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Non-commuting integrals of motion in XXZ model

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Index number: 250193

Bachelor thesis
under supervision of
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Wrocław
University
of Science
and Technology

Wrocław 2021

Abstract

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Introduction

1.1 Motivation

1.2 Structure

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:

$$H_{XXZ} = \frac{J}{2}\sum_{j=1}^{L}\left(S_j^+S_{j+1}^- + S_j^-S_{j+1}^+\right) + J\Delta\sum_{j=1}^{L}S_j^zS_{j+1}^z + \alpha H' \tag{2.1}$$

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

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

We set $J = 1$ and subsequently work in units of J.

It is perhaps important to note that, between spin operators in the Hamiltonian stands the tensor product, not regular composition of operators.

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 $m \in \mathbb{N}$ 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]. It allows us to classify integrals of motions for a given system size L. After doing so for accessible values of L, we then carry out finite size scaling to obtain information about the thermodynamic limit $L \to \infty$.

In our description and notation used, we follow the works of Mierzejewski, Prelovšek, and Prosen [1], Mierzejewski et al. [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. The importance of (Q)LIOMs is made clear by invoking the concept of spectral functions and Mazur bound.

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 $\mathcal{D}$. We can define an inner product on this space:

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

i.e. the Hilbert-Schmidt product, where $A_{nm} = \langle n|A|m\rangle$ and $H|n\rangle = E_n|n\rangle$. Moreover, we define the Hilbert-Schmidt norm of an operator to be $\|A\| = \sqrt{(A|A)}$. This product corresponds to the infinite temperature limit of averaging over a suitable ensemble (either canonical or grand canonical). Presented definitions are 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, $(A|\mathbb{1}) = \frac{1}{D}\operatorname{tr}(A) = 0$. 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:

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

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:*

$$H = \sum_n E_n \left|n\right\rangle\!\left\langle n\right|$$

Then a set of projection operators $P_n = \left|n\right\rangle\!\left\langle n\right|$ 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

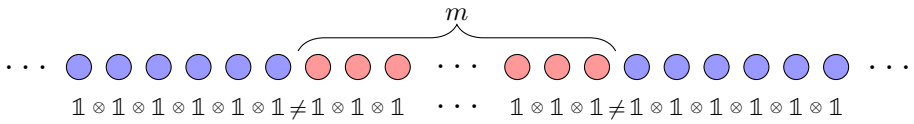

Figure 3.1: Illustration of an operator supported on m sites.

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:

$$S^z_{tot} = \sum_{i=1}^{L} S^z_i \tag{3.3}$$

The resulting $U(1)$ symmetry 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:

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

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, which do not posses the $U(1)$ symmetry of Hamiltonian. 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 $A \in \mathcal{V}_L^M$, employing the Heisenberg picture [2]:

$$\begin{aligned}\bar{A}^\tau =& \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, A_H(t) = \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, e^{iHt}Ae^{-iHt} = \sum_{m,n}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\, e^{iE_m t}\,|m\rangle\,\langle m|A|n\rangle\,\langle n|\,e^{-iE_n t} = \\ =& \sum_{m,n} A_{mn}\,|m\rangle\langle n|\,\frac{1}{\tau}\int_0^\tau \mathrm{d}t\, e^{i(E_m-E_n)t} = \sum_{m,n} A_{mn}\,|m\rangle\langle n|\,\frac{1}{\tau}\frac{1}{i\,(E_m-E_n)}\left(e^{i(E_m-E_n)\tau}-1\right) \\ =& \sum_{m,n} A_{mn}\,|m\rangle\langle n|\,e^{i(E_m-E_n)\tau/2}\times\frac{\sin\left((E_m-E_n)\,\tau\right)}{\tau\,(E_m-E_n)}\end{aligned} \tag{3.4}$$

What this procedure does is essentially a cut off (cf. Figure 3.2) 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 replace it with a simplified time averaging (henceforth time averaging):

Definition 3.3 (Simplified time averaging)

$$\bar{A}^\tau \equiv \sum_{m,n}\theta\left(\frac{1}{\tau}-|E_m-E_n|\right)A_{mn}\,|m\rangle\langle n| = \sum_{m,n}\theta^\tau_{mn}A_{mn}\,|m\rangle\langle n| \tag{3.5}$$

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]:

$$\bar{A} = \lim_{\tau\to\infty}\bar{A}^\tau = \sum_{\substack{m,n\\ E_m=E_n}} A_{mn}\,|m\rangle\langle n| \tag{3.6}$$

The quantity $\left(\bar{A}\middle|\bar{A}\right)$ is called the stiffness of operator A and corresponds to the infinite time limit of its autocorrelation function. In order to carry out the time averaging we need to express the operator in the basis of energy eigenstates and thus we need to perform exact diagonalization of the Hamiltonian. This is one of the main limiting factors of this procedure.

