = \frac{\mathrm{e}^{-\frac{H}{T}}}{\mathrm{tr}\,\mathrm{e}^{-\frac{H}{T}}}$$

statistical operator for chain at temperature T. Then the density matrix of the sub-system consisting of the first m lattice sites is

$$D_L(T) = \operatorname{tr}_{m+1...L} \rho_L$$





$$p_L = \frac{e^{-\frac{H}{T}}}{\operatorname{tr} e^{-\frac{H}{T}}}$$

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• Thermal average of an operator A acting non-trivially only on sites 1 to m

$$tr_{1...L}A\rho_L = tr_{1...m}A_{1...m}tr_{m+1...L}\rho_L$$
$$= tr_{1...m}A_{1...m}D_L(T)$$

where $A_{1...m}$ is the restriction of A to sites 1 to m





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• Thermal average of an operator A acting non-trivially only on sites 1 to m

$$\operatorname{tr}_{1...L} A \rho_L = \operatorname{tr}_{1...m} A_{1...m} \operatorname{tr}_{m+1...L} \rho_L$$
$$= \operatorname{tr}_{1...m} A_{1...m} D_L(T)$$

where $A_{1...m}$ is the restriction of A to sites 1 to m

• If we follow the common convention and use the same symbols for the local operators $e_{j\beta}^{\alpha}$ and for their restriction to the first *m* sites, we find the expression

$$D_{L_{\beta_1...\beta_m}}^{\alpha_1...\alpha_m}(T) = \operatorname{tr}_{1...m} e_1_{\beta_1}^{\alpha_1} \dots e_m_{\beta_m}^{\alpha_m} D_L(T)$$
$$= \langle e_1_{\beta_1}^{\alpha_1} \dots e_m_{\beta_m}^{\alpha_m} \rangle_T$$

for the matrix elements of the density matrix.



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• Thermal average of an operator *A* acting non-trivially only on sites 1 to *m*

$$\operatorname{tr}_{1...L} A \rho_L = \operatorname{tr}_{1...m} A_{1...m} \operatorname{tr}_{m+1...L} \rho_L$$
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for the matrix elements of the density matrix.

• Here we are interested in the unique (normalized) ground state $|\Psi_0\rangle$ of the system of finite even length. In the limit $T \rightarrow 0+$ the statistical operator ρ_L converges to the projector $|\Psi_0\rangle\langle\Psi_0|$ onto the ground state, and the formula for the density matrix elements turns into

$$D_{L\beta_{1}...\beta_{m}}^{\alpha_{1}...\alpha_{m}} = \lim_{T \to 0+} D_{L\beta_{1}...\beta_{m}}^{\alpha_{1}...\alpha_{m}}(T)$$
$$= \langle \Psi_{0} | e_{1\beta_{1}}^{\alpha_{1}} \dots e_{m\beta_{m}}^{\alpha_{m}} | \Psi_{0} \rangle$$

Density matrix of a finite segment



• We use a trick suggested in [KMT99] in order to express this entirely in terms of data related to the monodromy matrix $T(\lambda)$

$$e_{j\beta}^{\alpha} = t^{j-1}(0)T_{\beta}^{\alpha}(0)t^{-j}(0)$$

It follows that

$$D_{L_{\beta_1\dots\beta_m}}^{\alpha_1\dots\alpha_m} = \langle \Psi_0 | T_{\beta_1}^{\alpha_1}(0) \dots T_{\beta_m}^{\alpha_m}(0) t^{-m}(0) | \Psi_0 \rangle$$

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• In order to apply the techniques developed in [GKS04] for the finite-temperature case we regularize the expression by introducing inhomogeneity parameters ξ_j , j = 1, ..., m, in the following way. Define an 'inhomogeneous density matrix'

$$D_{L\beta_{1}...\beta_{m}}^{\alpha_{1}...\alpha_{m}}(\xi_{1},\ldots,\xi_{m}) = \frac{\langle\{\lambda\}|T_{\beta_{1}}^{\alpha_{1}}(\xi_{1}-\frac{\eta}{2})\ldots T_{\beta_{m}}^{\alpha_{m}}(\xi_{m}-\frac{\eta}{2})|\{\lambda\}\rangle}{\langle\{\lambda\}|\{\lambda\}\rangle\prod_{j=1}^{m}\Lambda_{0}(\xi_{j}-\frac{\eta}{2})}$$

where $|\{\lambda\}\rangle$ is the (unnormalized) Bethe ansatz ground state. Then

$$D_{L_{\beta_1...\beta_m}}^{\alpha_1...\alpha_m} = \lim_{\xi_1,...,\xi_m \to \frac{\eta}{2}} D_{L_{\beta_1...\beta_m}}^{\alpha_1...\alpha_m}(\xi_1,\ldots,\xi_m)$$

