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# Eigenmodes in nearly integrable quantum chains

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**Abstract**

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**Keywords:** *integrals of motion, ETH, nearly integrable systems, spin chains*

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# Contents

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# 1
# Introduction

## 1.1 Nearly integrable quantum systems

One of the most widely disputed problems in modern physics is the reconciliation of irreversible thermodynamics [1, 2] with unitary, time-reversible dynamics predicted by quantum mechanics [3, 4]. In other words, it is the question of whether a generic, isolated quantum system can and will 'forget' about its initial, nonequilibrium state. In recent years, this problem has attracted the attention of many physicists, especially taking into account experimental evidence of the loss of information, or thermalization, in isolated systems [5–9]. Understanding this phenomenon is a crucial first step to controlling it, and perhaps to the creation of sought-after, robust systems which do not exhibit such behavior. After all, 'forgetting' about the initial state is equivalent to scrambling of quantum information and decoherence, which has been known for a long time to be one of the most important hindrances to a functional and scalable quantum computer [10, 11]. Given the multitude of possible applications of such a device, both purely scientific and commercial, controlling thermalization in isolated systems could be the next groundbreaking achievement [12].

**Preventing thermalization** A possible theoretical explanation of the thermalization in isolated quantum systems has been proposed in seminal papers by Deutsch [13] and Srednicki [14] in form of an ansatz for matrix elements of local quantum observables $A_{mn} = \langle m|A|n\rangle$ (in eigenbasis $H\,|n\rangle = \varepsilon_n\,|n\rangle$ of some Hamiltonian), known as **Eigenstate Thermalization Hypothesis** (ETH)

$$A_{mn} = A(\bar{\varepsilon})\delta_{mn} + \mathrm{e}^{-S(\bar{\varepsilon})/2} f_A(\bar{\varepsilon},\omega) R_{mn} \tag{1.1}$$

where $\bar{\varepsilon} = (\varepsilon_n + \varepsilon_m)/2$, $\omega = \varepsilon_n - \varepsilon_m$ and $S(\bar{\varepsilon})$ is the thermodynamic entropy at energy $\bar{\varepsilon}$, $A(\bar{\varepsilon})$ and $f_A(\bar{\varepsilon},\omega)$ are some smooth functions of their parameters and $R_{mn}$ is a random real or complex variable. The origin of ETH is the Random Matrix Theory [15, 16], but it was the key insight of Deutsch and Srednicki that connected it directly to statistical mechanics. Unraveling the physics behind equation (1.1), we have that, for generic systems, long-time (thermalized) expected values of local observables are related to the predictions of Gibbsian ensembles known from equilibrium statistical physics [17]. Diagonal matrix elements $A_{nn} \simeq A(\varepsilon_n)$ are smooth functions of energy and coincide with the microcanonical average at energy $\varepsilon_n$, whereas the off-diagonal matrix elements and fluctuations of the diagonal ones are postulated to decrease exponentially with system size [18]. While ETH has been shown to hold analytically in only a few selected systems [19], numerical clues can be found in various systems with many-body interactions such as hard-core bosons, interacting spin chains [20–23] and fermions [24, 25].

Given the lack of a definitive answer to the question of when ETH holds and the fact that our ultimate goal is preventing thermalization, it is desirable to look for systems that explicitly violate this hypothesis. There are a few known classes of such systems: quantum integrable models, systems with 'scars', which freeze thermalization for some infrequent, but physically relevant states [26, 27], quantum time crystals with broken time-translation symmetry [28, 29] and systems with many-body interactions together with some form of disorder [30]. As the thermalization in those systems is slowed down or even completely stopped, in principle they could preserve information about the initial state for an arbitrarily long time. This behavior is in stark contrast with what is usually observed in interacting, many-body systems, namely fast dynamics on the time scales of tens of femtoseconds [31]. In this thesis, we shall concern ourselves only with the case of **quantum integrable models**.

**Robustness of integrability** In quantum mechanics, as opposed to classical mechanics, a unique definition of integrability is yet to emerge [32, 33]. Nevertheless, a common practice is to take as a sufficient condition of integrability the presence of an extensive number (increasing linearly with the system size) of local observables that are integrals of motion, i.e. commute with the Hamiltonian, called LIOMs for short. The significance of such systems is at least twofold. First, as already mentioned, they can provide a new method of storage of information, encoded in expectation values of LIOMs, which can pave the way for the creation of the sought-after quantum memory. Second, they are among a few quantum many-body systems that are susceptible to analytical methods and so provide a rich playground for both theoretical physicists and mathematicians. Tools such as Algebraic Bethe Ansatz [34–36] or Generalized Hydrodynamics [37–41] lead to considerable insight regarding the nature of integrable systems.

Unfortunately, it is often the case for integrable systems such as Heisenberg, Hubbard or Lieb-Linger models whose integrability relies on a certain set of fine-tuned parameters. Any deviation from these parameters, eg. in the form of some perturbation, can very easily destroy the integrability. Exactly this situation takes place in most experimental setups (albeit some signatures of integrability were observed [42], suggesting sufficient proximity to an integrable system), even though the capabilities and precision of control have reached remarkable levels [43]. Therefore, **more realistic systems are expected to be described by nearly integrable systems**, containing some non-negligible perturbations that impact integrability [44, 45]. This renders all the formalism for investigations of purely integrable systems inapplicable and forces one to rely mostly on numerical methods (for a recent review see Bertini et al. [39]). A general expectation for such nearly integrable systems is such, that in the thermodynamic limit, an arbitrarily small perturbation should restore generic chaotic dynamics, which leads to thermalization [46]. However, there are some reports about surviving traces of integrability, for example in the form of residual quasiconserved quantities [45]. In most cases numerical methods can only access finite systems and indirect transitions to infinite system sizes, such as finite-size scaling, pose great difficulties when executed properly, eg. first thermodynamic limit and then infinite time limit [47, 48]. Therefore, it is important to first gain a deep understanding of **weakly-perturbed finite systems**. Such endeavor immediately raises a few questions: How strong should a perturbation in a finite systems be to destroy integrability and how to efficiently describe resulting slow dynamics? Recently, those and other similar questions have been asked concerning the phenomena of ergodicity breaking phase transitions [49, 50]. Insight from experiments with ultracold atomic gases suggest also another way for nearly integrable systems to emerge, namely generic, chaotic one- and quasi-one-dimensional systems that exhibit approximately integrable dynamics on experimentally relevant timescales, because of a lack of rapid local thermalization [51, 52].

In classical mechanics, answers to those types of questions are given by the Hamiltonian perturbation theory [53]. There, the distinction between integrable and non-integrable systems is well understood. It is known, that for classical systems with $n$ degrees of freedom to be integrable, it is sufficient to have $n$ integrals of motion $\{H, F_i\} = 0,\ i \in \{1, \ldots, n\}$ that are in involution, i.e. $\{F_i, F_j\} = 0$ for any $i, j \in \{1, \ldots, n\}$. Then, dynamics are restricted to an $n$-dimensional torus in the phase space. The fate of such invariant tori under integrability-breaking perturbations is given by the famous Kolmogorov-Arnold-Moser theorem (KAM) [54–56], stating that for systems with finite degrees of freedom, majority of the invariant tori occupying the phase space survive the influence of small perturbations. However, as of now, there is no equivalent of this result in quantum mechanics. Nevertheless, such quantum systems are very intriguing as they can facilitate robust prethermalization plateaux, i.e. dynamics that at intermediate times resemble that of integrable models (at least for suitably weak perturbations), even though the system eventually thermalizes at longer times [57–60].

## 1.2 Motivation and aim of this dissertation

As argued in the previous section, nearly integrable quantum systems constitute an important relaxation of constraints imposed on ordinary integrable systems, facilitating experimental realizations. They form the broader context this thesis is set in and the main motivation. However, to keep it finite in size, we restrict our attention to two concrete problems.

First, we provide a pedagogical introduction to the so-called **Krylov subspace methods** which allow us to leverage the sparsity of local observables in order to avoid the limitations originating from the exponential growth of many-body Hilbert space. Following the exposition by Trefethen and Bau [61], in Chapter 2 we start our journey seemingly far away from physics, investigating a general algorithm called Arnoldi iteration, which original aim was to reduce a matrix to 'almost triangular' or Hessenberg form. Along the way we discover that, as a byproduct, Arnoldi iteration produces a remarkably good approximation of extremal eigenvalues and eigenvectors. Contrary to most physics texts and in the spirit of the pedagogical nature of this chapter, we try to derive all results when possible and motivate them thoroughly when not. Setting course back to physics, next, we assume that our matrices are Hermitian and observe how the Arnoldi iteration simplifies tremendously, producing the well known

Lanczos iteration [62]. Then, going beyond just groundstate calculations, we show how to slightly modify Lanczos iteration to be able to compute an approximation of action of any analytic function of hermitian matrix on a vector. Applying this scheme to the function $f(x) = \exp(-ixt)$, we obtain an efficient way of calculating pure state time evolution, called the Krylov propagator [63]. At the end of Chapter 2, we outline the recent concept of Quantum Typicality [64] and derive a numerical procedure for efficient calculation of correlation functions, without the need for Exact Diagonalization. All algorithms described in chapter 2 were implemented using the Armadillo linear algebra library [65] and Intel MKL.

Our second topic of interest is the **spin transport in the long-range anisotropic Heisenberg model.** Existence of many interesting features of quantum many-body systems, such as ballistic dynamics in Heisenberg spin chains [39, 66], exotic frustrated magnetism [67], peculiar phase transitions [68, 69] and entangled spin liquids [70] depends strongly on the type and range of interaction present in them, so it is safe to say that it plays a crucial role. In the last few years, considerable development of experimental techniques has occurred, allowing for unprecedented manipulation of the interactions. Platforms such as individually controlled Rydberg atoms, or optical lattices provide insight into the properties of quantum many-body systems. Whereas optical lattice facilitates mostly fermionic systems [71–74], Rydberg atoms can be used to simulate pure spin systems. Models such as Ising or XY emerge naturally from their properties [43], and the ability to control range of interactions make them suitable for the simulation of long-range models [75]. Using time-periodic driving one can turn naturally existing Hamiltonian into some other, effective one - the so-called Floquet Hamiltonian. So far, this method has been applied with great success to create tunable XXZ model [76], strongly distance selective interactions [77], and tunable XYZ models [78, 79]. Progress in experimental methods sparked theoretical interest in long-range models [80–91], yet their dynamical properties are still largely unknown, which explains our interest in long-range anisotropic Heisenberg model in this thesis. In Chapter 3, motivated by experiments with density expansion in cold atoms [92–94], we study the dynamics of spin domains using the Krylov propagator, followed by Exact Diagonalization studies of the optical conductivity. Chapter 4 is devoted to investigating a class of local observables exhibiting similar properties to the spin current, using a numerical procedure searching for most conserved operators [95]. It is worth noting that the results presented in Chapters 3 and 4 have been recently published in Mierzejewski et al. [96].

In the remainder of this chapter, we provide a short introduction to the long-range anisotropic Heisenberg model and other quantities of interest in this thesis.

## 1.3 Long range anisotropic Heisenberg model and spin current

In this thesis, we study the paradigmatic quantum model of magnetism, the anisotropic Heisenberg model, but enriched with a long-range exchange $J(r) = J/r^{\alpha}$. The full Hamiltonian, defined on a one-dimensional lattice with periodic boundary conditions, reads

$$H = \sum_{\ell=1}^{L} \sum_{r=1}^{r_{\max}} J(r) \left[ \frac{1}{2} \left( S_\ell^+ S_{\ell+r}^- + S_\ell^- S_{\ell+r}^+ \right) + \Delta S_\ell^z S_{\ell+r}^z \right] \tag{1.2}$$

where $r_{\max}$ is taken to be $\lceil L/2 \rceil - 1$, to avoid double counting of hoppings. Unless stated otherwise, we will work in units where $J = 1$. The spin$-\frac{1}{2}$ operators are defined in the usual way

$$S^a_\ell = \underbrace{\mathbb{1} \otimes \mathbb{1} \otimes \ldots \mathbb{1}}_{\ell-1} \otimes S^a \otimes \underbrace{\mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{L-\ell} \tag{1.3}$$

where $a \in \{+, -, z\}$, $S^+ = S^x + iS^y$, $S^- = (S^+)^\dagger$, $\mathbb{1}$ is a $2 \times 2$ identity matrix and operators $S^x, S^y, S^z$ are defined in terms of corresponding Pauli matrices and obey the $\mathfrak{su}(2)$ algebra commutations relations

$$\left[S^a, S^b\right] = i\varepsilon_{abc} S^c \tag{1.4}$$

From equation (1.3) it is evident, that the Hilbert space $\mathcal{H}$ our Hamiltonian acts on is the tensor product of $L$ copies of single spin spaces $\mathfrak{h}_\ell \cong \mathbb{C}^2$,

$$\mathcal{H} = \bigotimes_{\ell=1}^{L} \mathfrak{h}_\ell \tag{1.5}$$

As $\dim_{\mathbb{C}}(\mathfrak{h}) = 2$, the total dimension is $2^L$. For numerical calculations, we shall use the so-called **Ising basis**, consisting of eigenstates of the $S^z_{\text{tot}} = \sum_{\ell=1}^{L} S^z_\ell$ operator. As on each site we can only have spin up or down, an efficient representation of such states is achieved using binary numbers.

Our main interest is in the spin transport in this system. To this end, we first notice that the total magnetization, or $z$ component of the total spin $S^z_{\text{tot}}$ is a conserved quantity. It can be shown by directly evaluating the commutator $[H, S^z_{\text{tot}}] = 0$, or by just observing that both spin-flip and interaction terms do not change the number of up/down spins when acting on a state from the Ising basis. Thus, we can write down a well-defined continuity equation for the evolution of local spin density

$$\frac{\mathrm{d}}{\mathrm{d}t} S^z_\ell(t) + \boldsymbol{\nabla} \cdot j^\sigma_\ell(t) = 0 \tag{1.6}$$

where $\boldsymbol{\nabla} \cdot j^\sigma_\ell(t) = j^\sigma_{\ell+1}(t) - j^\sigma_\ell$ is the discrete divergence of the spin current and $S^z_\ell(t) = e^{iHt} S^z_\ell e^{-iHt}$. The time derivative in the above equation is given by the Heisenberg equation

$$\frac{\mathrm{d}}{\mathrm{d}t} S^z_\ell(t) = i[H, S^z_\ell(t)] \tag{1.7}$$

Combining equations (1.6) and (1.7), we get

$$j^\sigma_{\ell+1} - j^\sigma_\ell = i[S^z_\ell, H] \tag{1.8}$$

This equation is simple in principle, however, its solution can get tedious in case of more complicated operator densities.

Fortunately, there is a trick that yields a simple expression for the current associated with an arbitrary conserved, extensive operator. Let $X = \sum_{\ell=1}^{L} x_l$ be such quantity, with $x_\ell$ being its local density and $j^x = \sum_{\ell=1}^{L} j^x_\ell$ being the current. Then define the polarization operator

$$P = \sum_{\ell=1}^{L} \ell x_\ell \tag{1.9}$$

We will now calculate its derivative in two ways, first using the continuity equation and second using the Heisenberg picture. For brevity, we suppress the explicit time dependence of operators.

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \sum_{\ell=1}^{L} \ell \frac{\mathrm{d}x_\ell}{\mathrm{d}t} = \sum_{\ell=1}^{L} \ell j_\ell^x - \underbrace{\sum_{\ell=1}^{L} \ell j_{\ell+1}^x}_{\ell \to \ell-1} = \sum_{\ell=1}^{L} \left[\ell j_\ell^x - (\ell-1)\, j_\ell^x\right] = \sum_{\ell=1}^{L} j_\ell^x = j^x \tag{1.10}$$

$$\frac{\mathrm{d}P}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \sum_{\ell=1}^{L} \ell \left(e^{iHt} x_\ell e^{-iHt}\right) = \sum_{\ell} \left(\ell e^{iHt} i[H, x_\ell] e^{-iHt}\right) = e^{iHt} \left(i \sum_{\ell} \ell [H, x_\ell]\right) e^{-iHt} \tag{1.11}$$

From the two equations above we can read off a compact expression for the current operator in Schrödinger picture

$$j^x = i \sum_{\ell=1}^{L} \ell [H, x_\ell] \tag{1.12}$$

Substituting $x_\ell = S_\ell^z$ we now quickly derive

$$\begin{aligned}
j^\sigma &= i \sum_{\ell=1}^{L} [H, S_\ell^z] = i \sum_{\ell,\ell'=1}^{L} \sum_{r=1}^{r_{\max}} \ell J(r) \left(\frac{1}{2}\left[S_{\ell'}^+ S_{\ell'+r}^-, S_\ell^z\right] + \frac{1}{2}\left[S_{\ell'}^- S_{\ell'+r}^+, S_\ell^z\right] + \Delta \cancel{\left[S_{\ell'}^z S_{\ell'+1}^z, S_\ell^z\right]}\right) \\
&= \frac{i}{2} \sum_{\ell,\ell'=1}^{L} \sum_{r=1}^{r_{\max}} \ell J(r) \left(\delta_{\ell,\ell'+r} S_{\ell'}^+ S_{\ell'+r}^- - \delta_{\ell,\ell'} S_\ell^+ S_{\ell'+r}^- - \delta_{\ell'+r,\ell} S_{\ell'}^- S_\ell^+ + \delta_{\ell',\ell} S_\ell^- S_{\ell'+r}^+\right) \\
&= \frac{i}{2} \sum_{\ell'=1}^{L} \sum_{r=1}^{r_{\max}} J(r) \left((\ell'+r) S_{\ell'}^+ S_{\ell'+r}^- - \ell' S_{\ell'}^+ S_{\ell'+r}^- - (\ell'+r) S_{\ell'}^- S_{\ell'}^+ + \ell' S_{\ell'}^- S_{\ell'+r}^+\right) \\
&= \frac{i}{2} \sum_{\ell=1}^{L} \sum_{r=1}^{r_{\max}} \frac{J}{r^{\alpha-1}} \left(S_\ell^+ S_{\ell+r}^- - S_\ell^- S_{\ell+r}^+\right)
\end{aligned} \tag{1.13}$$

which is our desired spin current. It will be the quantity of central interest in Chapter 3.

Before we finish the introductory chapter, let us notice two symmetries shared by the Hamiltonian (1.2) and spin current (1.13), which are particularly useful for numerical calculations. First of them we have just met – it manifests itself as the conservation of magnetization, i.e. $[H, S_{\text{tot}}^z] = 0$. This $U(1)$ symmetry allows us to decompose the full Hilbert space into parts consisting of states with the same total $z$-component of spin. In more mathematical terms, we have the following

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

i.e., the full Hilbert space with $\dim \mathcal{H} = 2^L$ can be decomposed into the direct sum of its proper subspaces $\mathcal{H}_j$ such that $\dim \mathcal{H}_j = \binom{L}{j}$ and all states in a given subspace correspond to the same eigenvalue of $S_{\text{tot}}^z$ operator. The index $j$ denotes the number of sites with spin up. It turns out that the Ising basis we use as a default for numerical calculations in spin systems is already the 'correct' basis, as it is enough to just sort the states according to the number of spins pointing up. This yields a manifestly block diagonal structure of the Hamiltonian matrix (cf. Figure 2.2 with a matrix of nearest neighbors Heisenberg model).

Because we have assumed periodic boundary conditions, both the Hamiltonian and the spin current are invariant under translations by any number of sites - that is under the action of $\mathbb{Z}_L$ cyclic group. This symmetry allows us to further decompose the Hilbert space using the eigenbasis of $T$, the one-site translation operator defined on the Ising basis as

$$T\left|\sigma_1, \sigma_2, \ldots, \sigma_L\right\rangle = \left|\sigma_L, \sigma_1, \ldots, \sigma_{L-1}\right\rangle \tag{1.14}$$

where $\sigma_\ell \in \{\downarrow, \uparrow\}$. It is easy to see that $T$ is unitary, thus its eigenvalues must lie on the unit circle in the complex plane [97]. In a finite chain of length $L$ we have $T^L = \mathbb{1}$ and the eigenvalues of $T$ are quantized, i.e. of the form $\mathrm{e}^{ik}$, where $k \in \left\{0, \frac{2\pi}{L}, \ldots, \frac{2\pi}{L}(L-1)\right\}$. As a consequence, the Hilbert space can be decomposed into the direct sum of eigenspaces of $T$

$$\mathcal{H} = \bigoplus_{m=0}^{L-1} \mathcal{H}_m, \text{ where } (\forall \left|\psi\right\rangle \in \mathcal{H}_m)\left(T\left|\psi\right\rangle = \exp\left(i\frac{2\pi}{L}m\right)\left|\psi\right\rangle\right) \tag{1.15}$$

and once again the Hamiltonian and the spin current are block diagonal in this basis, which each block being about $L$ times smaller than the full Hilbert space. The practical construction of the momentum states is more complicated than that of the magnetization states, although is not that difficult. We refer the reader to Sandvik [62] for a beautiful and detailed explanation. Importantly, we also have $[T, S^z_{\text{tot}}] = 0$ and thus the two symmetries are compatible. Using both of them at the same time, the size of the largest block is reduced to $\binom{L}{L/2}\frac{1}{L}$, which is still exponentially large in $L$, but much smaller than the full Hilbert space of dimension $2^L$.

To end this chapter we note that these two symmetries are not the only ones present in this model. For a comprehensive treatment of this topic, together with details of numerical implementation, we once again refer the reader to the standard text on this topic, namely Sandvik [62].

# 2

# Krylov subspace methods for quantum many-body systems

One of the two purposes of this thesis is to develop and test a set of numerical tools based on the Krylov subspace methods, which is a family of **iterative** methods concerned with projecting high dimensional problems into smaller dimension subspaces and solving them therein. Given a finite-dimensional vector space $\mathcal{H} \cong \mathbb{C}^m$, a vector $\mathbf{v} \in \mathbb{C}^m$ and a linear operator $A \in \mathbb{C}^{m \times m}$, represented as a matrix, the **k-th Krylov subspace** $\mathcal{K}_k$ is defined as

$$\mathcal{K}_k := \operatorname{span}\{\, \mathbf{v}, A\mathbf{v}, A^2\mathbf{v}, \dots, A^{k-1}\mathbf{v}\,\} \subseteq \mathbb{C}^m \tag{2.1}$$

The maximal dimension of a Krylov subspace is bounded from above by $\operatorname{rank}(A) + 1$ [98].

This chapter serves as a pedagogical introduction to the core ideas of these methods, including some of the usually omitted mathematical details. For the initial part of this exposition, we follow the excellent textbook of numerical linear algebra by Trefethen and Bau [61], whereas for further applications to quantum many-body physics, we rely on the excellent treatments of the topic found in Sandvik [62] and PhD thesis by Crivelli [99].

We start this chapter by quickly sketching the problems with **direct** algorithms such as Exact Diagonalization (ED), and quickly follow with the fundamental iterative algorithm for sparse general matrices, the Arnoldi iteration. Its output admits several possible interpretations, however, we shall focus on the problem of locating extremal eigenvalues. Afterward, we restrict our attention to the class of Hermitian matrices, to which of course all typical tight-binding Hamiltonians belong to, and describe the Lanczos algorithm, which allows for efficient calculation of the ground state eigenvalue and eigenvector, and thus the ground state properties of a system. Yet in this work, we are mainly interested in infinite temperature calculations, for which in principle sampling of the whole spectrum is required. To this end, in subsequent sections, we develop a scheme for the time evolution of an arbitrary state, called the Krylov propagator [63], and in the last section combine it with the idea of Dynamical Quantum Typicality (DQT), which states that a single pure state can have the same properties as an ensemble density matrix [100–102]. This will produce a numerical algorithm for the efficient calculation of time-dependent correlation functions without the need for Exact Diagonalization.

## 2.1 Problems with Exact Diagonalization

The most straightforward numerical method for studying discrete quantum many-body systems is without a doubt Exact Diagonalization (ED) [103]. It belongs to the family of the so-called direct algorithms (cf. Fig 2.1) and allows one to obtain a numerically exact set of eigenvalues and eigenvectors and subsequently compute any desired properties of the system, be it thermal expectation values, time evolution, Green's functions, etc. Unfortunately, the starting point of any ED calculation is the expression of the Hamiltonian as a dense matrix, in the Hilbert space basis of choice. Taking into account the fact that the dimension many-body Hilbert space grows exponentially with the size of the system, the memory cost quickly becomes prohibitive, even when exploiting conservation laws and related symmetries. For example, in the case of a spin chain of length L, with the on-site basis dimension being 2, the full dimension of the Hilbert space would be $\mathcal{D} = 2^L$. Taking a modest length of 25 sites gives $2^{25} = 33554432 \approx 3.36 \cdot 10^7$ basis states and a memory footprint of the Hamiltonian matrix of around 9PB (using double-precision floating point numbers), which is 9000 times more than the typical consumer hard drive capacity of 1TB. Even assuming some kind of distributed memory platform allowing for handling such large matrices, the computational complexity of ED, requiring $O(\mathcal{D}^3)$ operations, is the next major hurdle. Therefore, it is exceedingly difficult to probe the thermodynamic limit physics and ED calculations suffer from finite size effects.

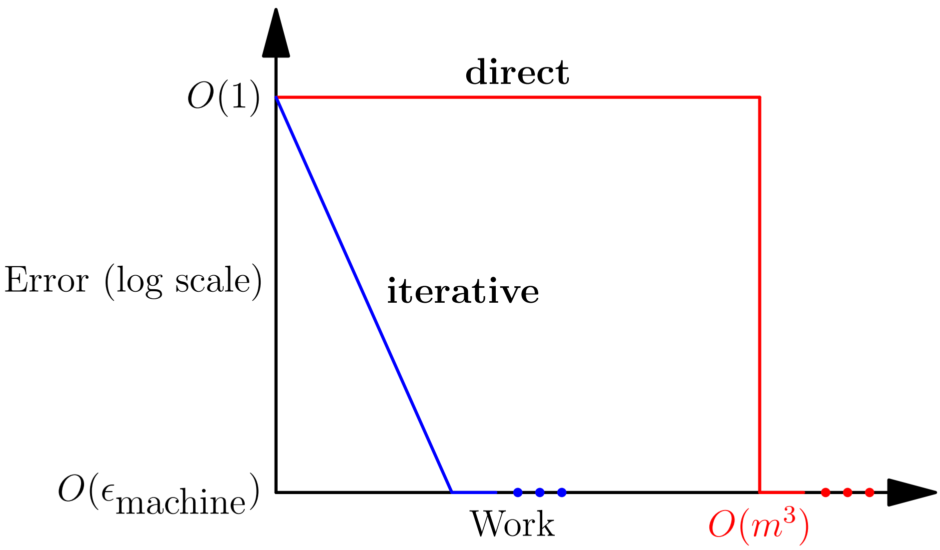



Figure 2.1: Schematic representation of the difference between direct (such as Exact Diagonalization) and iterative (such as Lanczos iteration) algorithms. The advantage of iterative methods comes from the fact that they can be stopped midway after desired precision is reached. On the other hand, direct algorithms require all $O(m^3)$ operations before any results can be extracted. Figure reproduced from Trefethen and Bau [61].

