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Tensor Networks in Condensed Matter

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Nothing produced such odd results
as trying to get even.

Franklin P. Jones (1908-1980)

Zusammenfassung

Diese Doktorarbeit ist dem Studium der Quantenvielteichentheorie gewidmet. Die dazugehörige Forschung wurde im Rahmen der *Matrix Product States* (MPS) und deren Generalisierung in höheren Dimensionen, *Projected Entangled Pair States* (PEPS) durchgeführt. Im ersten Teil dieser Arbeit beschäftigen wir uns näher mit den mathematischen Eigenschaften solcher Tensornetzwerkzustände. Die ersten Kapitel behandeln eindimensionale Systeme. Dabei nutzen wir die Verbindungen zwischen MPS und Quantenkanälen um mehrere neue Ergebnisse, wie zum Beispiel die Quanten-Wielandt-Ungleichung oder die Konditionen für die Konstruktion lokal-invarianter Zustände unter einer Symmetriegruppe zu beweisen. Kapitel 5-7 sind höherdimensionalen Systemen gewidmet. Hier definieren wir die Bedingungen für die Herstellung invarianter PEPS . Im zweiten Teil der Arbeit gehen wir auf die Anwendung in kondensierter Materie ein. Das achte Kapitel zeigt mehrere Methoden quasi-lösbare Hamiltonoperatoren mit Zweikörperwechselwirkung und SU(2)-Symmetrie zu konstruieren, während wir im neunten Kapitel darlegen, dass diese Tensornetzwerkzustände als Labor für die Kondensierte-Materie-Theorie genutzt werden können: Zum Beispiel in der Charakterisierung der String-Order, der Verallgemeinerung des Lieb-Schultz-Mattis-Theorems, dem Beweis neuer Theoreme die versuchen die Quantenverschränkung mit Magnetisierung oder mit Langstreckeninteraktion in Verbindung zu setzen und vielem mehr.

This thesis is devoted to the study of quantum many-body systems. This investigation is performed in the framework of *Matrix Product States* (MPS) and their generalization to higher dimensions, *Projected Entangled Pair States* (PEPS). In the first part of the work, we discuss the mathematical properties of such tensor network states in depth. In the first chapters we deal with one-dimensional systems, for which we use the connections between MPS and completely positive maps to prove several new results, such as the quantum version of the Wielandt's inequality or the construction of locally invariant states under a symmetry group. Chapters 5-7 are dedicated to higher-dimensional systems, for which we provide the conditions to construct invariant PEPS. The second part of the thesis is dedicated to applications in condensed matter. In chapter 8 we provide several methods of constructing quasi-solvable Hamiltonians with two-body interactions, while in chapter 9 we show that these tensor network states can be used as a laboratory for theoretical condensed matter in, for instance, the characterization of the string-order, the generalization of the Lieb-Schultz-Mattis theorem, the demonstration of new theorems relating entanglement to magnetisation or to long-range interactions, etc.

Abstract

This Thesis contributes to the development of the theory of tensor network states in many–body systems. The first part is dedicated to improving our comprehension of the mathematical properties of such states; in the second part, these properties are employed to obtain results in condensed matter and quantum magnetism. The cornerstone of these advances is the possibility of a local characterization of global features. Properties such as the uniqueness of the ground state, the existence of a non–vanishing spectral gap above this ground state, or the characterization of symmetries are encoded in the tensor. This is based on the connection between Matrix Product States and completely positive maps in one–dimensional systems. For higher–dimensional networks, where such a connection does not exist, one can attempt to transform the question into the former one–dimensional problem.

We prove a quantum generalization of the Wielandt's inequality, well–known in the context of classical channels and Markov chains. This inequality provides an upper bound for the number of spins which must be gathered in order to find a gapped parent Hamiltonian which has the Matrix Product State as a unique ground state. The bound, surprisingly, depends only on the tensor's physical and bond dimensions, and not on the explicit entries of the tensor. Many previous results on Matrix Product States depended on the existence of this upper bound.

With this in hand, we provide a local characterization of the symmetries in both Matrix Product States and Projected Entangled Pair States. As almost every interesting Hamiltonian in condensed matter exhibits some kind of symmetry, to be able to locally characterize these symmetries in the tensors is a key question. Furthermore, we employ this characterization to systematically construct quasi–solvable $SU(2)$–invariant Hamiltonians with two–body interactions.

Finally, we apply the advances achieved in Matrix Product States' and Projected Entangled Pair States' theories to characterize the existence of string order in one–dimensional systems (proposing as well an extension to higher dimensions), to provide generalizations of existing theorems in the context of tensor networks, and to exploit the simplicity of the structure of these states in order to make use of them as a theoretical laboratory for condensed matter. An example of this would be the proved relationship between fractional magnetization and entanglement, or the proposed one which links long–range interacting Hamiltonians to the entanglement of their ground states.

Contents

Introduction

This work is devoted to the study of quantum spin many–body systems, and their properties and applications in condensed matter. The spectral resolution of Hamiltonians acting on many–body systems is a highly complex problem, because of the exponential growth of the associated Hilbert space with the number of particles. This exponential growth is a valuable characteristic for the purposes of quantum information theory, since it permits an exponential speed–up in quantum computation tasks, and in condensed matter it is also a never–ending source of unexpected behaviours and surprising results, such as phase transitions [WOVC06, VWC09], fractionalization of physical quantities [AMU75, KDP80, Lau81, Gre94, OYA97], and rare matter phases (for instance, certain glass structures [Sch91, Ell90]). These examples show that the resolution of Hamiltonians acting on many–body systems is a mathematical problem of the utmost importance in several fields of Physics.

Nevertheless, it is difficult to deal with these systems, because they are hardly tractable by classical means, so new mathematical techniques must be developed. Thankfully, the fact that many of the interactions in Nature are *local*, translates into a non–uniform distribution of the ground states of such Hamiltonians in the Hilbert space. Or, in other words, one requires, on average, an exponentially long time to entangle a state by evolving a non–entangled one by means of a local–interacting Hamiltonian. Therefore, an effective management of the problem demands a *local treatment* of such states, which is precisely the objective pursued throughout this work by means of *tensor networks*.

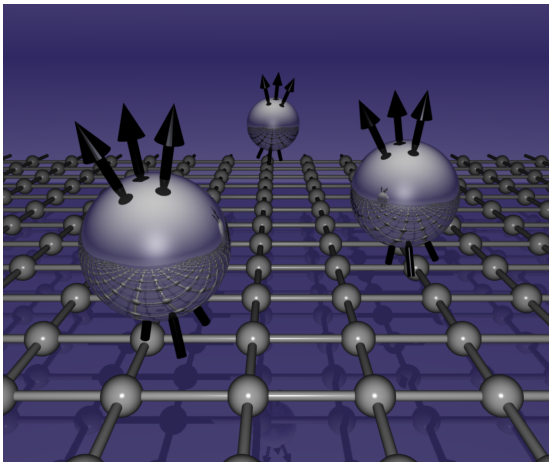
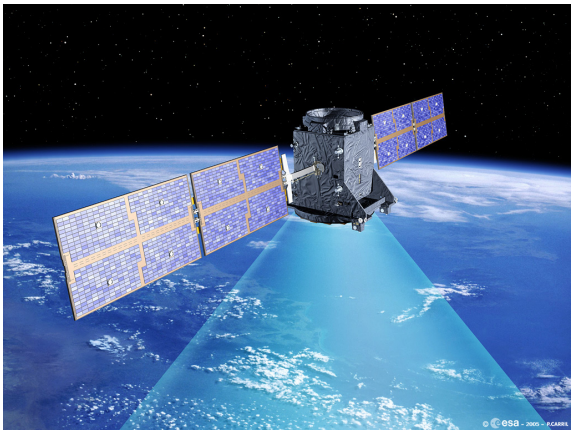


Figure 1: Fractional quantum Hall effect is probably the best–known fractionalization effect. (Image based on [TAN+10])

Although there are many different kinds of tensor networks (for instance, the MERA states proposed by G. Vidal [Vid07]), here we use this term to refer to both *Matrix Product States* and *Projected Entangled Pair States*. These state Ansätze fulfil the local structure requirement mentioned above, and they are the keystone of



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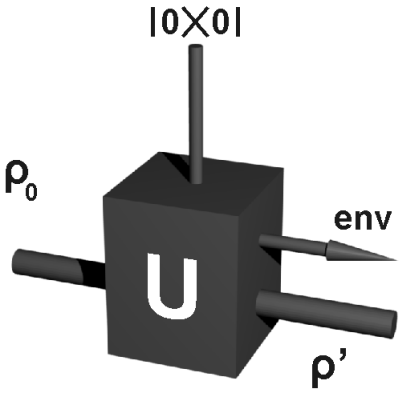


(b)

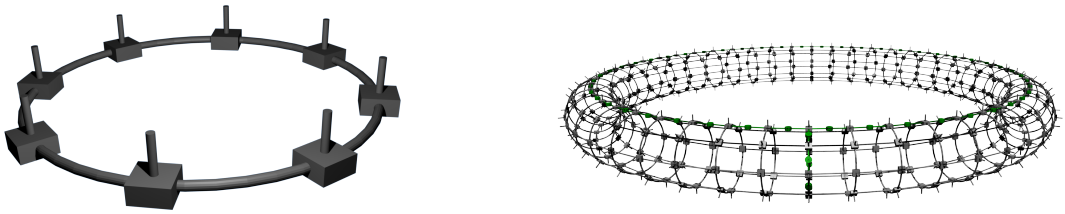
Figure 2: (a) A group at Padova University recently published an experiment in which individual photons are reflected off a satellite orbiting almost 1500 kms above the Earth, one step closer to the construction of a quantum channel between space and Earth and the establishment of a truly secure communication system [ea08] (Credit: ESA). (b) The representation by means of a quantum channel of any quantum operation.

the hereby presented work.

The idea of Matrix Product States originally appeared in the framework of the Density Matrix Renormalization Group (DMRG) method, developed for the resolution of one–dimensional systems with short–range interactions at zero temperature. This method's mathematical foundations in terms of the current language of tensor networks were established by Östlund *et al.* [ÖR95], by taking White's algorithm [Whi92, Whi93] as a starting point. Afterwards, techniques based on this work have successfully extended DMRG to more general situations, such as representations of mixed states, systems at non–zero temperature [VGRC04], and larger dimensions [VC04a, MVC09]. It is precisely in the field of numerical analysis where these tensor network Ansätze have found their most enthusiastic public and have been more widely implemented, since DMRG enables an understanding of the physical properties of quantum many–body systems with groundbreaking precision.

As inferred from above, this Matrix Product States formalism was developed from the DMRG without fully understanding the grounds of its success, and this question was not solved even after the formulation by Östlund and Rommer. This comprehension came later, when the connection between Matrix Product States and quantum information was established [FNW92, PGVWC07, VPC04], in particular with the theory on *quantum channels* or *completely positive maps*.

A large number of modern developments in Matrix Product States stem from



(a) (b)

Figure 3: **Tensor networks**. (a) A Matrix Product State with periodic boundary conditions is represented by a ring of tensors. (b) A Projected Entangled Pair State with periodic boundary conditions on a two–dimensional square lattice, *i.e.* with the topology of a torus.

the application of the techniques available in completely positive maps. These techniques have been particularly successful in establishing a local description (*i.e.* in terms of the local tensor) of global properties, such as the necessary and sufficient conditions for these Matrix Product States to be unique ground states of local gapped frustration–free Hamiltonians [FNW92, PGVWC07], the characterization of the symmetries of the state [SWPGC09], or the decay–law fulfilled by two–point correlation functions [FNW92].

A couple of complementary quantum information–based works by Verstraete *et al.* [VC06] and Hastings [Has07a] finally drew attention to the real relevance of the Matrix Product States formalism in the framework of many–body systems. These two seminal works established that the ground state of every one–dimensional gapped Hamiltonian is faithfully described by a Matrix Product State. As a consequence, they provide not only a definite explanation of the reason why the DMRG method succeeds with such great accuracy, but also an explicit evidence of the relevance of the tiny corner of the Hilbert space generated by the Matrix Product States in order to describe the usual quantum states constructed by means of many–body Hamiltonians. This idea is one of the cornerstones of this work, as shown below.

Although we started by mentioning general tensor networks, we have only discussed one–dimensional systems in the previous paragraphs. One could expect higher–dimensional systems to show a richer and more complex behaviour, but a more difficult mathematical description and treatment as well. Therefore, a previous extensive grasp of the one–dimensional problem is not only useful, but also necessary. Then, Projected Entangled Pair States were proposed as a generalization of Matrix Product States for higher dimensions [VC04a, PGVCW08], providing an efficient description of quantum states, as well. Unfortunately, there exists no connection between Projected Entangled Pair States and completely positive maps, which makes the mathematical treatment of the former much more challenging.

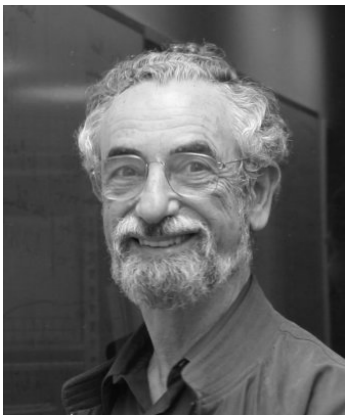
This results, as a consequence, in Matrix Product States' features not being directly translatable into characteristics of Projected Entangled Pair States.

Even thought we have so far referred to many–body systems in general, it is beyond doubt that the main target of the machinery described above are *spin systems*. Of all the questions which can be studied in spin systems, the microscopic description of *magnetism* is the most relevant one. Since its publication, W. Heisenberg's well–known spin model, $H = \sum_i S_i \cdot S_{i+1}$, has become the archetypal model in the study of microscopic spin dynamics. Its physical relevance increased when Mattheis [Mat61a, Mat61b] and Paul [Pau60b, Pau60a] showed that both the ground states and the elementary excited states of every chain of molecules where the valence electrons occupy nondegenerate s–orbitals are well described by an effective Heisenberg Hamiltonian, which couples nearest–neighbour spins antiferromagnetically and neglects all the electronic degrees of freedom [Mat81]. On the other hand, if two or more valence states are allowed to conduct electrons on each atom, one might expect [LM66] that an effective Heisenberg Hamiltonian with ferromagnetic nearest–neighbour interactions describes the magnetic degrees of freedom of the chain (but not the electronic ones).

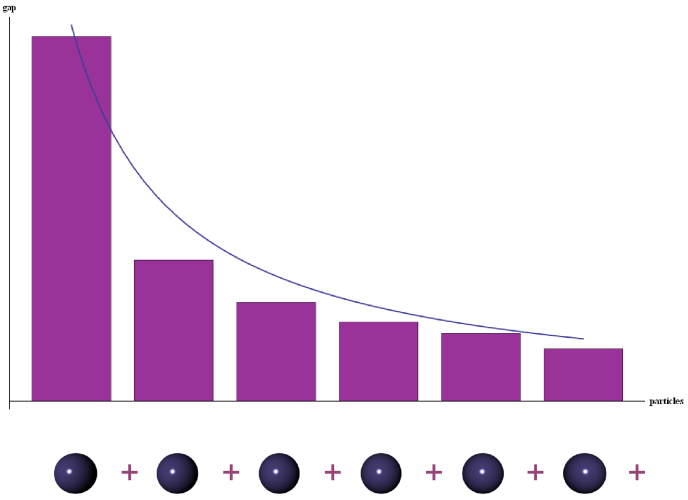
Figure 4: Werner Heisenberg in 1927 (Credit: AIP Niels Bohr Library)

The list of well–known names associated with the development of the quantum theory of magnetism is long. Nevertheless, Elliot H. Lieb stands out for his contributions to the establishment of the mathematical foundations of this theory. His name is associated with many of the best–known results in the field [Aue98], as we will show throughout this Thesis. For instance, the Lieb–Schultz–Mattis Theorem [LSM61] is especially relevant in this work. It shows that the gap above the ground state of every $SU(2)$–invariant many–body Hamiltonian composed by semi–integer spins vanishes in the thermodynamic limit. This Theorem turned out to be the most relevant support for the Haldane hypothesis [Hal83a, Hal83b], by establishing a connection between the microscopic bosonic or fermionic character of spins with an $SU(2)$–invariant interactions, and a macroscopic property: the existence of a non–trivial spectral gap above the unique ground state of the Hamiltonian. However, a completely general formal proof of this type of results is actually difficult to obtain, and requires an unfathomable mathematical machinery of functional analysis and algebra [Has04, NS07].

Consequently, one might wonder why not employ the results obtained for tensor networks to advance in the mathematical foundations of quantum magnetism with



(a)



(b)

Figure 5: (a) Elliot H. Lieb. (b) The Lieb–Schultz–Mattis Theorem states that the gap over the ground state of an $SU(2)$–invariant Hamiltonian with semi–integer spin vanishes in the thermodynamic limit, being upper–bounded by $\propto \frac{1}{N}$.

spin systems. Up until recently, the mathematical properties of tensor networks had not been mastered well enough for this task. Therefore, during the last three decades, we have been availing ourselves of Matrix Product States as a source of examples and counter–examples to support some hypotheses and discard others.

Let us review some of the most relevant examples. For instance, Majumdar and Ghosh [MG69, Maj70] provided the first (unexpected) example of translational invariant Hamiltonian with a continuous local $SU(2)$ symmetry, but with gap and (faster than) exponentially decaying correlation functions. Afterwards, Affleck *et al.* proposed in their seminal work [AKLT88] an exactly solvable gapped model, widely known as *AKLT model*, which proved to be not only a major theoretical advance, by introducing the parent Hamiltonian method of constructing frustration–free Hamiltonians which expose this state as a ground state, but also the first support for the Haldane hypothesis. Haldane proposed that the Heisenberg Hamiltonian corresponding to a system constituted by integer spins is gapped, while the one corresponding to semi–integer spins is gapless, statement which was against the common belief at that time. To support his hypothesis, he provided several obscure quantum field theory–based arguments [Hal83a, Hal83b], so this did not convince the condensed matter community. The Lieb–Schultz–Mattis Theorem mentioned above proved the second part of his statement corresponding to semi–integer spins.

The most general one–dimensional $SU(2)$–invariant nearest–neighbour interact-

ing Hamiltonian for spin 1 is the *bilinear–biquadratic model*:

$$H = \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + \beta (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$$

when $\beta = 0$, this model corresponds to the Heisenberg Hamiltonian which, according to the Haldane hypothesis, must have a unique massive ground state. However, the Hamiltonian had already been solved for $\beta = -1$ in the so–called *Takhtajan–Babudjian model*, by means of the Bethe Ansatz [Bab82, Bab83, Tak82], showing a unique gapless ground state. For $\beta < -1$ this presents a two–fold dimerized ground state. For $\beta = 1$ the model has an exact $SU(3)$ symmetry and it is massless [Aff86]. The Heisenberg Hamiltonian is between these two points. Therefore, there is no evidence that allows us to expect a massive phase in $-1 < \beta < 1$, which is the reason of the initially scarce acceptance of the Haldane hypothesis. The AKLT model corresponds to $\beta = \frac{1}{3}$. Its authors analytically proved the uniqueness of the ground state and the existence of a non–trivial spectral gap above this ground state [AKLT88]. Hence, this was the confirmation of the existence of a massive phase and an indication of the trueness of the Haldane hypothesis.

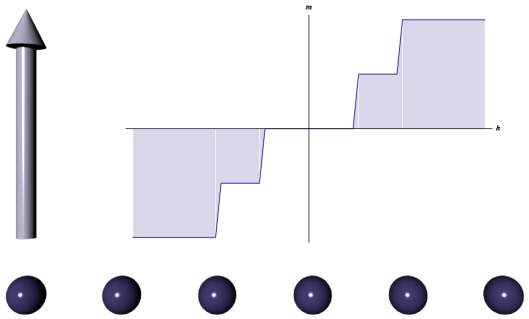


Figure 6: The Oshikawa–Yamanaka–Affleck Theorem predicts the existence, under certain circumstances, of plateaux with fractional magnetization when a magnetic field is applied on a one–dimensional spin system.

These two examples illustrate, in quite an accurate way, the manner in which tensor networks have usually been employed. As pointed out above, the knowledge of the mathematical properties of these states was not mature enough to overcome the task of rigorously proving in this framework theorems on spin systems and quantum magnetism. Nevertheless, the theories of Matrix Product States and Projected Entangled Pair States flourished during the last decade [FNW92, VC04a, VC04b, VC06, PGVWC07, Has07a, PGVCW08, PGWS$^+$08, SWPGC09, PGSGG$^+$10] and we are currently poised to finally face up to this obstacle in this Thesis.

The present work is split into two parts, the first one containing both already established and recently developed results about Matrix Product States and Projected Entangled Pair States; the second one is dedicated to the applications of the previous results to problems in spin systems and magnetism. This work is organized in the following manner:

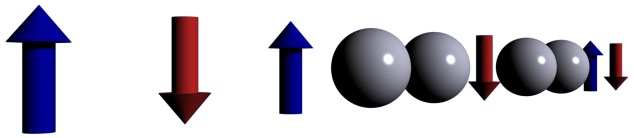


Figure 7: The correlation function of the AKLT state decays exponentially, which means no long–range order. However, it only has contribution of states for which every spin up is followed by an spin down in the $|1, m_s\rangle$ basis, with any number of spins in the state $|0\rangle$ between them. This gives a sort of hidden order, very much related with the symmetry of the system, called string order.

- Chapters 1–4 are consigned to the study of states in one–dimensional systems by means of Matrix Product States, providing a concise but complete summary of the theory of these tensor networks, where previous results and the recent developments are superposed. There are three reasons to opt for this structure in lieu of a more specific one centred on the newer results: firstly, this enables us to view the results in context, allowing a better comprehension of their meaning; secondly, there is a lack of updated reviews about the topic, with results spread over many papers with significantly different notations; finally, there are results well–known among the tensor networks community but unrecognised by other communities, which could, in principle, be interested in this topic. The new results are mainly concentrated in Chapter 2, where both a complete description of the concept of injectivity and the proof of the quantum Wielandt's inequality are provided, and Chapter 4, where we characterize the necessary and sufficient conditions to construct invariant Matrix Product States under symmetry groups. These results appear in [SPGWC10] and [SWPGC09], respectively. The other results are extracted from [FNW92, PGVWC07, BJKW00, Wol09].

- Chapters 5–7 are devoted to states in higher–dimensional systems, specially two–dimensional many–body systems. We follow a structure of contents similar to the previous Chapter, not only for the reasons put forward in the last paragraph, but also to explicitly present the differences between Matrix Product States and Projected Entangled Pair States, founded on the absence of connections between the latter and completely positive maps. The new results are condensed in Chapters 5 and 7 and they can be found in [PGSGG$^+$10]. The other results are mainly based on [PGVCW08].

- In Chapter 8, two methods of constructing quasi–solvable $SU(2)$–invariant Hamiltonians with two–body interactions are provided. The $SU(2)$ symmetry is the most natural one in spin–interacting systems, so it is reasonable to search for exactly solvable models showing this symmetry. Furthermore, the interactions usually occur by means of two–body operators, so it is also natural to seek Hamiltonians with this type of structure. The first method permits us to construct Hamiltonians with a given structure and the Matrix Product State as an eigenstate, and not only as a ground state [SWPGC09]. The second method is an exact renormalization group technique which is complementary to the previous one, since it allows us to find all possible strongly frustration–free Hamiltonians with nearest–neighbour interactions [TS10].

- Chapter 9 contains several results connecting the theory of Matrix Product States with the quantum theory of magnetism, and condensed matter in general. In Section 9.3 we prove that the existence of string order in a quantum state is intimately related to the presence of local symmetries [PGWS$^+$08]. In Section 9.5, we provide a proof of the Lieb–Schultz–Mattis Theorem (see Fig. 5b) and its generalization for $U(1)$ symmetry, known as Oshikawa–Yamanaka–Affleck Theorem (see Fig. 6), in the context of tensor networks [SWPGC09, PGSGG$^+$10]. Sections 9.4 and 9.2 show, in the first case, an application of the results about symmetries in Projected Entangled Pair States [PGSGG$^+$10] to topological quantum computation and, in the second case, a dichotomy theorem about the ground state of frustration–free Hamiltonians. The last two Sections exhibit the best illustrations of the idea introduced above: the use of tensor networks as a laboratory to *experiment* with theoretical condensed matter, attempting to extrapolate the results to the general Hilbert space (these results will appear in a paper now in preparation). For instance, in Section 9.6 we show a theorem which relates the fractional magnetization of a state to the entanglement present in this state. In Section 9.7, we prove that, under certain conditions, the states which are unique ground states of a gapped Hamiltonian with long–range interactions, display long–range entanglement.

De omni re scibili...
et quibusdam aliis.

François Voltaire
(1694-1778)

1

One dimensional systems: Matrix Product States

1.1 Introduction

This first Chapter is devoted to one–dimensional quantum spin many–body systems. As already argued in the Introduction, the spectral resolution of Hamiltonians acting on many–body systems is a very interesting but highly complex problem, because of the exponential growth of the associated Hilbert space with the number of particles. In quantum information theory, this allows an exponential speed–up in quantum computation tasks, and in condensed matter is a never–ending source of unexpected behaviours and surprising results, such as phase transitions [WOVC06, VWC09], fractionalization of physical quantities [AMU75, KDP80, Lau81, Gre94, OYA97], and rare matter phases, like certain glass structures [Sch91, Ell90].

The Matrix Product States formalism was developed from the Density Matrix Renormalization Group (DMRG), the best–known numerical method to compute ground state properties of many–body systems, without a full comprehension of the grounds of its success. This method allows us to analyse the low–energy spectrum of one–dimensional spin systems efficiently and with unprecedented precision, which enables us to understand the main properties of the different phases of condensed matter systems.

DMRG was originally proposed for 1D quantum (zero temperature) systems with short–range interactions [Whi92, Whi93]. However, the method has been extended to many other situations [PHKW99], and even to higher dimensions [VC04a, MVC09]. As pointed out above, the reason why the method worked so well was not

entirely understood in the original paper by White [Whi92], until the connection with MPS was proposed by Östlund et al. [ÖR95]. However, a complete and coherent theoretical picture was only reached when the underlying connections with quantum information theory was established [FNW92, PGVWC07, VPC04], in particular with the theory of completely positive maps.

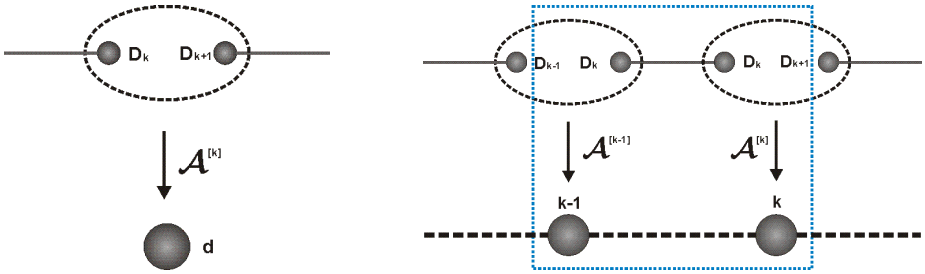
As a consequence, a large number of results in condensed matter theory stems from the application of the techniques available in completely positive maps to Matrix Product States. These techniques, which are introduced in this Chapter, have been particularly successful in establishing a local description (*i.e.* in terms of the tensor) of global features, a *leitmotiv* in the forthcoming chapters.

In this Chapter, we provide a complete overview about Matrix Product States, from the Ansätze which end with the construction of such states, to the main characteristics shown by them. We include recent developments, updating the results shown in previous reviews [PGVWC07]. The structure of the Chapter is as follows:

- Many of the properties of the Matrix Product States straightforwardly follow from the construction of these states. Therefore, in Section 1.2, we describe in detail one of the possible construction methods: the Valence Bond Solid state. This approach is physically intuitive and constitutes a solid background for the correct understanding of the forthcoming results.

- We characterize the freedom in the representation of Matrix Product States in Section 1.3. As a consequence, the question about which the most adequate representation naturally emerges, and it is treated. We show that there exists a canonical form with block–diagonal structure coming from the classification of complete positive maps [FNW92, PGVWC07]. We explicitly distinguish between states with open and states with periodic boundary conditions, discussing the inherent features associated with both of them. The results of this Section are mainly taken from [PGVWC07]. Nonetheless, some of the proofs have been slightly changed and some additional lemmas have been included to make the Chapter more accessible for the condensed matter community.

