Women in Mathematics Day 2006

Correlation Functions of Quantum Spin Chains

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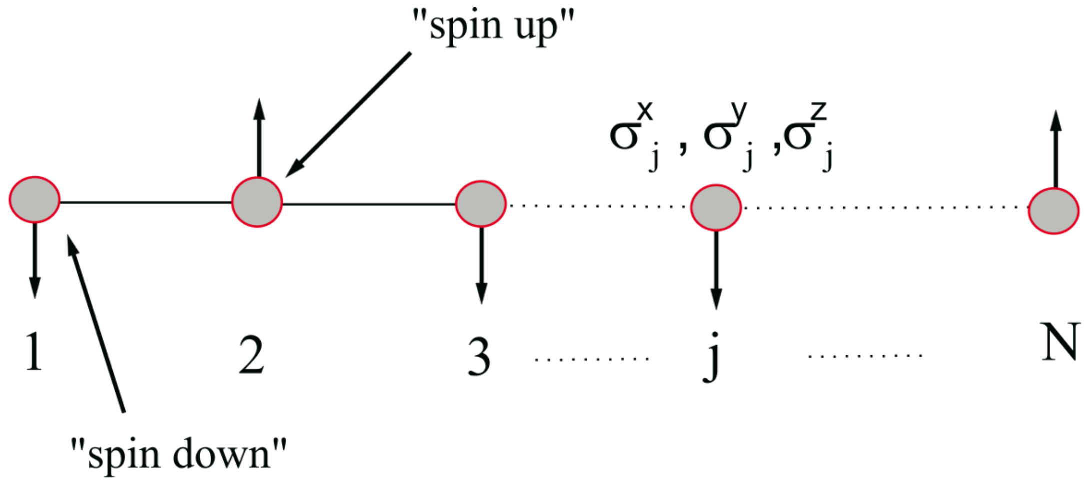
I.WHAT ARE QUANTUM SPIN CHAINS?



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

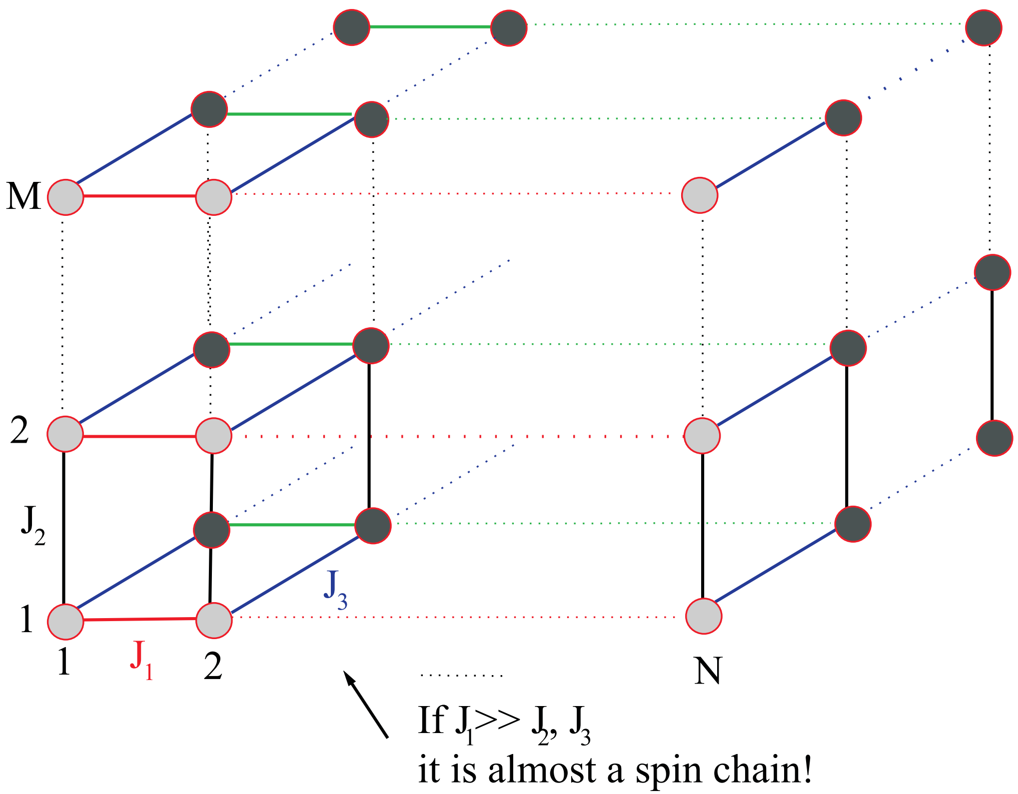
(W. Heisenberg '28, H. Bethe '31)

$$H = \sum_{m=1}^{N} \left\{ \underbrace{\sigma_m^x \sigma_{m+1}^x}_{X} + \underbrace{\sigma_m^y \sigma_{m+1}^y}_{X} + \underbrace{\Delta\left(\sigma_m^z \sigma_{m+1}^z - 1\right)}_{Z} \right\}$$