Integral representation



• The inhomogeneous density matrix element for the ground state of the chain of finite length

$$D_{L\beta_{1}...\beta_{m}}^{\alpha_{1}...\alpha_{m}}(\xi_{1},...,\xi_{m}) = \left[\prod_{j=1}^{|\alpha^{+}|} \int_{\mathcal{C}} \frac{d\omega_{j}}{2\pi i(1+\mathfrak{a}(\omega_{j}))} \prod_{k=1}^{x_{j}-1} \operatorname{sh}(\omega_{j}-\xi_{k}-\eta) \prod_{k=x_{j}+1}^{m} \operatorname{sh}(\omega_{j}-\xi_{k})\right]$$
$$\left[\prod_{j=|\alpha^{+}|+1}^{m} \int_{\mathcal{C}} \frac{d\omega_{j}}{2\pi i(1+\overline{\mathfrak{a}}(\omega_{j}))} \prod_{k=1}^{y_{j}-1} \operatorname{sh}(\omega_{j}-\xi_{k}+\eta) \prod_{k=y_{j}+1}^{m} \operatorname{sh}(\omega_{j}-\xi_{k})\right]$$
$$\frac{\det(-G(\omega_{j},\xi_{k}))}{\prod_{1\leq j\leq k\leq m} \operatorname{sh}(\xi_{k}-\xi_{j}) \operatorname{sh}(\omega_{j}-\omega_{k}-\eta)}$$

where $\overline{\mathfrak{a}} = 1/\mathfrak{a}$ and where the function $G(\omega, \xi)$ has to be calculated from the linear integral equation

$$G(\lambda,\xi) = \frac{\operatorname{sh}(\eta)}{\operatorname{sh}(\lambda-\xi)\operatorname{sh}(\lambda-\xi-\eta)} + \int_{\mathbb{C}} \frac{d\omega G(\omega,\xi)}{2\pi(1+\mathfrak{a}(\omega))} K_{\eta}(\lambda-\omega)$$

Integral representation



• The inhomogeneous density matrix element for the ground state of the chain of finite length

$$D_{L\beta_{1}...\beta_{m}}^{\alpha_{1}...\alpha_{m}}(\xi_{1},...,\xi_{m}) = \left[\prod_{j=1}^{|\alpha^{+}|} \int_{\mathbb{C}} \frac{d\omega_{j}}{2\pi i(1+\mathfrak{a}(\omega_{j}))} \prod_{k=1}^{x_{j}-1} \operatorname{sh}(\omega_{j}-\xi_{k}-\eta) \prod_{k=x_{j}+1}^{m} \operatorname{sh}(\omega_{j}-\xi_{k})\right]$$
$$\left[\prod_{j=|\alpha^{+}|+1}^{m} \int_{\mathbb{C}} \frac{d\omega_{j}}{2\pi i(1+\overline{\mathfrak{a}}(\omega_{j}))} \prod_{k=1}^{y_{j}-1} \operatorname{sh}(\omega_{j}-\xi_{k}+\eta) \prod_{k=y_{j}+1}^{m} \operatorname{sh}(\omega_{j}-\xi_{k})\right]$$
$$\frac{\det(-G(\omega_{j},\xi_{k}))}{\prod_{1\leq j\leq k\leq m} \operatorname{sh}(\xi_{k}-\xi_{j}) \operatorname{sh}(\omega_{j}-\omega_{k}-\eta)}$$

where $\overline{\mathfrak{a}} = 1/\mathfrak{a}$ and where the function $G(\omega, \xi)$ has to be calculated from the linear integral equation

$$G(\lambda,\xi) = \frac{\operatorname{sh}(\eta)}{\operatorname{sh}(\lambda-\xi)\operatorname{sh}(\lambda-\xi-\eta)} + \int_{\mathcal{C}} \frac{d\omega G(\omega,\xi)}{2\pi(1+\mathfrak{a}(\omega))} K_{\eta}(\lambda-\omega)$$

