XXZ spin chain with generic boundaries.

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Beyond integrability.
The mathematics and physics of integrability and its breaking in low-dimensional strongly correlated quantum phenomena
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The XXZ spin-1/2 Heisenberg chain

Open chain XXZ chain

$$H = \sum_{m=1}^{N-1} \left(\sigma^x_m \sigma^x_{m+1} + \sigma^y_m \sigma^y_{m+1} + \Delta\,(\sigma^z_m \sigma^z_{m+1} - 1)\right)$$
$$-h^x_- \sigma^x_1 - h^y_- \sigma^y_1 - h^z_- \sigma^z_1 - h^x_+ \sigma^x_N - h^y_+ \sigma^y_N - h^z_+ \sigma^z_N$$

$h^a_\pm$, $a = x, y, z$ - boundary magnetic fields.

Due to the $U(1)$ symmetry of the bulk Hamiltonian **5 generic complex parameters**

Motivations

- All the attributes of the integrability but one: there was no exact solution for generic boundary terms.
- A simple model for the interaction with an environment
- Relation with open **Asymmetric Simple Exclusion Process** (ASEP)
- We need eigenstates, overlaps, form factors, correlation functions
- The key element of the correlation functions analysis for models solvable by the **Algebraic Bethe Ansatz** is the Slavnov determinant formula for the overlaps of on-shell and off-shell Bethe vectors (asymptotic analysis, numerical computation of structure factors etc.). Is there a similar way to compute overlaps without ABA?

$$\langle \{\mu\}_{\mathrm{off-shell}} | \{\lambda\}_{\mathrm{on-shell}} \rangle = p(\{\lambda\}, \{\mu\}) \det \left[\frac{\partial \tau(\mu_j, \{\lambda\})}{\partial \lambda_k} \right].$$

Quantum inverse scattering method

L.D. Faddeev, E.K. Sklyanin, L.A. Takhtajan (1979):

1. Yang-Baxter equation:

$$R_{12}(\lambda_{12})\ R_{13}(\lambda_{13})\ R_{23}(\lambda_{23}) = R_{23}(\lambda_{23})\ R_{13}(\lambda_{13})\ R_{12}(\lambda_{12}).$$

We consider the trigonometric solution with $\Delta = \cosh\eta$

2. Monodromy matrix.

$$M_a(\lambda) = R_{aN}(\lambda - \xi_N - \eta) \dots R_{a1}(\lambda - \xi_1 - \eta) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}_{[a]}$$

ξ_j are generic inhomogeneity parameters: $\xi_j \neq \xi_k + \epsilon\eta$, $\epsilon = 0, \pm 1$.

Reflection equation

Cherednik 1984

$$R_{12}(\lambda-\mu)\,K_1(\lambda)\,R_{12}(\lambda+\mu)\,K_2(\mu)=K_2(\mu)\,R_{12}(\lambda+\mu)\,K_1(\lambda)\,R_{12}(\lambda-\mu).$$

General 2×2 solution (Ghoshal Zamolodchikov 1994):

$$K(\lambda;\zeta,\kappa,\tau)=\frac{1}{\sinh\zeta}\begin{pmatrix}\sinh(\lambda-\eta/2+\zeta) & \kappa e^{\tau}\sinh(2\lambda-\eta)\\ \kappa e^{-\tau}\sinh(2\lambda-\eta) & \sinh(\zeta-\lambda+\eta/2)\end{pmatrix}$$

Right boundary: $K^{+}(\lambda)=K^{-}(\lambda+\eta)$,

Quantum inverse scattering method, (Sklyanin 1988)

$$\mathcal{U}_-(\lambda)=M(\lambda)K_-(\lambda)\widehat{M}(\lambda)=M(\lambda)K_-(\lambda)\sigma_0^y M^{t_0}(-\lambda)\sigma_0^y=\begin{pmatrix}\mathcal{A}_-(\lambda) & \mathcal{B}_-(\lambda)\\ \mathcal{C}_-(\lambda) & \mathcal{D}_-(\lambda)\end{pmatrix}$$

