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Non-commuting integrals of motion in XXZ model

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Contents

Introduction

In this work we will describe ... [1]

Throughout this thesis we will work in units such that $\hbar = 1$.

Spin operator algebra:

$$\left[S_i^{\alpha}, S_k^{\beta}\right] = i\delta_{i,k}\epsilon_{\alpha\beta\gamma}S_i^{\gamma}$$
$$S_i^{\pm} = S_i^x \pm iS_i^y$$
$$\left[S_i^+, S_k^+\right] = 2\delta_{i,k}S_i^z$$
$$\left[S_i^z, S_k^{\pm}\right] = \pm\delta_{i,j}S_i^{\pm}$$

Heisenberg Hamiltonian:

$$H_{XXZ} = \frac{1}{2}\sum_{j=1}^{L}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + \Delta\sum_{j=1}^{L} S_j^z S_{j+1}^z + \alpha H' \tag{1.1}$$

where H' is the perturbation that breaks integrability for nonzero α:

$$H' = \sum_{j=1}^{L} S_j^z S_{j+2}^z \tag{1.2}$$

Quantity that is plotted in Figures 4–14:

- With extrapolation to thermodynamic limit:

$$R_l(\tau, \alpha) = \frac{\lambda_l(L \to \infty, \tau, \alpha)}{\lambda_l(L \to \infty, \tau \to \infty, \alpha = 0)} \tag{1.3}$$

- Without extrapolation to thermodynamic limit:

$$R_l^L(\tau, \alpha) = \frac{\lambda_l(L, \tau, \alpha)}{\lambda_l(L, \tau \to \infty, \alpha = 0)} \tag{1.4}$$

Energy current in integrable XXZ model:

$$J^E = \sum_i i\left[\beta_1\left(S_{i-1}^- S_i^z S_{i+1}^+\right) + \beta_2\left(S_{i-1}^z S_i^+ S_{i+1}^- + S_{i-1}^+ S_i^- S_{i+1}^z\right)\right] + \text{H.c.} \tag{1.5}$$

Spin LIOM for $\Delta = 1.0$:

$$\hat{O}_1 = \beta_3\sum_{i=1}^{L} S_i^+ + \text{H.c.} \tag{1.6}$$

Spin QLIOM for $\Delta = -0.5$:

$$\hat{O}_1 = \beta_4\sum_{i=1}^{L}\left(S_i^+ S_{i+1}^+ S_{i+2}^+\right) + \text{H.c.} \tag{1.7}$$

$$\left[J^E, S_{tot}^z\right] = 0 \text{ where } S_{tot}^z = \sum_i S_i^z$$

1.1 Model and method

We investigate a one dimensional XXZ Hamiltonian on a lattice of L sites with periodic boundary conditions.

$$H = J \sum_{j=1}^{L} \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + \Delta \sum_{j=1}^{L} S_j^z S_{j+1}^z \tag{1.8}$$

We are interested in systematic classification of all local and quasilocal CQs supported on 3 and 4 sites. To this end, we employ the algorithm first proposed in (relevant citation). Here we will present all derivations in a detailed manner. Consider the space $\mathcal{B}_L^m$ of local, traceless and translationally invariant observables supported on m sites, with inner product:

$$(A|B) = \frac{1}{2^L} \operatorname{tr}\!\left(A^\dagger B\right) \tag{1.9}$$

i.e. the Hilbert-Schmidt product. Traceless operators have zero overlap with the identity, $(A|\mathcal{I}) = \frac{1}{2^L} \operatorname{tr}(A) = 0$. Now we introduce an orthonormal basis of $\mathcal{A}_L^m$:

$$O_{\underline{s}} = \sum_{j=1}^{L} \sigma_j^{s_1} \sigma_{j+1}^{s_2} \cdots \sigma_{j+m-1}^{s_m} \tag{1.10}$$

where $\sigma_j^z \equiv \sqrt{2} S_j^z$, $\sigma_j^\pm \equiv S_j^\pm$, $\sigma_j^0 \equiv \mathcal{I}$, $\underline{s} = (s_1, s_2, \ldots s_m)$ and $s_j \in \{+, -, z, 0\}$ while $s_{1,m} \in \{+, -, z\}$. For a fixed m, there are exactly $N_m = 3 \cdot 4^{m-2} \cdot 3$ such operators and they satisfy an orthonormality condition i.e $\left(O_{\underline{s}} | O_{\underline{s}'}\right) = \delta_{\underline{s}, \underline{s}'}$.

