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Non-commuting integrals of motion in XXZ model

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Abstract

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Contents

Introduction

1.1 Motivation

1.2 Organization

XXZ model

We investigate a one dimensional XXZ Hamiltonian on a one-dimensional lattice of L sites with periodic boundary conditions. Throughout this thesis we will work in units such that $\hbar = 1$.

Spin operator algebra:

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

Write about tensor product, Hilbert space structure and such

Heisenberg Hamiltonian:

$$H_{XXZ} = J\sum_{j=1}^{L}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) + \Delta\sum_{j=1}^{L}S_j^zS_{j+1}^z + \alpha H' \tag{2.1}$$

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

$$H' = \sum_{j=1}^{L}S_j^zS_{j+2}^z \tag{2.2}$$

Integrals of motion

The problem of our interest is the systematic classification of all local and quasilocal integrals of motion (LIOMs and QLIOMs) supported on $\mathbb{N} \ni m \leq L/2$ sites in a model given by 1-D tight-binding Hamiltonian H. To this end, we employ the algorithm first proposed in Mierzejewski, Prelovšek, and Prosen [1]. In our description and notation used, we will follow the works of Mierzejewski, Prelovšek, and Prosen [1, 2] and Mierzejewski, Kozarzewski, and Prelovšek [3]. The aim of this thesis is to provide a pedagogical introduction to the topic, so all derivations are presented in full detail, together with a simple proof of correctness for the algorithm.

3.1 Preliminaries

Space of observables Consider the vector space $\mathcal{V}_L$ of traceless and translationally invariant observables, acting on a Hilbert space of dimension 2^L. We can define an inner product on this space:

$$(A|B) = \frac{1}{2^L}\operatorname{tr}\left(A^\dagger B\right) = \frac{1}{2^L}\sum_{mn} A_{nm} B^*_{nm} \tag{3.1}$$

i.e. the Hilbert-Schmidt product, where $A_{nm} = \langle n|A|m\rangle$ and $H|n\rangle = E_n|n\rangle$. This definition is correct, as we work only with finite dimensional Hilbert spaces and taking the trace is an linear operation. We require the operators to be traceless, because they have zero overlap with the identity, $(A|\mathcal{I}) = \frac{1}{2^L}\operatorname{tr}(A) = 0$. Now we consider a subspace $\mathcal{V}_L^m$ of m-local operators and a direct sum $\mathcal{V}_L^M = \bigoplus_{m=1}^M \mathcal{V}_L^m$ being a subspace of operators supported on up to M sites. We also define a basis of $\mathcal{V}_L^M$ consisting of operators $O_s \in \mathcal{V}_L^M$ satisfying the following properties:

$$\begin{aligned}
&(O_s|O_t) = \delta_{s,t} && \text{(orthonormality)}\\
&\left(\forall A \in \mathcal{V}_L^M\right)\left(A = \sum_s (O_s|A)\, O_s\right) && \text{(completeness)}\\
&\left(\forall A \in \mathcal{V}_L\right)\left(A = A^M + A^\perp = \sum_s (O_s|A)\, O_s + A^\perp\right), \text{ such that } (\forall s)\left(\left(O_s|A^\perp\right) = 0\right) && (3.2)
\end{aligned}$$

Locality We begin with a definition of integral of motion in quantum mechanics.

Definition 3.1 *Let H be a Hamiltonian operator. Then, any observable O fulfilling the equation:*

$$[H, O] = 0$$

*is an **integral of motion**.*

It is easy to see, that there are many such observables. Let us consider the following

Example 3.1 *Take H to be any Hamiltonian operator. By spectral theorem, it can be written is diagonal form:*

$$H = \sum_n E_n |n\rangle\langle n|$$

Then a set of projection operators $P_n = |n\rangle\langle n|$ is a family of IOMs. Eigenstates of a Hamiltonian are in general very nonlocal.