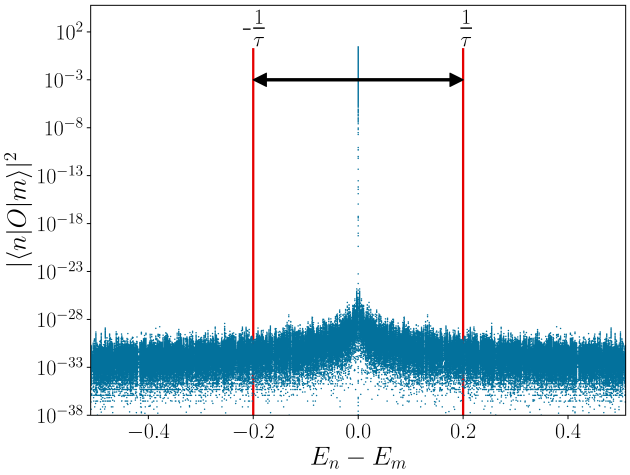

Figure 3.2: Illustration of averaging procedure as defined by equation (3.3). The sum of matrix elements is restricted by the theta function to the region between the two red lines. In the case of operator in question, we see that only the matrix elements corresponding to differences of energies very close to zero contribute to the time average.

Observing that $\left(\theta^\tau_{mn}\right)^2 = \theta^\tau_{mn}$ 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* $A, B \in \mathcal{V}_L$

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

and

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

Proof.

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

■

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:

$$\begin{aligned}\left[H, \bar{A}^\tau\right] &= \sum_n \sum_{k,p} E_n \theta^\tau_{kp} A_{kp} \left[|n\rangle\langle n|, |k\rangle\langle p|\right] \\ &= \sum_{k,p} \left(E_k - E_p\right) \theta^\tau_{kp} A_{kp} |k\rangle\langle p| \xrightarrow{\tau\to\infty} 0 \end{aligned} \tag{3.7}$$

The last limit follows directly from equation (3.6). 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 $A \in \mathcal{V}_L^M \nRightarrow \bar{A} \in \mathcal{V}_L^M$, that is the truncation of matrix elements modifies the support of an operator. 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 $\bar{A} \in \mathcal{V}_L^M$, then it is local. Second possibility is that it can be written as a convergent series of operators from $\mathcal{V}_L^m$ 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 $\mathcal{V}_L^M$. 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

$$K^\tau_{st} = \left(\bar{O_s}^\tau \middle| \bar{O_t}^\tau\right) \tag{3.8}$$

This matrix is Hermitian by design. However, the models we usually consider posses time-reversal symmetry, and so we may assume that it is real and symmetric. Therefore, the spectral theorem guarantees existence of an orthogonal matrix U that diagonalizes it. In other words, $D = UK^\tau U^T$ is diagonal and we have the following relations:

$$\begin{aligned}&\sum_{s,t} U_{ns} K^\tau_{st} U^T_{tm} = \delta_{nm} \lambda_n \in \mathbb{R}, \quad \lambda_n \text{ — eigenvalue of } K^\tau \\ &UU^T = U^T U = \mathbb{1} \implies \sum_s U_{ns} U^T_{sm} = \delta_{mn} \\ &UK = DU \implies \sum_s U_{ns} K^\tau_{st} = \sum_s \delta_{ns} \lambda_s U_{st} = \lambda_n U_{nt}\end{aligned} \tag{3.9}$$

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

$$Q_n = \sum_s U_{ns} \bar{O}^\tau_s \tag{3.10}$$

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 (3.10). Their orthogonality can be shown by direct calculation:

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

■

The last two equalities, marked with $\triangleq$, follow from properties (3.9). We can learn something more about the eigenvalues of K^{τ} matrix from a simple corollary to Proposition 3.2.

Corollary 3.1 *K^{τ} is a positive semi-definite matrix.*

Proof. Let Q_n be defined as in (3.10). 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^{τ} is a positive semi-definite matrix. ■

This corollary provides us with a lower bound on spectrum of matrix K^{τ}.

Let us now examine the support of Q_n. By (3.2) and making use of Proposition 3.1 and properties (3.9), we can decompose into M-local part and nonlocal part:

$$\begin{aligned}Q_n &= \sum_s (O_s|Q_n)\,O_s + Q_s^{\perp} = \sum_{s,t} U_{nt}\left(O_s\middle|\bar{O}^{\tau}_t\right)O_s + Q_n^{\perp} \\ &= \sum_{s,t} U_{nt}\left(\bar{O}^{\tau}_s\middle|\bar{O}^{\tau}_t\right)O_s + Q_n^{\perp} = \sum_{s,t} U_{nt}K_{ts}O_s + Q_n^{\perp} \\ &= \sum_s \left(\sum_t U_{nt}K^{\tau}_{ts}\right)O_s + Q_n^{\perp} = \sum_s \lambda_n U_{ns}O_s + Q_n^{\perp} = Q_n^M + Q_n^{\perp}\end{aligned} \tag{3.11}$$

