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SEMS Seminar Series

Correlation Functions of Quantum Spin Chains

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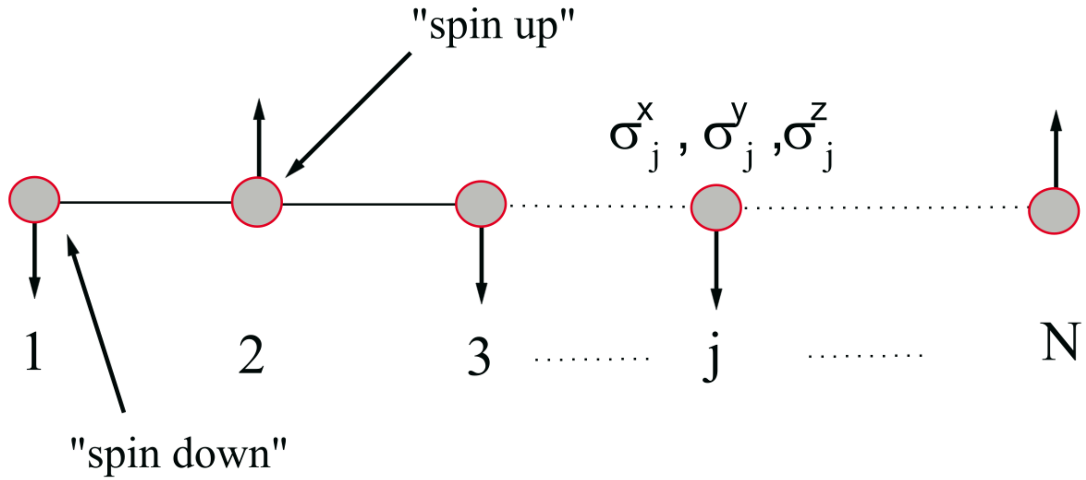
I.WHAT ARE QUANTUM SPIN CHAINS?



- The best known cases are the spin 1/2 XXX and XXZ chains

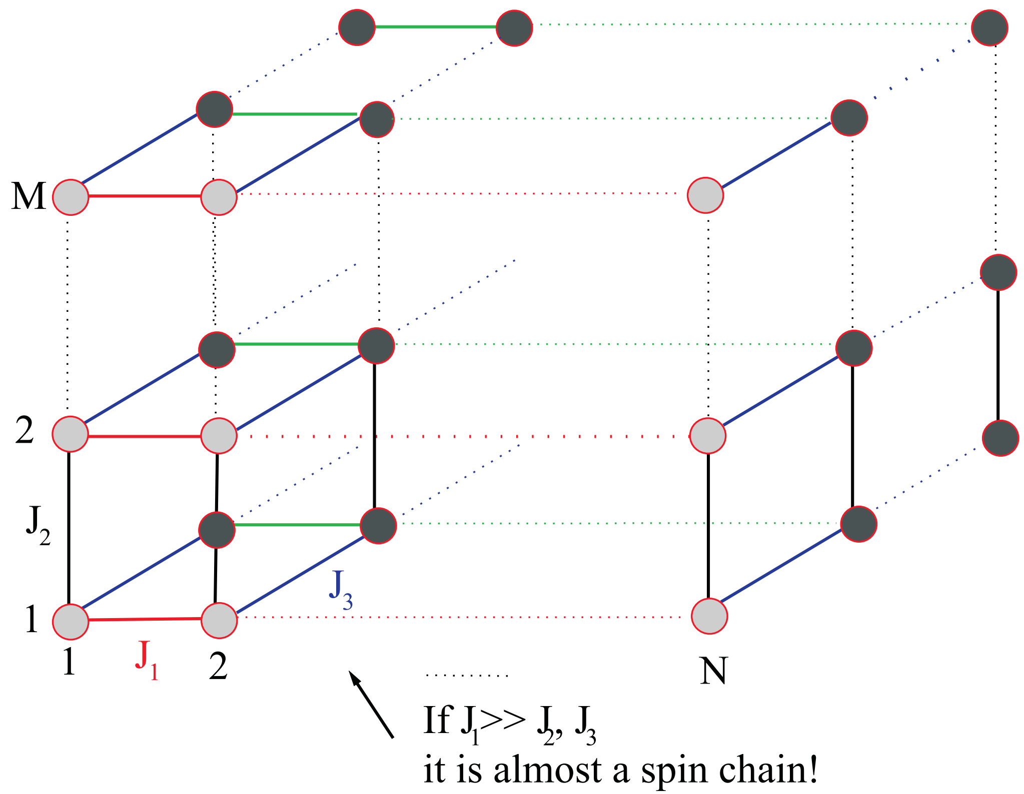
(W. Heisenberg '28, H. Bethe '31)