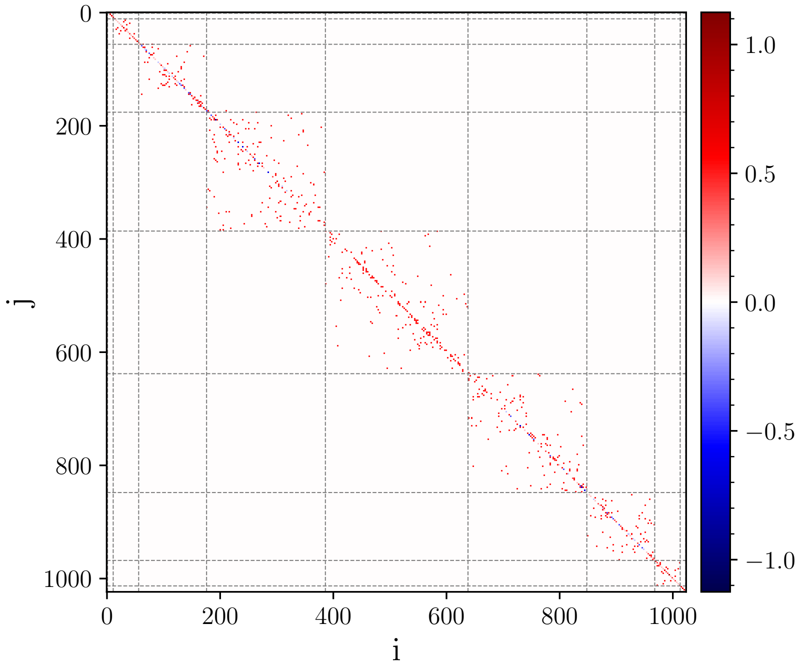



Figure 2.2: Ising basis representation of matrix of the XXZ Hamiltonian $H = J\sum_i \left[\frac{1}{2}\left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + \Delta S_i^z S_{i+1}^z\right]$ on 10 sites, with $J = 1$ and $\Delta = 0.5$. Basis states are sorted according to the magnetization which yields the block structure emphasized by dashed lines. The filling factor $\mu$ is approximately 0.005.

A closer investigation of the Hamiltonian matrix, expressed in the Ising basis, quickly reveals the inefficiency of dense storage. Looking at Figure 2.2, we see that most of the matrix elements are zero. Only about $\mu \propto \mathcal{D}$ out of $\mathcal{D}^2$ matrix elements are non-zero. Hence, a numerical scheme leveraging this sparsity is highly desirable. This is exactly what the Krylov subspace algorithms do, by the virtue of requiring only a ”black box” computation of matrix-vector product, which can be fairly easily implemented in a way requiring only $O(\mu\mathcal{D})$ operations.

## 2.2 Calculation of ground state

Our goal in this section is to develop the Lanczos algorithm for ground-state search of Hermitian matrices, and along the way to understand how and why it works.

### 2.2.1 Arnoldi iteration

The Lanczos algorithm is a special case of a more general algorithm, called Arnoldi iteration, designed to transform a general, non-Hermitian matrix $A \in \mathbb{C}^{m\times m}$ via a orthogonal [1] similarity transformation to a Hessenberg form $A = QHQ^\dagger$. Such transformation always exists [104]. A square, $m \times m$ matrix $H$ is said to be in **upper Hessenberg form** if $\forall i, j \in \{1, \ldots, n\} : i >$

[1] Orthogonal in this context means that $Q^\dagger Q = I_{m\times m}$

$j+1 \implies (A)_{i,j} = 0$. It is said to be in **lower Hessenberg form** if its transpose is in upper Hessenberg form. A Hessenberg matrix differs from a triangular one by one additional super- or subdiagonal. Such form is desirable because many numerical algorithms in linear algebra experience considerable speedup from leveraging the triangular structure of a matrix, and sometimes those benefits carry over to this almost-triangular case. A particularly important strength of the Arnoldi iteration is that it can be interrupted before completion (cf Fig. 2.1), thus producing only an approximation of the Hessenberg form in a situation where $m$ is so large, that full computations are infeasible (eg. in quantum many-body physics).

Assume now that we can only compute the first $n < m$ columns of the equation $AQ = QH$. Let $Q_n$ be the restriction of $Q$ to $n$ columns and let them be denoted by $\mathbf{q_1}, \mathbf{q_2}, \dots \mathbf{q_n} \in \mathbb{C}^m$. Denoting by $\tilde{H}_n$ the $(n+1) \times n$ upper left section of H, which is also a Hessenberg matrix, we can write down the following $n$-step approximation to the full decomposition

$$AQ_n = Q_{n+1}\tilde{H}_n \tag{2.2}$$

From this equation we can deduce an $n+1$ term recurrence relation for the column $\mathbf{q_{n+1}}$, however it is perhaps best illustrated with a simple example in the first place.

**Example 2.1** *Let $A \in \mathbb{C}^{3\times3}$, $AQ = QH$ be the Hessenberg decomposition and corresponding matrix elements be denoted by lowercase letters. We consider the approximation for $n = 2$, i.e. $AQ_2 = Q_3\tilde{H}_2$. On the right-hand side*

$$AQ_2 = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \\ q_{31} & q_{32} \end{bmatrix} = \begin{bmatrix} a_{11}q_{11} + a_{12}q_{21} + a_{13}q_{31} & a_{11}q_{12} + a_{12}q_{22} + a_{13}q_{32} \\ a_{21}q_{11} + a_{22}q_{21} + a_{23}q_{31} & a_{21}q_{12} + a_{22}q_{22} + a_{23}q_{32} \\ a_{31}q_{11} + a_{32}q_{21} + a_{33}q_{31} & a_{31}q_{12} + a_{32}q_{22} + a_{33}q_{32} \end{bmatrix}$$
$$= \begin{bmatrix} (A\mathbf{q_1})_1 & (A\mathbf{q_2})_1 \\ (A\mathbf{q_1})_2 & (A\mathbf{q_2})_2 \\ (A\mathbf{q_1})_3 & (A\mathbf{q_2})_3 \end{bmatrix}$$

*On the left-hand side*

$$Q_3H_2 = \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{21} & q_{22} & q_{23} \\ q_{31} & q_{32} & q_{33} \end{bmatrix} \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \\ 0 & h_{32} \end{bmatrix} = \begin{bmatrix} q_{11}h_{11} + q_{12}h_{21} & q_{11}h_{12} + q_{12}h_{22} + q_{13}h_{32} \\ q_{21}h_{11} + q_{22}h_{21} & q_{21}h_{12} + q_{22}h_{22} + q_{23}h_{32} \\ q_{31}h_{11} + q_{32}h_{21} & q_{31}h_{12} + q_{32}h_{22} + q_{33}h_{32} \end{bmatrix}$$
$$= \begin{bmatrix} h_{11}(\mathbf{q_1})_1 + h_{21}(\mathbf{q_2})_1 & h_{12}(\mathbf{q_1})_1 + h_{22}(\mathbf{q_2})_1 + h_{32}(\mathbf{q_3})_1 \\ h_{11}(\mathbf{q_1})_2 + h_{21}(\mathbf{q_2})_2 & h_{12}(\mathbf{q_1})_2 + h_{22}(\mathbf{q_2})_2 + h_{32}(\mathbf{q_3})_2 \\ h_{11}(\mathbf{q_1})_3 + h_{21}(\mathbf{q_2})_3 & h_{12}(\mathbf{q_1})_3 + h_{22}(\mathbf{q_2})_3 + h_{32}(\mathbf{q_3})_3 \end{bmatrix}$$

*From the above calculation and 2.2 we can read off two identities*

$$A\mathbf{q_1} = h_{11}\mathbf{q_1} + h_{21}\mathbf{q_2}$$
$$A\mathbf{q_2} = h_{21}\mathbf{q_1} + h_{22}\mathbf{q_2} + h_{32}\mathbf{q_3}$$

*Therefore we get, assuming $\mathbf{q_1}$ is known,*

$$\mathbf{q_2} = \frac{A\mathbf{q_1} - h_{11}\mathbf{q_1}}{h_{21}}$$
$$\mathbf{q_3} = \frac{A\mathbf{q_2} - h_{21}\mathbf{q_1} - h_{22}\mathbf{q_2}}{h_{32}}$$

Generalizing the above example, we arrive at the desired $n+1$ term recurrence relation for $\mathbf{q_{n+1}}$

$$\mathbf{q_{n+1}} = \frac{A\mathbf{q_n} - \sum_{m=1}^{n} h_{mn}\mathbf{q_m}}{h_{n+1,n}} \tag{2.3}$$

We can now easily cast the above recurrence into a pseudocode algorithm:

---

**Algorithm 1** Arnoldi iteration

---

**Input:** $\mathbf{v} \in \mathbb{C}^m$, $A \in \mathbb{C}^{m\times m}$, number of steps $n$

**Output:** columns of $Q_n$, matrix elements of $H_n$

```
 1: q_1 = v/‖v‖                ▷ components of v are usually drawn from uniform distribution
 2: for i = 1 : n − 1 do
 3:     q = A q_i
 4:     for j = 1 : i do
 5:         h_ji = cdot(q_j, q)            ▷ cdot is the complex dot product on C^m.
 6:         q = q − h_ji q_j               ▷ In exact arithmetic, this ensures orthogonality.
 7:     end for
 8:     h_{i+1,i} = ‖q‖
 9:     q_{i+1} = q/h_{i+1,i}
10: end for
```

---

Step 9 of the Algorithm 1 may be questionable, as we are dividing by a norm of a vector, which after all can be equal to zero. However, in practical applications of Arnoldi iteration, it usually means that our calculations have converged and the iterations may be stopped.

Examining closely the Arnoldi iteration algorithm, we notice that it is essentially the Gram-Schmidt procedure applied to the vectors $\{\,\mathbf{v}, A\mathbf{v}, \ldots, A^{n-1}\mathbf{v}\,\}$ and hence the vectors $\{\,\mathbf{q_1}, \mathbf{q_2}, \ldots, \mathbf{q_n}\,\}$ form an orthonormal basis of the Krylov subspace $\mathcal{K}_n$. The orthonormality condition is concisely expressed by the fact that $Q_n^\dagger Q_{n+1}$ is the $n \times (n+1)$ identity matrix. Multiplying the left-hand side of equation (2.2) by $Q_n^\dagger$ we get

$$Q_n^\dagger A Q_n = \underbrace{Q_n^\dagger Q_{n+1}}_{\mathrm{Id}_{n\times(n+1)}} \tilde{H}_n = H_n \in \mathbb{C}^{n\times n} \tag{2.4}$$

where $H_n$ is the Hessenberg matrix $\tilde{H}_n$ with its last row removed.

To understand the meaning of matrix $H_n$ from the point of view of linear algebra, consider the following reasoning. Imagine we are given an endomorphism of the space $\mathbb{C}^m$, represented in the standard basis by a matrix $A$. We would like to restrict it to an endomorphism of the Krylov subspace $\mathcal{K}_n$, $n < m$. Of course, as $\mathbf{q} \in \mathcal{K}_n \implies \mathbf{q} \in \mathbb{C}^m$, we can calculate the action of $A$ on a vector from Krylov subspace in a straightforward way. However, the resulting vector $A\mathbf{q}$ is not guaranteed to be an element of $\mathcal{K}_n$. We need to orthogonally project it back to the subspace. Such projection is realized by $Q_n Q_n^\dagger \in \mathbb{C}^{m\times m}$ and hence, with respect to the standard basis on $\mathbb{C}^m$, the desired restriction can be written as $Q_n Q_n^\dagger A$. Transforming it to the basis given by columns of $Q_n$ we get $Q_n^{-1}\left(Q_n Q_n^\dagger A\right) Q_n = Q_n^\dagger A Q_n$. Thus, matrix $H_n$ is the orthogonal projection of $A$ to the subspace $\mathcal{K}_n$, represented in the basis $\{\,\mathbf{q_1}, \mathbf{q_2}, \ldots, \mathbf{q_n}\,\}$.

$H_n$ is once again a square matrix, so we can talk about its eigenvalues $\{\theta_i\}_{i=1}^n$ in the usual fashion. These numbers are called the *Arnoldi eigenvalues estimates at step n*, or the *Ritz* *values with respect to* $\mathcal{K}_n$. Given the interpretation above, we may suspect that they would be related to the eigenvalues of the original matrix $A$. Indeed, as we shall see in a moment, some of the Ritz values are extremally good approximations of some of the original eigenvalues.

### 2.2.2 Polynomial approximation and eigenvalues

By carrying out the Arnoldi iterations for successive steps, and at each step $n$ (or at just some of the steps) calculating the eigenvalues of the Hessenberg matrix $H_n$, we are left with sequences of Ritz values. Some of them often converge rapidly to, what we reasonably assume, are eigenvalues of the original matrix $A$. However, in practice, the maximal accessible $n$ is much smaller than $m$, so we cannot expect to find all eigenvalues. As it turns out, Arnoldi iteration typically finds extremal eigenvalues, which fortunately are those that we are interested in.

Before we will understand the details, let us introduce a different, seemingly unrelated problem of *polynomial approximation*. We can take any $\mathbf{q} \in \mathcal{K}_n$ and using the defining basis of Krylov subspace $\mathcal{K}_n$(Definition 2.1), expand is as

$$\begin{aligned}\mathbf{q} &= a_0\mathbf{v} + a_1A\mathbf{v} + a_2A^2\mathbf{v} + \ldots + a_{n-1}A^{n-1}\mathbf{v} \\ &= \left(a_0\mathbb{1} + a_1A + a_2A^2 + \ldots + a_{n-1}A^{n-1}\right)\mathbf{v}\end{aligned}$$

Utilizing the special structure of vectors from $\mathcal{K}_n$, we can define a polynomial $p(z) = a_0 + a_1z + a_2z^2 + \ldots + a_{n-1}z^{n-1}$, and concisely write our vector as $\mathbf{q} = p(A)\mathbf{v}$. As the vector $\mathbf{q}$ was arbitrary, we have established an isomorphism between the $n$-th Krylov subspace and the space of complex polynomials of maximal degree $n-1$. We are now ready to state the problem:

**Arnoldi Approximation Problem**

Given a matrix $A \in \mathbb{C}^{m\times m}$ and a vector $\mathbf{v} \in \mathbb{C}^m$, find
$p \in P^n := \{\, a_0 + a_1z + \ldots + a_{n-1}z^{n-1} + z^n \mid a_0, a_1, \ldots a_{n-1} \in \mathbb{C}\,\}$
such that $\|p(A)\mathbf{v}\|_2$ is minimized.

Remarkably, the Arnoldi approximation is the exact solution to this problem. This fact is interesting enough that we state it here as a theorem and, following Trefethen and Bau [61], provide a complete proof.

**Theorem 2.1** *If* $dim(\mathcal{K}_n) = n$*, i.e. matrix having columns* $\mathbf{v}, A\mathbf{v}, \ldots, A^{n-1}\mathbf{v}$ *is of rank* $n$*, then the Arnoldi Approximation Problem has a unique solution* $p^n \in P^n$*, given by the characteristic polynomial of the matrix* $H_n$*, defined by* (2.4)*.*

**Proof.** We start with an observation, that given a polynomial $p \in P^n$, the vector $p(A)\mathbf{v}$ can be written as $p(A)\mathbf{v} = A^n\mathbf{v} - Q_n\mathbf{r}$ for some $\mathbf{r} \in \mathbb{C}^n$. To see that, note that $(A^n\mathbf{v} - p(A)\mathbf{v}) \in \mathcal{K}_n$ and columns of $Q_n$ form an orthonormal basis of $\mathcal{K}_n$. Now, we can recast our problem into a slightly different language, namely finding a vector in $\mathcal{K}_n$ that is the closest in the sense of $L_2$ norm to $A^n\mathbf{v}$. In short:

$$\mathbf{r}^* = \min_{\mathbf{r}\in\mathbb{C}^n} \|A^n\mathbf{v} - Q_n\mathbf{r}\|$$

To achieve that, we need to have $p(A)\mathbf{v} \perp \mathcal{K}_n$, that is $p(A)\mathbf{v}$ must be orthogonal to all basis vectors spanning $\mathcal{K}_n$. This is consisely expressed as $Q_n^\dagger p(A)\mathbf{v} = \mathbf{0} \in \mathbb{C}^n$.

Now, we know that the Hessenberg factorization $A = QHQ^\dagger$ exists, and is approximated by $n$ steps of the Arnoldi iteration. Thus, the matrices $Q$ and $H$ can have the following block structure:

$$Q = \begin{bmatrix} Q_n & V \end{bmatrix}, \quad H = \begin{bmatrix} H_n & 0_{n\times(m-n)} \\ Y & 0_{(m-n)\times(m-n)} \end{bmatrix} \tag{2.5}$$

where $V \in \mathbb{C}^{m\times(m-n)}$ is a matrix with orthonormal columns, which are also orthogonal to columns of $Q_n$, and matrix $Y \in \mathbb{C}^{(m-n)\times n}$ has only the upper-right entry different from zero (the one from the last row of $\tilde{H}_n$). Using the Hessenberg factorization we can write our condition as $Q_n^\dagger Q p(H) Q^\dagger \mathbf{v} = \mathbf{0}$, and because equation (2.5) introduces partitions into *conformable* blocks, we can use the rules of block-matrix algebra to simiplify it further [105].

First, let us investigate closely the structure of $p(H)$. We observe that

$$\begin{aligned}
H^2 &= \begin{bmatrix} H_n & 0_{n\times(m-n)} \\ Y & 0_{(m-n)\times(m-n)} \end{bmatrix}^2 = \begin{bmatrix} H_n^2 & 0_{n\times(m-n)} \\ YH_n & 0_{(m-n)\times(m-n)} \end{bmatrix} \\
H^3 &= \begin{bmatrix} H_n & 0_{n\times(m-n)} \\ Y & 0_{(m-n)\times(m-n)} \end{bmatrix}^3 = \begin{bmatrix} H_n^3 & 0_{n\times(m-n)} \\ YH_n^2 & 0_{(m-n)\times(m-n)} \end{bmatrix} \\
&\dots \\
H^n &= \begin{bmatrix} H_n & 0_{n\times(m-n)} \\ Y & 0_{(m-n)\times(m-n)} \end{bmatrix}^n = \begin{bmatrix} H_n^n & 0_{n\times(m-n)} \\ YH_n^{n-1} & 0_{(m-n)\times(m-n)} \end{bmatrix}
\end{aligned}$$

Thus $p(H)$ can be written as

$$\begin{aligned}
p(H) &= a_0\mathbb{1} + a_1 H + a_2 H^2 + \ldots + a_{n-1}H^{n-1} + H^n \\
&= \begin{bmatrix} a_0\mathbb{1} + a_1 H_n + a_2 H_n^2 + \ldots + a_{n-1}H_n^{n-1} + H_n^n & 0_{n\times(m-n)} \\ a_0\mathbb{1} + a_1 Y + a_2 YH_n + \ldots + a_{n-1}YH_n^{n-2} + YH_n^{n-1} & 0_{(m-n)\times(m-n)} \end{bmatrix} \\
&= \begin{bmatrix} p(H_n) & 0 \\ \tilde{Y} & 0 \end{bmatrix}
\end{aligned}$$

We have now all the pieces to simplify the orthogonality condition:

$$\begin{aligned}
\mathbf{0} &= Q_n^\dagger Q p(H) Q^\dagger \mathbf{v} \\
&= \begin{bmatrix} Q_n^\dagger \end{bmatrix} \begin{bmatrix} Q_n & V \end{bmatrix} \begin{bmatrix} p(H_n) & 0_{n\times(m-n)} \\ \tilde{Y} & 0_{(m-n)\times(m-n)} \end{bmatrix} \begin{bmatrix} Q_n^\dagger \\ U^\dagger \end{bmatrix} \mathbf{v} \\
&= \begin{bmatrix} \mathbb{1}_{n\times n} & 0_{n\times(m-n)} \end{bmatrix} \begin{bmatrix} p(H_n) & 0_{n\times(m-n)} \\ \tilde{Y} & 0_{(m-n)\times(m-n)} \end{bmatrix} \begin{bmatrix} Q_n^\dagger \\ U^\dagger \end{bmatrix} \mathbf{v} \\
&= \begin{bmatrix} p(H_n) & 0_{n\times(m-n)} \end{bmatrix} \begin{bmatrix} Q_n^\dagger \\ U^\dagger \end{bmatrix} \mathbf{v} \\
&= p(H_n) Q_n^\dagger \mathbf{v}
\end{aligned}$$

As a final step, notice that by construction the first row of $Q_n^\dagger$ is $\mathbf{v}/\|\mathbf{v}\|$, and all the remaining rows are orthogonal to $\mathbf{v}$, therefore only the first column of $H_n$, or the first $n$ elements of the first column of $H$ are required to be 0. By Caylel-Hamilton theorem, this is guaranteed if we take $p = p^n$, where $p^n$ is the characteristic polynomial of $H_n$. For the uniqueness part, suppose that there exists another polynomial, say $q^n$ such that $q^n \perp \mathcal{K}_n$. But then $p^n - q^n$ is a nonzero polynomial of degree $n-1$ (because $p^n$, $q^n$ are monic) such that $(p^n - q^n)(A)\mathbf{v} = \mathbf{0}$, and hence vectors $\mathbf{v}, A\mathbf{v}, \ldots, A^{n-1}\mathbf{v}$ are linearly dependent, which violates assumption that $\dim(\mathcal{K}_n) = n$.

■

This theorem allows us to interpret the Arnoldi eigenvalues estimates $\{\theta_i\}$ as the roots of the optimal polynomial. Following the above proof, it is relatively easy to see that they are scale-invariant, i.e. if $A \to \alpha A$ for some $\alpha \in \mathbb{C}$, then $\{\theta_i\}_{i=1}^n \to \{\alpha\theta_i\}_{i=1}^n$ and invariant under unitary transformations, i.e. if $A \to UAU^\dagger$ and $\mathbf{v} \to U\mathbf{v}$ for some unitary $U$, then the Arnoldi estimates are unchanged. Furthermore, owing to the properties of monic polynomials, they are also translationally invariant, namely if $A \to A + \alpha\mathbb{1}$ for some $\alpha \in \mathbb{C}$, then $\{\theta_i\}_{i=1}^n \to \{\theta_i + \alpha\}_{i=1}^n$.

In the end, we see that the direct purpose of Arnoldi iteration is to solve a polynomial approximation problem and not to find eigenvalues. However, those two problems have enough in common, that the Arnoldi iteration produces some correct eigenvalues as a 'by-product'. We can reason along the following lines. If our task is to find a polynomial $p \in P^n$ minimizing $\|p(A)\|$, it may be a good idea to select a polynomial that has roots close to the eigenvalues of $A$. In an extreme situation, when there exists a diagonalization of $A$ and it posses only $n \ll m$ distinct eigenvalues, the minimal polynomial[2] will coincide with the characteristic polynomial computed via Arnoldi iteration after $n$ steps and the Arnoldi eigenvalue approximations will be exact, provided we start from $\mathbf{v}$ having nonzero overlap with all eigenvectors of $A$. In most practical situations, however, the agreement is only approximate, namely Arnoldi eigenvalues are close to real eigenvalues, and computed polynomial is such that $\|p(A)\|$ is small.

There is more to this story than we have told here, particularly a nice geometric interpretation of Algorithm 1 via *Arnoldi lemniscates*, which illustrates why extremal eigenvalues are found first, however, we shall not concern ourselves with those matters any further. Interested readers are once again referred to Trefethen and Bau [61], whereas we turn our attention to the case of utmost interest in quantum mechanics, namely Arnoldi iteration for Hermitian matrices.

### 2.2.3 Restriction to Hermitian matrices: Lanczos iteration

After the mathematical detour of the previous section, armed with a deeper understanding of Krylov subspace and Arnoldi iteration, we are ready to investigate the algorithms that are of direct relevance to condensed matter physics, starting with Lanczos iteration. From this point onwards, we shall return to the favored by physicists Dirac bra-ket notation, namely $|v\rangle \equiv \mathbf{v}$ and $\langle v| = \mathbf{v}^\dagger$. Moreover, we assume the matrix $A$ to be Hermitian, as in most use cases it will be the Hamiltonian of our system.

It immediately follows from (2.4) that, given $A$ is Hermitian, the Hessenberg matrix $H_n$ will also be Hermitian. But a matrix that is both Hessenberg and Hermitian, must of course

[2] A minimal polynomial of matrix $A$ is a polynomial $p$ of the smallest degree such that $p(A) = 0$. It always divides the characteristic polynomial.

be tridiagonal! Indeed, to see this directly, let us write the equation for matrix elements $(H_n)_{ij}$ of $H_n$:

$$(H_n)_{ij} = \sum_{r,s}(Q_n^\dagger)_{ir}(A)_{rs}(Q_n)_{sj} = \langle q_i|A|q_j\rangle \tag{2.6}$$

where $|q_i\rangle, |q_j\rangle$ are respectively $i$-th and $j$-th columns of matrix $Q_n$. From the recurrence relation (2.3) we know that $A|q_j\rangle \in \text{span}\{|q_1\rangle, \ldots, |q_{j+1}\rangle\}$, and that it is orthogonal to all $|q_i\rangle$ with $i > j+1$. Therefore $(H_n)_{ij} = 0$ for $i > j+1$. Similarly, by taking the Hermitian conjugate of equation (2.6), we get

$$(H_n)_{ij} = \langle q_j|A^\dagger|q_i\rangle \triangleq \langle q_j|A|q_i\rangle \tag{2.7}$$

where $\triangleq$ follows from assumed hermiticity of $A$. Repeating the above reasoning we quickly obtain that $(H_n)_{ij} = 0$ also for $j > i+1$ and hence the matrix is tridiagonal. In literature the diagonal is usually denoted by $\alpha_i \equiv (H_n)_{ii}$, whereas the sub- and superdiagonal are denoted by $\beta_i \equiv (H_n)_{i,i+1} = (H_n)_{i+1,i}$. The relation for $|q_{n+1}\rangle$ becomes a 3-step recurrence:

$$|q_{n+1}\rangle = \frac{A|q_n\rangle - \beta_{n-1}|q_{n-1}\rangle - \alpha_n|q_n\rangle}{\beta_n} \tag{2.8}$$

This has a tremendous impact on the practical applications of the algorithm, as both computational and memory costs decrease significantly. We are now ready to state the simplified version of the Algorithm 1. Another important observation is that $\alpha_n$'s are diagonal elements

**Algorithm 2** Lanczos iteration

**Input:** $|v\rangle \in \mathbb{C}^m$, $A \in \mathbb{C}^{m\times m}$ such that $A^\dagger = A$, number of steps $n$

**Output:** columns of $Q_n$, tridiagonal matrix $H_n$

$\beta_0 = 0$
$|q_0\rangle = \mathbf{0} \in \mathbb{C}^m$
$|q_1\rangle = |v\rangle / \||v\rangle\|$
**for** $i = 1 : n-1$ **do**
    $|q\rangle = A|q_i\rangle$
    $\alpha_i = \langle q_i|q\rangle$
    $|q\rangle = |q\rangle - \beta_{i-1}|q_{i-1}\rangle - \alpha_i|q_i\rangle$
    $\beta_i = \||q\rangle\|$
    $|q_{i+1}\rangle = |q\rangle / \beta_i$
**end for**

of a Hermitian matrix, and $\beta_n$'s are norms of the vector $|q\rangle$ in subsequent iterations, both of which are real. Therefore, even if our Hamiltonian is complex, the numbers $\alpha_n$ and $\beta_n$ can be stored as vectors of real floating point numbers, decreasing memory requirements even further. Matrix $Q_n$ is of dimension $m \times n$, so keeping it in full in the memory can still be costly. Fortunately, at each step of the Lanczos iteration, no more than three vectors are necessary $(|q\rangle, |q_i\rangle, |q_{i-1}\rangle)$ so the storage of full matrix $Q_n$ is reduntant. Extremal eigenvalues are then obtained by explicit diagonalization of the constructed matrix $H_n = V_n D_n (V_n)^\dagger$, which can be done efficiently using specialized routines for tridiagonal matrices. However, this approach has its drawbacks when we are interested also in the ground state eigenvector, which will be the case in further applications.