1. Reflection algebra

$$R_{12}(\lambda-\mu)\,(\mathcal{U}_-)_1(\lambda)\,R_{12}(\lambda+\mu-\eta)\,(\mathcal{U}_-)_2(\mu)$$
$$=(\mathcal{U}_-)_2(\mu)\,R_{12}(\lambda+\mu-\eta)\,(\mathcal{U}_-)_1(\lambda)\,R_{12}(\lambda-\mu)$$

2. Transfer matrix:

$$\mathcal{T}(\lambda)=\mathrm{tr}_0\{K_+(\lambda)\,\mathcal{U}_-(\lambda)\},\qquad [\mathcal{T}(\lambda),\mathcal{T}(\mu)]=0.$$

3. Quantum determinant

$$\frac{\det_q\mathcal{U}_-(\lambda)}{\sinh(2\lambda-2\eta)}=\mathcal{A}_-(\epsilon\lambda+\eta/2)\mathcal{A}_-(\eta/2-\epsilon\lambda)+\mathcal{B}_-(\epsilon\lambda+\eta/2)\mathcal{C}_-(\eta/2-\epsilon\lambda)$$
$$=\mathcal{D}_-(\epsilon\lambda+\eta/2)\mathcal{D}_-(\eta/2-\epsilon\lambda)+\mathcal{C}_-(\epsilon\lambda+\eta/2)\mathcal{B}_-(\eta/2-\epsilon\lambda),$$

where $\epsilon=\pm 1$, Quantum determinant is a central element of the reflection algebra

$$[\det_q\mathcal{U}_-(\lambda),\mathcal{U}_-(\mu)]=0.$$

Notations:

$$\mathbf{A}(\lambda) = (-1)^N \frac{\sinh(2\lambda+\eta)}{\sinh 2\lambda} g_+(\lambda) g_-(\lambda) a(\lambda) d(-\lambda)$$

$$d(\lambda) = a(\lambda-\eta), \quad a(\lambda) = \prod_{n=1}^{N} \sinh(\lambda - \xi_n),$$

$$g_\pm(\lambda) = \frac{\sinh(\lambda+\alpha_\pm \pm \eta/2)\cosh(\lambda \mp \beta_\pm \pm \eta/2)}{\sinh\alpha_\pm \cosh\beta_\pm},$$

$\alpha_\pm$ and $\beta_\pm$ give a different parametrisation for the boundary parameters:

$$\sinh\alpha_\pm \cosh\beta_\pm = \frac{\sinh\zeta_\pm}{2\kappa_\pm}, \qquad \cosh\alpha_\pm \sinh\beta_\pm = \frac{\cosh\zeta_\pm}{2\kappa_\pm}.$$

Hamiltonian

In the homogeneous limit:

$$H = \frac{2(\sinh\eta)^{1-2N}}{\text{tr}\{K_+(\eta/2)\}\,\text{tr}\{K_-(\eta/2)\}}\frac{d}{d\lambda}\mathcal{T}(\lambda)_{|\lambda=\eta/2} + \text{constant.}$$

$$= \sum_{i=1}^{N-1}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \cosh\eta\,\sigma_i^z\sigma_{i+1}^z)$$

$$+ \frac{\sinh\eta}{\sinh\zeta_-}\left[\sigma_1^z\cosh\zeta_- + 2\kappa_-(\sigma_1^x\cosh\tau_- + i\sigma_1^y\sinh\tau_-)\right]$$

$$+ \frac{\sinh\eta}{\sinh\zeta_+}\left[(\sigma_N^z\cosh\zeta_+ + 2\kappa_+(\sigma_N^x\cosh\tau_+ + i\sigma_N^y\sinh\tau_+)\right].$$

Two obstacles: No reference state! $|0\rangle$, such that $\mathcal{C}_-(\lambda)|0\rangle = 0$, $\forall\lambda$ and K_+ mixes all the operators...