Now we are ready to derive central result, stating why this actually algorithm works. Combining the fact that $(Q_n|Q_n) = \lambda_n$(see proof of Proposition 3.2) with (3.11) we obtain:

$$\begin{aligned}\lambda_n = (Q_n|Q_n) &= \left(Q_n^M + Q_n^{\perp}\middle|Q_n^M + Q_n^{\perp}\right) = \left(Q_n^M\middle|Q_n^M\right) + \left(Q_n^{\perp}\middle|Q_n^{\perp}\right) + \underbrace{2\left(Q_n^M\middle|Q_n^{\perp}\right)}_{=0\ (\text{cf. }(3.2))} \\ &= \left(\sum_s \lambda_n U_{ns}O_s\middle|\sum_t \lambda_n U_{nt}O_t\right) + \left\|Q_n^{\perp}\right\|^2 = \lambda_n^2 \sum_{s,t} U_{ns}\,(O_s|O_t)\,U^T_{tn} + \left\|Q_n^{\perp}\right\|^2 \\ &= \lambda_n^2 + \left\|Q_n^{\perp}\right\|^2\end{aligned} \tag{3.12}$$

Rearranging the above equality we get that $\lambda_n - \lambda_n^2 = \left\|Q_n^{\perp}\right\|^2 \geq 0$, which together with Corollary 3.1 gives $\lambda_n \in [0,1]$.

From now on, we will focus on the case $\tau \to \infty$, as it guarantees that $\bar{O}_s$'s and hence Q_n's commute with the Hamiltonian. Consequently, we finally arrive at a classification scheme for the support of Q_n's.

Definition 3.4 (Classification of IOMs) *An integral of motion Q_n is called:*

- *local:* $\lambda_n = 1 \implies \left\|Q_n^{\perp}\right\| = 0 \implies Q_n \in \mathcal{V}_L^M$
- *quasilocal:* $\lambda_n \in (0,1) \implies \left\|Q_n^{\perp}\right\| > 0 \implies Q_n \in \mathcal{V}_L$
- *generic nonlocal:* $\lambda_n = 0 \implies \|Q_n\| = 0$

The procedure outlined above works for a fixed system size L. In principle, to asses the character of an integral of motion, we need to examine how λ_n behaves in the thermodynamic limit. To achieve this, we execute this algorithm for a few accessible values of L and then proceed with finite size scaling. However, in this thesis we will examine both the $L \to \infty$ case and $L = 14$ case, that is largest system size for exact diagonalization that we were able to attain. We will end the discussion about the algorithm with a short summary on support of Q_n:

$$\begin{aligned} Q_n &= Q_n^M + Q_n^\perp \\ \|Q_n\|^2 &= \lambda_n \\ \left\|Q_n^M\right\|^2 &= \lambda_n^2 \\ \left\|Q_n^\perp\right\|^2 &= \lambda_n - \lambda_n^2 \end{aligned} \tag{3.13}$$

Proof of corectness Suppose we have an operator $\mathcal{V}_L^M \ni A = \sum_s u_s O_s$, where $u_s \in \mathbb{R}$ for all s. We can identify this operator from $\mathcal{V}_L^M$ with a vector $\vec{u} \in \mathbb{R}^{\dim \mathcal{V}_L^M}$. Using this picture, the stiffness of A can be calculated as follows:

$$\left(\bar{A}\middle|\bar{A}\right) = \sum_{s,t} u_s \left(\bar{O}_s\middle|\bar{O}_t\right) u_t = \sum_{s,t} u_s K_{st} u_t = \vec{u}^T K \vec{u} \tag{3.14}$$

Thus, a problem in quantum mechanics is reduced to a problem in linear algebra. Because all eigenvalues of K matrix are real, we can sort the corresponding operators (defined with columns of U matrix, i.e. eigenvectors of K) by their magnitude. We then say that the larger the eigenvalue, the 'better' the integral of motion is. But can we be sure, that the maximal eigenvalue obtained from the algorithm corresponds to the 'best' possible integral of motion? To put it another way, if the procedure detects neither local nor quasilocal integrals of motion, does that necessarily mean they do not exist for a given system? The answer to this question lies within the subsequent

Proposition 3.3 *Let λ be the maximal eigenvalue of K. Then the following equality holds:*

$$\lambda = \max_{\substack{\vec{v} \in \mathbb{R}^{\dim \mathcal{V}_L^M} \\ \|v\|=1}} \vec{v}^T K \vec{v}$$