- In Section 1.4, we describe states in the thermodynamic limit. These states, named Finitely Correlated States, were proposed in the seminal work [FNW92] as a generalization of the relevant findings from [AKLT88]. It is in this limit where, in fact, the connections with the completely positive maps turn out to be more relevant, so the Section is opened with a summary of the most relevant results about quantum channels [Wol09]. With this in hand, we discuss the properties of the Finitely Correlated States in the natural framework of the reduced density matrix, providing calculations for expectation values of local operators and the computation of two–point correlation functions.



(a) (b)

Figure 1.1: **Matrix Product States construction**. (a) Two virtual Hilbert spaces of dimensions D_k and D_{k+1} are mapped to a Hilbert space of dimension d by means of a linear map $\mathcal{A}^{[k]}$. (b) The maps are applied to two consecutive sites connected by a maximally entangled state. By successive applications, a Matrix Product State with open boundary conditions is generated.

1.2 Construction of Matrix Product States

In this Section, we provide a constructive definition of Matrix Product States (MPS) with Open Boundary Conditions (OBC). We show the existence of a *canonical form* for the representations of Matrix Product States, which will prove to be a key tool for the rest of this Thesis. We also show that a translational invariant state always admits a site–independent representation of the matrices.

1.2.1 A constructive definition of Matrix Product States and the Valence Bond Picture

Let us consider a pure quantum state $|\psi\rangle \in \mathbb{C}^{\otimes d^N}$ in an N–site spin system, with each of the spins associated to a d–dimensional Hilbert space. There are different methods of constructing the matrix product Ansatz, each of which with its advantages and disadvantages. Here, we use the *Valence Bond Picture* (VBP) [PGVWC07, VC04b], since this is a very intuitive approach. Let us consider N aligned local spins (d–dimensional Hilbert spaces), such that each of them has a couple of ancillary D–dimensional spins, as shown in Fig. 1.1a. These ancillas are called **virtual spins** throughout this work. Let us assume that every pair of virtual spins, one of them corresponding to site $k-1$ and the other to k (neighbouring physical spins), is in an unnormalized maximally entangled state $|\chi\rangle = \sum_{\alpha=1}^{D} |\alpha,\alpha\rangle$, which is called **bond** and gives the construction its name (see Fig. 1.1b). Let us define the site–dependent linear maps $\mathcal{A}^{[k]} : \mathbb{C}^{D_k} \otimes \mathbb{C}^{D_{k+1}} \to \mathbb{C}^d$, where k labels each

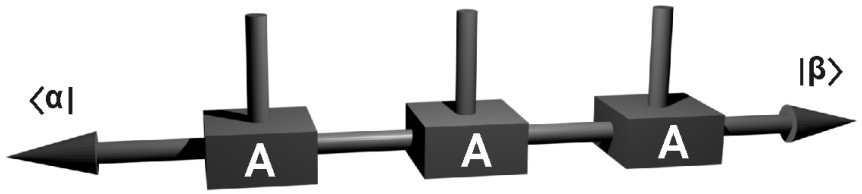


Figure 1.2: **MPS–OBC**. Tensor network representation of a Matrix Product State with open boundary conditions. The vectors encoding such boundary conditions are represented by the cones in the extremities.

site. This map depends on $d \cdot D_k \cdot D_{k+1}$ parameters and can be written for site k as

$$\mathcal{A}^{[k]} = \sum_{i_k=1}^{d} \sum_{\alpha,\beta} A^{[k]}_{i_k,\alpha,\beta} \, |i_k\rangle\langle\alpha,\beta| \tag{1.1}$$

where $|i\rangle \in \mathbb{C}^d$ is a basis of the physical Hilbert space, and $|\alpha\rangle \in \mathbb{C}^{D_{k-1}}$ and $|\beta\rangle \in \mathbb{C}^{D_k}$denote the states of two ancillary spins, which encode the boundary conditions, as illustrated in Fig. 1.2. Let us now apply the map twice, as shown in Fig. 1.1b:

$$|\psi^{(2)}_{\alpha,\beta}\rangle = (\mathcal{A}^{[k-1]} \otimes \mathcal{A}^{[k]})\Big(|\alpha\rangle \sum_{\gamma=1}^{D_k} |\gamma,\gamma\rangle \, |\beta\rangle\Big) =$$

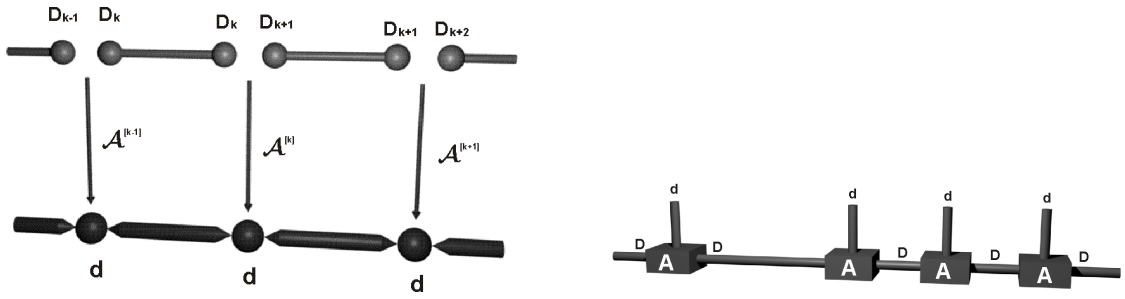
$$\Big(\sum_{\substack{i_{k-1},i_k \\ \mu_1,\mu_2,\nu_1,\nu_2}} A^{[k-1]}_{i_{k-1},\mu_1\nu_1} A^{[k]}_{i_k,\mu_2\nu_2} \, |i_{k-1}\, i_k\rangle\langle\mu_1\, \nu_1| \, \langle\nu_2\, \mu_2| \Big) \Big(|\alpha\rangle \sum_{\gamma=1}^{D_k} |\gamma,\gamma\rangle \, |\beta\rangle\Big) =$$

$$\sum_{\substack{i_{k-1},i_k \\ \gamma}} A^{[k-1]}_{i_{k-1},\alpha\gamma} A^{[k]}_{i_k,\gamma\beta} \, |i_{k-1}\, i_k\rangle = \sum_{i_{k-1},i_k=1}^{d} \langle\alpha| \, A^{[k-1]}_{i_{k-1}} A^{[k]}_{i_k} \, |\beta\rangle \; |i_{k-1}\, i_k\rangle$$

where in the last equality we have rewritten the sum as a product of matrices. By repeating the process over N sites, one straightforwardly gets:

$$|\psi^{(N)}_{\alpha,\beta}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \langle\alpha| \, A^{[1]}_{i_1} \cdots A^{[N]}_{i_N} \, |\beta\rangle \; |i_1 \ldots \, i_N\rangle \tag{1.2}$$

The states which can be represented by the structure given in Eq. 1.2 constitute the set of **Matrix Product States with open boundary conditions** (MPS–OBC) (see Fig. 1.2). In these states, there is a set of d matrices $\{A^{[k]}_{i_k} \in \mathcal{M}_{D_k,D_{k+1}}\}^d_{i_k=1}$ for every site k, and the vectors $\langle\alpha|$ and $|\beta\rangle$ encode the boundary conditions. The maximum of the dimensions of the ancillary Hilbert spaces, $D = \max_k D_k$, is generally denominated **bond dimension** or **virtual dimension**. Every MPS–OBC can be represented by square matrices with bond dimension D by



(a) (b)

Figure 1.3: **Representations of MPS**. (a) Representation of an MPS constructed by means of the VBP, in which two virtual Hilbert spaces of dimensions D_k and D_{k+1} are mapped to a Hilbert space of dimension d by means of a linear map $\mathcal{A}$. (b) Representation of the MPS as a tensor network: the vertical *leg* represents the physical Hilbert space (spin), while the two horizontal ones are the bonds.

padding the remaining matrix entries with zeros. This is especially relevant when the MPS has periodic boundary conditions, as we will see in the following Section. In Fig. 1.3, we show the two most common graphical representations of MPS: with the physical spins and the ancillary differentiated, and as a three-legged tensor, where one corresponds to the physical spin and the other to the virtual ones.

It is also common in the literature to replace $\langle\alpha|\, A^{[1]}_{i_1} \to A^{[1]}_{i_1} \in \mathcal{M}_{1,D_1}$, *i.e.* the first matrix is a row–vector which contains the information about the boundary condition. This also applies to its counterpart $A^{[N]}_{i_N}\,|\beta\rangle$.

Let us note that the total Hilbert space has dimension d^N, while the dimension of the Hilbert subspace generated by the MPS is smaller than $d \cdot D^2 \cdot N$, where D is the bond dimension defined above, *i.e.* the number of required parameters grows linearly with N, instead of exponentially. This allows an efficient simulation of many–body quantum states which are writeable as MPS, something which cannot be done with a general state. Moreover, these states show a local structure (they are described in terms of local tensors) and present non–trivial correlations, as shown in Subsubsection 1.4.3.4.

Finally, let us remark that the mean field Ansatz $|\psi\rangle = |\phi\rangle^{\otimes N}$, *i.e.* the product states, can be understood as an MPS with bond dimension $D = 1$.

1.3 Canonical form for Matrix Product States

We have shown the structure of an MPS–OBC in the previous Section. However, one can expect that there is freedom in the choice of the matrices $A^{[k]}_{i_k}$ in Eq. 1.2. In this Section, we establish *all* possible degrees of *freedom of choice*, showing as well that the matrices representing every MPS–OBC can be expressed in a block–diagonal form, which is called *canonical form*. This is a consequence of the deep relationship

between MPS and quantum channels, which is widely discussed in Section 1.4. The existence of such a canonical form has relevant consequences for the proof of several features of MPS, as shown in the following sections.

1.3.1 Matrix Product States with open boundary conditions

In this Subsection, we show that the matrices which define an MPS can be written in a *canonical form*. This canonical form turns out to be keystone in the proofs of several theorems. We also show the freedom in the choice of the matrices describing an MPS. The Ansatz for an N–particle MPS–OBC in Eq. 1.2 can be written as:

$$|\psi^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} A_{i_1}^{[1]} \cdots A_{i_N}^{[N]} \, |i_1 \ldots i_N\rangle \tag{1.3}$$

where $A_{i_k}^{[k]} \in \mathcal{M}_{D_k,D_{k+1}}$, $1 < k < N$, and the replacements $\langle\alpha| \, A_{i_1}^{[1]} \to A_{i_1}^{[1]} \in \mathcal{M}_{1,D_1}$ and $A_{i_N}^{[N]} \, |\beta\rangle \to A_{i_N}^{[N]} \in \mathcal{M}_{D_{N-1},1}$ have been used. This notation is employed here since it allows us to write the theorems in a more compact form. Then, the existence of a canonical form is ensured by the following Theorem:

Theorem 1 (Canonical form with OBC) *Let us consider any N–site quantum state $|\psi\rangle$ with physical dimension d, $|\psi\rangle \in (\mathbb{C}^d)^{\otimes N}$. Then, there always exists a $D \leq d^{\lfloor \frac{N}{2} \rfloor}$ MPS–OBC representation with the structure shown in Eq. 1.3, such that:*

1. $\sum_{i=1}^{d} A_i^{[k]} A_i^{[k]\dagger} = \mathbb{1}_{D_k}$, $1 \leq k \leq N$
2. $\sum_{i=1}^{d} A_i^{[k]\dagger} \Lambda^{[k-1]} A_i^{[k]} = \Lambda^{[k]}$, $1 \leq k \leq N$, $\Lambda^{[k]} \in \mathcal{M}_{D_{k+1}}$ *being diagonal, strictly positive (and hence, full–rank) and with* $\mathrm{tr}\left[\Lambda^{[k]}\right] = 1$. *Particularly,* $\Lambda^{[0]} = \Lambda^{[N]} = 1$.

Any representation of an MPS–OBC fulfilling these conditions is said to be in the ***canonical form***. □

Proof The complete proof can be found in [Vid03], but let us summarize the main idea here in the form shown in [PGVWC07]. The local decomposition can be obtained by successive application of Schmidt or singular value decompositions (SVD) on $|\psi\rangle$. The fact that there exists a decomposition fulfilling conditions 1. and 2. is obtainable by exploiting the freedom $A_i^{[k]} A_i^{[k+1]} = (A_i^{[k]} X)(X^{-1} A_i^{[k+1]})$, for every invertible X. The following Theorem ensures the existence of these matrices. ■

The following Theorem is proven in [SWPGC09]. The proof, which shows that the entire freedom in any MPS–OBC is given by local matrix multiplication in the space of virtual spins, is not difficult but it is long and is not transcribed here.

Theorem 2 (Freedom in the choice of matrices (OBC)) *Let us consider a state* $|\psi\rangle \in (\mathbb{C}^d)^{\otimes N}$ *with an MPS–OBC representation given by*

$$|\psi\rangle = \sum_{i_1,\ldots,i_N} B_{i_1}^{[1]} \cdots B_{i_N}^{[N]} |i_1 \ldots i_N\rangle$$

Then, there exist, in general, non–square matrices Y_k *and* Z_k*, with* $Y_k Z_k = \mathbb{1}$*, such that, by defining*

$$A_i^{[1]} = B_i^{[1]} Z_1 \qquad A_i^{[N]} = Y_{N-1} B_i^{[N]}$$
$$A_i^{[k]} = Y_{k-1} B_i^{[k]} Z_k, \qquad 1 < k < N$$

the new matrices also describe $|\psi\rangle$ *and they are in the canonical form. Additionally, the multiplication by invertible matrices provides the only freedom of choice.* □

There are several consequences that derive from these theorems, which can be summarized as follows

- The canonical form is unique by construction, up to permutations and degeneracies in the Schmidt decomposition.
- Any state whose reduced density matrix fulfils rank $\left[\rho^{[n]}\right] \leq D$, $1 \leq n \leq N$, can be written as an MPS–OBC with bond dimension smaller than or equal to D.
- The only freedom in the representation of an MPS–OBC is local matrix multiplication.
- The proof of Theorem 2 is constructive and actually provides the method for obtaining the canonical form.

The following examples show the MPS–OBC which represent the W–state and the Majumdar–Ghosh state:

Example 1 The W–state for N sites is defined as

$$|W_N\rangle = |1\overbrace{0\ldots0}^{N-1}\rangle + \cdots + |\overbrace{0\ldots0}^{N-1}1\rangle.$$

This state, which is translational invariant, appears as the ground state of the ferromagnetic XX–model with strong transverse magnetic field. This state admits a

site–dependent representation with $D = 2$ given, for $1 < k < N$, by:

$$A_0^{[1]} = \begin{pmatrix} 1 & 0 \end{pmatrix} \qquad A_1^{[1]} = \begin{pmatrix} 0 & 1 \end{pmatrix}$$
$$A_0^{[k]} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad A_1^{[k]} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$
$$A_0^{[N]} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad A_1^{[N]} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

□

Example 2 The Majumdar–Ghosh model, published in [MG69], was the first example of translational invariant Hamiltonian with a continuous local $SU(2)$ symmetry, gap and faster than exponentially decaying correlation function. The ground state is a two–fold degenerate manifold essentially formed by a dimerized state and its one–site–displaced state. The matrices describing the $2N$–particle (non–translational invariant) dimerized state is given, for $1 \leq k \leq N$, by:

$$A_0^{[2k-1]} = \begin{pmatrix} 1 & 0 \end{pmatrix} \qquad A_1^{[2k-1]} = \begin{pmatrix} 0 & 1 \end{pmatrix}$$
$$A_0^{[2k]} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad A_1^{[2k]} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

□

1.3.2 Matrix Product States with periodic boundary conditions

In this Subsection, we focus on a very particular and important kind of boundary conditions: periodic boundary conditions (PBC). These can be considered as a particular case of OBC, where the extremities of the chain are connected, transforming it into a ring (see Fig. 1.4). Then, a maximally entangled state connecting the extremities is introduced. As a consequence, Eq. 1.2 can be rewritten as

$$|\psi_{\alpha,\beta}^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[A_{i_1}^{[1]} \cdots A_{i_N}^{[N]} |\beta\rangle\langle\alpha|\right] |i_1 \ldots i_N\rangle$$
$$\Big\downarrow \sum_{\alpha,\beta} \delta_{\alpha,\beta}$$
$$|\psi^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[A_{i_1}^{[1]} \cdots A_{i_N}^{[N]}\right] |i_1 \ldots i_N\rangle \qquad (1.4)$$

Therefore, the states with the structure given by Eq. 1.4 represent the family of **Matrix Product States with periodic boundary conditions** (MPS–PBC) (see

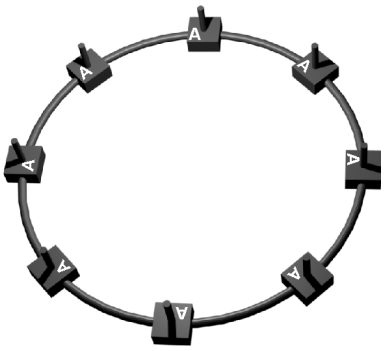


Figure 1.4: **MPS–PBC**. Tensor network representation of a Matrix Product State with periodic boundary conditions. The extremities of the chain are identified, transforming it into a ring.

Fig. 1.4). As stated above, PBC are physically implemented in a ring where the extremities are identified, instead of in an open chain. Mathematically, it corresponds to replacing the vectors in the ends of the open chain by a trace.

These boundary conditions are relevant in condensed matter when the system length reaches the **thermodynamic limit** (macroscopic number of particles). When the number of particles is large, it is reasonable to consider that the measured properties are local and, hence, that we work far from the boundaries. Therefore one can essentially forget about the surface effects by introducing PBC. They are also broadly employed in condensed matter because of the better convergence properties which many functions have in this topology (a torus).

In particular, the study of *translational invariant systems* is of the utmost importance in condensed matter theory, since it is connected, by means of *Noether's Theorem* [Noe18], to a conserved quantity: the **momentum** (in this case, as the translational invariance is on a lattice, it is more suitable to talk about **quasi–momentum**). This is a very relevant tool in the spectral resolution of Hamiltonians, which has as a consequence that almost every solvable Hamiltonian shows this symmetry. Although the symmetries in MPS–PBC are discussed in detail in Chapter 4, let us now discuss translational invariant MPS (TI–MPS), since they are closely related to PBC. The aim of this Section is to establish the properties of such states, as well as the characterization of their matrix description, a relevant task since the main results shown in this Thesis are all about TI–MPS.

Let us start by defining translational invariant states. We provide here two definitions: the first one is the strict mathematical definition, while the second one, which is more restrictive, is also physically more intuitive definition, which is the one taken in condensed matter.

Definition 1 (Translational invariant state 1) A state $|\psi^{(N)}\rangle \in (\mathbb{C}^d)^{\otimes N}$ with periodic boundary conditions is called **translational invariant** (TI) if this is an eigenvector of the translation operator τ. As (with these boundary conditions) the operator is idempotent, $\tau^N = \mathbb{1}$, the eigenvalues are complex phases. □

The Definition above establishes the mathematical condition for a state to be translational invariant. However, a more restrictive definition of translational invariant state is also widely used (including in this work).

Definition 2 (Translational invariant state 2) A state $|\psi^{(N)}\rangle \in (\mathbb{C}^d)^{\otimes N}$ with periodic boundary conditions is called **(strongly) translational invariant** when it is an eigenstate of the translation operator with eigenvalue $+1$. □

The latter corresponds more accurately to the physical idea of translational invariance in condensed matter, since no global phase appears after a one–site translation. In any case, whether the definition of TI–state used in a theorem is the one provided by Definition 1 or Definition 2 will be specified in the corresponding section to avoid confusion.

It is clear that, by taking the matrices which define the MPS–PBC as site–independent, *i.e.* $A_i^{[k]} = A_i$, $\forall k$, the state is translational invariant in the sense of Definition 2. The following Theorem [PGVWC07, Theorem 3] shows that the converse is also true and that any TI–state can always be written by means of a site–independent set of matrices.

Theorem 3 (Site–independent representation of TI–states) *Every TI–MPS defined on a finite chain has a site–independent MPS representation*

$$|\psi^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[A_{i_1}\cdots A_{i_N}\right]\ |i_1\ldots i_N\rangle \tag{1.5}$$

where $A_i^{[k]} = A_i$. Starting from the site–dependent representation with bond dimension D, the TI–representation could require a bond dimension ND, which increases with the length of the chain. □

Proof Let us start with the site–dependent representation of the state given by the matrices $A_i^{[k]}$ and let us consider the following d matrices:

$$B_i = N^{-\frac{1}{N}} \begin{pmatrix} 0 & A_i^{[1]} & 0 & \cdots & 0 \\ 0 & 0 & A_i^{[2]} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & A_i^{[N-1]} \\ A_i^{[N]} & 0 & 0 & \cdots & 0 \end{pmatrix}$$

which leads to

$$\sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[B_{i_1}\cdots B_{i_N}\right]\ |i_1\ldots i_N\rangle =$$

$$\sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[A_{i_1}^{[1]}\cdots A_{i_N}^{[N]}\right]\ |i_1\ldots i_N\rangle = |\psi^{(N)}\rangle$$

where we have used translational invariance in the last step. Therefore, from the construction of B–matrices, one can see that the TI–representation could require a bond dimension which grows with the number of particles. However, there are many relevant cases in which D can be chosen independently of the number of particles.■

The W–state is an example in which it is necessary to increase the bond dimension with the length of the ring when a site–independent representation for the MPS is required. We also show here the translational invariant representation of the Majumdar–Ghosh state.

Example 3 As we stated in Example 1, the W–state is translational invariant, but there is no translational invariant number–of–particles–independent representation (in particular, with $D = 2$, which is the dimension used in case of a non–translational invariant representation). In fact, it is proven in [PGVWC07, Corollary 1] that $D \geq \mathcal{O}(N^{\frac{1}{3}})$, so the translational invariant representation requires a bond dimension which increases with the number of particles. □

Example 4 In Example 2, we provided the matrices for the dimerized state. However, the Majumdar–Ghosh state also can be described with a translational invariant representation (in the sense of Definition 2) given by the Kraus operators:

$$A_0^{[1]} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & \frac{-1}{\sqrt{2}} \\ 0 & 0 & 0 \end{pmatrix} \qquad A_1^{[1]} = \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

This example also illustrates that the bond dimension must be increased when we represent the translational invariant state. □

From this point on, we call the matrices which describe a TI–MPS **Kraus operators**. The reason lies within the deep connections between these matrices and the Kraus operators which describe quantum channels. This will become clear in Sections 1.4 and 2.2.

Once it is established that it is always possible to take a site–independent representation for any translational invariant state, let us prove that one can always decompose the matrices of a TI–MPS into a canonical form. The proof of the following Theorem (this is essentially the proof of [PGVWC07, Theorem 4] with some slight changes for the sake of clarity) is constructive and provides the method to actually obtaining such a canonical form.

Theorem 4 (Canonical form with TI) *Let us consider any N–site quantum TI–MPS $|\psi\rangle \in (\mathbb{C}^d)^{\otimes N}$ with physical dimension d and bond dimension D, and let us assume that it has a site–independent representation with the structure shown in Eq. 1.5. Then, the Kraus operators A_i can be written in a block–diagonal form as*

$$A_i = \begin{pmatrix} \lambda_1 A_i^1 & 0 & \cdots & 0 \\ 0 & \lambda_2 A_i^2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n A_i^n \end{pmatrix} \tag{1.6}$$

with $1 \geq \lambda_k > 0$, and every block fulfils the following conditions:

1. $\sum_{i=1}^d A_i^k A_i^{k\dagger} = \mathbb{1}_D$, $1 \leq k \leq n$, *usually called gauge condition.*

2. $\sum_{i=1}^d A_i^{k\,\dagger} \Lambda^k A_i^k = \Lambda^k$, $1 \leq k \leq n$, Λ^k *being diagonal, strictly positive (and hence, full–rank) and with* $\mathrm{tr}\left[\Lambda^k\right] = 1$.

3. $\mathbb{1}$ *is the only fixed point of the operator* $\mathcal{E}_k(X) = \sum_{i=1}^d A_i^k X A_i^{k\,\dagger}$, $1 \leq k \leq n$.

Any representation of an MPS–PBC fulfilling these conditions is in the ***canonical form****. The bond dimension of the TI–MPS in the canonical form is always smaller than or equal to D.* □

Proof We can assume w.l.o.g. that the spectral radius of $\mathcal{E}$ is 1 since, in any other case, we can always redefine the Kraus operators by multiplying them by a constant. Let us denote the fixed point of $\mathcal{E}$ by $X \geq 0$, *i.e.* $\mathcal{E}(X) = X$. If X is *invertible*, then by denoting $B_i = X^{-\frac{1}{2}} A_i X^{\frac{1}{2}}$, the gauge condition $\sum_{i=1}^d B_i B_i^\dagger$ is fulfilled.

Otherwise, X is *not invertible*, but it is positive and can be expanded on an orthonormal basis as $X = \sum_\alpha \lambda_\alpha |\alpha\rangle\langle\alpha|$ with $\lambda_\alpha > 0$. Let us denote by $P_R = \sum_\alpha |\alpha\rangle\langle\alpha|$ the projector onto the subspace R spanned by $\{|\alpha\rangle\}$. By means of Lüder's theorem (see Theorem 8), the fixed point must fulfil $[A_i, X] = 0$, which is trivially equivalent to $[A_i, P_R X] = P_R[A_i, X] + [A_i, P_R]X = [A_i, P_R]X = 0$. Let us denote $X^{-1} = \sum_\alpha \lambda_\alpha^{-1} |\alpha\rangle\langle\alpha|$, so multiplying the previous expression by the left, we obtain

$$[A_i, P_R] X X^{-1} = [A_i, P_R] P_R = 0 \;\Rightarrow\; A_i P_R = P_R A_i P_R \tag{1.7}$$

Let us call $P_R^\perp = \mathbb{1} - P_R$, then

$$\begin{aligned} |\psi^{(N)}\rangle = & \sum_{i_1,\ldots,i_N=1}^d \mathrm{tr}\left[P_R A_{i_1} \cdots A_{i_N}\right] |i_i \ldots i_N\rangle + \\ & + \sum_{i_1,\ldots,i_N=1}^d \mathrm{tr}\left[P_R^\perp A_{i_1} \cdots A_{i_N}\right] |i_i \ldots i_N\rangle \end{aligned} \tag{1.8}$$

By means of Eq. 1.7, the first term of Eq. 1.8 becomes $\mathrm{tr}[P_R A_{i_1} P_R \cdots P_R A_{i_N} P_R]$, which corresponds to a TI–MPS with bond dimension $\dim R$. Analogously, by replacing $P_R = \mathbb{1} - P_R^\perp$, we get that $P_R^\perp A_i = P_R^\perp A_i P_R^\perp$, and we can rewrite the second term in Eq. 1.8 as a TI–MPS with Kraus operators $C_i = P_R^\perp A_i P_R^\perp$. Therefore, we can trivially rewrite the initial state with matrices

$$A_i \hookrightarrow \begin{pmatrix} B_i & 0 \\ 0 & C_i \end{pmatrix}$$

By repeating the process, we end up with a block–diagonal representation of the matrices $A_i \hookrightarrow \bigoplus_{k=1}^n B_i^k$, in which property 1. is fulfilled in every block and the fixed point is invertible.

Let us now prove by contradiction that these blocks also fulfil property 3. Let us assume that there exists another hermitian fixed point $Y_k \neq \mathbb{1}$ for $\mathcal{E}_k(Y_k) = \sum_{i=1}^d B_i^k Y_k B_i^{k\,\dagger} = Y_k$. Then, this fixed point can be expanded as $Y_k = \sum_\alpha \lambda_\alpha^{(k)} |\alpha\rangle\langle\alpha|$ with $\lambda_1^{(k)} \geq \cdots \geq \lambda_n^{(k)}$. Obviously, $\tilde{Y}_k = \mathbb{1} - \frac{1}{\lambda_1^{(k)}} Y_k$ is also a positive fixed point, since both $\mathbb{1}$ and Y_k are fixed points, but this is not full–rank, which contradicts the initial hypothesis.

