Faculty of Fundamental Problems of Technology
Wrocław University of Science and Technology

Non-commuting integrals of motion in XXZ model

Jakub Pawłowski
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prof. dr hab. Marcin Mierzejewski

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Abstract

Apparent incompatibility of classical irreversible thermodynamics with unitary quantum dynamics has for a long time been a topic of intensive research. One possible approach to reconciliation between these two fields in generic nonintegrable systems is given by *Eigenstate Thermalization Hypothesis*. On the other hand, in integrable systems thermalization is hindered by the existence of extensive number of (quasi)local integrals of motions, (Q)LIOMs. In this work we investigate a class of *noncommuting* (Q)LIOMs originating from symmetries of spin-1/2 XXZ model present for certain values of anisotropy parameter. However, it is the boundary between chaotic and integrable systems that is the most interesting, as it is still largely unknown. To this end, a weak integrability-breaking perturbation is introduced and the relaxation of aforementioned noncommuting (Q)LIOMs is studied. We report a novel Gaussian-like decay of autocorrelation functions, together with a linear, instead of the expected quadratic, scaling of relaxation times with perturbation strength. This result is a consequence of the origin of these noncommuting quantities being the macroscopical degeneracy of many-body spectra for high-symmetry anisotropy values.

Keywords: *integrals of motion, ETH, integrability breaking, XXZ model*

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Introduction

1.1 Thermalization in closed systems

Of all long-standing problems that have bothered physicists, the relationship between micro and macro worlds is perhaps one of the most disputed ones. On the one hand, we have a remarkably successful theory of statistical mechanics and the seemingly irreversible laws of thermodynamics [1, 2]. On the other hand, we have no less successful theory of quantum mechanics, which predicts the reversibility of microscopic dynamics [3, 4]. One can then pose a question, when and why a far-from equilibrium isolated quantum system can be accurately described using equilibrium statistical mechanics?

Eigenstate Thermalization Hypothesis It was already suggested by John von Neumann in 1929 that a proper way of thinking about thermalization of quantum systems is by looking at physical observables instead of wave functions or density matrices of the whole system [5]. Following the review article by D'Alessio et al. [6], we say that an observable undergoes thermalization if it evolves with time towards the prediction of microcanonical ensemble and stays in the vicinity of it for majority of future times. The question is, what is necessary for this thermalization to happen? To answer it, let us imagine that we have an isolated quantum system in a pure state $|\psi_{\text{initial}}\rangle$. We want to investigate evolution of some observable O under time-independent Hamiltonian H with eigenstates $|n\rangle$ and corresponding energies E_n. Writing the time-dependent wave function as $|\psi(t)\rangle = \sum_n C_n \mathrm{e}^{-iE_n t} |n\rangle$, $C_n = \langle n|\psi_{\text{initial}}\rangle$, we have

$$\begin{aligned} O(t) = \langle\psi(t)|O|\psi(t)\rangle &= \sum_{m,n} C_m^* C_n \mathrm{e}^{i(E_m - E_n)t} O_{mn} \\ &= \sum_n |C_n|^2 O_{nn} + \sum_{n \neq m} C_m^* C_n \mathrm{e}^{i(E_m - E_n)t} O_{mn} \end{aligned} \tag{1.1}$$

where $O_{mn} = \langle m|O|n\rangle$. We immediately see that, assuming absence of degeneracy, long-time average of the off-diagonal part must be equal to zero and what remains is the diagonal part. This is a prediction of the so-called *diagonal ensemble* [7]. It basically means that the system 'remembers' its initial conditions via the constant coefficients $|C_n|^2$. At first, it is not clear how we could reach the prediction of microcanonical ensemble. Moreover, the time necessary for the second term to vanish in many-body systems could easily exceed the age of our universe [6]. Nevertheless, such thermal relaxation was observed in experiments with isolated cold atomic gasses [8, 9, 10, 11, 12].

This is where an insight from Random Matrix Theory (RMT), pioneered by Wigner [13] in context of nuclear physics, comes into play. He observed that if we were to write a Hamiltonian in a generic and not fine-tuned basis, it would essentially be a random matrix (subject to symmetry constraints). It can then be shown within RMT formalism [14], that matrix elements of an Hermitian operator O in eigenbasis of a random Hamiltonian can be written as

$$O_{mn} \approx \bar{O}\delta_{mn} + \sqrt{\frac{\overline{O^2}}{\mathcal{D}}} R_{mn} \tag{1.2}$$

where $\bar{O} = \frac{1}{\mathcal{D}}\sum_i O_i$, $O = \sum_i O_i |i\rangle\langle i|$, $\mathcal{D}$ it the dimension of the underlying Hilbert space and R_{mn} is either a real or a complex (depending on the symmetries of the Hamiltonian) random variable with zero mean and unit variance. Using equation (1.2), we can then disentangle the prediction of the diagonal ensemble from the initial conditions

$$\sum_n |C_n|^2 O_{nn} \approx \bar{O} \sum_n |C_n|^2 = \bar{O} \tag{1.3}$$

obtaining a result consistent with the microcanonical ensemble, albeit without energy dependence so equivalent to the infinite temperature limit. Furthermore, off-diagonal elements are exponentially small in system size, so in order for the second term in average of (1.1) to vanish, it is necessary only for the matrix elements with largest contribution to the expected value to average to zero. This can happen on much shorter timescales that would be required for eliminating matrix elements between all eigenstates [6].

Nonetheless, it is not yet enough, as RMT misses two crucial points in order to be able to relate it to real systems. First, the expectation values should depend on energy and second, relaxation times should be observable dependent. These shortcomings were fixed in groundbreaking works of Deutsch [15] and Srednicki [16], giving rise to the *Eigenstate Thermalization Hypothesis* (ETH) It is often stated in form of an *ansatz* for matrix elements of observables expressed in eigenbasis of a Hamiltonian [17]

$$O_{mn} = O(\bar{E})\delta_{mn} + \mathrm{e}^{-S(\bar{E})/2} f_O(\bar{E}, \omega) R_{mn} \tag{1.4}$$

where $\bar{E} = (E_n + E_m)/2$, $\omega = E_n - E_m$ and $S(\bar{E})$ is the thermodynamic entropy at energy $\bar{E}$. Both $O(\bar{E})$ and $f_O(\bar{E}, \omega)$ are smooth functions of their parameters and $O(\bar{E})$ is equivalent to the expected value in microcanonical ensemble. Finally, as in RMT, R_{mn} is a random real or complex variable. At the moment it is unknown in general whether the ETH holds for a given observable in a given system, however it is expected to be valid for all physical observables [6]. Numerical clues for the validity of ETH have been found in many correlated lattice models for example hard core bosons, interacting spin chains [18, 19, 20, 21], and fermions [22, 23]. For more details on ETH see the review by D'Alessio et al. [6], on which this part of Introduction is based.

Generalized Gibbs Ensemble In a generic system exhibiting ETH, after thermalization, the expectation values of observables can be calculated using a density matrix from relevant

Gibbs ensembles (because of the equivalence of ensembles one can use either the microcanonical, canonical or grand canonical one). For example, in the grand canonical ensemble $\hat{\rho} \propto \mathrm{e}^{-(H-\mu N)/kT}$ and $\bar{O} \approx \mathrm{tr}(O\hat{\rho})$. However, there exists a class of models, called *integrable*[1], for which the ETH does not hold. There is no unique definition of quantum integrability, but for our purposes it will be enough to characterize such systems by existence of an extensive number of (quasi)local operators $\{\hat{I}_k\}$ that commute with the Hamiltonian and with each other[2]. Just as in classical mechanics the existence of integrals of motion imposes a constraint on phase space available to a system, the lack of thermalization in integrable quantum systems can be attributed to the existence of an extensive number of conservation laws, instead of only a few like in nonintegrable ones (such as energy or momentum). Remarkably, it was shown by Rigol et al. [24] that the usual approach employed in statistical mechanics, namely maximizing many-body entropy $S = k_B\,\mathrm{tr}(-\hat{\rho}\ln(\hat{\rho}))$ subject to constraints, yields a very successful result. It is now known as the Generalized Gibbs Ensemble (GGE)

$$\hat{\rho}_{\mathrm{GGE}} = \frac{\exp(-\sum_k \lambda_k I_k)}{\mathrm{tr}[\exp(-\sum_k \lambda_k I_k)]} \tag{1.5}$$

where I_k are the integrals of motion and λ_k are Lagrange multipliers fixed by requiring that $\mathrm{tr}(\hat{\rho}_{\mathrm{GGE}} I_k) = \langle I_k \rangle (t=0)$. In generic nonintegrable models where the only integrals of motion are the Hamiltonian and particle number operator, GGE reduces to the usual grand canonical ensemble. Many numerical tests have been carried out suggesting that integrable systems, in general, do not relax to thermal equilibrium and that GGE accurately describes the properties of few-body observables after thermalization [7, 24, 25, 26]. Nonetheless, finding agreement with predictions from thermal equilibrium does not necessarily mean that the model is nonintegrable, as there are fine-tuned states that relax towards predictions of thermal equilibrium despite integrability of underlying system [8, 27, 28].

1.2 Motivation and aim of this dissertation

As ETH is anticipated to be valid in generic nonintegrable systems, so is GGE likely to describe thermalization in a generic integrable system. However, on the contrary to nonintegrable models, the classification of appropriate conserved quantities in integrable models is in general a difficult task [6]. This problem is our main interest in Chapter 2, where following Mierzejewski, Prelovšek, and Prosen [29] we describe in detail an algorithm allowing for systematic classification of all conserved quantities in a system given by a tight-binding Hamiltonian. As a further motivation for the search of integrals of motion, in Chapter 2 we also introduce the well-known concept of Mazur bound [30, 31] and a rather new phenomenological tool for studying quantum many-body systems — integrated spectral function [32]. As an application of the introduced methodology, we study the energy current and two *noncommuting* conserved quantities in paradigmatic spin-1/2 XXZ model.

Complete integrability is not a common property in the quantum world. Many systems require fine-tuning of their parameters to achieve this, with perhaps a single exception given by systems

[1] A very brief review of integrability is presented in Appendix A.
[2] For relevant definitions see Section 2.1.

exhibiting many-body localization. Furthermore, we usually do not have precise enough control over real-world systems to perform such fine tuning, so full integrability is rarely seen (albeit some signatures of it were observed in an experiment [33]). It is thus desirable to investigate *almost* integrable systems, where the integrability-breaking perturbation is small. In classical systems, the solution to this problem lies within the KAM theorem, however no such conclusive result exists in the quantum world (for details see Appendix A). In such weakly perturbed quantum systems, the number of conserved quantities usually behaves like in generic nonintegrable models, so integrals of motion from parent integrable model start to decay. Investigating long-time behavior of the autocorrelation functions of aforementioned energy current and two noncommuting observables in spin-1/2 XXZ model is the subject of Chapter 3. In case of the titular noncommuting integrals of motion, we report a novel result about a linear scaling of relaxation time with perturbation strength and Gaussian, instead of the expected exponential [34], decay of relevant autocorrelation functions.

The remainder of this chapter is devoted to a short introduction to the Heisenberg model and its modification, namely the titular XXZ model.

1.3 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 an external magnetic field and those which have a nonzero magnetic moment without external field [35]. First group consists of paramagnetic and diamagnetic systems. In the former, a nonzero net magnetic moment comes from alignment of valence electrons' spins in the direction of the external magnetic field. In the latter, we deal with an inductive effect in which the external field induces magnetic dipoles opposing the field that 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. The 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 [36].

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 itinerant magnetism. In this chapter, we deal with the former of two models. First, a physics-motivated derivation of Heisenberg model is be presented. Afterwards, on our way to XXZ model, we discuss the mathematical details and various modifications of original model. Our review of this topic is based on the books by Spałek [35] and thesis by Ng [37].

1.3.1 Heisenberg-Dirac exchange interaction

Coulomb interaction 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. To facilitate these two degrees of freedom, we say that i-th electron's wave function lives in a Hilbert space which is a tensor product of spacial wave functions' space and spin wave functions' space, i.e. $\mathcal{H}_i \cong L^2(\mathbb{R}^3) \otimes \mathfrak{h}_i$, where $L^2(\mathbb{R}^3)$ is the usual space of square-integrable functions on $\mathbb{R}^3$, and $\mathfrak{h}_i \cong \mathbb{C}^2$ is a two-dimensional vector space spanned by $|\uparrow\rangle = \binom{1}{0}$ and $|\downarrow\rangle = \binom{0}{1}$. The combined wave function 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 $\mathcal{H}_{\text{spin}} \cong \mathfrak{h}_1 \otimes \mathfrak{h}_2$.

The Hamiltonian of two interacting electrons is given by

$$H_C = \underbrace{-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2}_{\text{free particles}} + \underbrace{V(\boldsymbol{r}_1, \boldsymbol{r}_2)}_{\text{interaction}} \tag{1.6}$$

where in the case of Coulomb interaction we have $V(\boldsymbol{r}_1, \boldsymbol{r}_2) = \frac{\mathrm{e}^2}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|}$. 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 action is restricted to the $\mathcal{H}_{\text{space}}$ part of the full Hilbert space. This is a crucial observation that leads to the development of Heisenberg model. We shall now seek a way to replace this Hamiltonian by an equivalent one acting only on $\mathcal{H}_{\text{spin}}$.

Two-electron wave function It is time to invoke the Pauli exclusion principle, which requires the composite wave function of two electrons to be antisymmetric under the exchange of pairs of coordinates (both spatial and spin degrees of freedoms are treated like coordinates). Because Hamiltonian 1.6 does not depend explicitly on spin, the total wave function 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 wave functions (unnormalized) are of the form

$$\psi^{(s)}_{\text{space}} = \psi_1(\boldsymbol{r}_1) \otimes \psi_2(\boldsymbol{r}_2) + \psi_2(\boldsymbol{r}_1) \otimes \psi_1(\boldsymbol{r}_2) \tag{1.7}$$

$$\psi^{(a)}_{\text{space}} = \psi_1(\boldsymbol{r}_1) \otimes \psi_2(\boldsymbol{r}_2) - \psi_2(\boldsymbol{r}_1) \otimes \psi_1(\boldsymbol{r}_2) \tag{1.8}$$

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

$$\psi^{(s)}_{\text{spin}} = |\uparrow\uparrow\rangle\,,\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\,,\ |\downarrow\downarrow\rangle \tag{1.9}$$

$$\psi^{(a)}_{\text{spin}} = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \tag{1.10}$$

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

Possible two-electron wave functions 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 the energy of Coulomb interaction in these states is given by

$$\langle\varphi|H_C|\varphi\rangle = \left\langle \psi^{(s)}_{\text{space}} \middle| H_C \middle| \psi^{(s)}_{\text{space}} \right\rangle = E^{(s)} \tag{1.11}$$

$$\langle\chi|H_C|\chi\rangle = \left\langle \psi^{(a)}_{\text{space}} \middle| H_C \middle| \psi^{(a)}_{\text{space}} \right\rangle = E^{(a)} \tag{1.12}$$

In general we have that $E^{(s)} \neq E^{(a)}$. We can argue that this is the case with Coulomb potential, because it blows up to infinity at $\boldsymbol{r}_1 \to \boldsymbol{r}_2$, whereas the antisymmetric wave function vanishes at this point. It is thus energetically favorable for our system to pick the one of the two possible wave functions.