$$H = \sum_{m=1}^{N} \left\{ \underbrace{\sigma^x_m \sigma^x_{m+1}}_{X} + \underbrace{\sigma^y_m \sigma^y_{m+1}}_{X} + \underbrace{\Delta\left(\sigma^z_m \sigma^z_{m+1} - 1\right)}_{Z} \right\}$$

$\Delta \equiv$ anisotropy parameter ($\Delta = 1$ corresponds to the XXX chain)

II.WHY STUDY THEM?

- Even though materials are 3-dimensional sometimes a 1-dimensional approximation can be quite accurate.



- They are 1-dimensional models, therefore easier to study than more realistic (3-dimensional) theories. In addition, the advance of nanotechnology makes it now possible to identify and study quasi-one-dimensional systems in the lab.
- Despite their simplicity (integrability) they are able to reproduce some realistic features of one-dimensional magnetic material.
- The property of integrability makes it possible (a priori) to compute all relevant physical quantities exactly.
- These computations are in general highly non-trivial mathematical problems. For this reason lots of work have been done (especially in the last 30 years) to develop new analytical methods.
- The development of these methods has revealed very beautiful underlying mathematical structures (for example, quantum groups). The study of these has become a research subject in itself.

III.WHY CORRELATION FUNCTIONS?

• Everything that can be measured is related to correlation functions. The knowledge of all correlation functions is the solution of any physical theory.

• For instance, quantities that are easily accessible experimentally and that characterize well the magnetic properties of a material are the so-called structure factors:

$$S^{\alpha\beta}(q,w) = \frac{1}{N}\sum_{j,j'=1}^{N} e^{iq(j-j')}\int_{-\infty}^{\infty} dt\, e^{iwt}\langle S_j^{\alpha}(t)S_{j'}^{\beta}(0)\rangle.$$

• Correlation functions can be expressed in terms of form factors by means of an expansion of the form

$$\langle S_j^{\alpha}S_{j'}^{\beta}\rangle \sim \sum_n \langle \text{vac}|S_j^{\alpha}|n\rangle\langle n|S_{j'}^{\beta}|\text{vac}\rangle$$

• Expanding correlation functions in terms of form factors has proven to be very efficient from a numerical point of view (J.-S. Caux, J.-M. Maillet et al. 2005). Hence obtaining simple formulae for the form factors is essential.

IV. FORM FACTORS AND CORRELATION FUNCTIONS OF QUANTUM SPIN CHAINS

- The objects we are interested in are correlation functions and form factors (expectation values) of local operators, say $\mathcal{O} = S_j^{\alpha}$ or $\mathcal{O} = S_j^{\alpha} S_k^{\beta}$ at zero temperature.

$$\langle \mathcal{O} \rangle = \frac{\mathrm{tr}_{\mathcal{H}}(\mathcal{O} e^{-H/kT})}{\mathrm{tr}_{\mathcal{H}}(e^{-H/kT})} \underset{T \to 0}{=} \frac{\langle \Psi_g | \mathcal{O} | \Psi_g \rangle}{\langle \Psi_g | \Psi_g \rangle}$$

- Here $|\Psi_g\rangle$ is the ground state of the system.
- In the context of integrable quantum spin chains, two main approaches exist which allow the computation of form factors and correlation functions:

- In the first approach (Jimbo, Miwa '95) form factors and correlation functions are expressed in terms of q-deformed vertex operators and can be obtained as solutions to q-deformed KZ equations. The main idea is to exploit the symmetries of the model in order to deduce a set of equations whose solutions are the correlation functions.