The same argumentation can be used to prove that the dual channel (see Definition 5) $\mathcal{E}^*(X) = \sum_{i=1}^d B_i^{k\,\dagger} X B_i^k$ has a unique strictly positive fixed point Z_k. This is diagonalizable, $\Lambda_k = U_k Z_k U_k^\dagger$, so we can redefine $\tilde{B}_i^k = U_k B_i^k U_k^\dagger$ and the new Kraus operators fulfil property 2. without actually changing properties 1. and 3. ∎

The proof contains tools which come from completely positive maps (cp maps) which are explained with further details in Section 1.4, but this simple proof already allows us to glimpse their power.

Note that, in the Theorem, some λ_j appear in the matrix while, in the proof, they do not appear explicitly. In fact, they emerge from the very first line of the proof. The operator $\mathcal{E}$ is a cp linear map and hence it admits a *spectral decomposition* $\mathcal{E}(X_k) = \lambda_k X_k$ (eigenvalue equation), with $1 \geq \lambda_k > 0$ due to positivity. Then, the blocks in the decomposition correspond to invariant subspaces of the linear map. As a consequence, the canonical form above is essentially the idea of expanding an operator T into its eigenbasis.

Finally, let us clarify the reason for always considering positive fixed points. The following Lemma[1] shows that this is completely general:

Lemma 1 (Fixed points can be taken positive) *If $X \neq 0$ is a fixed point of a completely positive linear map $\mathcal{E}$, $\mathcal{E}(X) = \sum_k A_k^\dagger X A_k = X$, then X can be written as a (complex) linear combination of positive fixed points.* □

Proof Firstly, let us note that $X = \frac{1}{2}(X + X^\dagger) - \frac{i}{2}(iX - iX^\dagger)$, and that $\mathcal{E}(X) = X \Leftrightarrow \mathcal{E}(X^\dagger) = X^\dagger$. By linearity, this means that the fixed point can be expressed

[1] In fact, this Lemma is a consequence of the quantum version of the Perron–Frobenius Theorem (see [EHK78, Lemma 5.2] and [Rus02]).

as a linear combination of two hermitian fixed points, so we can take wlog X as hermitian. Let us now show that every hermitian fixed point can be written as a combination of positive fixed points, $X = \frac{1}{2}(\sqrt{X^2} + X) - \frac{1}{2}(\sqrt{X^2} - X)$, where the positive root is taken for all the eigenvalues (this means that $\sqrt{X^2} = |X|$, where $|X|$ must be understood as the absolute value of all eigenvalues of X). By Lüder's theorem, X^2 is obviously a fixed point, since $[X^2, A_i] = \{X, [X, A_i]\} = 0$. Therefore, our objective is to prove that if $X^2 \geq 0$ is a fixed point of a complete positive map, then $X \geq 0$ is also a fixed point. By hypothesis, $0 =: [X^2, A_i] = \{X, [X, A_i]\}$. Let us work in the basis in which X is diagonal, so $X = \sum_i^r x_i \, |i\rangle\langle i|$. Then, in coordinates, $(x_j + x_k)\langle j| \, Y \, |k\rangle = 0$, where $Y = [X, A_i]$. If $|j\rangle$ or $|k\rangle$ are in the support of X, then $(x_j + x_k) > 0$ and $\langle j| \, Y \, |k\rangle = 0$. Otherwise, $\langle j| \, Y \, |k\rangle = 0$ by definition, because $Y = [X, A_i]$. This proves that $[X, A_i] = 0$ if $X \geq 0$, which means that X is also a fixed point and the lemma follows straightforwardly. ∎

Finally, in the proof of the Theorem we assume that there is only one fixed point corresponding to an eigenvalue 1. The general case is slightly more complicated and yields a further decomposition into a superposition of periodic states. We explain such a decomposition, and its consequences, with further details in Section 1.4.

By reproducing the structure shown when we studied MPS–OBC, the natural question is now the freedom in the choice of Kraus operators. The following Theorem shows that the essential gauge freedom arises from multiplying the Kraus operators by an invertible matrix.

Theorem 5 (Gauge freedom for PBC) *Let $|\psi_A^{(N)}\rangle$ and $|\psi_B^{(N)}\rangle$ be two TI–MPS with N sites and generated by Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ and $\{B_i \in \mathcal{M}_D\}_{i=1}^d$, respectively. Then, if these two states are equal, i.e. $|\psi_A^{(N)}\rangle = e^{i\theta} \, |\psi_B^{(N)}\rangle$, with sufficiently large N, there exists an invertible X such that $A_i = e^{i\frac{\theta}{N}} X B_i X^{-1}$ $\forall i$.* □

The proof of this Theorem is shown in Subsection 5.3.1 instead of here, since we require the mathematical tools described in Section 2.2. We also explain there the meaning of *sufficiently large N*.

1.4 Finitely correlated states

In this Section, we introduce the concept of *quantum channel*: a communication channel which can transmit quantum information. Mathematically, it is a complete positive trace–preserving map mapping density operator spaces. We show several mathematical results in quantum channels from which the Kraus representation theorem stands out, since it allows the connection with TI–MPS [FNW92]. This Theorem establishes that every complete positive map can be described by a set of matrices, called Kraus operators (this is the reason why we denominate the matrices describing MPS in this way). If these matrices are used to describe a TI–MPS,

then many characteristics of the complete positive map are reflected in relevant features of TI–MPS. For instance, it is well–known [Mur90] that Kraus operators are representations of the generators of a finite–dimensional C^*–algebra, and that there always exists a basis in which these representations are block–diagonal, directly connecting this point of view to the canonical form [EHK78]. Another feature inherited by MPS connects the total decoherence of any state by successive uses of a quantum channel with the existence of a local Hamiltonian, such that it has the MPS as a unique ground state with a non–trivial spectral gap above it.

This framework provides an efficient description of TI–MPS in the thermodynamic limit, *i.e.* the limit in which the number of particles tends to infinity. In particular, we will focus here on a very relevant subset of TI–MPS called *finitely correlated states*, firstly defined in [FNW92].

The description of the states in the thermodynamic limit is provided in the natural language of the reduced density matrix, which is employed for the efficient computation of expectation values and correlation functions, finally proving the *exponential clustering* feature put forward in Section 1.2.

1.4.1 A bit about quantum channels

In this Subsection, we define the concept of quantum channel and show some relevant results on complete positive maps which are employed in the rest of this Thesis. In lieu of proving the theorems here, we provide references to the original papers, as well as more recent works, for the interested reader.

Let us start by defining the concept of quantum channel by specifying the intuitive physical properties which a general transformation between density matrices must show [Pre98, Wol09]:

Definition 3 (Quantum channel) A **quantum channel** is a general transformation $\mathcal{E}$ between states defined in the bounded operator spaces $\rho \in \mathcal{B}(\mathcal{H}_1)$ and $\mathcal{E}(\rho) \in \mathcal{B}(\mathcal{H}_2)$, where the Hilbert spaces $\mathcal{H}_{1,2}$ are finite–dimensional, such that it is:

1. *Trace preserving.* If $\mathcal{E}(\rho)$ is interpreted as a density matrix, then $\mathrm{tr}\,[\mathcal{E}(\rho)] = \mathrm{tr}\,[\rho] = 1$, so the transformation must preserve the trace.

2. *Linear.* Non–linear transformations can in general violate causality, so all transformations between states must be linear.

3. *Completely positive.* $\mathcal{E}(\rho)$ is a density matrix, so it is positive. Therefore, $\mathcal{E}$ maps positive operators into positive operators. The map $\mathcal{E}$ is called **completely positive** when the operator $\mathbb{1}\otimes\mathcal{E}$ is positive, *i.e.* when $(\mathbb{1}\otimes\mathcal{E})\rho_{AB} \geq 0$, for all $\rho_{AB} \in \mathcal{B}(\mathcal{H}_A \otimes \mathcal{H}_B)$. □

In general, we consider cases where the initial and final Hilbert spaces are isomorphic, *i.e.* $\mathcal{H}_1 \simeq \mathcal{H}_2$, but this is not necessary.

It is also possible to define a quantum channel in a general mathematical formalism of operator algebras [Wol09, Section 1.3], without making use of the density matrix formalism.

Complete positivity comes from the fact that, if we consider an initial bipartite system $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ with Alice and Bob sharing an entangled state, in which Alice makes nothing and Bob applies a quantum operation, the output must be a permited (positive) state as well. There are operations, such as the partial transpose, which may yield non–positive states. So the complete positivity is a necessary condition. Nonetheless, given a linear trace–preserving map $\mathcal{E}$, verifying whether this transformation is completely positive from the definition above is very difficult. However, there is a much simpler criterion [Wol09, Proposition 1.2] which arises from the definition:

Lemma 2 (Complete positivity criterion) *A transformation $\mathcal{E} \in \mathcal{B}(\mathcal{H})$, $\dim\mathcal{H} = D$, is **completely positive** iff*

$$\tau := (\mathbb{1}_D \otimes \mathcal{E})(\,|\Omega\rangle\langle\Omega|\,) \geq 0$$

*where $|\Omega\rangle \in \mathcal{H} \otimes \mathcal{H}$ is a maximally entangled state and τ is usually called **Choi–Jamiołkowski operator**.* □

Let us now enunciate the Kraus representation theorem, which is a key result in quantum channels and a cornerstone for the results showed in this Thesis, owing to the fact that it allows the connection between quantum channels and MPS:

Theorem 6 (Kraus representation theorem) *A linear map $\mathcal{E} : \mathcal{B}(\mathcal{H}_1) \to \mathcal{B}(\mathcal{H}_2)$ with $\dim\mathcal{H}_1 = D_1$ and $\dim\mathcal{H}_2 = D_2$ is **completely positive** iff it can be represented in the form*

$$\mathcal{E}(\cdot) = \sum_{k=1}^{d} A_k^\dagger \cdot A_k$$

$A_k \in \mathcal{M}_{D_1,D_2}$, with the following properties:

1. *Normalization. $\mathcal{E}$ is **trace preserving** iff $\sum_{k=1}^{d} A_k A_k^\dagger = \mathbb{1}$ and **unital** iff $\sum_{k=1}^{d} A_k^\dagger A_k = \mathbb{1}$.*
2. *Kraus rank. The minimal number of Kraus operators $\{A_k \in \mathcal{M}_{D_1,D_2}\}_{k=1}^{d}$ is $r = \operatorname{rank}[\tau] \leq D_1 \cdot D_2$, where τ is the Choi–Jamiołkowski operator defined in Lemma 2, and r is called **Kraus rank**, **Choi rank** or **Kraus–Choi rank**.*
3. *Orthogonality. There is a representation with $d = \operatorname{rank}[\tau]$ for which the Kraus operators are orthogonal in the Hilbert–Schmidt sense, i.e. $\operatorname{tr}\left[A_i A_j^\dagger\right] \propto \delta_{ij}$.*
4. *Unitary freedom. Two sets of Kraus operators $\{A_k\}$ and $\{B_k\}$ represent the same linear map $\mathcal{E}$ iff they are related by a unitary blend U, i.e. $B_j = \sum_k U_{jk} A_k$ (where the smaller set is padded with zeros).* □

PROOF The original proof is published in [BK83, Kra87] but there is an elegant proof closer to the language used here in [Wol09, Theorem 2.1]. ∎

The composition of two quantum channels $\mathcal{E}_1$ and $\mathcal{E}_2$, $\mathcal{E}_2(\mathcal{E}_1(\cdot))$, with Kraus operators A and B respectively, is obviously another quantum channel, $(\mathcal{E}_1 \circ \mathcal{E}_2)(\cdot)$, whose Kraus operators are nothing but the product of the Kraus operators of the individual channels, $B_j A_i$. Therefore, if a quantum channel $\mathcal{E}$ with $D_1 = D_2 = D$ is considered, the N–times composition with itself, *i.e.* $\mathcal{E}^N(\cdot)$, has the set of products $\{A_{i_1} \cdots A_{i_N}\}$ as Kraus operators.

The matrices which define an MPS can be used as Kraus operators defining a complete positive map and vice versa. The fact that the Kraus operators defining the N–times composition of a quantum channel with itself also describe the coefficients of the TI–MPS, allows the MPS to inherit the strong mathematical techniques developed for the composition of complete positive maps, which are especially relevant for the study of the thermodynamic limit of TI states. This finally clarifies the reason why we denominate the matrices which define the MPS *Kraus operators*. As a final remark about the connections between completely positive maps and MPS, the trace–preserving condition immediately reminds us of the canonical form shown in Section 1.3.

The **Kraus rank** $r = \operatorname{rank}[\tau]$ defined above is the rank of τ as an operator and this must not be confused with the rank of $\mathcal{E}$ as a linear map, since they are not equivalent. For instance, the **ideal channel** $\mathcal{E} : \rho \to \rho$ is obviously full–rank as a linear map, since $\mathcal{E}$ is invertible, but the Kraus rank is $r = 1$, since it can be represented by means of only one Kraus operator $A = \mathbb{1}$. In the same way, the channel $\mathcal{E}(\cdot) \equiv \operatorname{tr}[\cdot] = \sum_{k=1}^{D} \langle k| \cdot |k\rangle$ has rank 1 as a linear map, but Kraus rank D.

Let us focus now on the last property in Theorem 6, in which the freedom in the choice of Kraus operators in order to describe the same quantum channel is established. The unitary blend which relates equivalent quantum channels is not generally equivalent to the multiplication by invertible matrices allowed by MPS. In fact, two representations of the same quantum channel produce in general different MPS and, conversely, two equivalent representations of MPS produce non–equivalent quantum channels.

The *physical representation* of a quantum channel (Fig. 1.5) consists of an initial state, defined by the density matrix ρ_0 which interacts with an environment in an initial state $|0\rangle\langle 0|$ in such a way that the total system (state + environment) is closed, being the interaction modelled by a unitary matrix U. Finally, we trace out the environment producing a final state with density matrix ρ'. Mathematically,

$$\rho' = \mathcal{E}(\rho_0) = \operatorname{tr}_{\text{env}}\left[U\left(\rho_0 \otimes |0\rangle\langle 0|\right) U^\dagger\right] \tag{1.9}$$

As a complete positive trace–preserving map, the Kraus representation theorem ensures that it can be represented by means of Kraus operators. Let us now relate the unitary U to them. If $\{|i\rangle\}$ is an orthonormal basis, then the Kraus operators

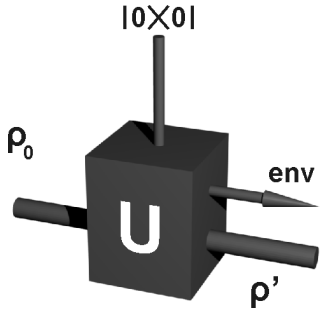


Figure 1.5: **Quantum channel**. Any quantum transformation can be represented by a quantum channel, and it can be understood as the initial state interacting with an environment by means of a unitary transformation.

[Pre98, Section 3.2] of the quantum channel 1.9 are given by

$$A_i = \mathrm{tr}_{\mathrm{env}} \left[U \left(\mathbb{1} \otimes |i\rangle\langle 0| \right) \right]$$

One can straightforwardly check that $\sum_i A_i A_i^\dagger = \mathbb{1}$ with this definition.

It is possible to prove by means of *Stinespring's representation theorem* [Wol09, NC00] that the process described above is nothing but a quantum channel fulfilling the conditions required in Definition 3 and vice versa, every quantum channel can be associated to a state–environment interaction picture.

One can always assume w.l.o.g. [PGVWC07, Theorem 2.5] that every completely positive map $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, with $\dim \mathcal{H} = D$, has spectral radius 1 and at least one positive fixed point $\mathcal{E}(\Lambda) = \Lambda$ with $0 \leq \Lambda \in \mathcal{M}_D$ associated to this eigenvalue. However, if the eigenspace associated to the eigenvalue 1 is degenerate, then there is a convex set of fixed points with at most D^2 extreme points. Let us now enunciate a couple of very powerful theorems related to fixed points of quantum channels.

Theorem 7 (Carathéodory's theorem) *Let us consider a d–dimensional real vector space and a convex set* Ω *in it, generated by the extreme points* $\Lambda = \{\Lambda_i\}_{i=1}^{\chi}$, $\chi > d$. *Then, every point in* Ω *can be expressed as a convex combination of, at most,* $d+1$ *extreme points from* Λ. □

Proof The original reference is [Car11], but a more modern proof can be found in [Eck93]. ■

Obviously, the d+1 extreme points are not global, but depend on the point described. Before enunciating the second theorem, known as Lüder's Theorem, let us define the *commutant of a set* of matrices.

Definition 4 (Commutant) Let $\mathcal{K} = \{A_i \in \mathcal{M}_D\}$ be a set of matrices. Then, the **commutant** of $\mathcal{K}$ is the set of operators which commute with all elements in $\mathcal{K}$, *i.e.* $\{X \mid [X, A_i] = 0, \forall i\}$. □

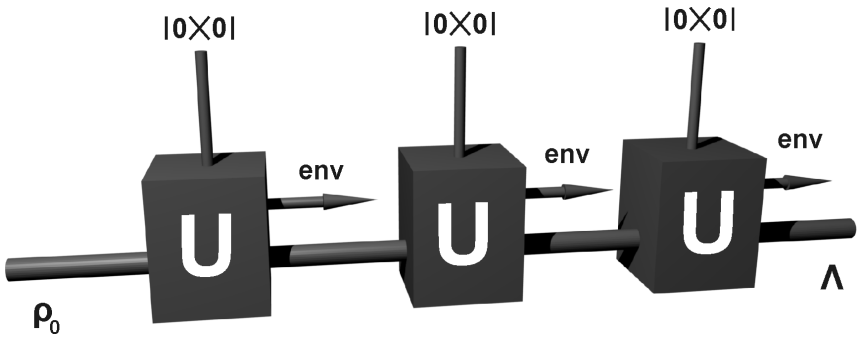


Figure 1.6: **Fixed point**. The fixed point of a quantum channel is the final state resulting after many applications of the quantum channel. If the quantum channel is very decoherent, then the final state is independent of the initial one.

The commutant is obviously never an empty set, since it always contains the identity.

Theorem 8 (Lüder's Theorem) *The set of fixed points $\mathcal{P}$ of a quantum channel coincides with the commutant of the set of Kraus operators which define it.* □

Proof A proof of this Theorem can be found in [BJKW00]. ■

Let us now define *dual channel*.

Definition 5 (Dual channel) Let $\mathcal{E} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$, with $\mathcal{B}(\mathcal{H}) \subseteq \mathcal{M}_D$, be a quantum channel. Then, its **dual channel** $\mathcal{E}^*$ is defined as the quantum channel fulfilling $\mathrm{tr}\,[\mathcal{E}(X)Y] = \mathrm{tr}\,[X\mathcal{E}^*(Y)]$, for all positive X and Y. The Kraus representation of the channel $\mathcal{E}(\cdot) = \sum_k A_k^\dagger \cdot A_k$ leads to $\mathcal{E}^*(\cdot) = \sum_k A_k \cdot A_k^\dagger$. □

1.4.2 Finitely correlated states

In this Subsection, we start focussing on infinite systems. We recall the definition of *finitely correlated states*, firstly introduced by M. Fannes *et al* in [FNW92], in which a successful generalization of the findings in [AKLT88] is provided. The authors introduced several techniques excerpted from complete positive maps, providing a mathematical background for the TI–MPS in the thermodynamic limit. The results shown here are mainly based on the point of view and notation used in [PGVWC07]. The **finitely correlated states** are *translational invariant* states defined on an *infinite chain*, *i.e.* in the thermodynamic limit. They are constructed by means of a completely positive trace–preserving map $\mathbb{E} : \mathcal{B}(\mathbb{C}^D) \to \mathcal{B}(\mathbb{C}^D \otimes \mathbb{C}^d)$ and the fixed–point density operator Λ of the map $\Lambda = \mathrm{tr}_d[\mathbb{E}(\Lambda)]$ (see Fig. 1.6). In the language used in Subsection 1.2.1, $\mathbb{C}^D$ is the Hilbert space associated to the virtual spin and $\mathbb{C}^d$ is the Hilbert space corresponding to the physical spin.

The most important finitely correlated states are the *purely generated* ones, where the map $\mathbb{E}(\cdot) = V^\dagger \cdot V$ is generated by a *partial isometry* $V : \mathbb{C}^D \otimes \mathbb{C}^d \to \mathbb{C}^D$,

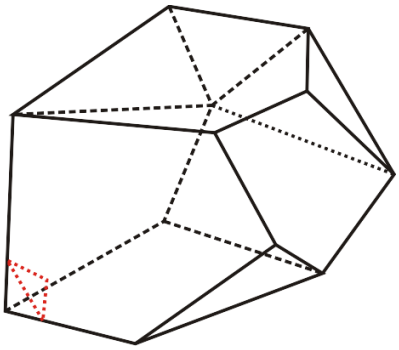


Figure 1.7: **MPS in the Hilbert Space**. Although the set of Matrix Product States with fixed bond dimension is a tiny corner of the total Hilbert space, this is a very important corner, since ground states of local Hamiltonians are well described by them [VC06, Has07a].

with $VV^\dagger = \mathbb{1}_D$, $V^\dagger V = P$, and P a projector with rank smaller than or equal to D. The isometry can be related to the Kraus operators by the invertible relationship:

$$V = \sum_{i=1}^{d} \sum_{\alpha,\beta=1}^{D} (A^i)_{\alpha,\beta} \, |\alpha\rangle\langle\beta \, i| \qquad (1.10)$$

The isometry conditions are directly translated into the canonical form conditions shown in Theorem 4, and the fixed points of $\mathcal{E}$ and $\mathbb{E}$ coincide. Let us enunciate a couple of theorems proven in [FNW92] which show some important properties of the finitely correlated states.

Theorem 9 (Density of FCS) *The set of purely generated finitely correlated states is* ***weakly dense*** *within the set of all translational invariant states on the infinite chain.* □

In order to explain the meaning of *weakly dense*, let us consider a set $P = \{\rho_k\}$ in certain Hilbert space $\mathcal{H}$ and a bounded functional $\mathbb{F} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H}')$ ($\mathcal{H}$ and $\mathcal{H}'$ two finite–dimensional Hilbert spaces), then the set P is **weakly dense** in $\mathcal{H}$ if, for any $\mathbb{F}$, there exists a sequence of elements in P such that $\lim_{\rho_k \in P} \mathrm{tr}\,[\mathbb{F}(\rho_k - \rho)] \to 0$. Under this perspective, Theorem 9 means that, by considering funtionals such as multiplication by local operators, one can find a sequence of finitely correlated states which approximate expectation values accurately, which is translated into the fact that they are an adequate Ansatz for numerical calculations of, for instance, ground state energies or correlation functions. This is a complementary result to the ones proven by F. Verstraete et al [VC06] and M. Hastings [Has07a], in which it is proven that the ground state of every gapped Hamiltonian can be well described by MPS (see Fig. 1.7).

Theorem 10 (Ergodicity) *A finitely correlated state is* ***ergodic****, i.e. an extreme point within all possible translational invariant states, iff the completely positive map* $\mathcal{E}$ *has a non–degenerate eigenvalue* 1. □

This Theorem implies that every finitely correlated state can be decomposed into a combination of ergodic finitely correlated states with a unique decomposition, since they are extreme points of a convex hull.

Let us establish a connection with the canonical form in Theorem 4. As we stated above, the isometry condition is deeply related to the canonical form. In the basis which gives the canonical form, the Kraus operators are written with a block diagonal structure in which each block is multiplied by the correspondent eigenvalue of $\mathcal{E}$, whose modulus is smaller than or equal to 1. When we multiply the Kraus operators to construct the state, the multiplicative constants accumulate, while the norm of the block remains stable. This results in a suppression of the blocks corresponding to eigenvalues with modulus smaller than 1, which is exponential in the length of the chain. Then, the states in the canonical form correspond, in the thermodynamic limit, to ergodic finitely correlated states.

We have now the necessary mathematical background to study the case where the completely positive map has other eigenvalues of modulus 1, which were ignored in the proof of Theorem 4. Every ergodic finitely correlated state can be decomposed into the sum of p p-periodic states, each of them corresponding to a root of unity $\exp(\frac{2\pi i}{p}m)$, with $0 \leq m \leq p-1$, in the spectrum of $\mathcal{E}$. This statement is strictly enunciated in the following Theorem, which improves [PGVWC07, Theorem 5].

Theorem 11 (Periodic decomposition) *Let* $|\psi\rangle \in (\mathbb{C}^d)^{\otimes N}$ *be a TI–MPS generated by the set of Kraus operators* $\{A_k \in \mathcal{M}_D\}_{k=1}^d$ *and such that they have only one block in the canonical representation. Let us assume that the map* $\mathcal{E}$ *has* $1 \leq p \leq D^2$ *eigenvalues with modulus one, then we have the dichotomy*

- *If* p *is a factor of* N*, then* $|\psi\rangle$ *can be decomposed into* p *p-periodic different and injective states with a* D_l*–dimensional representation, such that* $\sum_{l=1}^p D_l = D$*.*
- *Otherwise* $|\psi\rangle = 0$*. This is not a restriction in the thermodynamic limit.* □

Proof The Theorem is a consequence of the spectral properties of the complete positive map $\mathcal{E}$ proven in [FNW92]. It was proven that, if the identity is the only fixed point of $\mathcal{E}$, then there exists a $p \in \mathbb{N}$ such that the powers $\{\omega^k = e^{i\frac{2\pi k}{p}}\}_{k=1}^p$ are all the eigenvalues of $\mathcal{E}$ with modulus 1 and each of them is a simple root.

Moreover, there is a unitary $U = \sum_{k=1}^p \omega^k P_k$, where P_k is a complete set of orthogonal projectors $\sum_{k=1}^p P_k = \mathbb{1}$, such that $\forall X \in \mathcal{M}_D$, $\mathcal{E}(XP_k) = \mathcal{E}(X)P_{k-1}$ (k is a cyclic index). We assume w.l.o.g. that these projectors are diagonalized in the canonical basis. It is straightforward to show that the latter implies that

$$A_j P_k = P_{k-1} A_j, \qquad \forall j,k \tag{1.11}$$

This, together with the decomposition of the trace as $\mathrm{tr}\,[\cdots] = \sum_{k=1}^{p} \mathrm{tr}\,[P_k \cdots P_k]$, leads to a decomposition of the state into a superposition of MPS $|\psi_k\rangle$, *i.e.* $|\psi\rangle = \sum_{k=1}^{p} |\psi_k\rangle$, with site–dependent matrices $A(k)_i^{[j]} = P_{k+j-1} A_{i_j} P_{k+j}$. This means that each state $|\psi_k\rangle$ is p–periodic and, as $P_k P_l = \delta_{kl} P_k$, this is non–zero iff p is a factor of N.

This proves that $\mathcal{E}^p$ has exactly a p–fold degeneracy of the eigenvalue 1. Moreover, the space of fixed points is generated by $\{P_k\}$, since

$$\mathcal{E}^p(X) = \sum_{j,k} P_j \mathcal{E}^p(P_j X P_k) P_k \qquad (1.12)$$

while the space of fixed points of the dual channel is generated by $\{P_k \Lambda P_k\}$.

We use this to show that the states $|\psi_k\rangle$ are injective and different. Let us start with *injectivity*: an MPS is injective if the associated completely positive map shows only one eigenvalue of modulus 1 and the correspondent eigenvector Λ is full–rank (see Definition 8 for further details). To see this, it is sufficient to show that the associated complete positive map $\mathcal{E}_k^p(X) = P_k \mathcal{E}^p(P_k X P_k) P_k$, with $X = P_k X P_k$, has P_k as the only fixed point, $P_k \Lambda P_k$ as the only fixed point of the dual channel and no other eigenvalues of modulus 1. This is obvious, however, from Eq. 1.12 and the results found on the set of fixed points.