It turns out that the Lanczos iteration can approximate not only eigenvalues, but also corresponding eigenvectors. They are the eigenvectors of the tridiagonal matrix $H_n$, transformed back to the original Hilbert space. Given the full Hessenberg decomposition, we would have

$$A = QHQ^\dagger = Q(VDV^\dagger)Q^\dagger = (QV)D(QV)^\dagger \tag{2.9}$$

Restriction to $n$-step iteration produces an approximation $A \approx (Q_n V_n) D_n (Q_n V_n)^\dagger$. The simplest form of Lanczos iteration presented in Algorithm 2 is sufficient to obtain only the ground state eigenvector with machine precision because eigenvectors of excited states are plagued by the loss of orthogonality stemming from the nature of floating point numbers. We shall have a brief look at this problem at the end of this section.

The ground state vector $|\psi_0\rangle$ can be then read of as the first column $Q_n V_n$. However, there is a problem. To conserve memory, we have not constructred the whole matrix $Q_n$ explicitly, but only three of its columns at a given time and hence do not have access to the matrix product $Q_n V_n$. We need a second pass of the Lanczos iteration, with a single line added for iterative calculation of the first column. It can be summarized by the the following piece of pseudocode:

**Algorithm 3** Second pass of Lanczos iteration, for calculating ground state eigenvector

**Input:** $|\psi_0\rangle = \mathbf{0} \in \mathbb{C}^m$, matrix $V_n$ from Alg. 2, rest of input data from Alg. 2

**Output:** columns of $Q_n$, tridiagonal matrix $H_n$

$\beta_0 = 0$
$|q_0\rangle = \mathbf{0} \in \mathbb{C}^m$
$|q_1\rangle = |v\rangle / \||v\rangle\|$
**for** $i = 1 : n-1$ **do**
  $|\psi_0\rangle = |\psi_0\rangle + (V_n)_{i,1} |q_i\rangle$ ▷ this is the only difference from Alg. 2
  $|q\rangle = A|q_i\rangle$
  $\alpha_i = \langle q_i|q\rangle$
  $|q\rangle = |q\rangle - \beta_{i-1}|q_{i-1}\rangle - \alpha_i |q_i\rangle$
  $\beta_i = \||q\rangle\|$
  $|q_{i+1}\rangle = |q\rangle / \beta_i$
**end for**

To finish this section, let us discuss quickly the convergence properties of Lanczos iteration. We have one free parameter, namely the number of iterations $n$. If we had carried out the full Arnoldi iteration, as described in 1, the orthogonality of subsequent columns of matrix $Q_n$ would be guaranteed by the explicit Gram-Schmidt procedure and we in principle could continue it up to $n = m$ obtaining the full Hessenberg decomposition. However, restricting ourselves to a three-step recurrence in Lanczos iteration we rely on mathematical identities to force the orthogonality of $|q_i\rangle$ with all previous vectors. Those are valid in exact arithmetic, but can quickly break down when using floating point numbers, as it is done in practice. Therefore, the iteration is unstable and should be stopped as soon as the desired accuracy is reached. Taking $E_n^1$ to be the lowest eigenvalues of $H_n$, the convergence criterion can be defined as $|E_{n+1}^1 - E_n^1|/|E_n^1| < \varepsilon$ for some small $\varepsilon$, e.g. $10^{-14}$. As long as it is nondegenerate, the convergence usually happens quite quickly for both the lowest eigenvalue and corresponding eigenvector. To reliably obtain higher eigenstates one needs to perform reorthogonalization, but it requires keeping the matrix $Q_n$ in memory which can be very costly.

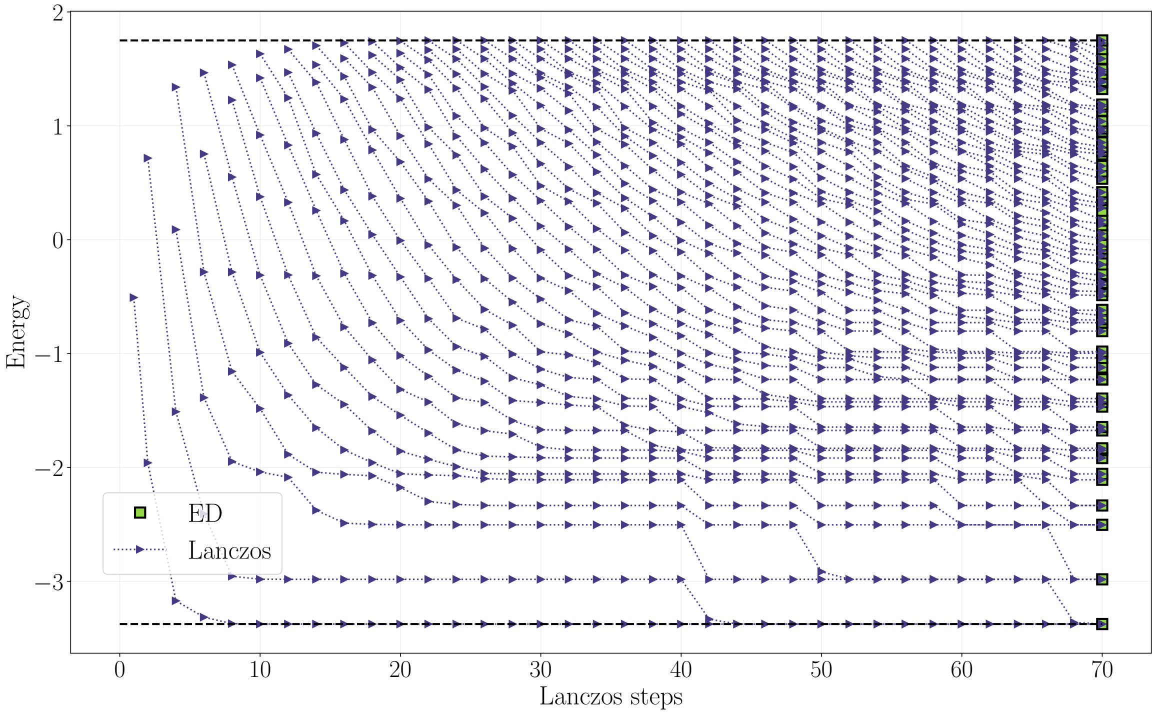



Figure 2.3: Plot of Arnoldi eigenvalues as a function of Lanczos steps, for a XXZ chain on 8 sites in the subspace with 0 total magnetization. The extremal eigenvalues converge very quickly to the values matching Exact Diagonalization. The numerical instability of Lanczos iteration is especially visible for a few lowest eigenvalues, where multiple ghosts start appearing. After $\binom{8}{4} = 70$ Lanczos steps, we should observe the exact spectrum emerging from Arnoldi approximates. However, we see that the ground state is triple degenerated, instead of unique as it should be.

This instability can manifest itself in an interesting way, namely in the form of additional eigenvalues, called Lanczos 'ghosts'. They are spurious copies of already found eigenvalues, which start apperating after too many iteration steps (cf. Fig. 2.3) They are difficult to understand rigorously, however Trefethen and Bau [61] offers a nice heuristic explanation. Reaching convergence of some Arnoldi approximated eigenvalue to the true eigenvalue of A causes annihilation of the corresponding eigenvector component in the vector $|q\rangle$. However, rounding errors originating from floating-point arithmetic cause $|q\rangle$ to again develop a component in the direction of the eigenvector and thus, after a certain number of iterations, the appearance of another Arnoldi approximated eigenvalue is necessary to annihilate it. This can go on and on producing more and more Lanczos 'ghosts'. Fortunately, for all further applications in this thesis, we will only require the lowest eigenstate, so we can avoid most of the instability problems by stopping the iteration sufficiently quickly.

## 2.3 Time evolution via the Krylov propagator

Even though the original purpose of Lanczos iteration was to approximate boundaries of the spectrum of matrices and solve systems of linear equation [106, 107], it can also be employed to evaluate functions of Hermitian matrices. Given any unitary (or orthogonal) decomposition of the matrix $A = QHQ^\dagger$, and an analytic function $f$[3], we have $f(A) = Qf(H)Q^\dagger$. And indeed, Lanczos iteration gives us such decomposition, albeit an approximate one $A \approx Q_n H_n Q_n^\dagger$. Because of this approximate character and convergence problems discussed at the end of the previous section, the global approximation of $f(A)$ via Lanczos iteration is a hopeless endeavor. However, the goal of this section is to calculate time evolution, which boils down to the evaluation of how the time-evolution operator $\exp\left(-i\hat{H}t\right)$ acts on some state $|v\rangle$ in the Hilbert space for a given Hamiltonian $\hat{H}$. It is thus enough to restrict our attention to the problem of calculating $f(A)|v\rangle$, for which the Lanczos iteration turns out to be an excellent tool.

Let us now assume that the matrix $A$ is our Hamiltonian $\hat{H}$, acting on Hilbert space $\mathcal{H} \cong \mathbb{C}^m$ and $|v\rangle \in \mathcal{H}$ is some fixed state. Using the approximate factorization derived from (2.9), we get

$$f(\hat{H})\,|v\rangle \approx (Q_n V_n) f(D_n) (Q_n V_n)^\dagger \,|v\rangle \tag{2.10}$$

where $D_n$ is a real diagonal matrix, so $f(D_n)$ is easy to compute. Previously, we have started the construction of the Krylov subspace basis from some random vector. Now, let us change this slighlty and start from the vector $|v\rangle$ instead, which we assume to be normalized. Then, the first column of $Q_n$ will be $|v\rangle$, whereas all subsequent columns will be orthogonal (up to some numerical errors), yielding $Q_n^\dagger\,|v\rangle = |e_1\rangle$, which is the first vector in canonical basis of $\mathbb{C}^n$, i.e. $|e_1\rangle = [1, 0, 0, \ldots, 0]$. Equation (2.10) then simplifies to

$$f(\hat{H})\,|v\rangle \approx Q_n(V_n f(D) V_n^\dagger) Q_n^\dagger\,|v\rangle = Q_n(V_n f(D) V_n^\dagger)\,|e_1\rangle = Q_n f(H_n)\,|e_1\rangle \tag{2.11}$$

Moreover, $f(H_n)\,|e_1\rangle$ is just the first column of $f(H_n)$, because $(f(H_n)\,|e_1\rangle)_i = \sum_j (f(H_n))_{i,j}\,\delta_{1,j} = (f(H_n))_{i,1}$. So we do not need to compute the full matrix, but only a single vector of the form

$$(f(H_n))_{i,1} = \sum_j (V_n)_{i,j}\, f(D_n)_j \left(V_n^\dagger\right)_{j,1} = \sum_j (V_n)_{i,j}\,(V_n^*)_{1,j}\, f(D_n)_j \tag{2.12}$$

where the diagonal matrix $f(D_n)$ is treated as a vector. Assuming that $f(D_n)$ is already computed, it boils down to a single dot product for each element of the column.

We are now ready to apply this procedure to the problem of interest, namely the time-evolution of a pure state $|\psi(t)\rangle$ in the interval $(t, \Delta t)$. It is described by the Schrödineger equation $i\partial_t\,|\psi(t)\rangle = \hat{H}\,|\psi(t)\rangle$, having a formal solution

$$|\psi(t+\Delta t)\rangle = \exp\left(-i\hat{H}\Delta T\right)|\psi(t)\rangle\,, \tag{2.13}$$

under the assuption that $\hat{H}$ does not depend explicitly on time. The exact exponentiation of the matrix amounts to exact diagonalization which, as mentioned at the beginning of this

[3] A function $f$ is real (complex) analytic if and only if its Taylor series about $x_0$ converges in some neighborhood of $x_0$ pointwise to the function, for every $x_0$ in the domain.

chapter, is a difficult task. However, by letting $f(\hat{H}) = \exp\left(-i\hat{H}\Delta t\right)$ and $|v\rangle = |\psi(t)\rangle$ in equation (2.11) we get an approximation of the action of the time evolution operator on a state, called the **Krylov based propagator** [108], which was originally proposed in the 1980's by Park and Light [63] and has been since used with great success to investigate many different systems [109–112]. The final equation reads

$$|\psi(t+\Delta t)\rangle = \exp\left(-i\hat{H}\Delta T\right)|\psi(t)\rangle \approx Q_n \exp\left(-iH_n\Delta t\right) Q_n^\dagger |\psi(t)\rangle \tag{2.14}$$

$$= Q_n \exp\left(-iH_n\Delta t\right)|e_1\rangle = \sum_{j=1}^{n} \left(f(H_n)\right)_{j,1}|q_j\rangle \tag{2.15}$$

where $|q_j\rangle$ are columns of the unitary (orthogonal) matrix $Q_n$. Because of this orthogonality, the approximation error is bounded from above by the last coefficient $\left(f(H_n)\right)_{n,1}$, i.e.

$$\Big\||\psi(t+\Delta t)\rangle_{\text{exact}} - |\psi(t+\Delta t)\rangle_{\text{Krylov}}\Big\| \leq \left|\left(f(H_n)\right)_{n,1}\right| \tag{2.16}$$

assuming that $\||\psi(t)\rangle\| = 1$. There also exists an estimate of the sufficient dimension of Krylov subspace [113]

$$n \lessapprox 1.5\rho_{\hat{H}}\Delta t > 10 \tag{2.17}$$

where $\rho_{\hat{H}}$ is the spectral radius of Hamiltonian and can be calculated as the difference between the highest and lowest eigenvalue. It is now very simple to cast these expressions into a concrete algorithm

---

**Algorithm 4** Krylov propagator

---

**Input:** input data from Algorithm 2, with $|v\rangle = |\psi(t)\rangle$, time step $\Delta t$

**Output:** propagated state $|\psi(t+\Delta t)\rangle$

1: Run Alg. 2, obtaining eigenvalues $D_i$

2: Calculate $\left(f(H_n)\right)_{i,1}$ using eq. (2.12)

3: Run modified Alg. 3, with $\left(f(H_n)\right)_{i,1}$ instead of $(V_n)_{i,1}$

---

We finish this section with a remark, that the real-time propagator is not the only function of the Hamiltonian which can be calculated using Lanczos techniques. Fairly often encounterd are also the imaginary-time propagator $\exp\left(-\beta H\right)$ and pure state Green's function of some obervable $Q$: $\langle\psi_{\epsilon_0}|\, Q \left(\omega + i\eta + \epsilon_0 + H\right)^{-1} Q\, |\psi_{\epsilon_0}\rangle$ [114]. However, we will not need them for this thesis.

## 2.4 Correlation functions and Quantum Typicality

We are now ready to introduce **time dependent correlation functions** and a method of calculating them using already developed Krylov subspace machinery. This function is defined for a pair of operators $A, B$ as

$$\tilde{C}_{AB}(t) \equiv \mathrm{Re}\langle A(t)B\rangle = \mathrm{Re}\,\mathrm{Tr}\left(\hat{\rho}A(t)B\right) \tag{2.18}$$

where $\hat{\rho} = e^{-\beta H}/\mathcal{Z}$, $\mathcal{Z} = \mathrm{Tr}\left(e^{-\beta H}\right)$ is the canonical ensemble at temperature $T = 1/\beta$, and $A(t) = e^{i\hat{H}t}Ae^{-i\hat{H}t}$ is understood via the Heisenberg picture. In this thesis we are interested only in the infinite temperature properties, so $\hat{\rho} \to \frac{1}{\mathcal{D}}\mathbb{1}$, where $\mathcal{D}$ is the dimension of Hilbert space, however, lets us keep the temperature finite for a while, so we can see the results of subsequent developments in full. Correlation functions allow us to probe the complex dynamics of interacting many-body systems and within Linear Response Theory are directly related to the transport properties [115], so they have been an object of intense study [116–122]. We can use a complete set of eigensetates $|n\rangle$ of the Hamiltonian $\hat{H}$ in order to transform the correlation function into the so-called spectral representation

$$\begin{aligned}
\langle A(t)B\rangle &= \frac{1}{\mathcal{Z}}\operatorname{Tr}\left(A(t)Be^{-\beta H}\right) = \frac{1}{\mathcal{Z}}\operatorname{Tr}\left(e^{i\hat{H}t}Ae^{-i\hat{H}t}Be^{-\beta H}\right) \\
&= \frac{1}{\mathcal{Z}}\sum_{k}\sum_{m,n}\langle k|\,|n\rangle\langle n|\,e^{i\hat{H}t}Ae^{-i\hat{H}t}\,|m\rangle\langle m|\,Be^{-\beta H}\,|k\rangle \\
&= \frac{1}{\mathcal{Z}}\sum_{k}\sum_{m,n}\delta_{k,n}e^{i(\varepsilon_n-\varepsilon_m)t}e^{-\beta\varepsilon_k}\,\langle n|A|m\rangle\,\langle m|B|k\rangle \\
&= \frac{1}{\mathcal{Z}}\sum_{m,n}e^{i(\varepsilon_n-\varepsilon_m)t}e^{-\beta\varepsilon_n}\,\langle m|A|n\rangle^*\,\langle m|B|n\rangle
\end{aligned} \tag{2.19}$$

which is useful for calculations using Exact Diagonalization. Unfortunately, we have already established that ED calculations suffer greatly from the exponential growth of the Hilbert space. We would like to have a more efficient method for calculating $C_{AB}(t)$, capable of accessing larger systems sizes, far beyond the reach of ED. The question is, how the Krylov subspace methods developed so far can help us? After all, we only know how to find the ground state and calculate the time evolution of any state, whereas calculating a correlation function requires taking the trace over a full ensemble of states. This is where the concept of **(Dynamical) Quantum Typicality** ((D)QT) comes into play, which broadly speaking postulates that a set of states with a common feature e.g. the same energy, should give a narrow distribution of some other feature e.g. expected value of some observable [64]. For pedagogical purposes, we shall now briefly review two approaches to (D)QT, first in Sec. 2.4.1 following the article by Popescu et al. [102] focusing on a conceptual point of view, and second in Sec. 2.4.2 following Bartsch and Gemmer [64] and Steinigeweg et al. [123], giving us a concrete numerical tool for evaluating correlation functions, complete with rigorous error analysis.

### 2.4.1 General Canonical Principle

Roughly speaking, Quantum Typicality is an attempt to replace the fundamental postulate of statistical mechanics [1], the equal *a priori* probability postulate, by a fundamentally different principle, referring not to statistical ensembles or time averages, but to individual states. Another key characteristic of this new postulate, dubbed **general canonical principle** [102] or **canonical typicality** [101] is the existence of a rigorous mathematical proof, unlike in the case of equal *a prior* probability postulate. Let us now consider an isolated quantum system, called the universe $U$, partitioned into two components, the system $S$ and the much larger environment $E$. In the language of Hilbert spaces, this decomposition is $\mathcal{H}_U = \mathcal{H}_S \otimes \mathcal{H}_E$ such that $\mathcal{D}_s = \dim(\mathcal{H}_S) \ll d_E = \dim(\mathcal{H}_E)$. We can also impose some global constraint $R$ for the universe, represented as restriction of the allowed states to some subspace $\mathcal{H}_R \subseteq \mathcal{H}_S \otimes \mathcal{H}_E$.

We take the restricted universe to be in a maximally entangled state

$$\rho_R = \frac{1}{\mathcal{D}_R}\mathbb{1}_R \tag{2.20}$$

capturing our lack of knowledge about the system and being consistent with our intuition from statistical mechanics, about assigning *a priori* equal probability to each pure state. Now, we define a canonical state of our system $S$, as the density matrix obtaiend from $\rho_R$ by tracing out the degrees of freedom of the environment $E$

$$\rho_S^{\mathrm{C}} = \mathrm{Tr}_E\left(\rho_R\right) \tag{2.21}$$

The crucial insight of canonical typicality is that we can take the universe to be in some pure state $\rho_R = |\psi\rangle\langle\psi|$ and the state of the system

$$\rho_S(\psi) = \mathrm{Tr}_R\left(|\psi\rangle\langle\psi|\right) \tag{2.22}$$

will be very close to the canonical state $\rho_S^{\mathrm{C}}$. Moreover, this 'closeness' can be quanitfied very precisely, using a mathematical result from the asymptotic theory of finite dimensional normed spaces called Levy's lemma [124], which tells us about the properties of typical points on high-dimensional hyperspheres. Because of normalization, pure quantum states can be represented as the point of a hypersphere, hence the lemma is applicable. Let us now introduce some concepts necessary for the precise statement of the result. A precise notion of distance between two objects requires a metric and in our case a suitable metric will be induced by a norm on the vector space of operators. There are two norms relevant for this problem, the **trace norm**

$$\|\rho\|_1 = \mathrm{Tr}\,|\rho| = \mathrm{Tr}\left(\sqrt{\rho^\dagger\rho}\right) \tag{2.23}$$

and the **Hilbert-Schmidt norm**

$$\|\rho\|_2 = \sqrt{\mathrm{Tr}\left(\rho^\dagger\rho\right)}\,. \tag{2.24}$$

The trace norm is used directly in the preciste statements of the general canonical principle, because $\|\rho_1 - \rho_2\|_1$ quantifies how hard is to tell apart $\rho_1$ and $\rho_2$ using measurements. Indeed, it can be shown that $\|\rho\|_1 = \sup_{\|A\|\leq 1}\mathrm{Tr}(\rho A)$, where $\|\cdot\|$ is the operator norm. The Hilbert-Schmidt norm is used during the proof, as it is a bit easier to manipulate and can be easily related to the trace norm using Jensen's inequality [125] for convex functions applied to $\phi(x) = x^2$. Taking $\{\lambda_i\}_{i=1}^{\mathcal{D}}$ to be the eigenvalues of $\rho$ we have

$$\begin{aligned}\|\rho\|_1^2 &= \left(\sum_{i=1}^{\mathcal{D}}|\lambda_i|\right)^2 = \mathcal{D}^2\left(\sum_{i=1}^{\mathcal{D}}\frac{1}{\mathcal{D}}|\lambda_i|\right)^2 = \mathcal{D}^2\phi\left(\sum_{i=1}^{\mathcal{D}}\frac{1}{\mathcal{D}}|\lambda_i|\right)\\ &\leq \mathcal{D}^2\sum_{i=1}^{\mathcal{D}}\frac{1}{\mathcal{D}}\phi\left(\lambda_i\right) = \mathcal{D}\sum_{i=1}^{\mathcal{D}}|\lambda_i|^2 = \mathcal{D}\|\rho\|_2^2\end{aligned} \tag{2.25}$$

Hence, $\|\rho\|_1 \leq \sqrt{\mathcal{D}}\|\rho\|_2$. We shall meet the Hilbert-Schmidt norm again in the next section, when discussing the algorithm searching for local integrals of motion. The precise theorem establishing the typicality is as follows

**Theorem 2.2** *Let $V$ be a function assigning to each subset of $\mathcal{H}_U$ its volume (in the sense of a suitable Haar measure [124]). Then, the following inequality holds*

$$\frac{V\left[\{|\psi\rangle \in \mathcal{H}_R \mid \frac{1}{2}\|\rho_S(\psi) - \rho_S^{\mathrm{C}}\|_1 \geq \eta\}\right]}{V\left[\{|\psi\rangle \in \mathrm{H}_R\}\right]} \leq \eta' \tag{2.26}$$

*where*

$$\begin{aligned}\eta &= \epsilon + \frac{1}{2}\sqrt{\frac{\mathcal{D}_S}{\mathcal{D}_E^{\mathrm{eff}}}}\\ \eta' &= 4e^{-\frac{2}{9\pi^3}\mathcal{D}_R\epsilon^2}\end{aligned}$$

*and the effective dimension of environment subspace is* $\mathcal{D}_E^{\mathrm{eff}} = \frac{1}{\mathrm{Tr}\left(\rho_E^2\right)} \geq \frac{\mathcal{D}_R}{\mathcal{D}_S}$, *where* $\rho_E = \mathrm{Tr}_S\left(\rho_R\right)$.

Mathematically inclined readers are referred to Popescu et al. [126] for the full proof of this theorem, but for us it is important what this theorem means, namely that all but exponentially rare pure states of the universe are on the level of the system indistinguishable from the canonical state $\rho_S^{\mathrm{C}}$. For our purposes in this thesis, we are interested in the case where the constraint $R$ is that the total energy in the universe is close to some fixed value $E$. Assuming that the system is weakly coupled with the environment, it becomes a standard exercise in statistical mechanics to show that the canonical state is the Gibbs canonical ensemble

$$\rho_S^{\mathrm{C}} \propto \exp\left(-\frac{H_S}{k_B T}\right) \tag{2.27}$$

where $H_s$ is the Hamiltonian of the system and $T$ is the temperature set by the energy $E$.