Proof. Assume the converse, i.e. there exists such $\vec{u} \in \mathbb{R}^{\dim \mathcal{V}_L^M}$ that $\vec{u}^T K \vec{u} > \lambda$ and $\|u\| = 1$. Let $\{\vec{v}_n\}_n$ be a orthonormal basis consisting of eigenvectors of K. We can express $\vec{u}$ in this basis as $\sum_n u_n \vec{v}_n$ for $u_n \in \mathbb{R}$. Then we have:

$$\begin{aligned} \vec{u}^T K \vec{u} &= \left(\sum_n u_n \vec{v}_n^T\right) K \left(\sum_m u_m \vec{v}_m\right) = \sum_{n,m} u_n u_m \lambda_m \underbrace{\vec{v}_n^T \vec{v}_m}_{\delta_{mn}} \\ &= \sum_n u_n^2 \lambda_n \leq \sum_n u_n^2 \lambda = \lambda \sum_n u_n^2 = \lambda \end{aligned}$$

Obtained contradiction concludes the proof. ■

3.3 Spectral function and Mazur bound

Spectral function After we have learned about local and quasilocal IOMs and how to find them, it is perhaps the time to ask why are they actually important? To answer this question in a convincing manner we will follow the discussion in Vidmar et al. [4] and introduce the concept of spectral functions.

Suppose that we have an observable $A \in \mathcal{V}_L^M$ and we are interested in studying its time evolution. An obvious choice would be to calculate its autocorrelation function $(A(t)|A)$, where the time dependence of $A(t)$ is understood via the Heisenberg picture i.e. $A(t) = \exp(iHt)\, A \exp(-iHt)$. However, this quantity is rather unpleasant to work with. Instead, we will investigating the Fourier transform of autocorrelation function, formally defined as:

Definition 3.5 (Spectral function)

$$S(\omega) = \lim_{\varepsilon \to 0^+} \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}t \; e^{i\omega t - |t|\varepsilon} \, (A(t)|A)$$

The limit in the definition is present in order to ensure proper convergence of the integral and ω corresponds to $\frac{1}{\tau}$ from earlier discussion. To connect this quantity with numerical calculations and to smoothen out any fluctuations, we can once again integrate it, but this time over a finite frequency window:

$$I(\omega) = \int_{-\omega}^{\omega} \mathrm{d}\omega' \; S(\omega') = \frac{1}{D} \sum_{m,n} \theta \left(\omega - |E_m - E_n|\right) A_{mn}^2 \tag{3.15}$$

It turns out that this quantity is equal to the square of Hilbert-Schmidt norm of time averaged operator $\bar{A}^{\frac{1}{\omega}}$, which fits nicely within the previously discussed framework. Because all observables of interest are traceless and normalized to unity, we have this two important limits

$$\lim_{\omega \to \infty} I(\omega) = \frac{1}{\mathcal{D}} \sum_{m,n} A_{mn}^2 = \|A\|^2 = 1 \tag{3.16}$$

$$\lim_{\omega \to 0^+} I(\omega) = \frac{1}{\mathcal{D}} \sum_{\substack{m,n \\ E_m = E_n}} A_{mn}^2 = \|\bar{A}\|^2 \tag{3.17}$$

For frequencies small (long times) in comparison with system's characteristic energy scale, spectral function of an observable $A \in \mathcal{V}_L^M$ attains the following approximation:

$$S(\omega \ll J) \simeq D_A \delta(\omega) \tag{3.18}$$

where $D_A = \lim_{\omega \to 0^+} I(\omega)$ is the stiffness of an observable. Let us now imagine that we have a complete set of orthogonal (Q)LIOMs $(Q_n|Q_m) \propto \delta_{nm}$. It was shown by Mazur [5] and Suzuki [6] that the stiffness D_A of arbitrary observable A has its origin in the projections on these Q_n:

$$D_A = \sum_n D_n = \sum_n \frac{(A|Q_n)^2}{(Q_n|Q_n)} \tag{3.19}$$

Therefore, by calculating the overlap between our observable and all the (Q)LIOMs, we can infer about the long time behavior of its spectral function and thus its autocorrelation function. It is here that the importance of (Q)LIOMs becomes evident, as the overlap with generic nonlocal conserved quantities vanishes in the thermodynamic limit [7]. Because autocorrelation function of LIOMs is constant, its Fourier transform is a Dirac delta, which explains the form of equation (3.18).

Mazur bound If we know only a subset of the full set of (Q)LIOMs, this equality turns into a very useful lower bound for stiffness, called the *Mazur bound*. We will now proceed with a derivation of this bound for the case of one (Q)LIOM, in the spirit of a more modern discussion from Ilievski et al. [8].