Once it is proven that they are injective, showing that they are different is trivial by contradiction. For simplicity's sake, let us argue in the case of two 2–periodic states, but the argumentation can be straightforwardly extended to the general case. Let us assume that there are two equal states, and by making use of the uniqueness of the canonical form for injective TI–MPS, one has that $\mathrm{rank}\,[P_1] = \mathrm{rank}\,[P_2] = D$ and $P_1 A_i A_j P_1 = U P_2 A_i A_j P_2 U^\dagger$, $\forall i, j$. Then, in addition to matrices $P_1 = \sum_{i=1}^{D} |i\rangle\langle i|$ and $P_2 = \sum_{i=D+1}^{2D} |i\rangle\langle i|$, also the matrix

$$\Lambda = \sum_{i=1}^{2D} |i\rangle\langle i + D|$$

is trivially a fixed point of $\mathcal{E}^2$, contradicting that they are injective. ∎

This Theorem brings us to the definition of *pure finitely correlated states*:

Definition 6 (Pure FCS) A finitely correlated state is **pure** when this is purely generated and 1 is the only eigenvalue of $\mathcal{E}$ with modulus 1. □

Therefore, pure finitely correlated states are the bricks from which one can construct the rest of finitely correlated states, and they match the TI–MPS whose canonical form has only one block corresponding to an eigenvalue of $\mathcal{E}$ with modulus 1.

Let us remark that the results shown for chains with finite length are more general than the ones shown in the theory of finitely correlated states. It is meant that finitely correlated states can be recovered by taking the thermodynamic limit

in the theory developed for finite chains. However, in this process the same finitely correlated state could arise from different TI–MPS; for instance, those with a non–equivalent composition of blocks corresponding to eigenvalues with modulus smaller than 1, because the blocks are suppressed in the process.

1.4.3 Reduced density matrix and expectation values

In this Subsection, we construct the expression for the n–particle reduced density matrix corresponding to a TI–MPS in the thermodynamic limit. We provide the expression in terms of both Kraus operators and the partial isometry V, defined in Eq. 1.10. We make use of this to define as well the expression for expectation values of local operators in the framework of TI–MPS. Finally, we compute the two–point correlation function, proving an important property of the MPS which is *exponential clustering*, *i.e.* the correlation function decays exponentially.

1.4.3.1 Reduced density matrix from Kraus operators

We start by constructing the reduced density matrix in terms of the Kraus operators. In general, the definition of the reduced density matrix for a compact region R (which in the one–dimensional case means an n–particle block) is

$$\rho^{(n)} = \lim_{N\to\infty} \mathrm{tr}_{R^c}[\,|\psi^{(N)}\rangle\langle\psi^{(N)}|\,] \tag{1.13}$$

where the trace is taken over the complementary region of R, R^c. This is the general definition of the n–particle reduced density matrix. Let us now apply this to TI–MPS (Fig. 1.8 gives a graphical idea of the process). As the state is translational invariant, we can consider w.l.o.g. that the region R is constituted by the first n particles, so

$$\begin{aligned}
\mathrm{tr}_{R^c}[\,|\psi^{(N)}\rangle\langle\psi^{(N)}|\,] &= \mathrm{tr}_{R^\perp}\Big[\sum_{\substack{i_1,\dots,i_N\\ j_1,\dots,j_N}}^{d} \mathrm{tr}\,[A_{i_1}\cdots A_{i_N}]\,\overline{\mathrm{tr}\,[A_{j_1}\cdots A_{j_N}]}\,|i_1\dots i_N\rangle\langle j_1\dots j_N|\Big] \\
&= \sum_{\substack{i_1,\dots,i_N\\ j_1,\dots,j_N}}^{d} \mathrm{tr}\,[A_{i_1}\cdots A_{i_N}]\,\mathrm{tr}\left[\bar{A}_{j_1}\cdots\bar{A}_{j_N}\right]\,|i_1\dots i_n\rangle\langle j_1\dots j_n| \\
&\qquad\qquad \delta_{i_{n+1},j_{n+1}}\cdots\delta_{i_N,j_N} \\
&= \sum_{\substack{i_1,\dots,i_n\\ j_1,\dots,j_n}}^{d} \mathrm{tr}\left[(A_{i_1}\otimes\bar{A}_{j_1})\cdots(A_{i_n}\otimes\bar{A}_{j_n})\mathbb{E}_{\mathbb{1}}^{N-n}\right]\,|i_1\dots i_n\rangle\langle j_1\dots j_n|
\end{aligned} \tag{1.14}$$

where $\mathbb{E}_{\mathbb{1}} = \sum_{i=1}^{d} A_i\otimes\bar{A}_i$ is a representation of the dual quantum channel $\mathcal{E}^*$ (see Definition 5) written as a linear map acting on a vector space instead of on a space of

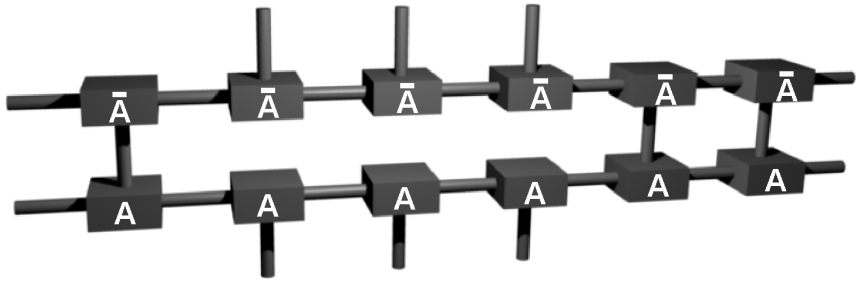


Figure 1.8: **Reduced density matrix**. Representation of the n–particle reduced density matrix constructed from an MPS. The physical legs of the two states are contracted except in the support of the reduced density matrix.

matrices. As they are linear maps, the entries of $\mathbb{E}_{\mathbb{1}}$ are automatically determined once one chooses how to do the mapping $\rho \leftrightarrow |\rho\rangle$. In this case, we chose the partial transpose in the second subspace. Therefore, if $\rho = \sum_{\alpha,\beta} \rho_{\alpha\beta} |\alpha\rangle\langle\beta|$, then $|\rho\rangle = \sum_{\alpha,\beta} \rho_{\alpha\beta} |\alpha,\beta\rangle$. Once this is chosen, the definition for $\mathbb{E}_{\mathbb{1}}$ straightforwardly follows from $\mathcal{E}^*$. Let us define this matrix:

Definition 7 (Transfer matrix) The matrix representation of the dual channel $\mathcal{E}^*$ given by $\mathbb{E}_{\mathbb{1}} = \sum_{i=1}^{d} A_i \otimes \bar{A}_i$, is called **transfer matrix** in the language of MPS.□

Obviously, $\mathbb{E}_{\mathbb{1}}^\dagger$ is the representation as a linear mapping of the quantum channel $\mathcal{E}$ itself, so the spectra of the quantum channel and its dual are related by conjugation. The term *left eigenvectors* of $\mathbb{E}_{\mathbb{1}}$ is commonly used when one refers to the eigenvectors of $\mathbb{E}_{\mathbb{1}}^\dagger$.

It is clear by construction that the spectra of $\mathcal{E}^*$ (and hence, the spectrum of $\mathcal{E}$ by conjugation) and $\mathbb{E}$ are equal. This means that, if λ_k and Λ_k are an eigenvalue and its corresponding eigenvector of $\mathcal{E}^*$, *i.e.* $\mathcal{E}^*(\Lambda_k) = \lambda_k \Lambda_k$, then $\mathbb{E}_{\mathbb{1}} |\Lambda_k\rangle = \lambda_k |\Lambda_k\rangle$.

We assume that there is only one eigenvalue λ of $\mathcal{E}^*$ such that $|\lambda| = 1$ (otherwise, one can decompose the state into pure finitely correlated states and apply this to each block). The fixed point is $\mathbb{1}$, due to the gauge condition $\sum_i A_i A_i^\dagger = \mathbb{1}$, while we call Λ the fixed point of the channel. Then, from the polar decomposition [NC00] of $\mathbb{E}_{\mathbb{1}}$, one can easily write[2]

$$\mathbb{E}_{\mathbb{1}} = |\mathbb{1}\rangle\langle\Lambda| + \mathcal{O}(|\lambda_2|) \qquad (1.15)$$

where λ_2 is the second largest eigenvalue in modulus. The second term in Eq. 1.15 is obviously suppressed in the thermodynamic limit,

$$\lim_{N\to\infty} \mathbb{E}_{\mathbb{1}}^N = |\mathbb{1}\rangle\langle\Lambda| \qquad (1.16)$$

[2]The polar decomposition ensures that every matrix M can be written as $M = UA$, with U unitary and $A \geq 0$. This is the key for proving that every matrix $M = \sum_i \lambda_i |r_i\rangle\langle l_i|$, where $M^\dagger M |r_i\rangle = \lambda_i^2 |r_i\rangle$ and $M M^\dagger |l_i\rangle = \lambda_i^2 |l_i\rangle$.

Therefore, by taking the thermodynamic limit in Eq. 1.14 and replacing Eq. 1.16 in the resultant expression, one obtains

$$\begin{aligned}\rho^{(n)} &= \sum_{\substack{i_1,\ldots,i_n\\ j_1,\ldots,j_n}}^{d} \langle\Lambda|\,(A_{i_1}\otimes\bar{A}_{j_1})\cdots(A_{i_n}\otimes\bar{A}_{j_n})\,|\mathbb{1}\rangle\,|i_1\ldots i_n\rangle\langle j_1\ldots j_n| \\ &= \sum_{\substack{i_1,\ldots,i_n\\ j_1,\ldots,j_n}}^{d}\sum_{\alpha,\beta=1}^{D} \Lambda_\alpha\langle\alpha|\,A_{i_1}\cdots A_{i_n}\,|\beta\rangle\langle\beta|\,A^\dagger_{j_n}\cdots A^\dagger_{j_1}\,|\alpha\rangle\,|i_1\ldots i_n\rangle\langle j_1\ldots j_n|\end{aligned}$$

Therefore, by using that $\sum_{\beta=1}^{D}|\beta\rangle\langle\beta| = \mathbb{1}_D$ together with the properties of the trace, one finally obtains

$$\rho^{(n)} = \sum_{\substack{i_1,\ldots,i_n\\ j_1,\ldots,j_n}}^{d} \mathrm{tr}\left[A^\dagger_{j_n}\cdots A^\dagger_{j_1}\Lambda A_{i_1}\cdots A_{i_n}\right]\,|i_1\ldots i_n\rangle\langle j_1\ldots j_n| \qquad (1.17)$$

which is the expression for the ***n*–particle reduced density matrix** in a very large spin chain (thermodynamic limit). The fixed point Λ encodes *exactly* the entanglement between the block and the rest of chain in the thermodynamic limit.

One can easily check that $\mathrm{rank}\left[\rho^{(n)}\right] \leq D^2$ from Eq. 1.17. Let us define the vectors $|\psi^{(n)}_{\alpha\beta}\rangle = \sum_{i_1,\ldots,i_n}\langle\alpha|\,A_{i_1}\cdots A_{i_n}\,|\beta\rangle\,|i_1\ldots i_n\rangle$, then Eq. 1.17 is nothing but

$$\rho^{(n)} = \sum_{\alpha,\beta=1}^{D}\Lambda_\alpha\,|\psi^{(n)}_{\alpha\beta}\rangle\langle\psi^{(n)}_{\alpha\beta}|$$

which clearly has rank smaller than or equal to D^2.

1.4.3.2 Reduced density matrix from partial isometry

We provide here another expression for the reduced density matrix in terms of the isometry V defined in Subsection 1.4.2. This does not provide any mathematical advantage, but it sometimes turns out to be more convenient, for instance, for the construction of states which are invariant under the action of a group (see Chapter 4). Let us prove the following Lemma:

Lemma 3 (Reduced density matrix (isometry)) *If the partial isometry $V : \mathbb{C}^D\otimes\mathbb{C}^d\to\mathbb{C}^D$ is defined as in Eq. 1.10, then the* ***n*–particle reduced density matrix** *can be written as:*

$$\rho^{(n)} = \mathrm{tr}_{\mathbb{C}^D}\left[(V^\dagger\otimes\mathbb{1}_d^{\otimes(n-1)})\cdots(V^\dagger\otimes\mathbb{1}_d)V^\dagger\Lambda V(V\otimes\mathbb{1}_d)\cdots(V\otimes\mathbb{1}_d^{\otimes(n-1)})\right] \qquad (1.18)$$

where Λ is the fixed point and the partial trace is taken over the first (virtual) subspace. □

PROOF The proof straightforwardly follows from the definition of V in Eq. 1.10:

$$(V^\dagger \otimes \mathbb{1}_d^{\otimes(n-1)}) \cdots (V^\dagger \otimes \mathbb{1}_d) V^\dagger \Lambda V (V \otimes \mathbb{1}_d) \cdots (V \otimes \mathbb{1}_d^{\otimes(n-1)}) = A_{j_n}^\dagger \cdots A_{j_1}^\dagger \Lambda A_{i_1} \cdots A_{i_n} \otimes |i_1 \dots i_n\rangle\langle j_1 \dots j_n|$$

by tracing out the first subspace, we directly obtain Eq. 1.17. ∎

1.4.3.3 Expectation values

The calculation of expectation values, one of the main and most common tasks in quantum mechanics, is an almost effortless exercise in the framework of MPS. The objective is to compute the scalar product $\langle T \rangle_{|\psi\rangle} = \langle\psi| T |\psi\rangle = \mathrm{tr}\left[T |\psi\rangle\langle\psi|\right]$ in the thermodynamic limit, where the operator T is composed of tensor products of local operators T_i with **interaction length** $\boldsymbol{n}$, *i.e.* acting non–trivially on n particles:

$$T = \overbrace{T_1 \otimes \cdots \otimes T_n}^{T^{(n)}} \otimes \mathbb{1}_{rest}$$

Let us calculate the scalar product for $n < N < \infty$ sites, evaluating later the thermodynamic limit. As we are considering translational invariant states, the position of the operator is not important. By following the same reasoning that we used in this Subsection,

$$\begin{aligned}
\langle T \rangle_{|\psi^{(N)}\rangle} &= \mathrm{tr}\left[T |\psi^{(N)}\rangle\langle\psi^{(N)}|\right] \\
&= \sum_{\substack{i_1,\dots,i_N \\ j_1,\dots,j_N}} \mathrm{tr}\left[(A_{i_1} \otimes \bar{A}_{j_1}) \cdots (A_{i_n} \otimes \bar{A}_{j_n}) \mathbb{E}_{\mathbb{1}}^{N-n}\right] \langle j_1 \dots j_n| T^{(n)} |i_1 \dots i_n\rangle \\
&= \mathrm{tr}\left[\mathbb{E}_{T_1} \cdots \mathbb{E}_{T_n} \mathbb{E}_{\mathbb{1}}^{N-n}\right]
\end{aligned}$$

where

$$\mathbb{E}_T = \sum_{i,j=1}^{d} (T)_{ji} A_i \otimes \bar{A}_j \qquad (1.19)$$

As T is hermitian and the scalar product $\langle T \rangle_{|\psi^{(N)}\rangle}$ is real as a consequence, one can also write the expression in terms of $\bar{\mathbb{E}}_X = \sum_{i,j=1}^{d} (X)_{ij} \bar{A}_i \otimes A_j$. We are interested in the thermodynamic limit so, by using Eq. 1.16, we obtain

$$\lim_{N\to\infty} \langle T \rangle_{|\psi^{(N)}\rangle} = \langle\Lambda| \mathbb{E}_{T_1} \cdots \mathbb{E}_{T_n} |\mathbb{1}\rangle \qquad (1.20)$$

This is the analytical structure of the **expectation value** of a local operator constituted by the tensor product of n operators in the thermodynamic limit. This calculation is generally very efficient, since the multiplication of matrices is efficient too. Furthermore, the support of the operators is usually small (*i.e.* n is small) and the T_i are often equal, which notably simplifies the calculations.

Here, the fact that the MPS is in the canonical form was used, so the right eigenvector is $|\mathbb{1}\rangle$, but this is of course not necessary and the calculations can be made exactly in the same way by calculating the corresponding right eigenvector $|\lambda_R\rangle$ and right eigenvector $\langle\lambda_L|$. However, some issues must be taken into account if we do not work in the canonical form. For instance, if the maximum eigenvalue of the transfer matrix is not normalized to 1, then it is necessary to divide the RHS by $\langle\psi|\psi\rangle$ in Eq. 1.20.

1.4.3.4 Two–point correlation functions

This Subsubsection consists essentially of the proof of one of the main properties of the MPS: *exponential clustering*. This means that the two–point correlation function of MPS either has an infinite range or decays exponentially. This is the reason why MPS are not a good Ansatz for very entangled systems, such as critical systems near the transition point. In that case, other more suitable Ansätze, such as the Multiscale Entanglement Renormalization Ansatz (MERA) [Vid04, Vid07], are often used. Let us prove the following Theorem:

Theorem 12 (Exponential clustering) *Let us consider a TI–MPS $|\psi\rangle$ on an infinite chain and the operators $T_i^{(1)}$ and $T_{i+\Delta}^{(2)}$ sited in positions i and $i+\Delta$. Then, the* ***two-point correlation function*** $\mathcal{C}_\Delta(|\psi\rangle) = \langle T_i^{(1)} T_{i+\Delta}^{(2)}\rangle_{|\psi\rangle} - \langle T_i^{(1)}\rangle_{|\psi\rangle}\langle T_{i+\Delta}^{(2)}\rangle_{|\psi\rangle}$ *decays exponentially on approaching the thermodynamic limit.* □

Proof We start working on a finite system for N particles, evaluating afterwards the thermodynamic limit, and studying finally the asymptotic behaviour $\Delta \gg 1$. By using the techniques developed in Subsubsection 1.4.3.3 for the calculation of expectation values, one can straightforwardly obtain:

$$\mathcal{C}_{\Delta,N}(|\psi\rangle) = \mathrm{tr}\left[\mathbb{E}_{T^{(1)}}\mathbb{E}_{\mathbb{1}}^{\Delta-1}\mathbb{E}_{T^{(2)}}\mathbb{E}_{\mathbb{1}}^{N-\Delta-1}\right] - \mathrm{tr}\left[\mathbb{E}_{T^{(1)}}\mathbb{E}_{\mathbb{1}}^{N-1}\right]\mathrm{tr}\left[\mathbb{E}_{T^{(2)}}\mathbb{E}_{\mathbb{1}}^{N-1}\right]$$

where we have used the cyclic properties of the trace to place $\mathbb{E}_{T^{(1)}}$ in the first site. By using Eq. 1.15, *i.e.* $\mathbb{E}_{\mathbb{1}} = \sum_{i=1}^{D^2}\lambda_i |\lambda_i^R\rangle\langle\lambda_i^L|$, with $1 = \lambda_1 > \lambda_2 \geq \cdots \geq \lambda_{D^2}$, we take the thermodynamic limit:

$$\begin{aligned}
\lim_{N\to\infty}\mathcal{C}_{\Delta,N}|\psi\rangle &= \lim_{N\to\infty}\langle\lambda_1^L|\mathbb{E}_{T^{(1)}}\mathbb{E}_{\mathbb{1}}^{\Delta-1}\mathbb{E}_{T^{(2)}}|\lambda_1^R\rangle - \langle\lambda_1^L|\mathbb{E}_{T^{(1)}}|\lambda_1^R\rangle\langle\lambda_1^L|\mathbb{E}_{T^{(2)}}|\lambda_1^R\rangle \\
&\quad + \mathcal{O}(\lambda_2^{N-\Delta-1}) \\
&= \sum_{i=1}^{D^2}\lambda_i^{\Delta-1}\langle\lambda_1^L|\mathbb{E}_{T^{(1)}}|\lambda_i^R\rangle\langle\lambda_i^L|\mathbb{E}_{T^{(2)}}|\lambda_1^R\rangle - \langle\lambda_1^L|\mathbb{E}_{T^{(1)}}|\lambda_1^R\rangle\langle\lambda_1^L|\mathbb{E}_{T^{(2)}}|\lambda_1^R\rangle \\
&= \sum_{i=2}^{D^2}\lambda_i^{\Delta-1}\langle\lambda_1^L|\mathbb{E}_{T^{(1)}}|\lambda_i^R\rangle\langle\lambda_i^L|\mathbb{E}_{T^{(2)}}|\lambda_1^R\rangle
\end{aligned}$$

We are interested in analysing the asymptotic behaviour of the correlation function, so we take the approximation $\Delta \gg 1$:

$$\mathcal{C}_\Delta(\,|\psi\rangle) \xrightarrow{\Delta\gg 1} \lambda_2^{\Delta-1}\langle\lambda_1^L|\,\mathbb{E}_{T^{(1)}}\,|\lambda_2^R\rangle\langle\lambda_2^L|\,\mathbb{E}_{T^{(2)}}\,|\lambda_1^R\rangle$$

As $\lambda_2 < 1$, it means that, asymptotically, $\mathcal{C}_\Delta(\,|\psi\rangle)$ decays exponentially, property known as exponential clustering. ∎

For the sake of clarity in the notation, we have slightly simplified the proof by assuming that there is no periodic decomposition, *i.e.* there is only one eigenvalue with maximum module. Otherwise, the analysis must be performed over each pure component.

Product states, which are the simplest Ansatz to approximate states due to their lack of entanglement, produce quite accurate results for some numerical calculations. This is because the great majority of the many–body states which are relevant in Nature (such as ground states of Hamiltonians) are low-entangled. However, they do have non–trivial correlations. This fits perfectly to the properties of MPS: on the one hand, exponential clustering provides them short-range correlations; on the other hand, they keep a quite simple local structure which facilitates calculations. This makes them an advantageous Ansatz to approximate one–dimensional states [Has06, VC06].

Il libro della natura è scritto
in lingua matematica.
Galileo Galilei (1564-1642)

2

Injectivity and quantum Wielandt's inequality

2.1 Introduction

There is a deep relationship between MPS and quantum channels, as we already pointed out in Chapter 1. This Chapter is essentially dedicated to exploiting such a relationship, especially by means of a mathematical property, called *injectivity*, which leads to relevant consequences in the physical properties of both the quantum channels, discussed in this Chapter, and the states, shown in Chapter 3.

Every quantum operation can be encoded in a quantum channel, where there is an input state transformed by the channel into an output state. An essential question is to study the properties of such an output state after a large number of applications of the quantum channel. In general, after the application of the channel, a certain **decoherence** of the initial state emerges, *i.e.* part of the information about the input state is missing and, even knowing in detail both the final state and the quantum channel, a complete information about the input state is unrecoverable. One can already glimpse in this point that the loss of information after a reiterative implementation of the quantum operation is deeply related to the fixed–point properties of the channel, especially to the number of fixed points. For instance, if a quantum channel has only one fixed point, then a total decoherence of the input state is produced, since the final state is totally independent of the initial one. On the other extreme is the ideal channel, $T(\rho) = \rho$, *El Dorado* for the quantum communication, for which no loss of information is produced.

The question above has a long history in classical channels, since this kind of long–term behaviour was already a subject of intensive research in the framework of Markov chains and discrete dynamical systems. It is directly connected to the celebrated Wielandt's inequality [Wie50], which establishes an upper bound for the number of times that a classical channel must be applied until all information about the original state is completely lost.

The results shown in this Chapter are essentially extracted from [SPGWC10], and it is structured as follows:

- In the first two Sections, we provide a physical definition of the concept of *injectivity*, since this definition is straightforwardly generalizable to higher dimensions. We simultaneously show the consequences for the associated quantum channel when described by the Kraus operators of an MPS with such a property. We later define in Section 2.3 *strong irreducibility*, a property apparently different from injectivity but, as we will prove, actually equivalent. The advantage of the description based on strong irreducibility lies in the fact that it is a local characterization of the injectivity, *i.e.* stemming from the eigenvalues of the transfer matrix.

- In Section 2.4, we make a brief introduction to classical channels. We put forward as well a relevant result in this field, known as *Wielandt's inequality* [Wie50]. This inequality provides a bound for the number of times that a classical channel must be applied on any initial state to ensure that there is a non–trivial probability to reach any possible state of the classical system. The most impressive feature of this result is, however, that the bound does not depend on the entries of the classical channel, but only on a quadratic polynomial of the the matrix dimension.

- Finally, we prove in Section 2.5 an extension of this result for quantum channels, providing an upper bound for the number of times that it must be applied until we get a total decoherence of the initial quantum state. Similarly, the bound depends only on the physical and virtual dimensions of the quantum channel. This result allows us to prove a dichotomy theorem on the zero-error capacity of quantum channels, as well as other results in condensed matter (see Section 9.2).

2.2 Injectivity

In this Subsection, we define a property of the MPS called *injectivity* from a physical point of view (we will see in the following sections that there are other equivalent definitions), since it is clear and straightforwardly generalizable to higher dimensions. Injectivity has a natural physical interpretation, as well as several relevant physical consequences which are described in detail in Chapter 3. We also prove

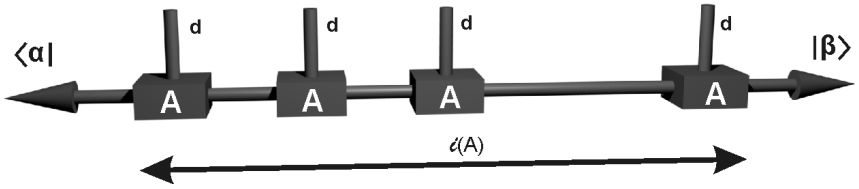


Figure 2.1: **Injectivity**. A Matrix Product State is injective with injectivity length $i(A)$ if for the MPS–OBC constructed for $i(A)$ sites, different boundary conditions (linearly independent), represented by the cones in the figure, give rise to different states (linearly independent), and this does not happen for $i(A) - 1$ spins.

that this property is equivalent to the fact that the associated quantum channel eventually reaches full Kraus rank. This is convenient for showing that injectivity is independent of the representation used for both the MPS and the quantum channel.

In this Chapter, we make intensive use of several mathematical techniques developed in the fields of completely positive maps and matrix analysis, especially stochastic matrices. As this could be difficult for a reader with a background in condensed matter, we will try to keep this Chapter as self–contained as possible. Nevertheless, the effort to understand the proofs is quite fruitful, since both the techniques and the obtained results have relevant implications in condensed matter in general, and in the theory of tensor networks in particular, as shown in the following chapters.

Let us start by defining injectivity from a physical point of view:

Definition 8 (Injectivity for MPS) Let $\{|\alpha\rangle \in \mathbb{C}^D\}$ be an orthonormal basis and $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ the Kraus operators defining an MPS. Let us also consider the D^2 states for N particles defined as

$$|\psi_{\alpha\beta}^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \langle\alpha| A_{i_1} \cdots A_{i_N} |\beta\rangle |i_1 \ldots i_N\rangle \qquad (2.1)$$

Then, we say that the MPS is **injective** (with *injectivity length* smaller than or equal to N) if there exists a finite N such that the vector space spanned by the vectors in Eq. 2.1 has dimension D^2, *i.e.* if $\dim \mathrm{span}\left[\{|\psi_{\alpha\beta}^{(N)}\rangle\}\right] = D^2$ (Fig. 2.1). □

We already pointed out in Subsection 1.4.3 that $\mathrm{rank}\,[\rho]^{(N)} \leq D^2, \forall N$. Hence, by Definition 8, an MPS is injective iff there is an N such that $\mathrm{rank}\,[\rho]^{(N)} = D^2$, *i.e.* the maximum rank is reached. In general in any MPS, the properties of the *bulk* are completely determined by the behaviour at the *boundary*[1], which is related to the existance an area law (see [PGVWC07]), *i.e.* that the entanglement between a

[1]This is a condensed matter example of the celebrated Holographic principle [Bou02]. This principle was originally proposed by Gerard 't Hooft and it states, in few words, that the description of a volume of space cabe be thought of as encoded on the boundary of the region.

compact block and the rest of the chain depends on the length of the interaction surface and not on the volume of the region. In injective MPS, this relationship between the properties of the bulk and at the bounday are especially relevant.

We already put forward the concept of injectivity length in Definition 8, but let us define it clearly:

Definition 9 (Injectivity length) An MPS defined by the Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ has **injectivity length** N, if N is the minimal number of sites for which $\operatorname{rank}[\rho]^{(N)} = D^2$. □

Let us now prove a Lemma which connects this property to the injectivity of a linear map. This is obviously the feature which names the property.