M. Jimbo and T. Miwa (1995,1996) [integral representations for the n-point correlations for the XXZ spin chain].

H.E. Boos, V.E. Korepin (2001); H.E. Boos, V.E. Korepin, Y. Nishiyama and M. Shiroishi (2002); H.E. Boos, V.E. Korepin and F.A. Smirnov (2003); K. Sakai, M. Shiroishi, Y. Nishiyama and M. Takahashi (2003); G. Kato, M. Shiroishi, M. Takahashi and K. Sakai (2003,2004); M. Takahashi, G. Kato and M. Shiroishi (2004); H. Boos, M. Jimbo, T. Miwa, F. Smirnov and Y. Takeyama (2004,2005) [formulae in terms of ζ-functions for correlation functions of the XXX and XXZ chains (initially for 2th, 3th and 4th-neighbour correlations)].

$\Rightarrow$ I will not follow this approach here!

- The other approach (N. Kitanine, J.-M. Maillet and V. Terras ’99) combines the algebraic Bethe ansatz technique (which provides a construction scheme for the quantum states) and the solution of the inverse scattering problem (which allows to write local operators on the chain in terms of the same objects the quantum states are made of).

N. Kitanine, J.-M. Maillet and V. Terras (1999); J.-M. Maillet and V. Terras (2000) [solution of the inverse scattering problem].

N. Kitanine, J.-M. Maillet, N.A. Slavnov and V. Terras (1999-2005) [integral representations for correlation functions and form factors of the spin 1/2 XXZ chain (dynamical correlation functions, roots of unity...)].

J.-S-Caux, J.-M. Maillet et al. (2005) [numerical applications].

F. Göhmann, A. Klümper et al. (2004, 2005) [correlation functions at finite T].

- Our main contribution has been the use of this technique for the computation of form factors of mixed spin chains (different spin representations at different sites), e.g. impurity systems and alternating spin chains.

V. ALGEBRAIC BETHE ANSATZ

- The algebraic Bethe ansatz technique (L.D Faddeev, E.K. Sklyanin and L.A. Takhtajan '79) provides a closed algebraic setup which allows the simultaneous construction of the conserved charges of a quantum spin chain (including the Hamiltonian), and of its eigenstates.

- The starting point of this construction is a so-called R-matrix,

$$R_{\text{XXX}}^{(\frac{1}{2},\frac{1}{2})}(\lambda) = \begin{pmatrix} \frac{\lambda - \frac{i}{2}(\sigma^z+1)}{\lambda - i} & -\frac{i}{\lambda - i}\sigma^- \\ -\frac{i}{\lambda - i}\sigma^+ & \frac{\lambda - \frac{i}{2}(1-\sigma^z)}{\lambda - i} \end{pmatrix} \in \mathbb{C}^2 \otimes \mathbb{C}^2$$

- R-matrices are solutions of the Yang-Baxter equations. These equations are a consequence of integrability.

$$R_{12}^{(s_1,s_2)}(\lambda) R_{13}^{(s_1,s_3)}(\lambda+\mu) R_{23}^{(s_2,s_3)}(\mu) = R_{23}^{(s_2,s_3)}(\mu) R_{13}^{(s_1,s_3)}(\lambda+\mu) R_{12}^{(s_1,s_2)}(\lambda)$$

- The quantum monodromy matrix is then defined as

$$T^{(\frac{1}{2})}_{0;1\ldots N}(\lambda;\{\xi\}) = \underbrace{R^{(\frac{1}{2},s_N)}_{0N}(\lambda-\xi_N)\cdots R^{(\frac{1}{2},s_1)}_{01}(\lambda-\xi_1)}_{\in \quad V_0\otimes V_1\otimes\ldots\otimes V_N \ \text{with}\ V_0=\mathbb{C}^2\ \text{and}\ V_j=\mathbb{C}^{2s_j+1}}$$

$$= \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}; \quad t^{(1/2)}(\lambda,\{\xi\}) = (A+D)(\lambda)$$

- We can regard the algebraic Bethe ansatz as providing a highly non-trivial map

$$\sigma_j^\alpha \mapsto \{A,B,C,D\}$$

The inverse scattering problem consists of finding the inverse of this map.