### 2.4.2 Dynamical Quantum Typicality

Another approach to Quantum Typicality is not concerned directly with quantum states, but with expectation values of quantum observables instead. It was shown that for states drawn from a particular distribution in Hilbert space, the expectation values of a generic observable $Q$ are very similar [127]. This result was further extended in the case of a unitarly invariant probability distribution, that is normalized states of the form

$$|\psi\rangle = \sum_{i=1}^{\mathcal{D}} c_i\,|i\rangle \tag{2.28}$$

where $\mathrm{Re}\,c_i$ and $\mathrm{Im}\,c_i$ are drawn from multidimensional Gaussian distribuion with zero mean, and $\{|i\rangle\}_{i=1}^{\mathcal{D}}$ is an arbitrary basis. Technicaly, because $\sum_{i=1}^{\mathcal{D}}|c_i|^2 = 1$, the coefficients are not independent, thus the full distribution is not necessarily Gaussian. However, Central Limit Theorem ensures that for $\mathcal{D}$ suitably large the distribution is indeed close to Gaussian, with the standard deviation equal $1/\sqrt{2\mathcal{D}}$ [128]. Using the **Hilbert space average method**, analytical expressions for both the average HA and variance HV of $\langle\psi|Q|\psi\rangle$ were derived [64]. They are as follows

$$\mathrm{HA}\left[\,\langle\psi|Q|\psi\rangle\right] = \frac{\mathrm{Tr}\left(Q\right)}{\mathcal{D}} \tag{2.29}$$

$$\mathrm{HV}\left[\,\langle\psi|Q|\psi\rangle\right] = \frac{1}{\mathcal{D}+1}\left(\frac{\mathrm{Tr}\left(Q^2\right)}{\mathcal{D}} - \left(\frac{\mathrm{Tr}\left(Q\right)}{\mathcal{D}}\right)^2\right) \tag{2.30}$$

Proof of the above equations is not difficult conceptually, however, requires evaluation of rather cumbersome integrals over high-dimensional hyperspheres so we shall refrain from spelling it out in full. Interested readers can find all the details in a book by Gemmer et al. [128]. Let us now take $Q(t) = \hat{\rho}A(t)B$ and define a quantity

$$\alpha = \mathcal{D} \langle \psi | \sqrt{\hat{\rho}} A(t) B \sqrt{\hat{\rho}} | \psi \rangle \tag{2.31}$$

Note that because density matrix $\hat{\rho}$ is positive semi-definite and Hermitian, the square root $\sqrt{\hat{\rho}}$ exists and is well defined. The next step is to plug $\alpha$ into equations (2.29) and (2.30)

$$\mathrm{HA}\left[\alpha\right] = \mathrm{Tr}\left(\sqrt{\hat{\rho}}A(t)B\sqrt{\hat{\rho}}\right) = \mathrm{Tr}\left(\hat{\rho}A(t)B\right) = \frac{\mathrm{Tr}\left(e^{-\beta H}A(t)B\right)}{\mathcal{Z}} \tag{2.32}$$

$$\begin{aligned}\mathrm{HV}\left[\alpha\right] &= \frac{\mathcal{D}^2}{\mathcal{D}+1}\left(\frac{\mathrm{Tr}\left((\sqrt{\hat{\rho}}A(t)B\sqrt{\hat{\rho}})^2\right)}{\mathcal{D}} - \left(\frac{\mathrm{Tr}\left(\sqrt{\hat{\rho}}A(t)B\sqrt{\hat{\rho}}\right)}{\mathcal{D}}\right)^2\right) \\ &\leq \frac{\mathcal{D}}{\mathcal{D}+1}\mathrm{Tr}\left(\hat{\rho}A(t)B\hat{\rho}A(t)B\right) < \mathrm{Tr}\left(\hat{\rho}A(t)B\hat{\rho}A(t)B\right)\end{aligned} \tag{2.33}$$

Looking at eq. (2.32) we immediately see the desired way of calculating the correlation function.

$$\tilde{C}_{AB}(t) = \mathrm{Re}\,\frac{\mathrm{Tr}\left(e^{-\beta H}A(t)B\right)}{\mathcal{Z}} = \mathrm{Re}\,\frac{\mathcal{D}}{\mathcal{Z}}\langle\psi|e^{-\frac{\beta H}{2}}e^{iHt}Ae^{-iHt}Be^{\frac{-\beta H}{2}}|\psi\rangle + \mathrm{Re}\,\epsilon \tag{2.34}$$

where $\epsilon$ is the error we made by using just one random state $|\psi\rangle$. Let us massage this expression a bit more by introducing two auxiliary states $|\psi_\beta(t)\rangle = e^{-iHt}e^{-\frac{-\beta H}{2}}|\psi\rangle$ and $|\phi_\beta(t)\rangle = e^{-iHt}Be^{-\frac{-\beta H}{2}}|\psi\rangle$. We can also calculate the partition function using the random state $|\psi\rangle$ as

$$\mathcal{Z} = \mathrm{Tr}\left(e^{-\beta H}\right) = \mathcal{D}\langle\psi|e^{-\beta H}|\psi\rangle = \mathcal{D}\langle\psi_\beta(0)|\psi_\beta(0)\rangle \tag{2.35}$$

Combining (2.34) and (2.35), we arrive at the final expression, as seen in literature [116, 121, 122]

$$\tilde{C}_{AB}(t) = \mathrm{Re}\,\frac{\langle\psi_\beta(t)|A|\phi_\beta(t)\rangle}{\langle\psi_\beta(0)|\psi_\beta(0)\rangle} + \mathrm{Re}\,\epsilon \tag{2.36}$$

We have successfully shifted time evolution and the action of the density matrix to state vectors instead of operators, hence we may apply the Krylov time propagator, studied in the previous section, to calculate both real and imaginary time evolution. Apart from that, the only other numerical calculations are sparse matrix-vector multiplication[4] and inner products of vectors, which are much less demanding than full exact diagonalization.

The final thing left is to estimate the error $\epsilon$, in order to show that this approach makes sense. From eq. (2.33) it is clear that the Hilbert Space Average of $\epsilon$ is zero, as

$$\mathrm{HA}(\epsilon) = \mathrm{HA}\left(\alpha - \mathrm{Tr}\left(\hat{\rho}A(t)B\right)\right) = 0 \tag{2.37}$$

[4]Matrices representing local observables will also be sparse.

Equation (2.33), for Hilber Space Variance, allows us to estimate the standard deviation

$$\begin{aligned}
(\sigma(\epsilon))^2 &= \mathrm{HV}\left[\epsilon\right] = \mathrm{HV}\left[\alpha\right] < \mathrm{Tr}\left(\hat{\rho}A(t)B\hat{\rho}A(t)B\right) \\
&= \sum_{m,n} \frac{e^{-\beta\varepsilon_m}}{\mathcal{Z}} \langle m|A(t)B|n\rangle \frac{e^{-\beta\varepsilon_n}}{\mathcal{Z}} \langle n|A(t)B|m\rangle \\
&< \sum_{m,n} \frac{e^{-\beta\varepsilon_m}}{\mathcal{Z}} \langle m|A(t)B|n\rangle \frac{e^{-\beta\varepsilon_0}}{\mathcal{Z}} \langle n|A(t)B|m\rangle \\
&= \frac{1}{\mathrm{Tr}\left(e^{-\beta(H-\varepsilon_0)}\right)} \sum_{m} \frac{e^{-\beta\varepsilon_m}}{\mathcal{Z}} \langle m|A(t)BA(t)B|m\rangle \\
&= \frac{1}{\mathrm{Tr}\left(e^{-\beta(H-\varepsilon_0)}\right)} \mathrm{Tr}\left(\hat{\rho}A(t)BA(t)B\right)
\end{aligned} \tag{2.38}$$

Where the red inequality follows from the fact that the Boltzmann factor is a strictly decreasing function and assuming that the spectrum of $H$ is ordered in increasing fashion. Defining the effective dimension $\mathcal{D}_{\text{eff}} \equiv \mathrm{Tr}\left(e^{-\beta(H-\varepsilon_0)}\right)$, we finally obtain the upper bound on a standard deviation of error as

$$\sigma\left(\mathrm{Re}\,\epsilon\right) < \sqrt{\frac{\mathrm{Re}\langle A(t)BA(t)B\rangle}{\mathcal{D}_{\text{eff}}}} \tag{2.39}$$

From this bound, we see that at infinite temperature, the error is exponentially suppressed in system size, and thus for suitably large systems even a single pure state $|\psi\rangle$ is enough to obtain a very good approximation of the correlation function. It becomes progressively worse with lower temperature, however as the mean error is 0 we can always average over a few random states. Fortunately, in this thesis, we are only interested in case $\beta \to 0$, so usually a single run will be enough.

As an example application, in figure 2.4 we present the infinite-temperature spin current autocorrelation functions in the nearest-neighbor Heisenberg model, obtained by setting $r_{\max} = 1$ in equations (1.2) and (1.13).

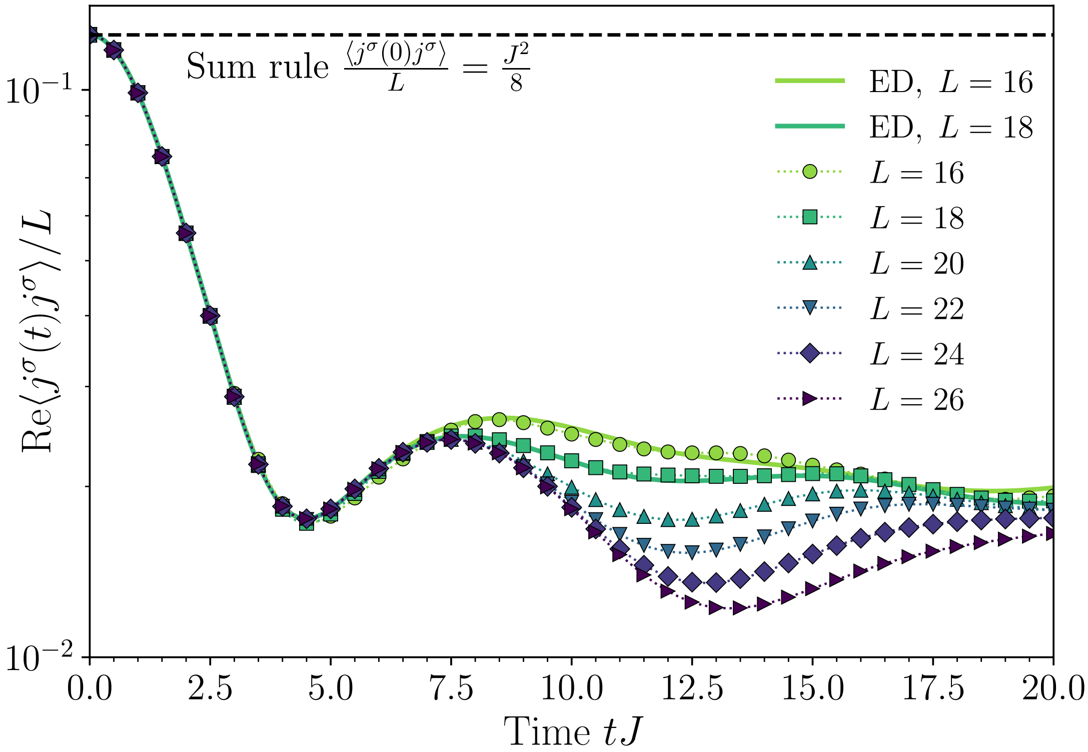



Figure 2.4: Infinite-temperature autocorrelation function of spin current $j_\sigma$ in isotropic Heisenberg model ($J = 1,\ \Delta = 1$), evaluated using Exact Diagonalization for $L = 16,\ 18$ and Dynamical Quantum Typicality with Krylov propagator for $L = 16,\ 18,\ 20,\ 22,\ 24,\ 26$. Already for a modest size of $L = 18$ lattice sites we observe a very good agreement between ED and DQT calculation for a single pure state. Because of eq. (2.39), we expect this agreement to be exponentially better for larger system sizes.

# 3

# Spin transport in long-range anisotropic Heisenberg model

After all the technicalities of the previous chapter, we are finally ready to study spin transport in the long-range anisotropic Heisenberg model. The main motivation of this investigation is the fact that this model admits two limits exhibiting ballistic spin transport (cf. Fig. 3.1), namely the free particles with nearest-neighbor hopping for $\alpha \to \infty$, $\Delta = 0$ and the Haldane-Shastry model with $J_{\mathrm{HS}(r)} = J \sin^2(\pi/L) / \sin^2(\pi r/L)$ for $\alpha = 2$ [129, 130]. In the latter case, this limit is only strictly valid in the thermodynamic limit, since $\sin^{-2}(r/L) \propto r^{-2}$ for $r \ll L$. In both of these limiting models the spin current $j^\sigma$ commutes with the Hamiltonian and thus is strictly conserved. Hence, even though the Hamiltonian (1.2) is not integrable for arbitrary $\alpha$, one could suspect that it will be *nearly integrable*, in the sense described in the introduction, and support interesting transport properties. Using spin density expansion and linear response theory of optical conductivity, in this chapter we will show that this is indeed the case and the spin transport is *quasibalistic* along a sharp line in the parameter space $\Delta \simeq \exp(-\alpha + 2)$, which continuously connects the two limiting cases mentioned above.

Results described in this chapter were first presented in chapters II and III of Mierzejewski et al. [96].

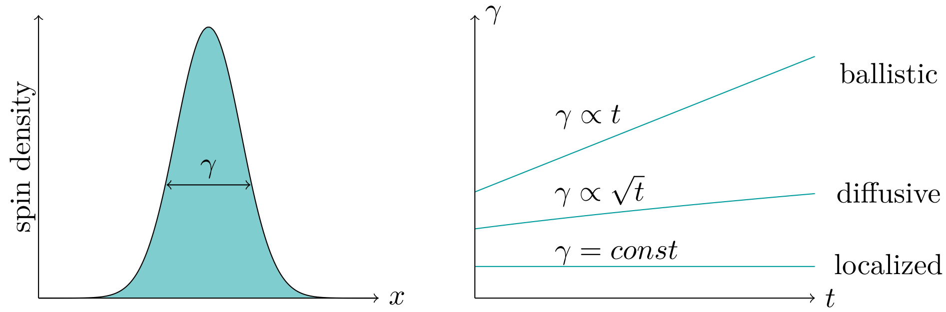



Figure 3.1: Illustration of different types of transport. On the left panel, we have some initial spin density characterized by width $\gamma$. On the right panel, we have the dependence of $\gamma$ on time in three different cases.

## 3.1 Spin density expansion

Taking inspiration from experimental studies of cold atoms [92–94, 131], we consider an initial state in the form of a spin domain wall

$$|\psi(0)\rangle = |\underbrace{\uparrow\uparrow\uparrow\uparrow\uparrow}_{x}\underbrace{\downarrow\downarrow\downarrow\ldots\downarrow}_{L-x}\rangle\,,\; x=5 \tag{3.1}$$

and study the dynamics of spin expansion by measuring the time dependence of the magnetization profile $M_\ell(t) = \langle\psi(t)|S^z_\ell|\psi(t)\rangle$. Such a product state initial configuration is desirable for two reasons. First, it is relatively accessible in experiments, e.g. using higher-order optical Stark shifts to rotate individual spins [132]. Second, from the theoretical point of view, by assuming open boundary conditions and choosing $x = 5$, we localize the domain wall close to the edge of the system, which allows us to avoid finite-size effects for longer times. Moreover, the dynamics generated by the Hamiltonian (1.2) conserve the total magnetization and hence we can restrict ourselves to the subspace of states with just 5 spins up. This considerably reduces the dimensionality of the problem and allows us to study systems as large as $L = 45$ with $\binom{45}{5} \approx 1.2\times10^6$ states, characterized by the total magnetization $M_{\rm tot} = -35/2$. To put this into perspective, the full Hilbert space of such system has dimension $2^{45}$ which is $O(10^7)$ larger and thus completely inaccessible without additional techniques.

For the time evolution, we use the Krylov propagator introduced in detail in the previous chapter. A sample magnetization profile obtained for $\alpha = 3.5$ and $\Delta = 1.0$ is shown in Fig. 3.2. In order to quantitatively investigate the spin transport in this setup, we introduce

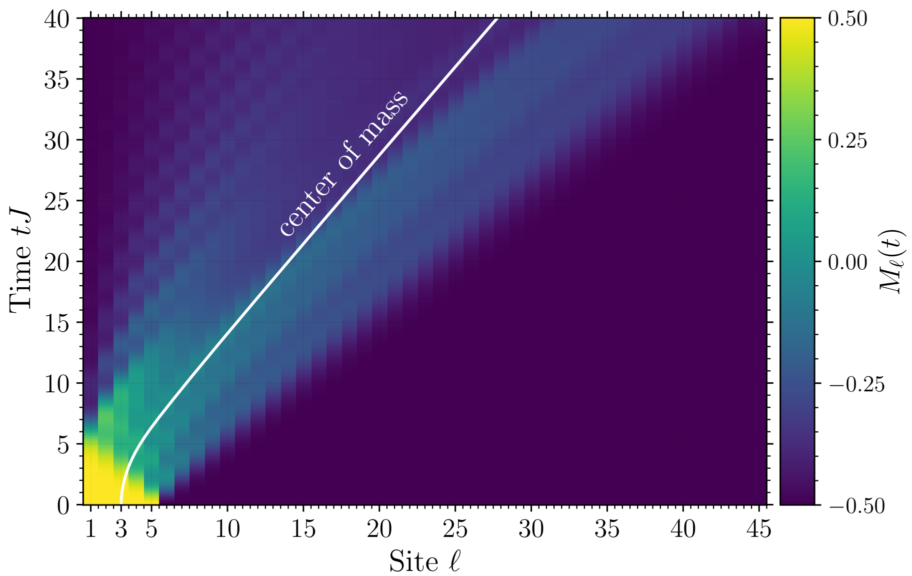



Figure 3.2: Time dependence of magnetization profile $M_\ell(t)$ for $\alpha = 3.5$ and $\Delta = 1.0$. The evolution of the center of mass, initially at $r_{\rm cm}(t=0) = 3$, is marked by a white line.

the so-called **center of mass**, defined as the first density moment of the magnetization profile

$$r_{\rm cm}(t) = \frac{\sum_{\ell=1}^{L} \ell\,(M_\ell(t)+1/2)}{\sum_{\ell=1}^{L}(M_\ell(t)+1/2)} = \frac{\sum_{\ell=1}^{L} \ell\,(M_\ell(t)+1/2)}{M_{\rm tot}+L/2} \tag{3.2}$$

In Fig. 3.2, an example of time evolution of center of mass is shown. Examining $r_{\mathrm{cm}}(t)$ calculated for two values of $\Delta = 0.2,\ 0.5$ and various values of $\alpha \in \{2.0, 2.5, \ldots, 5.0\}$ (cf. Fig. 3.3), we observe a first hint of non-trivial transport properties of the model, namely non-monotonic dependence of $r_{\mathrm{cm}}(t)$ on $\alpha$.

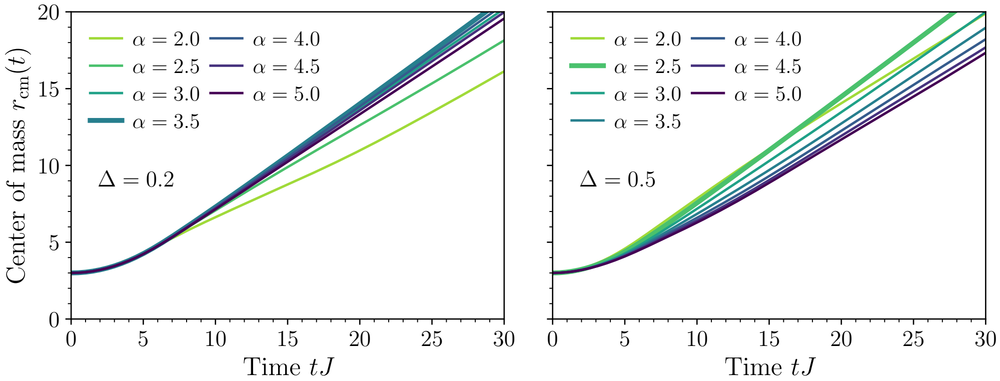



Figure 3.3: Time dependence of the center of mass $r_{\mathrm{cm}}(t)$ for $\Delta = 0.2$ (left panel) and $\Delta = 0.5$ (right panel) and various values of interaction decay $\alpha$. The line corresponding to the fastest-moving center of mass is thicker than the rest.

To see this better, in Fig. 3.4 we look at the velocity obtained from the time derivative of the center of mass

$$\nu_{\mathrm{cm}}(t) = \frac{\mathrm{d}r_{\mathrm{cm}}(t)}{\mathrm{d}t}. \tag{3.3}$$

We observe that for both values of $\Delta$, there is a clear maximum of the velocity of the expansion

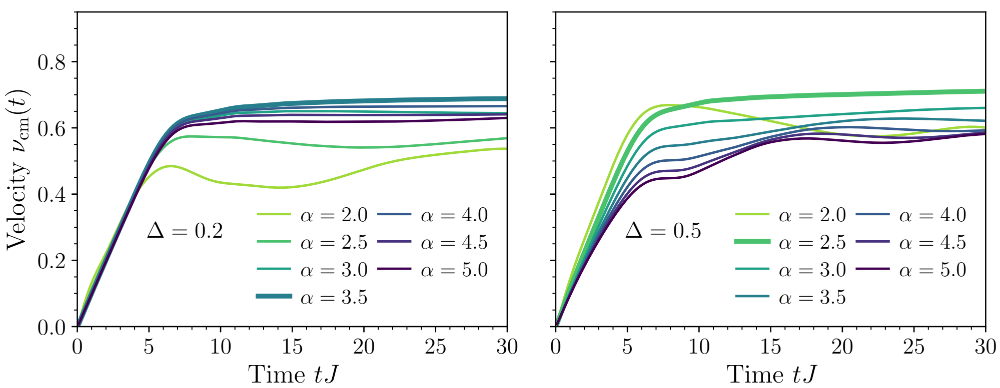



Figure 3.4: Time dependence of the velocity $\nu_{\mathrm{cm}}(t)$ for $\Delta = 0.2$ (left panel) and $\Delta = 0.5$ (right panel) and various values of interaction decay $\alpha$. The line corresponding to the largest velocity is again thicker than the rest.

at some intermediate value of $\alpha$. Investigating further the dependence of velocity on the parameters of the model, we calculate the average velocity $\bar{\nu}_{\mathrm{cm}}$ on the interval $t \in [20, 30]$ and plot it as a function of $\alpha$ for various values of $\Delta$ (cf. left panel of Fig. 3.5). The non-monotonic behavior is now evident, as for a fixed $\Delta$, there exists a value of $\alpha = \alpha_{\nu_{\max}}(\Delta)$, such that the average velocity has a maximum (for $\Delta = 0.0$ the optimal $\alpha$ is shifted to infinity). Equivalently, for each $\alpha$ there exists an optimal value of $\Delta = \Delta_{\nu_{\max}}(\alpha)$.

In the right panel of Fig. 3.5 we look at the dependence of average velocity on both parameters of the model. Moreover, we superimpose the points corresponding to the optimal anisotropies $\Delta_{\nu_{\max}}(\alpha)$. Curiously, these points seem to lie very close to an exponential curve, given by $\Delta_{\mathrm{O}} = \exp(-\alpha + 2)$. Furthermore, as seen in the left panel, the average velocity is approximately constant for $\alpha \geq 2$ and equal to $\bar{\nu} \simeq J/\sqrt{2}$ along this line. Such velocity is a characteristic of ballistic transport in the nearest neighbors free-fermion model [93, 133], corresponding via Jordan-Wigner transformation to our model with $\alpha \to \infty$ and $\Delta = 0$. Therefore, we suspect that the optimal line $\Delta_{\nu_{\max}}(\alpha)$, present in this interacting system and indicating **quasibalistic** transport, is a transient remnant of the transport properties of the free fermions.

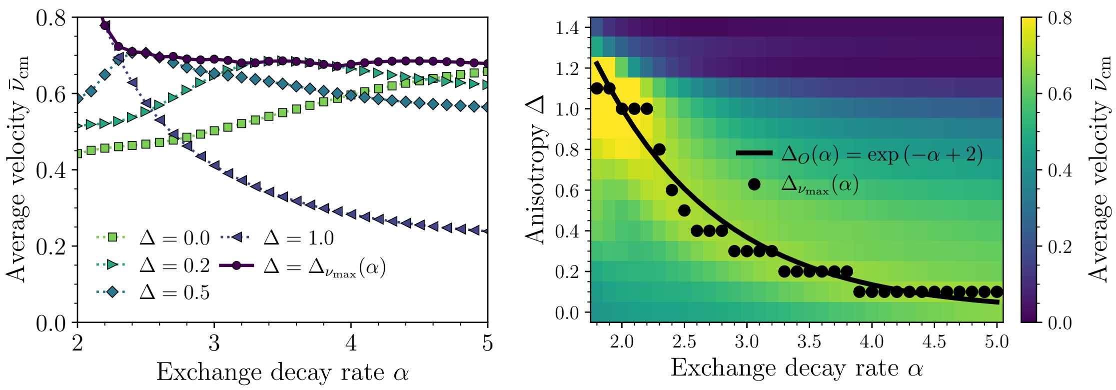



Figure 3.5: Left panel: average velocity $\bar{\nu}_{\mathrm{cm}}$ as a function of $\alpha$ for various values of $\Delta$. Right panel: heatmap of the average velocity $\bar{\nu}_{\mathrm{cm}}$ as a function of $\alpha$ and $\Delta$. The points corresponding to the optimal anisotropies $\Delta_{\nu_{\max}}(\alpha)$ are marked with black dots, while the solid line indicates the optimal line $\Delta = \Delta_{\mathrm{O}} = \exp(-\alpha + 2)$.

## 3.2 Optical conductivity

In this section, we approach the problem of spin transport in the long-range Heisenberg model from the perspective of **linear response theory**. We study the **optical conductivity** [1] $\sigma(\omega)$ of the model, which is a measure of the response of the system to an external electromagnetic field. In the linear response regime, the optical conductivity is given by the Kubo formula, which for infinite temperature reads

$$\sigma(\omega) = \frac{\pi}{L\mathcal{Z}} \sum_{n,m} |\langle n|j^{\sigma}|m\rangle|^2 \delta(\omega - \epsilon_m + \epsilon_n) \tag{3.4}$$

where $\mathcal{Z}$ is the number of states in the Hilbert space, $L$ is the system size and $j^{\sigma}$ is the spin current operator (1.13), derived in Chapter 1. For the derivation of the Kubo formula and

[1] The optical conductivity is also known as the spin conductivity. Technically, as shown in the appendix A, this the *real* part of the optical conductivity, but it is enough to study it as the real part and the imaginary part are related via the Kramers-Kronig relation.

the optical conductivity, see Appendix A. As the sum in Eq. (3.4) runs uniformly over all many-body eigenstates $H|n\rangle = \epsilon_n |n\rangle$ of the Hamiltonian, this quantity probes the whole eigenspectrum. Equation 3.4 suggests a simple numerical procedure for calculating the optical conductivity. First, one needs to diagonalize the Hamiltonian $H$ and obtain the eigenstates $|n\rangle$ and eigenvalues $\epsilon_n$. Then, one needs to calculate the matrix elements of the spin current operator $\langle n|j^\sigma|n\rangle$ between all pairs of eigenstates. Finally, the optical conductivity is obtained by summing over all pairs of eigenstates, weighted by the corresponding matrix elements and the $\delta$ function. It is only the last step that requires some care, as the $\delta$ function is not a regular function and would require some binning of the discrete spectrum. We avoid this, by instead considering the **integrated conductivity**

$$\mathcal{I}(\Omega) = \frac{1}{\mathcal{S}_{\text{tot}}} \int_{-\Omega}^{\Omega} \mathrm{d}\omega\, \sigma(\omega) = \frac{\pi}{L\mathcal{Z}\mathcal{S}_{\text{tot}}} \sum_{n,m} |\langle n|j^\sigma|m\rangle|^2 \theta(\Omega - |\epsilon_m - \epsilon_n|) \tag{3.5}$$

where $\theta(x)$ is the Heaviside step function and $\mathcal{S}_{\text{tot}}$ is the sum rule

$$\mathcal{S}_{\text{tot}} = \int_{-\infty}^{\infty} \mathrm{d}\omega\, \sigma(\omega) = \frac{\pi}{L\mathcal{Z}} \sum_{n,m} |\langle n|j^\sigma|m\rangle|^2 \tag{3.6}$$

It is easy to see that the integrated conductivity $\mathcal{I}(\Omega)$ is a regular function of $\Omega$, and contains the information about the fraction of the spectral weight contained in the frequency window $[-\Omega, \Omega]$. Equation (3.5) is now straightforward to evaluate numerically.

We evaluate the integrated conductivity (3.5) for the long-range Heisenberg model with periodic boundary conditions, and system sizes up to $L = 20$. We also restrict the calculations to the subspace of zero total magnetization, i.e. the largest sector with $\binom{L}{L/2}$ states. Leveraging the periodic boundary conditions, we perform the calculations separately for each momentum sector and then add the results together.