• For the chain at finite T with external magnetic field h replace the auxiliary function with the solution of

$$\ln \mathfrak{a}(\lambda) = -\frac{h}{T} - \frac{2J \operatorname{sh}^2(\eta)}{T \operatorname{sh}(\lambda) \operatorname{sh}(\lambda + \eta)} - \int_{\mathfrak{C}} \frac{\mathrm{d}\omega}{2\pi} K_{\eta}(\lambda - \omega) \ln(1 + \mathfrak{a}(\omega))$$

Multiple integrals numerically



• Numerical evaluation of multiple integrals for m = 3, temperature case





- Multiple integrals for T, h = 0: M. Jimbo et al. 92, M. Jimbo and T. Miwa 96, N. Kitanine et al. 00
- Were considered rather useless for practical calculations, since the numerical costs grow exponentially with the number of integrations for multiple integral
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- What is behind?

Theorem (H. E. Boos et al. 05). The inhomogeneous correlation functions of the isotropic Heisenberg chain at T, h = 0 depend on a single transcendental function

$$\psi_0(\xi_1,\xi_2) = 2i \partial_x \ln \left[\frac{\Gamma(\frac{1}{2} + \frac{ix}{2})\Gamma(1 - \frac{ix}{2})}{\Gamma(\frac{1}{2} - \frac{ix}{2})\Gamma(1 + \frac{ix}{2})} \right]_{x=\xi_1 - \xi_2}$$

which is proportional to the two-spinon scattering phase (for XXZ two functions, for XYZ three).



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• Why do ζ-functions appear?

$$\psi_0(\xi_1,\xi_2) = 4\sum_{k=0}^{\infty} (-1)^k (\xi_1 - \xi_2)^{2k} \zeta_a(2k+1), \qquad \zeta_a(z) = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{k^z} = \begin{cases} (1-2^{1-z})\zeta(z) & \text{if } z \neq 1\\ \ln 2 & \text{if } z = 1 \end{cases}$$



Consider the inhomogeneous emptiness formation probability for the XXX chain

$$D_{11}^{11}(\xi_1,\xi_2)(\xi_1-\xi_2) = \int_C \frac{d\omega_1}{2\pi(1+\mathfrak{a}(\omega_1))} \int_C \frac{d\omega_2}{2\pi(1+\mathfrak{a}(\omega_2))} \det(G(\omega_j,\xi_k)) \underbrace{\frac{(\omega_1-\xi_1-i)(\omega_2-\xi_2)}{\omega_1-\omega_2-i}}_{=:r(\omega_1,\omega_2)}$$
$$= \frac{1}{2} \int_C \frac{d\omega_1}{2\pi(1+\mathfrak{a}(\omega_1))} \int_C \frac{d\omega_2}{2\pi(1+\mathfrak{a}(\omega_2))} \det(G(\omega_j,\xi_k)) \left(r(\omega_1,\omega_2)-r(\omega_2,\omega_1)\right)$$



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$$=\frac{1}{2}\int_{C}\frac{d\omega_{1}}{2\pi(1+\mathfrak{a}(\omega_{1}))}\int_{C}\frac{d\omega_{2}}{2\pi(1+\mathfrak{a}(\omega_{2}))}\det(G(\omega_{j},\xi_{k}))(r(\omega_{1},\omega_{2})-r(\omega_{2},\omega_{1}))$$

Here

$$r(\omega_1, \omega_2) - r(\omega_2, \omega_1) = \frac{(\omega_1 - \xi_1 - i)(\omega_2 - \xi_2)}{\omega_1 - \omega_2 - i} + \frac{(\omega_2 - \xi_1 - i)(\omega_1 - \xi_2)}{\omega_1 - \omega_2 + i} = \frac{P(\omega_1, \omega_2)}{1 + (\omega_1 - \omega_2)^2}$$



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$$=\frac{1}{2}\int_{C}\frac{d\omega_{1}}{2\pi(1+\mathfrak{a}(\omega_{1}))}\int_{C}\frac{d\omega_{2}}{2\pi(1+\mathfrak{a}(\omega_{2}))}\det(G(\omega_{j},\xi_{k}))(r(\omega_{1},\omega_{2})-r(\omega_{2},\omega_{1}))$$