Proposition 3.4 (Mazur bound for a single (Q)LIOM) *Let $A \in \mathcal{V}_L^M$ be an arbitrary observable and Q be a (quasi)local conserved quantity. Then the following inequality holds:*

$$D_A = \left(\bar{A}\middle|\bar{A}\right) \geq \frac{(A|Q)^2}{(Q|Q)}$$

Proof. We define a new observable $\mathcal{A} = \bar{A} - \alpha Q$ for $\alpha \in \mathbb{R}$. Obviously, square of the norm of this quantity is positive i.e. $\|\mathcal{A}\|^2 = \mathrm{tr}(\mathcal{A}\mathcal{A})/\mathcal{D} \geq 0$. On the other hand, we can carry out an explicit computation of the norm:

$$\begin{aligned} \|\mathcal{A}\|^2 &= \left(\bar{A} - \alpha Q\middle|\bar{A} - \alpha Q\right) = \left(\bar{A}\middle|\bar{A}\right) - \left(\bar{A}\middle|Q\right) - \alpha \left(Q\middle|\bar{A}\right) + \alpha^2 (Q|Q) \\ &= \left(\bar{A}\middle|\bar{A}\right) - 2\alpha (A|Q) + \alpha^2 (Q|Q) \geq 0 \end{aligned}$$

Between the first and the second line we have used the fact that $\big(\bar{A}\big|\bar{B}\big) = \big(\bar{A}\big|B\big) = \big(A\big|\bar{B}\big)$(cf. Proposition 3.1) and $\bar{Q} = Q$ for a conserved quantity. Let us now substitute $\alpha = \frac{(A|Q)}{(Q|Q)}$ to the above inequality.

$$D_A = \big(\bar{A}\big|\bar{A}\big) \geq 2\frac{(A|Q)}{(Q|Q)}(A|Q) - \frac{(A|Q)^2}{(Q|Q)^2}(Q|Q) = \frac{(A|Q)^2}{(Q|Q)}$$

■

It is perhaps worth noting, that the derivation Mazur bound for a single (Q)LIOM is almost equivalent to the proof of the Cauchy-Schwarz inequality, found in any linear algebra textbook. By following exactly the same procedure, we can easily generalize this results to a set of orthogonal conserved quantities $\{Q_n\}$:

$$D_A = \big(\bar{A}\big|\bar{A}\big) \geq \sum_n \frac{(A|Q_n)^2}{(Q_n|Q_n)} \tag{3.20}$$

We have already seen that Mazur inequality turns into an equality, if the set $\{Q_n\}$ is complete. However, up until a few years ago, it was not clear how to systematically identify such a complete set in interacting models. This have changed with the work of Mierzejewski, Prelovšek, and Prosen [1], where the algorithm described in details in Section 3.2 was first proposed. We will now show that the following proposition holds:

Proposition 3.5 (Saturation of Mazur bound) *The set $\{Q_n\}$ of (Q)LIOMs obtained from the algorithm in Section 3.2 is complete, that is it saturates the Mazur bound.*

Proof. Consider once again an arbitrary observable $\mathcal{V}_L^M \ni A = \sum_n a_n O_n$, $(\forall n)(a_n \in \mathbb{R})$. We are interested in computing its stiffness $D_A = \big(\bar{A}\big|\bar{A}\big)$, where $\bar{A} = \sum_n a_n \bar{O}_n$. Inverting the relation (3.10), we can write $\bar{O}_n = \sum_s U_{ns}^T Q_s = \sum_s U_{sn} Q_s$ and thus the following:

$$\bar{A} = \sum_n a_n \bar{O}_n = \sum_n a_n \sum_s U_{sn} Q_s = \sum_s \underbrace{\left(\sum_n a_n U_{sn}\right)}_{v_s} Q_s = \sum_s v_s Q_s$$

Now, let us express the overlap $\big(\bar{A}\big|Q_k\big)$ in two ways:

1. $\big(\bar{A}\big|Q_k\big) = \sum_s v_s \underbrace{(Q_s|Q_k)}_{=\lambda_s \delta_{sk}} = v_k \lambda_k$
2. $\big(\bar{A}\big|Q_k\big) = \big(A\big|\bar{Q}_k\big) = (A|Q_k)$

We are finally ready to make a direct calculation of stiffness of A:

$$D_A = \big(\bar{A}\big|\bar{A}\big) = \sum_{sk} v_s v_k (Q_s|Q_k) = \sum_{sk} v_s v_k \delta_{sk} \lambda_k = \sum_{\substack{s \\ \lambda_s > 0}} v_s^2 \lambda_s$$

$$= \sum_{\substack{s \\ \lambda_s > 0}} v_s^2 \lambda_s^2 \frac{1}{\lambda_s} = \sum_{\substack{s \\ \lambda_s > 0}} \frac{(A|Q_s)^2}{(Q_s|Q_s)}$$

Therefore, the Mazur bound is saturated by our construction and the proof is concluded. ■

We will finish the section with an example of an application of Mazur bound. To this end, we can consider the topic of ballistic linear response [8]. Let J be an extensive current, for example the spin current. From Kubo linear response theory we have the following well-known expression for the real (non-dissipative) part of dynamical spin conductivity [9]:

$$\sigma'(\omega) = 2\pi D_J \delta(\omega) + \sigma_J^{reg}(\omega) \tag{3.21}$$

If there exists a (quasi)local conserved quantity Q such that $(J|Q) > 0$, the Mazur bound implies that $D_J > 0$. Such nonzero value of spin current stiffness is an indicator of *ballistic* DC transport (i.e. without scattering, cf. Figure 3.3) — $\sigma'(0)$ diverges.