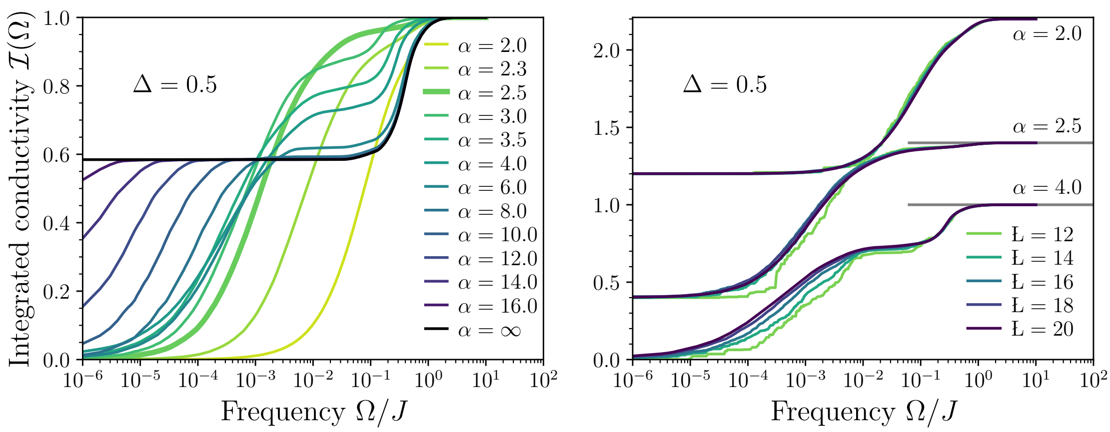



Figure 3.6: Left panel: Integrated conductivity $\mathcal{I}(\Omega)$ as a function of frequency window $\Omega$ for various values of $\alpha$ and $\Delta = 0.5$. The thicker line denotes the result for optimal decay parameter $\alpha$. Right panel: Size dependence of the integrated conductivity $I(\Omega)$ for $\alpha = 2.0,\ 2.5,\ 4.0$ and $\Delta = 0.5$, illustrating the effects of finite size. For clarity, we added a vertical shift to distinguish the curves for different decay parameters.

Looking at the left panel of Fig. 3.6, we observe that the integrated conductivity for $\alpha \to \infty$ is exhibiting a **Drude peak** behavior at $\Omega \to 0$, and a distinct incoherent (regular) spectrum for $0.1 \lesssim \Omega/J \lesssim 1.0$, which is consistent with the results for the nearest neighbor Heisenberg model [134]. As $\alpha$ is decreased (the range of the interactions increases), but remains $\alpha \gtrsim 10$, the Drude peak becomes suppressed, while the regular part of the spectrum is still more or less the same. However, an interesting feature appears in the spectrum for $\alpha \lesssim 10$, namely the incoherent part starts shifting towards lower frequencies. For anisotropy $\Delta = 0.5$, this behavior is most pronounced for $\alpha = 2.5$, where the integrated conductivity is $\mathcal{I}(\Omega) \simeq 1$ for all $\Omega/J < 0.01$, which means that most of the spectral weight is contained in the frequency window $[-0.01, 0.01]$. This in turn implies ballistic-like spin transport for extremely long times up to $tJ \simeq 100$, similar to the case of noninteracting particles, as there we have $\sigma(\omega) \propto \delta(\omega) \implies I(\Omega) = 1$ for $\Omega > 0$. Furthermore, we once again observe some kind of non-monotonic behavior, as decreasing the decay parameter beyond $\alpha \approx 2.5$ shifts the incoherent part of the spectrum back towards higher frequencies.

To quantitatively investigate this effect across the parameter space, in Fig. 3.7 we present heatmaps of the integrated conductivity $\mathcal{I}(\Omega)$ on the $(\alpha, \Omega)$ plane, for different values of the anisotropy $\Delta$. Moreover, with a solid black line we denote the the value $\Omega = \Omega^*$, for which the integrated conductivity is $\mathcal{I}(\Omega^*) = 0.9$, i.e. 90% of the sum rule $S_{\text{tot}}$.

As in the case of average velocity during a spin expansion experiment, for every value of $\Delta$, we can find a value of $\alpha$ for which the quantity telling about transiency of ballistic transport admits extremal value. Here, it is the $\Omega^*$ that becomes minimal, and in fact surprisingly small, implying transient ballistic spin transport. Once again, we can proceed in reverse, and extract the optimal anisotropy $\Delta_\sigma = \Delta_\sigma(\alpha)$ as a function of the decay parameter $\alpha$, for which $\Omega^*$ is minimal. We can thus directly compare the optimal anisotropies obtained from the two different quantities, namely the average velocity and the integrated conductivity.

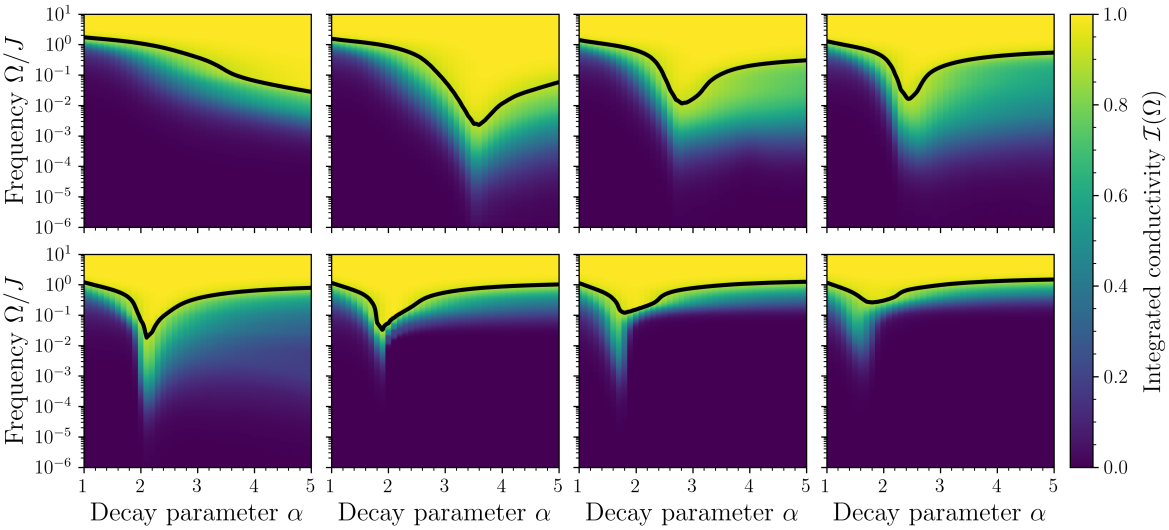



Figure 3.7: Heatmaps of the integrated conductivity $\mathcal{I}(\Omega)$ on the $(\alpha, \Omega)$ plane. Black solid line denotes the value $\Omega = \Omega^*$, for which the integrated conductivity is $I(\Omega^*) = 0.9$.

The results are presented in Fig. 3.8, and we observe an excellent agreement between $\Delta_\sigma$ obtained from linear response theory, that is low frequency (long time) dynamics, of a system with periodic boundary conditions, and the optimal anisotropy $\Delta_O(\alpha)$, inferred from the short-time spin domain expansion in a chain with open boundary conditions. This is a strong indication that the transient ballistic spin transport is a generic feature of the long-range Heisenberg model, and not an artifact of the finite system size. It is further supported by the finite-size analysis of the integrated conductivity, presented in the right panel of Fig. 3.6, where we observe that $\mathcal{I}(\Omega)$ for $\alpha = 2.0$ is almost independent of the system size, and for larger values of $\alpha$, the incoherent part of the spectrum is shifted towards even lower frequencies.

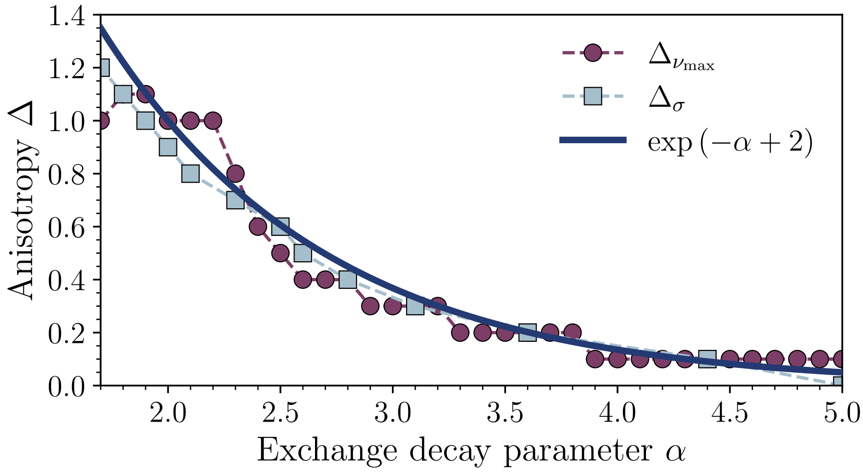



Figure 3.8: Optimal values of anisotropy $\Delta$, as a function of decay parameter $\alpha$, obtained from the average velocity of spin expansion and integrated conductivity. The solid line denotes the optimal line $\Delta_\mathrm{O} = \exp(-\alpha + 2)$.

It is worth mentioning, that in Mierzejewski et al. [96], we have also looked into a generalized version of the aforementioned Haldane-Shastry model, with the exchange interaction of the form $J_{\mathrm{HS}(\alpha)} \propto 1/\sin^\alpha(\pi r/L)$. We have shown that it exhibits very similar behavior, with the integrated conductivity close to the one obtained for the long-range Heisenberg model, and the optimal anisotropy following the same exponential curve. Moreover, we have investigated two other models, namely the next-nearest neighbor Heisenberg model (i.e. (1.2) with $r_{\max} = 2$), and the long-range $t$-$V$ spinless fermion model. Contrary to the nearest-neighbor case, the long-range $t$-$V$ model is not related to the long-range Heisenberg model via the Jordan-Wigner transformation, and thus the two models are not equivalent. The former case yielded results similar to the long-range Heisenberg model for small values of anisotropy $\Delta \in [0, 0.2]$, while for larger values of $\Delta$, the integrated conductivity was rather featureless. It is consistent with our main results, as is this parameter regime, the optimal decay is $\alpha \gtrsim 3.5$, rendering the terms with $r > 2$ insignificant. In the latter case of spinless fermions, the quasibalistic transport was all but absent. Therefore, it is expected that this phenomenon is unique to the long-range Heisenberg model. For more details about those results, that go beyond the scope of this thesis, the interested reader is referred to the original research article.

# 4
# Slowly decaying eigenmodes

In the previous chapter, we have numerically shown the existence of optimal anisotropy $\Delta_O = \exp(-\alpha + 2)$, which ensures slow relaxation of the spin current $j^\sigma$ (1.13) and consequently quasiballistic spin transport. Here, we will demonstrate that this feature is not unique to the spin current, but exhibited also by a class of other, *local* operators. To this end, we will employ an algorithm devised by Mierzejewski et al. [95], originally designed to identify local integrals of motion in integrable tight-binding models. As the model we are considering in this work is not integrable, we are not expecting to find strictly conserved quantities, but only so-called **local slowly relaxing operators (LSROs)**. We will interpret the discovered observables in terms of fermionic currents, describing particle hopping with various ranges. Moreover, we will also show how to improve the numerical efficiency of the algorithm, by utilizing symmetry subspaces and the Dynamical Quantum Typicality approach to correlation functions[1] (cf. section 2.4.2).

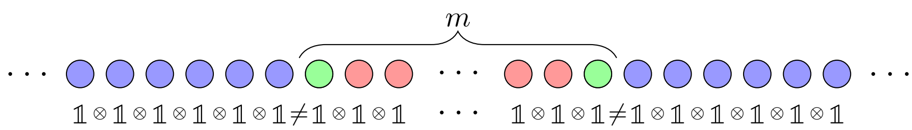
## 4.1 Detecting local slowly relaxing operators

### 4.1.1 Theoretical description

Let us start by introducing in detail the original algorithm for detecting local integrals of motion (LIOMs), following the original article by [95]. In principle, finding a **complete set of LIOMs** is a conceptually nontrivial task, however, this procedure reduces it to a simple application of linear algebra [95]. In this section, unless stated otherwise, by $H$ we will denote an arbitrary tight-binding Hamiltonian with periodic boundary conditions on $L$ sites, having eigenstates $H|n\rangle = \epsilon_n |n\rangle$. Moreover, for any operator $A$ we define $A_{mn} \equiv \langle m|A|n\rangle$.

In order to employ techniques from linear algebra, we need to have a linear space of some kind. This role is played by the space of *local, traceless, and translationally invariant* observables, supported on up to $M$ sites and acting on vectors from a Hilbert space $\mathcal{H}$ of dimension $\mathcal{D}$. We will denote this space by $\mathcal{V}_M$. Its building blocks are the spaces $\mathcal{V}^m$, of operators supported on exactly $m$ sites, i.e. of the form

[1] And why it, unfortunately, fails in this case.




where blue circles correspond to single-site identity operators, green circles to an arbitrary single-site operator except for the identity and red circles to an arbitrary single-site operator. If we were to allow identity operators on green sites, we would have obtained a $(m-1)$-local operator. It is easy to see that an arbitrary linear combination of operators from $\mathcal{V}^m$ is again an element of $\mathcal{V}^m$, hence $\mathcal{V}^m$ is a linear space. Therefore, the full space

$$\mathcal{V}_M = \bigoplus_{m=1}^{M} \mathcal{V}^m \tag{4.1}$$

is also a linear space. We will always assume that $0 \leq M \leq L/2$.

Using the infinite temperature correlation function (cf. Eq. (2.18)) we can endow this space with an inner product

$$\mathcal{V}_M \times \mathcal{V}_M \ni (A, B) \mapsto (A|B) \equiv \frac{1}{\mathcal{D}} \operatorname{Tr}\left(AB^\dagger\right) = \frac{1}{D} \sum_{n,m=1}^{D} A_{nm} B^*_{nm} \in \mathbb{C} \tag{4.2}$$

called the **Hilbert-Schmidt inner product** and inducing the **Hilbert-Schmidt norm** $\|A\| = \sqrt{(A|A)}$. It is worth noting, that if we let the first operator be time-dependent, and consider the Hilbert-Schmidt inner product as a function of time, we obtain the infinite temperature correlation function (2.18). Because we only consider finite systems in this thesis, we do not need to worry about situations where the trace is not well defined. The pair $(\mathcal{V}_M, (\cdot|\cdot))$ is then a finite-dimensional Hilbert space. We are now able to state more precisely what we mean by a complete set of LIOMs. It is a set of local observables $\{Q_\beta : [Q_\beta, H] = 0\}$, such that for any observable $A$ we have

$$\lim_{t\to\infty} (A(t)|A) = \sum_\beta \frac{(Q_\beta|A)^2}{(Q_\beta|Q_\beta)} \tag{4.3}$$

i.e. the completeness is understood as the saturation of the Mazur bound [135].

The mathematical stage is now set, so let us proceed further toward the algorithm. As $\mathcal{V}_M$ is a linear space, it possesses a basis $\{O_\gamma\}$, which with the help of the inner product can be made into an orthonormal basis $(O_\gamma|O_{\gamma'}) = \delta_{\gamma\gamma'}$. We can also think of this space as an orthogonal subspace of the space $\mathcal{V}$ of all possible operators acting on $\mathcal{H}$, in the sense that

$$(\forall A \in \mathcal{V})(A = A^M + A^\perp = \sum_\gamma (O_\gamma|A)\, O_\gamma + A^\perp), \text{ such that } (\forall\gamma)((O_\gamma|A^\perp) = 0) \tag{4.4}$$

We will describe an example of such a basis in the next section, but for now, it is enough that it exists.

Next, we would like to determine the conserved part of all the basis operators $O_\gamma$. We do this by considering the infinite time average

$$\begin{aligned}\bar{O}_\gamma = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\, O_\gamma(t) &= \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\, \mathrm{e}^{iHt}O_\gamma \mathrm{e}^{-iHt} \\ &= \sum_{m,n}(O_\gamma)_{mn}\left|m\right\rangle\!\left\langle n\right| \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^\tau \mathrm{d}t\, \mathrm{e}^{i(\epsilon_m-\epsilon_n)t} \\ &= \sum_{\substack{n,m\\ \epsilon_n=\epsilon_m}} (O_\gamma)_{mn}\left|m\right\rangle\!\left\langle n\right| \end{aligned} \tag{4.5}$$

This time-averaging amounts to a cut-off, removing all matrix elements between non-degenerate eigenstates of the Hamiltonian. A crucial property of this operation is that it is an orthogonal projection in the space of operators, i.e. $\left(\bar{O}_\gamma\middle|\bar{O}_{\gamma'}\right) = \left(\bar{O}_\gamma\middle|O_{\gamma'}\right)$. This will in the end will allow us to distinguish between different types of conserved quantities. However, our ultimate goal concerns LSROs in a system that is not integrable, which dictates the need for performing also a finite-time averaging. Unfortunately, a simple omission of the limit in Eq. (4.5) destroys the projective character of this operation. To remedy this, we introduce a parameter $\tau$ and define effective time averaging [136] as

$$\bar{O}_\gamma^\tau = \int_{-\infty}^{\infty}\mathrm{d}t\, O_\gamma(t)\frac{\sin(t/\tau)}{\pi t} \tag{4.6}$$

By considering the Fourier transform of the $\sin(x)/x$ function, it can be shown that this expression is equivalent to (see Appendix B for details)

$$\bar{O}_\gamma^\tau = \sum_{n,m}\underbrace{\theta\left(\frac{1}{\tau}-|\epsilon_n-\epsilon_m|\right)}_{\theta_{nm}^\tau}(O_\gamma)_{mn}\left|m\right\rangle\!\left\langle n\right| \tag{4.7}$$

and because for Heaviside theta function we have $\theta(x)^2 = \theta(x)$, the projective character is restored. Properties the $\theta$-function ensure that the $\tau\to\infty$ limit of Eq. (4.7) agrees with Eq. (4.5). Notice also the similarity of this expression to the integrated conductivity (3.5). Indeed, the parameter $1/\tau$ can be interpreted as $\Omega$, giving the frequency cut-off for the matrix elements. Thus, for finite $\tau$, $\left(\bar{O}_\gamma^\tau\middle|\bar{O}_{\gamma'}^\tau\right)$ can be related to the low-frequency spectrum of the correlation function $\langle O_\gamma(t)O_{\gamma'}\rangle$. We shall return to this idea later on.

Let us now calculate the commutator of $O_\gamma^\tau$ with the Hamiltonian

$$\begin{aligned}\left[H,\bar{O}_\gamma^\tau\right] &= \sum_n\sum_{k,p}\epsilon_n\theta_{kp}^\tau(\bar{O}_\gamma)_{kp}[\left|n\right\rangle\!\left\langle n\right|, \left|k\right\rangle\!\left\langle p\right|] \\ &= \sum_{k,p}(\epsilon_k-\epsilon_p)\,\theta_{kp}^\tau(\bar{O}_\gamma)_{kp}\left|k\right\rangle\!\left\langle p\right| \xrightarrow{\tau\to\infty} 0\end{aligned} \tag{4.8}$$

We see that the operator obtained from infinite-time averaging is an integral of motion. Unfortunately, this procedure modifies the support of the operator and in general $\bar{O}_\gamma \notin \mathcal{V}_M$, i.e. its locality is lost.

Having calculated the time-averaged basis $\{\bar{O}_\gamma^\tau\}$, we would like to perform in a systematic way the decomposition 4.4. We need the overlaps between the basis operators before and after the time-averaging. Because of the projective character of the time-averaging, they are given by the pairwise inner products of the time-averaged operators, which we collect into a matrix $K^\tau$, with elements

$$K_{\gamma\gamma'}^\tau = \left(\bar{O}_\gamma^\tau\middle|\bar{O}_{\gamma'}^\tau\right) = \frac{1}{\mathcal{D}}\sum_{n,m}\theta_{nm}^\tau(O_\gamma)_{nm}(O_{\gamma'})_{nm}^* \tag{4.9}$$

This matrix is Hermitian by design, and in the case of systems with time-reversal symmetry, it is also real, thus symmetric. By the spectral theorem, there exists a unitary matrix $U^\tau$ that transforms it via a similarity transformation to a diagonal matrix $D^\tau$

$$\sum_{\gamma,\gamma'} U^\tau_{\beta\gamma} K^\tau_{\gamma\gamma'} (U^\tau)^*_{\beta'\gamma'} = \delta_{\beta\beta'}\lambda^\tau_\beta \in \mathbb{R}, \quad \lambda_\beta \text{ — eigenvalue of } K^\tau \tag{4.10}$$

$$U^\tau (U^\tau)^\dagger = (U^\tau)^\dagger U^\tau = \mathbb{1} \implies \sum_\gamma (U^\tau)_{\beta\gamma} (U^\tau)^*_{\beta'\gamma} = \delta_{\beta\beta'} \tag{4.11}$$

$$U^\tau K^\tau = D^\tau U^\tau \implies \sum_\gamma U^\tau_{\beta\gamma} K^\tau_{\gamma\gamma'} = \sum_\gamma \delta_{\beta\gamma}\lambda^\tau_\gamma U^\tau_{\gamma\gamma'} = \lambda^\tau_\beta U^\tau_{\beta\gamma'} \tag{4.12}$$

Using the columns of $U^\tau$, which are just the eigenvectors of $K^\tau$, we can construct a new set of operators

$$Q^\tau_\beta = \sum_\gamma U^\tau_{\beta\gamma} \bar{O}^\tau_\gamma \tag{4.13}$$

Let us note a few properties of the newly defined quantities. First, they are orthogonal

$$\begin{aligned}\left(Q^\tau_\beta \middle| Q^\tau_{\beta'}\right) &= \sum_{\gamma,\gamma'} U^\tau_{\beta\gamma} \left(\bar{O_\gamma}^\tau \middle| \bar{O_{\gamma'}}^\tau\right) (U^\tau)^*_{\beta'\gamma'} = \sum_{\gamma'} \left(\sum_\gamma U^\tau_{\beta\gamma} K^\tau_{\gamma\gamma'}\right) (U^\tau)^*_{\beta'\gamma'} \\ &= \lambda^\tau_\beta \sum_{\gamma'} U^\tau_{\beta\gamma'} (U^\tau)^*_{\beta'\gamma'} = \lambda^\tau_\beta \delta_{\beta\beta'}\end{aligned} \tag{4.14}$$

where the last two equalities follow from (4.12) and (4.11) respectively. From the fact that $\left(Q^\tau_\beta \middle| Q^\tau_\beta\right) = \lambda^\tau_\beta$ and that $(\cdot|\cdot)$ is an inner product, we immediately deduce that $K^\tau$ is positive semidefinite. We are now ready to consider the desired decomposition into the part that is supported on at most $M$ sites and the remaining, nonlocal part

$$\begin{aligned}Q^\tau_\beta &= \sum_\gamma \left(O_\gamma \middle| Q^\tau_\beta\right) O_\gamma + (Q^\tau_\beta)^\perp = \sum_{\gamma,\gamma'} U^\tau_{\beta\gamma'} \left(O_\gamma \middle| \bar{O}^\tau_{\gamma'}\right) O_\gamma + (Q^\tau_\beta)^\perp \\ &= \sum_{\gamma,\gamma'} U^\tau_{\beta\gamma'} \left(\bar{O}^\tau_\gamma \middle| \bar{O}^\tau_{\gamma'}\right) O_\gamma + (Q^\tau_\beta)^\perp = \sum_{\gamma,\gamma'} U^\tau_{\beta\gamma'} K^\tau_{\gamma\gamma'} O_\gamma + (Q^\tau_\beta)^\perp \\ &= \sum_\gamma \left(\sum_{\gamma'} U^\tau_{\beta\gamma'} K^\tau_{\gamma\gamma'}\right) O_\gamma + (Q^\tau_\beta)^\perp = \sum_\gamma \lambda^\tau_\beta U^\tau_{\beta\gamma} O_\gamma + (Q^\tau_\beta)^\perp = (Q^\tau_\beta)^M + (Q^\tau_\beta)^\perp\end{aligned} \tag{4.15}$$

Everything we did so far holds for an arbitrary value of $\tau$. However, let us for a moment restrict it to $\tau \to \infty$, dropping the superscript. This guarantees that the operators $Q_\beta$ are integrals of motion. We have one step left to complete the algorithm and obtain a classification scheme for the integrals of motion. We need to determine how much of the operator $Q_n$ is contained in the $M$-local part $Q^M_\beta$. In other words, we want to calculate $\|Q^\perp_\beta\|$. Consider the following calculation

$$\begin{aligned}\lambda_\beta = (Q_\beta|Q_\beta) &= \left(Q^M_\beta + Q^\perp_\beta \middle| Q^M_\beta + Q^\perp_\beta\right) = \left(Q^M_\beta \middle| Q^M_\beta\right) + \left(Q^\perp_\beta \middle| Q^\perp_\beta\right) + 2\underbrace{\left(Q^M_\beta \middle| Q^\perp_\beta\right)}_{=0} \\ &= \left(\sum_\gamma \lambda_\beta U_{\beta\gamma} O_\gamma \middle| \sum_{\gamma'} \lambda_\beta U_{\beta\gamma'} O_{\gamma'}\right) + \left\|Q^\perp_\beta\right\|^2 = \lambda^2_\beta \sum_{\gamma,\gamma'} U_{\beta\gamma} \left(O_\gamma | O_{\gamma'}\right) U^*_{\beta\gamma'} + \left\|Q^\perp_\beta\right\|^2 \\ &= \lambda^2_\beta + \left\|Q^\perp_\beta\right\|^2\end{aligned} \tag{4.16}$$

Rearranging the terms, we obtain the desired formula

$$\left\| Q_\beta^\perp \right\|^2 = \lambda_\beta^2 - \lambda_\beta = \lambda_\beta(\lambda_\beta - 1) \geq 0 \tag{4.17}$$

Thus, the spectrum of the matrix $K$ is contained in the interval $[0, 1]$ and determines the classification of the integrals of motion. We have three classes:

- local: $\lambda_\beta = 1 \implies \left\| Q_\beta^\perp \right\| = 0 \implies Q_\beta \in \mathcal{V}_M$
- quasilocal: $\lambda_\beta \in (0, 1) \implies \left\| Q_\beta^\perp \right\| > 0 \implies Q_\beta \in \mathcal{V}$
- generic nonlocal: $\lambda_\beta = 0 \implies \|Q_\beta\| = 0$

Let us now give a physical interpretation of these results. The procedure outlined above can be carried out for, in principle, arbitrary but finite systems size $L$. However, to understand the character of the integrals of motion, we need to take the thermodynamic limit $L \to \infty$. In practical calculations, we are always limited to finite, $M$-local basis of operators. Thus, the output of the algorithm is not the set of true integrals of motion $\{Q_\beta\}$, but rather the set $\{Q_\beta^M/\lambda_n\} \equiv \{I_\beta\}$ (as eigenvectors obtained from numerical procedures are usually normalized). If a particular $\lambda_\beta = 1$, this is not a problem, as we have $\|Q_\beta^M\| = 1$, and the true LIOM is $M$-local. However, if for a given $\beta$ we have $0 < \lambda_\beta < 1$, then $\|Q_\beta^M\| < 1$. It is only if this norm stays non-zero in the thermodynamic limit, we can say that the operator is quasilocal. Then the $Q_\beta^M$ can be regarded as an $M$-local approximation of the true LIOM $Q_\beta$. Numerous studies have confirmed their relevance in the theory of integrable systems [137–140], however, we shall not deal with them any further. In fact, we shall not even deal with LIOMs, as the system we are interested in here is not integrable. Nevertheless, even without integrability, this algorithm will produce a sequence of operators $\{I_\beta\}$, with the largest possible norm, often called **stiffness**. We will refer to them as **local slowly relaxing operators (LSROs)** and they will play a central role in section 4.2. We shall also relax the restriction $\tau \to \infty$ and look at the LSROs at finite values of $\tau$.