We define the infinite time averaging of an operator $A \in \mathcal{A}_L^m$, employing the Heisenberg picture:

$$\overline{A} = \lim_{\tau \to \infty} \frac{1}{\tau} \int dt\, A_H(t) = \lim_{\tau \to \infty} \frac{1}{\tau} \int dt\, e^{iHt} A e^{-iHt} =$$

$$\sum_{n,m} \lim_{\tau \to \infty} \frac{1}{\tau} \int dt\, e^{iE_m t} |m\rangle \langle m|A|n\rangle \langle n| e^{-iE_n t} =$$

$$\sum_{n,m} \langle m|A|n\rangle |m\rangle\langle n| \lim_{\tau \to \infty} \frac{1}{\tau} \int dt\, e^{i(E_m - E_n)t} = \sum_{n,m}^{E_n = E_m} \langle m|A|n\rangle |m\rangle\langle n| \tag{1.11}$$

It is evident from equation (1.11) that large degeneracy of energy spectrum will be important to the structure of time-averaged operators. Moreover, time averaging in such form is an orthogonal projection in the Hilbert space of operators. From that follows a crucial property i.e $\left(\overline{A}|\overline{B}\right) = \left(\overline{A}|B\right)$.

Here continues a detailed derivation of the algorithm. And something about fermions.

We conducted preliminary studies for small values of L, without assuming translational invariance. Available resources allowed us to make unrestricted search for $L = 8, 9, 10, 11, 12$ in case of $m = 3$ and $L = 8, 9, 10, 11$ in case of $m = 4$. Nevertheless, operators that maximized stiffness for given L and Δ turned out to be translationally invariant. Therefore, we restrict our considerations to translationally invariant operators only. This allowed us to obtain numerical results for L up to 14 in case of $m = 3$ and up to 13 in case of $m = 4$. To study the case of $L = 16$ we considered a subspace of $\mathcal{A}_L^m$ spanned by basis operators $\overline{O}_{\underline{s}}$ that have nonzero coefficients in operator with largest stiffness for $L = 14$. Then we diagonalized the resulting 2×2 correlation matrix to obtain the stiffness.

Operators with corresponding to largest eigenvalues of K matrix

1.2 Operators with largest stiffness

In this section we list operators with leading eigenvalues.

Fermions with $m = 3$:

- $\hat{O}_{max} = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+ \mathcal{I}_{i+2}) + \alpha_2 (S_i^+ S_{i+1}^z S_{i+2}^+) \Big)$ for even L and $\Delta = \pm 1.0$

- $\hat{O}_{max} = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+ \mathcal{I}_{i+2}) + \alpha_2 (S_i^+ \mathcal{I}_{i+1} S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^+ S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^z S_{i+2}^+) +$

  $\alpha_5 (S_i^+ S_{i+1}^+ S_{i+2}^z) \Big)$ for odd L and $\Delta = \pm 1.0$

- $\hat{O}_{max} = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+ \mathcal{I}_{i+2}) + \alpha_2 (S_i^+ S_{i+1}^z S_{i+2}^+) \Big)$ for $L = 8, 12$ and $\Delta = \pm 0.5$

- $\hat{O}_{max} = \sum_{i=1}^{L} (-1)^i \alpha_1 \Big(S_i^+ S_{i+1}^+ \mathcal{I}_{i+2} \Big)$ for $L = 10, 14$ and $\Delta = \pm 0.5$

- $\hat{O}_{max} = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+ \mathcal{I}_{i+2}) + \alpha_2 (S_i^+ \mathcal{I}_{i+1} S_{i+1}^+) + \alpha_3 (S_i^z S_{i+1}^+ S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^z S_{i+2}^+) +$

  $\alpha_5 (S_i^+ S_{i+1}^+ S_{i+2}^z) \Big)$ for $L = 9, 11, 13$ and $\Delta = \pm 0.5$

Fermions with $m = 4$:

- $\hat{O}_{max} = \sum_{i=1}^{L}$

Spins with $m = 3$:

- $\hat{O}_{max} = \sum_{i=1}^{L} \alpha_1 \Big(S_i^+ \mathcal{I}_{i+1} \mathcal{I}_{i+2} \Big)$ for all L and $\Delta = 1.0$ $\quad \alpha_1 = \pm \frac{1}{\sqrt{L}}$

- $\hat{O}_{max} = \sum_{i=1}^{L} (-1)^i \alpha_1 \Big(S_i^+ \mathcal{I}_{i+1} \mathcal{I}_{i+2} \Big)$ for even L and $\Delta = -1.0$ $\quad \alpha_1 = \pm \frac{1}{\sqrt{L}}$

- $\hat{O}_{max} = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ \mathcal{I}_{i+1} \mathcal{I}_{i+2}) + \alpha 2 (S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^z S_{i+2}^+) +$

  $\alpha_5 (S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6 (S_i^z S_{i+1}^+ S_i^z) + \alpha_6 (S_i^+ S_{i+1}^z S_{i+2}^z) \Big)$ for odd L and $\Delta = -1.0$