No usual Algebraic Bethe Ansatz $\longrightarrow$ **Separation of variables** (Sklyanin 1985)

Gauge transformation

Cao et al (2003): 8-vertex scheme, following Baxter 1972 and Faddeev Takhtadjan 1979. **Gauge transformation** to diagonalize the boundary matrices.

$$G(\lambda|\beta) = \begin{pmatrix} 1 & e^{-\lambda+\beta\eta} \\ 0 & 1 \end{pmatrix}.$$

For our approach we need K_+ triangular and K_- generic, one parameter is enough. If one of the boundary matrices is triangular no gauge transform is needed.

Gauge transformed two-row monodromy matrix

$$\mathcal{U}_-(\lambda|\beta) = G^{-1}(\lambda - \eta/2|\beta)\,\mathcal{U}_-(\lambda)\,G(\eta/2 - \lambda|\beta) = \begin{pmatrix} \mathcal{A}_-(\lambda|\beta) & \mathcal{B}_-(\lambda|\beta) \\ \mathcal{C}_-(\lambda|\beta) & \mathcal{D}_-(\lambda|\beta) \end{pmatrix}$$

Quantum determinant:

$$\mathcal{U}_-(\lambda+\eta/2|\beta)\,\mathcal{U}_-(\eta/2-\lambda|\beta)=\frac{\det_q\mathcal{U}_-(\lambda)}{\sinh(2\lambda-2\eta)},$$

$$\mathcal{U}_-(\eta/2-\lambda|\beta)\,\mathcal{U}_-(\lambda+\eta/2|\beta)=\frac{\det_q\mathcal{U}_-(\lambda)}{\sinh(2\lambda-2\eta)}.$$

Transfer matrix:

$$\mathcal{T}(\lambda)=K_+^{(L)}(\lambda|\beta)_{11}\mathcal{A}_-(\lambda|\beta)+K_+^{(L)}(\lambda|\beta)_{22}\mathcal{D}_-(\lambda|\beta)$$
$$+K_+^{(L)}(\lambda|\beta)_{21}\mathcal{B}_-(\lambda|\beta)+K_+^{(L)}(\lambda|\beta)_{12}\mathcal{C}_-(\lambda|\beta),$$

where $K_+^{(L)}(\lambda|\beta)$ gauge transformed boundary matrix

Gauge fixing: we need $K_+^{(L)}(\lambda|\beta)_{12}=0$

$$\beta\eta=\tau_+(-1)^k(\beta_+-\alpha_+)+i\pi k,$$

Eigenstates of $\mathcal{B}$

The following states form a basis and are eigenstates of $\mathcal{B}_-(\lambda|\beta)$:

$$|h_1, \ldots, h_N, \beta\rangle = \prod_{n=1}^{N} \left(\frac{\mathcal{D}_-(\xi_n + \eta\,|\beta)}{\mathsf{D}_-(\xi_n + \eta)} \right)^{h_n} |0\rangle, \quad h_j = 0, 1$$

$$\mathcal{B}_-(\lambda|\beta)|\mathbf{h}, \beta\rangle = \mathsf{B}_{\mathbf{h}}(\lambda|\beta)|\mathbf{h}, \beta\rangle,$$

$$\mathsf{B}_{\mathbf{h}}(\lambda|\beta) = (-1)^N a_{\mathbf{h}}(\lambda) a_{\mathbf{h}}(-\lambda) \times \frac{\sinh(2\lambda - \eta)\left(2\kappa_- \sinh\left[(N + \beta + 1)\eta - \tau_-\right] - e^{\zeta_-}\right)}{2\sinh\zeta_-}.$$

$$a_{\mathbf{h}}(\lambda) = \prod_{n=1}^{N} \sinh(\lambda - \xi_n + h_n\eta)$$

Separate states

Let $\alpha(\lambda)$ be an arbitrary polynomial. We call **separate states** the states defined as

$$|\alpha\rangle = \sum_{h_1,\dots,h_N=0}^{1} \prod_{a=1}^{N} \alpha(\xi_a + h_a\eta)\, \mathcal{N}(\mathbf{h}) |h_1, \dots, h_N, \beta\rangle,$$