Lemma 4 (Injectivity of $\Gamma_N(X)$) *An MPS defined by the Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ is injective iff the linear map $\Gamma_N : \mathcal{M}_D \to (\mathbb{C}^d)^{\otimes N}$ defined by*

$$\Gamma_N(X) = \sum_{i_1,\ldots,i_N=1}^{d} \operatorname{tr}\left[A_{i_1}\cdots A_{i_N} X\right] |i_1 \ldots i_N\rangle \tag{2.2}$$

is injective. □

Proof The proof follows from the decomposition $X = \sum_{\alpha,\beta=1}^{D} X_{\alpha\beta} |\alpha\rangle\langle\beta|$, which transforms Γ_N into

$$\Gamma_N(X) = \sum_{\alpha,\beta=1}^{D} X_{\beta\alpha} |\psi_{\alpha\beta}^{(N)}\rangle$$

where $|\psi_{\alpha\beta}^{(N)}\rangle$ is given in Eq. 2.1. This map is injective iff the vectors $|\psi_{\alpha\beta}^{(N)}\rangle$ are linearly independent which, by Definition 8, proves the Lemma. ■

Let us now show that, once injectivity is reached, this property does not vanish by adding additional particles, *i.e.* if an MPS is injective for N particles, then it also is for $N+1$ particles.

Lemma 5 (Persistence of injectivity) *If Γ_N is injective, then Γ_{N+1} is also injective.* □

Proof The proof can be found in Section 2.5. ■

Lemma 4 is important, since it allows us to connect injectivity to another relevant property of quantum channels: having *eventually full Kraus rank*. We prove below that this is equivalent to injectivity. Let us first start by introducing some notation.

We define $S_N(A) \subseteq \mathcal{M}_D$ as the linear space spanned by all possible products of exactly N Kraus operators, $A_{k_1} A_{k_2} \ldots A_{k_N}$, and denote by $A_k^{(N)}$ the elements of $S_N(A)$. There is a one-to-one correspondence between a quantum channel $\mathcal{E}$ and its Choi–Jamiołkowski matrix τ defined in Lemma 2. It is readily verified that $\operatorname{rank}\left[\tau(\mathcal{E}^N)\right] = \dim\left[S_N(A)\right]$.

Let us now define when a quantum channel has eventually full Kraus rank. Note that the Kraus rank was already defined in Theorem 6.

Definition 10 (Eventually full Kraus rank) A quantum channel $\mathcal{E}$ is said to have **eventually full Kraus rank** if there exists some $N \in \mathbb{N}$ such that $S_N(A) = \mathcal{M}_D$, *i.e.* if $\operatorname{rank}\left[\tau(\mathcal{E}^N)\right] = D^2$. We denote by $i(A)$ the minimum N for which that condition is satisfied. Obviously, if $\mathcal{E}$ fulfills this property, then $S_N(A) = \mathcal{M}_D$ for all $N \geq i(A)$. □

The last part of this Chapter consists in proving that a quantum channel is injective if and only if it eventually has full Kraus rank, and hence that the injectivity length is equal to $i(A)$. This equivalence leads to a characterization of injectivity and injectivity length by means of the calculation of the rank of the Jamiołkowski isomorphism which corresponds to a composition of channels, which is more convenient for several applications.

Lemma 6 (Equivalence between injectivity and eventual full Kraus rank) *Let us consider a quantum channel $\mathcal{E}$ generated by the Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^d$. Then, this quantum channel is injective with injectivity length N iff this has eventually full Kraus rank. Moreover, $i(A) = N$.* □

Proof We have to prove that Γ_N is injective iff $S_N(A) = \mathcal{M}_D$:

$\boxed{\Rightarrow}$

Let us prove this by contradiction by assuming that there exists $X_0 \neq 0$ such that $X_0 \notin S_N(A)$ and the scalar products $\operatorname{tr}\left[A_{i_1} \cdots A_{i_N} X_0\right] = 0$ for all $i_1, \ldots, i_N$. However, this means that $\Gamma_N(X_0) = 0$ and, as $X_0 \neq 0$, then the mapping Γ_N is not injective. This directly proves that $i(A) \leq N$.

$\boxed{\Leftarrow}$

Let us also prove this by contradiction and assume that there exists $X_0 \neq 0$ such that $\Gamma_N(X_0) = 0$. This means that $\operatorname{tr}\left[A_{i_1} \cdots A_{i_N} X_0\right] = 0$ for all $i_1, \ldots, i_N$, but this is none other than the Hilbert–Schmidt scalar product between $A_{i_1} \cdots A_{i_N}$ and $X_0^\dagger$, and this means that this is orthogonal to all components in $S_N(A)$, so $\dim\left[S_N(A)\right] < D^2$. Therefore, $i(A) \geq N$ which, together with the inequality proven above, concludes the Theorem. ■

This Theorem proves that injectivity is equivalent to the fact that the quantum channel eventually reaches full Kraus rank. This connection between the physical interpretation of injectivity and a property of the Kraus rank is very powerful, since the latter is a more convenient approach for proving the results which we will show in the following sections.

Let us remark that both injectivity and full Kraus rank are properties which require gathering spins to be checked. However, it would be relevant for many applications a local characterization of these properties, and this is what we provide in the following Section.

2.3 Strong irreducibility

In this Section, we define the idea of strong irreducibility of a quantum channel (or MPS). This connects directly to the properties of pure finitely correlated states discussed in Subsection 1.4.2, as well as to the canonical form. We will prove here some properties of the MPS, such as that two injective MPS in the thermodynamic limit are either proportional or orthogonal, and the interpretation of the fixed point which appears in the definition of the reduced density operator given in Eq. 1.17. In Section 2.5, we show the equivalence between strong irreducibility and an eventually full Kraus rank, and hence, with injectivity.

Let us start by defining when a quantum channel is strongly irreducible:

Definition 11 (Strong irreducibility) Let $\mathcal{E}(X) = \sum_{i=1}^{d} A_i^\dagger X A_i$ be a completely positive trace preserving map. Then, we say that this quantum channel is **strongly irreducible** if the two following conditions are fulfilled:

1. $\mathcal{E}$ has a unique maximum eigenvalue λ, with $|\lambda| = 1$.
2. The corresponding eigenvector, Λ, is a strictly positive operator, *i.e.* $\Lambda > 0$. □

This definition implies the convergence:

$$\lim_{N\to\infty} \mathcal{E}^N = \mathcal{E}^\infty \tag{2.3}$$

where $\mathcal{E}^\infty(X) := \Lambda \operatorname{tr}[X]$. Note that, as already stated in Section 1.4 , the generalized Frobenius Theorem proven in [EHK78, Theorem 2.5] (see footnote of Lemma 1) ensures that a trace–preserving complete positive map (TPCPM) always has an eigenvalue $\lambda = 1$ with eigenvector $\rho \geq 0$.

For strongly irreducible channels, it was already known [FNW92, Lemma 5.2] that there exists an upper bound for $i(A)$ related to the second eigenvalue λ_2 of $\mathcal{E}$, which is essentially $i(A) \lesssim O(\exp \frac{1}{\lambda_2})$.

Strong irreducibility is obviously equivalent to a unique block in the canonical form of the MPS, as one can deduce from the proof of Theorem 4 where, in addition, also the periodic components are removed (since there is only one eigenvalue with modulus 1). Therefore, the MPS associated with a strongly irreducible quantum channel is a pure finitely correlated state in the thermodynamic limit. These MPS are *weakly dense*, as shown in Theorem 9.

It is also remarkable that strong irreducibility is a *local property*, *i.e.* it is a characteristic of the tensor which can be tested without gathering many sites, as would happen when testing injectivity, or verifying whether a quantum channel eventually reaches full Kraus rank. However, we will prove in Subsection 2.5.1 that the three characteristics are equivalent, so this will provide us with a local characterization for injectivity which is, as pointed above, a many–particle property.

Let us now prove a couple of very interesting properties of TI–MPS associated to a strongly irreducible quantum channel. The first one is related to the orthogonality of these states in the thermodynamic limit:

Theorem 13 (Orthogonality of infinite MPS) *Let* $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ *and* $\{B_i \in \mathcal{M}_D\}_{i=1}^d$ *be two sets of Kraus operators of two strongly irreducible quantum channels and let us assume that they are in the canonical form. If* $|\psi_A^{(N)}\rangle$ *and* $|\psi_B^{(N)}\rangle$ *are the TI–MPS for* N *particles, then one has that*

$$\lim_{N\to\infty} \langle \psi_B^{(N)} | \psi_A^{(N)} \rangle = \begin{cases} e^{iN\theta} & \text{if } A_i = e^{i\theta} X B_i X^\dagger \text{ and } XX^\dagger = \mathbb{1} \\ 0 & \text{otherwise} \end{cases} \tag{2.4}$$

with exponentially small corrections in N *for finite cases.* □

Proof This theorem is a non–trivial consequence of the generalized Frobenius theorem and we provide here a proof based on the proof of [PGWS+08, Lemma 1]. First, let us recall that $\| |\psi_A^{(N)}\rangle \| = \| |\psi_B^{(N)}\rangle \| = 1$ up to exponentially small corrections in N. By adopting the same reasoning followed in calculation of the reduced density matrix from the Kraus operators in Subsection 1.4.3, one can straightforwardly show that

$$\langle \psi_B^{(N)} | \psi_A^{(N)} \rangle = \mathrm{tr}\left[\tilde{\mathbb{E}}^N\right]$$

where $\tilde{\mathbb{E}} = \sum_i A_i \otimes \bar{B}_i$. In addition, by following the same argumentation exposed in calculation of expectation values in Subsection 1.4.3, one can easily see that the spectrum of $\tilde{\mathbb{E}}$ is the same as that of the mapping $\tilde{\mathcal{E}}(X) = \sum_i A_i X B_i^\dagger$. Therefore, the goal is to prove that $|\lambda_k| < 1$ for all eigenvalues of $\tilde{\mathbb{E}}$. Note that one cannot adjust the eigenvalues of the mapping, since we are assuming that both states are in the canonical form and that there are no additional freedoms.

Let us consider the eigenvalue equation given by

$$\sum_{i=1}^d A_i X B_i^\dagger = \lambda X$$

then, denoting by Λ_B the fixed point $\mathcal{E}(\Lambda_B) = \sum_i B_i^\dagger \Lambda_B B_i = \Lambda_B$, we get

$$\begin{aligned} |\lambda| |\mathrm{tr}\left[X\Lambda_B X^\dagger\right]| &= \left| \sum_i \mathrm{tr}\left[A_i X B_i^\dagger \Lambda_B X^\dagger\right] \right| \\ &\leq \left| \sum_i \mathrm{tr}\left[X B_i^\dagger \Lambda_B B_i X^\dagger\right] \right|^{\frac{1}{2}} \left| \sum_i \mathrm{tr}\left[A_i^\dagger X \Lambda_B X^\dagger A_i\right] \right|^{\frac{1}{2}} = |\mathrm{tr}\left[X\Lambda_B X^\dagger\right]| \end{aligned}$$

where we have used the eigenvalue equation in the first equality; the Cauchy–Schwarz inequality for the Hilbert–Schmidt scalar product with weight Λ_B in the inequality; and the relations $\sum_i A_i A_i^\dagger = \mathbb{1}$ and $\sum_i B_i^\dagger \Lambda_B B_i = \Lambda_B$, coming from the canonical form, in the last equality.

If $|\lambda| = 1$, then the Cauchy–Schwarz inequality turns into an equality, which means that the vectors are parallel, so $\alpha \Lambda_B^{\frac{1}{2}} X^\dagger A_i = \Lambda_B^{\frac{1}{2}} B_i X^\dagger$. By multiplying the expression by the hermitian conjugate, taking traces and using again the gauge

condition for A_i and the fixed point condition for B_i, one straightforwardly shows that $|\alpha| = 1$, so $\alpha = e^{-i\theta}$.

As the Kraus operators describe strongly irreducible quantum channels, Λ_B is invertible, so

$$e^{-i\theta} X^\dagger A_i = B_i X^\dagger \Rightarrow \sum_{i=1}^{d} B_i X^\dagger X B_i^\dagger = X^\dagger X$$

Therefore, $X^\dagger X$ is a fixed point corresponding to the eigenvalue of modulus 1, but strong irreducibility implies that $\mathbb{1}$ is the only fixed point. Consequently, $X^\dagger X = \mathbb{1}$, which means that X is unitary, and hence $A_i = e^{i\theta} X B_i X^\dagger$. This means that $|\psi_A^{(N)}\rangle$ and $|\psi_B^{(N)}\rangle$ are equal up to a global phase.

If $|\lambda| < 1$, then the scalar product is exponentially suppressed with the length of the chain, which concludes the proof. ∎

This Theorem has the following Lemma as a corollary:

Lemma 7 (Quasi-orthogonality of general MPS) *Let us now consider a TI–MPS of the form* $|\psi^{(N)}\rangle = \sum_{r=1}^{m} \mu_r |\psi_r^{(N)}\rangle$ *with all* $|\psi_r^{(N)}\rangle$ *being different TI–MPS associated to strongly irreducible quantum channels. Then, for all* n*, there is a constant* $c > 0$ *such that the reduced density matrix of* n *sites,* $\rho^{(n)}$*, is in trace distance* $\exp[-c(N-n)]$ *close to* $\bigoplus_r |\mu_r|^2 \rho_r^{(n)}$*, where* $\rho_r^{(n)}$ *are the reduced density matrices for* n *particles of* $|\psi_r^{(N)}\rangle$*.* □

Proof This Lemma straightforwardly follows from Theorem 13. We only need to construct $|\psi^{(N)}\rangle\langle\psi^{(N)}|$, trace out the complementary region and use the fact that N is very large and that each $|\psi_r^{(N)}\rangle$ corresponds to a different TI–MPS. Then, Theorem 13 ensures the orthogonality of $|\psi_r^{(N)}\rangle$ and the Lemma follows. ∎

Let us now point out the physical interpretation of the fixed point of the complete positive map in terms of the eigenvalues of the reduce density matrix:

Theorem 14 (Physical interpretation of Λ) *Let* $|\psi^{(N)}\rangle$ *be a TI–MPS associated to a strongly irreducible quantum channel and let us assume that this is in the canonical form. If* $\rho^{(n)}$ *is the reduced density matrix for a block of* n *particles in the thermodynamic limit, then*

$$\operatorname{spec} \lim_{n\to\infty} \rho^{(n)} = \operatorname{spec} \Lambda \otimes \Lambda \tag{2.5}$$

i.e. Λ *is related to the eigenvalues of* $\rho^{(n)}$*.* □

Proof Let us start from Eq. 1.17 and use the eigenvector decomposition $\Lambda = \sum_{\alpha=1}^{D} \Lambda_\alpha |\alpha\rangle\langle\alpha|$, then

$$\rho^{(n)} = \sum_{\alpha\beta} \Lambda_\alpha |\psi_{\alpha\beta}^{(N)}\rangle\langle\psi_{\alpha\beta}^{(N)}|$$

Let us compute the scalar product $\langle\psi^{(N)}_{\alpha\beta}|\psi^{(N)}_{\gamma\delta}\rangle$

$$\begin{aligned}\langle\psi^{(N)}_{\alpha\beta}|\psi^{(N)}_{\gamma\delta}\rangle &= \sum_{i_1,\dots,i_n=1}^{d} \langle\alpha|\,\bar{A}_{i_1}\cdots\bar{A}_{i_n}\,|\beta\rangle\langle\gamma|\,A_{i_1}\cdots A_{i_n}\,|\delta\rangle \\ &= \sum_{i_1,\dots,i_n=1}^{d} \mathrm{tr}\left[(A_{i_1}\otimes\bar{A}_{i_1})\cdots(A_{i_n}\otimes\bar{A}_{i_n})\,|\delta\,\beta\rangle\langle\gamma\,\alpha|\,\right] \\ &= \mathrm{tr}\left[\mathbb{E}^n_{\mathbb{1}}\,|\delta\,\beta\rangle\langle\gamma\,\alpha|\,\right] \xrightarrow{n\gg 1} \mathrm{tr}\left[\,|\mathbb{1}\rangle\langle\Lambda|\;|\delta\,\beta\rangle\langle\gamma\,\alpha|\,\right] \\ &= \Lambda_\beta\delta_{\gamma\alpha}\delta_{\delta\beta}\end{aligned}$$

Therefore, the states $|\psi^{(N)}_{\alpha\beta}\rangle$ are orthogonal, but not orthonormal. So by replacing the norms, one obtains

$$\rho^{(n)} = \sum_{\alpha\beta}\Lambda_\alpha\Lambda_\beta\,|\tilde{\psi}^{(N)}_{\alpha\beta}\rangle\langle\tilde{\psi}^{(N)}_{\alpha\beta}|$$

where $|\tilde{\psi}^{(N)}_{\alpha\beta}\rangle = \frac{1}{\sqrt{\langle\psi^{(N)}_{\alpha\beta}|\psi^{(N)}_{\alpha\beta}\rangle}}\,|\psi^{(N)}_{\alpha\beta}\rangle$ are normalized and the Theorem follows. ∎

2.4 Classical channels and Wielandt's inequality

In this Section, we explain the concept of classical channels as a mathematical representation of a Markov process [Sen06]. We also show the natural description of these classical channels in terms of stochastic matrices [HJ91] and use this to enunciate a very beautiful theorem, which provides an upper bound for the number of times that a classical channel must be applied to have a non–trivial probability of being in any possible classical state of the system with a non–zero probability. This result, known as Wielandt's inequality [Wie50], has the special feature that the bound does not depend on the specific characteristics of the channel, but only on its dimension.

Let us start with a brief explanation about classical channels (a nice extension can be found in [NC00, Chapter 8]). The aim is to obtain the mathematical framework which describes the evolution of classical systems provided with a Markovian approximation, *i.e.* the evolution is memoryless, so only depends on the last step.

Let us consider a classical system with χ different states $\{\omega_i \in \Omega\}_{i=1}^{\chi}$ and a classical probability p_i of being in ω_i. Therefore, the information about the state can be summarized in a χ-dimensional vector of probabilities $\boldsymbol{p}$ such that $\sum_{i=1}^{\chi} p_i = 1$.

Once the classical system is defined, let us consider the evolution of such a system assuming a Markovian approximation. The evolution, as explained for quantum channels in Subsection 1.4.1, is modelled by a linear map due to the causality. Therefore, we want to describe the process as:

$$\boldsymbol{p}_2 = \mathbb{M}\,\boldsymbol{p}_1 \qquad (2.6)$$

The matrix $\mathbb{M}$ is an evolution operator, which obviously must fulfil several conditions in order to be called **classical channel**. The entry $\mathbb{M}_{ij}$ of this matrix is the probability of the state to end in state ω_i, provided that the system was initially in state ω_j. Therefore, the entries must be positive reals smaller than or equal to 1, $0 \leq \mathbb{M}_{ij} \leq 1$. Furthermore, $\boldsymbol{p}_2$ is also a probability vector and the entries must add up to 1, which means that each column of $\mathbb{M}$ must also add up to 1. These matrices are called **(left) stochastic matrices** and there are very powerful mathematical techniques developed for them.

Let us now introduce a couple of definitions. The first one describes when a classical channel is *irreducible* (see [HJ91, Definition 6.2.21]) and the second one, defines the notion of *primitivity* (see [HJ91, Definition 8.5.0]).

Definition 12 (Irreducible classical channel) Let us consider a classical channel $\mathbb{M} \in \mathcal{M}_d$, $d > 1$, then we say that this is **reducible** if there are a permutation matrix $P \in \mathcal{M}_d$ and an integer $1 \leq r \leq d-1$ such that

$$P\,\mathbb{M}\,P^{\dagger} = \begin{pmatrix} A & B \\ 0 & C \end{pmatrix}$$

where $B \in \mathcal{M}_r$, $D \in \mathcal{M}_{n-r}$ and $C \in \mathcal{M}_{r,n-r}$. Otherwise, the classical channel is said to be **irreducible**. □

We would like to highlight the apparent similarity between this Definition and the uniqueness of the block in the canonical form defined in Section 1.2. Furthermore, we also proved in Section 2.3 that this uniqueness of the block was equivalent to the quantum channel's strong irreducibility. This is the reason why we chose this name for the quantum case.

Let us now define primitivity, a notion firstly introduced by Frobenius in 1912:

Definition 13 (Primitive classical channel) Let us consider a classical channel $\mathbb{M} \in \mathcal{M}_d$, then we say that this is **primitive** if it is irreducible and has only one eigenvalue of maximum modulus. □

This property is also deeply connected to strong irreducibility for quantum channels. However, the connection with the asymptotic behaviour of the system is more interesting after applying the classical channel many times. The state after applying the channel k times is given by $\boldsymbol{p}_{k+1} = \mathbb{M}^k\,\boldsymbol{p}_1$, so the relevant features are the powers of the stochastic matrices. The following Theorem provides the connection between such powers and primitivity:

Theorem 15 (Primitivity implies that $\mathbb{M}^k > 0$) *Let $\mathbb{M} \in \mathcal{M}_d$ be a classical channel ($\mathbb{M} \geq 0$), then $\mathbb{M}$ is primitive iff there exists a finite integer $k \geq 1$ such that $\mathbb{M}^k > 0$. The minimum power k fulfilling this condition is called **classical index of primitivity** $p(\mathbb{M})$.* □

Proof See the proof in [HJ91, Theorem 8.5.2]. ■

The existence of an integer k such that $\mathbb{M}^k > 0$ has a very interesting physical meaning. If the matrix is strictly positive, it means that there is a non–trivial probability $p_i > 0$ of finding the system in every possible state ω_i, independently of the initial state, *i.e.* of the initial conditions. Therefore, *primitivity* is a property which is tightly related to *ergodicity*.

To conclude this summary about classical channels, let us enunciate the celebrated Perron–Frobenius theorem:

Theorem 16 (Perron–Frobenius theorem) *Let $\mathbb{M} \in \mathcal{M}_d$ be a primitive classical channel, then the following statements hold:*

- *There is a positive eigenvalue of $\mathbb{M}$, $q > 0$, called **Perron root** or **Perron–Frobenius eigenvalue**, such that the rest of the eigenvalues λ_i are in modulus smaller than q, i.e. $|\lambda_i| < q$, $\forall i$. This means that the spectral radius $\rho(\mathbb{M}) = q$.*
- *The eigenspace associated to the eigenvalue q is one–dimensional, with right eigenvector $\boldsymbol{\pi}$.*
- *The components of $\boldsymbol{\pi}$ are strictly positive.*
- *The Perron–Frobenius eigenvalue fulfils the inequality*

$$\min_i \sum_j \mathbb{M}_{ij} \leq q \leq \max_i \sum_j \mathbb{M}_{ij}$$

*The eigenvector $\boldsymbol{\pi}$ is called **stochastic eigenvector** or **Frobenius eigenvector**.* □

Let us connect this with the previous discussion. We can always choose a primitive channel to have a nondegenerate maximal eigenvalue of modulus 1. Therefore,

$$\lim_{k\to\infty} (\mathbb{M}^k)_{ij} = \boldsymbol{\pi}_j$$

which means that the long–term probability of being in a state ω_j is independent of the initial state. But this is nothing but the Ergodic Theorem [Pet89, Chapter 2].

Now that the main characteristics and properties of classical channels are described, let us answer the question proposed in the introduction of this Section: is there any bound, independent of the specific entries of the primitive channel, for the k defined in Theorem 15, *i.e.* for the minimum k, such that $\mathbb{M}^k > 0$? The answer was given by the celebrated result by H. Wielandt [Wie50], which provides a sharp upper bound for the number of times that the classical channel has to be applied.

Theorem 17 (Wielandt's inequality for stochastic matrices) *If $\mathbb{M} \in \mathcal{M}_d$ is a stochastic matrix (classical channel) such that $\mathbb{M} \geq 0$, then $\mathbb{M}$ is primitive iff $\mathbb{M}^{d^2-2d+2} > 0$.* □

Proof A nice proof of this Theorem can be found in [HJ91, Theorem 8.5.9]. ■

Wielandt proved that this result is sharp, by providing an example which requires exactly this number of steps to be positive. The classical channel that he proposed was

$$\mathbb{M} = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 1 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

If $d = \dim \mathbb{M}$, then $\mathbb{M}^k > 0$ only when $k \geq d^2 - 2d + 2$. Notwithstanding, one can correctly argue that this matrix is not stochastic, and this is because this was constructed as the adjacent matrix of a graph. However, the matrix can be normalized column by column, resulting in no change of the bound.

Wielandt's inequality has a multitude of applications in classical systems, especially through the connections with graph theory [Ram05]. Furthermore, by testing whether the inequality $\mathbb{M}^{d^2-2d+1} > 0$ holds, one obtains a simple method to check primitivity in a classical channel.

2.5 Quantum Wielandt's inequality

In this Section, we are interested in finding an equivalent result to the classical Wielandt's inequality shown in Section 2.4 for quantum channels. The question is not only mathematically natural, due to the parallelisms between classical and quantum channels that we exposed previously, but also physically relevant, due to the many results on MPS and quantum channels which depend on the existence of such an inequality.

We have structured this Section in the following way: we first introduce some notation and the extension of the concept of primitivity to quantum channels; then, we prove the equivalence among injectivity, eventually full Kraus rank, strong irreducibility and primitivity; we make use of this in order to prove a quantum version of Wielandt's inequality; finally, we prove a *dichotomy theorem* for the zero–error capacity of quantum channels, which is a very nice application of the quantum Wielandt's inequality. For other results see Chapter 9, especially Section 9.2.

Let us first introduce some additional notation before defining *primitivity*. We define $H_n(A, \varphi) := S_n(A) |\varphi\rangle \subseteq \mathbb{C}^D$ as the space spanned by vectors $A_{k_1} A_{k_2} \dots A_{k_n} |\varphi\rangle$, where $|\varphi\rangle \in \mathbb{C}^D$. That is, $\operatorname{rank}[\mathcal{E}^n(|\varphi\rangle\langle\varphi|)] = \dim\big[H_n(A, \varphi)\big]$.

Definition 14 (Primitive quantum channel) A quantum channel $\mathcal{E}$ is called **primitive** if there exists some $n \in \mathbb{N}$ such that for all $0 \neq |\varphi\rangle \in \mathbb{C}^D$, $H_n(A, \varphi) = \mathbb{C}^D$; in other words, if for every input density operator ρ, the output $\mathcal{E}^n(\rho)$ obtained after n applications of the channel has full rank. We denote by $q(\mathcal{E})$ the minimum n for which that condition is fulfilled, and we call it **(quantum) index of primitivity**.□

This is the natural extension of classical primitivity, since we are defining the existence of an $n \in \mathbb{N}$ such that, after the n-fold application of the quantum channel, every positive semidefinite operator is mapped onto a strictly positive operator.

Note that, if $\mathcal{E}$ is primitive, then $\mathcal{E}^m$ is also primitive for every $m \in \mathbb{N}$, so we have $H_n(A, \varphi) = \mathbb{C}^D$ for all $n \geq q(\mathcal{E})$.

2.5.1 Primitivity, eventually full Kraus rank and strong irreducibility are equivalent

In this Subsection, we prove the equivalence among primitivity, eventually full Kraus rank and strong irreducibility. This opens a lot of possibilities, since it means that all the characterizations shown in this Section are equivalent, and equivalent to injectivity by means of Lemma 6. This is the reason why we will refer to all these properties as injectivity in the rest of this work.

Let us start with the goal of this Subsection. We work here with quantum channels with any of the following properties:

(a) The quantum channel is primitive;

(b) The quantum channel has eventually full Kraus rank;

(c) The quantum channel is strongly irreducible.