Spin-spin interaction Under the Coulomb interaction, the symmetric and antisymmetric spin wave functions are not directly distinguished. It is the difference between spatial parts, together with Pauli exclusion principle that forces the choice of a given 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 wave functions and thus fix the spatial part. Let τ^x, τ^y, τ^z be the 2×2 Pauli matrices

$$\tau^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \tau^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \tau^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.13}$$

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 particular commutation and anticommutation relations

$$\left[\tau^j, \tau^k\right] = 2i\varepsilon_{jkl}\tau^l \tag{1.14}$$

$$\left\{\tau^j, \tau^k\right\} = 2\delta_{jk}\mathbb{1}_{2\times 2} \tag{1.15}$$

which in turn leads to the following important property

$$\begin{aligned}\left[\tau^j, \tau^k\right] + \left\{\tau^j, \tau^k\right\} &= \left(\tau^j\tau^k - \tau^k\tau^j\right) + \left(\tau^j\tau^k + \tau^k\tau^j\right) \\ i\varepsilon_{jkl}\tau^l + \delta_{jk}\mathbb{1}_{2\times 2} &= \tau^j\tau^k\end{aligned} \tag{1.16}$$

which shall be of use in Appendix D. We define an operator via a formal dot product

$$\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 = \tau_1^x \otimes \tau_2^x + \tau_1^y \otimes \tau_2^y + \tau_1^z \otimes \tau_2^z \tag{1.17}$$

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

$$\begin{aligned}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 |\uparrow\uparrow\rangle &= (\tau_1^x |\uparrow\rangle_1) \otimes (\tau_2^x |\uparrow\rangle_2) + (\tau_1^y |\uparrow\rangle_1) \otimes (\tau_2^y |\uparrow\rangle_2) + (\tau_1^z |\uparrow\rangle_1) \otimes (\tau_2^z |\uparrow\rangle_2) \\ &= \left(\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \otimes \left(\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) + \left(\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \otimes \left(\left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) + \left(\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \otimes \left(\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)\right) \\ &= \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right) + \left(\begin{smallmatrix} 0 \\ i \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 0 \\ i \end{smallmatrix}\right) + \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right) \otimes \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right) = |\uparrow\uparrow\rangle\end{aligned} \tag{1.18}$$

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 the 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 [38]. The proportionality constant is equal for spin$-s$ particles to $s(s+1)$ and thus all single spin-1/2 states are eigenvectors of these operators with eigenvalue 3/4. We can also construct the square of the total spin angular momentum operator $\boldsymbol{S}^2 = (\boldsymbol{S}_1 + \boldsymbol{S}_2)^2$ 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

$$s(s+1)\mathbb{1}_{2\times 2} = \boldsymbol{S}_1^2 + \boldsymbol{S}_2^2 + 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_1 = \frac{3}{2}\mathbb{1}_{2\times 2} + 2\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \tag{1.19}$$

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 $\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$.

Equivalent Hamiltonian After this detour into the 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 $\mathcal{H}_{\text{spin}}$

$$H_S = \frac{3E^{(a)} + E^{(s)}}{4} + \frac{E^{(a)} - E^{(s)}}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \tag{1.20}$$

It is easy to see that eigenvalues of H_S are $E^{(a)}$ for symmetric spin states (corresponding to $\psi^{(a)}_{\text{space}}$) and $E^{(s)}$ for antisymmetric spin state (corresponding to $\psi^{(s)}_{\text{space}}$). 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 $J = E^{(a)} - E^{(s)}$ and ignoring constant energy offset, we finally arrive at the Dirac-Heisenberg exchange interaction

$$H_S = \frac{J}{4}\boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \tag{1.21}$$

or expressed in terms of the usual spin operators

$$H_S = J\boldsymbol{S}_1 \cdot \boldsymbol{S}_2 \tag{1.22}$$

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.

1.3.2 One-dimensional XXZ model

Heisenberg model It now straightforward to generalize this exchange interaction to spins living on an arbitrary lattice, by summing the spin-disguised Coulomb interaction (1.22) over all pairs of spins

$$H = \frac{1}{2}\sum_{i\neq j} J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1.23}$$

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 the correlation between the spins of single particles located in atoms i and j (lattice sites), induced by the repulsive Coulomb interaction. In practical calculations, it is often assumed that electrons are well localized, and thus the value of the exchange integral falls off quickly enough with increasing distance between them that only the nearest neighbor interactions are important. Moreover, J_{ij} is also assumed to be the same between those nearest neighbors

$$J_{ij} = \begin{cases} J, & i \text{ is a nearest neighbor of } j \\ 0, & \text{otherwise} \end{cases} \tag{1.24}$$

These assumptions reduce Heisenberg Hamiltonian to its most popular form

$$H = -\frac{J}{2}\sum_{\langle i,j\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j \tag{1.25}$$

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

One-dimensional lattice From now on, we restrict 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 the visualization of periodic boundary conditions in one and two-dimensional cases, see Figure 1.1. 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 use the standard embedding [37]

$$\sigma_j = \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{j-1} \otimes\, \sigma \otimes \mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2} \tag{1.26}$$

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

Hamiltonian (1.25) in one dimension has the following form

$$H_{XXX} = J\sum_{j=1}^{L}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + S_j^z S_{j+1}^z\right) \tag{1.27}$$

where periodic boundary conditions are imposed by requiring that $S_{L+1}^{\alpha} = S_1^{\alpha}$. Sometimes it is also called the isotropic XXX model. A characteristic property of the XXX model is that is posses $SU(2)$ symmetry (rotation of spins), which causes difficulties in numerical studies. Therefore, breaking this symmetry is often desirable. This can be achieved by introducing anisotropy in the form of different exchange integrals for different directions. The resulting model is known in literature as the XYZ model

$$H_{XYZ} = \sum_{j=1}^{L}\left(J_x S_j^x S_{j+1}^x + J_y S_j^y S_{j+1}^y + J_z S_j^z S_{j+1}^z\right) \tag{1.28}$$

It is interesting to note that this is not only a mathematical trick to simplify numerical calculations, but the system described by this Hamiltonian was realized in practice [39]. To reduce the number of parameters, we can single out a particular direction. 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

$$H_{XXZ} = J\sum_{j=1}^{L}\left(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y\right) + J\Delta\sum_{j=1}^{L} S_j^z S_{j+1}^z \tag{1.29}$$

where Δ is the so-called anisotropy parameter. It is convenient to reexpress this model in terms of the spin-flip operators

$$S^+ = S^x + iS^y \tag{1.30}$$

$$S^- = S^x - iS^y \tag{1.31}$$

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

$$S^x = \frac{S^+ + S^-}{2} \tag{1.32}$$

$$S^y = \frac{S^+ - S^-}{2i} \tag{1.33}$$

and inserting them into (1.29) yields

$$H_{XXZ} = \frac{J}{2} \sum_{j=1}^{L} \left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ \right) + J\Delta \sum_{j=1}^{L} S_j^z S_{j+1}^z \tag{1.34}$$

which is the most common form of XXZ Hamiltonian. The isotropy could be restored by setting $\Delta = 1$. 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 [40] 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 [41, 42]. However, these solutions, as well as the so far unsuccessful attempts at solving it in two and more dimensions, are notoriously difficult and we do not use them in this thesis. Instead, when in need of concrete computations, we resort to much simpler numerical methods in the form of exact diagonalization [43].

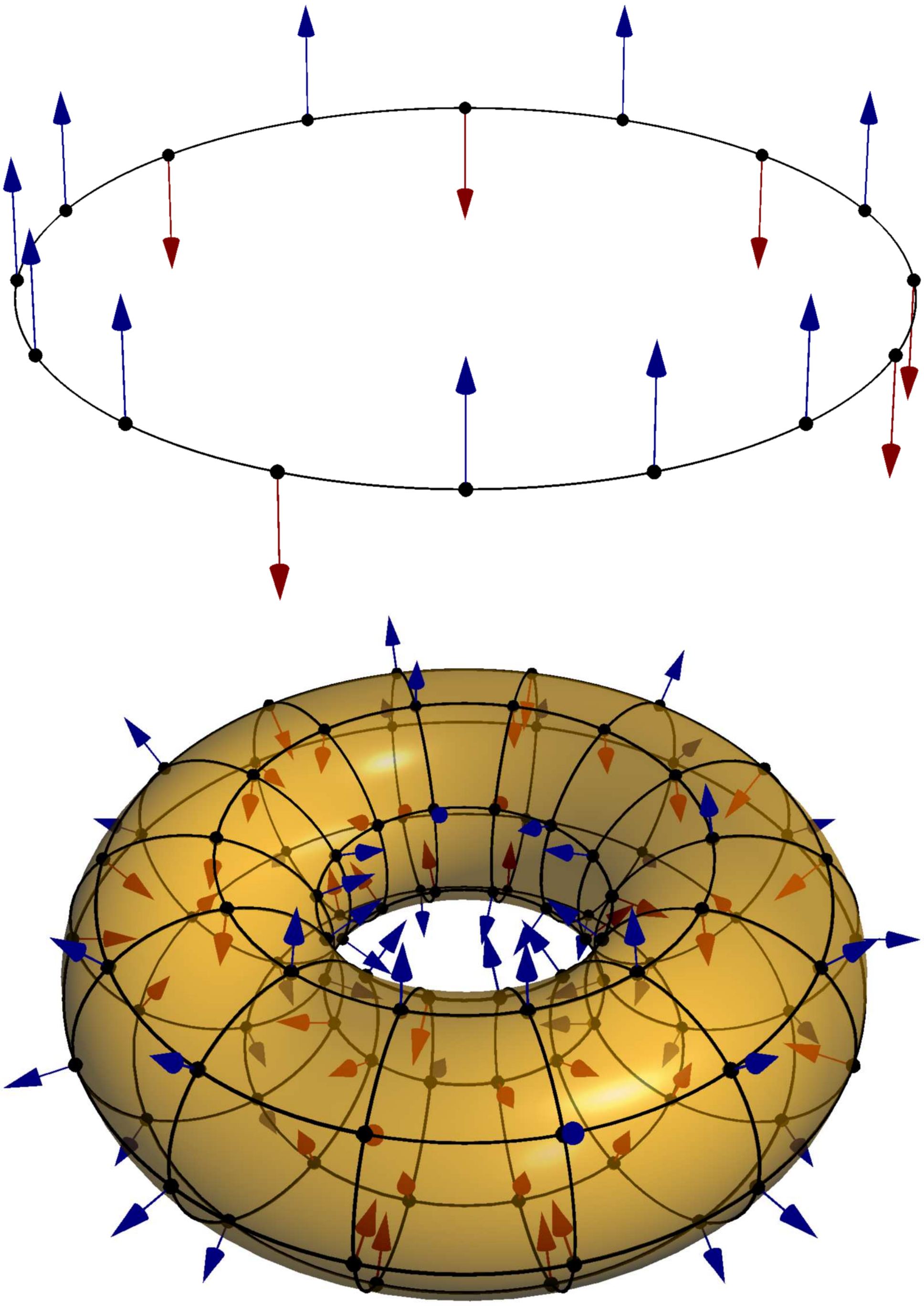

Figure 1.1: Visualization of periodic boundary conditions in 1-D (circle topology) and 2-D (torus topology).

2

Integrals of motion

The problem of our interest is the systematic classification of all local and quasilocal integrals of motion (LIOMs and QLIOMs) supported on up to $M \in \mathbb{N}$ 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 [29]. 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 principle this algorithm could be also applied to lattice systems in two and more dimensions, however as of now it is prevented by computational complexity of numerical approaches to such models.

In our description and used notation, we follow the works of Mierzejewski, Prelovšek, and Prosen [29], Mierzejewski et al. [44], and Mierzejewski, Kozarzewski, and Prelovšek [45]. 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 of the algorithm. The importance of (Q)LIOMs is be made clear by invoking the concepts of spectral functions and Mazur bound. Examples of application of this algorithm to the XXZ model conclude this chapter.

The algorithm introduced in this chapter was implemented in C++ with the help of Armadillo linear algebra library [46, 47].

2.1 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

Definition 2.1 (Hilbert-Schmidt product) *Let $A, B \in \mathcal{V}_L$. The Hilbert-Schmidt product of A and B is*

$$(A|B) = \frac{1}{\mathcal{D}} \operatorname{tr}\left(A^\dagger B\right) = \frac{1}{\mathcal{D}} \sum_{mn} A_{nm} B^*_{nm} \tag{2.1}$$

where $A_{nm} = \langle n|A|m\rangle$ and $|n\rangle, |m\rangle$ are eigenstates of some Hamiltonian, i.e. $H|n\rangle = E_n|n\rangle$. Moreover, we define the Hilbert-Schmidt norm of an operator to be $\|A\| = \sqrt{(A|A)}$.

The presented definitions are correct, as we work only with finite dimensional Hilbert spaces and taking the trace is a linear operation. We require the operators to be traceless, because they have zero overlap with the identity, $(A|\mathbb{1}) = \frac{1}{D}\operatorname{tr}(A) = 0$. Recall from statistical physics, that the average of an observable A over a canonical ensemble in a finite temperature is given by

$$\langle A\rangle_\beta = \frac{\operatorname{tr}\left(\mathrm{e}^{-\beta H}A\right)}{\operatorname{tr}(\mathrm{e}^{-\beta H})} \tag{2.2}$$

where $\beta = \frac{1}{kT}$. Taking the limit $\beta \to 0$, we obtain that $(A|B) = \langle AB\rangle_0$. Therefore, the Hilbert-Schmidt inner product corresponds to the infinite temperature limit of averaging over a suitable ensemble (either canonical or grand canonical). Now, 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 define a basis of $\mathcal{V}_L^M$ consisting of operators $O_s \in \mathcal{V}_L^M$ satisfying the following properties

$$(O_s|O_t) = \delta_{st} \qquad \text{(orthonormality)}$$

$$(\forall A \in \mathcal{V}_L^M)\,(A = \sum_s (O_s|A)\,O_s) \qquad \text{(completeness)}$$

$$(\forall A \in \mathcal{V}_L)\,(A = A^M + A^\perp = \sum_s (O_s|A)\,O_s + A^\perp),\ \text{such that}\ (\forall s)\Big(\Big(O_s\Big|A^\perp\Big) = 0\Big) \tag{2.3}$$

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

Definition 2.2 *Let H be a Hamiltonian operator. Then, any observable A commuting with the Hamiltonian*

$$[H, A] = 0$$

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

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

Example 2.1 *Take H to be any Hamiltonian operator. By spectral theorem, it can be written in diagonal form*

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

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

However, as it will become evident in Section 2.3 on spectral functions, 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 2.1. They can be thought of as being different from identity only on m consecutive sites. The XXZ Hamiltonian defined by equation (1.34) is an example of 2-local operator. On the other hand, a quasilocal operator can be represented as a convergent sum of operators with increasing support. In Section 2.2, a more precise definition of locality and quasilocality will be stated.

