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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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1 Introduction

Throughout this thesis, we assume the infinite temperature limit.

1.1 Motivation

1.2 Structure

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Heisenberg model of magnetism

It is well known, that we can divide magnetic materials into two broad groups: those which exhibit magnetic properties in reaction to external magnetic field and those which have a nonzero magnetic moment without external field [1]. First group consists of paramagnetic and diamagnetic systems. In the former, nonzero net magnetic moment comes from alignment of valence electrons' spins in the direction of external magnetic field. In the latter, we deal with an inductive effect in which external field induces magnetic dipoles opposing the field tha have induced them. Diamagnetism exists in all materials, however it is usually much weaker than other magnetism related effects and thus only detectable in the absence of them. Second group includes ferromagnets, which exhibit spontaneous magnetization below Curie temperature, and ferrimagnets, which are composed of two ferromagnetic sublattices with different spontaneous magnetization. There are also antiferromagnets, which are essentially a special case of ferrimagnets in which the two sublattices, below the so-called Néel temperature, have spontaneous magnetizations of equal magnitude but opposite directions [2].

There are two paradigmatic models of magnetism, namely the Heisenberg model, which describes magnetism of localized electrons and their magnetic moments (spins), and the Hubbard model which deals with magnetism of delocalized electrons, called the itinerant magnetism. In this thesis we will focus on a special case of the former of two models, namely the XXZ model.

2.1 Heisenberg-Dirac exchange interaction

We will now proceed with a derivation and a physical motivation of Heisenberg model. Our discussion will be based on the books by Spałek [1] and thesis by Ng [3]. The story begins with two electrons interacting with each other via Coulomb potential. An electron can be described by two quantities, its position in space and its spin. Two facilitate these two degrees of freedom, we say that i-th electron's wavefunction lives in a Hilbert space which is a tensor product of spacial wavefunction space $\mathcal{H}_i \cong L^2(\mathbb{R}^3) \otimes \mathfrak{h}_i$, where $L^2(\mathbb{R}^3)$ is the usual space of square-integrable functions on $\mathbb{R}^3$, and spin wavefunctions space $\mathfrak{h} \cong \mathbb{C}^2$ is a two-dimensional vector space spanned by $|\uparrow\rangle = \binom{1}{0}$ and $|\downarrow\rangle = \binom{0}{1}$. The combined wavefunction of a composite two-particle system it then an element of $\mathcal{H}_1 \otimes \mathcal{H}_2$, which can be decomposed into spacial and spin components, i.e $\mathcal{H}_1 \otimes \mathcal{H}_2 \cong \mathcal{H}_{\text{space}} \otimes \mathcal{H}_{\text{spin}}$, where $\mathcal{H}_{\text{space}} \cong L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$ and $\mathcal{H}_{\text{spin}} \cong \mathfrak{h}_1 \otimes \mathfrak{h}_2$.

Hamiltonian of two interacting electrons is given by:

$$H_C = \underbrace{-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2}_{\text{free particles}} + \underbrace{V(\boldsymbol{r}_1, \boldsymbol{r}_2)}_{\text{interaction}} \tag{2.1}$$

where in case of Coulomb interaction we have $V(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{e^2}{|r_1 - r_2|}$. Formally, this Hamiltonian acts on the space $\mathcal{H}_1 \otimes \mathcal{H}_2$. However, it depends only on the spatial coordinates $\boldsymbol{r}_1, \boldsymbol{r}_2$ and not on the spin coordinates, so essentially its actions is restricted to the $\mathcal{H}_{\text{space}}$ part of the full Hilbert space. This is a crucial observation that lead to the development of Heisenberg model. We will now seek a way to replace this Hamiltonian by an equivalent one acting only on $\mathcal{H}_{\text{spin}}$.

It is time to invoke the Pauli exclusion principle, which requires the composite wavefunction of two electrons to be antisymmetric under exchange of pairs of coordinates (both spatial and spin degrees of freedoms are treated like coordinates). Because Hamiltonian 2.1 does not depend explicitly on spin, the total wavefunction ψ can be expressed as tensor product $\psi_{\text{space}} \otimes \psi_{\text{spin}}$. Antisymmetric nature of ψ then requires one of these components to be antisymmetric (a) and the other to be symmetric (s). Spatial wavefunctions are of the form:

$$\psi^{(s)}_{\text{space}} = \psi_1(\boldsymbol{r}_1) \otimes \psi_2(\boldsymbol{r}_2) + \psi_2(\boldsymbol{r}_1) \otimes \psi_1(\boldsymbol{r}_2) \tag{2.2}$$

$$\psi^{(a)}_{\text{space}} = \psi_1(\boldsymbol{r}_1) \otimes \psi_2(\boldsymbol{r}_2) - \psi_2(\boldsymbol{r}_1) \otimes \psi_1(\boldsymbol{r}_2) \tag{2.3}$$

where $\psi_1, \psi_2 \in L^2(\mathbb{R}^3)$. Spin wavefunctions are elements of $\mathbb{C}^2$ and are given by:

$$\psi^{(s)}_{\text{spin}} = |\uparrow\uparrow\rangle\,,\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\,,\ |\downarrow\downarrow\rangle \tag{2.4}$$

$$\psi^{(a)}_{\text{spin}} = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \tag{2.5}$$

where $|\uparrow\uparrow\rangle$ is an usual shorthand notation for $|\uparrow\rangle_1 \otimes |\uparrow\rangle_2$. Moreover, symmetric spin wavefunctions constitute a triplet state, whereas antisymmetric one is a singlet state.

Possible two-electron wavefunctions are thus either $\varphi = \psi^{(s)}_{\text{space}} \otimes \psi^{(a)}_{\text{spin}}$ or $\chi = \psi^{(a)}_{\text{space}} \otimes \psi^{(s)}_{\text{spin}}$. Expected value of energy of Coulomb interaction in these states is given by:

$$\langle\varphi|H_C|\varphi\rangle = \left\langle \psi^{(s)}_{\text{space}} \middle| H_C \middle| \psi^{(s)}_{\text{space}} \right\rangle = E^{(s)} \tag{2.6}$$

$$\langle\chi|H_C|\chi\rangle = \left\langle \psi^{(a)}_{\text{space}} \middle| H_C \middle| \psi^{(a)}_{\text{space}} \right\rangle = E^{(a)} \tag{2.7}$$

Because $\psi^{(a)}_{\text{space}}$ is symmetric with respect to $(\boldsymbol{r}_1 - \boldsymbol{r}_2)$ we have $E^{(s)} > E^{(a)}$. Therefore, it is energetically favourable for our system to pick the total wavefunction that is antisymmetric in space and symmetric in spin coordinates.

Under the Coulomb interaction, symmetric and antisymmetric spin wavefunctions are not directly distinguished. It is the difference between spatial parts, together with Pauli exclusion principle that forces the choice of a triplet state. Let us now do something similar, but the other way around. We can formally recast the Coulomb Hamiltonian as a spin-spin interaction acting on $\mathcal{H}_{\text{spin}}$ that would distinguish between symmetric and antisymmetric spin wavefunctions and thus fix the spatial part. Let τ^x, τ^y, τ^z be the 2×2 Pauli matrices:

$$\tau^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2.8}$$

Together with a 2×2 identity matrix $\mathbb{1}$ they form a basis of vector space of Hermitian operators acting on a single spin Hilbert space. They are traceless and of unit determinant. By direct computation it can be checked that they satisfy a particular commutation and anticommutation relations:

$$\left[\tau^j, \tau^k\right] = 2i\varepsilon_{jkl}\tau^l \tag{2.9}$$

$$\left\{\tau^j, \tau^k\right\} = 2\delta_{jk}\mathbb{1}_{2\times 2} \tag{2.10}$$

which in turn leads to the following important property:

$$\begin{aligned}\left[\tau^j, \tau^k\right] + \left\{\tau^j, \tau^k\right\} &= \left(\tau^j\tau^k - \tau^k\tau^j\right) + \left(\tau^j\tau^k + \tau^k\tau^j\right) \\ i\varepsilon_{jkl}\tau^l + \delta_{jk}\mathbb{1}_{2\times 2} &= \tau^j\tau^k \end{aligned} \tag{2.11}$$

We define an operator via a formal dot product:

$$\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 = \tau_1^x \otimes \tau_2^x + \tau_1^y \otimes \tau_2^y + \tau_1^z \otimes \tau_2^z \tag{2.12}$$

where subscripts refer to which electron's Hilbert space they act on. Let us now examine how this operator acts on $|\uparrow\uparrow\rangle$ spin wavefunction:

$$\begin{aligned}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 |\uparrow\uparrow\rangle &= (\tau_1^x |\uparrow\rangle_1) \otimes (\tau_2^x |\uparrow\rangle_2) + (\tau_1^y |\uparrow\rangle_1) \otimes (\tau_2^y |\uparrow\rangle_2) + (\tau_1^z |\uparrow\rangle_1) \otimes (\tau_2^z |\uparrow\rangle_2) \\ &= \left(\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \otimes \left(\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) + \left(\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \otimes \left(\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) + \left(\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \otimes \left(\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \\ &= \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ i \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 0 \\ i \end{smallmatrix}\right) + \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right) = |\uparrow\uparrow\rangle \end{aligned}$$

So $|\uparrow\uparrow\rangle$ is an eigenvector of $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$ with an eigenvalue 1. Carrying out such computations for the three remaining states we get that all symmetric states are eigenvectors with eigenvalue 1, whereas the antisymmetric state is also an eigenvector, but with eigenvalue -3. We could have also obtained this result in a more elegant way by referring directly to quantum mechanics and algebra of spin angular momentum [4]. If we set $\hbar = 1$ (which from now on will always be the case), we have the usual spin vector operators $\boldsymbol{S}_i = (S_i^x, S_i^y, S_i^z)$ where $S_i^\alpha = \tau_i^\alpha/2$. Squares of these operators commute with all other S_i^α, hence are the Casimir operators of their algebras and by Schur's Lemma are proportional to the identity [5]. The proportionality constant is equal for spin$-s$ particles to $s(s+1)$ and thus all single spin states are eigenvectors of these operators with eigenvalue 3/4. We can also construct square of total spin angular momentum operator $\boldsymbol{S}^2 = (\boldsymbol{S}_1 + \boldsymbol{2}_2)^2$ for which our triplet (total spin $S = 1$) and singlet (total spin $S = 0$) are eigenvectors with eigenvalue $S(S+1)$. On the other hand, we can calculate $\boldsymbol{S}^2$ directly to obtain the following equation:

$$S(S+1) = \boldsymbol{S}_1^2 + \boldsymbol{S}_2^2 + 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_1 = \frac{3}{2} + 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \tag{2.13}$$

Rearranging it, replacing $\boldsymbol{S}_i$ by $\boldsymbol{\tau}_i/2$ and inserting appropriate values of S we recreate the previously obtained result on eigenvalues of $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$.