### 4.1.2 Details of implementation

Before proceeding further toward a concrete application of the procedure outlined above, let us first discuss some technical details of its implementation. The most demanding part, from the computational point of view, is the calculation of matrix elements (4.9). It requires explicit construction of matrices of all the basis operators $O_\gamma$, change of basis using Hamiltonian eigenstates, time averaging (4.7), and finally carrying out the trace of pairwise products. All those operations are constrained by the fact that the Hilbert space dimension grows exponentially. To keep the computational cost manageable, we can use symmetries of the system. In chapter 1, we have explored how the presence of a symmetry, manifested by the existence of an operator $S$, such that $[S, H] = 0$, can be used to decompose the Hilbert space into a direct sum of $s_{\max}$ smaller subspaces $\mathcal{H}_s$, consisting of states with a fixed eigenvalue $s$ of $S$. Given a compatible operator $A$, its matrix in the symmetry-adapted basis has a block-diagonal structure. It is easy to see that then, its trace is equal to the sum of traces of the individual blocks. Thus, instead of carrying out the algorithm in the full Hilbert space, we can perform it separately in each symmetry sector and then construct the matrix $K^\tau$ by summing the matrices of the individual sectors. However, there is a caveat. We require the basis operators $O_\gamma$ to be traceless, to avoid trivial overlaps with the identity operator, and normalized, to form an orthonormal basis. But they must be traceless and normalized with respect to the full space Hilbert-Schmidt inner product (4.2), not the one restricted to a symmetry sector. It is known from linear algebra, that given a collection of spaces equipped with an inner product, a unique way to define an inner product on the direct sum of those spaces is to consider the sum of the individual inner products [141]. Thus, we have the following identities

$$\Lambda_A \equiv \frac{1}{\mathcal{D}} \operatorname{Tr}(A) = \frac{1}{\mathcal{D}} \sum_{s=1}^{s_{\max}} \operatorname{Tr}(A^s) \tag{4.18}$$

$$\Gamma_A \equiv \|A\|^2 = \frac{1}{\mathcal{D}} \operatorname{Tr}\left(A^\dagger A\right) = \frac{1}{\mathcal{D}} \sum_{s=1}^{s_{\max}} \operatorname{Tr}\left((A^s)^\dagger A^s\right) \tag{4.19}$$

where by $A^s$ we denote the block of matrix of $A$ in the symmetry sector with eigenvalue $s$. Now, we are ready to derive the formula for the overlap matrix, using symmetry sectors. For brevity, we shall suppress the $\tau$ superscript.

$$\begin{aligned}
K_{\gamma\gamma'} &= \left(\frac{\bar{O}_\gamma - \Lambda_{O_\gamma}}{\Gamma_{O_\gamma}} \middle| \frac{\bar{O}_{\gamma'} - \Lambda_{O_{\gamma'}}}{\Gamma_{O_{\gamma'}}}\right) = \frac{1}{\mathcal{D}} \operatorname{Tr}\left(\frac{\bar{O}_\gamma - \Lambda_{O_\gamma}}{\Gamma_{O_\gamma}} \frac{\bar{O}_{\gamma'} - \Lambda_{O_{\gamma'}}}{\Gamma_{O_{\gamma'}}}\right) \\
&= \frac{1}{\mathcal{D}\Gamma_{O_\gamma}\Gamma_{O_{\gamma'}}} \left[\operatorname{Tr}\left(\bar{O}_\gamma \bar{O}_{\gamma'}\right) - \Lambda_{\gamma'} \operatorname{Tr}(O_\gamma) - \Lambda_\gamma \operatorname{Tr}(O_{\gamma'}) + \Lambda_\gamma \Lambda_{\gamma'} \mathcal{D}\right] \\
&= \frac{1}{\mathcal{D}\Gamma_{O_\gamma}\Gamma_{O_{\gamma'}}} \left[\operatorname{Tr}\left(\bar{O}_\gamma \bar{O}_{\gamma'}\right) - \Lambda_{\gamma'} \Lambda_\gamma \mathcal{D}\right] \\
&= \frac{1}{\mathcal{D}\Gamma_{O_\gamma}\Gamma_{O_{\gamma'}}} \left[\sum_{s=1}^{s_{\max}} \operatorname{Tr}\left(\bar{O}^s_\gamma \bar{O}^s_{\gamma'}\right) - \Lambda_{\gamma'} \Lambda_\gamma \mathcal{D}\right]
\end{aligned} \tag{4.20}$$

Algorithm 5 summarizes the procedure for finding LIOMs/LSROs, optimized using symmetry subspaces.

There is one more possible improvement to the algorithm. We have spent the better part of chapter 2 developing numerical methods that allow us to avoid using exact diagonalization. However, the algorithm presented above requires knowledge of the full eigenspectrum of the Hamiltonian. It turns out, that it is possible to escape this requirement, and instead rely on the Dynamical Quantum Typicality approach to correlation functions. We have already hinted at that relationship after introducing finite time averaging (4.7). To see this, let us calculate the Fourier transform of an infinite-temperature correlation function between two operators $A$ and $B$. It is a bit lengthy to carry out the calculation in a rigorous way, so the details are relegated to Appendix B. The result, written in spectral representation, is

$$\mathcal{F}\left[(A(t)|B)\right] = \frac{1}{\mathcal{D}} \sum_{n,m} A_{mn} B_{nm} \delta(\epsilon_m - \epsilon_n + \omega) \tag{4.21}$$

Let us now do one more step and consider the integral of $\mathcal{F}\left[(A(t)|B)\right]$ over some finite frequency window $[-\Omega, \Omega]$, akin to the integrated conductivity (3.5).

$$\begin{aligned}\mathcal{I}_{AB}(\Omega) &= \int_{-\Omega}^{\Omega} \mathrm{d}\omega\, \mathcal{F}\left[(A(t)|B)\right](\omega) = \frac{1}{\mathcal{D}} \sum_{n,m} A_{mn} B_{nm} \int_{-\Omega}^{\Omega} \mathrm{d}\omega\, \delta(\epsilon_m - \epsilon_n + \omega) \\ &= \frac{1}{\mathcal{D}} \sum_{n,m} A_{mn} B_{nm} \theta(\Omega + (\epsilon_m - \epsilon_n))\theta(\Omega - (\epsilon_m - \epsilon_n)) \\ &= \frac{1}{\mathcal{D}} \sum_{n,m} A_{mn} B_{nm} \theta(\Omega - |\epsilon_m - \epsilon_n|) \end{aligned} \tag{4.22}$$

This is a very important result, and the quantity $\mathcal{I}_{AB}(\Omega)$ goes by the name of the integrated spectral function [142]. It tells us that the matrix element of the overlap matrix $K^\tau$, for a pair of operators $A$ and $B$, is equal to the integrated Fourier transform of the infinite-temperature correlation function between $A$ and $B$. This means that we can calculate the matrix elements of $K^\tau$ by using the Dynamical Quantum Typicality and Lanczos-based approach, which should be more efficient than exact diagonalization. Unfortunately, this is not the case for the physical system considered in this thesis, i.e. the long-range Heisenberg model. The reason is that the efficiency of Lanczos-based correlation function calculation relies on the sparse structure of the Hamiltonian matrix. This is of course not the case for a power-law decaying interaction. Thus, we will not use this approach here, as its performance is worse than exact diagonalization. However, all the work is not in vain, as this method will surely prove useful for further research.

## 4.2 Fermionic currents in the long-range Heisenberg model

We are now ready to apply the algorithm described in the previous section to the long-range Heisenberg model. Let us stress again, that this model is not integrable, thus we do not expect to find any strictly conserved, local operator, i.e. LIOMs $I_\beta$ with $\lambda_\beta = 1$. Nevertheless, we can still hope to find a sequence of operators with large stiffness, indicating their slow relaxation.

In order to use the procedure, we need to construct a basis of the operator space $\mathcal{V}_M$. Our starting point is a set of traceless, translationally invariant operators $\{O'_\gamma\}$,

$$O'_\gamma = \frac{1}{\sqrt{L}} \sum_{\ell=1}^{L} (o_{\ell+1} o_{\ell+2} \dots o_{\ell+M}) \tag{4.23}$$

where $o_\ell \in \{\mathbb{1}_\ell, \sqrt{2}S^-_\ell, \sqrt{2}S^+_\ell, 2S^z_\ell\}$ are the single-site operators. It can be verified by direct calculation that they are orthonormal with respect to the Hilbert-Schmidt inner product, as required. However, they are not Hermitian. We have two possible ways to remedy this. First, is to consider **real operators** of the form $O_\gamma = (O'_\gamma + {O'_\gamma}^\dagger)$. The Hamiltonian (1.2) is an example of a real operator. The second option is to consider **imaginary operators**, defined as $O_\gamma = i(O'_\gamma - {O'_\gamma}^\dagger)$. The spin current (1.13) belongs to this class. Fortunately, operators belonging to different classes are orthogonal, so we can consider them separately. Here, we are seeking the most conserved operators, sharing some properties with the spin current, so we are going to focus on the imaginary operators. We numerically perform the steps described in Algorithm 5, initially for $\tau \to \infty$, using the basis of imaginary operators $\{O_\gamma\}$ and the Hamiltonian (1.2) and obtain a sequence of local, orthonormal observables $I_\beta = \sum_\gamma U_{\beta\gamma} O_\gamma$

**Algorithm 5** Algorithm for finding LIOMs/LSROs, optimized using symmetry subspaces

**Input:** $\{O_i\}_{i=1}^{N}$ — Basis of the operator space $\mathcal{V}_M$, tight-binding Hamiltonian $H$

**Output:** $\{I_i\}_{i=1}^{N}$ — most conserved operators (LIOMs/LSROs)

$\Gamma_{O_i} = 0$, $\Lambda_{O_i} = 0$, $K_{ij} = 0$ for all $i, j = 1, \ldots N$

**for** $s = 1 : s_{\max}$ **do**

  Generate and diagonalize $H^s$

  **for** $i = 1 : N$ **do**

    Generate $O_i^s$

    $\Gamma_{O_i} = \Gamma_{O_i} + \frac{1}{\mathcal{D}} \operatorname{Tr}\Big((O_i^s)^\dagger O_i^s\Big)$

    $\Lambda_{O_i} = \Lambda_{O_i} + \frac{1}{\mathcal{D}} \operatorname{Tr}(O_i^s)$

    Change basis and calculate $\bar{O}_i^s$ according to Eq. (4.7)

    **for** $j = i : N$ **do**

      Generate $O_j^s$, calculate $\bar{O}_j^s$ according to Eq. (4.7)

      $K_{ij} = K_{ij} + \frac{1}{\mathcal{D}} \operatorname{Tr}\Big(\bar{O}_i^s \bar{O}_j^s\Big)$

      $K_{ji} = K_{ji} + (1 - \delta_{ij}) K_{ij}$

    **end for**

  **end for**

**end for**

**for** $i, j = 1 : N$ **do**

  $K_{ij} = K_{ij} - \mathcal{D}\Lambda_{O_i}\Lambda_{O_j}$

  $K_{ij} = K_{ij} / (\mathcal{D}\Gamma_{O_i}\Gamma_{O_j})$

**end for**

Diagonalize $K$, obtaining eigenvalues $\{\lambda_i\}$ and eigenvectors $\{U_{ij}\}$

$\{Q_i^M\} = \sum_j U_{ij} O_j$

together with corresponding stifnesses $\lambda_\beta$. Figure 4.1 shows the dependence of the stiffness of the top 3 operators, on the parameters $\Delta$ and $\gamma$. These results were obtained for a system of $L = 16$ sites, with a maximal operator support of $M = 4$ using full Hilber space.

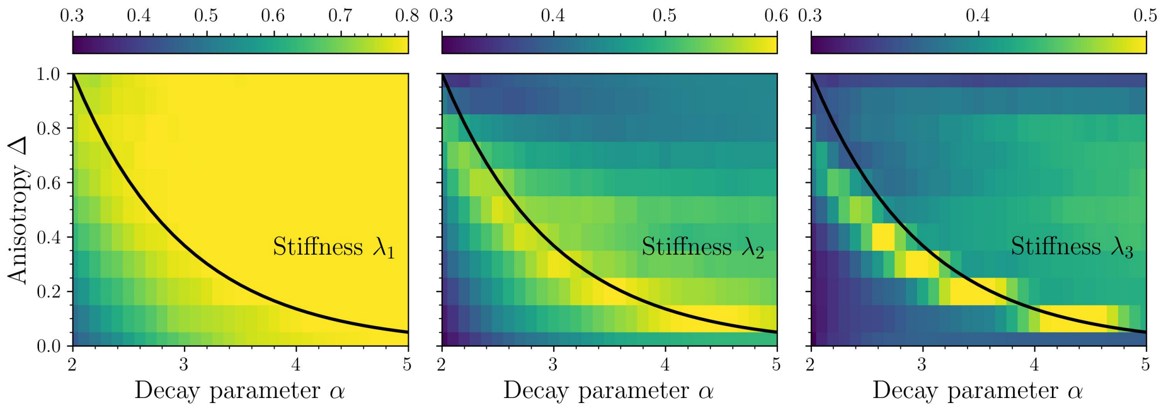



Figure 4.1: Heatmaps depicting the dependence of the stiffness of the top 3 operators on the parameters $\Delta$ and $\gamma$. From left to right we have $\lambda_1$, $\lambda_2$ and $\lambda_3$ respectively. The black line corresponds to the optimal anisotropy $\Delta_O(\alpha) = \exp(-\alpha + 2)$.

We see that $\lambda_2$ and $\lambda_3$ exhibit behavior resembling the initially investigated spin current, that is a clear maximum along the line of optimal anisotropy $\Delta_O(\alpha) = \exp(-\alpha + 2)$, whereas $\lambda_1$ is approximately constant above this line and sharply drops below it. As we are not aware of any mechanism explaining non-zero stiffness in the thermodynamic limit, we have also carried out a finite-size analysis of operators $I_2$ and $I_3$ for 3 points in the parameter space: below the optimal line $(\alpha, \Delta) = (3.5, 0.0)$, on the optimal line $(\alpha, \Delta) = (3.5, 0.2)$ and above the optimal line $(\alpha, \Delta) = (3.5, 0.8)$. The results are shown in Figure 4.2.

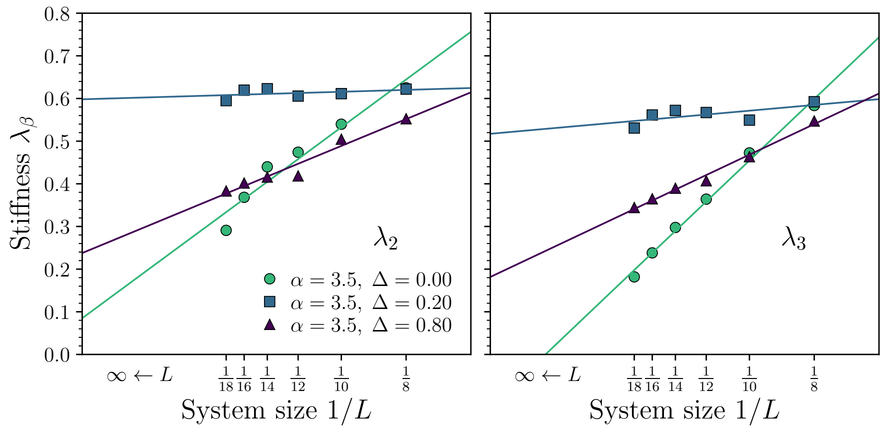



Figure 4.2: Finite size dependence of $\lambda_2$ (left panel) and $\lambda_3$ (right panel) for the optimal anisotropy $\alpha = 3.5$, $\Delta = 0.2$ and away from it $(\Delta = 0.0, 0.8)$.

We observe another feature manifesting itself along the line of optimal anisotropy. Not only the stiffness is the largest, but its dependence on the system size is also the weakest. Still, we know of no reason for it to stay finite in the thermodynamic limit, so we expect it to decay for systems much beyond our reach.

To learn more about the nature of the operators $I_1$, $I_2$, and $I_3$, we have also examined the contribution of each basis operator $O_\gamma$ to their structure. Specifically, we have calculated the projections $(O_\gamma|I_\beta)^2 = |U_{\gamma\beta}|^2$ and discovered that the largest contributions come from three imaginary (current-like) operators

$$O_1 = i\frac{2}{\sqrt{L}}\sum_{\ell=1}^{L}\left(S_\ell^+ S_{\ell+1}^- - \text{H.c.}\right)$$
$$O_2 = i\frac{4}{\sqrt{L}}\sum_{\ell=1}^{L}\left(S_\ell^+ S_{\ell+1}^z S_{\ell+2}^+ - \text{H.c.}\right)$$
$$O_3 = i\frac{8}{\sqrt{L}}\sum_{\ell=1}^{L}\left(S_\ell^+ S_{\ell+1}^z S_{\ell+2}^z S_{\ell+3}^+ - \text{H.c.}\right) \tag{4.24}$$

The adjective *fermionic* describing these currents stems from their image under Jordan-Wigner transformation, which maps them into currents describing particle hopping between first-, second-, and third-nearest neighbors in a system of spinless fermions. The dependence of the projections on the parameters is shown in Figure 4.3.

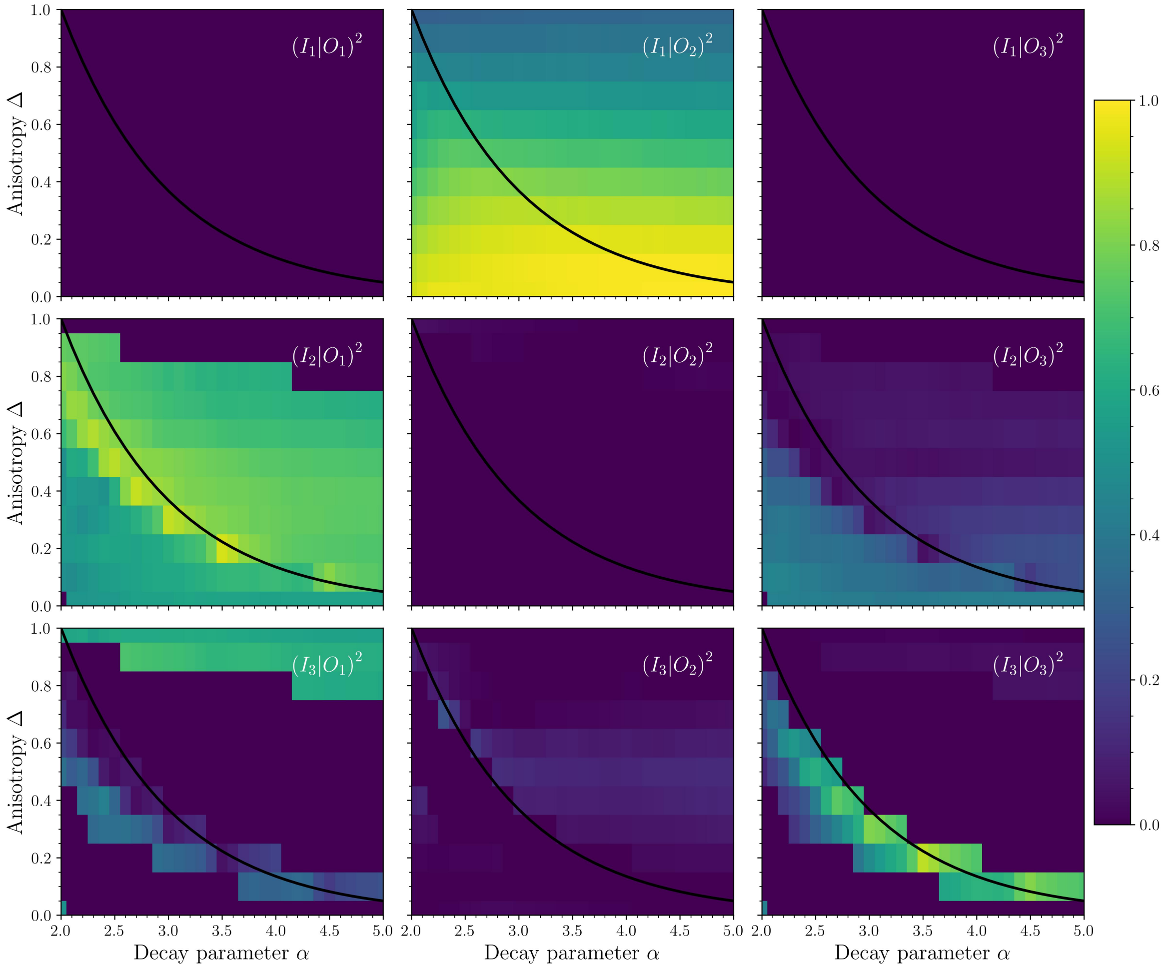



Figure 4.3: Projections of the LSROs $I_\beta$ on the local operators $O_\gamma$ defined in (4.24), i.e. $(O_\gamma|I_\beta)^2 = |U_{\gamma\beta}|^2$ for $\beta = 1, 2, 3$ and $\gamma = 1, 2, 3$.

We see that the best LSRO, $I_1$, has nonzero overlap only with $O_2$, which is even under the spin-flip transformation[2]. Both $O_1$ and $O_3$ are odd under this transformation, so they do not contribute to $I_1$. This is a consequence of the orthogonality between even and odd subspaces of operator space $\mathcal{V}_\mathrm{M}$ and in fact those two spaces can be considered separately to reduce the computational cost. Observing that $\lambda_1 \to 1$ as $\alpha \to \infty$ and $(O_2|I_1)^2 \to 1$ as $\Delta \to 0$, we can suspect that this LSRO is a remnant of the energy current operator [66], which in the nearest-neighbor Heisenberg model is a proper LIOM. Next, $I_2$ has a nonzero overlap only with $O_1$ and $O_3$, which are odd under spin flip. Moreover, the overlap $(O_1|I_2)^2$ is maximal along the line of optimal anisotropy. Similar behavior is observed for $I_3$, but now the overlap with $O_3$ is maximized for parameters on the line. However, there is a slight difference in comparison to the previous two LSROs. There are values of parameters for which $I_3$ has overlap with just the odd currents, whereas for others only with the even one. This is caused by the fact the $I_3$, defined as the operator with the third largest stiffness, can have a completely different structure depending on the parameters of the model. Nevertheless, the important fact is that for optimal anisotropy, it is the odd current that contributes the most. Curiously, even though this model cannot be mapped onto a fermionic system with two-body interactions, numerical evidence points to the existence of long-lived local, fermionic currents which are the most stable at the line of optimal anisotropy.

Finally, we consider the case $\tau < \infty$ and look at the eigenvalues of the overlap matrix $K^\tau$ as functions of $\Omega = 1/\tau$. Let us stop for a moment and see another interpretation of the eigenvalues of $K^\tau$

$$
\begin{aligned}
\lambda_\beta^\tau &= \left(Q_\beta^\tau \middle| Q_\beta^\tau\right) = \sum_{\gamma\gamma'} U_{\beta\gamma} \left(\bar{O}_\gamma^\tau \middle| \bar{O}_{\gamma'}^\tau\right) U_{\beta\gamma'}^* \\
&= \frac{1}{\mathcal{D}} \sum_{\gamma\gamma'} \sum_{n,m} \theta_{nm}^\tau \left(O_\gamma\right)_{nm} \left(O_{\gamma'}\right)_{mn} U_{\beta\gamma} U_{\beta\gamma'}^* \\
&= \frac{1}{\mathcal{D}} \sum_{n,m} \theta_{mn}^\tau \underbrace{\left[\sum_\gamma U_{\beta\gamma} \left(O_\gamma\right)_{nm}\right]}_{(I_\beta)_{nm}} \underbrace{\left[\sum_{\gamma'} U_{\beta\gamma'}^* \left(O_{\gamma'}\right)_{mn}\right]}_{(I_\beta)_{mn}^*} \\
&= \frac{1}{\mathcal{D}} \sum_{n,m} \theta_{nm}^\tau \left|\left(I_\beta\right)_{nm}\right|^2 = \mathcal{I}_{I_\beta I_\beta}\left(\frac{1}{\tau}\right)
\end{aligned}
\tag{4.25}
$$

This is precisely the integrated spectral function (4.22) of the operator $I_\beta$ at frequency $\Omega = 1/\tau$. Thus, by investigating the eigenvalues of $K^\tau$ we can study our LSROs on the same footing as the integrated conductivity in the previous chapter. $\Omega$-dependence of the eigenvalues of $K^\tau$ for the 3 operators with largest stiffnesses, $I_1$, $I_2$, and $I_3$, is shown in Figure 4.4.

The relaxation time of the first LSRO, $I_1$, is not very affected by the proximity to the optimal line, which is expected given its origin as a remnant of the energy current. However, for both $I_2$ and $I_3$ we can clearly see that the decay is the slowest for the parameters on the optimal line. We have thus shown, that the quasiballistic nature is not exclusive to the nonlocal spin current, but also to a broader class of current-like, local operators.

[2]Spin-flip transformation maps $S_\ell^z$ to $-S_\ell^z$. $S_\ell^+$ to $S_\ell^-$ and $S_\ell^-$ to $S_\ell^+$.

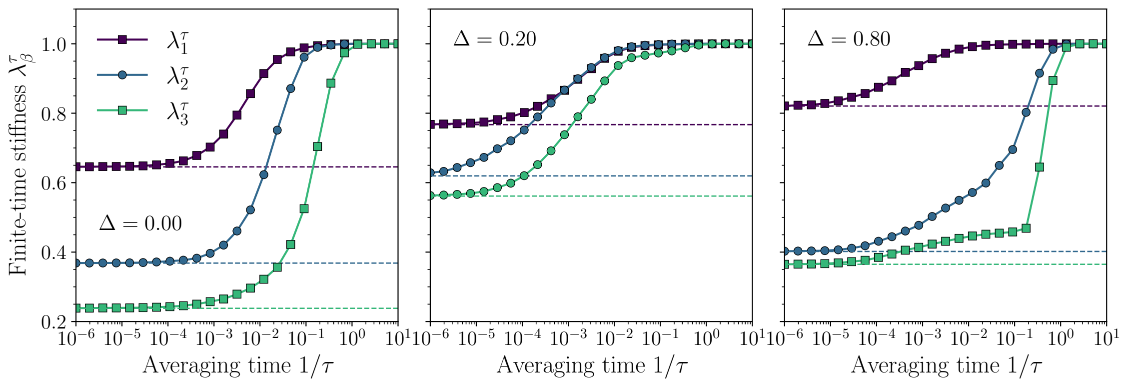



Figure 4.4: Eigenvalues of $K^\tau$ for the 3 operators with largest stiffnesses, $I_1$, $I_2$, and $I_3$, as a function of $\Omega = 1/\tau$. Dashed lines correspond to the $\tau \to \infty$ limit.

# 5 Summary

The overarching goal of the work presented in this thesis, serving as the background is to understand the properties of quantum systems that are close to integrability, as they facilitate real-world implementation, while still maintaining some desired properties of strictly integrable systems. To aid this development, there is a strong need for a robust set of theoretical tools that one could use for the investigation of such systems. As most of the sophisticated machinery developed for integrable systems cease to work for the case of nearly integrable systems, one has to resort to numerical methods. It is impossible to touch upon all the aspects of this topic in a short thesis, thus we had two concrete goals in mind.