with a Sklyanin mesure

$$\mathcal{N}(\mathbf{h}) = \prod_{1\le b<a\le N} \Big(\cosh 2\,(\xi_a + h_a\eta) - \cosh 2\,(\xi_b + h_b\eta) \Big) \equiv V(\{\cosh 2\,(\xi + h\eta)\}),$$

here $V(\{x\})$ is a Vandermonde determinant

This state will play the role of **off-shell Bethe vectors**

Transfer matrix eigenstates

Separation of variables permits to prove that
1. The spectrum of the transfer matrix is simple
2. If $\tau(\lambda)$ is an eigenvalue of the transfer matrix then the corresponding eigenstate is a separate state

$$|\tau\rangle = \sum_{h_1,\dots,h_N=0}^{1} \prod_{a=1}^{N} Q_\tau(\xi_a + h_a\eta)\,\mathcal{N}(\mathbf{h})|h_1,\dots,h_N,\beta\rangle,$$

With a function Q_τ satisfying

$$\frac{Q_\tau(\xi_a+\eta)}{Q_\tau(\xi_a)} = \frac{\tau(\xi_n)}{\mathbf{A}(-\xi_n)}$$

This relation reminds Baxter $T - Q$ relation (note that $\mathbf{A}(\xi_a) = 0$):

$$\tau(\xi_a)Q_\tau(\xi_a) = \mathbf{A}(-\xi_a)Q_\tau(\xi_a+\eta) + \mathbf{A}(\xi_a)Q_\tau(\xi_a-\eta).$$

T-Q relation

In general $Q_\tau(\xi_a + h_a\eta)$ are values of the Baxter Q operator satisfying T-Q **relation**.
Related question: are there **Bethe equation**?
Lemma Let boundary parameters be generic (Nepomechie's constraints are not satisfied).

$$\kappa_+ \neq 0, \kappa_- \neq 0, \quad Y^{(i,r)}(\tau_\pm, \alpha_\pm, \beta_\pm) \neq 0 \;\; \forall i \in \{0,1\}, r = 0, \ldots N$$

where

$$Y^{(i,r)}(\tau_\pm, \alpha_\pm, \beta_\pm) \equiv \tau_- - \tau_+ + (-1)^i \left[(N-1-r)\,\eta + (\alpha_- + \alpha_+ + \beta_- - \beta_+)\right]$$

Then for any eigenstate, the homogeneous Baxter equation

$$\tau(\lambda)Q(\lambda) = \mathbf{A}(\lambda)Q(\lambda-\eta) + \mathbf{A}(-\lambda)Q(\lambda+\eta),$$

has no non-trivial polynomial solution.

It's sufficient to compare leading behaviour at $\lambda \to \infty$

Inhomogeneous T-Q relation

We define:

$$F(\lambda) = F_0 \, (\cosh^2 2\lambda - \cosh^2 \eta) \prod_{b=1}^{N} (\cosh 2\lambda - \cosh 2\xi_b)(\cosh 2\lambda - \cosh 2(\xi_b + \eta))$$

with the obstacle term for the Baxter equation

$$F_0 = \frac{2\kappa_+\kappa_- \, (\cosh(\tau_+ - \tau_-) - \cosh(\alpha_+ + \alpha_- - \beta_+ + \beta_- - (N+1)\eta))}{\sinh \zeta_+ \sinh \zeta_-},$$

Theorem: Let the boundary parameters be generic. Then $\tau(\lambda)$ is an eigenvalue of the transfer matrix if and only if there is the unique polynomial solution $Q(\lambda)$ of the **inhomogeneous Baxter equation**

$$\tau(\lambda)Q(\lambda) = \mathbf{A}(\lambda)Q(\lambda - \eta) + \mathbf{A}(-\lambda)Q(\lambda + \eta) + F(\lambda).$$

$Q(\lambda)$ is a polynomial of degree N of $\cosh(2\lambda)$. Solving the corresponding Bethe equations for the roots of Q we obtain the **complete set of eigenstates!**.