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The polynomial $P(\omega_1, \omega_2)$ can be decomposed in such a way that

$$\frac{P(\omega_1, \omega_2)}{1 + (\omega_1 - \omega_2)^2} = -\frac{2}{3}(\omega_1 - \omega_2) + \frac{p(\omega_1) - p(\omega_2)}{1 + (\omega_1 - \omega_2)^2}$$

where

$$p(\omega) = \frac{2}{3}\omega^3 - (\xi_1 + \xi_2 + i)\omega^2 + \left[i(\xi_1 + \xi_2 + \frac{i}{3}) + 2\xi_1\xi_2\right]\omega$$



Then

$$D_{11}^{11}(\xi_1,\xi_2)(\xi_1-\xi_2) = \frac{1}{4} \sum_{P \in \mathfrak{S}^2} \operatorname{sign}(P) \int_C \frac{d\omega_1 G(\omega_1,\xi_{P1})}{\pi(1+\mathfrak{a}(\omega_1))} \int_C \frac{d\omega_2 G(\omega_2,\xi_{P2})}{\pi(1+\mathfrak{a}(\omega_2))} \left[-\frac{2}{3}\omega_1 + \frac{p(\omega_1)}{1+(\omega_1-\omega_2)^2} \right]$$



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This can be reduced by means of the integral equation for $G(\omega, \xi)$,

$$\int_{C} \frac{d\omega_2 G(\omega_2, \xi_{P2})}{\pi (1 + \mathfrak{a}(\omega_2))} \frac{1}{1 + (\omega_1 - \omega_2)^2} = G(\omega_1, \xi_{P2}) + \frac{1}{(\omega_1 - \xi_{P2})(\omega_1 - \xi_{P2} - i)}$$



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Finally (H. E. Boos, FG, A. Klümper, J. Suzuki 06)

$$D_{11}^{11}(\xi_1,\xi_2)(\xi_1-\xi_2) = \sum_{P\in\mathfrak{S}^2} \operatorname{sign}(P) \left[\frac{1}{12} (3\xi_{P1}-\xi_{P2}+i)\phi_1(\xi_{P1}) + \frac{1}{6}\phi_2(\xi_{P2}) - \frac{1}{6}\phi_1(\xi_{P1})\phi_2(\xi_{P2}) - \frac{1}{24} (\xi_{P1}-\xi_{P2})(1+(\xi_{P1}-\xi_{P2})^2)\psi(\xi_{P1},\xi_{P2}) \right]$$

where

$$\Psi(\xi_1,\xi_2) = \int_C \frac{d\omega}{\pi(1+\mathfrak{a}(\omega))} \frac{G(\omega,\xi_1)}{(\omega-\xi_2)(\omega-\xi_2-i)}, \qquad \phi_j(\xi) = \int_C \frac{d\omega\,\omega^{j-1}G(\omega,\xi)}{\pi(1+\mathfrak{a}(\omega))}$$



The functions ψ generalizes the 'two-spinon scattering phase' to finite temperature and magnetic field

 $\lim_{T\to 0}\lim_{h\to 0}\psi(\xi_1,\xi_2)=\psi_0(\xi_1,\xi_2)$

Instead of $\psi(\xi_1,\xi_2)$ we shall rather use the closely related expression

 $\gamma(\xi_1,\xi_2) = \left[1 + (\xi_1 - \xi_2)^2\right] \psi(\xi_1,\xi_2) - 1$

in terms of which our final formulae look neater. We also define $\lim_{h\to 0} \gamma(\xi_1, \xi_2) =: \gamma_0(\xi_1, \xi_2)$.



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in terms of which our final formulae look neater. We also define $\lim_{h\to 0} \gamma(\xi_1, \xi_2) =: \gamma_0(\xi_1, \xi_2)$. In the same limit the moments $\phi_j(\xi)$ become polynomials of order j-1 in ξ ,

$$\lim_{T \to 0} \lim_{h \to 0} \phi_j(\xi) = \phi_j^{(0)}(\xi) = (-i\partial_k)^{j-1} \left. \frac{2e^{ik\xi}}{1+e^k} \right|_{k=0}$$

Using these polynomials we define the 'normalized moments' $\varphi_j(\xi) = \phi_j(\xi) - \phi_j^{(0)}(\xi)$ which vanish for $T, h \to 0$. We further introduce the symmetric combinations

$$\Delta_n(\xi_1,\ldots,\xi_n) = \frac{\det(\varphi_j(\xi_k))\big|_{j,k=1,\ldots,n}}{\prod_{1\leq j< k\leq n}\xi_{kj}}$$

with the shorthand notation $\xi_{kj} = \xi_k - \xi_j$.