The first one was to provide a comprehensive introduction to the numerical methods, beyond the simplest exact diagonalization, that are used in the study of quantum many-body systems. To this end, we presented the Krylov subspace methods, which are designed to leverage the sparsity of matrix representations of physical observables, in order to speed up the computations. Starting from the very beginning, we introduced in detail the Arnoldi iteration, which is most often used to find the extremal eigenvalues of general, non-hermitian matrices, even though it does so rather accidentally. We then moved on to the case of hermitian matrices, where this procedure reduces to the well-known and versatile Lanczos iteration. As an immediate application of the Lanczos iteration, beyond just the ground state computations, the so-called Krylov propagator was presented, which allows one to compute the time evolution of a state vector, without the need for diagonalization of the Hamiltonian. Finally, we described, and partially derived, an approach to the correlation functions, based on the Krylov propagator and the concept of Quantum Typicality, which allows one to compute the correlation functions without explicitly carrying out the trace over all many-body states.

The second goal was to apply those methods to the study of the dynamics of the spin transport in the anisotropic Heisenberg model with power-law interaction $J(\alpha) = J/r^{\alpha}$, which is an important example of a long-range interacting system. Motivated by experimental setups, we started by considering the expansion of a domain-wall initial state and found a non-monotonic dependence of the center of mass velocity on the anisotropy parameter. By considering maximal velocities, we found a line in the parameter space, $\Delta_O(\alpha) = \exp(-\alpha + 2)$, for which the velocity of spin domain wall expansion is similar to the case of free nearest-neighbors particles, indicating short-time (high-frequency) ballistic transport. Next, we studied spin transport from the perspective of the linear response theory, by considering the optical conductivity and its integral over a frequency window. It revealed a regime of quasi-ballistic transport, where the spectral sum of the optical conductivity accumulated at frequencies below $\Omega^*/J \sim 10^{-3} - 10^{-2}$. As a result, along the line of optimal anisotropy, the spin transport is ballistic for surprisingly long times, up to $t \sim 1/\Omega^*$, which is in agreement with the results of the domain-wall expansion. We also investigated the properties of local, slowly relaxing observables (LSROs), obtained using a numerical algorithm designed to find local integrals of motion in integrable systems. For completeness, we provided a rather detailed description of the algorithm itself, together with a possible upgrade, replacing ED-based time averaging with Lanczos-based long-time correlation functions. Unfortunately, the upgraded approach turned out to be unsuitable for the purpose of this thesis, as matrices of long-range operators are no longer sparse and thus do not benefit from the Lanczos iteration. Nevertheless, using the original algorithm, we found that the best LSROs decay the slowest precisely for the optimal anisotropy, obtained from previous methods. Additionally, we showed that they can be understood in terms of projections onto current-like operators, corresponding via the Jordan-Wigner transformation to long-range fermionic hoppings, even though the Hamiltonian does not admit a representation in terms of two-body fermionic operators. Finally, using finite-time averaging version of the algorithm, we investigated the frequency dependence of the LSROs, akin to the optical conductivity, and found that the concentration of the spectral weight resembles the one of the optical conductivity.

The main result of this thesis, and the broader research published in [96], is the discovery of the line of optimal anisotropy, $\Delta_O(\alpha) = \exp(-\alpha + 2)$, along which the spin transport is ballistic for surprisingly long times $tJ \sim 10^{-2} - 10^{-3}$. This line smoothly interpolates between integrable two models with purely ballistic transport, namely free particles for $\alpha = \infty,\ \Delta = 0$ and Haldane-Shastry like model for $\alpha = 2,\ \Delta = 1$. It suggests that the long-range Heisenberg model can be thought of as nearly-integrable far beyond just the vicinity of the integrable limits, but rather for a whole line of parameters. Unfortunately, the precise microscopic origin of the optimal anisotropy is still unknown. A possible explanation would be that for $\delta = \exp(-\alpha + 2)$ this model is very close to some, more complicated, integrable model, in which the spin current is an integral of motion. Investigation of systems similar to the one studied in this thesis, from the perspective of the search for remnants of integrability, is a promising direction for future research.

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# A
# Optical conductivity in spin chains

The aim of this appendix is to derive the Kubo formula for the optical conductivity in spin chains, specifically the spectral representation of the real part, as given in Eq. (3.4). In the spirit of the pedagogical approach of this thesis, we shall present all the steps in detail. For simplicity, we consider the nearest-neighbor version of the Heisenberg model:

$$H = \underbrace{\frac{J}{2}\sum_{\ell=1}^{L}\left(S_\ell^+ S_{\ell+1}^- + S_\ell^- S_{\ell+1}^+\right)}_{H_0} + \underbrace{J\Delta\sum_{\ell=1}^{L} S_\ell^z S_{\ell+1}^z}_{H_{\text{int}}} - h\sum_{\ell=1}^{L} S_\ell^z \tag{A.1}$$

## A.1 Peierls phase

To discuss the linear *response*, we need to couple our model to some external field, in our case the electromagnetic field. Under the Jordan-Wigner transformation, the Hamiltonian (A.1) maps to a model of spinless fermions, with a density-density interaction term.

$$H_{\text{F}} = \frac{J}{2}\sum_{\ell=1}^{L}\left(c_\ell^\dagger c_{\ell+1} + c_{\ell+1}^\dagger c_\ell\right) + J\Delta\sum_{\ell=1}^{L}\left(n_\ell - \frac{1}{2}\right)\left(n_{\ell+1} - \frac{1}{2}\right) - h\sum_{\ell=1}^{L}\left(n_\ell - \frac{1}{2}\right) \tag{A.2}$$

where $n_\ell = c_\ell^\dagger c_\ell$. In this picture, the kinetic part of the fermionic Hamiltonian couple to the electromagnetic field via the so-called **Peierls phase**, which is a manifestation of the $U(1)$ gauge field. To understand how this happens in the formalism of second quantization, we need to return for a moment back to the first quantization picture for spinless fermions. This section is based on the book by Essler et al. [143]. A one-particle Hamiltonian in a 3-dimensional space is given by

$$h_1 = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \tag{A.3}$$

where $\mathbf{p}$ is the momentum operator and $V(x)$ is some external potential. In the presence of an electromagnetic 4-potential $(\Phi(\mathbf{x},t), A^\alpha(\mathbf{x},t)/c)$, the momentum operator is modified, via the minimal coupling, to the following form:

$$h_1 \to \frac{1}{2m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2 - e\,\Phi(\mathbf{x},t) + V(\mathbf{x}) \tag{A.4}$$

where $\Phi$ is the scalar potential and $\mathbf{A}$ is the vector potential. Moreover, we can choose the **radiation gauge** $\Phi(\mathbf{x}, t) = 0$. Now, let us proceed with the second quantization procedure in the standard fashion. Let $c_\ell^\dagger, c_\ell$ create and annihilate a particle in the Wannier state $\phi(\mathbf{x} - \mathbf{R}_\ell)$, corresponding to the $\ell$-th lattice site (we assume only a single band). Written using those operators, the one-particle part of the Hamiltonian *without* the electromagnetic field is

$$H_1 = \sum_{\ell,\ell'} t_{\ell\ell'} c_\ell^\dagger c_{\ell'} \tag{A.5}$$

where the hopping matrix elements are given by the matrix elements of the one-particle operator, between the Wannier states:

$$t_{\ell\ell'} = \int \mathrm{d}x^3\, \phi^*(\mathbf{x} - \mathbf{R}_\ell) \left( \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \right) \phi(\mathbf{x} - \mathbf{R}_{\ell'}) \tag{A.6}$$

From the above expression, we can see that the influence of the electromagnetic field enters the second-quantized Hamiltonian via the hopping integrals. Let us see now how this happens

$$\begin{aligned} t_{\ell\ell'} &\to \int \mathrm{d}x^3\, \phi^*(\mathbf{x} - \mathbf{R}_\ell) \left[ \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c}\mathbf{A} \right)^2 + V(\mathbf{x}) \right] \phi(\mathbf{x} - \mathbf{R}_{\ell'}) \\ &\triangleq \int \mathrm{d}x^3\, \phi^*(\mathbf{x} - \mathbf{R}_\ell) \mathrm{e}^{-ie\lambda/c} \left[ \frac{1}{2m} \left( \mathbf{p} - \frac{q}{c}(\mathbf{A} - \boldsymbol{\nabla}\lambda) \right)^2 + V(\mathbf{x}) \right] \mathrm{e}^{ie\lambda/c} \phi(\mathbf{x} - \mathbf{R}_{\ell'}) \end{aligned} \tag{A.7}$$

Note, that the equality denoted with $\triangleq$ is valid for any differentiable, complex gauge field $\lambda(\mathbf{x}, t)$. We choose it to be

$$\lambda(\mathbf{x}, t) = \int_{\mathbf{x}_0}^{\mathbf{x}} \mathrm{d}\mathbf{x}' \cdot \mathbf{A}(\mathbf{x}', t) \tag{A.8}$$

for an arbitrary reference point $\mathbf{x}_0$. Furthermore, we introduce modified Wannier functions

$$\tilde{\phi}(\mathbf{x} - \mathbf{R}_\ell) = \mathrm{e}^{ie\lambda(\mathbf{x},t)/c} \phi(\mathbf{x} - \mathbf{R}_\ell) \tag{A.9}$$

This way, we can write the modified hopping integrals as

$$t_{\ell\ell'}(t) = \int \mathrm{d}x^3\, \tilde{\phi}^*(\mathbf{x} - \mathbf{R}_\ell) \left[ \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) \right] \tilde{\phi}(\mathbf{x} - \mathbf{R}_{\ell'}) \tag{A.10}$$

thus recovering (almost) the original form of the hopping integral, but with the modified Wannier functions. We need a few more steps to get to the final result. First, let us assume that the Wannier functions are strongly localized, and that the vector potential varies slowly on the scale of the lattice constant. This permits the approximation

$$\tilde{\phi}(\mathbf{x} - \mathbf{R}_\ell) \approx \phi(\mathbf{x} - \mathbf{R}_\ell) \mathrm{e}^{ie\lambda(\mathbf{R}_\ell, t)/c} \tag{A.11}$$

We can also assume that the hopping integrals beyond nearest neighbors are negligible, and denote its nearest-neighbor value by $t$. Then, we can write the one-particle Hamiltonian as

$$H_1(t) = -t \sum_{\langle \ell,\ell' \rangle} \mathrm{e}^{iq(\lambda(\mathbf{R}_\ell, t) - \lambda(\mathbf{R}_{\ell'}, t))/c} c_\ell^\dagger c_{\ell'} \tag{A.12}$$

Phase appearing in the above expression is precisely the Peierls phase. This is a general result, valid for any lattice geometry and in the tight-binding approximation. However, in this thesis we are only interested in a one-dimensional, periodic lattice, so let us simplify a bit. We can slightly modify the gauge field and absorb the constant $-\frac{q}{c}$

$$\begin{aligned}\lambda_{\ell,\ell+1}(t) &= -\frac{q}{c}\int_{\mathbf{R}_\ell}^{\mathbf{R}_{\ell+1}} \mathrm{d}\mathbf{x}\cdot\mathbf{A}(\mathbf{x},t) = -\frac{q}{c}\int_{\mathbf{x}_0}^{\mathbf{R}_{\ell+1}} \mathrm{d}\mathbf{x}\cdot\mathbf{A}(\mathbf{x},t) - \frac{q}{c}\int_{\mathbf{R}_\ell}^{\mathbf{x}_0} \mathrm{d}\mathbf{x}\cdot\mathbf{A}(\mathbf{x},t)\\ &= -\frac{q}{c}\int_{\mathbf{x}_0}^{\mathbf{R}_{\ell+1}} \mathrm{d}\mathbf{x}\cdot\mathbf{A}(\mathbf{x},t) + \frac{q}{c}\int_{\mathbf{x}_0}^{\mathbf{R}_{\ell}} \mathrm{d}\mathbf{x}\cdot\mathbf{A}(\mathbf{x},t) = \frac{q}{c}\left[\lambda(\mathbf{R}_\ell,t) - \lambda(\mathbf{R}_{\ell+1},t)\right]\end{aligned} \quad \text{(A.13)}$$

and finally obtain the desired result

$$H_1(t) = -t\sum_{\ell=1}^{L} \mathrm{e}^{i\lambda_{\ell,\ell+1}(t)} c_\ell^\dagger c_{\ell+1} + \text{h.c.} \quad \text{(A.14)}$$

Before we return to the original problem, let us see what is the relation of $\lambda_{\ell,\ell+1}(t)$ to the electric field. We define the electric field in terms of the 4-potential as

$$\mathbf{E}(\mathbf{x},t) = -\boldsymbol{\nabla}\phi(\mathbf{x},t) - \frac{1}{c}\frac{\partial\mathbf{A}(\mathbf{x},t)}{\partial t} = -\frac{1}{c}\frac{\partial\mathbf{A}(\mathbf{x},t)}{\partial t} \quad \text{(A.15)}$$

where the gradient of scalar potential is zero, since we are working in the radiation gauge. As we consider a one-dimensional, periodic system, i.e. ring lattice, the electric field vector can be decomposed into the radial and azimuthal components $\mathbf{E}(\mathbf{x},t) = E(r,t)\mathbf{e}_\varphi$, where $\mathbf{e}_\varphi$ is the unit vector along the ring and $r$ is the distance from the center of the ring. Thus, we can choose the vector potential to have the same form $\mathbf{A}(\mathbf{x},t) = A(r,t)\mathbf{e}_\varphi$. Then, we can carry out the integration in (A.13) and obtain

$$\lambda(t) \equiv \lambda_{\ell,\ell+1}(t) = -\frac{qa_0}{c}A(R,t) \quad \text{(A.16)}$$

where $a_0 = 2\pi\frac{R}{L}$ is the lattice constant and $R$ is the radius of the ring.

## A.2 Linear response of the spin current

Now, we can return from the fermionic realm back to our spin chain. For the remainder of this section, we set the speed of light $c = 1$. Using new insight from the previous section and following Göhmann et al. [144], we can write our Heisenberg Hamiltonian, with the Peierls phase, as

$$H'(t) = \underbrace{\frac{J}{2}\sum_{\ell=1}^{L}\left(\mathrm{e}^{i\lambda(t)}S_\ell^+ S_{\ell+1}^- + \mathrm{e}^{-i\lambda(t)}S_\ell^- S_{\ell+1}^+\right)}_{H_\lambda(t)} + \underbrace{J\sum_{\ell=1}^{L} S_\ell^z S_{\ell+1}^z}_{H_{\text{int}}} - h\sum_{\ell=1}^{L} S_\ell^z \quad \text{(A.17)}$$

where the gauge field $\lambda(t)$ is related to time-dependent electric field $E(t)$ as

$$\frac{\partial\lambda(t)}{\partial t} = qa_0E(t) \quad \text{(A.18)}$$

Thus, in Fourier space, we have the relation

$$\lambda_{\mathrm{F}}(\omega) = \frac{iqa_0}{\omega}E_{\mathrm{F}}(\omega), \text{ where } \lambda_{\mathrm{F}}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{i\omega t}\lambda(t) \quad \text{(A.19)}$$

provided that the Fourier transform exists. We assume that the electric field is switched on adiabatically, and is asymptotically constant. In terms of the gauge field, this can be expressed as $|\lambda(t)| \leq \mathrm{e}^{\varepsilon t}$ for $t \to -\infty$ and $|\lambda(t)| \leq bt$ for $t \to \infty$, where $\varepsilon > 0$ and $b > 0$ are some constants. Then, in the $t \to \infty$ limit, we have

$$\mathrm{e}^{i(\mathrm{Re}(\omega)t + i\,\mathrm{Im}(\omega)t)}\lambda(t) \leq \mathrm{e}^{i\,\mathrm{Re}(\omega)t}\mathrm{e}^{-\,\mathrm{Im}(\omega)t}bt,$$

whereas in the $t \to -\infty$ limit, we have

$$\mathrm{e}^{i(\mathrm{Re}(\omega)t + i\,\mathrm{Im}(\omega)t)}\lambda(t) \leq \mathrm{e}^{i\,\mathrm{Re}(\omega)t}\mathrm{e}^{(-\,\mathrm{Im}(\omega)+\varepsilon)t}$$

Thus, the Fourier transform of the gauge field exists in the vertical strip $0 < \mathrm{Im}(\omega) < \varepsilon$, and technically, we should not think about purely real frequencies, but instead about the limit $\lim_{\epsilon\to 0^+} \omega + i\epsilon \equiv \omega + i0^+$.

Of course, application of such external field will induce a current in the system. We can obtain the corresponding current operator by inspecting the nearest-neighbor restriction of the long-range current (1.13) and noticing that the gauge field enters the Hamiltonian only through the Peierls phase, which is a scalar and commutes with the spin operators. Thus, the current density reads

$$\mathcal{J}^\sigma_\ell(t) = i\frac{J}{2}\left(\mathrm{e}^{i\lambda(t)}S^+_\ell S^-_{\ell+1} - \mathrm{e}^{-i\lambda(t)}S^-_\ell S^+_{\ell+1}\right) \tag{A.20}$$

and the total current is

$$\mathcal{J}^\sigma(t) = \sum_{\ell=1}^{L} J^\sigma_\ell(t) = i\frac{J}{2}\sum_{\ell=1}^{L}\left(\mathrm{e}^{i\lambda(t)}S^+_\ell S^-_{\ell+1} - \mathrm{e}^{-i\lambda(t)}S^-_\ell S^+_{\ell+1}\right) \tag{A.21}$$

Here, as in $H'(t)$, the time argument is an explicit time-dependence, not the Heisenberg picture one. Note that we reserve the script $\mathcal{J}^\sigma$ for current including Peierls phase, and keep the lowercase $j^\sigma$ for the current without it. To apply the reasoning typical for the linear response theory, we need to identify the perturbation $V(t)$, such that our time-dependent Hamiltonian reads is decomposed as $H' = H + V(t)$. However, we will only need this perturbation up to the first order, so let us expand $H_\lambda(t)$ into the power series in the gauge field $\lambda(t)$ as

$$\begin{aligned}
H_\lambda(t) &= \frac{J}{2}\sum_{\ell=1}^{L}\left[\mathrm{e}^{i\lambda(t)}S^+_\ell S^-_{\ell+1} + \mathrm{e}^{-i\lambda(t)}S^-_\ell S^+_{\ell+1}\right] \\
&= \frac{J}{2}\sum_{\ell=1}^{L}\left[\left(1 + i\lambda(t) + O(\lambda^2)\right)S^+_\ell S^-_{\ell+1} + \left(1 - i\lambda(t) + O(\lambda^2)\right)S^-_\ell S^+_{\ell+1}\right] \\
&= \frac{J}{2}\sum_{\ell=1}^{L}\left[S^+_\ell S^-_{\ell+1} + S^-_\ell S^+_{\ell+1}\right] + \frac{iJ}{2}\sum_{\ell=1}^{L}\left[S^+_\ell S^-_{\ell+1}\lambda(t) - S^-_\ell S^+_{\ell+1}\lambda(t)\right] + O(\lambda^2) \\
&= H_0 + \lambda(t)j^\sigma + O(\lambda^2)
\end{aligned} \tag{A.22}$$

Thus we have $H' = H + \lambda(t)j^\sigma + O(\lambda^2)$ and the perturbation is identified as, up to the first order, $V(t) = \lambda(t)j^\sigma$. Analogously, we can expand the current operator to obtain

$$\mathcal{J}^\sigma(t) = j^\sigma - \lambda(t)H_0 + O(\lambda^2) \tag{A.23}$$

We have now all the ingredients to proceed with the calculation of linear response. In what follows, we will need to work with observables depending on time via the Heisenberg picture. They will always be denoted with a subscript, denoting which Hamiltonian generates the time evolution, to differentiate them from the operators in the Schrödinger picture with explicit time-dependence. Despite the pedagogical character of this section, we will refrain from the full derivation of the Kubo linear response theory, as this would enlarge this long appendix even further. Instead, here we will only sketch the idea and present the final formula, whereas the interested reader is, as usual, referred to the literature for details [115, 145, 146]. Formal solution of the Schrödinger equation, with the Hamiltonian $H'(t) = H + V(t)$, is given by the unitary time evolution operator $U(t, t_0)$ which acting on the initial state $|\psi(t_0)\rangle$ yields the state at time $t$, $|\psi(t)\rangle = U(t, t_0)\,|\psi(t_0)\rangle$. Moreover, it fulfills the equation

$$i\partial_t U(t, t_0) = H'(t)U(t, t_0) \tag{A.24}$$

Let now $\rho(t)$ be the density operator at time $t$. We assume that our system, before the perturbation is switched on at time $t_0$, is in the thermal equilibrium thus $\rho(t < t_0) = \rho_0$, where $\rho_0$ denotes the canonical ensemble density operator, $\rho_0 = \mathrm{e}^{-\beta H} / \operatorname{Tr} \mathrm{e}^{-\beta H}$, where $\beta = 1/k_B T$ is the inverse temperature. Corresponding average will be denoted as $\langle \dots \rangle_0$. By expanding the density operator in the time-evolved basis of eigenstates of $H$, the unperturbed Hamiltonian, we obtain

$$\begin{aligned}\rho(t) &= \sum_n \frac{\mathrm{e}^{-\beta E_n}}{\operatorname{Tr} \mathrm{e}^{-\beta H}} |n(t)\rangle\langle n(t)| = \sum_n \frac{\mathrm{e}^{-\beta E_n}}{\operatorname{Tr} \mathrm{e}^{-\beta H}} U(t, t_0)\,|n\rangle\langle n|\,U^\dagger(t, t_0) \\ &= U(t, t_0)\rho_0 U^\dagger(t, t_0)\end{aligned} \tag{A.25}$$

The time-dependent average of any operator $A$ is then given using $\rho(t)$,

$$\langle A \rangle_t = \operatorname{Tr}\left(\rho(t)A\right) = \langle U^\dagger(t, t_0) A U(t, t_0)\rangle_0 \tag{A.26}$$

where for the last equality we have used the cyclic property of the trace. Core goal of the linear response theory is the calculation of the above quantity, up to linear order in the perturbation $V(t)$. The standard approach is to move to the so-called **interaction picture**, where the time evolution given by the unperturbed Hamiltonian is absorbed into the states and the observables, and the time evolution operator depends only on the perturbation. It facilitates a systematic way for the perturbative solution of the equation (A.24), yielding subsequent approximations to the time evolution operator. The first order of this expansion also goes under the name of the **Born approximation**. Omitting the details, we have

$$\begin{aligned}\langle A \rangle_t &= \langle A_H(t)\rangle_0 - i\int_{-\infty}^{t} \mathrm{d}t' \langle [A_H(t), (V(t'))_H(t')]\,\rangle_0 \\ &= \langle A_H(t)\rangle_0 + \int_{-\infty}^{\infty} \mathrm{d}t'\left(-i\theta(t - t')\langle [A_H(t), (V(t'))_H(t')]\,\rangle_0\right)\end{aligned} \tag{A.27}$$

This equation is known as the **Kubo formula**. We assume that the perturbation is turned on adiabatically, starting from the infinite past, i.e. $t_0 \to -\infty$. What is interesting about the above formula, is that it does not depend on neither full evolution operator $U(t, t_0)$ nor the evolution operator generated by the perturbation. Therefore, we are in thermodynamic equilibrium — both canonical ensemble and the time evolution are generated by the same, unperturbed Hamiltonian. This will, in a moment, yield some very useful simplifications. Let us finally take the current operator $\mathcal{J}^\sigma(t)$ as the observable $A$, and the perturbation $V(t) = \lambda(t) j^\sigma + O(\lambda^2)$. We have

$$\langle \mathcal{J}^\sigma(t) \rangle_t = \langle (\mathcal{J}^\sigma(t))_H(t) \rangle_0 + \int_{-\infty}^{\infty} \mathrm{d}t' \, (-i\theta(t-t') \langle [(\mathcal{J}^\sigma(t))_H(t), (V(t'))_H(t')] \, \rangle_0) \tag{A.28}$$

First, let us deal with the term that does not feel the perturbation at all

$$\begin{aligned} \langle (J^\sigma(t))_H(t) \rangle_0 &= \langle J^\sigma(t) \rangle_0 = \langle j^\sigma - \lambda(t) H_0 + O(\lambda^2) \rangle_0 \\ &= \langle j^\sigma \rangle_0 - \lambda(t) \langle H_0 \rangle_0 + O(\lambda^2) \qquad \text{(A.29)} \\ &= -\lambda(t) \langle H_0 \rangle_0 + O(\lambda^2) \qquad \text{(A.30)} \end{aligned}$$

In the first equality we got rid of the Heisenberg time dependence, by utilizing the equilibrium condition and the cyclic property of the trace. In the last line we got rid of $\langle j^\sigma \rangle_0$, which vanishes due to different parities of $j^\sigma$ and $H$ under spin-flip transformation. Now, for the second, more complicated term

$$\begin{aligned} &\int_{-\infty}^{\infty} \mathrm{d}t' \, (-i\theta(t-t') \langle [(\mathcal{J}^\sigma(t))_H(t), (V(t'))_H(t')] \, \rangle_0) = \\ &\int_{-\infty}^{\infty} \mathrm{d}t' \, (-i\theta(t-t') \langle [(\mathcal{J}^\sigma(t))_H(t-t'), V(t')] \, \rangle_0) = \\ &\int_{-\infty}^{\infty} \mathrm{d}t' \, \Big(-i\theta(t-t') [\mathrm{e}^{iH(t-t')} (j^\sigma - \cancel{\lambda(t') H_0 + O(\lambda^2)}) \mathrm{e}^{-iH(t-t')}, \lambda(t') j^\sigma] \Big) \\ &\int_{-\infty}^{\infty} \mathrm{d}t' \, (-i\theta(t-t') [(j^\sigma_H(t-t'), j^\sigma] \,) \, \lambda(t') \qquad \text{(A.31)} \end{aligned}$$

We passed from first to second line by using once again the equilibrium condition and the cyclic property of the trace. In the third line, the crossed out terms would produce a contribution of order $\lambda^2$ and higher, so we can safely omit them. The quantity in the parenthesis is important enough to deserve a name, so we define the **retarded Green's function** as

$$G^r_{j^\sigma j^\sigma}(t, t') := -i\theta(t-t') [(j^\sigma_H(t), j^{\sigma(t')}] \tag{A.32}$$

and the Kubo formula becomes

$$\langle \mathcal{J}^\sigma(t) \rangle_t = -\lambda(t) \langle H_0 \rangle_0 + \int_{-\infty}^{\infty} \mathrm{d}t' G^r_{j^\sigma j^\sigma}(t-t', 0) \lambda(t') \tag{A.33}$$