However, as it will become evident in Section 3.3 on spectral function, nonlocal operators are not important in the thermodynamic limit and we are only interested in the so called local (or quasilocal) integrals of motion. A working intuition behind local operators is perhaps best seen in Figure 3.1. They can be thought of as being different from identity only on m consecutive sites. XXZ Hamiltonian defined by equation (2.1) is an example of 2-local operator. On the other hand, quasilocal operator can be represented as a convergent sum of operators with increasing support. In Section 3.2, a precise definition of locality and quasilocality will be

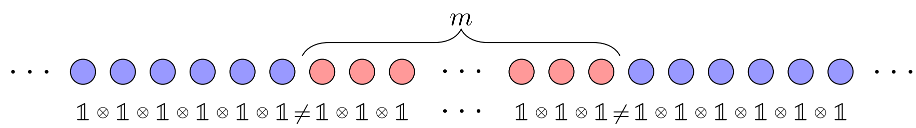

Figure 3.1: Illustration of an operator supported on m sites.

stated.

Noncommutativity In the case of XXZ model (also in general XYZ model) the Hamiltonian preserves the total z-component of spin, or in other words, it commutes with the total spin operator of the form:

$$S^z_{tot} = \sum_{i=1}^{L} S^z_i$$

This fact allows us to decompose the full Hilbert space into parts consisting of states with the same total z-component of spin. In more mathematical terms, we have the following:

$$\mathcal{H} = \bigoplus_{i=0}^{L} \mathcal{H}_i, \text{ where } \big(\forall \left|\psi\right\rangle \in \mathcal{H}_i\big)\big(S^z_{tot}\left|\psi\right\rangle = \frac{1}{2}(i-L)\left|\psi\right\rangle\big)$$

i.e. the full Hilbert space with $\dim \mathcal{H} = 2^L$ can be decomposed into the direct sum of its proper subspaces $\mathcal{H}_i$ such that $\dim \mathcal{H}_i = \binom{L}{i}$ and all states in a given subspace correspond to the same eigenvalue of S^z_{tot} operator. The index i denotes the number of sites with spin up. Now we are ready for

Definition 3.2 *Let O be an integral of motion. If O preserves total z-component of spin, i.e. $[S^z_{tot}, O] = 0$, then it is called a* ***commuting integral of motion****. Otherwise, it is called a* ***noncommuting integral of motion****.*

For the algorithm described in Section 3.2, we need to construct matrices of observables and express them in the Hamiltonian eigenbasis. If the operator in question is a commuting IOM, we can restrict ourselves to the fixed spin subspace and thus greatly reduce computational complexity, allowing us to investigate larger systems. Such operators, for example spin energy current, have already been studied [2]. Therefore, the main focus of this work is the investigation of existence and properties of much less known noncommuting IOMs. This forces us to remain in full Hilbert space and restricts system sizes that we are able to check.

3.2 (Q)LIOMs finding algorithm

We now introduce a finite time averaging of an operator $A \in \mathcal{V}^M_L$, employing the Heisenberg picture [2]:

$$\begin{aligned}
\bar{A}^\tau =& \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, A_H(t) = \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, e^{iHt} A e^{-iHt} = \sum_{m,n} \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, e^{iE_m t}\left|m\right\rangle \left\langle m|A|n\right\rangle \left\langle n\right| e^{-iE_n t} = \\
=& \sum_{m,n} A_{mn} \left|m\right\rangle\!\left\langle n\right| \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, e^{i(E_m-E_n)t} = \sum_{m,n} A_{mn}\left|m\right\rangle\!\left\langle n\right| \frac{1}{\tau}\frac{1}{i\,(E_m-E_n)}\left(e^{i(E_m-E_n)\tau}-1\right) \\
=& \sum_{m,n} A_{mn}\left|m\right\rangle\!\left\langle n\right| e^{i(E_m-E_n)\tau/2} \times \frac{\sin\left((E_m-E_n)\,\tau\right)}{\tau\,(E_m-E_n)}
\end{aligned} \tag{3.3}$$