Our first simple observation is that, if a quantum channel $\mathcal{E}$ eventually has full Kraus rank, then this implies that $\mathcal{E}$ is primitive, or stated quantitatively:

Lemma 8 (Full Kraus rank implies primitivity) *Let us consider a quantum channel $\mathcal{E}$ generated by the Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ which eventually reaches full Kraus rank. Then, $\mathcal{E}$ is primitive, and $q(\mathcal{E}) \leq i(A)$, where $q(\mathcal{E})$ is the quantum index of primitivity and $i(A)$ is the injectivity length.* □

Proof Take any $n \geq i(A)$. Then, by the definition of $i(A)$, the Choi–Jamiołkowski matrix $\tau(\mathcal{E}^n)$ has full rank. The channel can be written for any normalized vector $|\varphi\rangle \in \mathbb{C}$ as $\mathcal{E}^n(\,|\varphi\rangle\langle\varphi|\,) = \mathrm{tr}_1[\tau(\mathcal{E}^n) \cdot (\,|\bar{\varphi}\rangle\langle\bar{\varphi}| \otimes \mathbb{1})]$ [BL07, Section 5.3], or equivalently

$$\mathcal{E}^n(\,|\varphi\rangle\langle\varphi|\,) = (\langle\bar{\varphi}| \otimes \mathbb{1})\tau(\mathcal{E}^n)(\,|\bar{\varphi}\rangle \otimes \mathbb{1})$$

which also has full rank. ■

Before continuing the analysis of the relationships among the three properties above in the quantum context, let us connect them to the classical notion of primitivity. Given a stochastic matrix $\mathbb{M} = (m_{ij})$, let us consider the map $\mathcal{E}$ defined by the Kraus operators $A_{i,j} = \sqrt{m_{j,i}}\,|i\rangle\langle j|$. $\mathcal{E}$ has the property that for an operator ρ with entries $\rho_{i,j} = \delta_{i,j}p_i \geq 0$, $\rho' := \mathcal{E}(\rho)$ is diagonal with $\rho'_{i,j} = \delta_{i,j}p'_i$, with $\boldsymbol{p}' = \mathbb{M}\boldsymbol{p}$. Thus, $\mathcal{E}$ implements the stochastic map $\mathbb{M}$, *i.e.* the quantum channel reduces to

the classical channel when applied to diagonal density operators. Note that d is the number of positive entries of the stochastic matrix in the classical case, so the general quantum bound applied to a classical channel is worse than the classical one.

Let us consider a stochastic map (classical channel) $\mathbb{M}$, assume that this is primitive and denote by $p(\mathbb{M})$ its **classical index of primitivity**. Then,

Lemma 9 (Equivalence for classical channels) *Let us consider a primitive stochastic map $\mathbb{M}$ and construct its associated quantum channel $\mathcal{E}$ with Kraus operators A defined as above. Then, $\mathcal{E}$ is also primitive and the equality $q(\mathcal{E}) = p(\mathbb{M}) = i(A)$ holds.* □

Proof It is clear that $p(\mathbb{M}) \leq q(\mathcal{E})$ because $m_{i,j} = 0 \Rightarrow A_{i,j} = 0$ and we proved in Lemma 8 that $q(\mathcal{E}) \leq i(A)$. In order to show that $i(A) \leq p(\mathbb{M})$, we define $\tilde{A}_{i,j} = \sqrt{m_{j,i}} A_{i,j}$, where $A_{i,j}$ are the Kraus operators of the associated quantum channel, and $n = p(\mathbb{M}) - 1$, and take

$$\sum_{k_1,\ldots,k_n=1}^{D} \tilde{A}_{i,k_1}\tilde{A}_{k_1,k_2}\cdots\tilde{A}_{k_n,j}\,|i\rangle\langle j| = (A^{p(\mathbb{M})})_{i,j}\,|i\rangle\langle j| \neq 0.$$

Thus, $|i\rangle\langle j| \in S_{p(\mathbb{M})}(A)$ for all i, j. ■

We note that $q(\mathcal{E})$ is different from $i(A)$ in the general case. To see that, let us consider an example with $d = 3$, $D = 2$, and take as Kraus operators $\sigma_\alpha/\sqrt{3}$, where $\alpha = x, y, z$ labels the three Pauli matrices. Here $q(\mathcal{E}) = 1 < i(A) = 2$.

However, the following proposition shows that $i(A)$ is finite whenever $q(\mathcal{E})$ is. In fact, all three definitions above are equivalent.

Theorem 18 (Equivalence for quantum channels) *Given a quantum channel $\mathcal{E}$, the following statements are equivalent:*

(a) $\mathcal{E}$ is primitive;

(b) $\mathcal{E}$ has eventually full Kraus rank;

(c) $\mathcal{E}$ is strongly irreducible. □

Proof We denote by $\Lambda \geq 0$ an eigenoperator of $\mathcal{E}$ corresponding to the eigenvalue $\lambda = 1$.

(b) ⇒ (a)

This implication is given by Lemma 8.

(a) ⇒ (c)

We prove it by contradiction. Let us assume that $\mathcal{E}$ is not strongly irreducible. Then, we must have at least one of the following cases: (i) Λ is not full–rank; (ii) there exists another eigenoperator, Λ', corresponding to $\lambda = 1$; (iii) there is another eigenvalue, λ', with $|\lambda'| = 1$.

Since for all $n \in \mathbb{N}$, $\mathcal{E}^n(\Lambda) = \Lambda$, (i) automatically implies that $\mathcal{E}$ is not primitive. Besides, if we have (ii), choosing $\epsilon^{-1} = \max[\mathrm{spec}(\Lambda^{-1/2}\Lambda'\Lambda^{-1/2})]$ we have that $\tilde{\Lambda} = \Lambda - \epsilon\Lambda' \geq 0$ is not full–rank and thus we are back in (i). Moreover, it is proven in [FNW92, Proposition 3.3] that, if (i) and (ii) do not hold, the other possible eigenvalues of modulus 1 are the p-th roots of unity for $\mathbb{N} \ni p \leq D^2$. Therefore, we have (ii) for $\mathcal{E}^p$, and thus $\mathcal{E}^p$ cannot be primitive.

(c) ⇒ (b)

This implication can be deduced from [FNW92, Lemma 5.2], but we include a proof here for completeness. We prove it by contradiction. Let us assume that $\mathcal{E}$ is (i) strongly irreducible, but (ii) never gets full Kraus rank. If we have (i), then Λ is full–rank and Eq. 2.3 is fulfilled. Because of (ii), for all $n \in \mathbb{N}$ and $A_k^{(n)} \in S_n(A)$, there exists some $B_n \neq 0$ such that $\mathrm{tr}\left[A_k^{(n)} B_n\right] = 0$, $\forall k$. Thus,

$$\begin{aligned}\left|\mathrm{tr}\left[\Lambda B_n^\dagger B_n\right]\right| &= \left|\sum_{k_1,\ldots,k_n} \left|\mathrm{tr}\left[A_{k_1}\cdots A_{k_n} B_n\right]\right|^2 - \mathrm{tr}\left[\Lambda B_n^\dagger B_n\right]\right| \\ &= \left|\mathrm{tr}\left[\Omega(\mathcal{E}^n \otimes \mathbb{1})(\tilde{B}_n \Omega \tilde{B}_n^\dagger)\right] - \mathrm{tr}\left[\Omega(\mathcal{E}^\infty \otimes \mathbb{1})(\tilde{B}_n \Omega \tilde{B}_n^\dagger)\right]\right| \\ &\leq c_n \|\Omega\|_\infty \mathrm{tr}\left[\tilde{B}_n \Omega \tilde{B}_n^\dagger\right] = D c_n \mathrm{tr}\left[B_n^\dagger B_n\right]\end{aligned}$$

where $\tilde{B}_n = B_n \otimes \mathbb{1}$ and $\lim_n c_n = 0$. If Λ were full rank, then for all $X \geq 0$ one would have:

$$\mathrm{tr}\left[\Lambda X\right] \geq \frac{1}{\|\Lambda^{-1}\|_\infty} \mathrm{tr}\left[X\right]$$

where $\|\cdot\|_\infty$ is the operator norm, and we obtain a contradiction. ∎

As a consequence of Theorem 18 , we obtain that primitivity of a quantum channel can be decided by observing its spectral properties. In fact, this is the precise quantum analogue of the classical result that a stochastic matrix is primitive iff it has a unique eigenvalue of maximum modulus and a positive definite fixed point (cf. [HJ91]).

2.5.2 Quantum Wielandt's inequality

In this Subsection, the quantum extension of Wielandt's inequality is finally proven. In order to reach this inequality, which involves bounds for $q(\mathcal{E})$ and $i(A)$, we require some preliminary lemmas:

Lemma 10 (Bound to obtain a non–zero trace) *Let $\mathcal{E}$ be a primitive quantum channel on $\mathcal{M}_D$ with d Kraus operators $\{A_i\}$. Then, there is a $A^{(n)} \in S_n(A)$ with $n \leq D^2 - d + 1$ such that* $\mathrm{tr}\left[A^{(n)}\right] \neq 0$. □

PROOF Let us denote by $T_n(A)$ the span of all $S_m(A)$ with $m \leq n$. We just have to show that

(*) for any $n \in \mathbb{N}$, if $\dim T_n(A) < D^2$, then $\dim T_{n+1}(A) > \dim T_n(A)$.

Since $\dim T_1(A) = d$, we obtain by iteration that $T_{D^2-d+1} = \mathcal{M}_D$. This implies that a linear combination of the elements of $S_n(A)$ with various $n \leq D^2 - d + 1$ must be equal to the identity and thus, at least one of the elements must have non–zero trace.

In order to prove (*), we note that $T_n(A) \subseteq T_{n+1}(A)$ by definition. If they would be equal, then $T_m(A) = T_n(A)$ for all $m > n$. Thus, $\dim T_n(A) = D^2$ since the map $\mathcal{E}$ would not be primitive otherwise. ■

Lemma 11 (Bound for Kraus with non–zero eigenvalue) *Let $\mathcal{E}$ be a primitive quantum channel such that $A_1 |\varphi\rangle = \mu |\varphi\rangle$, with $\mu \neq 0$ and $\langle\varphi|\varphi\rangle = 1$. Then,*

(a) $H_{D-1}(A, \varphi) = \mathbb{C}^D$.

(b) If A_1 is not invertible, then for all $|\psi\rangle \in \mathbb{C}^D$, $|\varphi\rangle\langle\psi| \in S_{D^2-D+1}(A)$; □

PROOF Let us analyse both cases:

(a)

We define $K_n(A, \varphi)$ as the span of all $H_m(A, \varphi)$ with $m \leq n$. If $\dim K_n(A, \varphi) < D$, then $\dim K_{n+1}(A, \varphi) > \dim K_n(A, \varphi)$, since otherwise the map would not be primitive. Thus, $K_{D-1}(A, \varphi) = \mathbb{C}^D$. That is, for all $|\phi\rangle \in \mathbb{C}^D$, there exist matrices $A^{(n)} \in S_n(A)$, $n \leq D - 1$, such that (with $A^{(0)} \propto \mathbb{1}$)

$$|\phi\rangle = \sum_{n=0}^{D-1} A^{(n)} |\varphi\rangle = \sum_{n=0}^{D-1} A^{(n)} \frac{A_1^{D-k_n}}{\mu^{D-k_n}} |\varphi\rangle$$

and thus, $|\phi\rangle \in H_{D-1}(A, \varphi)$.

(b)

We write A_1 in the Jordan canonical form and divide it into two blocks. The first one, of size $\tilde{D} \times \tilde{D}$, consists of all Jordan blocks corresponding to non–zero eigenvalues, whereas the second one contains all those corresponding to zero eigenvalues. We denote by P the projector onto the subspace where the first block is

supported and by $r \leq D - \tilde{D}$ the size of the largest Jordan block corresponding to a zero eigenvalue. We have for every power r that:

$$A_1 P = P A_1, \quad A_1^r = A_1^r P. \tag{2.7}$$

We define $R_n(A) = PS_n(A)$ and show that $R_{D\tilde{D}}(A) = \mathcal{M}_{\tilde{D}\times D}$. For all $n \in \mathbb{N}$, $\dim R_{n+1}(A) \geq \dim R_n(A)$. The reason is that for any linearly independent set of matrices $A_k^{(n)} \in R_n(A)$, $A_1 A_k^{(n)} \in R_{n+1}(A)$ are also linearly independent, given that A_1 is invertible on its range. By following the reasoning of [PGVWC07, Appendix A] we get that, if $\dim R_{n+1}(A) = \dim R_n(A) =: D'$, then $\dim R_m(A) = D'$ for all $m > n$, which is incompatible with $\mathcal{E}$ being primitive unless $D' = \tilde{D}D$. Thus, for all $|\psi\rangle \in \mathbb{C}^D$, there exists $A \in S_{\tilde{D}D}$ with $|\varphi\rangle\langle\psi| = PA = A_1^r PA/\mu^r = A_1^r A/\mu^r = A' \in S_{\tilde{D}D+r}$. By using that $\tilde{D} \leq D - r$ and that $r \geq 1$ (since A_1 is supposed not to be invertible) we get $\tilde{D}D + r \leq D^2 - D + 1$, which concludes the proof. ∎

We have now the necessary tools to prove our main result.

Theorem 19 (Quantum Wielandt's inequality) *Let $\mathcal{E}$ be a primitive quantum channel on $\mathcal{M}_D$ with d Kraus operators. Then $q(\mathcal{E}) \leq i(A)$ and*

1. *if the span of Kraus operators $S_1(A)$ contains an **invertible element**, then $i(A) \leq D^2 - d + 1$,*
2. ***in general** $i(A) \leq (D^2 - d + 1)D^2$,*
3. *if the span of Kraus operators $S_1(A)$ contains a non–invertible element with at least **one non–zero eigenvalue**, then $i(A) \leq D^2$.* □

Proof The inequality $q(\mathcal{E}) \leq i(A)$ was already shown in Lemma 8, so let us prove the bounds.

1. If there is an invertible element, then it follows from [PGVWC07, Appendix A, Proposition 2] that $\dim S_{n+1}(A) > \dim S_n(A)$ until the full matrix space $\mathcal{M}_D$ is spanned and thus $i(A) \leq D^2 - d + 1$.

2. Let us denote by $\{A_k^{(n)}\}$ the Kraus operators of $\mathcal{E}^n$. According to Lemma 10, there is $n \leq D^2 - d + 1$ such that one of them, say $A_1^{(n)}$, has non–zero trace, and hence there exists $|\varphi\rangle \neq 0$ such that $A_1^{(n)}|\varphi\rangle = \mu|\varphi\rangle$ with $\mu \neq 0$. If $A_1^{(n)}$ is invertible, then 2. is implied by 1., so we assume that it is not invertible. According to Lemma 11(b), for all $|\psi\rangle$ and $|\chi\rangle \in \mathbb{C}^D$, we have $|\varphi\rangle\langle\psi| \in S_{D^2-D+1}(A^{(n)})$; and according to Lemma 11(a), with $D-1$ additional steps, any $|\chi\rangle \in \mathbb{C}^D$ can be generated, so $|\chi\rangle\langle\psi| \in S_{D^2}(A^{(n)}) = S_{nD^2}(A)$. This implies that $S_{nD^2}(A) = \mathcal{M}_D$, from which the general bound follows.

3. The argument which proves 3. is completely analogous. The main difference is that, in order to guarantee the existence of a Kraus operator with non–zero eigenvalue, we have to apply Lemma 10 for the general case 2. and to take the n–th power of the quantum channel for some $n \leq D^2 - d + 1$. ∎

We do not know whether, or in which cases, our bounds are sharp. A simple lower bound to $i(A)$ comes from the examples, showing that the classical Wielandt's inequality is sharp. In these cases $q(\mathcal{E}) = i(A) = D^2 - 2D + 2$. An upper bound that goes beyond this value is given by the next example.

Example 5 Let us consider the completely positive map described by the following Kraus operators $A_i \in \mathcal{M}_D$: $A_0 = \sum_{i=0}^{D-1} |i+1\rangle\langle i|$ and $A_1 = |1\rangle\langle D-1|$, with $|D\rangle = |0\rangle$. In this case, $i(A) = D^2 - D$, which is larger than the bound appearing in Wielandt's classical inequality whenever $D > 2$.

Let us prove this bound. Consider the case $D > 2$, since $D = 2$ is readily verifiable by inspection. Then $A_1^2 = 0$ and $A_1 A_0^k A_1 = A_1 \delta_{k,D-2}$. Therefore,

$$S_N(A) = \mathrm{span}\{A_0^N, A_0^k A_1 A_0^l\}$$

where $k, l = 0, \ldots, D-1$ fulfil the additional constraint that

$$k + l + 1 + n(D-1) + mD = N \tag{2.8}$$

for some $n, m \in \mathbb{N}_0$. The additional constraint comes from the fact that A_1 can stem from $A_1 A_0^{D-2} A_1$ or $A_1 A_0^{D-2} A_1 A_0^{D-2} A_1$ etc. which is a monomial of degree $1 + n(D-1)$. The fact that $A_0^{mD} = \mathbb{1}$ is taken care of by the additional factor mD. Now assume that $N = D(D-1) - 1$. Let us upper bound the number of linearly independent operators in $S_N(A)$. Clearly, for every chosen n and k, we get that l and m are fixed by the additional constraint. For $n = D-1$, the range of k is restricted to $k = 0, \ldots, D-3$ by Eq. 2.8. So we have at most $(D-2) + (D-1)D + 1 = D^2 - 1$ independent elements which cannot span the entire matrix algebra. Thus, $i(A) \geq D^2 - D$ (if the map is primitive). That this bound is sharp, and the map actually primitive, is seen by noting that, for $N = D^2 - D$, the constraint in Eq. 2.8 allows us to freely choose k and l, by adjusting n and m. However, then $A_0^k A_1 A_0^l$ runs through all matrix units which span the entire matrix algebra. □

We also note that, for small dimension $D = 2, 3$, there is always an element in $S_1(A)$ which has a non–zero eigenvalue. In other words, in these cases the first bound in Theorem 19 never applies in the absence of any of the other bounds. The fact that $S_1(A)$ has this property for $D = 2, 3$ stems from the classification of nilpotent subspaces [Fas97].

Let us assume that $S_1(A)$ would be a nilpotent subspace within the space of $D \times D$ matrices. Then, for $D = 2$, its dimension would have to be 1, so it could

not arise from the Kraus operators of a quantum channel. Similarly, for $D = 3$ there are (up to similarity transformations) two types of nilpotent subspaces [Fas97] with $d > 1$: one of dimension $d = 3$, the space of upper-triangular matrices, whose structure does not allow the trace-preserving property, and one of dimension $d = 2$ which only leads to quantum channels having a (in modulus) degenerate largest eigenvalue. Hence, if $S_1(A)$ is generated by the Kraus operators of a primitive quantum channel, then it cannot be nilpotent if $D = 2, 3$.

It is remarkable the fact that the injective TI–MPS with polynomial upper bound for the injectivity length are a set of measure zero, so if any random state is picked up from the set of injective TI–MPS, this state is going to be *generic* (see Definition 27), *i.e.* it reaches injectivity after gathering the minimal possible number of spins.

2.5.3 An application: zero-error capacity

Let us now point up in this Subsection an interesting application of the quantum Wielandt's inequality: a dichotomy theorem for the zero–error capacity of a quantum channel. The zero–error capacity C_0 of a noisy classical channel was already defined by Shannon in [Sha56] as follows:

Definition 15 (Zero–error capacity) The **zero–error capacity** C_0 of a noisy classical channel is the maximal real number such that there exists a sequence of codes of increasing block length fulfilling that the rate of transmission approaches C_0 and the probability of error after decoding is zero. □

Note the difference with the usual definition of capacity [NC00], where the probability of error approaches zero, instead of being zero.

This concept becomes important in situations where no error can be tolerated or when a fixed finite number of uses of the channel is available and it constitutes a central topic in information theory [KO98]. The definition can be straightforwardly translated to the case of quantum channels [MdA05], where a number of interesting results appear: the computation of this is QMA–hard [BS07] and it can be superactivated [CCH09] (see also [DS08, Dua09]).

We will show here a dichotomy behaviour for the power of a quantum channel with full–rank fixed point (e.g., a unital quantum channel) as a consequence of our quantum Wielandt's inequality. If we think of the power $\mathcal{E}^n$ as a channel describing the input–output relation after n units in time/space, then the subsequent result shows that there is a critical time/length $n = q(\mathcal{E})$ such that a successful transmission through $\mathcal{E}^n$ implies the possibility of a successful transmission to arbitrary $m \geq n$. By the quantum Wielandt's inequality, this critical value can be taken $(D^2 - d + 1)D^2$ and is therefore *universal*. It depends only on D and not on the channel itself.

Theorem 20 (Dichotomous behaviour of the zero–error capacity) *If $\mathcal{E}$ is a quantum channel with a full–rank fixed point, and we call $C_0(\mathcal{E})$ the 0–error classical capacity of $\mathcal{E}$, then either*[2] *$C_0(\mathcal{E}^n) \geq 1$ for all n or $C_0(\mathcal{E}^{q(\mathcal{E})}) = 0$.* □

Proof We split the problem into two cases:

(a)

Let us assume that the channel has two (or more) different fixed points. By following [Lin99], the set of fixed points of a quantum channel which has a full–rank fixed point is of the form $V\left[\bigoplus_i (\rho_i \otimes \mathcal{M}_{m_i})\right] V^\dagger$ where V is some unitary, the ρ_i's are density matrices with full–rank, and $\mathcal{M}_{m_i}$ is a full matrix algebra of dimension m_i. Consequently, if the direct sum is non–trivial, we can encode a classical bit in the corresponding projectors. If the direct sum is trivial, then the space of matrices is non–trivial, *i.e.* there is an $m_i \geq 2$, and we can encode one qubit in it. In either case $C_0(\mathcal{E}^n) \geq 1$ independent of n.

Similar statements hold if the channel has only one fixed point (which is, by assumption, full–rank) but another eigenvalue μ of magnitude one: since μ is a root of unity, *i.e.* there is an integer $p \leq D^2$ with $\mu^p = 1$, we have that $\mathcal{E}^p$ has several fixed points. So we can again safely encode a bit and $C_0(\mathcal{E}^n) \geq 1$ independent of n.

(b)

If the channel has just one fixed point and no other eigenvalue of magnitude one, then it is primitive by Proposition 18. So $\mathcal{E}^{q(\mathcal{E})}$ has the property that all output states are full–rank. This implies that $C_0(\mathcal{E}^n) = 0$ for all $n \geq q(\mathcal{E})$ [CCH09]. ■

[2] In fact, one can consider here even the one–shot zero–error capacity, that is, the one obtained with a single use of the channel.

Our job in life is to help people realize how rare and valuable each one of us really is, that each of us has something that no one else has, something inside that is unique to all time.

Fred Rogers (1928-2003)

3 Parent Hamiltonians

3.1 Introduction

In the previous chapters, we have focused on quantum states, especially on describing the construction of MPS and discussing their properties. However, condensed matter also concerns Hamiltonians, since they contain all information about the interactions among particles in the system. This Chapter revolves around the concept of *parent Hamiltonian*: a local TI Hamiltonian which is constructed from the MPS and has this as a ground state. Therefore, in the tensor network framework we observe the precisely opposite direction to the one usually followed in condensed matter: one starts with the state and then finds the Hamiltonian (showing certain relevant properties) which has it as a ground state, and not the opposite.

One of our main objectives in this Chapter, and a central topic in the rest of the Thesis, is to show that the characteristics of such a Hamiltonian can be determined by adjusting the local structure of the tensor, *i.e.* the parent Hamiltonian's features are encoded in the Kraus operators. In particular, connecting it to the results proven in previous chapters, we show that injectivity is the necessary and sufficient condition for the uniqueness of the ground state of the parent Hamiltonian and the key for the existence of a non–trivial spectral gap above it.

The relevance of such features is striking in condensed–matter–based implementations of quantum computers. The two–level system $\{|0\rangle, |1\rangle\}$ is the simplest model of quantum computer —where one may encode and process quantum information. Roughly speaking, the ground states of many–body systems play the role of $|0\rangle$–state and the first excited state the role of $|1\rangle$, while the quantum processing consists of excitations and desexitations of the system at low temperatures. The

uniqueness of the ground state allows the process to avoid phase errors in the desexcitation due to the indetermination of the ground state; and the existence of a spectral gap protects against environmental perturbations, *i.e.* thermal fluctuations which could generate flip errors $|0\rangle \leftrightarrow |1\rangle$.

This Chapter is essentially structured as follows:

- We provide in Section 3.2 the two definitions of parent Hamiltonian which can be found in the literature, discussing in which cases they are equivalent. We also show that parent Hamiltonians are *frustration–free*, a property which allows the local computation of the ground state energy. The problems associated with the idea of frustration–freeness in condensed matter, together with a property called *strong frustration–freeness*, are discussed.

- In Sections 3.3 and 3.4, we prove that injectivity is the necessary and sufficient condition for uniqueness, and the existence of a spectral gap in the sense pointed out above. As shown in Chapter 2, one can locally determine injectivity by means of its equivalence to strong irreducibility. Therefore, it becomes the first relevant example of a global feature which can be locally encoded in the tensors, complemented in the following Chapter with the characterization of symmetries.

- Finally, in the last Section, we also provide the definition of *kinsfolk Hamiltonian*, which is a broader family of Hamiltonians which have the MPS as an eigenstate, and not necessarily as the ground state. Therefore, every parent Hamiltonian is a kinsfolk Hamiltonian. These Hamiltonians are relevant in Chapter 8, where a systematic method to construct $SU(2)$–invariant two–body kinsfolk Hamiltonians is provided, together with a list of the most relevant ones.

3.2 Definition of Parent Hamiltonian

In this Section, we define the concept of *parent Hamiltonian*, as well as two properties of Hamiltonians called *frustration–freeness* and *strong frustration–freeness*, features that every parent Hamiltonian shows in particular. In condensed matter, geometrical frustration is a phenomenon which emerges when the geometrical properties of a crystal lattice or the existence of conflicting interactions forces forbid simultaneous local minimization of the ground state energy. This carries often as a consequence a degeneracy of the ground state and a high entanglement. The study of geometrically frustrated systems started with the investigations on the antiferromagnetic Ising model on a triangular lattice by H. Wannier in 1950 [Wan50], but the concept was not defined until 1977 by G. Toulouse [Tou77, VT77].