We stress once again, that $G^r_{j^\sigma j^\sigma}(t, t') = G^r_{j^\sigma j^\sigma}(t-t', 0)$ is valid *only* in thermodynamic equilibrium. As most transport experiments measure quantities in the frequency domain, we need to consider the Fourier transform of the Kubo formula

$$\mathcal{J}_{\mathrm{F}}(\omega) = q a_0 \int_{-\infty}^{\infty} \mathrm{d}t \, \mathrm{e}^{i\omega t} \frac{\langle \mathcal{J}^\sigma(t) \rangle_t}{a_0^3 L} \tag{A.34}$$

where $\mathcal{J}_{\mathrm{F}}(\omega)$ is the Fourier-transformed current per volume, expressed in physical units. We calculate

$$
\begin{aligned}
\mathcal{J}_{\mathrm{F}}(\omega) &= \frac{q}{a_0^2 L}\int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{i\omega t}\langle \mathcal{J}^\sigma(t)\rangle_t \\
&= -\frac{q}{a_0^2 L}\langle H_0\rangle \int_{-\infty}^{\infty} \mathrm{d}t\ \mathrm{e}^{i\omega t}\lambda(t) + \frac{q}{a_0^2 L}\int_{-\infty}^{\infty}\mathrm{d}t \int_{-\infty}^{\infty}\mathrm{d}t'\ \mathrm{e}^{i\omega t} G^r_{j^\sigma j^\sigma}(t-t',0)\lambda(t') \\
&= -i\frac{q^2}{a_0 L}\frac{\langle H_0\rangle_0 E_{\mathrm{F}}(\omega)}{\omega + i0^+} + \frac{q}{a_0^2 L}\int_{-\infty}^{\infty}\mathrm{d}t'' \int_{-\infty}^{\infty}\mathrm{d}t'\ \mathrm{e}^{i\omega(t'+t'')} G^r_{j^\sigma j^\sigma}(t'',0)\lambda(t') \\
&= -i\frac{q^2}{a_0 L}\frac{\langle H_0\rangle_0 E_{\mathrm{F}}(\omega)}{\omega + i0^+} + \frac{q}{a_0^2 L}\int_{-\infty}^{\infty}\mathrm{d}t''\mathrm{e}^{i\omega t''} G^r_{j^\sigma j^\sigma}(t'',0)\int_{-\infty}^{\infty}\mathrm{d}t'\ \mathrm{e}^{i\omega t'}\lambda(t') \\
&= -i\frac{q^2}{a_0 L}\frac{\langle H_0\rangle_0 E_{\mathrm{F}}(\omega)}{\omega + i0^+} + i\frac{q^2}{a_0 L} G^r_{j^\sigma j^\sigma}(\omega) E_{\mathrm{F}}(\omega) \\
&= \frac{q^2}{a_0}\left[\frac{i}{L(\omega+i0^+)}\left(-\langle H_0\rangle_0 + G^r_{j^\sigma j^\sigma}(\omega)\right)\right] E_{\mathrm{F}}(\omega)
\end{aligned} \tag{A.35}
$$

and recognize, that the final line is just the general form of the Ohm's law $\mathcal{J}_{\mathrm{F}}(\omega) = \frac{q^2}{a_0}\tilde{\sigma}(\omega)E_{\mathrm{F}}(\omega)$, with the complex **optical conductivity** $\tilde{\sigma}(\omega)$ given by the expression in the square bracket above. Assuming $\langle[j^\sigma(t), j^\sigma]\rangle$ to be bounded for $t\to\infty$, which is reasonable, the Fourier transform of the retarded Green's function is a holomorphic function in the upper half plane, and so it the optical conductivity. Hence, the real part and the imaginary part are not independent, but related by the Kramers-Kronig relations. We can therefore restrict our attention to just the real part of the conductivity. This is precisely what we have done in Chapter 3. Setting $\tilde{\sigma}'(\omega) \equiv \operatorname{Re}\tilde{\sigma}(\omega)$, we have

$$
\tilde{\sigma}'(\omega) = \frac{1}{L(\omega+i0^+)}\operatorname{Re}\left[iG^r_{j^\sigma j^\sigma}(\omega)\right] = -\frac{1}{L(\omega+i0^+)}\operatorname{Im}\left[G^r_{j^\sigma j^\sigma}(\omega)\right] \tag{A.36}
$$

The stage is now set for us to use one of the most powerful tools in the arsenal of statistical physics, namely the quantum version of the **fluctuation-dissipation theorem**. It relates the autocorrelation function of a physical quantity to the imaginary part of the response function $G^r_{j^\sigma j^\sigma}$, and is given by

$$
\langle j^\sigma_H(t)j^\sigma\rangle_0 = \frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\ \mathrm{e}^{-i\omega t}\frac{\operatorname{Im}G^r_{j^\sigma j^\sigma}(\omega)}{\mathrm{e}^{-\beta\omega}-1} = -\frac{L}{\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega\ \mathrm{e}^{-i\omega t}\frac{\omega\tilde{\sigma}'(\omega)}{\mathrm{e}^{-\beta\omega}-1} \tag{A.37}
$$

Applying the Fourier transform to both sides, we get

$$
\begin{aligned}
-\frac{\pi}{L}\int_{-\infty}^{\infty}\mathrm{d}t\ \mathrm{e}^{i\omega' t}\langle j^\sigma_H(t)j^\sigma\rangle_0 &= \int_{-\infty}^{\infty}\mathrm{d}t\int_{-\infty}^{\infty}\mathrm{d}\omega\,\mathrm{e}^{i(\omega'-\omega)t}\omega\frac{\tilde{\sigma}'(\omega)}{\mathrm{e}^{-\beta\omega}-1} \\
&= \int_{-\infty}^{\infty}\mathrm{d}\omega 2\pi\delta(\omega'-\omega)\omega\frac{\tilde{\sigma}'(\omega)}{\mathrm{e}^{-\beta\omega}-1} = 2\pi\omega'\frac{\tilde{\sigma}'(\omega')}{\mathrm{e}^{-\beta\omega'}-1}
\end{aligned} \tag{A.38}
$$

Rearranging and replacing $\omega'\to\omega$, we finally get the expression for the real part of the optical conductivity

$$
\tilde{\sigma}'(\omega) = \frac{1}{2L}\frac{1-\mathrm{e}^{-\beta\omega}}{\omega}\int_{-\infty}^{\infty}\mathrm{d}t\ \mathrm{e}^{i\omega t}\langle j^\sigma_H(t)j^\sigma\rangle_0 \tag{A.39}
$$

consistent with the result found in the literature [115, 144, 147]. We have to more steps to do, before we obtain the exact form of the optical conductivity used in Chapter 3, given by equation (3.4). First, we need to pass to the spectral representation of the current-current correlation function, to evaluate the Fourier integral. How to do it for zero temperature, including the delicate topic of convergence, is discussed in Appendix B. Extending the result to finite temperature is straightforward, and we get

$$\tilde{\sigma}'(\omega) = \frac{1}{L}\frac{1-\mathrm{e}^{-\beta\omega}}{\omega}\frac{\pi}{\mathcal{Z}}\sum_{n,m}\mathrm{e}^{-\beta E_n}\left|\langle n|j^\sigma|m\rangle\right|^2\delta(\omega+E_n-E_m) \tag{A.40}$$

To connect this to the infinite-temperature limit used in the main text, we define $\sigma(\omega) \equiv \tilde{\sigma}'(\omega)/\beta$ and calculate

$$\begin{aligned}\lim_{\beta\to 0}\sigma(\omega) &= \frac{\pi}{L\mathcal{D}}\frac{1}{\omega}\left(\lim_{\beta\to 0}\frac{1-\mathrm{e}^{-\beta\omega}}{\beta}\right)\sum_{n,m}\left|\langle n|j^\sigma|m\rangle\right|^2\delta(\omega+E_n-E_m)\\ &= \frac{\pi}{L\mathcal{D}}\sum_{n,m}\left|\langle n|j^\sigma|m\rangle\right|^2\delta(\omega+E_n-E_m)\end{aligned} \tag{A.41}$$

where we have used the fact that $\lim_{\beta\to 0}(1-\mathrm{e}^{-\beta\omega})/\beta = \omega$, and $\mathcal{D} \equiv \lim_{\beta\to 0}\mathcal{Z}$ is the number of states in the Hilbert space. The derivation of the final expression for the optical conductivity, given by equation (3.4), is now complete.

# B Two Fourier transforms

The goal of this appending is the calculation of two Fourier transforms, which appear in the main text. They originate from the definition of finite-time averaging (4.7) and the integrated spectral function (4.22).

## B.1 Fourier transform of the correlation function

Let us begin with the latter one, as it is simpler. We have, starting from the left-hand side of (4.21)

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

The $\varepsilon$ part in the exponent is a trick to make the integral converge, without assuming anything about the behavior of the correlation function at infinity. Let us massage it a bit further, by calculating the integral $\mathcal{I}$ explicitly.

$$\mathcal{I} = \lim_{\varepsilon\to0^+}\int_{-\infty}^{\infty}\mathrm{d}t\ e^{i(\epsilon_m-\epsilon_n+\omega)t-|t|\varepsilon} = \lim_{\varepsilon\to0^+}\left[\lim_{T_1\to-\infty}\int_{T_1}^{0}\mathrm{d}t\ e^{i(\epsilon_m-\epsilon_n+\omega-i\varepsilon)t}\right.$$
$$\left.+\lim_{T_2\to\infty}\int_0^{T_2}\mathrm{d}t\ e^{i(\epsilon_m-\epsilon_n+\omega+i\varepsilon)t}\right] = \lim_{\varepsilon\to0^+}\left[\lim_{T_1\to-\infty}\frac{1-e^{i(\epsilon_m-\epsilon_n+\omega)T_1}e^{\varepsilon T_1}}{i(\epsilon_m-\epsilon_n+\omega-i\varepsilon)}\right.$$
$$\left.+\lim_{T_2\to\infty}\frac{e^{i(\epsilon_m-\epsilon_n+\omega)T_2}e^{-\varepsilon T_2}-1}{i(\epsilon_m-\epsilon_n+\omega+i\varepsilon)}\right] = \lim_{\varepsilon\to0^+}\left[\frac{i}{\epsilon_n-\epsilon_m-\omega+i\varepsilon}+\frac{i}{\epsilon_m-\epsilon_n+\omega+i\varepsilon}\right]$$
$$= \lim_{\varepsilon\to0^+}\frac{2\varepsilon}{(\epsilon_m-\epsilon_n+\omega-i\varepsilon)(\epsilon_m-\epsilon_n+\omega+i\varepsilon)} = \lim_{\varepsilon\to0^+}\frac{2\varepsilon}{(\epsilon_m-\epsilon_n+\omega)^2+\varepsilon^2} \tag{B.2}$$

The obtained result is a limit of the so-called Poisson kernel. This happens to be a representation of Dirac $\delta$ in the form of a limit of a sequence of functions [148]

$$\lim_{\varepsilon\to0^+}\frac{1}{\pi}\frac{\varepsilon}{x^2+\varepsilon^2} = \delta(x) \tag{B.3}$$

Thus we get

$$\mathcal{I} = \lim_{\varepsilon\to0^+}\frac{2\varepsilon}{(\epsilon_m-\epsilon_n+\omega)^2+\varepsilon^2} = 2\pi\delta(\epsilon_m-\epsilon_n+\omega) \tag{B.4}$$

Inserting this result into equation (B.1) we arrive at

$$\mathcal{F}\left[(A(t)|B)\right] = \frac{1}{\mathcal{D}}\frac{1}{2\pi}\sum_{n,m}A_{mn}B_{nm}\lim_{\varepsilon\to0^+}\int_{-\infty}^{\infty}\mathrm{d}t\ e^{i\omega t-|t|\varepsilon}e^{i(\epsilon_m-\epsilon_n)t}$$
$$=\frac{1}{\mathcal{D}}\sum_{n,m}A_{mn}B_{nm}\delta(\epsilon_m-\epsilon_n+\Omega) \tag{B.5}$$

which is our desired results.

## B.2 Extension of Fourier transform to $L^2(\mathbb{R})$ and the Fourier transform of $\frac{\sin(x)}{x}$

Now, let us tackle the more difficult integral, necessary to show, that Eq. (4.6) and Eq (4.7) are equivalent. We start the usual way, by passing to spectral representation of the observable $A$

$$\bar{A}^\tau = \int_{-\infty}^{\infty}\mathrm{d}tA(t)\frac{\sin(t/\tau)}{\pi t} = \sum_{n,m}\langle n|A|m\rangle\,|n\rangle\langle m|\,\frac{1}{\pi}\int_{-\infty}^{\infty}\mathrm{d}t\ \mathrm{e}^{i(E_n-E_m)t}\frac{\sin(t/\tau)}{t} \tag{B.6}$$

where $H\,|n\rangle = E_n\,|n\rangle$ is the eigenbasis of our Hamiltonian. Our problem reduces to calculating the integral

$$I = \mathcal{F}\left[\frac{\sin(\alpha t)}{t}\right] = \int_{-\infty}^{\infty}\mathrm{d}t\ \mathrm{e}^{i\omega t}\frac{\sin(\alpha t)}{t} \tag{B.7}$$

where $\alpha = 1/\tau$ and $\omega = E_n - E_m$, which can be recognized as a Fourier transform of $\sin(\alpha t)/t$. Here is where things become a bit subtle. The Fourier transform is traditionally defined on functions belonging to the space $L^1 \equiv L^1(\mathbb{R})$ of Lebesgue-measurable, **integrable functions** [149], that is

$$L^1 = \left\{f:\mathbb{R}\to\mathbb{C}\ \Big|\ \int_{-\infty}^{\infty}\mathrm{d}t\ |f(t)| < \infty\right\} \tag{B.8}$$

It is a member of a larger family of spaces $L^p \equiv L^p(\mathbb{R}),\ p \in [1, \infty]$, defined as

$$L^p = \left\{ f : \mathbb{R} \to \mathbb{C} \mid \int_{-\infty}^{\infty} \mathrm{d}t \, |f(t)|^p < \infty \right\} \tag{B.9}$$

thus guaranteeing the existence of respective $L^p$ norms $\|f\|_p = \left(\int_{-\infty}^{\infty} tx \, |f(t)|^p\right)^{1/p}$. Unfortunately, the function $\sin(t)/t$ is not in $L^1$. To see it, note that $\int_{-\infty}^{\infty} \mathrm{d}t \ |\sin(t)/t| = 2\int_0^{\infty} \mathrm{d}t|\sin(t)/t|$ and consider the following

$$\begin{aligned}\int_{\pi}^{(N+1)\pi} \mathrm{d}t \, \left|\frac{\sin t}{t}\right| &= \sum_{k=1}^{N} \int_{k\pi}^{(k+1)\pi} \mathrm{d}t \, \left|\frac{\sin t}{t}\right| = \sum_{k=1}^{N} \int_0^{\pi} \mathrm{d}t' \, \frac{|\sin(t'+k\pi)|}{t'+k\pi} = \sum_{k=1}^{N} \int_0^{\pi} \mathrm{d}t' \, \frac{|\sin t'|}{t'+k\pi} \\ &\geq \sum_{k=1}^{N} \frac{1}{(k+1)\pi} \int_0^{\pi} \mathrm{d}t' \ \sin t' = \frac{2}{\pi} \sum_{k=1}^{N} \frac{1}{k+1},\end{aligned}$$

Thus, the integral is bounded from below by the harmonic series, which diverges. Now, the question is whether we can somehow make sesne of the integral $I$. It turns out, that even though the function is not integrable, it is **square integrable** — that is, it belongs to the space $L^2$ which can be seen by noting that

$$\int_{-\infty}^{\infty} \mathrm{d}t \, \left|\frac{\sin t}{t}\right|^2 = 2\left[\int_0^1 \mathrm{d}t \, \frac{\sin^2(t)}{t^2} + \int_1^{\infty} \mathrm{d}t \, \frac{\sin^2(t)}{t^2}\right] \tag{B.10}$$

and that the first integral is finite, while the second one is bounded from above by $\int_1^{\infty} \mathrm{d}t \ 1/t^2 = 1$. The space $L^2$ is unique among all the $L^p$ — it is the only *Hilbert space*, where the norm $\|\cdot\|_p$ is induced by an inner product

$$L^2 \times L^2 \ni (f, g) \to \langle f, g\rangle = \int_{-\infty}^{\infty} \mathrm{d}t \ f(t) g^*(t) \in \mathbb{C} \tag{B.11}$$

$g^*$ being the complex conjugate of $g$. We are going to work out an extension of the Fourier transform to the space $L^2$, using a classic **density argument**. To this end, we need the following theorem

**Theorem B.1 (Parseval-Plancherel)** *Let $f, g \in L^1 \cap L^2$, and let $\hat{f}, \hat{g}$ be respective Fourier transforms. Then*

$$\langle f, g\rangle = \frac{1}{2\pi}\langle \hat{f}, \hat{g}\rangle \ .$$

The proof on this theorem is not difficult, but it would require us to introduce some new notions and deviate too much from the scope of this thesis. Thus, we shall take it for granted and the reader is encouraged to look it up in any textbook on Fourier analysis [149, 150]. Now, we are ready for

**Theorem B.2** *$L^1 \cap L^2$ is a dense subset of $L^2$.*

**Proof.** We need to show, that for any $f \in L^2$, there exists a sequence $\{f_n\}_{n=1}^{\infty}$ of functions in $L^1 \cap L^2$ such that $\lim_{n\to\infty} \|f_n - f\|_2 = 0$. So let us take an arbitrary function $f \in L^2$ and define a sequence of functions $\{f_n\}_{n=1}^{\infty}$ as follows

$$f_n(t) = \mathbb{1}_{[-n,n]}(t) f(t)$$

where $\mathbb{1}_{[-n,n]}$ is the indicator function of the interval $[-n,n]$. Obviously, $f_n \in L^2$ as $\|f_n\|_2 \leq \|f\|_2 \leq \infty$. We need to show that for every $n \in \mathbb{N} \setminus \{0\}$, $f_n \in L^1$. Indeed, we have

$$\|f_n\|_1 = \|\mathbb{1}_{[-n,n]} f\|_1 \leq \|\mathbb{1}_{[-n,n]}\|_2 \|f\|_2 = \sqrt{2n}\|f\|_2 < \infty$$

where the first inequality above is an application of the Hölder's inequality. As $\hat{f} \in L^1 \cap L^2$ Thus, $f_n \in L^1 \cap L^2$ as required. Now, we need to show that $\lim_{n\to\infty} \|f_n - f\|_2 = 0$. Notice, that for every $t \in \mathbb{R}$, the pointwise convergence in $\mathbb{R}$ holds

$$\lim_{n\to\infty} |f(t) - f_n(t)| = 0,$$

Also, we can dominate this sequence of real numbers by

$$|f(t) - f_n(t)|^2 \leq 2\left(|f(t)|^2 + |f_n(t)|^2\right) \leq 4|f(t)|^2$$

and $4|f|^2 \in L^1(\mathbb{R})$, so it is Lebesgue-integrable and by the Lebesgue Dominated Convergence Theorem,

$$\lim_{n\to\infty} \|f - f_n\|_2^2 = \lim_{n\to\infty} \int_{-\infty}^{\infty} |f(t) - f_n(t)|^2 \,\mathrm{d}t = \int_{-\infty}^{\infty} \left(\lim_{n\to\infty} |f(t) - f_n(t)|^2\right) \mathrm{d}t = 0 \qquad \blacksquare$$

Let $\hat{f}_n$ be the Fourier transform of $f_n$. By the Parseval-Plancherel theorem, $\|\hat{f}_n\|_2^2 = 2\pi\|f_n\|_2^2 \leq \infty$, so $\{\hat{f}_n\}_{n=1}^{\infty}$ is a sequence of functions in $L^2$. Let us now take $n \geq m$ and consider

$$\begin{aligned}\frac{1}{2\pi}\|\hat{f}_n - \hat{f}_m\|_2 &= \|f_n - f_m\|_2^2 = \|(\mathbb{1}_{[-n,n]} - \mathbb{1}_{[-m,m]})f\|_2^2 = \|(\mathbb{1}_{[-n,-m]} + \mathbb{1}_{[m,n]})f\|_2^2 \\ &\leq \|\mathbb{1}_{[-n,-m]}f\|_2 + \|\mathbb{1}_{[m,n]}f\|_2 \leq \|\mathbb{1}_{(-\infty,-m]}f\|_2 + \|\mathbb{1}_{[m,\infty)}f\|_2 \xrightarrow[m\to\infty]{} 0\end{aligned}$$

where the first equality is again due to the Parseval-Plancherel theorem. Thus, $\{\hat{f}_n\}_{n=1}^{\infty}$ is a Cauchy sequence in $L^2$, and since $L^2$ is complete, it converges to some function $\hat{f} \in L^2$. We now **define** the Fourier transform of $f \in L^2$ as the limit of this sequence, i.e.

$$\hat{f} \equiv \lim_{n\to\infty} \hat{f}_n = \lim_{n\to\infty} \int_{-\infty}^{\infty} f_n(t) e^{i\omega t} \mathrm{d}t \tag{B.12}$$

It is no longer an ordinary Lebesgue integral, but an $L^2$-limit of improper Riemann integrals. Of course, in case of Lebesgue integrable functions, the two definitions coincide.

All this work was to convince ourselves that it actually *makes sense* to talk about the Fourier transform of $\sin(x)/x$, which is not Lebesgue integrable. Now, with clear conscience, we can calculate it. Our task at hand is to calculate the integral

$$\lim_{n\to\infty} \underbrace{\int_{-n}^{n} \frac{\sin(\alpha t)}{t} \mathrm{e}^{i\omega t} \,\mathrm{d}t}_{I_n(\omega)} \tag{B.13}$$

Consider the above integrand, but as a function of the complex variable $z$. Since $\mathrm{e}^{i\omega z}\sin(\alpha z)/z$ is an entire function, we can apply the Cauchy-Goursat theorem [148] and deform the integration path. Instead of integrating over a real interval $[-n,n]$, we can integrate over the contour $\Gamma_n$ consisting of an interval $[-n,-1]$, a lower semicircle of radius 1 centered at 0 and an interval $[1,n]$. Now, because we avoided the problematic point $z = 0$, we are safe

First contour

to use the Euler's formula $2i\sin(\alpha z) = (e^{i\alpha z} - e^{-i\alpha z})$, obtaining

$$I_n(\omega) = \frac{1}{2i}\int_{\Gamma_n}\frac{1}{z}\left(\mathrm{e}^{i(\alpha+\omega)z} - \mathrm{e}^{i(-\alpha+\omega)z}\right)\mathrm{d}z \tag{B.14}$$

Introducing

$$\psi_n(\eta) = \frac{1}{2i}\int_{\Gamma_n}\frac{e^{i\eta z}}{z}\,\mathrm{d}z \tag{B.15}$$

we can write $I_n(\omega) = \psi_n(\alpha+\omega) - \psi_n(-\alpha+\omega)$. To evaluate $\psi_n(\eta)$, we have to close the contour. We are going to do it in two ways: first, considering a counter-clockwise, upper semicircle of radius $n$, centered at $z=0$, that we call $\Gamma_n^U$, and second, a clockwise, lower semicircle of radius $n$, also centered at $z=0$, that we call $\Gamma_n^L$.

Second contour

We start with the second case, as it is simpler. The integral of $e^{i\eta z}/z$ over $\Gamma_n + \Gamma_n^L$ vanishes by the Cauchy-Goursat theorem, since the integrand is holomorphic in the interior of the contour. Thus, we have

$$\psi_n(\eta) = \frac{1}{2i}\int_{\Gamma_n}\frac{e^{i\eta z}}{z}\,\mathrm{d}z = \frac{1}{2i}\int_{-\Gamma_n^L}\frac{e^{i\eta z}}{z}\,\mathrm{d}z \tag{B.16}$$

where $-\Gamma_n^L$ is the same contour as $\Gamma_n^L$, but traversed in the opposite direction. We can parametrize $\Gamma_n^L$ as $z = ne^{i\varphi}$, $\varphi \in [-\pi, 0]$ and the integral becomes

$$\begin{aligned}
\psi_n(\eta) &= \frac{1}{2\cancel{i}}\int_{-\pi}^{0}\frac{\exp(i\eta ne^{i\varphi})}{\cancel{ne^{i\varphi}}}\cancel{ine^{i\varphi}}\,\mathrm{d}\varphi = \frac{1}{2}\int_{-\pi}^{0}\exp\left(i\eta ne^{i\varphi}\right)\mathrm{d}\varphi \\
&\le \frac{1}{2}\max_{-\pi\le\varphi\le 0}\left|\exp\left(i\eta ne^{i\varphi}\right)\right|\underbrace{2\pi n}_{\text{Length of }\Gamma_n^L} = \pi n\max_{-\pi\le\varphi\le 0}|\exp(-n\eta\sin(\varphi))| \\
&\le \pi n\,|\exp(n\eta)| \xrightarrow{n\to\infty} 0, \text{ if } \eta < 0
\end{aligned} \tag{B.17}$$

Now it is clear why two different contours are necessary, as the above argument fails for $\eta \ge 0$. We can easily salvage the trivial case $\eta = 0$, as it is just $\psi_n(0) = 1/2\int_{-\pi}^{0}\mathrm{d}\varphi = \pi/2$, but for the case $\eta > 0$, we need the second contour $\Gamma_n^U$.

Inside the contour $\Gamma_n + \Gamma_n^U$, our function $\mathrm{e}^{i\eta z}/z$ is meromorphic, with a pole at $z=0$. By the Residue theorem [148, 149],

$$\int_{\Gamma_n+\Gamma_n^U}\frac{\mathrm{e}^{i\eta z}}{z}\,\mathrm{d}z = 2\pi i\,\mathrm{Res}\left(\frac{\mathrm{e}^{i\eta z}}{z}, 0\right) \tag{B.18}$$

and the residue can be easily calculated as $\mathrm{Res}\left(\mathrm{e}^{i\eta z}/z, 0\right) = \lim_{z\to 0} z\frac{\mathrm{e}^{i\eta z}}{z} = 1$. Thus,

$$\psi_n(\eta) = \frac{1}{2i}\int_{\Gamma_n}\frac{\mathrm{e}^{i\eta z}}{z}\,\mathrm{d}z = \pi - \frac{1}{2i}\int_{\Gamma_n^U}\frac{\mathrm{e}^{i\eta z}}{z}\,\mathrm{d}z \tag{B.19}$$

We now play the same game as before, parametrizing $\Gamma_n^U$ as $z = ne^{i\varphi}$, $\varphi \in [0, \pi]$, and bounding the integral from above. But this time, we have

$$\begin{aligned}
\frac{1}{2i}\int_{\Gamma_n^U}\frac{\mathrm{e}^{i\eta z}}{z}\,\mathrm{d}z &= \frac{1}{2i}\int_{0}^{\pi}\exp\left(i\eta ne^{i\varphi}\right)\mathrm{d}\varphi \le \frac{1}{2}\max_{0\le\varphi\le\pi}\left|\exp\left(i\eta ne^{i\varphi}\right)\right|\underbrace{2\pi n}_{\text{Length of }\Gamma_n^U} \\
&= \pi n\max_{0\le\varphi\le\pi}|\exp(-n\eta\sin(\varphi))| \le \pi n\,|\exp(-n\eta)| \xrightarrow{n\to\infty} 0, \text{ if } \eta > 0
\end{aligned} \tag{B.20}$$

Summarizing, the in the limit $n \to \infty$, we obtain

$$\lim_{n\to\infty} \psi_n(\eta) = \begin{cases} \pi & \text{if} \eta > 0 \\ \pi/2 & \text{if } \eta = 0 \\ 0 & \text{if } \eta < 0 \end{cases} = \pi\theta(\eta) \tag{B.21}$$

where $\theta(\eta)$ is the Heaviside step function and we define $\theta(0) = 1/2$. Finally, we get

$$\begin{aligned} \lim_{n\to\infty} I_n(\omega) &= \lim_{n\to\infty} \psi_n(\alpha+\omega) - \lim_{n\to\infty} \psi_n(-\alpha+\omega) \\ &= \pi\left[\theta(\alpha+\omega) - \theta(-\alpha+\omega)\right] = \pi\theta(\alpha - |\omega|) \end{aligned} \tag{B.22}$$

Substituting this result into (B.6), we arrive at the final expression

$$\bar{A}^\tau = \sum_{n,m} \theta\left(\frac{1}{\tau} - |E_n - E_m|\right) \langle n|A|m\rangle\, |n\rangle\langle m| \tag{B.23}$$

which is precisely Eq. (4.7).