What this procedure does is essentially a cut off figure illustrating the cut off of for matrix elements determined by the value of $E_m - E_n$ in relation to the averaging time τ. However, this expression is quite complicated and therefore we introduce a simplified time averaging (henceforth time averaging):

Definition 3.3

$$\bar{A}^{\tau} \equiv \sum_{m,n} \theta\left(\frac{1}{\tau} - |E_m - E_n|\right) A_{mn} |m\rangle\langle n| = \sum_{m,n} \theta^{\tau}_{mn} A_{mn} |m\rangle\langle n| \tag{3.4}$$

where θ is the Heaviside step function, is the time averaged version of operator A.

Going to the infinite time limit we obtain the time averaging from Mierzejewski, Prelovšek, and Prosen [1]:

$$\bar{A} = \lim_{\tau\to\infty} \bar{A}^{\tau} = \sum_{\substack{m,n \\ E_m = E_n}} A_{mn} |m\rangle\langle n| \tag{3.5}$$

Observing that $(\theta^{\tau}_{mn})^2 = \theta^{\tau}_{mn}$ and $\left(\bar{A}^{\tau}\right)_{mn} = \theta^{\tau}_{mn} A_{mn}$ we can easily show some crucial properties of the time averaging:

Proposition 3.1 *For any $A, B \in \mathcal{V}_L$*

$$\left(\bar{A}^{\tau}|\bar{B}^{\tau}\right) = \left(A|\bar{B}^{\tau}\right) = \left(\bar{A}^{\tau}|B\right)$$

and

$$\overline{\left(\bar{A}^{\tau}\right)}^{\tau} = \left(\bar{A}^{\tau}\right)$$

Proof.

$$\begin{aligned}
\left(\bar{A}^{\tau}|\bar{B}^{\tau}\right) &= \frac{1}{2^L} \sum_{mn} \left(\bar{A}^{\tau}\right)_{mn} \left(\bar{B}^{\tau}\right)^{*}_{mn} = \frac{1}{2^L} \sum_{mn} (\theta^{\tau}_{mn})^2 A_{mn} B^{*}_{mn} \\
&= \frac{1}{2^L} \sum_{mn} (\theta^{\tau}_{mn}) A_{mn} B^{*}_{mn} = \left(A|\bar{B}^{\tau}\right) = \left(\bar{A}^{\tau}|B\right) \\
\overline{\left(\bar{A}^{\tau}\right)}^{\tau} &= (\theta^{\tau}_{mn})^2 A_{mn} = \theta^{\tau}_{mn} A_{mn} = \left(\bar{A}^{\tau}\right)
\end{aligned}$$

■

These two facts reveal an interesting interpretation of the time averaging, namely that it can be thought of as an orthogonal projection in vector space $\mathcal{V}_L$. The involutive character of this operation explains, why we can consider $\bar{A}^{\tau}$ time independent in the time window $(0, \tau)$.

Let us now calculate the commutator of time-averaged operator with the Hamiltonian:

$$\begin{aligned}
\left[H, \bar{A}^{\tau}\right] &= \sum_{n} \sum_{k,p} E_n \theta^{\tau}_{kp} A_{kp} [|n\rangle\langle n|\,, |k\rangle\langle p|] \\
&= \sum_{k,p} (E_k - E_p)\, \theta^{\tau}_{kp} A_{kp} |k\rangle\langle p| \xrightarrow{\tau\to\infty} 0
\end{aligned} \tag{3.6}$$

The last limit follows directly from equation (3.5). We can see that the infinite time averaging procedure creates an integral of motion, i.e. $\left[H, \bar{A}\right] = 0$. Nonetheless it is not enough to just time average a local operator in order to get a local integral of motion, because in general $A \in \mathcal{V}^M_L \not\Rightarrow \bar{A} \in \mathcal{V}^M_L$. One possible approach to checking its locality would be to express this operator in the basis defined in (3.2). If for some M we have $\bar{A} \in \mathcal{V}^M_L$, then it is local. Second possibility is that it can be written as a convergent series of operators from $\mathcal{V}^m_L$ with increasing m — then it is quasilocal. Otherwise it is a generic nonlocal quantity. But can we do better than this direct approach?