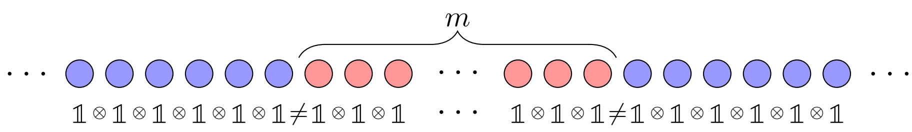

Figure 2.1: Illustration of an operator supported on m sites.

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

$$S^z_{tot} = \sum_{j=1}^{L} S^z_j \tag{2.4}$$

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

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

i.e. the full Hilbert space with $\dim \mathcal{H} = 2^L$ can be decomposed into the direct sum of its proper subspaces $\mathcal{H}_j$ 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 2.3 *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 2.2, 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 [44]. Therefore, the main focus of this work is the investigation of the 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 the full Hilbert space and restricts system sizes that we are able to check.

2.2 (Q)LIOMs finding algorithm

We now introduce a finite time averaging of an operator $A \in \mathcal{V}^M_L$, employing the Heisenberg picture [44]

$$\begin{aligned}
\bar{A}^\tau =& \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, A_H(t) = \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, \mathrm{e}^{iHt} A \mathrm{e}^{-iHt} = \sum_{m,n} \frac{1}{\tau}\int_0^\tau \mathrm{d}t\, \mathrm{e}^{iE_m t}\,|m\rangle\,\langle m|A|n\rangle\,\langle n|\,\mathrm{e}^{-iE_n t} = \\
=& \sum_{m,n} A_{mn}\,|m\rangle\langle n|\,\frac{1}{\tau}\int_0^\tau \mathrm{d}t\,\mathrm{e}^{i(E_m-E_n)t} = \sum_{m,n} A_{mn}\,|m\rangle\langle n|\,\frac{1}{\tau}\frac{1}{i\,(E_m-E_n)}\left(\mathrm{e}^{i(E_m-E_n)\tau}-1\right) \\
=& \sum_{m,n} A_{mn}\,|m\rangle\langle n|\,\mathrm{e}^{i(E_m-E_n)\tau/2} \times \frac{\sin\left((E_m-E_n)\,\tau\right)}{\tau\,(E_m-E_n)}
\end{aligned} \tag{2.5}$$

What this procedure does is essentially a cut-off (cf. Figure 2.2) 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 2.4 (Simplified time averaging)

$$\bar{A}^\tau \equiv \sum_{m,n} \theta\left(\frac{1}{\tau} - |E_m - E_n|\right) A_{mn} |m\rangle\langle n| = \sum_{m,n} \theta^\tau_{mn} A_{mn} |m\rangle\langle n| \tag{2.6}$$

where θ is the Heaviside step function.

Going to the infinite time limit, we obtain the time averaging from Mierzejewski, Prelovšek, and Prosen [29]

$$\bar{A} = \lim_{\tau\to\infty} \bar{A}^\tau = \sum_{\substack{m,n \\ E_m=E_n}} A_{mn} |m\rangle\langle n| \tag{2.7}$$

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. To carry out the time averaging, we need to express the operator in the basis of energy eigenstates and thus we need to perform an exact diagonalization of the Hamiltonian. This is one of the main limiting factors of this procedure. Observing

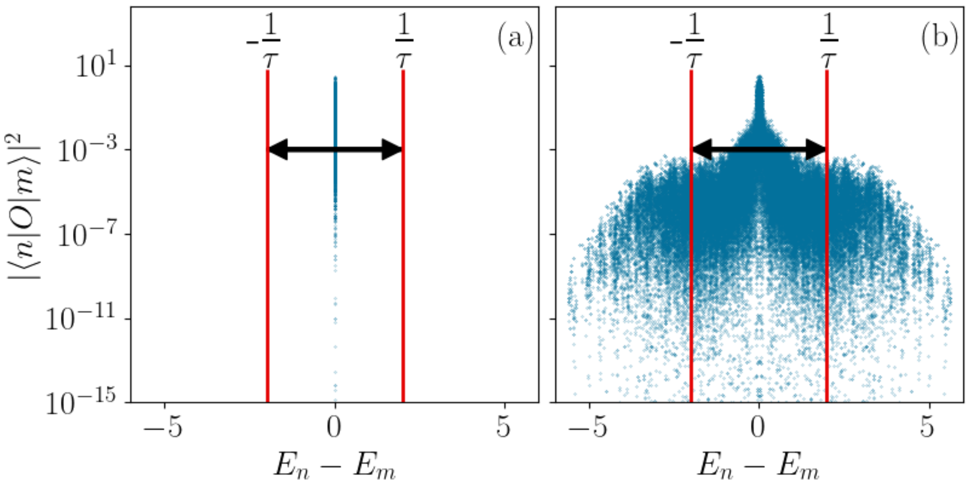

Figure 2.2: Illustration of averaging procedure as defined by equation (2.6) for $\tau = 1/2$. The sum of matrix elements is restricted by the θ function to the region between the two red lines. The operator O shown here is the $\hat{O}_1$ as defined in (2.33). Matrix elements in panel (a) are calculated for integrable XXZ model (1.34) with $\Delta = 1$ and in panel (b) for the perturbed XXZ model (3.1) with $\Delta = 1$ and perturbation strength $\alpha = 0.1$. Broadening of distribution of matrix elements is the reason why we need finite time averaging for investigating nonintegrable systems.

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 time averaging:

Proposition 2.1 *For any $A, B \in \mathcal{V}_L$*

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

Proof.

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

■

These two facts reveal an interesting interpretation of the time averaging, namely, that it can be thought of as an orthogonal projection in the 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 a time-averaged operator with the Hamiltonian

$$\begin{aligned}\left[H,\bar{A}^\tau\right] &= \sum_n\sum_{k,p} E_n\theta^\tau_{kp}A_{kp}[|n\rangle\langle n|\,,|k\rangle\langle p|]\\ &= \sum_{k,p}\left(E_k - E_p\right)\theta^\tau_{kp}A_{kp}\,|k\rangle\langle p| \xrightarrow{\tau\to\infty} 0\end{aligned} \tag{2.8}$$

The last limit follows directly from equation (2.7). 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 to get a local integral of motion, because in general $A \in \mathcal{V}^M_L \nRightarrow \bar{A} \in \mathcal{V}^M_L$, 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 (2.3). If for some M we have $\bar{A} \in \mathcal{V}^M_L$, then it is local. Second possibility is that it can be written as a convergent series of operators from $\mathcal{V}^m_L$ with increasing m — then it is quasilocal. Otherwise, it is a generic nonlocal quantity. But can we do better than this direct approach?

We begin our journey towards the answer to this question by fixing $0 \le M \le L/2$ and constructing a basis $\{O_s\}$ of $\mathcal{V}^M_L$. How to actually perform such construction will be shown in Section 2.4. Next, we find the time averages of all basis operators and build a matrix

$$K^\tau_{st} = \left(\bar{O_s}^\tau\middle|\bar{O_t}^\tau\right) \tag{2.9}$$

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. The spectral theorem then guarantees the 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

$$\sum_{s,t} U_{ns}K^\tau_{st}U^T_{tm} = \delta_{nm}\lambda_n \in \mathbb{R}, \quad \lambda_n \text{ — eigenvalue of } K^\tau \tag{2.10}$$

$$UU^T = U^TU = \mathbb{1} \implies \sum_s U_{ns}U^T_{sm} = \delta_{mn} \tag{2.11}$$

$$UK^\tau = DU \implies \sum_s U_{ns}K^\tau_{st} = \sum_s \delta_{ns}\lambda_s U_{st} = \lambda_n U_{nt} \tag{2.12}$$

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 $(0,\tau)$

$$Q_n = \sum_s U_{ns}\bar{O}^\tau_s \tag{2.13}$$

Proposition 2.2 *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 (2.13). 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 (2.12) and (2.11) respectively. We can learn something more about the eigenvalues of K^τ matrix from a simple corollary to Proposition 2.2.

Corollary 2.1 *K^τ is a positive semidefinite matrix.*

Proof. Let Q_n be defined as in (2.13). Then, from the defining properties of the 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 semidefinite matrix. ■

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

Let us now examine the support of Q_n. Making use of the basis definition (2.3), Proposition 2.1, and properties (2.10), (2.11),(2.12), we can decompose it into a part supported on up to M sites and a nonlocal part

$$\begin{aligned}Q_n &= \sum_s (O_s|Q_n)\,O_s + Q_s^\perp = \sum_{s,t} U_{nt}\left(O_s\middle|\bar{O}_t^\tau\right)O_s + Q_n^\perp\\ &= \sum_{s,t} U_{nt}\left(\bar{O}_s^\tau\middle|\bar{O}_t^\tau\right)O_s + Q_n^\perp = \sum_{s,t} U_{nt}K_{ts}O_s + Q_n^\perp\\ &= \sum_s\left(\sum_t U_{nt}K^\tau_{ts}\right)O_s + Q_n^\perp = \sum_s \lambda_n U_{ns}O_s + Q_n^\perp = Q_n^M + Q_n^\perp \end{aligned}\tag{2.14}$$

Now we are ready to derive the central result, stating why this actually algorithm works. Combining the fact that $(Q_n|Q_n) = \lambda_n$ (see proof of Proposition 2.2) with (2.14) we obtain

$$\begin{aligned}\lambda_n = (Q_n|Q_n) &= \left(Q_n^M + Q_n^\perp\middle|Q_n^M + Q_n^\perp\right) = \left(Q_n^M\middle|Q_n^M\right) + \left(Q_n^\perp\middle|Q_n^\perp\right) + \underbrace{2\left(Q_n^M\middle|Q_n^\perp\right)}_{=0\text{ (cf. (2.3))}}\\ &= \left(\sum_s \lambda_n U_{ns}O_s\middle|\sum_t \lambda_n U_{nt}O_t\right) + \left\|Q_n^\perp\right\|^2 = \lambda_n^2\sum_{s,t} U_{ns}\,(O_s|O_t)\,U^T_{tn} + \left\|Q_n^\perp\right\|^2\\ &= \lambda_n^2 + \left\|Q_n^\perp\right\|^2\end{aligned}\tag{2.15}$$

Rearranging the above equality, we get that $\lambda_n - \lambda_n^2 = \left\|Q_n^\perp\right\|^2 \geq 0$, which together with Corollary 2.1 gives $\lambda_n \in [0,1]$.

From now on, we shall restrict our considerations to the case $\tau \to \infty$, as it guarantees that $\bar{O}_s$ and hence Q_n commutes with the Hamiltonian. Consequently, we finally arrive at a classification scheme for the support of Q_n.

Definition 2.5 (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 assess 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 examine both the $L \to \infty$ case and, depending on operator, either $L = 14$ or $L = 16$ case, because these are the 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 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. (2.8)). However, the time averaging procedure expands the support of initially local basis operators O_s. In actual computation we are using the basis of operators supported on up to M sites at all times, therefore the operator obtained from the eigenvectors of K matrix is the Q_n^M operator. If $\lambda_n = 1$, then $\|Q_n^{\perp}\| = 0 \implies Q_n^{\perp} = 0$ and $Q_n = Q_n^M$. Hence, Q_n^M operator, which structure we know, is strictly conserved. On the other hand, if $\lambda_n \in (0,1)$, then $\|Q_n^{\perp}\| > 0 \implies Q_n^{\perp} \neq 0$ 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 the 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 concrete definition of quasilocality [1] [49]

Definition 2.6 (Quasilocality) *A conserved operator $Q \in \mathcal{V}_L$ is called quasilocal, if for some $M \in \mathbb{N}$ there exist a local operator $A \in \mathcal{V}_L^M$, such that*

$$\lim_{L\to\infty} \frac{(Q|A)}{(Q|Q)} > 0$$

i.e. Q has finite overlap with A in thermodynamic limit.

If $\|Q_n^{\perp}\| > 0$, and $\lim_{L\to\infty} \lambda_n \neq 0$, then the Q_n^M operator obtained from the algorithm is precisely the local operator from definition 2.6. We will end the discussion about the algorithm with a short summary on support of Q_n:

$$\begin{aligned} &Q_n = Q_n^M + Q_n^{\perp} \\ &\|Q_n\|^2 = \lambda_n \\ &\|Q_n^M\|^2 = \lambda_n^2 \\ &\|Q_n^{\perp}\|^2 = \lambda_n - \lambda_n^2 \end{aligned} \tag{2.16}$$

[1] Some authors refer to this condition as *pseudolocality*, while reserving the name *quasilocality* for a stronger condition. For details see Ilievski et al. [48].

Proof of correctness 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 $\boldsymbol{u} \in \mathbb{R}^{\dim \mathcal{V}_L^M}$. Using this picture, the stiffness of A can be calculated as follows

$$\left(\bar{A}\middle|\bar{A}\right) = \sum_{s,t} u_s \left(\bar{O}_s\middle|\bar{O}_t\right) u_t = \sum_{s,t} u_s K_{st} u_t = \boldsymbol{u}^T K \boldsymbol{u} \tag{2.17}$$

Thus, the problem in quantum mechanics is reduced to the problem in linear algebra. Because all eigenvalues of K matrix are real, we can sort the corresponding operators (defined by 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, i.e. it has larger projection on a local basis. 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 2.3 *Let λ be the maximal eigenvalue of K. Then the following equality holds*

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

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

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

Obtained contradiction concludes the proof. ■

2.3 Spectral functions and Mazur bound

Spectral functions 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 follow the discussion in Vidmar et al. [32] and introduce the concept of spectral function.