After this detour into the world of quantum mechanics of spin, let us return to the problem at hand. We have established that triplet states and singlet state are eigenvectors of $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$ operators with eigenvalues 1 and -3 respectively. Consider now the following Hamiltonian acting on $\mathcal{H}_{\text{spin}}$:

$$H_S = \frac{3E^{(a)} + E^{(s)}}{4} + \frac{E^{(a)} - E^{(s)}}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \tag{2.14}$$

It is easy to see that eigenvalues of H_S are $E^{(a)}$ for symmetric spin states (corresponding to $\psi_{\text{space}}^{(a)}$) and $E^{(s)}$ for antisymmetric spin state (corresponding to $\psi_{\text{space}}^{(s)}$). We have thus obtained a Hamiltonian that is equivalent to H_C, yet acting on space $\mathcal{H}_{\text{spin}}$ rather than $\mathcal{H}_{\text{space}}$. Setting $J = E^{(s)} - E^{(a)}$ and ignoring constant energy offset, we finally arrive at the Dirac-Heisenberg exchange interaction:

$$H_S = -\frac{J}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \tag{2.15}$$

or, expressed in terms of usual spin operators:

$$H_S = -J\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \tag{2.16}$$

Constant J is called the exchange integral and its sign determines the nature of system described by this Hamiltonian. If $J > 0$, then symmetric triplet states have lower energy and we say that the ground state is ferromagnetic. On the other hand, if $J < 0$ then antisymmetric singlet state has lower energy and the ground state is antiferromagnetic.

2.2 One-dimensional XXZ model

It now straightforward to generalize this exchange interaction to spins living on an arbitrary lattice, by summing the spin-disguised Coulomb interaction (2.16) over all pairs of spins.

$$H = -\frac{1}{2}\sum_{i\neq j} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{2.17}$$

The factor $\frac{1}{2}$ is introduced to mitigate double-counting of pairs. This is the so called Heisenberg (Heisenberg-Dirac) Hamiltonian. What this Hamiltonian does is describe correlation between spins of single particles located in atoms i and j (lattice sites), induced by repulsive Coulomb interaction. If we were to carry out more formal second-quantization of original Hamiltonian (2.1), we could have obtained a more concrete expression for the exchange integral. Assuming that one electron is in a state described by wavefunction $\varphi_i(\boldsymbol{r}_1)$ and second one in $\varphi_j(\boldsymbol{r}_2)$ then we would have [1]:

$$J_{ij} = \int \mathrm{d}^3\boldsymbol{r}_1 \mathrm{d}^3\boldsymbol{r}_2\ \varphi_i^*(\boldsymbol{r}_1)\varphi_j^*(\boldsymbol{r}_2)\frac{e^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}\varphi(\boldsymbol{r}_1)\varphi_j(\boldsymbol{r}_2) \tag{2.18}$$

In practical calculations it is often assumed that electrons are well localized, and thus the value of this integral falls off quickly enough with increasing distance between them that only the nearest neighbors interactions are important. Moreover, J_{ij} is also assumed to be the same between those nearest neighbors:

$$J_{ij} = \begin{cases} J, & i \text{ is a neighbor of } j \\ 0, & \text{otherwise} \end{cases} \tag{2.19}$$

These assumptions reduce Heisenberg Hamiltonian to its most popular form:

$$H = -\frac{J}{2}\sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{2.20}$$

where summation index $\langle i, j\rangle$ indicates that this sum should be performed over all pairs of nearest neighbors (with repetitions).

From now on we will be restricting our attention to the case of one-dimensional lattices and nearest neighbors interaction. First, let us set up the stage. We are interested in studying a one-dimensional chain of L spin-1/2 interacting fermions with periodic boundary conditions, i.e. arranged in a circular ring. For visualization of periodic boundary conditions in one and two-dimensional cases see Figure 2.1. The underlying Hilbert space is then a 2^L-dimensional tensor product of L single spin spaces $\mathcal{H}_{\text{spin}} = \bigotimes_{j=1}^{L} \mathfrak{h}_j$. To upgrade a single spin operator σ to this product space we will use the standard embedding:

$$\sigma_j = \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{j-1} \otimes \sigma \otimes \mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2} \tag{2.21}$$

Subscript j means that even though this operator formally acts on $\mathcal{H}_{\text{spin}}$, it acts in a nontrivial way only on $\mathfrak{h}_j$.

Real world systems usually exhibit some degree of anisotropy, which means that it can be more difficult to achieve magnetization in one direction than in some other direction. To capture this behavior, we can slightly generalize the Heisenberg Hamiltonian:

$$H_{XYZ} = \sum_{j=1}^{L} \left(J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z \right) \tag{2.22}$$

where periodic boundary conditions are imposed by requiring that $S_{L+1}^{\alpha} = S_1^{\alpha}$. Obtained model is known in literature as the XYZ model. However, it is often the case that a single direction is preferred. We can then choose it to be the z direction and set $J_x = J_y \equiv J \neq J_z \equiv J\Delta$. As a result we get the titular XXZ model:

$$H_{XXZ} = J \sum_{j=1}^{L} \left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right) + J\Delta \sum_{j=1}^{L} S_j^z S_{j+1}^z \tag{2.23}$$

It is convenient to reexpress this model in terms of the so-called spin-flip operators:

$$S^+ = S^x + iS^y \tag{2.24}$$

$$S^- = S^x - iS^y \tag{2.25}$$

They get their name from the easily checked fact that $S^+ \left|\downarrow\right\rangle = \left|\uparrow\right\rangle$ and $S^- \left|\uparrow\right\rangle = \left|\downarrow\right\rangle$. Inverting these relations:

$$S^x = \frac{S^+ + S^-}{2} \tag{2.26}$$

$$S^y = \frac{S^+ - S^-}{2i} \tag{2.27}$$

and inserting them into (2.23) yields:

$$H_{XXZ} = \frac{J}{2} \sum_{j=1}^{L} \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + J\Delta \sum_{j=1}^{L} S_j^z S_{j+1}^z \tag{2.28}$$

which is the most common form of this Hamiltonian. We could restore the isotropy by setting $\Delta = 1$, obtaining yet another version of this model, called the isotropic XXX model. A curious property of XXX model is that is posses $SU(2)$ symmetry (rotation of spins), which will be useful for us in the future. Unless stated otherwise, we will work in units such that $J = 1$.

Heisenberg model, despite its apparent simplicity, is exceedingly difficult to analyze. Nevertheless, the one-dimensional XXX version was diagonalized analytically by Hans Bethe [6] in 1931, by means of the now famous *Bethe ansatz*. Even more remarkably, Rodney Baxter in 1971 expanded upon the Bethe ansatz and solved the general XYZ model in one-dimension [7, 8]. However, these solutions, as well as the so far unsuccessful attempts at solving it in two and more dimensions, are notoriously difficult and we will not use them in this thesis. Instead, when in need of concrete computations, we will resort to much simpler numerical methods in form of exact diagonalization [9].

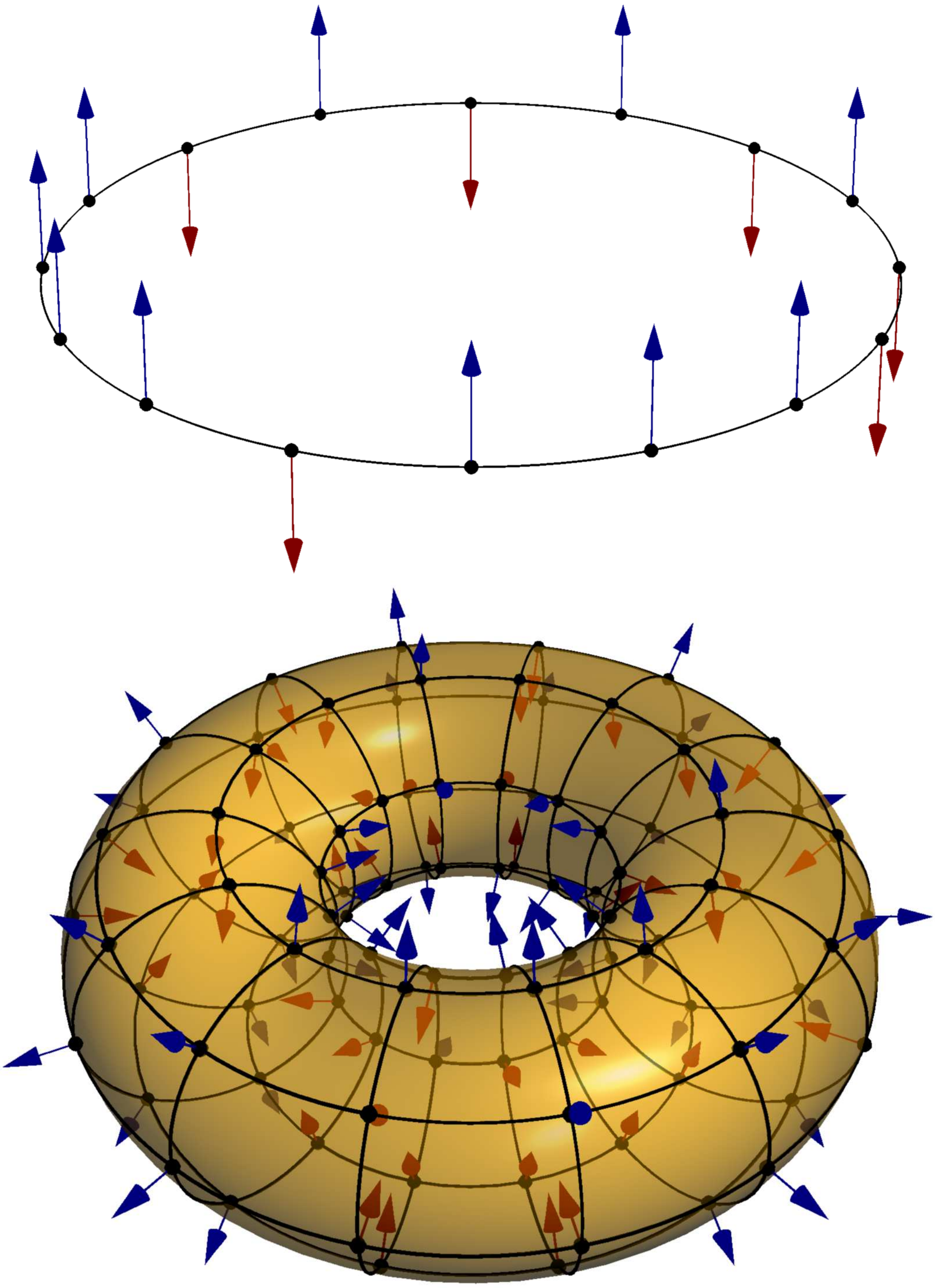

Figure 2.1: Visualization of periodic boundary conditions in 1-D (circle topology) and 2-D (torus topology).