To answer this question, we fix $0 \leq M \leq L/2$ and construct a basis $\{O_s\}$ of $\mathcal{V}^M_L$. How to actually perform such construction will be shown in Section 3.4. Next, we find time averages of all basis operators and build a matrix

$$K_{st} = \left(\bar{O_s}^{\tau}|\bar{O_t}^{\tau}\right) \tag{3.7}$$

This matrix is symmetric by design, as considered operators are Hermitian and thus of the form $O + O^\dagger$ or $i\left(O - O^\dagger\right)$. Therefore, the spectral theorem guarantees existence of an unitary matrix U that diagonalizes it. In other words, $D = UKU^\dagger$ is diagonal and we have the following relations:

$$\begin{aligned}
&\sum_{s,t} U_{ns} K_{st} U^T_{tm} = \delta_{nm}\lambda_n \in \mathbb{R}, \quad \lambda_n \text{ — eigenvalue of } K \\
&UU^\dagger = U^\dagger U = \mathbb{1} \implies \sum_s U_{ns} U^T_{sm} = \delta_{mn} \\
&UK = DU \implies \sum_s U_{ns} K_{st} = \sum_s \delta_{ns}\lambda_s U_{st} = \lambda_n U_{nt}
\end{aligned} \tag{3.8}$$

With the help of the U matrix (eigenvectors of K) we can define a new set of rotated operators that are time-independent in the window $(0, \tau)$:

$$Q_n = \sum_s U_{ns} \bar{O}^\tau_s \tag{3.9}$$

Proposition 3.2 *Operators Q_n are orthogonal, i.e. $(Q_n|Q_m) \propto \delta_{nm}$*

Proof. Let Q_n, Q_m be two operators defined as in (3.9). Their orthogonality can be shown by direct calculation:

$$\begin{aligned}
(Q_n|Q_m) &= \sum_{s,t} U_{ns}\left(\bar{O}_s{}^\tau|\bar{O}_t{}^\tau\right)U^T_{tm} = \sum_t \left(\sum_s U_{ns}K_{st}\right)U^T_{tm} \\
&\triangleq \lambda_n \sum_t U_{nt}U^T_{tm} \triangleq \lambda_n\delta_{mn}
\end{aligned}$$

■

The last two equalities, marked with $\triangleq$ follow from properties (3.8). We can learn something more about the eigenvalues of K matrix from a simple corollary to Proposition 3.2.

Corollary 3.1 *K is a positive semi-definite matrix.*

Proof. Let Q_n be defined as in (3.9). Then, from the defining properties of inner product we have that $(Q_n|Q_n) \geq 0$. However, we also have that $(Q_n|Q_n) = \lambda_n$. Combining these two equations, we get that $(\forall n)\,(\lambda_n \geq 0)$. Therefore K is a positive semi-definite matrix. ■

This corollary provides us with a lower bound on spectrum of matrix K.

Let us now examine the support of Q_n. By (3.2) and making use of Proposition 3.1 and properties (3.8), we can decompose into M-local part and nonlocal part:

$$\begin{aligned}
Q_n &= \sum_s (O_s|Q_n)\,O_s + Q^\perp_s = \sum_{s,t} U_{nt}\left(O_s|\bar{O}^\tau_t\right)O_s + Q^\perp_n \\
&= \sum_{s,t} U_{nt}\left(\bar{O}^\tau_s|\bar{O}^\tau_t\right)O_s + Q^\perp_n = \sum_{s,t} U_{nt}K_{ts}O_s + Q^\perp_n \\
&= \sum_s\left(\sum_t U_{nt}K_{ts}\right)O_s + Q^\perp_n = \sum_s \lambda_n U_{ns}O_s + Q^\perp_n = Q^M_n + Q^\perp_n
\end{aligned} \tag{3.10}$$