- $\hat{O}_{max} = \sum_{i=1}^{L} \alpha_1 \Big(S_i^+ S_{i+1}^+ S_{i+2}^+ \Big)$ for all L and $\Delta = -0.5$

- $\hat{O}_{max} = \sum_{i=1}^{L} (-1)^i \alpha_1 \Big(S_i^+ \mathcal{I}_{i+1} \mathcal{I}_{i+2} \Big)$ for even L and $\Delta = 0.5$

- $\hat{O}_{max} = \sum_{i=1}^{L} (-1)^i \Big(\alpha_1 (S_i^+ \mathcal{I}_{i+1} \mathcal{I}_{i+2}) + \alpha 2 (S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^- S_{i+2}^+) +$

  $\alpha_5 (S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6 (S_i^z S_{i+1}^+ S_i^z) + \alpha_6 (S_i^+ S_{i+1}^z S_{i+2}^z) \Big)$ for odd L and $\Delta = 0.5$

Konwencja w kodzie: $0 \longleftrightarrow \mathcal{I}$, $1 \longleftrightarrow S^+$, $2 \longleftrightarrow S^z$, $3 \longleftrightarrow S^-$

Spin operators supported on up to $m = 3$ sites:

- $\hat{O}_1 = \alpha_1 \sum_{i=1}^{L} S_i^+ + \text{H.c.}$, for all L and $\Delta = 1.0$ $\quad \alpha_1 = \pm \frac{1}{\sqrt{L}}$

- $\hat{O}_1 = \alpha_1 \sum\limits_{i=1}^{L} (-1)^i S_i^+ + \text{H.c., for even } L \text{ and } \Delta = -1.0 \quad \alpha_1 = \pm\frac{1}{\sqrt{L}}$

- $\hat{O}_1 = \sum\limits_{i=1}^{L} \Big(\alpha_1(S_i^+) + \alpha_2(S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3(S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4(S_i^+ S_{i+1}^- S_{i+2}^+) +$

  $\alpha_5(S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6(S_i^z S_{i+1}^+ S_i^z) + \alpha_7(S_i^+ S_{i+1}^z S_{i+2}^z) \Big) + \text{H.c., for odd } L \text{ and } \Delta = -1.0$

- $\hat{O}_1 = \alpha_1 \sum\limits_{i=1}^{L} \Big(S_i^+ S_{i+1}^+ S_{i+2}^+ \Big) + \text{H.c., for all } L \text{ and } \Delta = -0.5 \quad \alpha_1 = \pm\frac{1}{\sqrt{L}}$

- $\hat{O}_1 = \alpha_1 \sum\limits_{i=1}^{L} (-1)^i \Big(S_i^+ S_{i+1}^+ S_{i+2}^+ \Big) + \text{H.c., for even } L \text{ and } \Delta = 0.5$

- $\hat{O}_1 = \sum\limits_{i=1}^{L} \Big(\alpha_1(S_i^+) + \alpha_2(S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3(S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4(S_i^+ S_{i+1}^- S_{i+2}^+) +$

  $\alpha_5(S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6(S_i^z S_{i+1}^+ S_i^z) + \alpha_7(S_i^+ S_{i+1}^z S_{i+2}^z) \Big) + \text{H.c., for odd } L \text{ and } \Delta = 0.5$

Fermion operators supported on up to $m = 3$ sites:

- $\hat{O}_1 = \sum\limits_{i=1}^{L} \Big(\alpha_1(S_i^+ S_{i+1}^+) + \alpha_2(S_i^+ S_{i+1}^z S_{i+2}^+) \Big) + \text{H.c., for even } L \text{ and } \Delta = \pm 1.0$

- $\hat{O}_1 = \sum\limits_{i=1}^{L} \Big(\alpha_1(S_i^+ S_{i+1}^+) + \alpha_2(S_i^+ \mathcal{I}_{i+1} S_{i+2}^+) + \alpha_3(S_i^z S_{i+1}^+ S_{i+2}^+) + \alpha_4(S_i^+ S_{i+1}^z S_{i+2}^+) +$

  $\alpha_5(S_i^+ S_{i+1}^+ S_{i+2}^z) \Big) + \text{H.c., for odd } L \text{ and } \Delta = \pm 1.0$

- $\hat{O}_1 = \sum\limits_{i=1}^{L} \Big(\alpha_1(S_i^+ S_{i+1}^+) + \alpha_2(S_i^+ S_{i+1}^z S_{i+2}^+) \Big) + \text{H.c., for } L = 8, 12 \text{ and } \Delta = \pm 0.5$

- $\hat{O}_1 = \alpha_1 \sum\limits_{i=1}^{L} (-1)^i \Big(S_i^+ S_{i+1}^+ \Big) + \text{H.c., for } L = 10, 14 \text{ and } \Delta = \pm 0.5$