3

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 [10]. 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 [10], Mierzejewski et al. [11], and Mierzejewski, Kozarzewski, and Prelovšek [12]. The aim of this chapter 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. Examples of application of the algorithm to the XXZ model conclude this chapter.

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 $H\,|n\rangle = E_n\,|n\rangle$. 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:

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

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 $P_n = |n\rangle\langle n|$ 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 (**??**) 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 stated.

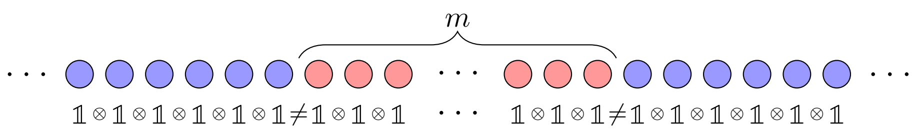

Figure 3.1: Illustration of an operator supported on m sites.

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

$$S^z_{tot} = \sum_{j=1}^{L} S^z_j \tag{3.3}$$

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:

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

i.e. the full Hilbert space with $\dim \mathcal{H} = 2^L$ can be decomposed into the direct sum of its proper subspaces $\mathcal{H}_j$ such that $\dim \mathcal{H}_j = \binom{L}{j}$ and all states in a given subspace correspond to the same eigenvalue of S^z_{tot} operator. The index j 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 [11]. 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 $A \in \mathcal{V}^M_L$, employing the Heisenberg picture [11]:

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

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)

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

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 [10]:

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

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

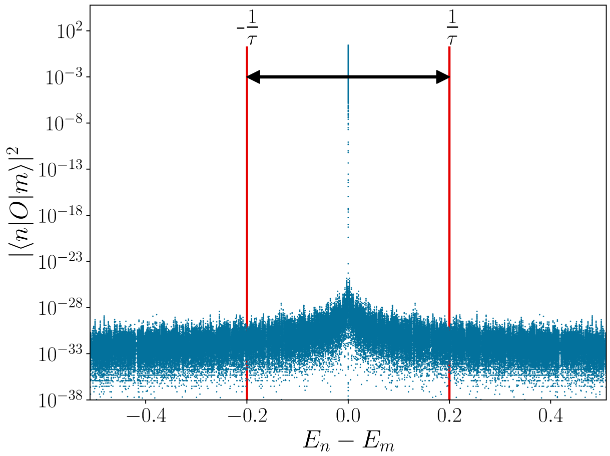

Figure 3.2: Illustration of averaging procedure as defined by equation (3.5). The sum of matrix elements is restricted by the theta function to the region between the two red lines. In the case of operator shown here, we see that only the matrix elements corresponding to differences of energies very close to zero contribute to the time average.

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.

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 $A, B \in \mathcal{V}_L$*

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

and

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

Proof.

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

■

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:

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

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 $A \in \mathcal{V}_L^M \not\Rightarrow \bar{A} \in \mathcal{V}_L^M$, 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

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

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:

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

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 $(0, \tau)$:

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

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:

$$\begin{aligned}
(Q_n|Q_m) &= \sum_{s,t} U_{ns} \left(\bar{O_s}^\tau \middle| \bar{O_t}^\tau\right) U_{tm}^T = \sum_t \left(\sum_s U_{ns} K_{st}^\tau\right) U_{tm}^T \\
&\triangleq \lambda_n \sum_t U_{nt} U_{tm}^T \triangleq \lambda_n \delta_{mn}
\end{aligned}$$

■

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 a part supported on up to M sites and a nonlocal part:

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

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:

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

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. 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, because that is largest system size for exact diagonalization that we were able to achieve.

It is important not to loose the physical interpretation of these results amidst all the formal development. Operator $Q_n = \sum_s U_{ns} \bar{O}_s = Q_n^M + Q_n^{\perp}$ is always an integral of motion, because it is a linear combination of infinite-time averaged operators (cf. (3.7)). However, the time averaging procedure expands the support of initially local basis operators O_s. In actual computations we are using the basis of operators supported on up to M sites at all times, therefore the operators obtained from the eigenvectors of K matrix are Q_n^M operators. If $\lambda_n = 1$, then $\left\| Q_n^{\perp} \right\| = 0 \implies Q_n^{\perp} = 0$ and $Q_n = Q_n^M$. Therefore, Q_n^M operator, which structure we know, is strictly conserved. On the other hand, if $\lambda_n \in (0, 1)$, then $\left\| Q_n^{\perp} \right\| > 0 \implies Q_n^{\perp} \neq 0$ and $Q_n \neq Q_n^M$. This means that the operator that we really get from the algorithm is not a conserved quantity.

It is an local approximation, or equivalently a projection of true quasilocal integral of motion Q_n on a basis supported on up to M sites. Moreover, we can construct a convergent series of operators with increasing support and system size, such that their norm approaches unity. In thermodynamic limit we obtain a strictly conserved quantity that is *quasilocal*. This discussion motivates a rather formal definition of quasilocality [13, 14]:

Definition 3.5 *An operator sequence* $\{X_L\}_{L\in\mathbb{N}}$*,* $X_L \in \mathrm{End}(\mathcal{H}^{\otimes L})$ *which can be written as:*

$$X_L = \sum_{M\leq L} \sum_{i=0}^{L-1} \mathcal{S}^i (q_M \otimes \mathbb{1}^{\otimes(L-r)})$$

where $q_M \in \mathrm{End}(\mathcal{H}^{\otimes M})$ *and there exist such constants* $\gamma, \zeta > 0$ *that*

$$\|q_M\| \leq \gamma e^{-\zeta M}$$

is called quasilocal.

In the above definition, $\mathcal{H} = \mathbb{C}^2$ is the single spin Hilbert space, $\mathrm{End}(V)$ is the space of endomorphism on vector space V, that is linear maps from V to V and $\mathcal{S}^i$ is the periodic left-shift operator defined as

$$\mathcal{S}\left(\tau^{s_0} \otimes \tau^{s_1} \otimes \cdots \tau^{s_{n-2}} \otimes \tau^{s_{n-1}}\right) = \tau^{s_1} \otimes \tau^{s_2} \otimes \cdots \tau^{s_{n-1}} \otimes \tau^{s_0}$$

However, in subsequent parts of this thesis we will use the Definition 3.4, while keeping in mind its interpretation. 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. [15] and introduce the concept of spectral functions.

Suppose that we have a real 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 3.6 (Spectral function)

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

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:

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

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

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

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

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 [16] and Suzuki [17] 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 [18]. 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. [19].

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. $\|\mathcal{A}\|^2 = \mathrm{tr}(\mathcal{A}\mathcal{A})/2^L \geq 0$. 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 $\left(\bar{A}\middle|\bar{B}\right) = \left(\bar{A}\middle|B\right) = \left(A\middle|\bar{B}\right)$(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.

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

■

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 $\{Q_n\}$:

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

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 [10], where the algorithm described in details in Section 3.2 was first proposed. We will now show that the following proposition holds [11]:

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 $D_A = \left(\bar{A}\middle|\bar{A}\right)$, where $\bar{A} = \sum_n a_n \bar{O}_n$. Inverting the relation (3.10), we can write $\bar{O}_n = \sum_s U^T_{ns} Q_s = \sum_s U_{sn} Q_s$ 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 $\left(\bar{A}\middle|Q_k\right)$ in two ways:

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

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

$$D_A = \left(\bar{A}\middle|\bar{A}\right) = \sum_{sk} v_s v_k \left(Q_s|Q_k\right) = \sum_{sk} v_s v_k \delta_{sk} \lambda_k = \sum_{\substack{s \\ \lambda_s > 0}} v_s^2 \lambda_s$$
$$= \sum_{\substack{s \\ \lambda_s > 0}} v_s^2 \lambda_s^2 \frac{1}{\lambda_s} = \sum_{\substack{s \\ \lambda_s > 0}} \frac{(A|Q_s)^2}{(Q_s|Q_s)}$$

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.

Example 3.2 *We consider the topic of ballistic linear response [19]. 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 [20]:*

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

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.

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 base on the work of Mierzejewski, Prelovšek, and Prosen [10].

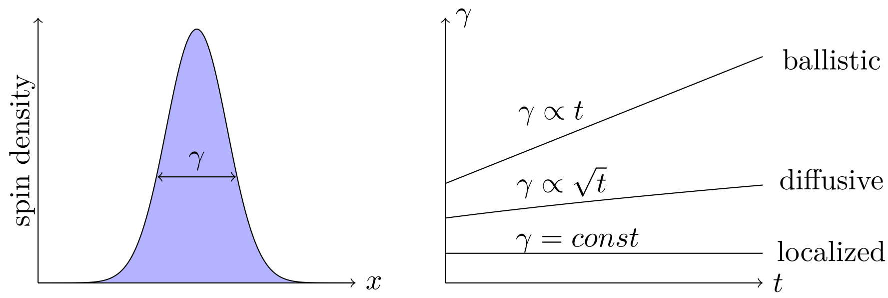

Figure 3.3: Illustration of different types of transport. On the left panel, we have some initial spin density characterized by width γ. On the right panel, we have the dependence of γ on time in three different cases.

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:

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

In the expression above we have $\sigma_j^z \equiv 2S_j^z$, $\sigma_j^{\pm} \equiv \sqrt{2}S_j^{\pm}$, $\sigma_j^0 \equiv \mathbb{1}_{2\times 2}$ 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. The index j indicates first site of the support. As a matter of mathematical precision, the notation for $O_{\underline{s},j}$ used here (and frequently in physics literature) is a bit of simplification. It is important to remember that becaues of embedding (2.21), there are tensor products between σ_j's, i.e. we have the following:

$$O_{\underline{s},j} = \underbrace{\mathbb{1}_{2\times 2}\otimes\cdots\otimes\mathbb{1}_{2\times 2}}_{j-1}\otimes\,\sigma_j^{s_1}\otimes\sigma_{j+1}^{s_2}\otimes\cdots\otimes\sigma_{j+m-1}^{s_m}\otimes\underbrace{\mathbb{1}_{2\times 2}\otimes\cdots\otimes\mathbb{1}_{2\times 2}}_{L-j-m+1} \tag{3.23}$$

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 $N_m = 3\cdot 4^{m-2}\cdot 2$ (excluding shifts i.e. different values of j for the same $\underline{s}$) operators constituting a m-local basis (for $m=1$ we have $N_1 = 3$). Moreover, they are orthonormal *by design*, i.e. $(O_{\underline{s},j}|O_{\underline{s}'}, j') = \delta_{\underline{s},\underline{s}'}\delta_{j,j'}$ (see Appendix C for proof). 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 $D_M = \sum_{m=1}^M N_m = 3\cdot 4^{M-1}$. To include all possible shifts, this value needs to multiplied by the number of sites L. Such construction can be implemented in practice by considering all possible M-digit numbers written in base 4 (as there are 4 'building blocks': $\sigma^{\pm}, \sigma^z, \mathbb{1}$).