TODO: finall results on support and proof of correctness

3.3 Spectral function

One may ask a question, why are local (and quasilocal) IOMs actually important. To answer this question in a convincing manner we will follow the discussion in Vidmar et al. [4] and introduce spectral functions. Suppose that we have an observable

$$\left(\bar{A}^\tau \mid \bar{B}^\tau\right) = \lim_{\varepsilon \searrow 0} \int_{-\frac{1}{\tau}}^{\frac{1}{\tau}} \mathrm{d}\omega \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}t e^{i\omega t - |t|\varepsilon} \frac{\left\langle A^\dagger B(t)\right\rangle}{L} \tag{3.11}$$

3.4 Case of $M = 3$ in the XXZ model

After explaining how and why to look for LIOMs and QLIOMs, let us now turn to an example.

Now we introduce an orthonormal basis of $\mathcal{A}_L^m$:

$$O_{\underline{s}} = \sum_{j=1}^{L} \sigma_j^{s_1} \sigma_{j+1}^{s_2} \cdots \sigma_{j+m-1}^{s_m} \tag{3.12}$$

where $\sigma_j^z \equiv \sqrt{2} S_j^z$, $\sigma_j^\pm \equiv S_j^\pm$, $\sigma_j^0 \equiv \mathcal{I}$, $\underline{s} = (s_1, s_2, \dots s_m)$ 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 $\left(O_{\underline{s}} | O_{\underline{s'}}\right) = \delta_{\underline{s},\underline{s'}}$.

Decomposition into 4 mutually orthogonal sectors

3.5 Commuting LIOM: Spin energy current

In order to test our (Q)LIOM 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 Zotos, Naef, and Prelovsek [5]. We start with the general XYZ Hamiltonian with periodic boundary conditions:

$$H_{XYZ} = \sum_{i=1}^{L} \left(J_x S_i^x S_{i+1}^x + J_x S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z \right) \tag{3.13}$$

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

$$H_{XYZ} = \sum_{i=1}^{L} h_{i,i+1} \tag{3.14}$$

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:

$$\frac{\mathrm{d}h_{i,i+1}(t)}{\mathrm{d}t} + \boldsymbol{\nabla} \cdot j_i^E(t) = 0 \tag{3.15}$$

where $\boldsymbol{\nabla} \cdot j_i^E(t) \equiv j_{i+1}^E(t) - j_i^E(t)$ is the discrete divergence of spin energy current density and $h_{i,i+1}(t) = e^{iH_{XYZ}t} h_{i,i+1} e^{-iH_{XYZ}t}$. On the other hand, time evolution of an arbitrary operator is determined by the Heisenberg equations:

$$\frac{\mathrm{d}h_{i,i+1}(t)}{\mathrm{d}t} = i[H_{XYZ}, h_{i,i+1}(t)] \tag{3.16}$$

Combining equations (3.15) and (3.16) we obtain the defining equations for the spin energy current density:

$$j_{i+1}^E - j_i^E = -i[H_{XYZ}, h_{i,i+1}] = i[h_{i,i+1}, H_{XYZ}] = i \sum_{k=1}^{L} [h_{i,i+1}, h_{k,k+1}] \tag{3.17}$$

Similar equations can be written for any operator being a sum of local operators such as the total spin operator or particle number operator in fermionic models. Detailed solution to the equation (3.17) is shown in Appendix A. For the XXZ model we get the following expression:

$$\begin{aligned} j_i^E &= i\Big(\underbrace{2J S_{i-1}^- S_i^z S_{i+1}^+ + J\Delta S_{i-1}^z S_i^+ S_{i+1}^- + J\Delta S_{i-1}^+ S_i^- S_{i+1}^z}_{O_i} \\ &\quad - \underbrace{\left(2J S_{i-1}^+ S_i^z S_{i+1}^- + J\Delta S_{i-1}^z S_i^- S_{i+1}^+ + J\Delta S_{i-1}^- S_i^+ S_{i+1}^z\right)}_{O_i^\dagger} \Big) \\ &= i\left(O_i - O_i^\dagger\right) \end{aligned}$$