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 shall investigate the Fourier transform of the autocorrelation function, formally defined as

Definition 2.7 (Spectral function)

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

The limit in the definition is present 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

$$I(\omega) = \int_{-\omega}^{\omega} \mathrm{d}\omega' \; S(\omega') = \frac{1}{\mathcal{D}} \sum_{m,n} \theta\left(\omega - |E_m - E_n|\right) A_{mn}^2 \tag{2.18}$$

For the derivation of equation (2.18) see Appendix B. 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 these two important limits

$$\lim_{\omega\to\infty} I(\omega) = \frac{1}{\mathcal{D}} \sum_{m,n} A_{mn}^2 = \|A\|^2 = 1 \tag{2.19}$$

$$\lim_{\omega\to 0^+} I(\omega) = \frac{1}{\mathcal{D}} \sum_{\substack{m,n \\ E_m = E_n}} A_{mn}^2 = \|\bar{A}\|^2 \tag{2.20}$$

For frequencies small (long times) in comparison with the system's characteristic energy scale, spectral function of an observable $A \in \mathcal{V}_L^M$ can be approximated as follows

$$S(\omega \ll J) \simeq D_A \delta(\omega) \tag{2.21}$$

where $D_A = \lim_{\omega\to 0^+} I(\omega) = \left(\bar{A}\middle|\bar{A}\right)$ is the stiffness of A. 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 [30] and Suzuki [31] that the stiffness D_A of arbitrary observable A has its origin in the projections on these Q_n

$$D_A = \sum_n D_n = \sum_n \frac{(A|Q_n)^2}{(Q_n|Q_n)} \tag{2.22}$$

Therefore, by calculating the overlap between our observable and all (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 [50]. Because autocorrelation function of LIOMs is constant, its Fourier transform is a Dirac delta, which explains the form of equation (2.21).

Mazur bound If we know only a subset of the full set of (Q)LIOMs, equality (2.22) 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. [48].

Proposition 2.4 (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*

$$D_A = \left(\bar{A}\middle|\bar{A}\right) \geq \frac{(A|Q)^2}{(Q|Q)} > 0$$

Proof. We define a new observable $\mathcal{A} = \bar{A} - \alpha Q$ for $\alpha \in \mathbb{R}$. Clearly, 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 $\left(\bar{A}\middle|\bar{B}\right) = \left(\bar{A}\middle|B\right) = \left(A\middle|\bar{B}\right)$(cf. Proposition 2.1) and $\bar{Q} = Q$ for a conserved quantity. Let us now substitute $\alpha = \frac{(A|Q)}{(Q|Q)}$ to the above inequality.

$$D_A = \left(\bar{A}\middle|\bar{A}\right) \geq 2\frac{(A|Q)}{(Q|Q)}(A|Q) - \frac{(A|Q)^2}{(Q|Q)^2}(Q|Q) = \frac{(A|Q)^2}{(Q|Q)} > 0$$

The last equality follows from Definition 2.6 and (quasi)locality of 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-Schwartz inequality, found in any linear algebra textbook. By following exactly the same procedure, we can easily generalize this result to a set of orthogonal conserved quantities $\{Q_n\}$

$$D_A = \left(\bar{A}\middle|\bar{A}\right) \geq \sum_n \frac{(A|Q_n)^2}{(Q_n|Q_n)} \tag{2.23}$$

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 [29], where the algorithm described in details in Section 2.2 was first proposed. We shall now show that the following proposition holds [44]

Proposition 2.5 (Saturation of Mazur bound) *The set $\{Q_n\}$ of (Q)LIOMs obtained from the algorithm in Section 2.2 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 (2.13), 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

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

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

We finish this section with an example of an application of Mazur bound.

Example 2.2 *Consider the topic of ballistic linear response [48]. 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 [51]*

$$\sigma'(\omega) = 2\pi D_J \delta(\omega) + \sigma_J^{reg}(\omega) \tag{2.24}$$

If there exists a (quasi)local conserved quantity Q such that $(J|Q) > 0$, the Mazur bound implies that $D_J > 0$. Such a nonzero value of spin current stiffness is an indicator of ballistic DC transport (i.e. without scattering, cf. Figure 2.3) — $\sigma'(0)$ diverges.

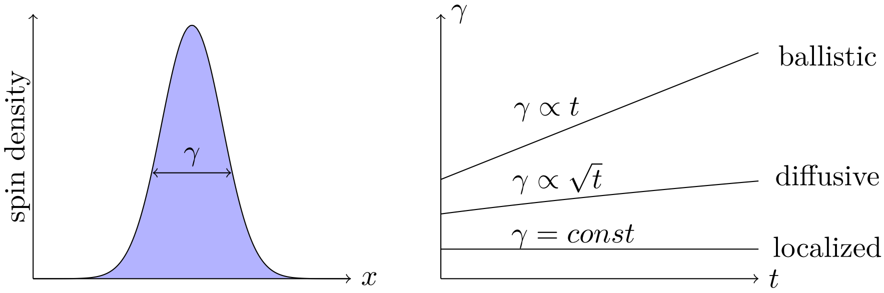

Figure 2.3: Illustration of different types of transport. On the left panel, we have some initial spin density characterized by width γ. On the right panel, we have the dependence of γ on time in three different cases.

2.4 (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 1.3. The subsequent considerations are based on the work of Mierzejewski, Prelovšek, and Prosen [29].

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

$$O_{\underline{s},j} = \sigma_j^{s_1}\sigma_{j+1}^{s_2}\cdots\sigma_{j+m-1}^{s_m} \tag{2.25}$$

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 the first and the last operator in a sequence we have $s_{1,m} \in \{+,-,z\}$, because the identity there would correspond to an $(m-1)$-local operator. The index j indicates the first site of support. As a matter of mathematical precision, the notation for $O_{\underline{s},j}$ used here (and frequently in the physics literature) is a bit of simplification. It is important to remember that because of embedding (1.26), there are tensor products between σ_j, i.e. we have the following

$$O_{\underline{s},j} = \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{j-1} \otimes\, \sigma_j^{s_1} \otimes \sigma_{j+1}^{s_2} \otimes \cdots \otimes \sigma_{j+m-1}^{s_m} \otimes \underbrace{\mathbb{1}_{2\times 2} \otimes \cdots \otimes \mathbb{1}_{2\times 2}}_{L-j-m+1} \tag{2.26}$$

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 D 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 see 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': $\sigma^+, \sigma^-, \sigma^z, \mathbb{1}_{2\times 2}$).

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 the symmetries of the system in question, the XXZ model. They allow us to decompose the matrix K (cf. (2.9)) and usually reduce the computational effort. First and perhaps the most important one is implied by the fact already discussed in Section 2.1 — conservation of magnetization. We could restrict our considerations to a subspaces of $\mathcal{V}_L^M$ comprised of operators such that $[S^z_{tot}, O_{\underline{s}}] = 0$. Yet, we will not be able to use 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.

2.4.1 Commuting LIOM: Spin energy current

In order to test our (Q)LIOM finding algorithm and the correctness of its implementation, we first investigate the known case of energy current in Spin$-1/2$ XXZ model [44] and see whether it is detected or not. For the sake of completeness, derivation of spin energy current for the general XYZ model is be presented, following the definitions in Zotos, Naef, and Prelovsek [50]. We start with the general XYZ Hamiltonian with periodic boundary conditions (1.28). It is easy to see that this Hamiltonian can be represented as a sum of operators supported on two consecutive sites

$$H_{XYZ} = \sum_{k=1}^{L} h_{k,k+1} \tag{2.27}$$

where $h_{k,k+1} = J_x S^x_k S^x_{k+1} + J_y S^y_k S^y_{k+1} + J_z S^z_k S^z_{k+1}$ 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

$$\frac{\mathrm{d}h_{k,k+1}(t)}{\mathrm{d}t} + \boldsymbol{\nabla} \cdot j^E_k(t) = 0 \tag{2.28}$$

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

$$\frac{\mathrm{d}h_{k,k+1}(t)}{\mathrm{d}t} = i[H_{XYZ}, h_{k,k+1}(t)] \tag{2.29}$$

Combining equations (2.28) and (2.29) we obtain the defining equations for the spin energy current density

$$j^E_{k+1} - j^E_k = -i[H_{XYZ}, h_{k,k+1}] = i[h_{k,k+1}, H_{XYZ}] = i\sum_{r=1}^{L} [h_{k,k+1}, h_{r,r+1}] \tag{2.30}$$

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 (2.30) is shown in Appendix C. For the XXZ model, we get the following expression

$$\begin{aligned} j^E_k &= i\Bigg(\underbrace{\frac{J^2}{2} S^-_{k-1} S^z_k S^+_{k+1} + \frac{J^2\Delta}{2} S^z_{k-1} S^+_k S^-_{k+1} + \frac{J^2\Delta}{2} S^+_{k-1} S^-_k S^z_{k+1}}_{O_k} \\ &\quad - \underbrace{\left(\frac{J^2}{2} S^+_{k-1} S^z_k S^-_{k+1} + \frac{J^2\Delta}{2} S^z_{k-1} S^-_k S^+_{k+1} + \frac{J^2\Delta}{2} S^-_{k-1} S^+_k S^z_{k+1}\right)}_{O^\dagger_k}\Bigg) \\ &= i\left(O_k - O^\dagger_k\right) \end{aligned}$$

Thus we see that it is an imaginary operator. Moreover, it is also a commuting operator because it consists of a sum of equal number of S^+ and S^-. Obtaining the extensive energy current operator is now simply the matter of summing over all lattice sites

$$J^E = \sum_{k=1}^{L} j^E_k \tag{2.31}$$

As the energy current commutes with the Hamiltonian [50], 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

$$J^E = \sum_{k=1}^{L} i\left[\beta_1\left(S^-_{k-1} S^z_k S^+_{k+1}\right) + \beta_2\left(S^z_{k-1} S^+_k S^-_{k+1} + S^+_{k-1} S^-_k S^z_{k+1}\right)\right] + \text{H.c.} \tag{2.32}$$

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 2.4). Thus, according to Definition 2.5, it is a local integral of motion.

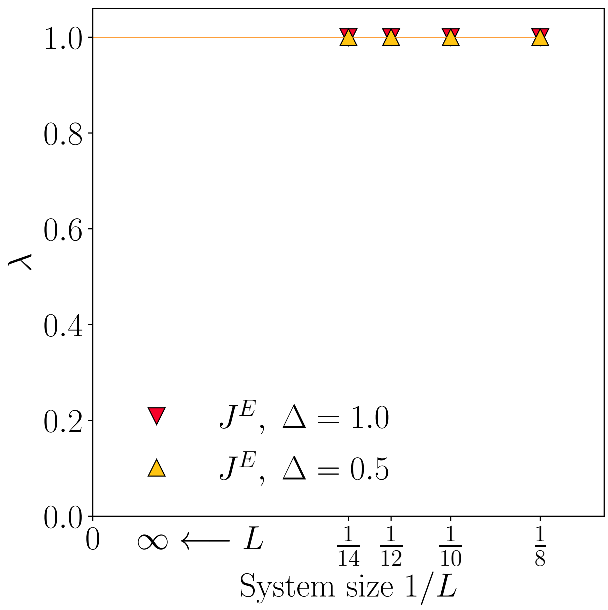

Figure 2.4: Eigenvalues of generalized stiffness matrix corresponding to the energy current operator as a function of inverse system size. Solid line is the extrapolation to thermodynamic limit. Calculations performed for $\Delta = 1.0$ and $\Delta = 0.5$.

2.4.2 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 an unrestricted search for $L \in \{8, 9, 10, 11, 12\}$. Nevertheless, the 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 $\hat{O}_2$ (2.34)). Therefore, we restricted our further considerations to such operators only. This allowed us to quite easily obtain numerical results for L up to 14. After quite lengthy calculations, we were also able to obtain some results for $L = 16$. We will focus on two concrete cases of operators, corresponding to largest eigenvalues of the 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 spectrum exhibits massive degeneracies, because eigenstates with different S^z_{tot} correspond to the same energies [52, 53].

For the case of $\Delta = 1.0$, the XXZ model reduces to the isotropic Heisenberg model (1.27) possessing $SU(2)$ symmetry. As a consequence of this symmetry, the conservation of total magnetization (S^z_{tot} operator (2.4)) implies the conservation of analogously defined S^x_{tot} and S^y_{tot} and therefore the following quantity

$$\hat{O}_1 = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} S_j^+ + \text{H.c.} \tag{2.33}$$

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 an analogously defined imaginary operator, we would obtain the S^y_{tot}, but due to

$SU(2)$ symmetry results would be the same.

The case of $\Delta = 0.5$ is much more difficult. It was shown by Zadnik, Medenjak, and Prosen [54] 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 exists a 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 $UH_{XXZ}(\Delta)U = -H_{XXZ}(-\Delta)$. It follows then, that if Q is a conserved quantity for Δ, then $\tilde{Q} = UQU$ is a conserved quantity for $-\Delta$. This is the reason we present numerical results only for even values of L. For $\Delta = 0.5$ the action of this operator produces a simple factor of $(-1)^i$ and the operator of interest reads

$$\hat{O}_2 = \frac{1}{\sqrt{L}} \sum_{j=1}^{L} (-1)^j \left(S_j^+ S_{j+1}^+ S_{j+2}^+\right) + \text{H.c.} \tag{2.34}$$

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 [48, 54, 55].

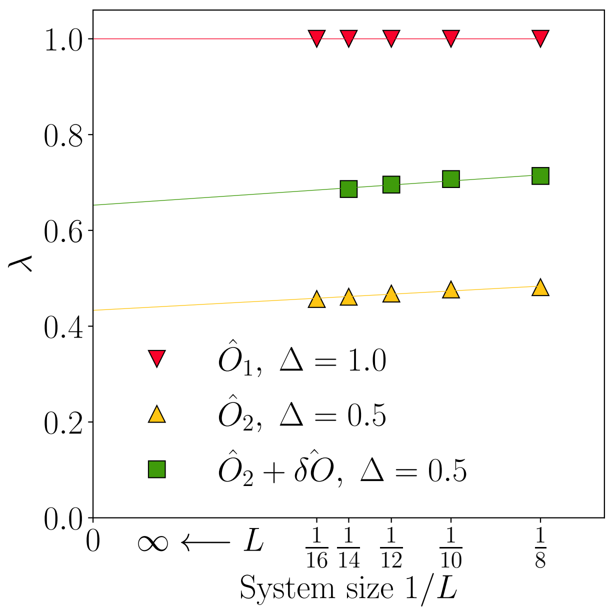

Figure 2.5: Eigenvalues of generalized stiffness matrix corresponding to the two noncommuting integrals of motion, as a function of inverse system size. Solid lines represent the extrapolation to the thermodynamic limit. Note that the operator $\hat{O}_2$ exhibits quasilocality and its stiffness in the thermodynamic limit is $\lambda_{L\to\infty} \approx 0.43$. Stiffness of $\hat{O}_2 + \delta\hat{O}$ in thermodynamic limit is $\lambda_{L\to\infty} \approx 0.65$

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 2.5. Comparing it with Definition 2.5 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. Looking at Figure 2.5 we see that stiffness of this new projection is larger than that of the old one. However, contribution of $\delta\hat{O}$ to the overall stiffness is smaller than that of $\hat{O}_2$.