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 $[S_{tot}^z, O_{\underline{s}}] = 0$. Yet, we will not be able to make use of that symmetry here, as in this work we are interested 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 [11] 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 [18]. We start with the general XYZ Hamiltonian with periodic boundary conditions (2.22). It is easy to see that this Hamiltonian can be represented as a sum of operators supported on two consecutive sites:

$$H_{XYZ} = \sum_{k=1}^{L} h_{k,k+1} \tag{3.24}$$

where $h_{k,k+1} = J_x S_k^x S_{k+1}^x + J_x S_k^y S_{k+1}^y + J_z S_k^z S_{k+1}^z$ 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:

$$\frac{\mathrm{d}h_{k,k+1}(t)}{\mathrm{d}t} + \boldsymbol{\nabla} \cdot j_k^E(t) = 0 \tag{3.25}$$

where $\boldsymbol{\nabla} \cdot j_k^E(t) \equiv j_{k+1}^E(t) - j_k^E(t)$ 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:

$$\frac{\mathrm{d}h_{k,k+1}(t)}{\mathrm{d}t} = i[H_{XYZ}, h_{k,k+1}(t)] \tag{3.26}$$

Combining equations (3.25) and (3.26) we obtain the defining equations for the spin energy current density:

$$j_{k+1}^E - j_k^E = -i[H_{XYZ}, h_{k,k+1}] = i[h_{k,k+1}, H_{XYZ}] = i \sum_{r=1}^{L} [h_{k,k+1}, h_{r,r+1}] \tag{3.27}$$

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 equation (3.27) is shown in Appendix B. For the XXZ model we get the following expression:

$$\begin{aligned} j_k^E &= i\Big(\underbrace{2JS_{k-1}^- S_k^z S_{k+1}^+ + J\Delta S_{k-1}^z S_k^+ S_{k+1}^- + J\Delta S_{k-1}^+ S_k^- S_{k+1}^z}_{O_k} \\ &\quad - \underbrace{\left(2JS_{k-1}^+ S_k^z S_{k+1}^- + J\Delta S_{k-1}^z S_k^- S_{k+1}^+ + J\Delta S_{k-1}^- S_k^+ S_{k+1}^z\right)}_{O_k^\dagger} \Big) \\ &= i\left(O_k - O_k^\dagger\right) \end{aligned}$$

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:

$$J^E = \sum_{k=1}^{L} j_k^E \tag{3.28}$$

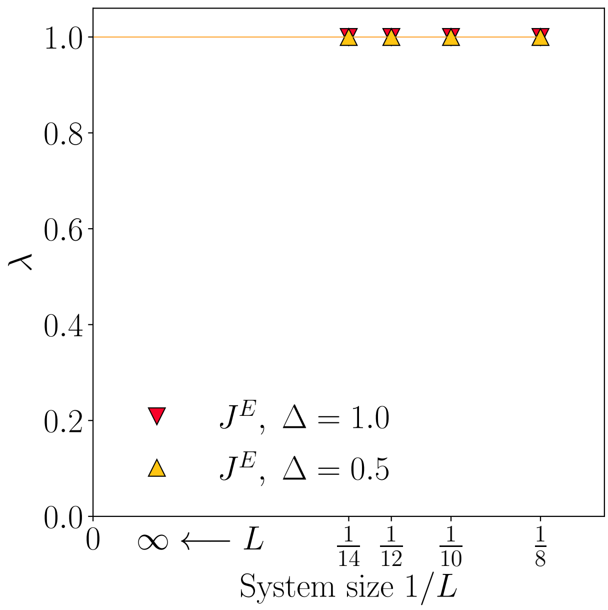

Figure 3.4: Eigenvalues of generalized stiffness matrix corresponding to the energy current operator as a function of inverse system size. Solid line is the extrapolation to thermodynamic limit. Calculations performed for $\Delta = 1.0$ and $\Delta = 0.5$.

As the energy current commutes with the Hamiltonian [18], 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:

$$J^E = \sum_{i=k}^{L} i\left[\beta_1\left(S^-_{k-1}S^z_kS^+_{k+1}\right) + \beta_2\left(S^z_{k-1}S^+_kS^-_{k+1} + S^+_{k-1}S^-_kS^z_{k+1}\right)\right] + \text{H.c.} \tag{3.29}$$

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 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 either translationally invariant or translationally invariant with a sign flip (see $\hat{O}_2$ (3.32)). Therefore, we restrict our further considerations to such 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 this values of Δ parameter, the many-body energy spectra exhibits massive degeneracies, because eigenstates with different S^z_{tot} correspond to the same energies [21, 22].

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

$$H = J \sum_{i=1}^{L} \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + S_i^z S_{i+1}^z \right) \tag{3.30}$$

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 the following quantity:

$$\hat{O}_1 = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} S_i^+ + \text{H.c.} \tag{3.31}$$

where the prefactor is introduced for the sake of normalization. Note that this operator is actually the S^x_{tot}, however this form shows that $\hat{O}_1$ is an example of a real operator. If we were to consider analogously defined imaginary operator, we would obtain the S^y_{tot}, but due to $SU(2)$ symmetry the results would be the same.

The case of $\Delta = 0.5$ is much more difficult. It was shown by Zadnik, Medenjak, and Prosen [13] 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 for even system sizes, in thermodynamic limit, there exist an unitary operator $U = (\mathbb{1}_{2\times 2} \otimes \tau^z)^{\otimes L/2}$, 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 $-\Delta$. This the reason why we present numerical results only for even values of L. For $\Delta = 0.5$ the actions of this operator produces a simple factor of $(-1)^i$ and the operator of interest reads:

$$\hat{O}_2 = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} (-1)^i \left(S_i^+ S_{i+1}^+ S_{i+2}^+ \right) + \text{H.c.} \tag{3.32}$$

This is once again a real operator. Detailed discussed of this topic is far beyond the scope of this thesis and can be found in [13, 14].

Both $\hat{O}_1$ and $\hat{O}_2$ are noncommuting operators, what can be seen easily from the fact that they consist of products of either just S^+ operators or S^- operators. 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 strictly conserved, local integral of motion, whereas $\hat{O}_2$ is a projection of a quasilocal integral of motion on a basis supported on up to 3 sites. To further illustrate the concept of quasilocality, we can consider a projection of this QLIOM on a basis supported on up to 4 sites, which results in an operator of the form $\hat{O}_2 + \delta\hat{O}$, where $\delta\hat{O}$ is the complicated 4-local part, which exact form is not important. Looking at Figure 3.5 we see that stiffness of this new projection is larger that the old one. However, contribution of $\delta\hat{O}$ to the overall stiffness is smaller than that of $\hat{O}_2$, which is in agreement with Definition 3.5.

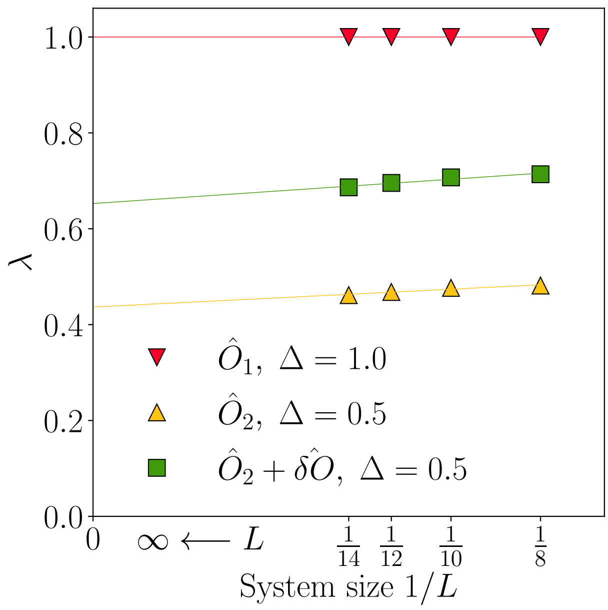

Figure 3.5: Eigenvalues of generalized stiffness matrix corresponding to the two noncommuting integrals of motion, as a function of inverse system size. Solid lines represent the extrapolation to the thermodynamic limit. Note that the operator $\hat{O}_2$ exhibits quasilocality and its stiffness in the thermodynamic limit is $\lambda_{L\to\infty} \approx 0.44$. Stiffness of $\hat{O}_2 + \delta\hat{O}$ in thermodynamic limit is $\lambda_{L\to\infty} \approx 0.65$

4

Relaxation of integrals of motions in weakly perturbed XXZ model

So far we have focused on investigating properties of an *integrable* XXZ spin-1/2 chain. Write, this part after the introduction to avoid repetition. It is important to note, that the methodology in this chapter follows the work of Mierzejewski et al. [11], however the results about relaxation of noncommuting integrals of motion are original and at the moment of writing this thesis not found elsewhere in literature.