Obtaining the energy current operator is now simply the matter of summing over all the lattice sites:

$$J^E = \sum_{i=1}^{L} j_i^E \tag{3.18}$$

Tutaj dalej o tym że komutuje z H, stała funkcja autokorelacji i jak zanika przy zaburzeniu. Ale dopiero po rozdziale o algorytmie żeby notacja była ustalona

Numerical results

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.

scratchpad

5.1 Meetings

27.10.2021 meeting:

- integrability of Heisenberg model for $\alpha = 0.0$ is Bethe ansatz?
  - bethe ansatz and existence of extensive number of IOMs
- sources for motivation and history in intro
  - From Chaos to Quantum Thermalization...
  - arXiv:2012.07849
- best way to introduce Heisenberg model?
  - follow Dirac as in Spalek book
- source for nonlocal operators stiffness vanishing in thermodynamic limit
  - just use Zotos1997
- is extrapolation with 1/L just finite size scaling?
  - yes

03.11.2021 meeting:

- is this algorithm valid for any lattice model? or just 1-D

5.2 Other

Quantity that is plotted in Figures 4–14:

- With extrapolation to thermodynamic limit:

$$R_l(\tau, \alpha) = \frac{\lambda_l(L \to \infty, \tau, \alpha)}{\lambda_l(L \to \infty, \tau \to \infty, \alpha = 0)} \tag{5.1}$$

- Without extrapolation to thermodynamic limit:

$$R_l^L(\tau, \alpha) = \frac{\lambda_l(L, \tau, \alpha)}{\lambda_l(L, \tau \to \infty, \alpha = 0)} \tag{5.2}$$

Energy current in integrable XXZ model:

$$J^E = \sum_i^L i\left[\beta_1\left(S_{i-1}^- S_i^z S_{i+1}^+\right) + \beta_2\left(S_{i-1}^z S_i^+ S_{i+1}^- + S_{i-1}^+ S_i^- S_{i+1}^z\right)\right] + \text{H.c.} \tag{5.3}$$

Spin LIOM for $\Delta = 1.0$:

$$\hat{O}_1 = \beta_3 \sum_{i=1}^L S_i^+ + \text{H.c.} \tag{5.4}$$

Spin QLIOM for $\Delta = -0.5$:

$$\hat{O}_1 = \beta_4 \sum_{i=1}^L \left(S_i^+ S_{i+1}^+ S_{i+2}^+\right) + \text{H.c.} \tag{5.5}$$

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

5.3 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 $\Delta = -1.0$ $\quad \alpha_1 = \pm\frac{1}{\sqrt{L}}$