Let us denote the support of the reduced density matrix $\rho^{(n)}$ as $S_n = \text{supp}\ \rho^{(n)}$. Now, we can provide the first definition of parent Hamiltonian:

Definition 16 (Parent Hamiltonian 1) Let us consider a TI–MPS $|\psi^{(N)}\rangle$ and its reduced density matrix for $n < N$ particles, $\rho^{(n)}$. Let us assume that $\{|v_i\rangle\}_{i=1}^{r}$, $r \geq 1$, is an orthonormal basis for $\ker \rho^{(n)}$. By taking any positive linear combination of projectors, one can construct the following local interactions:

$$h(\boldsymbol{a}) = \sum_{i=1}^{r} a_i \, |v_i\rangle\langle v_i| \tag{3.1}$$

with $a_i > 0$. Hence, $\ker h = S_n$. Then, if τ is the *translation operator*, we call the following operator a **parent Hamiltonian**:

$$H^{(N)} = \sum_{i=1}^{N} \tau_i(h) \otimes \mathbb{1}_{\text{rest}} \tag{3.2}$$

where N is the number of spins contained in the chain and n, the number of particles in the support of h, is called the **interaction length** of H. □

This construction is consistent with the original definition proposed in [AKLT88], where the authors put forward the AKLT state and its parent Hamitonian. Nevertheless, there is an alternative definition based on the posterior developments on finitely correlated states in [FNW92]:

Definition 17 (Parent Hamiltonian 2) Let us consider a TI–MPS $|\psi^{(N)}\rangle$ generated by the set of Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^{d}$ and let us construct the vectorial space $\mathcal{G}_n = \langle \Gamma_n(X) \rangle_X$, *i.e.* the vectorial space spanned by the support of the $\Gamma_n(X)$ (see Eq. 2.2)

$$\mathcal{G}_n = \{ |\psi^{(n)}\rangle_X = \sum_{i_1,\ldots,i_n} \operatorname{tr}\left[X A_{i_1} \cdots A_{i_n}\right] |i_1 \ldots i_n\rangle | \forall X \in \mathcal{M}_D \} \tag{3.3}$$

Let us consider *any* positive operator $h \geq 0$, such that $\operatorname{supp} h = \mathcal{G}_n^{\perp}$, the orthogonal subspace. A **parent Hamiltonian** is then constructed as in Eq. 3.2. □

Both definitions are equivalent if the state is *injective*, since the support of $\rho^{(n)}$ coincides with the support of $\Gamma_n(X)$. Let us explicitly show that in the following Lemma:

Lemma 12 (Equivalence between definitions) *In general, $S_n \subseteq \mathcal{G}_n$. The equality holds when the state reaches injectivity for at most $n-1$ sites.* □

Proof Let us consider a sufficiently large N, and rewrite the state as $|\psi^{(N)}\rangle = \sum_{a,b} |\psi_{ab}^{(n)}\rangle \otimes |\psi_{ba}^{(N-n)}\rangle$. Therefore, the reduced density matrix is

$$\rho^{(n)} = \sum_{ab} |\psi_{ab}^{(n)}\rangle\langle\psi_{a'b'}^{(n)}| \underbrace{\operatorname{tr}\left[|\psi_{ba}^{(N-n)}\rangle\langle\psi_{b'a'}^{(N-n)}| \right]}_{\alpha_{aba'b'}}$$

We can now prove $\boxed{\subseteq}$ by rewriting any element from $\mathcal{G}_n$ as:

$$\sum_{ab}\sum_{i_1,\ldots,i_n} X_{ab}\langle b|\, A_{i_1}\cdots A_{i_n}\,|a\rangle\,|i_1\ldots i_n\rangle = \sum_{ab} X_{ab}\,|\psi^{(n)}_{ba}\rangle$$

which proves that the support of $\rho^{(n)}$ is contained in $\mathcal{G}_n$. Let us now assume *injectivity*, or in other words, that the D^2 vectors $|\psi^{(N-n)}_{ab}\rangle$ are linearly independent. Then, the Gram–Schmidt decomposition theorem ensures that there exists an invertible matrix Y such that

$$|\tilde{\psi}^{(N-n)}_{kl}\rangle = \sum_{ab}(Y^{-1})_{kl,ab}\,|\psi^{(N-n)}_{ab}\rangle$$
$$\langle\tilde{\psi}^{(N-n)}_{kl}|\tilde{\psi}^{N-n}_{ab}\rangle = \delta_{ka}\delta_{lb}$$

Therefore,

$$\begin{aligned}|\psi^{(N)}\rangle\langle\psi^{(N)}| \;=& \sum_{\substack{ab\\a'b'}} |\psi^{(n)}_{b'a'}\rangle\langle\psi^{(n)}_{ba}|\;\otimes\sum_{\substack{kl\\k'l'}} Y_{a'b',k'l'}\,|\tilde{\psi}^{(N-n)}_{k'l'}\rangle\langle\tilde{\psi}^{(N-n)}_{kl}|\,(\bar{Y})_{ab,kl}\\ &\sum_{\substack{kl\\k'l'}}\sum_{\substack{ab\\a'b'}} Y_{a'b',k'l'}\,|\psi^{(n)}_{b'a'}\rangle\langle\psi^{(n)}_{ba}|\,(\bar{Y})_{ab,kl}\otimes\,|\tilde{\psi}^{(N-n)}_{k'l'}\rangle\langle\tilde{\psi}^{(N-n)}_{kl}|\end{aligned}$$

By defining $|\tilde{\psi}^{(n)}_{kl}\rangle = \sum_{ab} Y_{ab,kl}\,|\psi^{(n)}_{ba}\rangle$, then

$$\rho^{(n)} = \sum_{\substack{kl\\k'l'}} |\tilde{\psi}^{(n)}_{k'l'}\rangle\langle\tilde{\psi}^{(n)}_{kl}|\,\delta_{kk'}\delta_{ll'} = \sum_{kl}|\tilde{\psi}^{(n)}_{kl}\rangle\langle\tilde{\psi}^{(n)}_{kl}|$$

Therefore, $\mathrm{supp}\rho^{(n)} = \langle\{\,|\tilde{\psi}^{(n)}_{kl}\rangle\}\rangle = \mathcal{G}_n$. If the state is not injective, then the last equality is not true because Y is not invertible. ∎

As a consequence, one must specify which definition of parent Hamiltonian is being considered in each particular problem if the states are not injective.

Note that, due to the method used to construct the Hamiltonian, it is clear that $h_i\otimes\mathbb{1}_{\mathrm{rest}}\,|\psi^{(N)}\rangle = 0$. As both $h_i \geq 0$ and $H\geq 0$, this means that $H\,|\psi^{(n)}\rangle = 0$ and that $|\psi^{(n)}\rangle$ is a ground state. Therefore, this very simple method allows us to construct a parent Hamiltonian which has the MPS as a ground state.

The Hamiltonian is obviously not unique, since there is a freedom of choice in its coefficients (provided that they are positive) or, in other words, both definitions establish constraints on the support of the Hamiltonian, but they do not specify the vector in this vector space. This provides some leeway for finding Hamiltonians with a specific structure, such as those which are invariant under some group, as shown in Chapter 4, or those with two–body interaction, as discussed in Chapter 8.

We pointed out above that every term of H annihilates the state, *i.e.* it is the ground state not only of H, but also of each $h_i\otimes\mathbb{1}_{\mathrm{rest}}$. The following definition arises from this:

Definition 18 (Frustration–free Hamiltonian) Let us consider a TI local (not necessarily parent) Hamiltonian on a ring of N d–dimensional spins with the structure $H = \sum_{i=1}^{N} \tau_i(h) \otimes \mathbb{1}_{\text{rest}}$, with τ the translation operator, h has interaction length n and sites $N+1$ and 1 are identified. Then, we say that H is **frustration–free** with respect to its ground state $|\psi_0\rangle$, if the latter minimizes the energy locally, *i.e.* if

$$\langle\psi_0| H |\psi_0\rangle = \inf_{\psi} \langle\psi| H |\psi\rangle = N \inf_{\psi} \langle\psi| h \otimes \mathbb{1}_{\text{rest}} |\psi\rangle \qquad (3.4)$$

□

The following Lemma relates this Definition with the characteristics of the parent Hamiltonian described above.

Lemma 13 (Properties of frustration–free Hamiltonians) *A TI local Hamiltonian $H^{(N)} = \sum_{i=1}^{N} \tau_i(h) \otimes \mathbb{1}_{rest}$ is frustration–free with respect to its ground state $|\psi\rangle$ iff $h \otimes \mathbb{1}_{rest} |\psi\rangle = 0$ with $h \geq 0$.* □

Proof We must prove that $h \otimes \mathbb{1}_{\text{rest}} |\psi\rangle = 0$ with $h \geq 0 \Leftrightarrow \ker h \subseteq \text{supp}\rho^{(n)}$.

$\boxed{\Rightarrow}$

By simple calculations

$$(h \otimes \mathbb{1}_{\text{rest}}) |\psi\rangle = 0 \Rightarrow \text{tr}_{\ker h} \left[(h \otimes \mathbb{1}_{\text{rest}}) |\psi\rangle\langle\psi| (h \otimes \mathbb{1}_{\text{rest}}) \right] = 0$$
$$\Rightarrow (h \otimes \mathbb{1}_{\text{rest}}) \rho^{(n)} (h \otimes \mathbb{1}_{\text{rest}}) = 0 \overset{h \geq 0}{\Longrightarrow} \text{supp}\ \rho^{(n)} \supseteq \ker h$$

which proves the implication.

$\boxed{\Leftarrow}$

This is trivial by definition. ■

Some contradictions between the idea of frustration–freeness in condensed matter and the definition derived from Eq. 3.4 could appear, due to the explicit dependence of Definition 18 on the number of particles N. Let us illustrate the idea with the following example:

Example 6 Let us consider the antiferromagnetic spin–$\frac{1}{2}$ Ising model described by the Hamiltonian $H = -J \sum_{i=1}^{N} \sigma_i \sigma_{i+1}$, with $J < 0$ and the sites $N+1$ identified with site 1.

If N is even, the Hamiltonian is called *Néel antiferromagnet*, since its energy is minimized by a state in which the spins are anti–aligned, so the spins live in a bipartite lattice, and this is known as *Néel order*. Therefore, in this case, the Hamiltonian is frustration–free in the sense given by Eq. 3.4. The ground state is obviously 2–fold degenerate and the translational invariant linear combination (in the sense of Definition 2) has an MPS representation given by the Kraus operators $\{\sigma^+, \sigma^-\}$.

In case of an odd N, a kink produced by two contiguous aligned spins appears in the ground state, generating a $2N$–fold degeneracy in the ground state. The state is *frustrated* in this case, but it still shows a Néel order[1]. This simple example shows that frustration actually depends on the number of particles. □

Let us now consider a stronger version of the frustration–freeness condition.

Definition 19 (Strongly frustration–free Hamiltonian) We say that a Hamiltonian $H^{(N)} = \sum_{i=1}^{N} \tau_i(h) \otimes \mathbb{1}_{\text{rest}}$ is **strongly frustration–free** if it is frustration–free for all $N \geq N_0$. □

It is straightforward to see that every parent Hamiltonian is strongly frustration–free, but not every frustration–free Hamiltonian is strongly frustration–free, as shown in the Example above. A lot of effort was put into relating ground states of frustration–free Hamiltonians to MPS: it is proven in [Has06] that all gapped Hamiltonians can be approximated by frustration–free Hamiltonians by increasing the interaction length to the order of $\mathcal{O}(\log N)$, while in [VC06] it was shown that they can be faithfully approximated by MPS. However, one can wonder which kind of Hamiltonian has *exactly* a size–independent MPS representation as ground state. This question remains unsolved, even though we provide an advance in the question in Section **??** by showing a dichotomous behaviour in the bond dimension of the ground state of any strongly frustration–free Hamiltonian: either its ground state is an MPS with bond dimension D independent of the number of particles N, or $D \geq \mathcal{O}(N^{\frac{1}{5}})$.

3.3 Uniqueness of the ground state

In this Section, we set up a very successful idea which will turn out to be our *modus operandi* in the rest of this Thesis: the codification of the physical properties of the couple state–Hamiltonian in the structure of the local tensors, *i.e.* the Kraus operators. The case shown in this Section is probably the most surprising one, since we relate injectivity to the necessary and sufficient condition for *uniqueness* in the ground state of the parent Hamiltonian. Therefore, by analysing the spectrum of the transfer matrix $\mathbb{E}$ of the MPS (let us recall the equivalence between injectivity and strong irreducibility), one can predict whether it is possible or not to construct a parent Hamiltonian with such an MPS as a unique ground state.

Furthermore, as shown in the next Section, injectivity also implies the existence of a *gap* over the ground state, as well as the exponential decay of the correlation functions, what we called *exponential clustering* in Theorem 12.

Let us explicitly expose this in the following two theorems. The first one shows that injectivity is a sufficient condition and is proven in [PGVWC07, Theorem 10].

[1] Defining the order parameter for the Néel order as $\sum_i (-1)^i \sigma_i$, it is still non–vanishing for the ground states above.

Theorem 21 (Injectivity ⇒ uniqueness for TI–MPS) *Let us consider a TI–MPS* $|\psi^{(N)}\rangle$ *generated by the Kraus operators* $\{A_i \in \mathcal{M}_D\}_{i=1}^d$ *and let us assume that this state has injectivity length* $L_0 \leq \frac{N}{2}$*. Then, this state is the unique ground state of a parent Hamiltonian* $H^{(N)}$ *with interaction length* $n \geq L_0 + 1$*.* □

Proof Let us prove this by contradiction by assuming that there is another ground state $|\phi\rangle$ of the Hamiltonian $H^{(N)}$. Then, $|\phi\rangle \in \mathcal{G}_N$, *i.e.* the state can be written as $|\phi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{tr}\left[XA_{i_1}\cdots A_{i_N}\right] |i_1 \ldots i_N\rangle$. By using translational invariance, one can choose the first position in any spin, so $|\phi\rangle$ may also be written as:

$$|\phi\rangle = \sum_{i_1,\ldots i_N} \mathrm{tr}\left[A_{i_1}\cdots A_{i_{L_0}} Y A_{i_{L_0+1}}\cdots A_{i_N}\right] |i_1\cdots i_N\rangle$$

As $N \geq 2L_0$, by means of injectivity in the products $A_{i_{L_0+1}}\cdots A_{i_N}$, it follows that $XA_{i_1}\cdots A_{i_{L_0}} = A_{i_1}\cdots A_{i_{L_0}}Y$ for every $i_1,\ldots,i_{L_0}$. But by using again the fact that the system has full Kraus rank for L_0 sites, one can always find coefficients $a_{i_1\ldots i_{L_0}}$ such that $\sum_{i_1,\ldots,i_{L_0}} a_{i_1\ldots i_{L_0}} A_{i_1}\cdots A_{i_{L_0}} = \mathbb{1}$, so this means that $X = Y$ and X commutes with every matrix (since they can be generated by linear combinations of the products $A_{i_1}\cdots A_{i_{L_0}}$). Therefore, $X \propto \mathbb{1}$ and $|\phi\rangle \propto |\psi\rangle$, which proves the Theorem. ■

Obviously, there is an equivalent theorem for MPS–OBC (see [PGVWC07, Theorem 9]) but, as we stated in the first Chapter, we focus on TI–MPS in this work. We are exploiting here the equivalence between injectivity and the fact that the quantum channel reaches full Kraus rank when the system size reaches the injectivity length, as proven in Theorem 18.

The reason why in the Theorem it is required that $n \geq L_0 + 1$, while it does not seem so evident in the proof, is in Lemma 12. While $n < L_0 + 1$, there might be states which are in the ground space of H, but not in $\mathcal{G}_N$.

Let us now prove that injectivity is also a necessary condition. The absence of injectivity can be due to the existence of more than one block in the canonical form, or to the the existence of a periodic decomposition of the TI–MPS (see Theorem 11). We will prove that, in any of these cases, there exists no local frustration–free Hamiltonian which has the MPS as a unique ground state.

Let us assume for the moment that the absence of injectivity is due to the existence of $b \geq 2$ blocks in the canonical form, labelled by $A_i^1,\ldots,A_i^b$ with dimensions $D_1 \geq \cdots \geq D_b$ and each of them injective in the corresponding subspace. We denote by L_0 the injectivity length, which is the maximum of the injectivity lengths of the blocks and, as shown in Subsection 2.5.2, $L_0 \leq (D_1^2 - d + 1)D_1^2$.

We can clearly write $|\psi^{(N)}\rangle = \sum_{j=1}^b |\psi_j^{(N)}\rangle$, where

$$|\psi_j^{(N)}\rangle = \lambda_j^N \sum_{i_1,\ldots,i_N} \mathrm{tr}\left[A_{i_1}^j\cdots A_{i_N}^j\right] |i_1\ldots i_N\rangle$$

where λ_j is the eigenvalue which corresponds to the j-block, as shown in Eq. 1.6.

We require a previous Lemma, proven in [PGVWC07, Proposition 4], to prove the main theorem:

Lemma 14 (Direct sum of subspaces) *If $n \geq 3(b-1)(L_0+1)$, then the sum $\bigoplus_{j=1}^{b} \mathcal{G}_n^{(j)}$ is direct.* □

Proof We start by grouping spins in $3(b-1)$ blocks, each of them of, at least, L_0+1 spins. Let us consider the case $b=2$ and prove it by induction. We assume, on the contrary, that the sum is not direct (*i.e.* there is a common vector to both subspaces), so there exist two non–zero matrices X, Y such that

$$\sum_{i_1,i_2,i_3} \mathrm{tr}\left[A^1_{i_1} X A^1_{i_2} A^1_{i_3}\right] |i_1 i_2 i_3\rangle = \sum_{i_1,i_2,i_3} \mathrm{tr}\left[A^2_{i_1} Y A^2_{i_2} A^2_{i_3}\right] |i_1 i_2 i_3\rangle$$

Let us now consider an arbitrary matrix Z, then there exist complex numbers $\mu^i_{i_1}$, $\rho^i_{i_2}$ such that $Z = \sum_{i,i_1,i_2} \mu^i_{i_1}\rho^i_{i_2} A^1_{i_1} X A^1_{i_2}$, where we have used injectivity together with the polar decomposition given in [PGVWC07, Proposition 3][2]. Denoting by $W = \sum_{i,i_1,i_2} \mu^i_{i_1}\rho^i_{i_2} A^2_{i_1} Y A^2_{i_2}$, we have that $\sum_{i_3} \mathrm{tr}\left[Z A^1_{i_3}\right] |i_3\rangle = \sum_{i_3} \mathrm{tr}\left[W A^2_{i_3}\right] |i_3\rangle$, which implies that $\mathcal{G}^{A^1}_{L_0+1} \subseteq \mathcal{G}^{A^2}_{L_0+1}$. By hypothesis, $\mathrm{size}\,(A^1) \geq \mathrm{size}\,(A^2)$, but this is compatible with the inclusion if $\mathrm{size}\,(A^1) = \mathrm{size}\,(A^2)$ and $\mathcal{G}^{A^1}_{L_0+1} = \mathcal{G}^{A^2}_{L_0+1}$. If we take now the same local Hamiltonian, by hypothesis of injectivity in each block, both $|\psi_{A^1}\rangle$ and $|\psi_{A^2}\rangle$ must be its *only* ground state, which contradicts the initial hypothesis. Let us now introduce the induction step, starting with $\sum_{j=1}^{b+1} |w^j\rangle = 0$, where

$$\mathcal{G}^{A^j}_{3b(L_0+1)} \ni |w^j\rangle = \sum_{i_1,\ldots,i_{3b}} \mathrm{tr}\left[A^j_{i_1} W^j A^j_{i_2} \cdots A^j_{i_{3b}}\right] |i_1 \ldots i_{3b}\rangle$$

Our goal is to prove that $W^j = 0$ for every j. Let us prove it by contradiction by assuming that there exists a j such that $W^j \neq 0$, and denoting by $|\tilde{w}\rangle$ the states $|\tilde{w}^j\rangle = \left(\mathbb{1}_{[1,2]} \otimes h_{\mathcal{G}^{A^{b+1}}_{[3]}} \otimes \mathbb{1}_{[4,\ldots,3b]}\right) |w^j\rangle$. Then, $\sum_{j=1}^{b} |\tilde{w}^j\rangle = 0$, and by induction hypothesis, $|\tilde{w}^j\rangle = 0$. Now,

$$|\tilde{w}^j\rangle = \sum_{i_1,\ldots,i_{3b}} \mathrm{tr}\left[A^j_{i_1} W^j A^j_{i_2} X^j_{i_3} A^j_{i_4} \cdots A^j_{i_{3b}}\right] |i_1 \ldots i_{3b}\rangle$$

where there is a i_3 such that $X^j_{i_3} \neq 0$ because of injectivity in each block. By employing again injectivity together with [PGVWC07, Proposition 3], there exist complex numbers such that $\mathbb{1} = \sum_{i,i_1,i2} \mu^i_{i_1}\rho^i_{i_2} A^j_{i_1} W^j A^j_{i_2}$. Therefore, after multiplying everything by the left with $\langle i'_1 i'_2 i'_3| \otimes \mathbb{1}_{\mathrm{rest}}$,

$$\sum_{i_4,\ldots,i_{3b}} \mathrm{tr}\left[X^j_{i_3} A^j_{i_4} \cdots A^j_{i_{3b}}\right] |i_4 \ldots i_{3b}\rangle = 0$$

[2] This proposition states that, given a matrix $X \neq 0$ and a matrix Y, there always exist matrices R_i and S_i such that $Y = \sum_i R_i X S_i$.

for every i_3. But, due to the injectivity in each block, this means that $X^j_{i_3} = 0$, which is the desired contradiction. ∎

Finally, we can prove that, in the absence of injectivity, every parent Hamiltonian containing this state as a ground state has a degenerate ground space, *i.e.* injectivity is also a necessary condition for uniqueness.

Theorem 22 (Uniqueness ⇒ injectivity) *Let us consider an MPS $|\psi^{(N)}\rangle$ on an N–particle ring whose canonical form is composed by b different blocks, as described above. Let us assume that $N \geq 3(b-1)(L_0+1)+n$ and $H \geq 0$ is a frustration–free n–local TI–Hamiltonian with $|\psi^{(N)}\rangle$ as a ground state, i.e. $H|\psi^{(N)}\rangle = 0$, then $|\psi_j^{(N)}\rangle$, the state generated by the j–th block, is also a ground state for every j.* □

Proof Let us denote by h the local term of the Hamiltonian H. Then, it is clear that $0 = (h \otimes \mathbb{1}_{\text{rest}})|\psi^{(N)}\rangle = \sum_{j=1}^{b}(h \otimes \mathbb{1}_{\text{rest}})|\psi_j^{(N)}\rangle$. Since $(h \otimes \mathbb{1}_{\text{rest}})|\psi_j^{(N)}\rangle \in (\mathbb{C}^d)^{\otimes L} \otimes \mathcal{G}^{(j)}_{N-n}$, one can conclude by means of Lemma 14 that $(h \otimes \mathbb{1}_{\text{rest}})|\psi_j^{(N)}\rangle = 0$, for every j. ∎

This Theorem proves that there is a degeneration of the ground space in the absence of injectivity. However, it is possible to prove [PGVWC07, Theorem 12] that there always exists a parent Hamiltonian whose ground space is $\ker H = \text{span}\left[|\psi_j^{(N)}\rangle\right]$.

The proof for states which admit periodic decomposition can be avoided by the following reasoning. Let us assume a finite N, then, as proven in Theorem 11, the period p must be a factor of N, since otherwise the state $|\psi^{(N)}\rangle = 0$. Therefore, by coupling p sites together, the periodic decomposition is removed and we are back in the case of multiple blocks in the canonical form.

It was proven in Theorem 21 that, if the injectivity length is L_0, then the uniqueness of the parent Hamiltonian's ground state is ensured when the interaction length $n > L_0$. However, we will now show a theorem which ensures that, in some cases, the uniqueness already holds for $n = L_0$.

Theorem 23 (Intersection property) *Let us call $\mathcal{G}_n = \text{supp}\,\rho^{(n)}$, where $\rho^{(n)}$ is the reduced density matrix for $n \geq L_0$ particles of the TI–MPS $|\psi^{(N)}\rangle$, which has injectivity length L_0. If the* ***intersection condition***

$$\mathcal{G}_{L_0+1} = \mathcal{G}_{L_0} \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes \mathcal{G}_{L_0} \qquad (3.5)$$

holds, then the state $|\psi^{(N)}\rangle$ is the only ground state of the parent Hamiltonian $H = \sum_{i=1}^{N} \tau_i(h^{(L_0)} \otimes \mathbb{1}_{rest})$, where $h^{(L_0)}$ has support on L_0 particles. □

Proof The proof can be found in [FNW92, Lemma 5.5 and Theorem 5.8]. ∎

There are many important examples which fulfil Property 3.5. The most relevant one is the AKLT state [AKLT88], whose injectivity length is $L_0 = 2$, but it is the

only ground state of a parent Hamiltonian with interaction length $n = 2$. The generalization of this state for larger spins was proposed in [FNW92, Section 7.3], and it is discussed in detail in Chapter 4 and, along with other new examples, in Chapter 8. It is possible to prove that these states share the properties of AKLT and that they are the only ground states of parent Hamiltonians with nearest–neighbour interactions.

3.4 Gap

In Section 3.3, the equivalence between injectivity and uniqueness has been established, but the system could still be **gapless**, *i.e.* the energy gap between the ground state and the first excited state could be infinitesimally small. However, we show in this Section an argument proven in [FNW92] which ensures the existence of a non–trivial gap above the ground state for parent Hamiltonians constructed from injective states.

Let us prove a useful Lemma to define the gap in terms of H and its square.

Lemma 15 (Gap of a general Hamiltonian) *Let us consider a Hamiltonian H with a one–dimensional ground space and ground state energy 0. Then, the **energy gap** ϵ_0 above the ground space is the largest γ such that*

$$H^2 \geq \gamma H \tag{3.6}$$

Therefore, if we call $\chi = \{\gamma \mid H^2 - \gamma H \geq 0\}$, then $\epsilon_0 = \sup \chi$. □

PROOF Let us write the Hamiltonian in the eigenbasis as $H = \sum_i \lambda_i |\phi_i\rangle\langle\phi_i|$, with $0 = \lambda_0 < \lambda_1 \leq \cdots$, where the first strict inequality is due to the uniqueness of the ground state. Let us assume, for the sake of simplicity, that $\lambda_1 > 0$ is the energy of the first excited state, then

$$H^2 - \gamma H = \sum_i (\lambda_i^2 - \gamma\lambda_i) |\phi_i\rangle\langle\phi_i|$$

We are searching the larger γ which makes all these coefficients positive, so So one must analyse

$$\lambda_i^2 - \gamma\lambda_i \geq 0 \Rightarrow \gamma \leq \lambda_i, i \geq 1 \Rightarrow \gamma = \lambda_1 = \epsilon_0$$

which proves the Lemma. ■

The following Lemma is also useful:

Lemma 16 (Frustration–free Hamiltonians as two–body projectors) *To study the existence of a gap in an n–local frustration–free Hamiltonian, it is enough to study the case of nearest–neighbour interaction $\tilde{H} = \sum_i \tau_i(P)$, where P is a projector on the kernel of $\tilde{h} = \sum_{j=0}^{p} \tau_j(h)$, being p any integer such that $p \geq n$.* □

PROOF See [PGVWC07, Subsection 4.2] for the argumentation. ∎

We are now in the position to enunciate the main Theorem:

Theorem 24 (Injectivity ⇒ Gap) *Let us consider the parent Hamiltonian H corresponding to an injective TI–MPS $|\psi^{(N)}\rangle$ such that $H|\psi^{(N)}\rangle = 0$. Then, the* ***gap*** *ϵ_0 over the ground state is lower bounded by*

$$\epsilon_0 \geq 1 - \mathcal{O}(|\lambda_2|) \tag{3.7}$$

where $|\lambda_2| < 1$ is the modulus of the second eigenvalue of $\mathcal{E}$. □

PROOF This Theorem is proven in [FNW92, Theorem 6.4]. ∎

The second eigenvalue is always smaller than 1, so the gap is always positive.

In both [FNW92, Theorem 6.4] and [PGVWC07, Section 4.2], the Theorem is enunciated in a slightly more general way than here. Both consider the possibility that the injectivity length is larger than 1, which takes us to the necessity of blocking several spins to ensure uniqueness, as pointed out in Theorem 22. If it is necessary to block p sites, then Eq. 3.7 is corrected by replacing $|\lambda_2| \hookrightarrow |\lambda_2|^p$.

3.5 Kinsfolk Hamiltonian

In this Section, we have focused on finding local Hamiltonians which have an MPS as a unique ground state. The importance of finding Hamiltonians which have a unique ground state in condensed matter and quantum information was already pointed up in the Introduction and previous chapters. However, it is also mathematically and physically relevant to procure Hamiltonians in which other eigenstates are known. We define in this Section a generalization of the concept of parent Hamiltonian which is extensively used in Chapter 8.

Definition 20 (Kinsfolk Hamiltonian) Let us consider an n–particle–supported TI–Hamiltonian $H^{(N)} = \sum_{i=1}^{N} \tau_i(h^{(n)} \otimes \mathbb{1}_{\text{rest}})$ and an MPS $|\psi^{(N)}\rangle$. We say that $H^{(N)}$ is a **kinsfolk Hamiltonian** of $|\psi^{(N)}\rangle$ if the latter is an eigenstate of $H^{(N)}$. □

Obviously, every parent Hamiltonian is a kinsfolk Hamiltonian, for which $|\psi^{(N)}\rangle$ is particularly the ground state of $H^{(N)}$. The opposite, however, is not true.

Finding kinsfolk Hamiltonians is not as trivial as finding parent Hamiltonians with the VBS picture, so it is necessary to find new techniques to construct them. It is possible to prove (see Section 8.2) that for every kinsfolk Hamiltonian it holds that

$$\text{tr}\left[\rho^{(n)} h^{(n)\,2}\right] - \text{tr}^2\left[\rho^{(n)} h^{(n)}\right] = 0 \tag{3.8}$$

where $\rho^{(n)}$ is the reduced density matrix for n particles of the MPS $|\psi^{(N)}\rangle$.

We provide in Section 8.2 some examples of kinsfolk Hamiltonians computed using Eq. 3.8, together with a detailed discussion of the proof that the MPS in question is an excited state.

C'est véritablement utile, puisque c'est joli.

Antoine de Saint–Exupéry
(1900-1944)

4 Symmetries

4.1 Introduction

As we already showed through previous chapters, Matrix Product States (MPS) encapsulate many of the physical properties of quantum spin chains. Their importance stems from the fact that with a simple tensor, A, one can fully describe relevant states of N spins, which, in principle, would require to deal with an exponential number of parameters when written in a basis of the many–body Hilbert space $\mathcal{H}^{\otimes N}$. Thus, all the physical properties of such states are contained in A. Therefore, it is important to obtain methods to extract the physical properties directly from such a tensor, without having to resort to an explicit basis decomposition in $\mathcal{H}^{\otimes N}$.