4.1 Adding perturbation to the Hamiltonian

We are now going to weakly break integrability by adding a suitable perturbation. New Hamiltonian has the following form:

$$H_{XXZ} = \frac{1}{2}\sum_{j=1}^{L}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + \Delta\sum_{j=1}^{L} S_j^z S_{j+1}^z + \alpha H' \tag{4.1}$$

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

$$H' = \sum_{j=1}^{L} S_j^z S_{j+2}^z \tag{4.2}$$

In such system, only two conserved quantities remain — the Hamiltonian H_{XXZ} itself and the total magnetization S^z_{tot}. All other integrals of motions cease to be conserved and decay with a finite relaxation time τ. We are interested in investigating this decay and the timescales involved. However at first we should establish a range of values of parameter α so its small enough that H' remains a perturbation but large enough to be relevant for finite system sizes accessible numerically. To this end we take the previously discussed (Q)LIOMs $J^E, \hat{O}_1, \hat{O}_2$ and investigate their behavior under finite-time averaging (as defined in (3.5)) generated by perturbed Hamiltonian. More precisely, we calculate the finite-time autocorrelation function (finite-time stiffness) $\lambda_A^\tau = \left(\bar{A}^\tau \middle| \bar{A}^\tau\right)$ as a function of inverse system size. In order to relate this to the discussion of spectral functions in Section 3.3, we will from now on use the cutoff frequency $\omega = \frac{1}{\tau}$, instead of the time of averaging τ.

what about $\hat{O}_1, \hat{O}_2$? They do not exhibit such nice decay

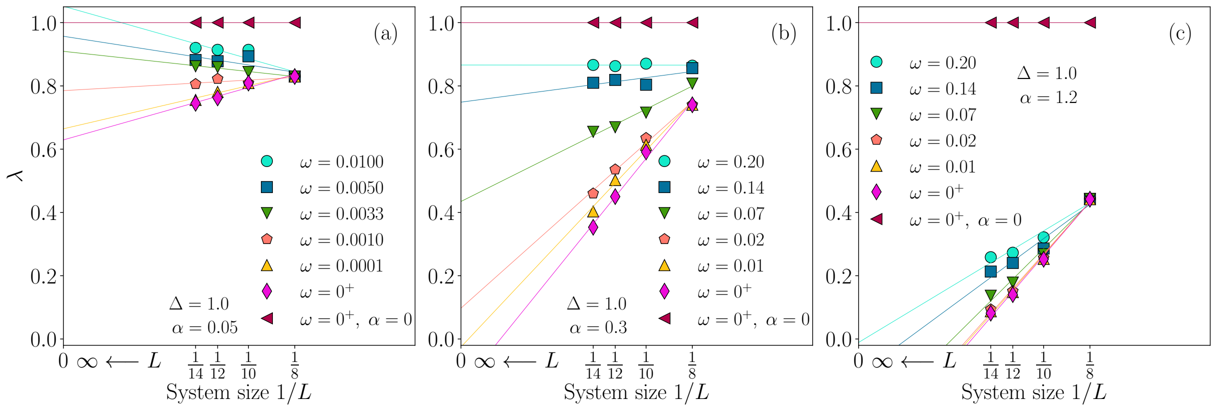

Figure 4.1: Finite time stiffness of J^E as a function of time for the perturbed Hamiltonian. Perturbation strength increase from left to right $\alpha = 0.05, 0.3, 1.2$. (a) Perturbation is too weak and even for very small ω the stiffness does not vanish. (b) Optimal perturbation, stiffness vanish for suitably small cutoff frequency.
(c) Perturbation too strong, stiffness vanish almost immediately.

4.2 Relaxation of known (Q)LIOMs

After establishing the range of perturbation strengths relevant to our problem, we can now investigate how our (Q)LIOMs decay with time. We will apply the formalism of spectral functions described in Sections 3.3. Since we are interested in the low-ω (long times) part of integrated spectral function $I(\omega)$, it is convenient to normalize it. Therefore, let us define the following [11]:

$$R_{\hat{A}}(\omega, \alpha) = \frac{I(\omega, \alpha)}{\lim_{\omega \to 0^+} I(\omega, \alpha = 0)} = \frac{\sum_{n,m} \theta\left(\omega - |E_n - E_m|\right) \left|\langle m|\hat{A}|n\rangle\right|^2}{\sum_{\substack{n,m \\ E_n = E_m}} \left|\langle m|\hat{A}|n\rangle\right|^2} \tag{4.3}$$

This normalization of $I(\omega)$ assures that $\lim_{\omega \to 0^+} R_{\hat{A}}(\omega, \alpha) = 0$ and $\lim_{\omega \to \infty} R_{\hat{A}}(\omega, \alpha) = 1$. Let us now study this quantity for operators in question.

4.2.1 Relaxation of energy current

$\Delta = 0.5$? We begin with the case energy current J^E for $\Delta = 1.0$, as derived in Section 3.4.1. In the integrable parent model it is a conserved quantity, so we have the following:

$$\left(J^E(t)\middle|J^E\right) = const \implies S(\omega) \propto \delta(\omega) \implies R_{J^E}(\omega, \alpha = 0) = 1$$

After moving away from integrable regime, the autocorrelation function starts to decay, so the δ-peak broadens and $R_{J^E}(\omega, \alpha = 0)$ is no longer equal to one, but approaches zero as time increases. We will look simultaneously at two different situations, results for $L = 14$ and results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$. Figure 4.2 shows $R(\alpha, \omega)$ as a function of ω for different α. We immediately see the expected outcome, as the stronger the perturbation the faster the current decays. However, an interesting thing happens when plot the same data, but as a function of rescaled frequency ω/α^2. Numerical results visible on Figure 4.3 show a convincing collapse of curves for different values of perturbation strength. This may suggest an universal dependence of $R(\omega, \alpha)$ on ω and α:

$$R(\omega, \alpha) \simeq \tilde{R}(\omega/\alpha^2) \tag{4.4}$$

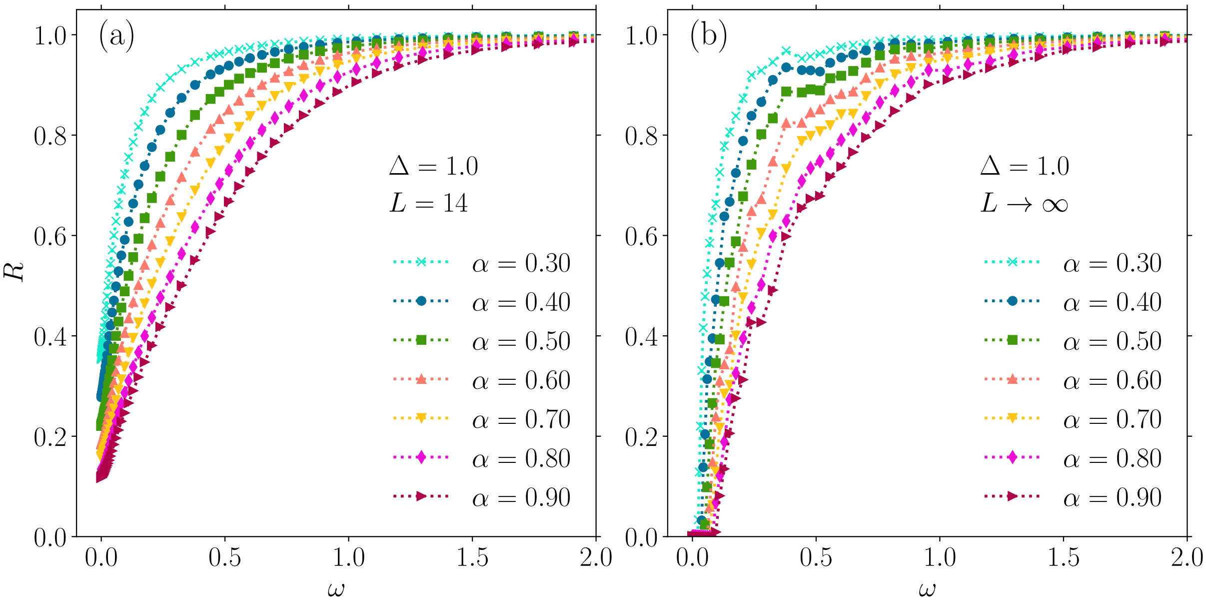

Figure 4.2: Normalized integrated spectral function as a function of cutoff frequency. (a) Results for $L = 14$. Low frequency limit does not approach 0 because of finite size effects. (b) Results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$. Note the expected observation, namely stronger perturbation leads to faster decay.

Moreover, this relation can be reasonably well approximation by a one parameter fit (black dashed line on Figure 4.3):

$$\tilde{R}(\omega/\alpha^2) \simeq \frac{2}{\pi} \arctan\left(\frac{\omega}{\gamma\alpha^2}\right) \tag{4.5}$$

where γ is the fitting parameter. It implies that the relaxation of energy current is exponential in nature. To see this, let us calculate $I(\omega)$ for such decay $\left(J^E(t)\middle|J^E\right) \propto e^{-|t|/\tau_1}$. Double-sided exponential has well defined Fourier transform, so we can drop the $\epsilon \to 0^+$ limit from the integral.

$$\begin{aligned} S(\omega) &\propto \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{-|t|/\tau_1} e^{i\omega t} = \frac{1}{2\pi}\left[\int_{-\infty}^{0} \mathrm{d}t\, e^{(1/\tau_1 + i\omega)t} + \int_{0}^{\infty} \mathrm{d}t\, e^{(-1/\tau_1 + i\omega)t}\right] \\ &= \frac{1}{2\pi}\left[\frac{\tau_1}{1 + i\omega\tau_1} + \frac{\tau_1}{1 - i\omega\tau_1}\right] = \frac{1}{\pi}\frac{\tau_1}{1 + \omega^2\tau_1^2} \end{aligned} \tag{4.6}$$

Integrating $S(\omega)$ over a frequency window we obtain:

$$I(\omega) \propto \frac{1}{\pi}\int_{-\omega}^{\omega} \mathrm{d}\omega'\, \frac{\tau_1}{1 + \omega^2\tau_1^2} = \frac{2}{\pi}\arctan(\tau_1\omega)$$

which after normalization yields the desired results (4.5). Furthermore, we learn that the characteristic relaxation time $\frac{1}{\tau_1} \propto \alpha^2$ and the proportionality coefficient is universal and does not depend on α. The quadratic scaling shown on Figure 4.3 is actually not the best possible for this set of numerical data. Choosing the rescaling coefficient to be $\frac{3}{2}$ allows for almost perfect collapse of all the curves (see Figure 4.4). However, it is expected to be a consequence of working with rather small system sizes, because in was shown in Mierzejewski et al. [11] using memory function formalism, that quadratic scaling is indeed the appropriate one.

4.2.2 Relaxation of noncommuting (Q)LIOMs

Let us now proceed with the same analysis, but for the $\hat{O}_1$ and $\hat{O}_2$ operators.

What to show here?

