

# Factorization of density matrix elements of higher spin chains at $T > 0$

Junji Suzuki

Shizuoka University

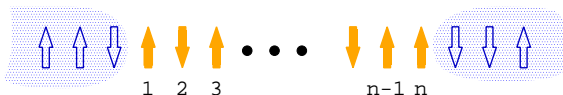
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Based on Collaboration with  
A. Klümper, F. Göhmann, D. Nawrath, A. Seel ...

# Reduced Density Matrix Elements

A measure of correlations in finite segments of quantum spin chains.

- (reduced) Density Matrix Elements (DME)



$$D_n := \langle E_1 \otimes E_2 \cdots \otimes E_n \rangle$$

$$(D_n)_{\alpha_1, \alpha_2, \dots, \alpha_n}^{\beta_1, \beta_2, \dots, \beta_n} := \langle E_{\beta_1}^{\alpha_1} E_{\beta_2}^{\alpha_2} \cdots E_{\beta_n}^{\alpha_n} \rangle \quad (E_{\beta}^{\alpha})_j^i := \delta_{\alpha, i} \delta_{\beta, j}$$

can be used to evaluate

- short correlation functions
- entanglement entropy



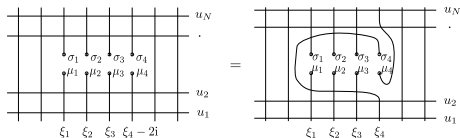
# Success story: $S = \frac{1}{2}$ at $T = 0$

- Multiple integral formula for  $D_n(\xi_1, \dots, \xi_n)$ 
  - ▶ Vertex Operator approach ( Jimbo et al.(1992-))
  - ▶  $q$ -KZ approach ( Jimbo and Miwa (1994))
  - ▶ QISM : Solving inverse problems ( Maillet et al (2000-))
- Factorize multiple integrals into sums of products of single integrals "by hand"
  - ▶ Boos Korepin Smirnov (2001-)
  - ▶ Sato Shiroishi Takahashi (2005) ( $n = 8$ )

## Conjecture (Boos-Korepin)

*Correlation functions at  $T = 0$  for  $S = \frac{1}{2}$  XXX model are described by  $(\ln 2)$  and Riemann's  $\zeta$  functions with odd arguments.*

reduced  $q$ -KZ equation uncovers the mystery  
(Boos et al (2004-))



Solution(Exponential formula)

- contains a transcendental fcn  $\omega$
- contains "Fermions"

It explains factorization, appearance of  $\zeta(2k+1)$  and so on. (M. Jimbo's talk in this conference)

# Status of DME $S = \frac{1}{2}, T > 0$

DME at  $T > 0$  (Göhmman et al., JPA 36 (2005) )

- Algebraic part : parallel to  $T = 0$  case.
- Trotter limit : NLIE  $\alpha$  (Kluemper et al. (1991), Destri-de Vega , (1995) )
- integrations contain "Fermi" (spinon) distribution functions  $\mathfrak{A}(:= 1 + \alpha)$ .

it can be explicitly factorized "by hand" (Wuppertal group (2006-) )

- DME = "algebraic" part + transcendental part ( $\omega \rightarrow$  finite  $T$  analogue).
- Exponential formulas are conjectured (Wuppertal group (2006, 2007) ) and partly proved ( "Kyoto" group (2008) )

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# Main Problem Today

## Problem

Consider the integrable isotropic  $S = 1$  chain with  $L$  sites.

$$H = \frac{J}{4} \sum_{j=1}^L [\vec{S}_{j-1} \cdot \vec{S}_j - (\vec{S}_{j-1} \cdot \vec{S}_j)^2]$$

Evaluate Density Matrix Elements  $D_n$  in  $L \rightarrow \infty$  or its “inhomogenous” generalization  $D_n(\xi_1, \dots, \xi_n)$ , at any  $T$  s in a “factorized” form.

# Aim of research

Common belief is..

- $S = \frac{1}{2}$  is fundamental. For example,  $\frac{1}{2} \otimes \frac{1}{2} = 0 \oplus 1$ .
- Description of  $S > \frac{1}{2}$  is mere a modification (at least for integrable cases)

What I believe is..

- Description of  $S > \frac{1}{2}$  using  $S = \frac{1}{2}$  is sometimes flawed.
- Each higher spins (composite particles) needs its own description of the Hilbert space.
- Natural description may offer an efficient formalism in numerics.

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- Natural description may offer an efficient formalism in numerics.