3

Relaxation of integrals of motions in weakly perturbed XXZ model

Thus far, we have focused on investigating properties of an *integrable* XXZ spin-1/2 chain. However, as mentioned in the introductory chapter, integrability is a rather rare occurrence. Therefore, this chapter is devoted to the study of (Q)LIOMs in the near-integrable XXZ model. For noncommuting integrals of motion, we identify two mechanisms that are at play during the decay of those observables, namely, the integrability breaking itself and the lifting of macroscopic degeneracy after shifting away from high symmetry values of anisotropy parameter Δ. Disentanglement of those two processes allows us to explain the origin of anomalous scaling of relaxation times.

Methodology in this chapter follows the work of Mierzejewski et al. [44], however the results about relaxation of noncommuting integrals of motion are original and at the moment of writing this thesis published as a preprint [56].

3.1 Adding perturbation to the Hamiltonian

We are now going to weakly break the integrability of XXZ model (1.34) by adding a perturbation in the form of next-nearest neighbor interaction. New Hamiltonian has the following form

$$H_{XXZ} = \frac{1}{2}\sum_{j=1}^{L}\left(S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+\right) + \Delta\sum_{j=1}^{L} S_j^z S_{j+1}^z + \alpha H' \tag{3.1}$$

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

$$H' = \sum_{j=1}^{L} S_j^z S_{j+2}^z \tag{3.2}$$

In such a 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 (cf. Figure 2.2). We are interested in investigating this decay and the timescales involved. To this end, we take the previously discussed (Q)LIOMs $J^E, \hat{O}_1, \hat{O}_2$

and examine their behavior under finite-time averaging (as defined in (2.6)) generated by the perturbed Hamiltonian. As an initial check, 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 the inverse system size. To relate this to the discussion of spectral functions in Section 2.3, from now on we use the cutoff frequency $\omega = \frac{1}{\tau}$, instead of the time of averaging τ. The perturbation should be strong enough, so that after taking the thermodynamic limit of the $\omega \to 0^+$ limit, stiffness vanishes. Results are shown in Figure 3.1. We see first hints that the behavior under perturbation for commuting and noncommuting operators differ. For perturbation strength $\alpha = 0.2$, the energy current stiffness does not decay in thermodynamic limit for $\omega \to 0^+$ and thus a stronger perturbation is needed. However, the stiffness of operators $\hat{O}_1, \hat{O}_2$ vanish even for finite size systems and smaller perturbations.

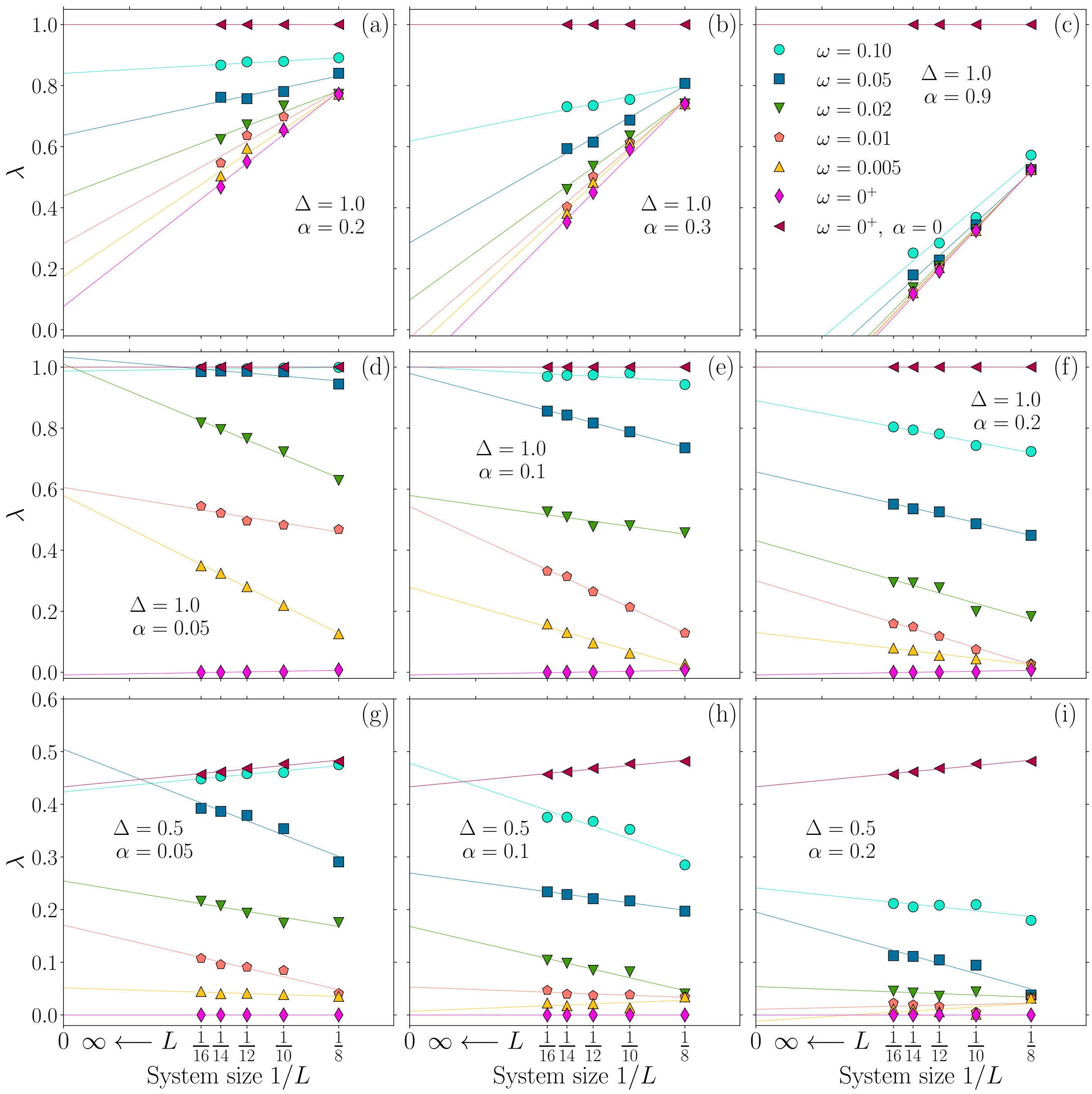

Figure 3.1: Finite-time stiffness operators as a function of time for the perturbed Hamiltonian. Panels (a)-(c) show results for J^E, (d)-(f) for $\hat{O}_1$ and (g)-(i) for $\hat{O}_2$. See text for detailed description.

3.2 Relaxation of known (Q)LIOMs

To investigate how our (Q)LIOMs decay with time, we apply the formalism of spectral functions described in Sections 2.3. Since we are interested in the low-ω (long times) part of the integrated spectral function $I(\omega)$, it is convenient to normalize it. Therefore, let us define the following [44]

$$R_{\hat{A}}(\omega,\alpha) = \frac{I(\omega,\alpha)}{\lim_{\omega\to 0^+} I(\omega,\alpha=0)} = \frac{\sum_{n,m}\theta\left(\omega - |E_n - E_m|\right)|\langle m|\hat{A}|n\rangle|^2}{\sum_{\substack{n,m\\E_n=E_m}} |\langle m|\hat{A}|n\rangle|^2} \tag{3.3}$$

This normalization of $I(\omega)$ assures that $\lim_{\omega\to\infty} R_{\hat{A}}(\omega,\alpha) = 1$. 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. As mentioned in previous section, we are looking for a vanishing of infinite-time stiffness in thermodynamic limit. Therefore, we shall take α as small as possible so that $\lim_{\omega\to 0^+} R_{\hat{A}}(\omega,\alpha) = 0$.

3.2.1 Relaxation of energy current

We begin with the case energy current J^E for $\Delta = 1.0$, as derived in Section 2.4.1. 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 the integrable regime, the autocorrelation function starts to decay,

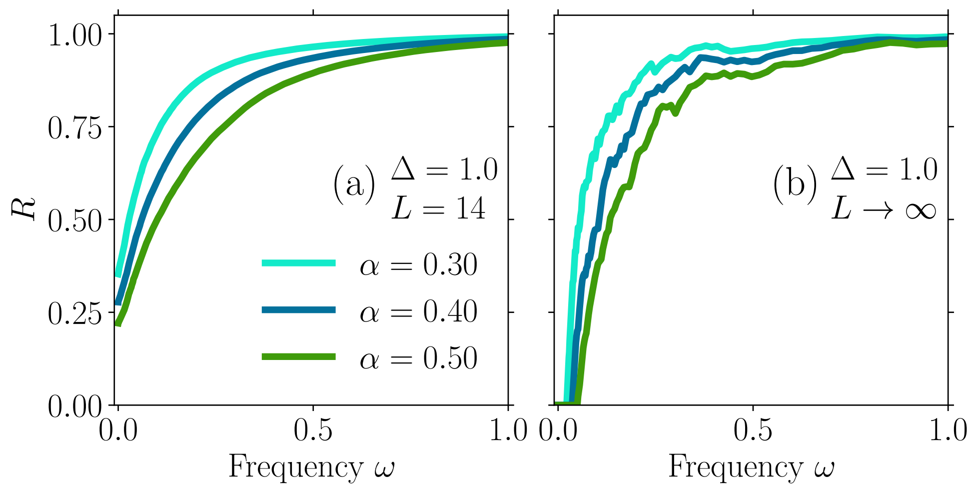

Figure 3.2: Normalized integrated spectral function as a function of cutoff frequency for J^E. (a) Results for $L = 14$. Low frequency limit does not approach 0 because of finite size effects. (b) Results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$. Note the expected observation, namely stronger perturbation leads to faster decay.

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 look simultaneously at two different situations, results for $L = 14$ and results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$. Figure 3.2 shows $R_{J^E}(\alpha,\omega)$ as a function of ω for $\alpha = 0.3, 0.4, 0.5$. We immediately see the expected outcome, as the stronger the perturbation, the faster the current decays. The fact that for finite L, $R_{J^E}(\alpha,\omega)$ does not

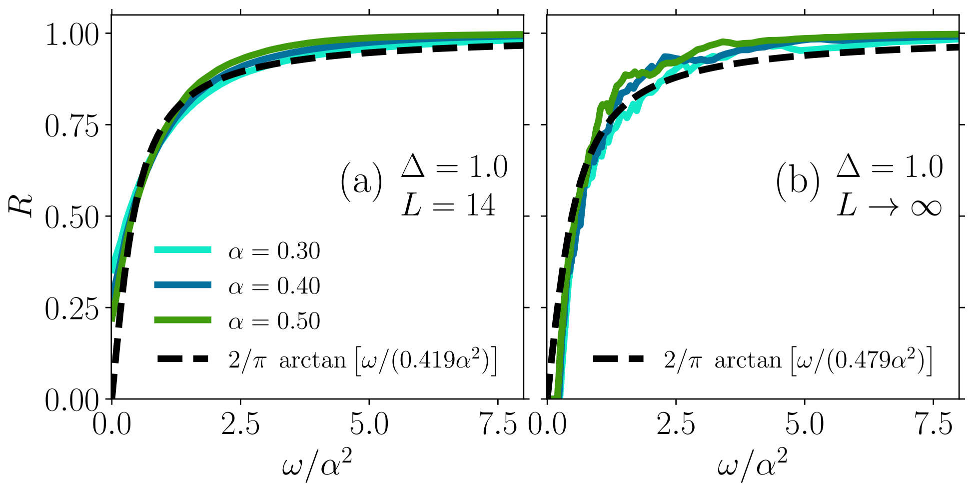

Figure 3.3: Normalized integrated spectral function as a function of rescaled cutoff frequency ω/α^2 for J^E. (a) Results for $L = 14$. (b) Results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$. Dashed black line corresponds to fit (3.5).

approach 0 in $\omega \to 0^+$ limit is consistent with results in Figure 3.1. However, an interesting thing happens when plotting the same data, but as a function of rescaled frequency ω/α^2. Numerical results visible on Figure 3.3 show a convincing collapse of the curves for different values of perturbation strength. This may suggest an universal dependence of $R(\omega, \alpha)$ on ω and α

$$R(\omega, \alpha) \simeq \tilde{R}(\omega/\alpha^2) \tag{3.4}$$

Moreover, this relation can be reasonably well approximation by a one parameter fit (black dashed line in Figure 3.3)

$$\tilde{R}(\omega/\alpha^2) \simeq \frac{2}{\pi} \arctan\left(\frac{\omega}{\gamma\alpha^2}\right) \tag{3.5}$$

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 $\left(J^E(t)\middle|J^E\right) \propto \mathrm{e}^{-|t|/\tau_j}$. Double-sided exponential has well defined Fourier transform, so we can drop the $\varepsilon \to 0^+$ limit from the integral

$$\begin{aligned} S(\omega) &\propto \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{-|t|/\tau_j}\mathrm{e}^{i\omega t} = \frac{1}{2\pi}\left[\int_{-\infty}^{0} \mathrm{d}t\ \mathrm{e}^{(1/\tau_j+i\omega)t} + \int_{0}^{\infty} \mathrm{d}t\ \mathrm{e}^{(-1/\tau_j+i\omega)t}\right] \\ &= \frac{1}{2\pi}\left[\frac{\tau_j}{1+i\omega\tau_j} + \frac{\tau_j}{1-i\omega\tau_j}\right] = \frac{1}{\pi}\frac{\tau_j}{1+\omega^2\tau_j^2} \end{aligned} \tag{3.6}$$

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

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

which after normalization yields the desired results (3.5). Furthermore, we learn that the characteristic relaxation time $\frac{1}{\tau_j} \propto \alpha^2$ and the proportionality constant is universal and does not depend on α. The quadratic scaling shown on Figure 3.3 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 3.4). However, it is expected to be a consequence of working with rather small system sizes, because it was shown in Mierzejewski et al. [44] using memory function formalism, that quadratic scaling is indeed the appropriate one.

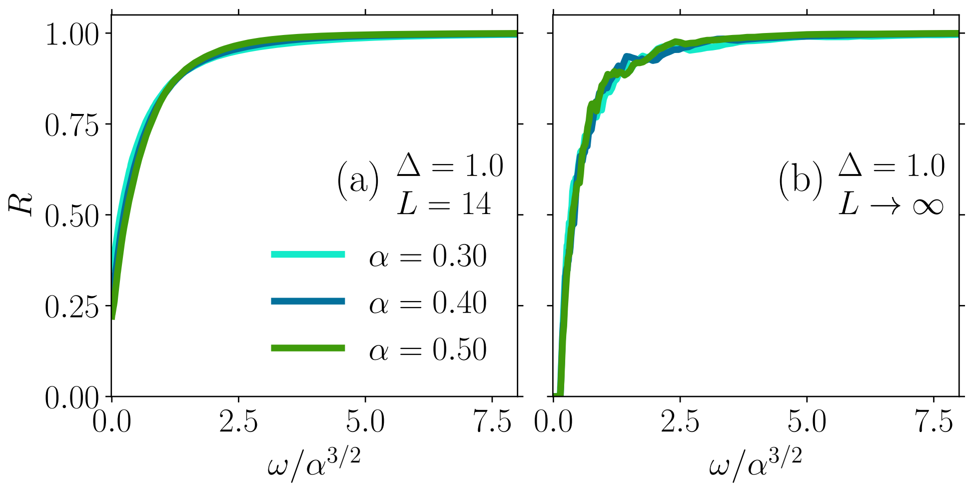

Figure 3.4: Normalized integrated spectral function as a function of rescaled cutoff frequency for J^E. The rescaling coefficient is chosen so as to obtain the best possible collapse of curves. (a) Results for $L = 14$. (b) Results extrapolated to thermodynamic limit from $L = 11, 12, 13, 14$.