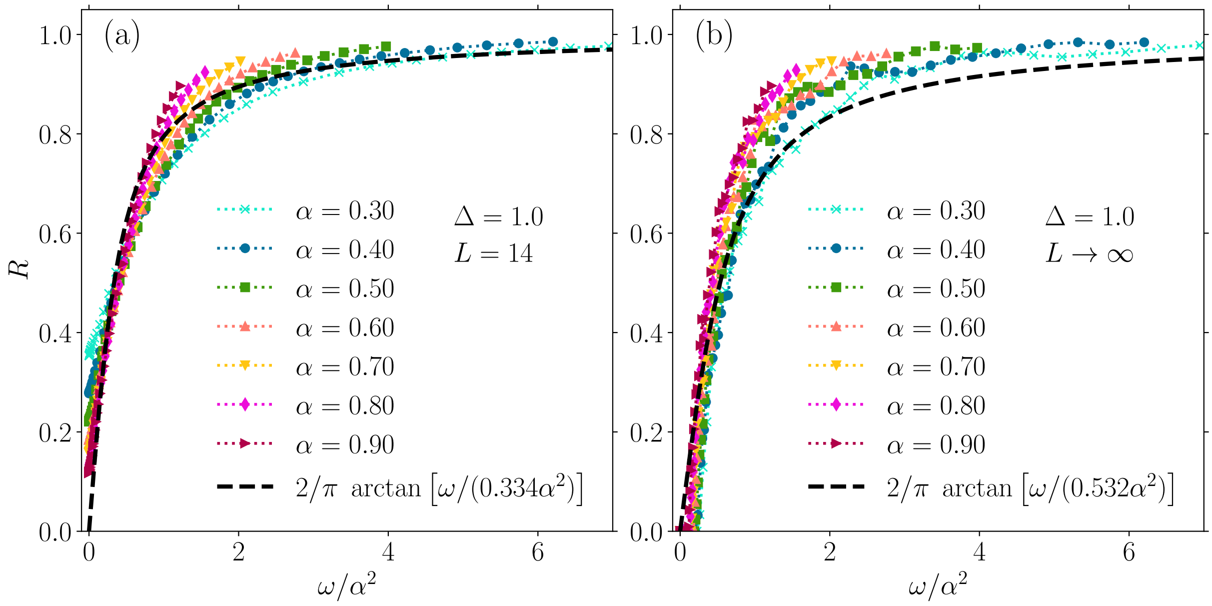

Figure 4.3: Normalized integrated spectral function as a function of rescaled cutoff frequency. (a) Results for $L = 14$. (b) Results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$. Dashed black line corresponds to fit (4.5).

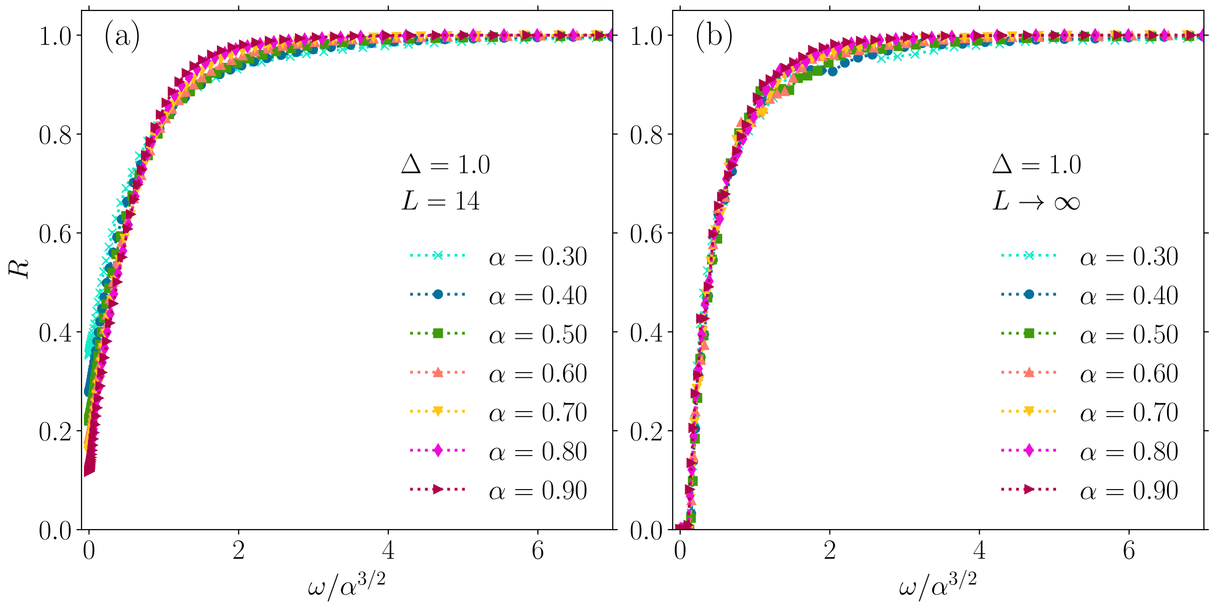

Figure 4.4: Normalized integrated spectral function as a function of rescaled cutoff frequency. The rescaling coefficient is chosen so as to obtain the best possible collapse of curves. (a) Results for $L = 14$. (b) Results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$.

- no scaling, quadratic scaling, linear scaling
- fitting error function, derivation of $I(\omega)$
- SU(2) breaking for $\Delta = 1.0$
- for $\Delta = 0.5$ too? why?
- loglog plots?
- comparison between SU(2) breaking and integrability breaking

Bibliography

[1] Józef Spałek. *Wst p do fizyki materii skondensowanej*. Wydawnictwo naukowe PWN, 2015. ISBN: 978-83-01-18800-9.

[2] Wolfgang Nolting. *Theoretical Physics 9: Fundamentals of Many-body Physics*. Springer International Publishing, 2018. ISBN: 9783319983264.

[3] Lenhard L Ng. "Heisenberg Model , Bethe Ansatz , and Random Walks". Harvard University, 2011.

[4] J. J. Sakurai and Jim Napolitano. *Modern Quantum Mechanics*. Cambridge University Press, Sept. 2017. ISBN: 9781108499996. DOI: 10.1017/9781108499996. URL: https://www.cambridge.org/core/product/identifier/9781108499996/type/book.

[5] Peter Woit. *Quantum theory, groups and representations: An introduction*. Jan. 2017. DOI: 10.1007/978-3-319-64612-1.

[6] Hans. Bethe. "Zur Theorie der Metalle - I. Eigenwerte und Eigenfunktionen der linearen Atomkette". In: *Zeitschrift für Physik* 71.3-4 (Mar. 1931), pp. 205–226. ISSN: 14346001. DOI: 10.1007/BF01341708. URL: https://link.springer.com/article/10.1007/BF01341708.

[7] Rodney. J. Baxter. "Eight-Vertex Model in Lattice Statistics". In: *Physical Review Letters* 26.14 (Apr. 1971), p. 832. ISSN: 00319007. DOI: 10.1103/PhysRevLett.26.832. URL: https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.26.832.

[8] Rodney J. Baxter. "One-dimensional anisotropic Heisenberg chain". In: *Annals of Physics* 70.2 (Apr. 1972), pp. 323–337. ISSN: 1096035X. DOI: 10.1016/0003-4916(72)90270-9.

[9] H. Q. Lin. "Exact diagonalization of quantum-spin models". In: *Physical Review B - Condensed Matter and Materials Physics* 42.10 (1990), pp. 6561–6567. ISSN: 01631829. DOI: 10.1103/PhysRevB.42.6561.

[10] Marcin Mierzejewski, Peter Prelovšek, and Tomaž Prosen. "Identifying local and quasilocal conserved quantities in integrable systems". In: *Physical Review Letters* 114.14 (2015), pp. 1–7. ISSN: 10797114. DOI: 10.1103/PhysRevLett.114.140601. arXiv: arXiv:1412.6974v2.

[11] Marcin Mierzejewski et al. "Approximate conservation laws in perturbed integrable lattice models". In: *Physical Review B - Condensed Matter and Materials Physics* 92.19 (Nov. 2015), pp. 1–7. ISSN: 1550235X. DOI: 10.1103/PhysRevB.92.195121. arXiv: 1508.06385. URL: https://link.aps.org/doi/10.1103/PhysRevB.92.195121.

[12] Marcin Mierzejewski, Maciej Kozarzewski, and Peter Prelovšek. "Counting local integrals of motion in disordered spinless-fermion and Hubbard chains". In: *Physical Review B - Condensed Matter and Materials Physics* 97.6 (2018), pp. 1–9. ISSN: 24699969. DOI: 10.1103/PhysRevB.97.064204. arXiv: 1708.08931.

[13] Lenart Zadnik, Marko Medenjak, and Tomaž Prosen. "Quasilocal conservation laws from semicyclic irreducible representations of $U_q(\mathfrak{sl}_2)$ in XXZ spin-1/2 chains". In: *Nuclear Physics B* 902 (Jan. 2016), pp. 339–353. ISSN: 0550-3213. DOI: https://doi.org/10.1016/j.nuclphysb.2015.11.023.

[14] Tomaž Prosen. “Quasilocal conservation laws in XXZ spin-1/2 chains: Open, periodic and twisted boundary conditions”. In: *Nuclear Physics B* 886 (2014), pp. 1177–1198. ISSN: 05503213. DOI: 10.1016/j.nuclphysb.2014.07.024. arXiv: 1406.2258.

[15] Lev Vidmar et al. “Phenomenology of Spectral Functions in Disordered Spin Chains at Infinite Temperature”. In: *Physical Review Letters* 127.23 (Dec. 2021), p. 230603. ISSN: 0031-9007. DOI: 10.1103/PhysRevLett.127.230603. arXiv: 2105.09336.

[16] Peter Mazur. “Non-ergodicity of phase functions in certain systems”. In: *Physica* 43.4 (Sept. 1969), pp. 533–545. ISSN: 00318914. DOI: 10.1016/0031-8914(69)90185-2.

[17] Masuo Suzuki. “Ergodicity, constants of motion, and bounds for susceptibilities”. In: *Physica* 51.2 (Jan. 1971), pp. 277–291. ISSN: 00318914. DOI: 10.1016/0031-8914(71)90226-6.

[18] Xenophon Zotos, Félix Naef, and Peter Prelovsek. “Transport and conservation laws”. In: *Physical Review B - Condensed Matter and Materials Physics* 55.17 (1997), pp. 11029–11032. ISSN: 1550235X. DOI: 10.1103/PhysRevB.55.11029. arXiv: 9611007 `[cond-mat]`.

[19] Enej Ilievski et al. “Quasilocal charges in integrable lattice systems”. In: *Journal of Statistical Mechanics: Theory and Experiment* 6.6 (June 2016), pp. 1–51. ISSN: 17425468. DOI: 10.1088/1742-5468/2016/06/064008. arXiv: 1603.00440.

[20] Xenophon Zotos and Peter Prelovšek. “Evidence for ideal insulating or conducting state in a one-dimensional integrable system”. In: *Physical Review B - Condensed Matter and Materials Physics* 53.3 (1996), pp. 983–986. ISSN: 1550235X. DOI: 10.1103/PhysRevB.53.983.

[21] Maurizio Fagotti. “On conservation laws, relaxation and pre-relaxation after a quantum quench”. In: *Journal of Statistical Mechanics: Theory and Experiment* 2014.3 (2014). ISSN: 17425468. DOI: 10.1088/1742-5468/2014/03/P03016. arXiv: 1401.1064.