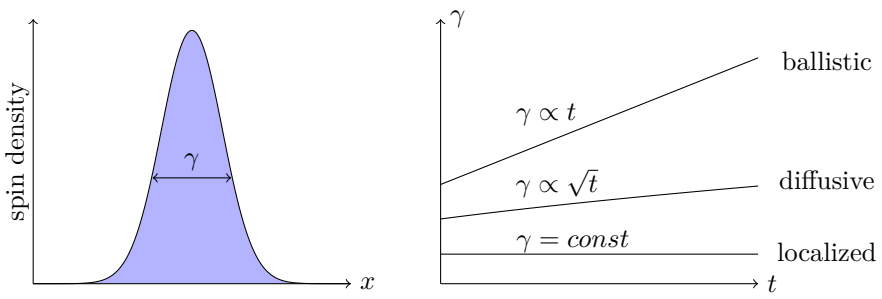

Figure 3.3: Illustration of different types of transport. On the left panel, we have some initial spin density characterized by width γ. On the right panel, we have the dependence of γ on time in three different cases.

3.4 (Q)LIOMs supported on up to 3 sites in the XXZ model

After explaining how and why to look for LIOMs and QLIOMs, let us now turn to a more concrete example of spin-1/2 XXZ model on one dimensional lattice of L sites with periodic boundary conditions, introduced already in Section 2. In the subsequent considerations we will be based on the work of Mierzejewski, Prelovšek, and Prosen [1].

Having chosen a concrete model, we can now give an explicit definition of a basis of a space of m-local observables $\mathcal{V}_L^m$. It is composed of operators of the form:

$$O_{\underline{s}} = \sum_{j=1}^{L} \sigma_j^{s_1} \sigma_{j+1}^{s_2} \cdots \sigma_{j+m-1}^{s_m} \tag{3.22}$$

In the expression above we have $\sigma_j^z \equiv \sqrt{2} S_j^z$, $\sigma_j^{\pm} \equiv S_j^{\pm}$, $\sigma^0 \equiv \mathbb{1}$ and $\underline{s} = (s_1, s_2, \ldots, s_m)$ where $s_j \in \{+, -, z, 0\}$ for $j \in \{2, 3, \ldots, m-1\}$. For first and last operator in a sequence we have $s_{1,m} \in \{+, -, z\}$, because an identity there would correspond to an $m-1$-local operator.
why no 1/L in my HS product? how it relates to slightly different definitions of sigmas? Operators constructed as in paper are normalized, here aren't As a matter of mathematical precision, the notation for $O_{\underline{s}}$ used here (and frequently in physics literature) is a bit of simplification. It is important to remember that implicitly, there are tensor products between σ_j's, i.e. we have the following:

$$O_{\underline{s}} = \sum_{j=1}^{L} \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{j-1} \otimes \sigma_j^{s_1} \otimes \sigma_{j+1}^{s_2} \otimes \cdots \otimes \sigma_{j+m-1}^{s_m} \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{L-j-m+1} \tag{3.23}$$

The single site identity operators ensure that the dimension of matrix of the operator is right. A simple combinatorial observation shows us, that there are $N_m = 3 \cdot 4^{m-2} \cdot 2$ operators constituting a m-local basis (for $m = 1$ we have $N_1 = 3$). Moreover, they are orthogonal (orthonormal?) *by design*, i.e. $\left(O_{\underline{s}} \middle| O_{\underline{k}}\right) \propto \delta_{\underline{s},\underline{k}}$.
Here proof of orthogonality(orthonormality), maybe an Appendix?
Fixing $M > 0$ (usually $M < L$), we can construct the basis of traceless operators spanning the space $\mathcal{V}_L^M = \bigoplus_{m=1}^{M} \mathcal{V}_L^m$. From the properties of direct sum of linear spaces we now that its cardinality is $D_M = \sum_{m=1}^{M} N_m = 3 \cdot 4^{M-1}$. Such construction can be implemented in practice by considering all possible M-digit numbers written in base 4 (as there are 4 'building blocks': $S^{\pm}, S^z, \mathbb{1}$).

Having put together this basis, we can now proceed with the rest of the (Q)LIOM finding algorithm. However, before that it is beneficial to discuss the influence of symmetries of system in question, the XXZ model. They allow us to decompose the matrix K (cf. (3.8)) and thus reduce the computational effort. First and perhaps the most important one is implied by the fact already discussed in Section 3.1 — conservation of magnetization. We could restrict our considerations to a subspaces of $\mathcal{V}_L^M$ comprised of operators such that $\left[S_{tot}^z, O_{\underline{s}}\right] = 0$. Yet, we will not be able to make use of that symmetry here, as in this work we are interested precisely in the *noncommuting* operators, i.e precisely those that break this symmetry. Furthermore, the XXZ model is time-reversal invariant, so the K matrix is real and symmetric. Therefore, we can divide our

operators into two orthogonal subspaces, either real or imaginary. Those subspaces are then spanned by operators of the form $O_{\underline{s}} + O_{\underline{s}}^\dagger$ or $i(O_{\underline{s}} - O_{\underline{s}}^\dagger)$ respectively. There is also one more useful symmetry, namely the $\mathbb{Z}_2$ spin-flip symmetry, however it remains out scope of this thesis.