Constrained case

1. Let the boundary parameters satisfy the following constraint:

$$\kappa_+ \neq 0, \kappa_- \neq 0, \quad \exists i \in \{0,1\} \quad : Y^{(i,2N)}(\tau_\pm, \alpha_\pm, \beta_\pm) = 0$$

Then $\tau(\lambda)$ is an eigenvalue of the transfer matrix if and only if there is the unique (up to overall normalization) polynomial solution $Q(\lambda)$ of the **homogeneous Baxter equation**

$$\tau(\lambda)Q(\lambda) = \mathbf{A}(\lambda)Q(\lambda - \eta) + \mathbf{A}(-\lambda)Q(\lambda + \eta),$$

$Q(\lambda)$ is a polynomial of degree N of $\cosh(2\lambda)$. Solving the corresponding Bethe equations for the roots of Q we obtain again the complete set of eigenstates.

2. More general constraint (for any integer $M = 0, \dots N-1$):

$$\kappa_+ \neq 0, \kappa_- \neq 0, \quad \exists i \in \{0,1\}, M \in \{0, ..., N-1\} : Y^{(i,2M)}(\tau_\pm, \alpha_\pm, \beta_\pm) = 0,$$

Then there are two sectors: one with **homogeneous** Baxter equations and $Q(\lambda)$ polynomial of degree M of $\cosh(2\lambda)$ and the second one with **inhomogeneous** Baxter equation and $Q(\lambda)$ polynomial of degree N.

Scalar products

The scalar product of any two separate states

$$\langle\omega| = \sum_{h_1,\ldots,h_N=0}^{1} \prod_{a=1}^{N} \omega(\xi_a + h_a\eta)\, \mathcal{N}(\mathbf{h}) \langle\beta, h_1, \ldots, h_N|,$$

$$|\rho\rangle = \sum_{h_1,\ldots,h_N=0}^{1} \prod_{a=1}^{N} \rho(\xi_a + h_a\eta)\, \mathcal{N}(\mathbf{h}) |h_1, \ldots, h_N, \beta\rangle,$$

Then

$$\langle\omega|\rho\rangle = Z(\beta) \frac{\det_N \mathcal{M}_{a,b}^{(\omega,\rho)}}{V(\{\cosh 2\xi\})}$$

$$\mathcal{M}_{a,b}^{(\omega,\rho)} = \sum_{h=0}^{1} \omega(\xi_a + h_a\eta)\rho(\xi_a + h_a\eta)\Big(\cosh 2\,(\xi_a + h_a\eta)\Big)^{(b-1)}.$$

Typical SOV result, difficult to use in the homogeneous limit

Toy example: anti-periodic XXX chain

XXX chain with anti-periodic boundary conditions

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

$$\sigma_{N+1}^z = -\sigma_1^z, \quad \sigma_{N+1}^{\pm} = \sigma_1^{\mp}$$

Transfer matrix: $\mathcal{T}(\lambda) = B(\lambda) + C(\lambda)$

Eigenstates of $D(\lambda)$:

$$|\mathbf{h}\rangle = \frac{1}{V(\{\xi\})} \prod_{n=1}^{N} \left(\frac{B(\xi_n)}{d(\xi_n + \eta)}\right)^{h_n} |0\rangle, \quad d(\lambda) = \prod_{n=1}^{N} (\lambda - \xi_n),$$

$$\langle \mathbf{h}| = \frac{1}{V(\{\xi\})} \langle 0| \prod_{n=1}^{N} \left(\frac{C(\xi_n)}{d(\xi_n - \eta)}\right)^{h_n},$$

Separate states

$$\langle\beta| = \sum_{h_1=0}^{1}\cdots\sum_{h_N=0}^{1}\prod_{a=1}^{N}\bar{\beta}(\xi_a - h_a\eta)\, V(\{\xi - h\eta\})\langle h_1, \ldots, h_N|,$$

$$|\alpha\rangle = \sum_{h_1=0}^{1}\cdots\sum_{h_N=0}^{1}\prod_{a=1}^{N}\alpha(\xi_a - h_a\eta)\, V(\{\xi - h\eta\})|h_1, \ldots, h_N\rangle,$$