[22] Marcin Mierzejewski, Jacek Herbrych, and Peter Prelovšek. “Ballistic transport in integrable quantum lattice models with degenerate spectra”. In: *Physical Review B - Condensed Matter and Materials Physics* 103.23 (2021). ISSN: 24699969. DOI: 10.1103/PhysRevB.103.235115.

[23] Frederick W. Byron and Robert W. Fuller. *Mathematics of Classical and Quantum Physics.* t. 1-2. Dover Publications, 1992. ISBN: 9780486671642.

Appendix A
Derivation of integrated spectral function

We want to prove equation (3.15), which gives a recipe for numerical calculation of integrated spectral function for arbitrary observable A. Our starting point is the definition of spectral function as stated in Definition 3.6:

$$
\begin{aligned}
S(\omega) &= \lim_{\varepsilon\to 0^+} \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t-|t|\varepsilon}\,(A(t)|A) = \lim_{\varepsilon\to 0^+} \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t-|t|\varepsilon}\frac{1}{2^L}\operatorname{tr}\left[\left(e^{iHt}Ae^{-iHt}\right)^{\dagger}A\right] \\
&= \lim_{\varepsilon\to 0^+} \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t-|t|\varepsilon}\frac{1}{2^L}\operatorname{tr}\left[e^{iHt}\left(\sum_m |m\rangle\langle m|\right)A\left(\sum_n |n\rangle\langle n|\right)e^{-iHt}A\right] \\
&= \frac{1}{2^L}\frac{1}{2\pi}\sum_{n,m}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t-|t|\varepsilon}\operatorname{tr}\left[e^{iE_m t}\,|m\rangle\langle m|\,A\,|n\rangle\langle n|\,e^{-iE_n t}A\right] \\
&= \frac{1}{2^L}\frac{1}{2\pi}\sum_{n,m}A_{mn}\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t-|t|\varepsilon}e^{i(E_m-E_n)t}\sum_k \underbrace{\langle k|m\rangle}_{=\delta_{km}}\,\langle n|A|k\rangle \\
&= \frac{1}{2^L}\frac{1}{2\pi}\sum_{n,m}|A_{mn}|^2\underbrace{\lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} \mathrm{d}t\; e^{i\omega t-|t|\varepsilon}e^{i(E_m-E_n)t}}_{\mathcal{I}}
\end{aligned}
\tag{A.1}
$$

Let us now deal with the integral $\mathcal{I}$:

$$
\begin{aligned}
\mathcal{I} &= \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}t\; e^{i(E_m-E_n+\omega)t-|t|\varepsilon} = \lim_{\varepsilon\to 0^+}\left[\lim_{T_1\to-\infty}\int_{T_1}^{0}\mathrm{d}t\; e^{i(E_m-E_n+\omega-i\varepsilon)t} + \lim_{T_2\to\infty}\int_{0}^{T_2}\mathrm{d}t\; e^{i(E_m-E_n+\omega+i\varepsilon)t}\right] \\
&= \lim_{\varepsilon\to 0^+}\left[\lim_{T_1\to-\infty}\frac{1-e^{i(E_m-E_n+\omega)T_1}e^{\varepsilon T_1}}{i(E_m-E_n+\omega-i\varepsilon)} + \lim_{T_2\to\infty}\frac{e^{i(E_m-E_n+\omega)T_2}e^{-\varepsilon T_2}-1}{i(E_m-E_n+\omega+i\varepsilon)}\right] \\
&= \lim_{\varepsilon\to 0^+}\left[\frac{i}{E_n-E_m-\omega+i\varepsilon}+\frac{i}{E_m-E_n+\omega+i\varepsilon}\right] = \lim_{\varepsilon\to 0^+}\frac{2\varepsilon}{(E_m-E_n+\omega-i\varepsilon)(E_m-E_n+\omega+i\varepsilon)} \\
&= \lim_{\varepsilon\to 0^+}\frac{2\varepsilon}{(E_m-E_n+\omega)^2+\varepsilon^2}
\end{aligned}
\tag{A.2}
$$

Obtained results is a limit of the so called Poisson kernel. This happens to be a representations of Dirac delta in form of a limit of a sequence of functions [23]:

$$
\lim_{\varepsilon\to 0^+}\frac{1}{\pi}\frac{\varepsilon}{x^2+\varepsilon^2} = \delta(x) \tag{A.3}
$$

Thus we get:

$$
\mathcal{I} = \lim_{\varepsilon\to 0^+}\frac{2\varepsilon}{(E_m-E_n+\omega)^2+\varepsilon^2} = 2\pi\delta(E_m-E_n+\omega) \tag{A.4}
$$

Inserting this results into equation (A.1) we get:

$$S(\omega) = \frac{1}{2^L}\frac{1}{2\pi}\sum_{n,m}|A_{mn}|^2 \lim_{\varepsilon\to 0^+}\int_{-\infty}^{\infty} \mathrm{d}t\ e^{i\omega t-|t|\varepsilon}e^{i(E_m-E_n)t} = \frac{1}{2^L}\sum_{n,m}|A_{mn}|^2\delta(E_m-E_n+\omega) \tag{A.5}$$

We are now ready to compute the integrated spectral function:

$$\begin{aligned} I(\omega) &= \int_{-\omega}^{\omega}\mathrm{d}\omega' S(\omega') = \frac{1}{2^L}\sum_{n,m}|A_{mn}|^2\int_{-\omega}^{\omega}\mathrm{d}\omega'\delta(E_m-E_n+\omega') \\ &= \frac{1}{2^L}\sum_{n,m}|A_{mn}|^2\theta(\omega+(E_m-E_n))\theta(\omega-(E_m-E_n)) \\ &= \frac{1}{2^L}\sum_{n,m}|A_{mn}|^2\theta(\omega-|E_m-E_n|) \end{aligned} \tag{A.6}$$

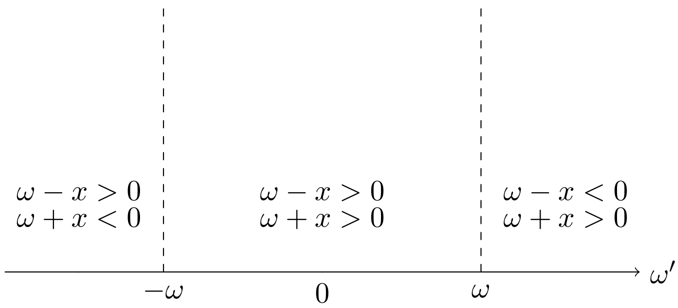

Figure A.1: Illustration of the equality $\int_{-\omega}^{\omega}\mathrm{d}\omega'\delta(x-\omega') = \theta(\omega+x)\theta(\omega-x) = \theta(\omega-|x|)$.

B Derivation of spin energy current

Equation (3.27) 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 $h_{k,k+1}$ into equation (3.27):

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

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.

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

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

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

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:

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

$$i\sum_{r=1}^{L} J_xJ_z\left[S_k^xS_{k+1}^x, S_r^zS_{r+1}^z\right] + i\sum_{r=1}^{L} J_xJ_z\left[S_k^zS_{k+1}^z, S_r^xS_{r+1}^x\right] =$$
$$= J_xJ_z\Big(S_k^xS_{k+1}^yS_{k+2}^z - S_k^zS_{k+1}^yS_{k+2}^x - \left(S_{k-1}^xS_k^yS_{k+1}^z - S_{k-1}^zS_k^yS_{k+1}^x\right)\Big)$$

$$i\sum_{r=1}^{L} J_yJ_z\left[S_k^yS_{k+1}^y, S_r^zS_{r+1}^z\right] + i\sum_{r=1}^{L} J_yJ_z\left[S_k^zS_{k+1}^z, S_r^yS_{r+1}^y\right] =$$
$$= J_yJ_z\Big(S_k^zS_{k+1}^xS_{k+2}^y - S_k^yS_{k+1}^xS_{k+2}^z - \left(S_{k-1}^zS_k^xS_{k+1}^y - S_{k-1}^yS_k^xS_{k+1}^z\right)\Big)$$

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

$$\begin{aligned} j_k^E &= J_xJ_y\left(S_{k-1}^yS_k^zS_{k+1}^x - S_{k-1}^xS_k^zS_{k+1}^y\right) \\ &+ J_xJ_z\left(S_{k-1}^xS_k^yS_{k+1}^z - S_{k-1}^zS_k^yS_{k+1}^x\right) \\ &+ J_yJ_z\left(S_{k-1}^zS_k^xS_{k+1}^y - S_{k-1}^yS_k^xS_{k+1}^z\right) \\ &= J_xJ_y\left(S_{k-1}^yS_k^zS_{k+1}^x - S_{k-1}^xS_k^zS_{k+1}^y\right) + \text{cyclic permutations of } (x,y,z) \end{aligned} \tag{B.1}$$

which is precisely the expression from Zotos, Naef, and Prelovsek [18]. However, in this work we are interested in the XXZ model with the Hamiltonian (**??**). To this end, we need to set $J_x, J_z = 2J,\ J_z = \Delta$ and substitute $S_k^x = \frac{S_k^+ + S_k^-}{2}$, $S_k^y = \frac{S_k^+ - S_k^-}{2i}$. After some more lengthy calculations, we finally arrive at the desired form of energy current density operator:

$$\begin{aligned} j_k^E &= i\Big(\underbrace{2JS_{k-1}^-S_k^zS_{k+1}^+ + J\Delta S_{k-1}^zS_k^+S_{k+1}^- + J\Delta S_{k-1}^+S_k^-S_{k+1}^z}_{O_k} \\ &\quad - \underbrace{\left(2JS_{k-1}^+S_k^zS_{k+1}^- + J\Delta S_{k-1}^zS_k^-S_{k+1}^+ + J\Delta S_{k-1}^-S_k^+S_{k+1}^z\right)}_{O_k^\dagger}\Big) \\ &= i\left(O_k - O_k^\dagger\right) \end{aligned} \tag{B.2}$$

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

C
Proof of orthonormality of basis (3.22)

We want to prove the following:

Proposition C.1 *Let $\{O_{\underline{s},j}\}$ be a set of operators defined as:*

$$O_{\underline{s},j} = \underbrace{\mathbb{1}_{2\times2} \otimes \cdots \otimes \mathbb{1}_{2\times2}}_{j-1} \otimes \sigma_j^{s_1} \otimes \sigma_{j+1}^{s_2} \otimes \cdots \otimes \sigma_{j+m-1}^{s_m} \otimes \underbrace{\mathbb{1}_{2\times2} \otimes \cdots \otimes \mathbb{1}_{2\times2}}_{L-j-m+1} \tag{C.1}$$

where $\sigma_j^z \equiv 2S_j^z$, $\sigma_j^\pm \equiv \sqrt{2}S_j^\pm$, $\sigma_j^0 \equiv \mathbb{1}_{2\times2}$ and $\underline{s} = (s_1, s_2, \ldots, s_m)$ where $s_j \in \{+,-,z,0\}$ for $j \in \{2,3,\ldots,m-1\}$, $s_{1,m} \in \{+,-,z\}$.