3.4.1 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] and see whether it is detected or not. 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 [7]. We start with the general XYZ Hamiltonian with periodic boundary conditions:

$$H_{XYZ} = \sum_{i=1}^{L} \left(J_x S_i^x S_{i+1}^x + J_x S_i^y S_{i+1}^y + J_z S_i^z S_{i+1}^z \right) \tag{3.24}$$

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

$$H_{XYZ} = \sum_{i=1}^{L} h_{i,i+1} \tag{3.25}$$

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:

$$\frac{\mathrm{d}h_{i,i+1}(t)}{\mathrm{d}t} + \boldsymbol{\nabla} \cdot j_i^E(t) = 0 \tag{3.26}$$

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:

$$\frac{\mathrm{d}h_{i,i+1}(t)}{\mathrm{d}t} = i[H_{XYZ}, h_{i,i+1}(t)] \tag{3.27}$$

Combining equations (3.26) and (3.27) we obtain the defining equations for the spin energy current density:

$$j_{i+1}^E - j_i^E = -i[H_{XYZ}, h_{i,i+1}] = i[h_{i,i+1}, H_{XYZ}] = i \sum_{k=1}^{L} [h_{i,i+1}, h_{k,k+1}] \tag{3.28}$$

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 (3.28) is shown in Appendix A. For the XXZ model we get the following expression:

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

Thus we see that it is an imaginary operator. Obtaining the energy current operator is now simply the matter of summing over all the lattice sites:

$$J^E = \sum_{i=1}^{L} j_i^E \tag{3.29}$$

As the energy current commutes with the Hamiltonian, it does not undergo time evolution and its autocorrelation function $\left(J^E(t) \middle| J^E(0)\right)$ is constant. Therefore, the corresponding spectral function is proportional to Dirac delta. After restricting our algorithm to the case of imaginary operators, we obtain the following:

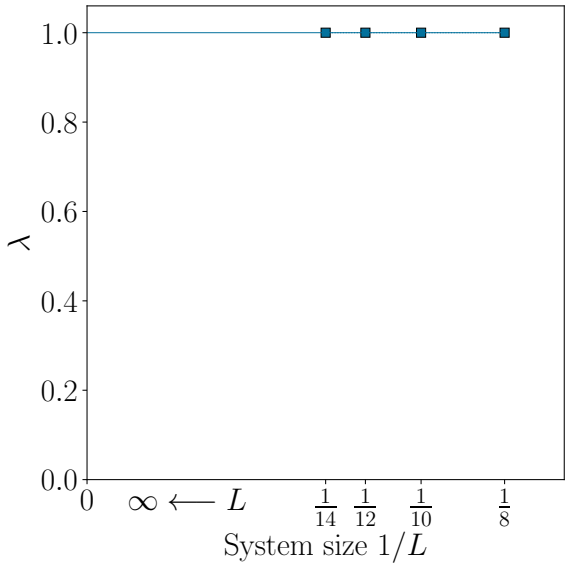

Figure 3.4: Eigenvalues of generalized stiffness matrix corresponding to the energy current operator as a function of inverse system size. Solid line is the extrapolation to thermodynamic limit. Calculations performed for $\Delta = 1.0$.

$$J^E = \sum_i^L i \left[\beta_1 \left(S^-_{i-1} S^z_i S^+_{i+1}\right) + \beta_2 \left(S^z_{i-1} S^+_i S^-_{i+1} + S^+_{i-1} S^-_i S^z_{i+1}\right)\right] + \text{H.c.} \tag{3.30}$$

where the coefficients β_1, β_2 are such that the operator is properly normalized. This is precisely the energy current operator as derived above. After taking the thermodynamic limit of the eigenvalue of K matrix corresponding to the energy current, we see that it equals precisely one (Figure 3.4). Thus, according to Definition 3.4, it is a local integral of motion.

3.4.2 Noncommuting (Q)LIOMs

Having checked the correctness of the algorithm and its implementation, we can now proceed with the main topic of this thesis, that is investigating the *noncommuting* integrals of motion. We conducted preliminary studies for small values of system size L, without assuming translational invariance. Available resources allowed us to make unrestricted search for $L \in \{8, 9, 10, 11, 12\}$. Nevertheless, noncommuting operators that maximized stiffness for given L and Δ turned out to be translationally invariant. Therefore, we restrict our further considerations to translationally invariant operators only. This allowed us to obtain numerical results for L up to 14. We will focus on two concrete cases of operators, corresponding to largest eigenvalues of generalized stiffness matrix for values of anisotropy parameter $\Delta = 1.0$ and $\Delta = 0.5$ respectively.