- $\hat{O}_{max} = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ \mathcal{I}_{i+1} \mathcal{I}_{i+2}) + \alpha 2 (S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^- S_{i+2}^+) +$
  $\alpha_5 (S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6 (S_i^z S_{i+1}^+ S_i^z) + \alpha_6 (S_i^+ S_{i+1}^z S_{i+2}^z) \Big)$ 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 $\Delta = 1.0 \quad \alpha_1 = \pm \frac{1}{\sqrt{L}}$
- $\hat{O}_1 = \alpha_1 \sum_{i=1}^{L} (-1)^i S_i^+ + \text{H.c.},$ for even L and $\Delta = -1.0 \quad \alpha_1 = \pm \frac{1}{\sqrt{L}}$
- $\hat{O}_1 = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+) + \alpha_2 (S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^- S_{i+2}^+) +$
  $\alpha_5 (S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6 (S_i^z S_{i+1}^+ S_i^z) + \alpha_7 (S_i^+ S_{i+1}^z S_{i+2}^z) \Big) + \text{H.c.},$ for odd L and $\Delta = -1.0$
- $\hat{O}_1 = \alpha_1 \sum_{i=1}^{L} \Big(S_i^+ S_{i+1}^+ S_{i+2}^+ \Big) + \text{H.c.},$ for all L and $\Delta = -0.5 \quad \alpha_1 = \pm \frac{1}{\sqrt{L}}$
- $\hat{O}_1 = \alpha_1 \sum_{i=1}^{L} (-1)^i \Big(S_i^+ S_{i+1}^+ S_{i+2}^+ \Big) + \text{H.c.},$ for even L and $\Delta = 0.5$
- $\hat{O}_1 = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+) + \alpha_2 (S_i^- S_{i+1}^+ S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^z S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^- S_{i+2}^+) +$
  $\alpha_5 (S_i^- S_{i+1}^- S_{i+2}^+) + \alpha_6 (S_i^z S_{i+1}^+ S_i^z) + \alpha_7 (S_i^+ S_{i+1}^z S_{i+2}^z) \Big) + \text{H.c.},$ for odd L and $\Delta = 0.5$

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

- $\hat{O}_1 = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+) + \alpha_2 (S_i^+ S_{i+1}^z S_{i+2}^+) \Big) + \text{H.c.},$ for even L and $\Delta = \pm 1.0$
- $\hat{O}_1 = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+) + \alpha_2 (S_i^+ \mathcal{I}_{i+1} S_{i+2}^+) + \alpha_3 (S_i^z S_{i+1}^+ S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^z S_{i+2}^+) +$
  $\alpha_5 (S_i^+ S_{i+1}^+ S_{i+2}^z) \Big) + \text{H.c.},$ for odd L and $\Delta = \pm 1.0$
- $\hat{O}_1 = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+) + \alpha_2 (S_i^+ S_{i+1}^z S_{i+2}^+) \Big) + \text{H.c.},$ for $L = 8, 12$ and $\Delta = \pm 0.5$

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

- $\hat{O}_1 = \sum_{i=1}^{L} \Big(\alpha_1 (S_i^+ S_{i+1}^+) + \alpha_2 (S_i^+ \mathcal{I}_{i+1} S_{i+1}^+) + \alpha_3 (S_i^z S_{i+1}^+ S_{i+2}^+) + \alpha_4 (S_i^+ S_{i+1}^z S_{i+2}^+) +$
  $\alpha_5 (S_i^+ S_{i+1}^+ S_{i+2}^z) \Big) + \text{H.c.}$, for $L = 9, 11, 13$ and $\Delta = \pm 0.5$

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Derivation of spin energy current

Equation (3.17) 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 (3.17):

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

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

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

Carrying out the calculation of remaining two non-trivial commutators, we arrive at the following equations:

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

Next step requires us to evaluate the sum over lattice sites to get rid of the Kronecker δ's. As before, one of the three parts of calculations is provided in full detail:

$$\begin{aligned}
& i \sum_{k=1}^{L} J_x J_y \left[S_i^x S_{i+1}^x, S_k^y S_{k+1}^y\right] + i \sum_{k=1}^{L} J_x J_y \left[S_i^y S_{i+1}^y, S_k^x S_{k+1}^x\right] = \\
& - J_x J_y \Big(\cancel{S_i^x S_i^y S_{i+1}^z} + S_i^x S_{i+1}^z S_{i+2}^y + S_{i-1}^y S_i^z S_{i+1}^x + \cancel{S_i^z S_{i+1}^y S_{i+1}^x} \Big) \\
& + J_x J_y \Big(\cancel{S_i^x S_i^y S_{i+1}^z} + S_i^y S_{i+1}^z S_{i+2}^x + S_{i-1}^x S_i^z S_{i+1}^y + \cancel{S_i^z S_{i+1}^y S_{i+1}^x} \Big) \\
& = J_x J_y \Big(S_i^y S_{i+1}^z S_{i+2}^x - S_i^x S_{i+1}^z S_{i+1}^y - \left(S_{i-1}^y S_i^z S_{i+1}^x - S_{i-1}^x S_i^z S_{i+1}^y \right) \Big)
\end{aligned}$$