Here $V(\{\xi\})$ is the Vandermonde determinant. $\alpha(\lambda)$ and $\beta(\lambda)$ arbitrary functions

Eigenstates are separate states $\langle Q_\tau|$ with a polynomial $Q_\tau(\lambda)$ if Baxter equation is satisfied

$$\tau(\lambda)Q_\tau(\lambda) = -a(\lambda)Q_\tau(\lambda - \eta) + d(\lambda)Q_\tau(\lambda + \eta)$$

Notations: $a(\lambda) = d(\lambda + \eta), \quad d(\lambda) = \prod_{n=1}^{N}(\lambda - \xi_n),$

Scalar products

Scalar product:

$$\langle\beta|\alpha\rangle = \frac{\det_N \mathcal{M}^{(\alpha,\beta)}}{V(\{\xi\})},$$

with

$$\mathcal{M}^{(\alpha,\beta)}_{a,b} = \xi_a^{b-1}\alpha(\xi_a)\bar{\beta}(\xi_a) + (\xi_a-\eta)^{b-1}\alpha(\xi_a-\eta)\bar{\beta}(\xi_a-\eta).$$

Main results: Let $\alpha(\lambda) = \prod_{j=1}^{M}(\lambda-\alpha_j)$ and $Q(\lambda) = \prod_{j=1}^{R}(\lambda-\lambda_j)$ then

- if $M < R$

$$\langle\alpha\,|Q\rangle = 0.$$

- If $M = R$ then the Slavnov formula can be applied:

$$\langle\alpha\,|Q\rangle = 2^{N-2M}\left(\prod_{n=1}^{M} d(\alpha_n)d(\lambda_n)\right)\mathcal{S}_M(\{\lambda\},\{\alpha\}).$$

- If $M>R$ then we obtain the generalized Slavnov formula

$$\langle\alpha\,|Q\rangle=(-1)^{M+R}2^{N-M-R}\left(\prod_{n=1}^{M}d(\alpha_n)\prod_{k=1}^{R}d(\lambda_k)\right)\,\mathcal{S}_{R,M}(\{\lambda\},\{\alpha\}).$$

$$\mathcal{S}_{M,M+S}(\{\lambda\},\{\alpha\})=\frac{\det_{M+S}\mathcal{H}}{V(\lambda_1,\dots,\lambda_M)V(\alpha_{M+S},\dots,\alpha_1)}$$

$$\mathcal{H}_{jk}=Q(\alpha_k-\eta)\frac{a(\alpha_k)}{d(\alpha_k)}\,t(\lambda_j-\alpha_k)+Q(\alpha_k+\eta)t(\alpha_k-\lambda_j),\quad \text{for}\quad j\leqslant M,$$

$$\mathcal{H}_{jk}=Q(\alpha_k-\eta)\frac{a(\alpha_k)}{d(\alpha_k)}\,\alpha_k^{j-M-1}+Q(\alpha_k+\eta)\,(\alpha_k+\eta)^{j-M-1},\quad \text{for}\quad j>M,$$

where $t(x)=\frac{\eta}{x(x+\eta)}$

The proof is very general and completely algebraic. **Similar technique works for the XXZ chain with generic boundaries** (to appear)

Conclusion and outlook

Main result: There is a **Slavnov-type formula** for the models solved by the Separation of Variables method: possibility to compute **form factors**, overlaps, correlation functions and it can be used for asymptotic and numerical analysis

Open questions:

- **Inhomogeneous Bethe equations:** classification of solutions.
- Connection between the **homogeneous** and **inhomogeneous** Baxter equations. Can we sacrifice polynomiality and retrieve **homogeneity**?
- Inhomogeneous Baxter equation appear in different frameworks: off-diagonal Bethe ansatz, separation of variables, modified algebraic Bethe ansatz (Belliard, Crampé). In the **classical limit**, what is the meaning of the inhomogeneous Baxter equation?