- $\hat{O}_1 = \sum\limits_{i=1}^{L} \Big(\alpha_1(S_i^+ S_{i+1}^+) + \alpha_2(S_i^+ \mathcal{I}_{i+1} S_{i+1}^+) + \alpha_3(S_i^z S_{i+1}^+ S_{i+2}^+) + \alpha_4(S_i^+ S_{i+1}^z S_{i+2}^+) +$

  $\alpha_5(S_i^+ S_{i+1}^+ S_{i+2}^z) \Big) + \text{H.c., for } L = 9, 11, 13 \text{ and } \Delta = \pm 0.5$

Energy current

In order to test our QLIOM finding algorithm and the correctness of its implementation, we investigate the known case of energy current in spin$-1/2$ XXZ model [2]. For the sake of completeness, derivation of spin energy current for the general XYZ model will be presented, following the definitions in [3]. We start with the XYZ Hamiltonian with periodic boundary conditions:

$$H_{XYZ} = \sum_{i=1}^{L} \left(J_x S_i^x S_{i+1}^x + J_x S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z \right) \tag{2.1}$$

It is easy to see that this Hamiltonian can be represented as a sum of operators supported on two consecutive sites:

$$H_{XYZ} = \sum_{i=1}^{L} h_{i,i+1} \tag{2.2}$$

where $h_{i,i+1} = J_x S_i^x S_{i+1}^x + J_x S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z$ and periodic boundary conditions require that $h_{L,L+1} = h_{L,1}$. The energy operator is a conserved quantity, thus the time evolution of its local density is given by the discrete continuity equation:

$$\frac{\mathrm{d} h_{i,i+1}(t)}{\mathrm{d}t} + \boldsymbol{\nabla} \cdot j_i^E = 0 \tag{2.3}$$

where $\boldsymbol{\nabla} \cdot j_i^E \equiv j_{i+1}^E - j_i^E$. On the other hand, time evolution of an arbitrary operator is determined by the Heisenberg equations:

$$\frac{\mathrm{d} h_{i,i+1}(t)}{\mathrm{d}t} = i[H_{XYZ}, h_{i,i+1}(t)] \tag{2.4}$$

Combining equations 2.3 and (2.4) we obtain the defining equations for the spin energy current:

$$j_{i+1}^E - j_i^E = -i[H_{XYZ}, h_{i,i+1}(t)] = i[h_{i,i+1}(t), H_{XYZ}] = i \sum_{k=1}^{L} [h_{i,i+1}, h_{k,k+1}] \tag{2.5}$$

Similar equations can be written for any operator being a sum of local operators (with support 2?) such as the total spin operator or particle number operator in Hubbard model. Equation (2.5) is conceptually simple, yet quite tedious to solve due to the amount of commutators present. Luckily, leveraging commutator properties to our advantage will allow us to simplify the calculations. Let us begin with inserting the definition of $h_{i,i+1}$ into equation (2.5):

$$\begin{aligned}
[h_{i,i+1}, h_{k,k+1}] =& \left[J_x S_i^x S_{i+1}^x + J_x S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z, J_x S_k^x S_{k+1}^x + J_x S_k^y S_{k+1}^y + J_z S_k^z S_{k+1}^z \right] \\
=& J_x J_y \left[S_i^x S_{i+1}^x, S_k^y S_{k+1}^y \right] + J_x J_z \left[S_i^x S_{i+1}^x, S_k^z S_{k+1}^z \right] + J_y J_x \left[S_i^y S_{i+1}^y, S_k^x S_{k+1}^x \right] \\
&+ J_y J_z \left[S_i^y S_{i+1}^y, S_k^z S_{k+1}^z \right] + J_z J_x \left[S_i^z S_{i+1}^z, S_k^x S_{k+1}^x \right] + J_z J_y \left[S_i^z S_{i+1}^z, S_k^y S_{k+1}^y \right]
\end{aligned}$$

By inspection it becomes clear that out of six terms present, only three will need to be directly evaluated, as commutators of the form xy will differ from yx by a sign and an index change.

$$\begin{aligned}
J_x J_y \left[S_i^x S_{i+1}^x, S_k^y S_{k+1}^y \right] =& J_x J_y \left(S_i^x \left[S_{i+1}^x, S_k^y S_{k+1}^y \right] + \left[S_i^x, S_k^y S_{k+1}^y \right] S_{i+1}^x \right) \\
=& J_x J_y \left(S_i^x \left(S_k^y \left[S_{i+1}^x, S_{k+1}^y \right] + \left[S_{i+1}^x, S_k^y \right] S_{k+1}^y \right) + \left(S_k^y \left[S_i^x, S_{k+1}^y \right] + \left[S_i^x, S_k^y \right] S_{k+1}^y S_{k+1}^y \right) \right)
\end{aligned}$$

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