- Here $\xi_1 \ldots \xi_N$ are the inhomogeneity parameters. Their presence simplifies certain computations. However a local Hamiltonian is only obtained for $\xi_j = -i/2 \quad \forall \quad i$.

• As a consequence of R satisfying Yang-Baxter equations, the monodromy matrix satisfies

$$R_{12}^{(\frac{1}{2},\frac{1}{2})}(\lambda)T_1^{(\frac{1}{2})}(\lambda+\mu)T_2^{(\frac{1}{2})}(\mu)=T_2^{(\frac{1}{2})}(\mu)T_1^{(\frac{1}{2})}(\lambda+\mu)R_{12}^{(\frac{1}{2},\frac{1}{2})}(\lambda)$$

it follows $\quad [t(\lambda),t(\mu)]=0 \quad$ (conserved commuting charges)

• The RTT-equations above imply various commutation relations amongst the operators $\{A,B,C,D\}$ which will be crucial for the computation of form factors and correlation functions.

- The transfer matrix $t^{(1/2)}(\lambda,\{\xi\})$ generates the Hamiltonian of the model

$$H \sim \left. \frac{d\log(t^{(1/2)}(\lambda,\{\xi\}))}{d\lambda} \right|_{\lambda=-i/2=\xi_1\ldots\xi_N}$$

- For the best known cases of the spin 1/2 XXX and XXZ chains

(W. Heisenberg '28, H. Bethe '31)

$$H = \sum_{m=1}^{N} \Big\{ \underbrace{\sigma^x_m \sigma^x_{m+1}}_{X} + \underbrace{\sigma^y_m \sigma^y_{m+1}}_{X} + \underbrace{\Delta\big(\sigma^z_m \sigma^z_{m+1} - 1\big)}_{Z} \Big\} \quad \text{acting on}$$

$\mathcal{H} \equiv V_1 \otimes \cdots \otimes V_N$ with $V_i \equiv \mathbb{C}^2$ and $\sigma^\alpha_a = \sigma^\alpha_{N+a}$

$\Delta \equiv$ anisotropy parameter ($\Delta = 1$ corresponds to the XXX chain)

- The matrices above are the Pauli matrices, which provide a 2-dimensional representation of the $su(2)$ algebra

$$\sigma_m^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_m \qquad \sigma_m^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_m \qquad \sigma_m^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_m$$

$$[\sigma^+, \sigma^-] = \sigma^z \qquad \text{and} \qquad [\sigma^z, \sigma^\pm] = \pm 2\sigma^\pm\,, \quad \sigma^\pm = \sigma^x \pm i\sigma^y$$

- Since $[H, t(\lambda)] = 0$, the eigenstates of H are those of $t(\lambda)$ and have the form

$$|\Psi(\{\lambda\})\rangle = B(\lambda_1) \cdots B(\lambda_\ell)|0\rangle \quad \text{with}$$

$$\prod_{k=1}^{\ell} \frac{\lambda_k - \lambda_j - i}{\lambda_k - \lambda_j + i} = -d(\lambda_j) \quad \text{Bethe ansatz equations}$$

• Here $|0\rangle$ denotes the completely ferromagnetic reference state (all spins up) and $d(\lambda)$ is the eigenvalue of $D(\lambda)$ on that state

$$D(\lambda)|0\rangle = d(\lambda)|0\rangle = \prod_{j=1}^{N} \left(\frac{\lambda - \xi_j + (s_j - 1/2)i}{\lambda - \xi_j - (s_j + 1/2)i} \right) |0\rangle$$

$$A(\lambda)|0\rangle = |0\rangle$$

• The knowledge of the ground state is the first step for the computation of correlation functions and form factors.

VI.THE INVERSE SCATTERING PROBLEM

- The next step in our problem is that of finding a realization of states and fields in terms of the same objects $\{A, B, C, D\}$.