$\Delta \equiv$ 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:

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

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

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

- 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 $\mathcal{O} = \sigma_j^\alpha$ or $\mathcal{O} = \sigma_j^\alpha \sigma_k^\beta$ 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 to compute correlation functions and form factors. They were initiated in M. Jimbo and T. Miwa '95 and N. Kitanine, J.-M. Maillet and V. Terras '99 respectively, and are both still actively pursued today. Here I will concentrate on the second one.

• The 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,

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

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

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

- The quantum monodromy matrix is then defined as

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

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

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

$$\sigma^\alpha_j \mapsto \{A,B,C,D\}$$

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 $\xi_j = -i/2 \quad \forall \quad i$.

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

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

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

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

$$H = \sum_{m=1}^{N} \Big\{ \underbrace{\sigma_m^x \sigma_{m+1}^x}_{X} + \underbrace{\sigma_m^y \sigma_{m+1}^y}_{X} + \underbrace{\Delta \big(\sigma_m^z \sigma_{m+1}^z - 1 \big)}_{Z} \Big\} \quad \text{acting on}$$

$\mathcal{H} \equiv V_1 \otimes \cdots \otimes V_N$ with $V_i \equiv \mathbb{C}^2$ and $\sigma_a^\alpha = \sigma_{N+a}^\alpha$

$\Delta \equiv$ 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

$$\sigma^x_m = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_m \quad \sigma^y_m = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_m \quad \sigma^z_m = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_m$$

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

- 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

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

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

- 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. In particular, for the spin 1/2 case:

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

$$\sigma_j^\alpha = \left[\prod_{k=1}^{j-1} t^{(\frac{1}{2})}(\xi_k)\right] \Lambda_\alpha^{(\frac{1}{2})}(\xi_j) \left[\prod_{k=1}^{j} t^{(\frac{1}{2})}(\xi_k)^{-1}\right] \qquad \alpha = \pm, z$$

$$\Lambda_\alpha^{(\frac{1}{2})}(u) := \mathrm{Tr}_0 \left[\sigma_0^\alpha T_{0;1\ldots N}^{(\frac{1}{2})}(u)\right], \qquad t^{(\frac{1}{2})}(u) := \mathrm{Tr}_0 \left[T_{0;1\ldots N}^{(\frac{1}{2})}(u)\right]$$

- The traces $\Lambda_\alpha^{(\frac{1}{2})}(u)$ are:

$$\Lambda_\alpha^{(\frac{1}{2})}(u) = \begin{cases} \dfrac{(A-D)(u)}{2}, & \alpha = z \\ C(u), & \alpha = + \\ B(u), & \alpha = - \end{cases}$$

- How do we generalize this program for higher spins? There is a well understood procedure for doing this which allows us to do the same analysis above for a chain having arbitrary spins s_j at every site $j = 1, \ldots, N$.

- The main ingredient needed in this generalization is the fusion mechanism developed in P.P. Kulish, N. Yu. Reshetikhin and E.K. Sklyanin '81, A.N. Kirillov and N. Yu. Reshetikhin '87 which allows to construct higher spin R-matrices, monodromy and transfer matrices in terms of their spin 1/2 counterparts.

VII. 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

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

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

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

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

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 are closed formula for all non-vanishing form factors of spin operators 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 functions ϕ_{j-1}).
- In order to obtain these formulae, highly non-trivial algebraic identities involving the functions $\Lambda^{(s)}(u, \{\lambda\})$ (eigenvalue of a spin s transfer matrix $t^{(s)}(u)$) need to be proven.

VIII. 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.
- Our results can be used for the study of specially interesting models, such as impurity systems and alternating chains.
- 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).

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

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

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

where

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

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

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

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

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

- 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 $S_j^{z,\pm}$.