Then this set is orthonormal, i.e. $(O_{\underline{s},j}|O_{\underline{s}',j'}) = \delta_{\underline{s},\underline{s}'}\delta_{j,j'}$.

Proof. Let τ^x, τ^y, τ^z be Pauli matrices as defined in (2.8). In this proof we will make use of the following properties of Pauli matrices:

$$\mathrm{tr}(\tau^\alpha) = 0 \implies \mathrm{tr}(\tau^\pm) = \mathrm{tr}(\tau^x \pm i\tau^y) = 0 \tag{C.2}$$

$$\tau^\alpha\tau^\beta = \delta_{\alpha\beta}\mathbb{1}_{2\times2} + i\varepsilon_{\alpha\beta\gamma}\tau^\gamma \tag{C.3}$$

$$\mathrm{tr}\left(\tau^\alpha\tau^\beta\right) = 2\delta_{\alpha\beta} \tag{C.4}$$

where $\alpha, \beta, \gamma \in \{x,y,z\}$ and $\varepsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol. We will begin with showing orthogonality. Consider the following inner product for $\underline{s} \neq \underline{s}'$:

$$\begin{aligned}(O_{\underline{s},j}|O_{\underline{s}',j}) =& \frac{1}{2^L}\,\mathrm{tr}\left((\mathbb{1}_{2\times2})^\dagger\,\mathbb{1}_{2\times2}\right)\cdots\mathrm{tr}\left((\mathbb{1}_{2\times2})^\dagger\,\mathbb{1}_{2\times2}\right)\cdot\mathrm{tr}\left(\left(\sigma_j^{s_1}\right)^\dagger\sigma_j^{s_1'}\right)\\ &\cdot\mathrm{tr}\left(\left(\sigma_{j+1}^{s_2}\right)^\dagger\sigma_{j+1}^{s_2'}\right)\cdots\mathrm{tr}\left(\left(\sigma_{j+m-1}^{s_m}\right)^\dagger\sigma_{j+m-1}^{s_m'}\right)\cdots\mathrm{tr}\left((\mathbb{1}_{2\times2})^\dagger\,\mathbb{1}_{2\times2}\right)\end{aligned} \tag{C.5}$$

Because $\underline{s} \neq \underline{s}'$, there must be an index i such that $s_i \neq s_i'$. Because trace is cyclic, we only need to consider four cases:

1. $s_i = 0$, $s_i' \in \{z,+,-\}$

$$\mathrm{tr}\left(\left(\sigma_{j+i-1}^{s_i}\right)^\dagger\sigma_{j+i-1}^{s_i'}\right) \propto \mathrm{tr}\left(\mathbb{1}_{2\times2}\tau_{j+i-1}^{s_i'}\right) = \mathrm{tr}\left(\tau_{j+i-1}^{s_i'}\right) = 0$$

2. $s_i = z$, $s_i' = +$

$$\mathrm{tr}\left(\left(\sigma_{j+i-1}^{s_i}\right)^\dagger\sigma_{j+i-1}^{s_i'}\right) \propto \mathrm{tr}\left(\tau_{j+i-1}^z\tau_{j+i-1}^+\right) = \left[\mathrm{tr}\left(\tau_{j+i-1}^z\tau_{j+i-1}^x\right) + i\,\mathrm{tr}\left(\tau_{j+i-1}^z\tau_{j+i-1}^y\right)\right] = 0$$

3. $s_i = z,\ s_i' = -$

$$\mathrm{tr}\Big(\big(\sigma^{s_i}_{j+i-1}\big)^\dagger \sigma^{s_i'}_{j+i-1}\Big) \propto \mathrm{tr}\Big(\tau^z_{j+i-1}\tau^-_{j+i-1}\Big) = \Big[\mathrm{tr}\Big(\tau^z_{j+i-1}\tau^x_{j+i-1}\Big) - i\,\mathrm{tr}\Big(\tau^z_{j+i-1}\tau^y_{j+i-1}\Big)\Big] = 0$$

4. $s_i = +,\ s_i' = -$

$$\begin{aligned}\mathrm{tr}\Big(\big(\sigma^{s_i}_{j+i-1}\big)^\dagger \sigma^{s_i'}_{j+i-1}\Big) \propto \mathrm{tr}\Big(\tau^-_{j+i-1}\tau^-_{j+i-1}\Big) &= \Big[\,\mathrm{tr}\Big(\tau^x_{j+i-1}\tau^x_{j+i-1}\Big) - \mathrm{tr}\Big(\tau^y_{j+i-1}\tau^y_{j+i-1}\Big) \\ &\quad - i\,\mathrm{tr}\Big(\tau^x_{j+i-1}\tau^y_{j+i-1}\Big) - i\,\mathrm{tr}\Big(\tau^y_{j+i-1}\tau^x_{j+i-1}\Big)\Big)\Big] \\ &= \Big[\,\underbrace{\mathrm{tr}\Big(\tau^x_{j+i-1}\tau^x_{j+i-1}\Big)}_{=2} - \underbrace{\mathrm{tr}\Big(\tau^y_{j+i-1}\tau^y_{j+i-1}\Big)}_{=2}\,\Big] = 0\end{aligned}$$

Therefore $(O_{\underline{s},j}|O_{\underline{s}',j}) = 0$. It is also easy to see that $(O_{\underline{s},j}|O_{\underline{s},j'}) = 0$, because in this case we would have in (C.5) a term of the form $\mathrm{tr}\Big(\sigma^{s_i}_{j+i-1}\mathbb{1}_{2\times2}\Big) = \mathrm{tr}\Big(\sigma^{s_i}_{j+i-1}\Big) \propto \mathrm{tr}\Big(\tau^{s_i}_{j+i-1}\Big) = 0$, where the last equality comes from (C.2). Thus the orthogonality is proven and we have $(O_{\underline{s},j}|O_{\underline{s}',j'}) \propto \delta_{\underline{s},\underline{s}'}\delta_{j,j'}$.

Now let us show that these operators are normalized:

$$\begin{aligned}(O_{\underline{s},j}|O_{\underline{s},j}) =& \frac{1}{2^L}\,\mathrm{tr}\left(\left(\mathbb{1}_{2\times2}\right)^\dagger \mathbb{1}_{2\times2}\right)\cdots\mathrm{tr}\left(\left(\mathbb{1}_{2\times2}\right)^\dagger \mathbb{1}_{2\times2}\right)\cdot\mathrm{tr}\Big(\big(\sigma^{s_1}_j\big)^\dagger\sigma^{s_1}_j\Big) \\ &\cdot\mathrm{tr}\Big(\big(\sigma^{s_2}_{j+1}\big)^\dagger\sigma^{s_2}_{j+1}\Big)\cdots\mathrm{tr}\Big(\big(\sigma^{s_m}_{j+m-1}\big)^\dagger\sigma^{s_m}_{j+m-1}\Big)\cdots\mathrm{tr}\left(\left(\mathbb{1}_{2\times2}\right)^\dagger \mathbb{1}_{2\times2}\right)\end{aligned} \tag{C.6}$$

We need to consider four cases $s_i \in \{0, z, +, -\}$.

1. $s_i = 0$

$$\mathrm{tr}\Big(\big(\sigma^{s_i}_{j+i-1}\big)^\dagger \sigma^{s_i}_{j+i-1}\Big) = \mathrm{tr}(\mathbb{1}_{2\times2}\mathbb{1}_{2\times2}) = \mathrm{tr}(\mathbb{1}_{2\times2}) = 2$$

2. $s_i = z$

$$\mathrm{tr}\Big(\big(\sigma^{s_i}_{j+i-1}\big)^\dagger \sigma^{s_i}_{j+i-1}\Big) = 4\,\mathrm{tr}\Big(S^z_{j+i-1}S^z_{j+i-1}\Big) = \mathrm{tr}\Big(\tau^z_{j+i-1}\tau^z_{j+i-1}\Big) = 2$$

3. $s_i = +$

$$\begin{aligned}\mathrm{tr}\Big(\big(\sigma^{s_i}_{j+i-1}\big)^\dagger \sigma^{s_i}_{j+i-1}\Big) &= 2\,\mathrm{tr}\Big(S^-_{j+i-1}S^+_{j+i-1}\Big) = \frac{1}{2}\,\mathrm{tr}\Big(\tau^-_{j+i-1}\tau^+_{j+i-1}\Big) = \frac{1}{2}\Big[\,\mathrm{tr}\Big(\tau^x_{j+i-1}\tau^x_{j+i-1}\Big) \\ &\quad + \mathrm{tr}\Big(\tau^y_{j+i-1}\tau^y_{j+i-1}\Big) - i\,\mathrm{tr}\Big(\tau^x_{j+i-1}\tau^y_{j+i-1}\Big) - i\,\mathrm{tr}\Big(\tau^y_{j+i-1}\tau^x_{j+i-1}\Big)\Big)\Big] \\ &= \frac{1}{2}\Big[\,\underbrace{\mathrm{tr}\Big(\tau^x_{j+i-1}\tau^x_{j+i-1}\Big)}_{=2} + \underbrace{\mathrm{tr}\Big(\tau^y_{j+i-1}\tau^y_{j+i-1}\Big)}_{=2}\,\Big] = 2\end{aligned}$$

4. $s_i = -$

$$\mathrm{tr}\Big(\big(\sigma^{s_i}_{j+i-1}\big)^\dagger \sigma^{s_i}_{j+i-1}\Big) = 2\,\mathrm{tr}\Big(S^+_{j+i-1}S^-_{j+i-1}\Big) = 2\,\mathrm{tr}\Big(S^-_{j+i-1}S^+_{j+i-1}\Big) = 2$$

In the end we get that $(O_{\underline{s},j}|O_{\underline{s},j}) = \frac{1}{2^L}2^L = 1$. Hence $(O_{\underline{s},j}|O_{\underline{s}',j'}) = \delta_{\underline{s},\underline{s}'}\delta_{j,j'}$ and the proof is finished.

■

Note that this proof holds only if we consider full Hilbert space of dimension 2^L. If we were to restrict our calculations to some subspace, a reorthogonalization procedure would be necessary [10].