3.2.2 Relaxation of noncommuting (Q)LIOMs

Let us now proceed with the same analysis, but for the $\hat{O}_1$ (2.33) and $\hat{O}_2$ (2.34) operators. Once again we shall look at the largest system size available to us, that is $L = 16$, as well as the case of extrapolation to thermodynamic limit from $L = 10, 12, 14, 16$. Figure 3.5 shows $R_\mu(\omega, \alpha)$, where $\mu = \hat{O}_1, \hat{O}_2$, as a function of ω for $\alpha = 0.05, 0.1, 0.2$. We have used weaker perturbations here, because Figure 3.1 suggested that it is enough to achieve the vanishing stiffness in thermodynamic limit. Indeed, this is the case and we observe that $\lim_{\omega\to 0^+} R_\mu(\omega, \alpha) = 0$ even for finite-size systems. Based on the discussion of energy current decay, the next logical step would be to rescale the frequency by α^2. In contrast to the energy current, we do not see any collapse (see Figure 3.6). Therefore, noncommuting operators do not follow the same universal scaling (3.4) as the energy current. However, as shown in Figure 3.7, it turns out that a reasonable collapse, working for both $\hat{O}_1$ and $\hat{O}_2$, may be observed for different scaling, namely ω/α. This suggests another kind of relation

$$R_\mu(\omega, \alpha) \simeq \tilde{R}_\mu(\omega/\alpha) \tag{3.7}$$

Moreover, the collapsed curves can be accurately fitted with an one-parameter error function (black dashed line in Figure 3.7)

$$\tilde{R}_\mu(\omega/\alpha) \simeq \operatorname{erf}\left(\frac{\omega}{\gamma\alpha}\right) \tag{3.8}$$

where the fitting parameter is denoted with γ and error function is defined as

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \mathrm{d}t\, \mathrm{e}^{-t^2} \tag{3.9}$$

This implies a Gaussian, instead of exponential, decay of the autocorrelation function, i.e. $\left(\hat{O}_\mu(t)\middle|\hat{O}_\mu\right) \propto \exp(-(t/\tau_\mu)^2)$. We can once again use the integrated spectral function to see that this is correct.

$$
\begin{aligned}
S(\omega) &\propto \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{-(t/\tau_\mu)^2}\mathrm{e}^{i\omega t} = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}t\ \exp\left(-\frac{1}{\tau_\mu^2}\left(t-\frac{i\omega\tau_\mu}{2}\right)^2 - \frac{\omega^2\tau_\mu^2}{4}\right) \\
&= \exp\left(-\frac{\omega^2\tau_\mu^2}{4}\right)\frac{1}{2\pi}\int_{-\infty+\frac{i\omega\tau_\mu}{2}}^{\infty+\frac{i\omega\tau_\mu}{2}} \mathrm{d}z\ \exp\left(-\frac{z^2}{\tau_\mu^2}\right) \\
&\triangleq \exp\left(-\frac{\omega^2\tau_\mu^2}{4}\right)\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}z\ \exp\left(-\frac{z^2}{\tau_\mu^2}\right) \\
&= \frac{\tau_\mu}{2\sqrt{\pi}}\mathrm{e}^{-(\omega\tau_\mu/2)^2}
\end{aligned} \tag{3.10}
$$

where between the first and second line a change of variables $z = t - \frac{i\omega\tau_\mu}{2}$ has been made, and the equality marked with $\triangleq$ can be justified by means of contour integration [57]. Now we can easily perform the integration over a finite frequency window

$$
\begin{aligned}
I(\omega) &\propto \frac{\tau_\mu}{2\sqrt{\pi}}\int_{-\omega}^{\omega} \mathrm{d}\omega'\ \mathrm{e}^{-(\omega/\tau_\mu)^2} = \frac{\tau_\mu}{2\sqrt{\pi}}\left[\int_{-\omega}^{0} \mathrm{d}\omega' \mathrm{e}^{-(\omega\tau_\mu/2)^2} + \int_{0}^{\omega} \mathrm{d}\omega' \mathrm{e}^{-(\omega\tau_\mu/2)^2}\right] \\
&= \frac{\tau_\mu}{2\sqrt{\pi}}\left[\frac{2}{\tau_\mu}\int_{-\frac{\omega\tau_\mu}{2}}^{0} \mathrm{d}x\ \mathrm{e}^{-x^2} + \frac{2}{\tau_\mu}\int_{0}^{\frac{\omega\tau_\mu}{2}} \mathrm{d}x\ \mathrm{e}^{-x^2}\right] \\
&= \frac{1}{\sqrt{\pi}}\left[\frac{\sqrt{\pi}}{2}\operatorname{erf}\left(\frac{\omega\tau_\mu}{2}\right) + \frac{\sqrt{\pi}}{2}\operatorname{erf}\left(\frac{\omega\tau_\mu}{2}\right)\right] \\
&= \operatorname{erf}\left(\frac{\omega\tau_\mu}{2}\right)
\end{aligned} \tag{3.11}
$$

where between the first and second lines a change of variables $x = \omega\tau_\mu/2$ has been made. We have thus obtained the desired result (3.8). On the contrary to the case of energy current, the scaling of decay rate is $\frac{1}{\tau_\mu} \propto \alpha$. This Gaussian relaxation of noncommuting integrals of motion under weak perturbation is the main finding of this work. One may ask a question about the origin of this anomalous scaling of characteristic time τ. As noted in Subsection 2.4.2, operators exhibiting such scaling are closely related to the massive degeneracies in the energy spectrum of H_{XXZ} for anisotropy $\Delta = 1.0$ and $\Delta = 0.5$, which is caused by states with different total magnetization S^z_{tot} but equal energies. This in turn, is caused by certain symmetries of the Hamiltonian, simple $SU(2)$ for the former case and much more complex $U_q(\mathfrak{sl}_2)$ for the latter case [1]. When adding perturbation (3.2), there are actually two mechanisms at play. We break integrability while simultaneously breaking symmetry and thus lifting the macroscopic degeneracy. We can disentangle these two mechanisms by studying behavior of $\hat{O}_1$ and $\hat{O}_2$ under a different perturbation, namely

$$
H'' = \delta\sum_{j=1}^{L} S^z_j S^z_{j+1} \tag{3.12}
$$

This is equivalent to the unperturbed Hamiltonian for $\Delta' = \Delta + \delta$, and allows us to eliminate degeneracy while preserving integrability. Results of this procedure are shown in Figure 3.8. We see almost the same behavior as for system with weakly broken integrability, i.e. the relaxation is Gaussian in nature with the characteristic decay rate inversely proportional to δ. It is not the lack of integrability but a lack of symmetry-related degeneracy, occurring for either $\alpha \neq 0$ or $\delta \neq 0$,

[1] Technically, this symmetry is present only for $\Delta = -0.5$, but this can be amended in thermodynamic limit for chains of even length, as discussed in Section 2.4.2.

that leads to this anomalous scaling. Lifting of this degeneracy happens already in first-order perturbation theory $|E_n - E_m| \propto \alpha, \delta$ hence the linear scaling in perturbation strength [53].

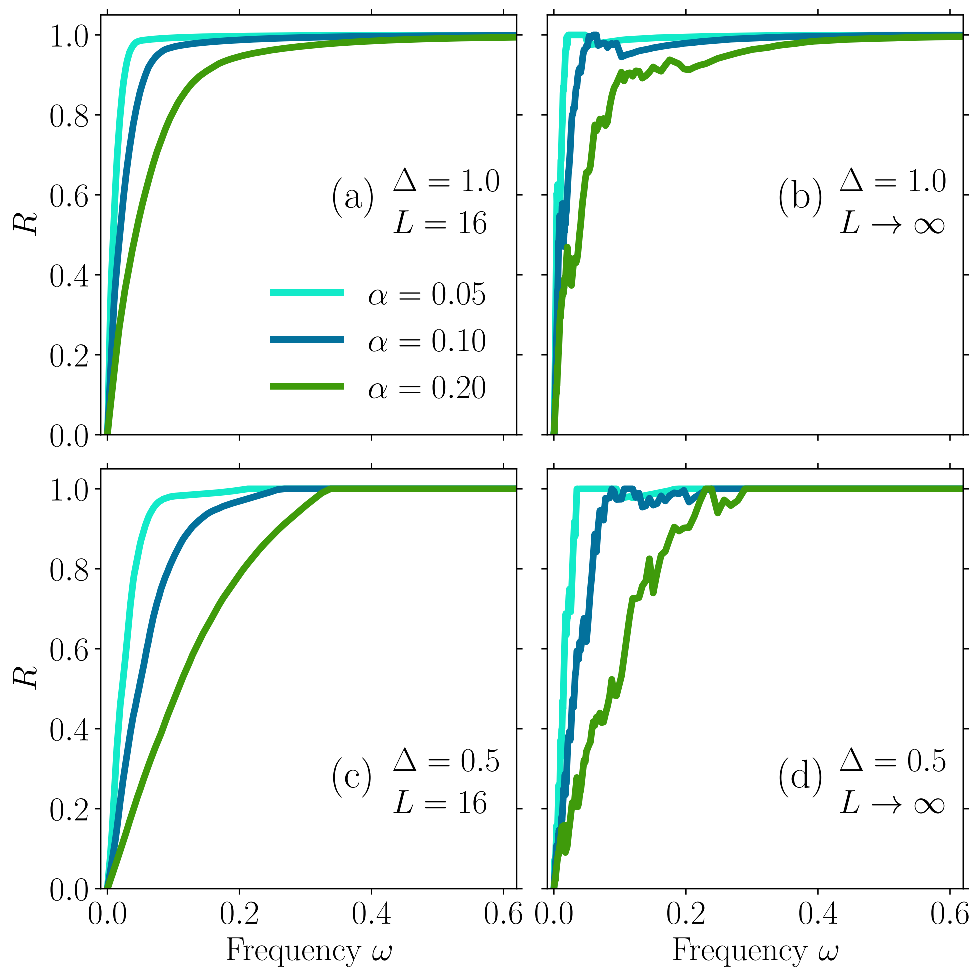

Figure 3.5: Normalized integrated spectral function as a function of cutoff frequency for $\hat{O}_1$ and $\hat{O}_2$. (a) Results for $L = 16$ and $\hat{O}_1$. (b) Results for $\hat{O}_1$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. (c) Results for $L = 16$ and $\hat{O}_2$. (d) Results for $\hat{O}_2$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. Note that low frequency limit for finite system does approach 0, as expected from Figure 3.1.

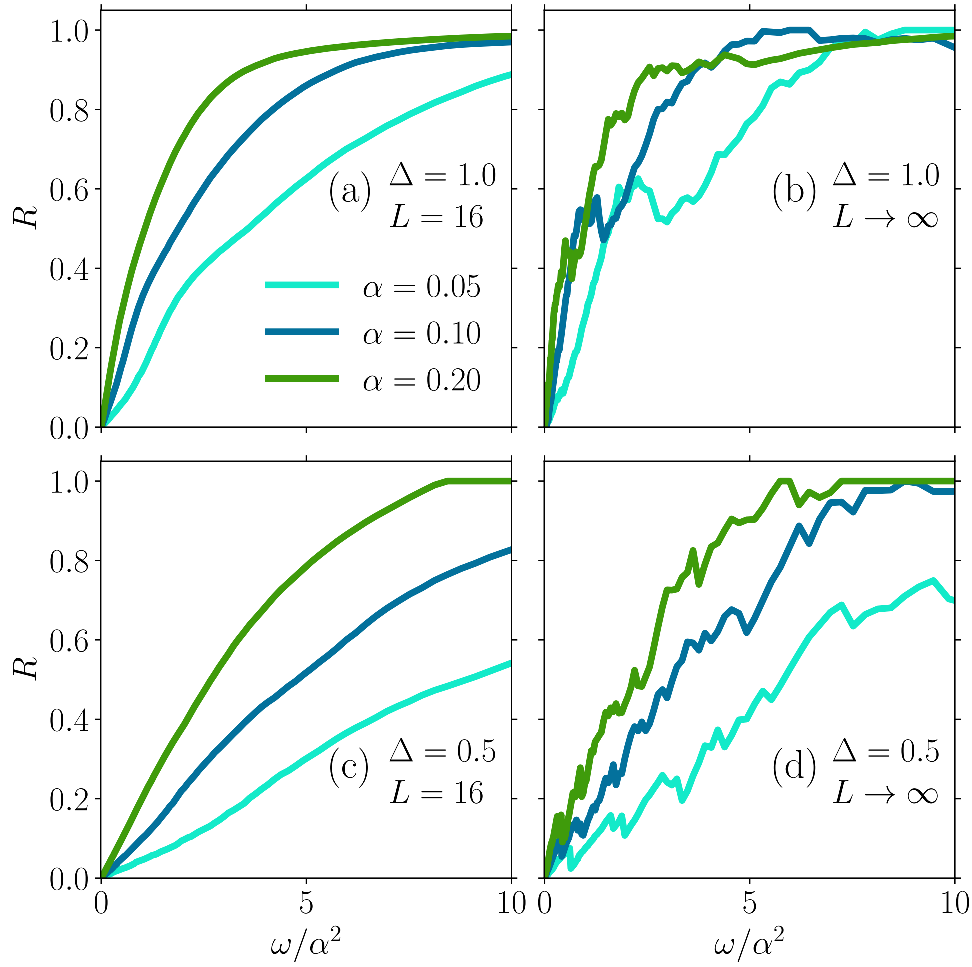

Figure 3.6: Normalized integrated spectral function as a function of rescaled frequency ω/α^2 for$\hat{O}_1$ and $\hat{O}_2$. (a) Results for $L = 16$ and $\hat{O}_1$. (b) Results for $\hat{O}_1$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. (c) Results for $L = 16$ and $\hat{O}_2$. (d) Results for $\hat{O}_2$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. On the contrary to the energy current, the curves do not collapse.