Emptiness formation probability for m = 3.

$$D_{111}^{111}(\xi_1,\xi_2,\xi_3) = \frac{1}{24} + \frac{1+5\xi_{12}\xi_{13}}{40\xi_{12}\xi_{13}}\Delta_1(\xi_1) + \frac{1+2\xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\Delta_2(\xi_1,\xi_2) + \frac{1}{60}\Delta_3(\xi_1,\xi_2,\xi_3) + \frac{1-\xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\gamma(\xi_1,\xi_2) - \frac{3+2\xi_{12}^2+5\xi_{13}\xi_{23}}{120\xi_{13}\xi_{23}}\gamma(\xi_1,\xi_2)\Delta_1(\xi_3) + \text{cyclic permutations.}$$



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In the limit of vanishing magnetic field $\Delta_j
ightarrow 0$, and our result reduces to

$$D_{111}^{111}(\xi_1,\xi_2,\xi_3) = \frac{1}{24} + \frac{1 - \xi_{13}\xi_{23}}{24\xi_{13}\xi_{23}}\gamma_0(\xi_1,\xi_2) + \text{cyclic permutations.}$$

Note that the only effect of taking the limit $T \to 0$ here is that the function $\gamma_0(\xi_1, \xi_2)$ changes into its zero temperature form.



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The two-point functions for m = 3.

$$\langle \boldsymbol{\sigma}_{1}^{z}\boldsymbol{\sigma}_{3}^{z} \rangle_{T,h} = \frac{2}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) - \frac{1}{6}(\Delta_{2})_{xx}(0,0) + \frac{1}{3}(\Delta_{2})_{xy}(0,0) - \frac{1}{6}\gamma_{xx}(0,0) + \frac{1}{3}\gamma_{xy}(0,0) \\ \langle \boldsymbol{\sigma}_{1}^{x}\boldsymbol{\sigma}_{3}^{x} \rangle_{T,h} = -\frac{1}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) + \frac{1}{12}(\Delta_{2})_{xx}(0,0) - \frac{1}{6}(\Delta_{2})_{xy}(0,0) - \frac{1}{6}\gamma_{xx}(0,0) + \frac{1}{3}\gamma_{xy}(0,0) \\ \langle \boldsymbol{\sigma}_{1}^{x}\boldsymbol{\sigma}_{3}^{x} \rangle_{T,h} = -\frac{1}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) + \frac{1}{12}(\Delta_{2})_{xx}(0,0) - \frac{1}{6}(\Delta_{2})_{xy}(0,0) - \frac{1}{6}\gamma_{xx}(0,0) + \frac{1}{3}\gamma_{xy}(0,0) \\ \langle \boldsymbol{\sigma}_{1}^{x}\boldsymbol{\sigma}_{3}^{x} \rangle_{T,h} = -\frac{1}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) + \frac{1}{12}(\Delta_{2})_{xx}(0,0) - \frac{1}{6}(\Delta_{2})_{xy}(0,0) - \frac{1}{6}\gamma_{xx}(0,0) + \frac{1}{3}\gamma_{xy}(0,0) \\ \langle \boldsymbol{\sigma}_{1}^{x}\boldsymbol{\sigma}_{3}^{x} \rangle_{T,h} = -\frac{1}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) + \frac{1}{12}(\Delta_{2})_{xx}(0,0) - \frac{1}{6}(\Delta_{2})_{xy}(0,0) - \frac{1}{6}\gamma_{xx}(0,0) + \frac{1}{3}\gamma_{xy}(0,0) \\ \langle \boldsymbol{\sigma}_{1}^{x}\boldsymbol{\sigma}_{3}^{x} \rangle_{T,h} = -\frac{1}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) + \frac{1}{12}(\Delta_{2})_{xx}(0,0) - \frac{1}{6}(\Delta_{2})_{xy}(0,0) - \frac{1}{6}\gamma_{xx}(0,0) + \frac{1}{3}\gamma_{xy}(0,0) \\ \langle \boldsymbol{\sigma}_{1}^{x}\boldsymbol{\sigma}_{3}^{x} \rangle_{T,h} = -\frac{1}{3}\Delta_{2}(0,0) - \frac{1}{3}\gamma(0,0) + \frac{1}{12}(\Delta_{2})_{xx}(0,0) - \frac{1}{6}(\Delta_{2})_{xy}(0,0) -$$