- For XXX quantum spin chains such realization has been found:

J.M. Maillet, V. Terras and N. Kitanine (1999); J.M. Maillet and V. Terras (2000)

$$S_j^\alpha = \left[\prod_{k=1}^{j-1} t^{(s_k)}(\xi_k)\right] \Lambda_\alpha^{(s_j)}(\xi_j) \left[\prod_{k=1}^{j} t^{(s_k)}(\xi_k)^{-1}\right] \qquad \alpha = \pm, z$$

$$\Lambda_\alpha^{(s)}(u) := \text{Tr}_0 \left[S_0^\alpha T_{0;1\ldots N}^{(s)}(u)\right], \qquad t^{(s)}(u) := \text{Tr}_0 \left[T_{0;1\ldots N}^{(s)}(u)\right]$$

- The traces $\Lambda_\alpha^{(s)}(u)$ were subsequently obtained by exploiting the fusion identities for quantum spin chains (see next page):

$$\Lambda_\alpha^{(s)}(u) = \sum_{k=1}^{2s} t^{(s-\frac{k}{2})}(u_k)\Lambda_\alpha^{(\frac{1}{2})}(u_{2k}-a)t^{(\frac{k-1}{2})}(u_k - a), \quad \alpha = \pm, z$$

$$u_k = u - \frac{ik}{2}; a = \frac{2s+1}{2}; \quad \Lambda_\alpha^{(\frac{1}{2})}(u) = \begin{cases} \frac{(A-D)(u)}{2}, & \alpha = z \\ C(u), & \alpha = + \\ B(u), & \alpha = - \end{cases}$$

- How do we obtain the eigenvalues of $t^{(s)}(u)$?

$$t^{(s)}(u)|\Psi(\{\lambda\})\rangle = \Lambda^{(s)}(u,\{\lambda\})|\Psi(\{\lambda\})\rangle$$

VII. FUSION

- A further important ingredient is the fusion procedure for quantum spin chains: a procedure for constructing higher spin objects (R-matrices, monodromy matrices ...) in terms of lower spin quantities (Clesbsch-Gordan decomposition).

P.P. Kulish, N. Yu. Reshetikhin and E.K. Sklyanin (1981) [fusion XXX chains]; A.N. Kirillov and N. Yu. Reshetikhin (1987) [fusion XXZ chains]; V.G. Drinfeld (1988) [quantum group approach]

- Several kinds of iterative relations follow from fusion:

$$t^{(s)}(x^+) = t^{(\frac{1}{2})}(x - is)t^{(s-\frac{1}{2})}(x) - \chi(x^- - is)t^{(s-1)}(x^-)$$

$$\chi(u) = A(u^+)D(u^-) - B(u^+)C(u^-) \quad \text{and} \quad u^{\pm} = u \mp i/2$$

• These iterative relations for the higher spin transfer matrices imply similar relations for their eigenvalues on a Bethe state and allow to find closed expressions for these eigenvalues:

$$\Lambda^{(s)}(u,\{\lambda\}) = \sum_{\alpha=0}^{2s} C_\alpha^{(s)}(u) \prod_{p=1}^{\ell} \frac{(u^+ - \lambda_p - is)(u^- - \lambda_p + is)}{(u^+ - \lambda_p - (\alpha - s)i)(u^- - \lambda_p - (\alpha - s)i)}$$

$$C_\alpha^{(s)}(u) = \prod_{k=\alpha}^{2s-1} d(u^+ - (k-s)i) \qquad \text{and} \qquad C_{2s}^{(s)}(u) = 1$$

VIII. FORM FACTORS

- We would like to compute the form factors (for spin s_j)

$$F_\ell^{z,\pm}(j,\{\mu\},\{\lambda\}) = \langle\psi(\{\mu\})|S_j^{z,\pm}|\psi(\{\lambda\})\rangle = \langle 0|\prod_{k=1}^{\ell} C(\mu_k) S_j^{z,\pm} \prod_{k=1}^{\tilde{\ell}} B(\lambda_k)|0\rangle$$

- There are two basic results we need to use: the action of operators A, D on a Bethe state

$$A(x)\,|\Psi(\{\lambda\})\rangle = \underbrace{\left[\prod_{k=1}^{\ell} \frac{\lambda_k - x - i}{\lambda_k - x}\right] |\Psi(\{\lambda\})\rangle}_{\text{direct term}}$$

$$\underbrace{+\sum_{p=1}^{\ell} \frac{i}{\lambda_p - x}\left[\prod_{k\neq p} \frac{\lambda_k - \lambda_p - i}{\lambda_k - \lambda_p}\right] B(x) \prod_{k\neq p} B(\lambda_k)\,|0\rangle}_{\text{indirect term}}$$

(similarly for $D(x)$).