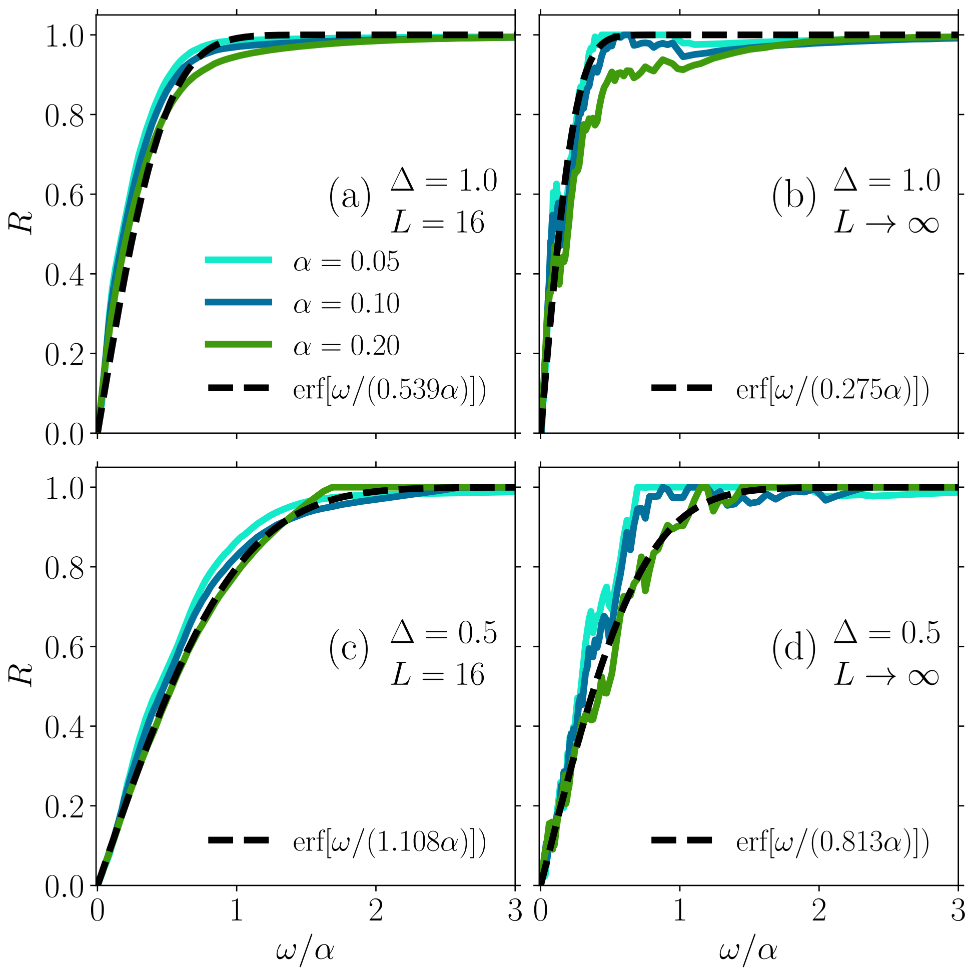

Figure 3.7: Normalized integrated spectral function as a function of rescaled frequency ω/α for$\hat{O}_1$ and $\hat{O}_2$. (a) Results for $L = 16$ and $\hat{O}_1$. (b) Results for $\hat{O}_1$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. (c) Results for $L = 16$ and $\hat{O}_2$. (d) Results for $\hat{O}_2$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. Note the convincing collapse of the curves for this scaling.

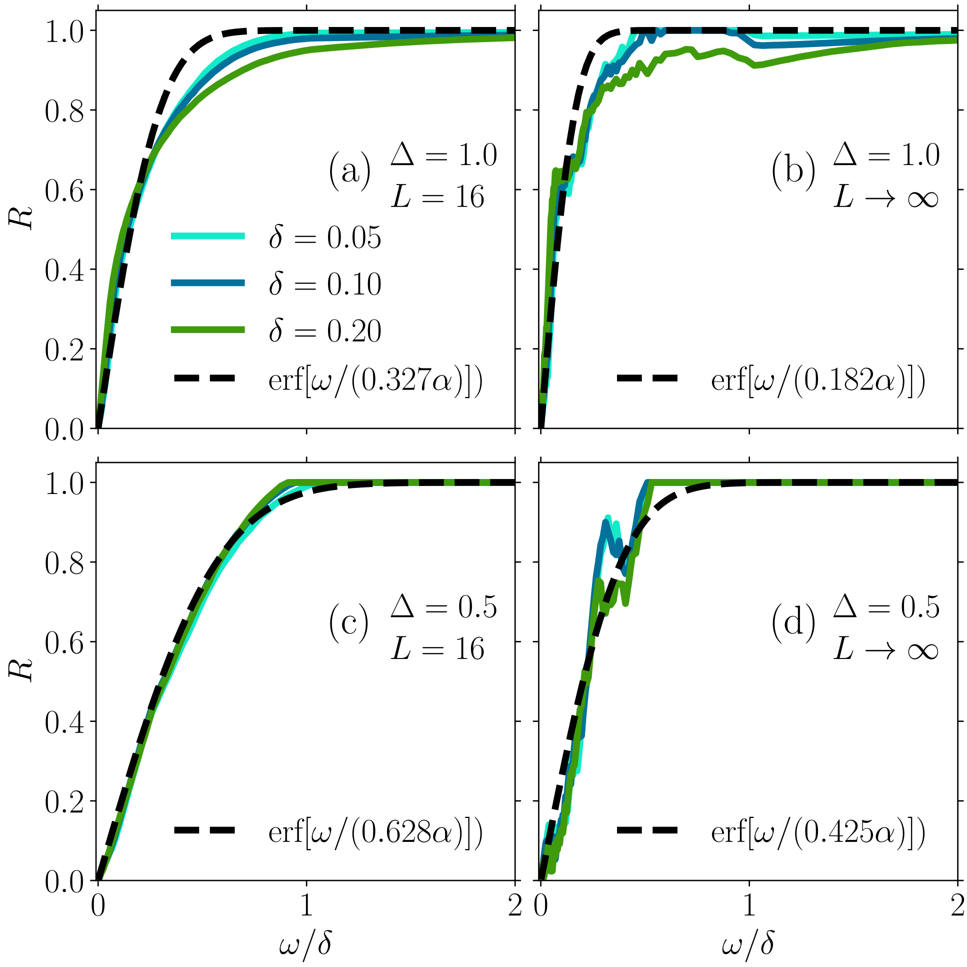

Figure 3.8: Normalized integrated spectral function as a function of rescaled frequency ω/δ for$\hat{O}_1$ and $\hat{O}_2$. Here the model remains integrable, it only the symmetry that is broken. (a) Results for $L = 16$ and $\hat{O}_1$. (b) Results for $\hat{O}_1$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. (c) Results for $L = 16$ and $\hat{O}_2$. (d) Results for $\hat{O}_2$ extrapolated to thermodynamic limit from $L = 10, 12, 14, 16$. Results are qualitatively similar to full integrability breaking case.

4
Summary

The aim of this work was to investigate the properties of noncommuting (quasi)local integrals of motion within the integrable spin-1/2 XXZ model with periodic boundary conditions on one-dimensional lattice. The case of commuting (Q)LIOMs has been studied extensively and it is now known that in nearly in the presence of integrability breaking perturbation, decay of their autocorrelation functions is exponential and the characteristic relaxation time scales quadratically with perturbation strength. On the other hand, the noncommuting (Q)LIOMs are much less studied. Even though their existence is a well-known fact that was formally proven, little has been known about their dynamics under weak integrability-breaking perturbation, which is often present in real-world systems.

Such a numerical study was realized in this thesis. To this end, a procedure allowing for systematic identification of all (Q)LIOMs present in a given model was described and implemented. It was then applied to the spin-1/2 chain with different values of anisotropy parameter, where to reduce the computational cost, the support of operators was restricted to 3 lattice sites. As a test case, a known commuting LIOM was identified, namely, the energy current operator. Apart from that, two nontrivial noncommuting conserved quantities were found, one local for $\Delta = 1.0$ and one quasilocal for $\Delta = 0.5$, in agreement with the existing analytical results. To study the decay of these quantities, the formalism of integrated spectral functions was introduced. With its help, the known results about exponential decay of energy current were confirmed. However, the key finding presented in this thesis is a novel result about the relaxation of noncommuting (Q)LIOMs. Both of them were found to decay in a Gaussian-like manner, with characteristic relaxation time scaling linearly with perturbation strength. This anomalous scaling was explained by observing, that it is not the breaking of integrability that is responsible for the decay, but shifting away from high-symmetry values of anisotropy parameter. Degeneracy resulting from symmetries is removed already in the first order of perturbation theory, hence the linear scaling.

The border between chaos and integrability in quantum many-body systems is still full of open problems, with as fundamental things as the concept of quantum integrability itself being a topic of debate. A highly sought-after result would perhaps be the quantum analogue of the famous KAM theorem, giving a concrete answer to the question about onset of chaos in perturbed integrable systems. However, in spite of numerous research, it seems that physicists still have a long road ahead of them. As for the work presented in this thesis, one of possible future directions is an extension of the used here approach to the case of two-dimensional lattice models, where considerable difficulties of computational nature await.

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A

Classical and quantum integrability

Classical integrability Before jumping head first into the quantum realm, it is perhaps valuable the state the problem of classical integrability, and the results therein. We consider this topic in the spirit of the classical discussion of Liouville and Arnold as presented in a monograph by Gutzwiller [58].

One usually begins the discussion of classical mechanics with the Lagrangian picture and then via Legendre transform moves on to the Hamiltonian picture, however we shall skip this for brevity and take the Hamiltonian picture as a starting point. A dynamical system at every given time t is described by its momentum p and position q. If we assume our system to have n degrees of freedoms, then its state can be specified as a point in a $2n$-dimensional space (n for momenta and n for coordinates) called the phase space. Dynamics are governed by a function of $H = H(p, q, t)$ called the Hamiltonian, which can be interpreted as the energy, and the so-called *Hamilton equations of motion*

$$\frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial H}{\partial q_j}, \quad \frac{\mathrm{d}q_j}{\mathrm{d}t} = \frac{\partial H}{\partial p_j} \tag{A.1}$$

Suppose that we have another function on a phase space, say $F = F(p, q)$, with a property that its value does not vary in time if we take as p and q solutions of equations (A.1). This is equivalent to the following condition

$$\begin{aligned} 0 = \frac{\mathrm{d}}{\mathrm{d}t} F(p, q) &= \frac{\partial F}{\partial p}\frac{\mathrm{d}p}{\mathrm{d}t} + \frac{\partial F}{\partial q}\frac{\mathrm{d}q}{\mathrm{d}t} \\ &= \frac{\partial H}{\partial p}\frac{\partial F}{\partial q} - \frac{\partial H}{\partial q}\frac{\partial F}{\partial p} = \{H, F\} \end{aligned} \tag{A.2}$$

where $\{\bullet, \bullet\}$ is the Poisson bracket. Vanishing of Poisson bracket with Hamiltonian is a necessary condition for F to be called an *integral of motion*. This property has a nice geometric interpretation. On the one hand, the vector field $(-\,\partial H/\partial q\,,\, \partial H/\partial p)$ in a phase space is tangent to surface $F(p, q) = const$. On the other hand, the vector field $(-\,\partial F/\partial q\,,\, \partial F/\partial p)$ is tangent to the energy surface $H(p, q) = E$. The trajectory of a dynamical system in a phase space is then located in the intersection of these two surfaces. Let us now imagine that we have a set $\{F_i\}_{i=1,\ldots,k}$ of such conserved quantities that are functionally independent (no function from this set can be expressed as a function of other functions from this set). It is not yet sufficient to enable us to solve the equations of motion. The integrals of motion must also be in *involution*, which means that for any $F_i, F_j \in \{F_i\}_{i=1,\ldots,k}$ we have $\{F_i, F_j\} = 0$. Existence of k integrals of motion restricts the dynamics of the system to a $(2n-k)$-dimensional subspace of the phase space, whereas the fact that they are in involution guarantees that this subspace has a simple internal structure. If there are at least n such conserved quantities, then a famous theorem by Liouville holds, which states a system with n degrees of freedom with n integrals of motion is integrable by quadratures. Then, there exists such a canonical transformation $(p, q) \to (F, \Theta)$, to the so-called angle-action variables, that $H(p, q) = H(F)$ and the equations of motions are solved by $F_j(t) = F_j^0$ and $\Theta(t)_j = \Omega_j t + \Theta_j(0)$ [59]. Moreover, it was proven with the help of topology that this restricted subspace has a shape of an n-dimensional torus, called the *invariant torus*. In general different initial conditions correspond to different invariant tori. Therefore, we see that integrability in classical mechanics has a very precise definition — differential equations governing time evolution can be solved explicitly with the help of action-angle variables. Then, the solutions to equations A.1 for integrable of motions exhibit periodic dynamics constrained to some invariant torus. On the other hand, solutions for nonintegrable systems, given sufficient time, explore the whole phase space.

KAM theorem Before we leave the classical world, let us ponder upon one more question. What happens to a classical integrable system under small perturbations? More precisely, how does the breakdown of invariant tori look like? The answer to this question lies within the remarkable KAM theorem, which was proven by a joint effort of Kolmogorov [60], Moser [61], and Arnold [62]. For a system with a finite number of degrees of freedom, it specifies, under some assumptions, that majority of the invariant tori that occupy[1] the phase space survive the influence of small perturbations. This entails the possibility of coexistence between chaos and regularity. Eventually, as perturbation grows, chaotic regions fill the phase space completely [6]. We end this part with a quote from Arnold's book [59] about the KAM theorem.

> *If an unperturbed system is nondegenerate, then for sufficiently small conservative Hamiltonian perturbations, most non-resonant invariant tori do not vanish, but are only slightly deformed, so that in the phase space of the perturbed system, too, there are invariant tori densely filled with phase curves winding around them conditionally-periodically, with a number of independent frequencies equal to the number of degrees of freedom. These invariant tori form a majority in the sense that the measure of the complement of their union is small when the perturbation is small.*

Quantum integrability After learning about classical integrability, which is a very mature subject, one may be surprised that the notion of quantum integrability is still vigorously debated among scientists. A conclusive answer to the question 'what does it mean for a quantum system to be integrable?' is yet to be found. In this paragraph, we outline the possible solutions following the reviews by Caux and Mossel [63] and Yuzbashyan and Shastry [64].