# Main problem Again

To be concrete , for  $S = 1$

- multiple integral formula at  $T = 0$  ✓
  - ▶ VO (Bougourzi et al., Konno, Idzumi )
  - ▶ QISM (Kitanine, Deguchi-Matsui )
- multiple integral formula at  $T > 0$ ?
- factorization at  $T \geq 0$  ?
- exponential formula at  $T > 0$  ?

## QTM

## Main tool : QTM framework

M. Suzuki (1985), M. Suzuki and Inoue (1987),  
Koma(1987), J.S. et al (1990), Klümper (1992)  
Map  $d$ -D quantum to  $d + 1$ -D  
classical. ( $d = 1$ )

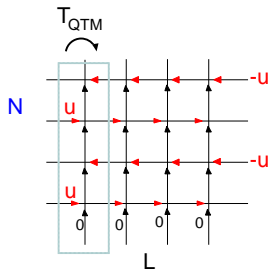
$$Z_{1D\text{Quantum}}(\beta, L) = Z_{2D}(N, L)$$

$$= \text{tr} T_{\text{QTM}}(u)^L$$

$$u = -\frac{\beta}{N}$$

## Theorem (M.Suzuki)

Only the largest eigenvalue of  
 $T_{\text{QTM}}$  contributes.

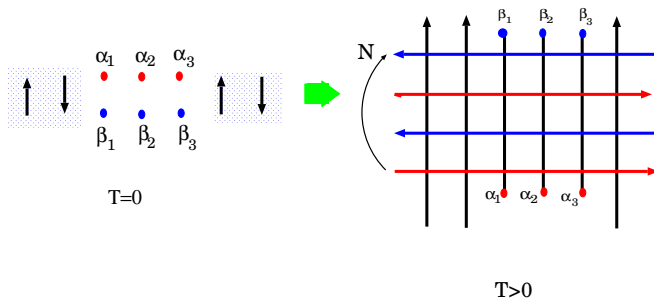


Neither summation nor variation  
necessary



DME in QTM formulation at  $T > 0$ 

In QTM framework you do not have to solve inverse problem (Göhhmann et al., JPA 36)

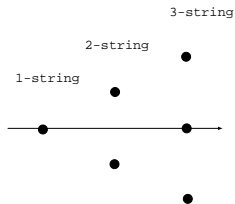


$$(D)_{\beta_1, \dots, \beta_n}^{\alpha_1, \dots, \alpha_n}(\xi_1, \dots, \xi_n) = \frac{\langle \Psi | T_{\beta_1}^{\alpha_1}(\xi_1) \cdots T_{\beta_n}^{\alpha_n}(\xi_n) | \Psi \rangle}{\langle \Psi | T_{\text{QTM}}(\xi_1) \cdots T_{\text{QTM}}(\xi_n) | \Psi \rangle} \Rightarrow \text{parallel to } T = 0!$$

# Bulk thermodynamics of $S > \frac{1}{2}$

Although Bethe ansatz roots characterizes highest weight states (Gaudin)...

composite states = strings  
 $\infty/\infty$ =highly singular



Numerics (Alcaraz et al '88)

- Ground state = 2S string
- Excited states = very complicated

Better not to deal with BAE roots directly..

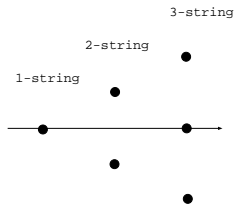
Other descriptions?



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## Conjecture(Reshetikhin '91)

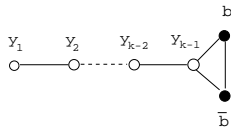
$$\mathcal{H}_{\text{spin}S} = \mathcal{H}_{\text{spinon}} \oplus \mathcal{H}_{\text{RSOS}_k}$$

Thermodynamics (JS '99): consists of two pieces.

- “RSOS” pieces. ( $1 \leq j \leq k-1$ )  
 $y_j, Y_j (:= 1 + y_j)$
- Spinon pieces  
 $b, \mathfrak{B} (:= 1 + b)$

They are nice objects, as

- 1 Good analyticity
- 2 They satisfy functional relations ( Klümper-Pearce transf )
- 3 The relations among nice objects lead to NLIE.
- 4 NLIE yields bulk quantities (specific heat..)



multiple integral formula  $S = 1, T \geq 0$ 

Not dealing with BAE roots directly

- Good: no need to deal with singular objects
- No good: problem with DME

The algebraic part of calculation of DME goes parallel to  $S = \frac{1}{2}$  case:

$$\langle T_{\beta_1}^{\alpha_1}(\xi_1) \cdots T_{\beta_n}^{\alpha_n}(\xi_n) \rangle \sim \sum_{\text{BAE roots } \{\mu_j\} \cup \text{others}} \mathcal{S}(\{\mu_j\})$$