- We will also need the expression of the scalar product of an arbitrary state $\langle\psi(\{\mu\})|$ and a Bethe state $|\psi(\{\lambda\})\rangle$:

V.E. Korepin, N.M. Bogoliubov and A.G. Izergin, Quantum inverse scattering method and correlation functions. Cambridge University Press (1993)

A.G. Izergin '87, V.E. Korepin '82, N.A. Slavnov '89.

$$\langle\psi(\{\mu\})|\psi(\{\lambda\})\rangle = \frac{\det H(\{\mu\},\{\lambda\})}{\prod_{i<j}(\lambda_i-\lambda_j)(\mu_j-\mu_i)}$$

$$H_{ab} = \frac{-i}{(\lambda_a-\mu_b)}\left[\prod_{i\neq a}(\lambda_i-\mu_b-i) - d(\mu_b)\prod_{i\neq a}(\lambda_i-\mu_b+i)\right]$$

- Employing these formulae and the reconstruction of $S_j^{z,\pm}$ in terms of $\{A, B, C, D\}$ we have found (work in collaboration with J.-M. Maillet)

$$F_\ell^z(j, \{\mu\}, \{\lambda\}) = \frac{\phi_j(\{\mu\})}{\phi_j(\{\lambda\})} \frac{s_j \det H - \sum_{p=1}^{\ell} \prod_{k=1}^{\ell} (\mu_k - \mu_p - i) \det \mathcal{Z}^{(p)}(\xi_j)}{\prod_{i<j} (\lambda_i - \lambda_j)(\mu_j - \mu_i)}$$

$$\phi_j(\{\mu\}) = \prod_{k=1}^{j} \Lambda^{(s_k)}(\xi_k, \{\mu\}); \qquad \xi_j^{\pm} = \xi_j \mp i/2$$

with

$$\mathcal{Z}^{(p)}(\xi_j)_{ab} = H_{ab} \qquad \text{for} \qquad b \neq p$$

$$\mathcal{Z}^{(p)}(\xi_j)_{ap} = \left[\prod_{k=1}^{\ell} \frac{\lambda_k - \xi_j^- - is_j}{\mu_k - \xi_j^- - is_j} \right] \left[\frac{-2is_j}{(\mu_a - \xi_j^- + is_j)(\mu_a - \xi_j^- - is_j)} \right]$$

- This is a closed formula for all non-vanishing form factors of S_j^z in an arbitrary spin s_j representation.
- It holds for XXX spin chains (and can be easily generalized to the XXZ case), irrespectively of the spin representations sitting at other sites of the chain (those only enter the function ϕ_j).
- As a consistency check, the total magnetization of the chain can be computed employing the formula above

$$\mu = \sum_{j=1}^{N} \frac{F_\ell^z(j, \{\lambda\}, \{\lambda\})}{\langle \psi(\{\lambda\}) | \psi(\{\lambda\}) \rangle} = \sum_{j=1}^{N} s_j - \ell$$

$$F_\ell^+(j,\{\lambda\},\{\mu\}) = \frac{\phi_{j-1}(\{\lambda\})}{\phi_{j-1}(\{\mu\})} \frac{\prod_{k=1}^{\ell+1}(\mu_k - \xi_j^- - is_j)}{\prod_{k=1}^{\ell}(\lambda_k - \xi_j^- - is_j)} \frac{\det \mathcal{C}(\xi_j)}{\prod_{i<j}(\lambda_i - \lambda_j)(\mu_j - \mu_i)}$$

$$F_\ell^-(j,\{\mu\},\{\lambda\}) = \frac{\phi_j(\{\mu\})\phi_{j-1}(\{\mu\})}{\phi_{j-1}(\{\lambda\})\phi_j(\{\lambda\})} F_\ell^+(j,\{\mu\},\{\lambda\})$$

with

$$\mathcal{C}_{ab}(\xi_j) = \begin{cases} H_{ab} & \text{for} \quad b \neq \ell+1 \\ \dfrac{-2is_j}{(\mu_a - \xi_j^- + is_j)(\mu_a - \xi_j^- - is_j)} & \text{for} \quad b = \ell+1 \end{cases}$$