Exponential formula



Conjecture. The density matrix of a finite sub-chain of length *m* of the infinite XXX Heisenberg chain at finite *T* (for h = 0) is determined by the vector

$$h_{m}(\lambda_{1},...,\lambda_{m}) = \frac{1}{2^{m}} e^{\Omega_{m}^{T}(\lambda_{1},...,\lambda_{m})} \mathbf{s}_{m}, \qquad \mathbf{s}_{m} = \prod_{j=1}^{m} s_{j,\bar{j}},$$

$$\Omega_{m}^{T}(\lambda_{1},...,\lambda_{m}) = \frac{(-1)^{(m-1)}}{4} \int \int \frac{d\mu_{1}}{2\pi i} \frac{d\mu_{2}}{2\pi i} \frac{\gamma_{0}(i\mu_{1},i\mu_{2})(\mu_{1}-\mu_{2})}{[1-(\mu_{1}-\mu_{2})^{2}]^{2}} \times \operatorname{tr}_{\mu_{1,2},2,2} \left\{ T\left(\frac{\mu_{1}+\mu_{2}}{2};\lambda_{1},...,\lambda_{m}\right) \otimes \left[T(\mu_{1};\lambda_{1},...,\lambda_{m}) \otimes T(\mu_{2};\lambda_{1},...,\lambda_{m}) \mathcal{P}^{-}\right] \right\},$$

through

$$h_m^{\varepsilon_1,\ldots,\varepsilon_m,\bar{\varepsilon}_m,\ldots,\bar{\varepsilon}_1}(\lambda_1,\ldots,\lambda_m) = D_{(3+\bar{\varepsilon}_1)/2,\ldots,(3+\bar{\varepsilon}_m)/2}^{(3-\varepsilon_1)/2,\ldots,(3-\varepsilon_m)/2}(\xi_1,\ldots,\xi_m) \cdot \prod_{j=1}^m (-\bar{\varepsilon}_j),$$

where $\lambda_j = -i\xi_j$ for j = 1, ..., m. By the integral over μ_1, μ_2 it is meant to take the residues at the poles $\lambda_1, ..., \lambda_m$ of the integrand.

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$$h_{m}^{\varepsilon_{1},...,\varepsilon_{m},\bar{\varepsilon}_{m},...,\bar{\varepsilon}_{1}}(\lambda_{1},...,\lambda_{m}) = D_{(3+\bar{\varepsilon}_{1})/2,...,(3+\bar{\varepsilon}_{m})/2}^{(3-\varepsilon_{1})/2,...,(3-\varepsilon_{m})/2}(\xi_{1},...,\xi_{m}) \cdot \prod_{j=1}^{m} (-\bar{\varepsilon}_{j}),$$

where $\lambda_j = -i\xi_j$ for j = 1, ..., m. By the integral over μ_1 , μ_2 it is meant to take the residues at the poles $\lambda_1, ..., \lambda_m$ of the integrand.

In the zero temperature limit this was proved in 2005 by H. E. Boos et al. by means of the reduced qKZ equation.



- Summary
 - (i) Multiple integral formula for density matrix (finite T, h, thermodynamic limit performed analytically, or ground state for finite L and twist Φ)
 - (ii) reduction (separation) of integrals for XXX even for finite T, h (finite L, Φ)
 - (iii) Finite temperature (finite length) exponential formula (h = 0) for XXX



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- Further results
 - (i) Multiple integral formulae for two-point function (resummation of density matrix elements) (FG, N. P. Hasenclever and A. Seel 05)
 - (ii) Limiting cases, Ising and XX, analytically from the integrals (FG and A. Seel 06)
 - (iii) Open XXZ chain with boundary fields (FG, M. Bortz and H. Frahm 05)
 - (iv) High order high temperature expansions (Z. Tsuboi and M. Shiroishi 05)
 - (v) Exponential formula for XXZ with T and h finite (H. E. Boos, FG, A. Klümper, J. Suzuki unpublished)
 - (vi) Inclusion of a disorder parameter and reformulation of the exponential formula in the spirit of CFT (H. E. Boos, M. Jimbo, T. Miwa, F. A. Smirnov, Y. Takeyama)
 - (vii) 'Phenomenological disorder parameter' for the finite temperature case (H. E. Boos, FG, A. Klümper, J. Suzuki unpublished)