- Zeros of  $Q$  (= BAE roots  $\{\mu_j\}$ ) are **not** encoded in  $\mathfrak{B}, Y_j!$ ,  $\mathfrak{B}(\mu_j) \neq 0$
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Still we can

- adopt narrower contours separated in the upper and lower half planes
- impose “subtle relations” among these contours
- introduce **one more** auxiliary function  $f, \tilde{f} := 1 + f$

### Theorem (Göhmann et al (2010))

$S = 1$  DME at  $T > 0$  has the following multiple integral formula

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

$$\left[ \prod_{j=1}^p \int_{\mathcal{C}} \frac{d\lambda_j}{2\pi i} F_{z_j}(\lambda_j) \right] \left[ \prod_{j=p+1}^{2m} \int_{\bar{\mathcal{C}}} \frac{d\lambda_j}{2\pi i} \bar{F}_{z_j}(\lambda_j) \right] \frac{\det_{2m} \Theta_{j,k}^{(p)}}{\prod_{1 \leq j < k \leq 2m} (\lambda_j - \lambda_k - 2i)}$$

# Factorization?

Still, improvement necessary..

- multiple integrals : too complicated to factorize into single loop integrals
- If  $\mathfrak{B}(\mu), Y$  already describe physics, only they should appear

Take other routes to find factorized expressions

- fusion of (already factorized) spin  $\frac{1}{2}$  DME
- use difference equations of  $q$ -KZ type at discrete points. (Aufgebauer et al (2012)  $S = \frac{1}{2}$ )

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# fusion of DME

The idea is trivially simple.

- evaluate  $D_{2m}$  of  $S = \frac{1}{2}$
- replace  $\omega_{\alpha,q}$  of  $S = \frac{1}{2}$  to  $\omega_{\alpha,q}$  of  $S = 1$
- proper combinations of  $D_{2m}$  give  $D_m$  of  $S = 1$  after proper normalization

The actual calculation is simple, not elegant but elephant.



$S = 1, m = 3$  result

convenient to present  $S = 1$  DME using  $SU(2)$  invariant projector

$$D_m^{S=1}(\xi_1, \dots, \xi_m) = \sum_{\alpha=1}^{N_m} \rho_{\alpha}^{S=1}(\xi_1, \dots, \xi_m) P_{\alpha}^{S=1}$$

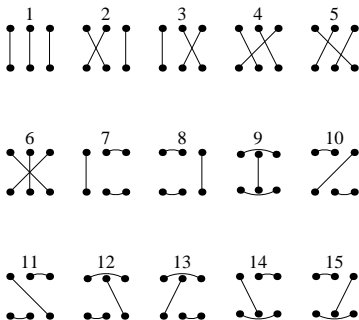
$$N_2 = 3, N_3 = 15 \dots$$

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example of projectors for  $S = 1, m = 3$



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factorized solution ( $\xi^{\pm} := \xi \pm i$ )

$$\begin{aligned} \rho_1^{S=1}(\xi_1, \xi_2, \xi_3) = & \frac{1}{27} + \frac{1}{N(\xi_1)N(\xi_2)N(\xi_3)} \left( c_1^{(1)}\omega(\xi_1^-, \xi_2^-) + c_2^{(1)}\omega(\xi_1^-, \xi_1^+) + c_3^{(1)}\omega(\xi_1^-, \xi_2^+) \right. \\ & + c_1^{(2)}\omega(\xi_1^-, \xi_1^+)\omega(\xi_2^-, \xi_3^-) + c_2^{(2)}\omega(\xi_1^-, \xi_2^-)\omega(\xi_2^+, \xi_3^-) + c_3^{(2)}\omega(\xi_1^-, \xi_1^+)\omega(\xi_2^-, \xi_3^+) \\ & + c_4^{(2)}\omega(\xi_1^+, \xi_3^-)\omega(\xi_2^-, \xi_3^+) + c_5^{(2)}\omega(\xi_1^-, \xi_2^-)\omega(\xi_1^+, \xi_3^+) + c_6^{(2)}\omega(\xi_2^-, \xi_3^+)\omega(\xi_2^+, \xi_3^-) \\ & + c_7^{(2)}\omega(\xi_1^-, \xi_1^+)\omega(\xi_2^-, \xi_2^+) + c_8^{(2)}\omega(\xi_2^-, \xi_3^-)\omega(\xi_2^+, \xi_3^+) + c_1^{(3)}\omega(\xi_1^-, \xi_1^+)\omega(\xi_2^-, \xi_3^+)\omega(\xi_2^+, \xi_3^-) \\ & + c_2^{(3)}\omega(\xi_1^-, \xi_2^+)\omega(\xi_1^+, \xi_3^-)\omega(\xi_2^-, \xi_3^+) + c_3^{(3)}\omega(\xi_1^-, \xi_1^+)\omega(\xi_2^-, \xi_2^+)\omega(\xi_3^-, \xi_3^+) \\ & \left. + c_4^{(3)}\omega(\xi_1^-, \xi_2^-)\omega(\xi_1^+, \xi_3^-)\omega(\xi_2^+, \xi_3^+) + c_5^{(3)}\omega(\xi_1^-, \xi_1^+)\omega(\xi_2^-, \xi_3^-)\omega(\xi_2^+, \xi_3^+) \right) \\ & + \text{permutations and negation} \end{aligned}$$