For the case of $\Delta = 1.0$, the XXZ model reduces to the isotropic XXX model possessing full $SU(2)$ symmetry:

$$H_{XXX} = \frac{J}{2} \sum_{i=1}^{L} \left(S^x_i S^x_{i+1} + S^y_i S^y_{i+1} + S^z_i S^z_{i+1}\right) \tag{3.31}$$

As a consequence of this symmetry, conservation of total magnetization (S^z_{tot} operator (3.3)) implies the conservation of analogously defined S^x_{tot} and S^y_{tot} and therefore their linear combination, i.e. the following quantity:

$$\hat{O}_1 = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} S^+_i + \text{H.c.} \tag{3.32}$$

where the prefactor is introduced for the sake of normalization. Operator $\hat{O}_1$ is an example of a real operator.

The case of $\Delta = 0.5$ is much more difficult. It was shown by Zadnik, Medenjak, and Prosen [10] that for special values of anisotropy parameter $\Delta \in S = \left\{\cos\left(\frac{2l}{2k-1}\pi\right)\right\}_{k,l\in\mathbb{N},\, l<k}$ one can use semicyclic irreducible representations of quantum group $U_q(\mathfrak{sl}_2)$ to generate a set of quasilocal integrals of motion that do not preserve magnetization. Even though the set S is a dense subset of the interval $[-1, 1]$ i.e. the gapless regime of XXZ spin-1/2 chain, it is not symmetric with respect to $\Delta = 0$. For example, considered here value of anisotropy parameter $\Delta = 0.5$ does not belong to this set, whereas $\Delta = -0.5$ do. However, it can be shown that there exist an unitary operator U, which action is equivalent to flipping the sign of parameter Δ, that is $UH_{XXZ}(\Delta)U = -H_{XXZ}(-\Delta)$. From that follows, that if Q is a conserved quantity for Δ, then $\tilde{Q} = UQU$ is a conserved quantity for $-\Delta$. Detailed discussed of this topic is far beyond the scope of this thesis and can be found in [10, 11]. It turns out, that for $\Delta = 0.5$ the actions of this operator produces a simple factor of $(-1)^i$ in the integral of motion:

$$\hat{O}_2 = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} (-1)^i \left(S_i^+ S_{i+1}^+ S_{i+2}^+\right) + \text{H.c.} \tag{3.33}$$

This is once again a real operator.

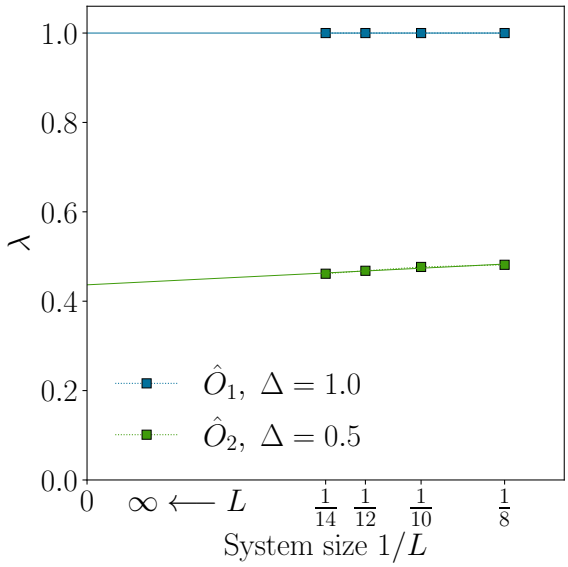

Figure 3.5: Eigenvalues of generalized stiffness matrix corresponding to the two noncommuting integrals of motion, as a function of inverse system size. Solid lines represent the extrapolation to the thermodynamic limit. Note that the operator $\hat{O}_2$ exhibits quasilocality and its stiffness in the thermodynamic limit is $\lambda_{L\to\infty} \approx 0.44$.

Both $\hat{O}_1$ and $\hat{O}_2$ are noncommuting (Q)LIOMs, what can be seen easily from the fact that they consist of just S^+ operators (not counting the Hermitian conjugate). Conducting an analysis with the help of the algorithm we indeed find these two operators among eigenvectors of the generalized stiffness matrix. Corresponding eigenvalues and their thermodynamic limit are shown in Figure 3.5. Comparing it with Definition 3.4 we see that $\hat{O}_1$ is a local integral of motion, whereas $\hat{O}_2$ is a quasilocal integral of motion.

Decay of integrals of motions under weak perturbation

So far we have focused on investigating properties of an *integrable* spin-1/2 chain.
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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:

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

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Derivation of spin energy current

Equation (3.28) 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 (3.28):

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

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.

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

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

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

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:

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

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

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

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 [7]. 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.