First contrasting difference between classical and quantum mechanics is how we count degrees of freedom. In the former, it corresponds to the number of pairs of conjugate variables necessary

[1]The more technical term is *foliate*.

to specify a point in a phase space, each variable admitting a continuum of possible values. In the latter, Heisenberg Uncertainty Principle prevents from constructing a quantum equivalent of a classical phase space. Furthermore, allowed energy levels very often constitute a discrete set and thus we can employ finite-dimensional Hilbert spaces with the dimensionality being the number of degrees of freedom. This alone prevents us from a straightforward application of classical integrability to quantum mechanics. Nonetheless, we can try in the spirit of Liouville integrability, consider a system to be integrable if it possesses a maximal set of conserved quantities (operators commuting with a Hamiltonian) of cardinality equal to the dimension of Hilbert space. Unfortunately, this simple criterion fails immediately, because by the spectral theorem, Hermitian Hamiltonians can be diagonalized and such maximal set can be built from projectors on its eigenstates i.e. $Q_n = |n\rangle\langle n|$. Therefore every system could be called integrable, even though the existence of these projector operators do not prevent thermalization of physical observables [6]. Shortcomings of this definition can be remedied by requiring the conserved quantities to be local (or, as recently discovered, quasilocal), that is acting in a nontrivial way only on some subspace of Hilbert space. As the projection operators are in general very nonlocal, they are rejected by this constraint. Moreover, we require the number of (quasi)local conserved charges to be extensive, that is, scaling with the system size. This allows for separation between integrable systems and nonintegrable ones, where this quantity is nonextensive. As mentioned in the Introduction, this definition is sufficient for considerations in this thesis.

For informational purposes, we shall now list some other possible approaches to the problem at hand. Mathematical physicists like to say that a system is integrable if it is exactly solvable, that means a full set of eigenstates can be constructed explicitly. A variety of techniques can be used to achieve that, for example, Fourier transform for noninteracting models, and quantum inverse scattering method for one dimensional models [65, 66, 67]. There are also approaches to integrability based on non-diffractive scattering (as it leads directly to non-ergodicity) [68], or eigenstate entanglement entropy [69]. Last but not least, an interesting viewpoint originates from the Berry-Tabor conjecture [70] about the distribution of energy levels spacings in quantum systems with integrable classical counterparts. We can take a set of normalized energies $\{e_i\}$ with mean spacing equal to unity, and define $s_i = e_{i+1} - e_i$, for which we are looking for an universal probability distribution $P(s)$ such that for a random choice of i, probability of having $s \leq s_i \leq s + \mathrm{d}s$ is $P(s)\mathrm{d}s$. It was shown to be a Poisson distribution [71]

$$P(s) = \exp(-s) \tag{A.3}$$

This result holds also for most integrable systems without the classical limit, but it can fail, usually due to extra symmetries of Hamiltonian and the resulting degeneracies [6]. Conversely, in chaotic systems Random Matrix Theory predicts emergence of the so-called Wigner-Dyson statistic. If we consider 2×2 Hamiltonians with entries being random numbers from suitable Gaussian distribution, the energy level spacing distribution is of the form [6]

$$P(s) = A_\beta \omega^\beta \exp\left[-B_\beta \omega^2\right] \tag{A.4}$$

where $\beta = 1$ if time-reversal symmetry is present and $\beta = 2$ otherwise. Constants A_β and B_β can be fixed by normalization and setting the mean energy level spacing. Remarkably, one can generalize this result to larger matrices by drawing them from a suitable Gaussian distribution [72]

$$P(H) \propto \exp\left[-\frac{\beta}{2a^2}\operatorname{tr}\left(H^2\right)\right] = \exp\left[-\frac{\beta}{2a^2}\sum_{ij} H_{ij}H_{ji}\right] \tag{A.5}$$

As previously, $\beta = 1$ for systems with time-reversal invariance, that is $H_{ij} \in \mathbb{R}$ and $H_{ij} = H_{ji}$, whereas $\beta = 2$ for systems without it, that is $H_{ij} \in \mathbb{C}$ and $H_{ij} = H^*_{ji}$. In the former case we have the so-called Gaussian Orthogonal Ensemble (GOE) and in the latter Gaussian Unitary Ensemble (GUE). As matrices from either GOE or GUE must be invariant under orthogonal and unitary transformation respectively, the equation (A.5) is quite natural, as $\operatorname{tr}\left(H^2\right)$ is such invariant [6]. A comparison between Poisson and GOE distributions is shown in Figure A.1. Another interesting difference between integrability and chaos becomes visible, namely, the repulsion of energy levels, manifested as a vanishing probability for $s = 0$ in GOE. One could take this as a definition of integrability, however it is probably more desirable to consider this as a consequence rather than a definition.

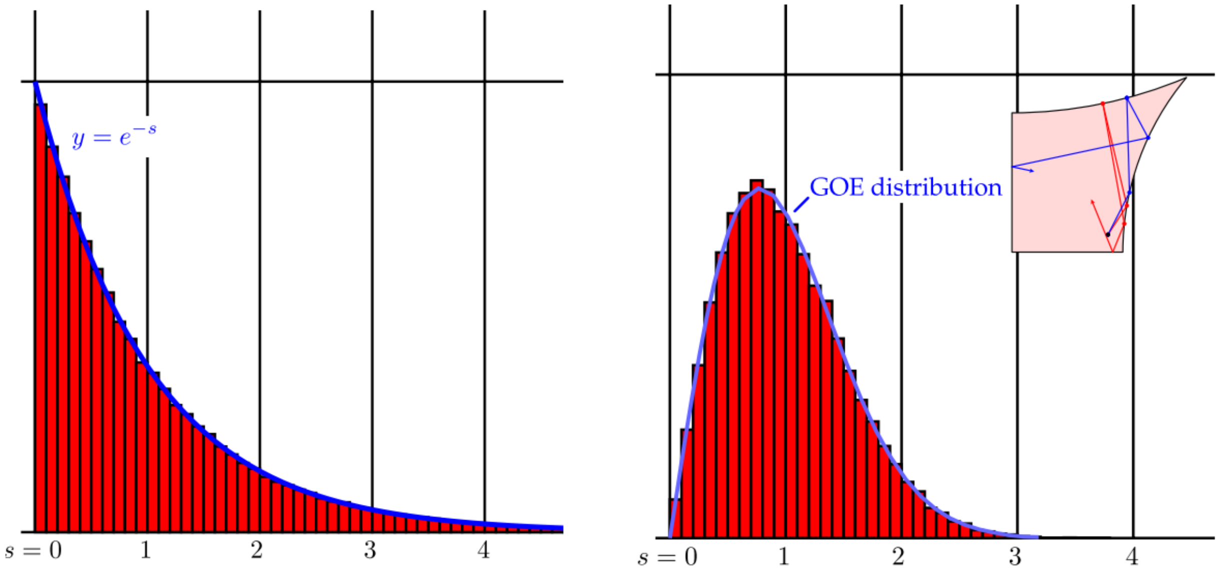

Figure A.1: (Left panel) Distribution of 250000 single-particle level spacings in an integrable system — rectangular box with fine-tuned sides. (Right panel) Distribution of 50000 single-particle level spacings in an nonintegrable system shown in the inset. Sourced from [6, 73].

As in classical mechanics, one may ask a question about the fate of an integrable system under influence of a weak perturbation. Thus far, we do not have a conclusive answer to this question, at least not in a form that would be analogous to the KAM theorem. There are results that show the existence of residual quasiconserved quantities, thus hinting towards a quantum KAM theorem [74]. However, it has been also reported that arbitrarily small perturbations in thermodynamic limit lead to quantum chaos and restoring of generic (dissipative) dynamics [75]. Therefore, as of now, the question of behavior on the border between integrable and chaotic regimes remains an open problem.

B

Derivation of integrated spectral function

We want to prove equation (2.18), which gives a recipe for the numerical calculation of the integrated spectral function for an arbitrary observable A. Our starting point is Definition 2.7

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

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

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

The obtained result is a limit of the so-called Poisson kernel. This happens to be a representations of Dirac delta in the form of a limit of a sequence of functions [76]

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

Thus we get

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

Inserting this result into equation (B.1) we get

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

We are now ready to compute the integrated spectral function

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

C Derivation of spin energy current

Equation (2.30) is conceptually simple, yet quite tedious to solve due to the number of commutators present. Luckily, leveraging the commutator properties to our advantage allow us to simplify the calculations. Let us begin with inserting the definition of $h_{k,k+1}$ into equation (2.30)

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

By inspection, it becomes clear that out of the 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 index change.

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

Carrying out the calculation of the remaining two nontrivial commutators, we arrive at the following equations

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

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 the calculations is provided in full detail

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

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

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

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

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

which is precisely the expression from Zotos, Naef, and Prelovsek [50]. However, in this work we are interested in the XXZ model with the Hamiltonian (1.34). To this end, we need to set $J_x, J_y = J$, $J_z = J\Delta$ 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

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

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.

D

Proof of orthonormality of basis

We want to prove the following

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

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

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

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 (1.13). In this proof we use the following properties of Pauli matrices

$$\mathrm{tr}\left(\tau^j\right) = 0 \implies \mathrm{tr}(\tau^\pm) = \mathrm{tr}(\tau^x \pm i\tau^y) = 0 \tag{D.2}$$

$$\tau^j\tau^k = \delta_{jk}\mathbb{1}_{2\times 2} + i\varepsilon_{jkl}\tau^l \tag{D.3}$$

$$\mathrm{tr}\left(\tau^j\tau^k\right) = 2\delta_{jk} \tag{D.4}$$

where $j,k,l \in \{x,y,z\}$ and ε_{jkl} is the Levi-Civita symbol. We begin with showing orthogonality. Consider the following inner product for $\underline{s} \neq \underline{s}'$

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

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

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

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

2. $s_i = z,\ s'_i = +$
$$\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s'_i}_{j+i-1}\right) \propto \mathrm{tr}\left(\tau^z_{j+i-1}\tau^+_{j+i-1}\right) = \left[\mathrm{tr}\left(\tau^z_{j+i-1}\tau^x_{j+i-1}\right) + i\,\mathrm{tr}\left(\tau^z_{j+i-1}\tau^y_{j+i-1}\right)\right] = 0$$
3. $s_i = z,\ s'_i = -$
$$\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s'_i}_{j+i-1}\right) \propto \mathrm{tr}\left(\tau^z_{j+i-1}\tau^-_{j+i-1}\right) = \left[\mathrm{tr}\left(\tau^z_{j+i-1}\tau^x_{j+i-1}\right) - i\,\mathrm{tr}\left(\tau^z_{j+i-1}\tau^y_{j+i-1}\right)\right] = 0$$
4. $s_i = +,\ s'_i = -$
$$\begin{aligned}\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s'_i}_{j+i-1}\right) \propto \mathrm{tr}\left(\tau^-_{j+i-1}\tau^-_{j+i-1}\right) &= [\,\mathrm{tr}\left(\tau^x_{j+i-1}\tau^x_{j+i-1}\right) - \mathrm{tr}\left(\tau^y_{j+i-1}\tau^y_{j+i-1}\right) \\ &\quad - i\,\mathrm{tr}\left(\tau^x_{j+i-1}\tau^y_{j+i-1}\right) - i\,\mathrm{tr}\left(\tau^y_{j+i-1}\tau^x_{j+i-1}\right))] \\ &= [\,\underbrace{\mathrm{tr}\left(\tau^x_{j+i-1}\tau^x_{j+i-1}\right)}_{=2} - \underbrace{\mathrm{tr}\left(\tau^y_{j+i-1}\tau^y_{j+i-1}\right)}_{=2}\,] = 0\end{aligned}$$

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 (D.5) a term of the form $\mathrm{tr}\left(\sigma^{s_i}_{j+i-1}\mathbb{1}_{2\times 2}\right) = \mathrm{tr}\left(\sigma^{s_i}_{j+i-1}\right) \propto \mathrm{tr}\left(\tau^{s_i}_{j+i-1}\right) = 0$, where the last equality comes from (D.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
$$\begin{aligned}(O_{\underline{s},j}|O_{\underline{s},j}) =& \frac{1}{2^L}\,\mathrm{tr}\left((\mathbb{1}_{2\times 2})^\dagger\,\mathbb{1}_{2\times 2}\right)\cdots\mathrm{tr}\left((\mathbb{1}_{2\times 2})^\dagger\,\mathbb{1}_{2\times 2}\right)\cdot\mathrm{tr}\left(\left(\sigma^{s_1}_j\right)^\dagger\sigma^{s_1}_j\right) \\ &\cdot\mathrm{tr}\left(\left(\sigma^{s_2}_{j+1}\right)^\dagger\sigma^{s_2}_{j+1}\right)\cdots\mathrm{tr}\left(\left(\sigma^{s_m}_{j+m-1}\right)^\dagger\sigma^{s_m}_{j+m-1}\right)\cdots\mathrm{tr}\left((\mathbb{1}_{2\times 2})^\dagger\,\mathbb{1}_{2\times 2}\right) \qquad \text{(D.6)}\end{aligned}$$

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

1. $s_i = 0$
$$\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s_i}_{j+i-1}\right) = \mathrm{tr}(\mathbb{1}_{2\times 2}\mathbb{1}_{2\times 2}) = \mathrm{tr}(\mathbb{1}_{2\times 2}) = 2$$
2. $s_i = z$
$$\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s_i}_{j+i-1}\right) = 4\,\mathrm{tr}\left(S^z_{j+i-1}S^z_{j+i-1}\right) = \mathrm{tr}\left(\tau^z_{j+i-1}\tau^z_{j+i-1}\right) = 2$$
3. $s_i = +$
$$\begin{aligned}\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s_i}_{j+i-1}\right) = 2\,\mathrm{tr}\left(S^-_{j+i-1}S^+_{j+i-1}\right) = \frac{1}{2}\,\mathrm{tr}\left(\tau^-_{j+i-1}\tau^+_{j+i-1}\right) &= \frac{1}{2}[\,\mathrm{tr}\left(\tau^x_{j+i-1}\tau^x_{j+i-1}\right) \\ + \mathrm{tr}\left(\tau^y_{j+i-1}\tau^y_{j+i-1}\right) - i\,\mathrm{tr}\left(\tau^x_{j+i-1}\tau^y_{j+i-1}\right) &- i\,\mathrm{tr}\left(\tau^y_{j+i-1}\tau^x_{j+i-1}\right)] \\ = \frac{1}{2}[\,\underbrace{\mathrm{tr}\left(\tau^x_{j+i-1}\tau^x_{j+i-1}\right)}_{=2} + \underbrace{\mathrm{tr}\left(\tau^y_{j+i-1}\tau^y_{j+i-1}\right)}_{=2}\,] = 2&\end{aligned}$$
4. $s_i = -$
$$\mathrm{tr}\left(\left(\sigma^{s_i}_{j+i-1}\right)^\dagger \sigma^{s_i}_{j+i-1}\right) = 2\,\mathrm{tr}\left(S^+_{j+i-1}S^-_{j+i-1}\right) = 2\,\mathrm{tr}\left(S^-_{j+i-1}S^+_{j+i-1}\right) = 2$$

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 the full Hilbert space of dimension 2^L. If we were to restrict our calculations to some subspace, a reorthogonalization procedure would be necessary [29].