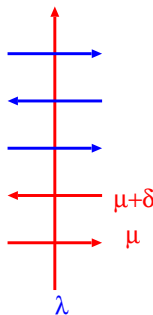
- $N(\xi)$  comes from normalization

$$N(\xi) = \frac{3}{4} + \frac{\omega(\xi^-, \xi^+)}{2}.$$

- $c_j^{(a)}$  are known rational functions of  $\xi_k^\pm$ .
- $\omega$  is  $(S = \frac{1}{2}) \times (S = 1)$  object

$$\omega(\lambda, \mu) \sim \frac{d}{d\delta} \ln \Lambda^{[1]}(\lambda, \mu)|_{\delta=0}$$

can be obtained only from  $\mathfrak{B}, Y$ : **no need** of  $\mathfrak{F}$



Almost what we want

# homogeneous and $T = 0$ limit of $S = 1$ result

One can take

- zero  $T$  limit

$$\omega_{T=0}^{S=1}(\lambda, \mu) = \omega_{T=0}^{S=\frac{1}{2}}(\lambda, \mu) + \frac{(\lambda - \mu)^2 + 4}{8} \frac{\pi(\lambda - \mu)}{2 \sin \frac{\pi}{2}(\lambda - \mu)}$$

- homogeneous limit  $\xi_j \rightarrow 0$

All  $\rho_\alpha^{S=1}$  are given by rational numbers and  $\pi^2, \pi^4, \dots$ ,  
example

$$8\rho_1^{S=1} = \frac{1879}{432} - \frac{3497}{1350}\pi^2 + \frac{53}{135}\pi^4 - \frac{11296}{637875}\pi^6$$

## Conjecture (Klümper et al 2013)

*The correlation functions at  $T = 0$  for the integrable  $S = 1$  (integer) spin chain of XXX-type are described by Riemann's  $\zeta$  functions with even arguments.*

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Still unsatisfactory..

- $\omega(\lambda, \mu)$  is  $(S = \frac{1}{2}) \times (S = 1)$  object.
- for  $S = \frac{1}{2}$ , homogeneous limit =  $\lim_{\lambda, \mu \rightarrow 0} \omega(\lambda, \mu)$
- for  $S = 1$ , homogeneous limit =  $\lim_{\lambda, \mu \rightarrow 0} \omega(\lambda + i, \mu - i)$ : needs singular object,

$$\omega(\lambda, \mu) - \frac{1}{2} = -\frac{(\lambda - \mu)^2 + 4}{2i} \frac{d}{d\delta} \ln \Lambda^{[1]}(\lambda, \mu)|_{\delta=0}$$

Question: Any proper  $(S = 1) \times (S = 1)$  object, free from singular objects?

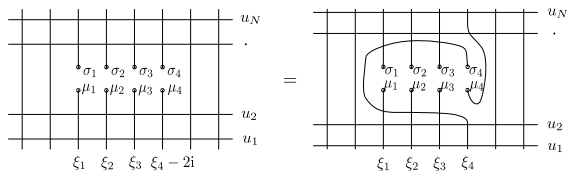
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The difference equation at discrete points (Aufgebauer et al (2012) ) gives a hint.