$$\begin{aligned}
& i \sum_{k=1}^{L} J_x J_z \left[S_i^x S_{i+1}^x, S_k^z S_{k+1}^z\right] + i \sum_{k=1}^{L} J_x J_z \left[S_i^z S_{i+1}^z, S_k^x S_{k+1}^x\right] = \\
& = J_x J_z \Big(S_i^x S_{i+1}^y S_{i+2}^z - S_i^z S_{i+1}^y S_{i+2}^x - \left(S_{i-1}^x S_i^y S_{i+1}^z - S_{i-1}^z S_i^y S_{i+1}^x \right) \Big)
\end{aligned}$$

$$\begin{aligned}
& i \sum_{k=1}^{L} J_y J_z \left[S_i^y S_{i+1}^y, S_k^z S_{k+1}^z\right] + i \sum_{k=1}^{L} J_y J_z \left[S_i^z S_{i+1}^z, S_k^y S_{k+1}^y\right] = \\
& = J_y J_z \Big(S_i^z S_{i+1}^x S_{i+2}^y - S_i^y S_{i+1}^x S_{i+2}^z - \left(S_{i-1}^z S_i^x S_{i+1}^y - S_{i-1}^y S_i^x S_{i+1}^z \right) \Big)
\end{aligned}$$

What now remains is to collect these parts and see that we finally arrive at the equation for the energy current density:

$$\begin{aligned} j_i^E &= J_x J_y \left(S_{i-1}^y S_i^z S_{i+1}^x - S_{i-1}^x S_i^z S_{i+1}^y\right) \\ &+ J_x J_z \left(S_{i-1}^x S_i^y S_{i+1}^z - S_{i-1}^z S_i^y S_{i+1}^x\right) \\ &+ J_y J_z \left(S_{i-1}^z S_i^x S_{i+1}^y - S_{i-1}^y S_i^x S_{i+1}^z\right) \\ &= J_x J_y \left(S_{i-1}^y S_i^z S_{i+1}^x - S_{i-1}^x S_i^z S_{i+1}^y\right) + \text{cyclic permutations of } (x, y, z) \end{aligned} \tag{A.1}$$

which is precisely the expression from Zotos, Naef, and Prelovsek [5]. However, in this work we are interested in the XXZ model with the Hamiltonian (2.1). To this end, we need to set $J_x, J_z = 2J$, $J_z = \Delta$ and substitute $S_i^x = \frac{S_i^+ + S_i^-}{2}$, $S_i^y = \frac{S_i^+ - S_i^-}{2i}$. After some more lengthy calculations, we finally arrive at the desired form of energy current density operator:

$$\begin{aligned} j_i^E = i\Big(&\underbrace{2JS_{i-1}^- S_i^z S_{i+1}^+ + J\Delta S_{i-1}^z S_i^+ S_{i+1}^- + J\Delta S_{i-1}^+ S_i^- S_{i+1}^z}_{O_i} \\ &- \underbrace{\left(2JS_{i-1}^+ S_i^z S_{i+1}^- + J\Delta S_{i-1}^z S_i^- S_{i+1}^+ + J\Delta S_{i-1}^- S_i^+ S_{i+1}^z\right)}_{O_i^\dagger}\Big) \end{aligned} \tag{A.2}$$

$$= i\left(O_i - O_i^\dagger\right) \tag{A.3}$$

It is evident that the energy current operator $J^E = \sum_{i=1}^L i\left(O_i - O_i^\dagger\right)$ has support of exactly 3 consecutive sites.