- This is a closed formula for all non-vanishing form factors of $S_j^{\pm}$ in an arbitrary spin s_j representation.
- It holds for XXX spin chains, irrespectively of the spin representations sitting at other sites of the chain (those only enter the function ϕ_{j-1}).
- In order to obtain these formulae, highly non-trivial algebraic identities involving the functions $\Lambda^{(s)}(u, \{\lambda\})$ need to be proven.
- These identities are shown below.

$$\sum_{k=1}^{2s} \Big[\Lambda^{(s-\frac{k}{2})}\,(\xi_j - ik/2, \{\lambda\})\,\Lambda^{(\frac{k-1}{2})}\left(\xi_j^- - i(k-2s)/2, \{\lambda\}\right)$$

$$\times\left[\prod_{p=1}^{\ell} b^{-1}(\lambda_p - \xi_j^- + i(k-s)) - d(\xi_j^- - i(k-s))\prod_{p=1}^{\ell} b^{-1}(\xi_j^- - i(k-s) - \lambda_p)\right]\Bigg]$$

$$= 2s\Lambda^{(s)}(\xi_j, \{\lambda\})$$

where

$$b(\lambda) = \frac{\lambda}{\lambda - i} \quad \text{and} \quad \xi_j^- = \xi_j + i/2$$

$$
\sum_{k=1}^{2s} \Big[\Lambda^{(s-k/2)}\,(\xi_j - ik/2, \{\lambda\})\,\Lambda^{((k-1)/2)}\left(\xi_j^- - i(k-2s)/2, \{\mu\}\right)
$$

$$
\times \left[\prod_{p\neq a} b^{-1}(\mu_p - \xi_j^- + i(k-s)) - d(\xi_j^- - i(k-s)) \prod_{p\neq a} b^{-1}(\xi_j^- - i(k-s) - \mu_p)\right]
$$

$$
\times \frac{-i}{(\mu_a - \xi_j^- + i(k-s))^2} \frac{\prod_{p=1}^{\tilde{\ell}} (\mu_p - \xi_j^- + i(k-s))}{\prod_{p=1}^{\ell} (\lambda_p - \xi_j^- + i(k-s))}\Bigg] =
$$

$$
\frac{\prod_{p=1}^{\tilde{\ell}} (\mu_p - \xi_j^- - is)}{\prod_{p=1}^{\ell} (\lambda_p - \xi_j^- + is)} \frac{(-2is)}{(\mu_a - \xi_j^- + is)(\mu_a - \xi_j^- - is)}
$$

- The proof can be carried out by using the explicit formulae for $\Lambda^{(s)}(u, \{\lambda\})$ obtained from fusion and certain properties of the function $d(x)$.
- These complicated expressions appear as a direct consequence of the reconstruction formulae for the operators $S_j^{z,\pm}$.

IX. CONCLUSIONS AND OUTLOOK

- The Algebraic Bethe ansatz technique, together with the solution of the inverse scattering problem can be successfully employed to compute form factors of spin operators for higher spins and mixed spin chains.

- The results I have presented today apply to XXX spin chains. The inverse scattering problem for higher spin representations remained so far unsolved for XXZ spin chains. We have now found a solution to this problem.

- Our results can be used for the study of specially interesting models, such as impurity systems and alternating chains, two kinds of systems whose thermodynamic properties have been extensively studied in the BA framework.

- Finally, we expect these results to be eventually useful for numerical computations. Recent results for the spin 1/2 case (J.-S. Caux, J.-M. Maillet et al. 2005) give us strong hope that this could be the case.

- The next natural step in this direction is to compute correlation functions (work in progress at the moment).