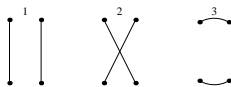


$$\xi_4 \in \{u_1, \dots, u_N\}$$



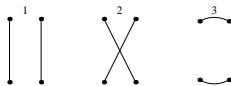
# difference equation at discrete points

Concentrate on  $m = 2$ :  $D_2(\xi_1, \xi_2) = \sum_{\alpha=1}^3 \rho_{\alpha}^{S=1}(\xi_1, \xi_2) P_{\alpha}$



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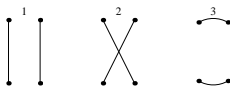


Difference equations

$$\begin{pmatrix} \rho_1(\xi_1 - 2i, \xi_2) \\ \rho_2(\xi_1 - 2i, \xi_2) \\ \rho_3(\xi_1 - 2i, \xi_2) \end{pmatrix} = L(\xi_1 - \xi_2) \cdot \begin{pmatrix} \rho_1(\xi_1, \xi_2) \\ \rho_2(\xi_1, \xi_2) \\ \rho_3(\xi_1, \xi_2) \end{pmatrix}$$

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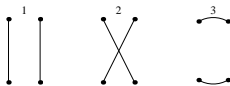
Change of variables

$$\begin{pmatrix} \rho_1(\xi_1, \xi_2) \\ \rho_2(\xi_1, \xi_2) \\ \rho_3(\xi_1, \xi_2) \end{pmatrix} = \begin{pmatrix} \frac{5\xi^2+36}{45(\xi^2+4)} & -\frac{\xi^2}{30(\xi^2+4)} & \frac{\xi^2+6}{15(\xi^2+4)} \\ -\frac{64}{45(\xi^2+4)} & \frac{3\xi^2-20}{60(\xi^2+4)} & -\frac{3\xi^2+28}{30(\xi^2+4)} \\ \frac{16}{45(\xi^2+4)} & \frac{3\xi^2+20}{60(\xi^2+4)} & -\frac{3\xi^2+8}{30(\xi^2+4)} \end{pmatrix} \begin{pmatrix} 1 \\ G(\xi_1, \xi_2) \\ H(\xi_1, \xi_2) \end{pmatrix}$$

$$\xi = \xi_1 - \xi_2$$

# difference equation at discrete points

Concentrate on  $m = 2$ :  $D_2(\xi_1, \xi_2) = \sum_{\alpha=1}^3 \rho_{\alpha}^{S=1}(\xi_1, \xi_2) P_{\alpha}$



Much simpler difference equation

$$\begin{pmatrix} 1 \\ \bar{G} \\ \bar{H} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{\xi(\xi-6i)}{(\xi-2i)(\xi+4i)} & 0 \\ -\frac{256i(\xi-i)}{3(\xi+2i)(\xi-2i)^2(\xi+4i)} & -\frac{\xi(\xi-6i)(\xi^2-2i\xi-4)}{(\xi-2i)^2(\xi+2i)(\xi+4i)} & \frac{\xi^2(\xi-6i)(\xi-4i)}{(\xi-2i)^2(\xi+2i)(\xi+4i)} \end{pmatrix} \begin{pmatrix} 1 \\ G \\ H \end{pmatrix}$$

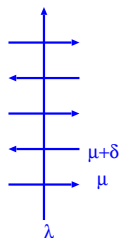
$$\bar{G} = G(\xi_1 - 2i, \xi_2)$$

$$G(\lambda, \mu) \sim (\Omega(\lambda - i, \mu - i) + \Omega(\lambda - i, \mu + i) + \Omega(\lambda + i, \mu - i) + \Omega(\lambda + i, \mu + i))$$

where  $\Omega(\lambda, \mu) = 2i \frac{\omega(\lambda, \mu) + 1/2}{(\lambda - \mu)^2 + 4}$ .

- $G$  is expressed by a  $(S = 1) \times (S = 1)$  object.
- homogeneous limit is in the physical strip of  $\Lambda^{[2]}(\lambda, \mu)$ .
- $H$  satisfies difference eq whose source term is  $G$ . Thus  $H$  is also proper  $(S = 1) \times (S = 1)$  object.

$$G(\lambda, \mu) \sim \frac{d}{d\delta} \ln \Lambda^{[2]}(\lambda, \mu)|_{\delta=0}$$



The simplicity of  $m = 2$  result at  $T = 0$  can be understood from

$$G(\lambda, \mu) \rightarrow 0$$

$$H(\lambda, \mu) \rightarrow \frac{1}{\sinh^2 \frac{\pi}{2}(\lambda - \mu)}$$

# Summary and Future problems

Our question was,  
can we play the same game for  $S > \frac{1}{2}$ ?

- multiple integral formula at  $T = 0$  ✓
- multiple integral formula at  $T > 0$  ✓
- factorization at  $T \geq 0$  ✓
- magnetic field?
- XXZ, XYZ?
- exponential formula at  $T > 0$  ?
- Mixed spin chains?
- scaling limit: space of operators in SUSYsG?

Thank you for your attention.