An important physical property of a TI state, $|\psi\rangle$, is the symmetry group under which it is invariant. That is, the group G such that

$$u_g^{\otimes N} |\psi\rangle = e^{i\theta_g} |\psi\rangle \tag{4.1}$$

where $g \in G$ and u_g is a unitary representation of the group on $\mathcal{H}$. We will show in this Section that this symmetry group is uniquely determined by the symmetry group of A (with a tensor product representation). Roughly speaking this means that by studying the symmetries of A we can obtain those for the whole state $|\psi\rangle$. This result allows us, for example, to shed a new light on string order [PGWS$^+$08], a key concept in strongly correlated states in many–body quantum systems.

The results shown in this Chapter are essentially extracted from [SWPGC09], and it is structured as follows:

- In Section 4.2, the question about the implementation of symmetries in MPS is introduced. We firstly solve the problem for discrete symmetries, extending

afterwards the result to any compact connected Lie group. The proof provided in this Section is general, improving on the one appeared in [PGWS$^+$08], which applied only for injective states.

- In Section 4.3, we provide a general method to construct the Kraus operators by means of Clebsch–Gordan coefficients once the way the symmetry acts on physical and virtual indices is specified. Finally, we focus on the relevant case of the $SU(2)$ symmetry, generalizing the results shown in [FNW92].
- We prove in the last Section that, when the chosen representations for the construction in the previous point are irreducible representations of a compact connected Lie group, then the state is injective. A counter–example for the converse statement is also provided, *i.e.* there are injective states which are invariant under reducible representations of the group.

4.2 Definition and characterization

In this Section we analyze the implications of a given *local* symmetry for an MPS. First, we show that the local symmetry transfers to the Kraus operators, generalizing the findings of [FNW92, PGWS$^+$08]. In a second step we show that the symmetry in the Kraus operators imposes that they are essentially uniquely defined in terms of Clebsch–Gordan coefficients. Finally, for the special case of $SU(2)$ one can simplify even further and analyse the qualitative differences between integer and semi–integer spins.

Firstly, let us remark that we focus in this Chapter on symmetries of *states* instead of *Hamiltonians*. There is, however, a close connection between both approaches. On the one hand, it is clear that the unique ground state of a symmetric Hamiltonian has to keep the symmetry. On the other hand, we have the following Lemma:

Lemma 17 (Symmetric parent Hamiltonians) *If an MPS $|\psi\rangle$ is invariant under a representation of a group, one can choose its parent Hamiltonian H invariant under the same representation.* □

Proof To see this, it is enough to notice that the symmetry in the state given by Eq. 4.1 implies the invariance of $\ker \rho^{(k)}$ under the same symmetry. Hence, the projector onto $\ker \rho^{(k)}$ yields an invariant h, so the parent Hamiltonian is also invariant. Moreover, in case of several invariant subspaces under the symmetry in $\ker \rho^{(k)}$, a positive linear combination of projectors onto each of such subspaces produces the most general family of parent Hamiltonians which are invariant under this representation of the symmetry. ■

It was proven in [PGWS$^+$08] that the Kraus operators which describe any *injective* state, symmetric under a group G, fulfil the condition $\sum_i u^g_{ij} A_i = U_g A_j U_g^\dagger$, where

u and U are representations of G. We provide in this Section a generalization in which injectivity is not required and which can be found in [SWPGC09].

The N appearing in the proof must be sufficiently large to reach full Kraus rank in every block of the canonical form after collecting $\frac{N}{5}$ spins.

We start by proving the case of discrete symmetries, extending the proof to continuous groups below.

Theorem 25 (Discrete symmetries) *Let $\{A_i\}_{i=1}^d$ be the Kraus operators, in the canonical form, which describe a TI–MPS $|\psi^{(N)}\rangle$ locally invariant under a single unitary u, i.e. $u^{\otimes N}|\psi^{(N)}\rangle = e^{i\theta}|\psi^{(N)}\rangle$. Then, the symmetry in the physical level can be replaced by a local transformation in the virtual level. This means that there exists a unitary U — which can be taken block diagonal with the same block structure as the A's in the MPS, and composed with a permutation matrix among blocks, i.e. $U = P(\oplus_b V_b)$ — such that*

$$\sum_j u_{ji} A_j = W U A_i U^\dagger \qquad \text{for } i = 1, \ldots, d \tag{4.2}$$

with $W = \oplus_b e^{i\theta_b} \mathbb{1}_b$. □

Proof We follow here the same reasoning as in the proof of Lemma 14. We collect the spins in five different blocks, each one of them with full Kraus rank in the corresponding subspace. Applying $u^{\otimes N}$ gives us the same MPS (we incorporate the global phase into the new matrices) with different matrices, which we call B, but with the same block diagonal form, and also (after gathering) with full Kraus rank. We now require the following Lemma, which is proven below.

Lemma 18 (Expansion of the same MPS) *For each block in the A's, for instance the one given by matrices A_i^1, there is a block in the B's, given by matrices B_i^1, which expands the same MPS.* □

Since both matrices are representations in the canonical form of the same injective MPS, by Theorem 5 [1], they must be related by a unitary and a phase: $V_1 A_i^1 V_1^\dagger = e^{i\theta_1} B_i^1$, which concludes the proof of the Theorem. ■

Proof (Lemma 18) Let us prove now the Lemma. By using that the state has full Kraus rank and summing with appropriate coefficients, it is possible to show that there exists a block diagonal $D \times D$ matrix $X \neq 0$ such that

$$\mathrm{tr}\left[A_{i_2}^1 \cdots A_{i_5}^1\right] = \mathrm{tr}\left[X B_{i_2} \cdots B_{i_5}\right], \quad \forall i_2, \ldots, i_5$$

[1] Theorem 5 is general, but here we are restricted to injective blocks, so [PGVWC07, Theorem 3.11] would be enough. The conditions for this Theorem that the canonical form in the OBC must be unique can be dropped by [LLPG+08, Equation 3]

Since $X \neq 0$, there exists one block, let us say X_1, different from 0. Then, summing with appropriate coefficients again we get that there exists a matrix $Y \neq 0$ such that

$$\mathrm{tr}\left[Y A^1_{i_3} A^1_{i_4} A^1_{i_5}\right] = \mathrm{tr}\left[X_1 B^1_{i_3} B^1_{i_4} B^1_{i_5}\right], \quad \forall i_3, i_4, i_5$$

We can now argue as in Lemma 5 to conclude the proof. ∎

If we have now a symmetry given by a compact connected Lie group G, that is, (4.1) holds for any $g \in G$ and a representation $g \mapsto u_g$, we obtain the following:

Theorem 26 (Continuous symmetries) *The map $g \mapsto P_g$, where P is the former permutation matrix, is a representation of G, and actually the trivial one. The maps $g \mapsto e^{i\theta^b_g}$ and $g \mapsto V^b_g$ are also representations of G.* □

Proof Let us start with the map $g \mapsto P_g$ for $g = g_2 g_1$. From Eq. 4.2 we get:

$$\begin{aligned} W_{g_2g_1} U_{g_2g_1} A_h U^\dagger_{g_2g_1} &= \sum_j u^{g_2g_1}_{jh} A_j = \\ \sum_{jk} u^{g_2}_{jk} u^{g_1}_{kh} A_j &= W_{g_2} W_{g_1,P_{g_2}} U_{g_2} U_{g_1} A_h U^\dagger_{g_1} U^\dagger_{g_2} \end{aligned} \tag{4.3}$$

where $W_{g_1,P_{g_2}}$ is the same unitary as W_{g_1} but with the blocks permuted according to permutation P_{g_2}. Since $P_{g'} W_g = W_{g,P_{g'}} P_{g'}$ and W_g commutes with all other terms appearing in Eq. 4.3, we can multiply successively and use the full Kraus rank (with L_0 the required block size), to get, for all $n \geq L_0$ and all X block–diagonal,

$$W^n_{g_2g_1} U_{g_2g_1} X U^\dagger_{g_2g_1} = (W_{g_2} W_{g_1,P_{g_2}})^n U_{g_2} U_{g_1} X U^\dagger_{g_1} U^\dagger_{g_2} \,. \tag{4.4}$$

By taking $X = \mathbb{1}_b$ for each block b, we get that $P_{g_2} P_{g_1}$ must be $P_{g_2g_1}$. But since we are assuming that the group G is connected, this in turn implies that $P_g = \mathbb{1}$ for all g. With this in hand, we can split Eq. 4.4 into blocks to get

$$e^{in\theta^b_{g_2g_1}} V^b_{g_2g_1} X V^{b\,\dagger}_{g_2g_1} = e^{in(\theta^b_{g_1}+\theta^b_{g_2})} V^b_{g_2} V^b_{g_1} X V^{b\,\dagger}_{g_1} V^{b\,\dagger}_{g_2} \tag{4.5}$$

for each b, each $n \geq L_0$ and each matrix X. By taking $X = \mathbb{1}$ we obtain

$$e^{in\theta^b_{g_2g_1}} = e^{in(\theta^b_{g_1}+\theta^b_{g_2})}$$

In particular, when $n = L_0$, we get that $L_0(\theta^b_{g_2g_1}) = L_0(\theta^b_{g_1} + \theta^b_{g_2}) + 2k_0\pi$, and when $n = L_0 + 1$, that $(L_0+1)(\theta^b_{g_2g_1}) = (L_0+1)(\theta^b_{g_1} + \theta^b_{g_2}) + 2k_1\pi$. By gathering both results, the L_0 can be removed and we obtain $\theta^b_{g_2g_1} = \theta^b_{g_1} + \theta^b_{g_2} + 2(k_1 - k_0)\pi$.

Finally, to show that $g \mapsto V^b_g$ is a representation, it is enough to notice that Eq. 4.5 implies that $V^{b\,\dagger}_{g_1} V^{b\,\dagger}_{g_2} V^b_{g_2g_1}$ commutes with every matrix. ∎

A trivial consequence of these theorems is the fact that having an *irreducible* representation U_g in the virtual level implies that the MPS has to be *injective*. We give an alternative proof of this fact in Section 4.4 without having to rely on the MPS canonical form. We also analyse there when the converse implication holds.

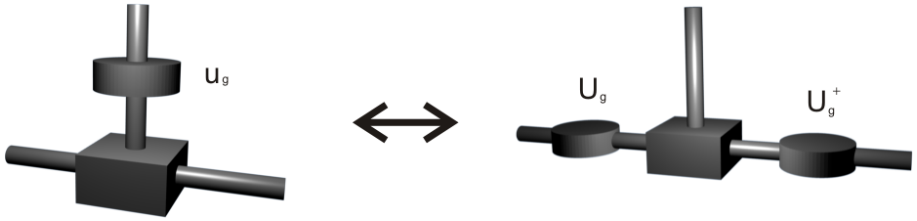


Figure 4.1: **Symmetry conditions on Kraus operators**. The unitary u_g applied on the physical level is reflected in the virtual bonds as pair of unitaries U_g.

4.3 Uniqueness of the construction method

Once the Theorem which provides the condition that the Kraus operators must fulfil in order to generate invariant MPS has been established, the next step is to provide a method for explicitly constructing such Kraus operators, showing that they always can be constructed by means of Clebsch–Gordan coefficients. To do that, it is more convenient to work with the isometry V defined in Eq. 1.10. From the definition, it is clear that the condition $\sum_i u_{ij}^g A_i = U_g A_j U_g^\dagger$ leads to

$$V(U_g \otimes u_g) = U_g V \qquad \forall g \tag{4.6}$$

where u is an irrep, U is in general a rerep, and V fulfils $VV^\dagger = \mathbb{1}_D$ and $V^\dagger V = P$. Notice that we have removed the dependence on the phase because it can always be absorbed into the physical representation by defining a new irrep $w_g \hookrightarrow e^{i\theta_g} u_g$. Besides, this phase is trivial for non–abelian groups like $SU(N)$, since there are no non–trivial one–dimensional representations for such groups. Let us remark that solving Eq. 4.6 is equivalent to solving the system $(U_g \otimes u_g)V^\dagger = V^\dagger U_g$, and the latter is traditionally the most common approach to write the problem [FNW92].

Let us write U_g as a direct sum of irreps, *i.e.* $\bigoplus_{j\in\tilde{\mathcal{X}}} v_g^j = W^\dagger U_g W$. It always can be performed by a unitary rotation W, but due to the gauge freedom in the Kraus operators, this W does not change the MPS and we can assume wlog that we are already in the correct basis. Therefore, the tensor product[2] $(U_g \otimes u_g) = \bigoplus_{j\in\tilde{\mathcal{X}}}(v_g^j \otimes u_g)$.

Given a compact group G, the tensor product of two *irreducible representations* (irreps) is reducible, and the *Clebsch–Gordan Theorem* ensures that it can always be decomposed as a direct sum:

$$C_j\ (v_g^j \otimes u_g) = \bigoplus_{i\in\mathcal{X}_j} w_g^{j,i}\ C_j \tag{4.7}$$

[2]Note that we interchange the direct sum and the tensor product. It depends on our choice for the basis of the tensor product, and in the worst case, it would be necessary to add first a flip operator F interchanging u and U, *i.e.* $(U_g \otimes u_g) = F(u_g \otimes U_g)F^\dagger$. Note that this F cannot be absorbed in the gauge freedom, so it has to be taken into account in calculations.

where C_j is a unitary matrix whose entries are called **Clebsch–Gordan coefficients** and $\mathcal{X}_j$ is the set of irreps in the decomposition of $(v_g^j \otimes u_g)$. Collecting everything together,

$$(U_g \otimes u_g) = \left(\bigoplus_{j\in\tilde{\mathcal{X}}} C_j^\dagger\right)\left(\bigoplus_{k\in\cup_i\tilde{\mathcal{X}}_j} w_g^{j,i}\right)\left(\bigoplus_{j\in\tilde{\mathcal{X}}} C_j\right) = C^\dagger\left(\bigoplus_{k,m\in\mathcal{T}} w_g^{k,m}\right)C \qquad (4.8)$$

where $\mathcal{T} = \bigcup_i \mathcal{X}_i$. For the sake of clarity of the notation, lets us assume that all equivalent irreps (let us recall that two unitary representations u_g and v_g are **equivalent** if they are related by a unitary matrix $u_g = wv_gw^\dagger$, for all g) are gathered together in an increasing dimension in both Eq. 4.8 and the decomposition of U. Therefore, the index k runs over different irreps, while the index m is runs over the equivalent representations. From Schur's lemma one can easily check that Eq. 4.6 has a non–trivial solution if $\mathcal{X} \subseteq \mathcal{T}$. Let us denote by $P_{i,j}$ the set of projectors which give $P_{i,j}^\dagger\left(\bigoplus_{k,m\in\mathcal{T}} w_g^{j,i}\right)P_{i,j} = w^{i,j}$, with $P_{k,l}^\dagger P_{i,j} = \delta_{i,k}\delta_{j,l}\mathbb{1}$ and $\sum_{i,j} P_{i_j}P_{i,j}^\dagger = 1_{dD}$. Additionally, let us also call $\phi_{m,n}^{(k,k')} = P_{k,m}^\dagger C P_{k',n}$. Obviously, the Schur's lemma ensures that $\phi_{m,n}^{(k,k')} \propto \delta_{k,k'}\mathbb{1}$.

Then, the solutions for Eq. 4.6 may be parametrized as follows:

$$V = \bigoplus_{k\in\mathcal{X}} M_k \otimes \mathbb{1}_{d_k} \qquad (4.9)$$

where the direct sum is taken over the different irreps in $\mathcal{X}$ and $M_k \in \mathcal{M}_{l_k,r_k}$ is an isometry for the k–th irrep with a number of rows l_k and columns r_k equal to the degeneracy of the irrep in $\mathcal{X}$ and $\mathcal{T}$, respectively. If there is an irrep such that $w_g \in \mathcal{X}$ but $w_g \notin \mathcal{T}$, then M is the zero matrix.

From this we can now conclude that the only non–trivial family of solutions for Eq. 4.6 is given by Eq. 4.9. The following Theorem shows the same in a more compact form:

Theorem 27 (Piecewise construction (MPS)) *Let us consider a group G and two representations u_g (irrep) and $U_g = \bigoplus_i U_g^{D_i}$ (each $U_g^{D_i}$ is also an irrep). Then, the structure of all possible maps V fulfilling $(U_g \otimes u_g)V = VU_g$ is*

$$V = \begin{pmatrix} \alpha_{11}V_{D_1}^{D_1} & \alpha_{12}V_{D_1}^{D_2} & \cdots & \alpha_{1n}V_{D_1}^{D_n} \\ \alpha_{21}V_{D_2}^{D_1} & \alpha_{22}V_{D_2}^{D_2} & \cdots & \alpha_{2n}V_{D_2}^{D_n} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n1}V_{D_n}^{D_1} & \alpha_{n2}V_{D_n}^{D_2} & \cdots & \alpha_{nn}V_{D_n}^{D_n} \end{pmatrix} \qquad (4.10)$$

where $V_{D_i}^{D_j}$ is a solution to $(U_g^{D_i} \otimes u_g)V_{D_i}^{D_j} = V_{D_i}^{D_j}U_g^{D_i}$. □

4.3.1 The case of $SU(2)$

Let us apply the results of the previous section to the case in which $G = SU(2)$. Our construction is a natural generalization of the one used in [FNW92, SZV10].

We consider from now on irreducible representations u_g of the symmetry on the physical spin. Nevertheless, a substantial part of the results can be straightforwardly extended to the reducible case. Hence, we are interested in analysing the restrictions that $SU(2)$ imposes on the general solution given by Theorem 27 to the equation

$$(U \otimes J)V = VU \tag{4.11}$$

where, with some abuse of notation, J is the $SU(2)$ irrep corresponding to spin J and $U = (i_1 \oplus \ldots \oplus i_n \oplus s_1 \oplus \ldots \oplus s_m)$ is a virtual representation composed of n integer irreps and m semi–integer irreps. Note that in the Clebsch–Gordan decomposition of $SU(2)$ all representations appear with multiplicity 1. Therefore, there is only one term in the sum in Eq. **??**. At this point one should distinguish the cases of integer or semi–integer J. If J is integer, zero is the only solution to $(i_j \otimes J)\Omega = \Omega s_k$ and $(s_k \otimes J)\Omega = \Omega i_j$ for all j, k, and we get in Eq. 4.10 a block diagonal structure:

$$V = \begin{pmatrix} \alpha_1^1 V_{i_1}^{i_1} & \cdots & \alpha_1^n V_{i_1}^{i_n} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \alpha_n^1 V_{i_n}^{i_1} & \cdots & \alpha_n^n V_{i_n}^{i_n} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \alpha_{n+1}^{n+1} V_{s_1}^{s_1} & \cdots & \alpha_{n+1}^{n+m} V_{s_1}^{s_m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \alpha_{n+m}^{n+1} V_{s_m}^{s_1} & \cdots & \alpha_{n+m}^{n+m} V_{s_m}^{s_m} \end{pmatrix}$$

The paradigmatic example in this case is the *AKLT* state [AKLT88], which corresponds to the case of $J = 1$, $U = 1/2$ in Eq. 4.11. In [FNW92, Section 7.3], the authors generalized the AKLT model to arbitrary integer J and irreducible U. We will call the resulting MPS **FNW states**. It is shown in [FNW92, Proposition 7.6] how, for $U = \frac{J}{2}$, FNW states are unique ground states of frustration–free nearest–neighbor interactions. An alternative construction focused on the restrictions imposed by the $SU(2)$ symmetry on the density matrix instead of the Kraus operators can be found in [DMDNS98].

If J is semi–integer, zero is the only solution to $(s_j \otimes J)\Omega = \Omega s_k$ and $(i_k \otimes J)\Omega = \Omega i_j$ for all j, k, and we get in Eq. 4.10 an off–diagonal structure:

$$V = \begin{pmatrix} 0 & \cdots & 0 & \alpha_1^{n+1} V_{i_1}^{s_1} & \cdots & \alpha_1^{n+m} V_{i_1}^{s_m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \alpha_n^{n+1} V_{i_n}^{s_1} & \cdots & \alpha_n^{n+m} V_{i_n}^{s_m} \\ \alpha_{n+1}^1 V_{s_1}^{i_1} & \cdots & \alpha_{n+1}^n V_{s_1}^{i_n} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \alpha_{n+m}^1 V_{s_m}^{i_1} & \cdots & \alpha_{n+m}^n V_{s_m}^{i_n} & 0 & \cdots & 0 \end{pmatrix}$$

It is clear that the virtual representations must be reducible now, which is very much related to the Lieb–Schultz–Mattis theorem, as we will show in Chapter 9. The paradigmatic example in this case is the *Majumdar–Ghosh model* [MG69], already introduced in Examples 2 and 4, which corresponds to $J = \frac{1}{2}$ and $U = \frac{1}{2} \oplus 0$. A generalization of this model for the case of arbitrary J and $U = F \oplus 0$, was recently proposed in [KM08].

In general, it is possible to find a set of representations which fits into any model with $SU(2)$ (or $U(1)$) symmetry, for instance [KSZ93, RSDMD98, RG08, Kum02, TS10].

4.4 Irreducibility implies injectivity

In this Section, we give a direct proof of the fact that an irreducible representation in the virtual level of a symmetric MPS implies that the MPS is injective. We also see that the reverse inclusion is not true in general, but it holds under some conditions on the Kraus operators.

We have to recall that, given a set $\mathcal{K} = \{A_1, \ldots, A_d\}$ of Kraus operators defining an MPS, we can define an associated quantum channel $\mathcal{E}$ as defined in Subsection 1.4.1, $\mathcal{E}(X) = \sum_{i=1}^{d} A_i^\dagger X A_i$. The symmetry in the MPS transfers then to the **covariance** of the channel, that is, $\mathcal{E}(U_g^\dagger X U_g) = U_g^\dagger \mathcal{E}(X) U_g$ for all X. We already proved in Section 2.2, that if $\mathcal{E}$ is trace–preserving and has $\mathbb{1}$ as its unique fixed point, then the MPS is injective. Moreover, it is trivial to see that if $\mathcal{E}$ is the ideal channel ($\mathcal{E}(X) = X$ for all X), then the MPS is a product state. Therefore, the desired result that *irrep implies injectivity* is a consequence of the following Theorem:

Theorem 28 (Irreducibility ⇒ injectivity) *Let us take a completely positive trace–preserving map $\mathcal{E} : \mathcal{M}_D \to \mathcal{M}_D$ that is covariant for an irrep of a compact connected Lie group G. Then, either $\mathcal{E}$ is the ideal channel, or the identity is its unique fixed point.* □

Proof Let us consider a fixed point Λ of $\mathcal{E}$. Then $U_g^\dagger \Lambda U_g$ is also a fixed point because of the covariance. Therefore, integrating under the Haar measure and using Schur's lemma, $\mathbb{1}$ is also a fixed point. A similar argument shows that $\mathcal{E}$ is also trace–preserving.

Now we can apply Lüders' theorem 8 , which ensures that the set of fixed points $\mathcal{P}$ of $\mathcal{E}$ coincides with the commutant $\mathcal{K}'$ of the set of Kraus operators of $\mathcal{E}$. This is trivially a C^*–subalgebra of $\mathcal{M}_D$. Moreover, we know by the classification of the C^*–subalgebras in $\mathcal{M}_D$ that there exists a unitary $V \in \mathcal{M}_D$ such that $V\mathcal{P}V^\dagger = \oplus_i (M_{n_i} \otimes \mathbb{1}_{n_i'}) = \mathcal{A}$.

The equivalent representation $V_g = V U_g V^\dagger$ is also an irrep and fulfils that $V_g \mathcal{A} V_g^\dagger = \mathcal{A}$. This means that the block structure of $\mathcal{A}$ remains invariant under the action of V_g by conjugation. Now we use that

$$V_g \mathcal{A} V_g^\dagger \subseteq \mathcal{A} \Leftrightarrow [J, \mathcal{A}] \subseteq \mathcal{A} \text{ for all } J \text{ generators .} \qquad (4.12)$$

This implies that J has the same block structure as $\mathcal{A}$. If there is more than one block, the representation is reducible. If $\mathcal{A} = M_n \otimes \mathbb{1}_{n'}$, then we use again Eq. 4.12: The Schmidt decomposition allows us to take $J = \sum_i A_i \otimes B_i$ where the B_i's form a basis of $M_{n'}$, with $B_1 = \mathbb{1}$. Then, Eq. 4.12 gives that $\sum_i [A_i, M_n] \otimes B_i = C \otimes \mathbb{1}$, which implies that A_i is proportional to $\mathbb{1}$ for all $i \geq 2$. This gives $J = \mathbb{1} \otimes X + Y \otimes \mathbb{1}$ and hence $V_g = V_1^g \otimes V_2^g$, which is reducible unless $\mathcal{A} = \mathbb{1}$ or $\mathcal{A} = M_N$ (which implies that $\mathcal{E}$ is the ideal channel). ∎

Although the implication in the opposite direction could also seem true, it is not, as shown by the following example.

Example 7 Let us consider the family of $SU(2)$ symmetric MPS of spin 1 with a reducible virtual representation $\frac{1}{2} \oplus \frac{3}{2}$ given by the following maps (see Section 4.3).

$$\tilde{V} = \begin{pmatrix} e^{i\alpha_{11}} \cos\theta_1 V_{\frac{1}{2}}^{\frac{1}{2}} & e^{i\alpha_{12}} \sin\theta_2 V_{\frac{1}{2}}^{\frac{3}{2}} \\ \\ e^{i\alpha_{21}} \sin\theta_1 V_{\frac{3}{2}}^{\frac{1}{2}} & e^{i\alpha_{22}} \cos\theta_2 V_{\frac{3}{2}}^{\frac{3}{2}} \end{pmatrix}$$

It is not difficult to check that the MPS is injective except for particular directions in space, such as those for which the isometry breaks into blocks, *i.e.* $\theta_i = n\frac{\pi}{2}$. □

Although the equivalence is not true in general, we can still give a sufficient condition which applies, for instance, to the AKLT and other FNW states. Let us recall from Theorems 25 and 26 that an injective symmetric MPS verifies

$$\sum_i u_{ij}^g A_i = e^{i\theta_g} U_g A_j U_g^\dagger \tag{4.13}$$

where in addition one may require that $\sum_i A_i A_i^\dagger = \mathbb{1}$.

Lemma 19 (Particular case where injectivity ⇒ irreducibility) *If u_g is irreducible and $\{A_i^\dagger A_j\}_{i,j}$ spans the whole space of matrices, then the virtual representation U_g of Eq. 4.13 is also irreducible.* □

Proof From (4.13) one gets

$$\sum_{i_1,i_2} \bar{u}_{i_1 j_1}^g u_{i_2 j_2}^g A_{i_1}^\dagger A_{i_2} = U_g A_{j_1}^\dagger A_{j_2} U_g^\dagger \, .$$

Integrating now with respect to the Haar Measure, the LHS is simplified by the irreducibility of u_g and the orthogonality relations. The result is $\delta_{j_1 j_2} \sum_i A_i^\dagger A_i = \delta_{j_1 j_2} \mathbb{1}$. This means that $\int_G U_g X U_g^\dagger \propto \mathbb{1}$, $\forall X \in \mathcal{M}_D$, since we can span the complete space of matrices. But this implies that U_g is an irrep by means of the inverse of Schur's lemma. ∎

If people don't believe that mathematics are simple, it's just because they don't realize how complicated life is.

John von Neumann
(1903-1957)

5

Multi–dimensional systems: Projected Entangled Pair States

5.1 Introduction

Projected Entangled Pair States emerge as the natural generalization of Matrix Product States to higher dimensions: where the latter are generated by matrices, *i.e.* a tensor with two legs in the virtual level, the former are constructed by means of multi–dimensional tensors [VC04a, PGVCW08].

In the construction, the tensors are placed forming a lattice with links (maximally entangled states) connecting sites. Distances among vertices are irrelevant for our purposes, with only the topological structure being of interest for us, *i.e.* the coordination number of each site, and with which other sites it is connected. Regardless, there exists a richness in the assortment of possible structures which makes these states in high dimensions even more fascinating and a never–ending source of unforeseen behaviours with often unpredictable consequences [Aue98].

Contrary to what happens for Matrix Product States, we cannot take advantage of a connection with completely positive maps, which leaves us with a much more complicated problem, but without a powerful mathematical *artillery*. This problem can sometimes be dodged by considering regular lattices susceptible of being transformed into one–dimensional problems where the results shown in previous chapters might be applied.

The representability of a state as a Projected Entangled Pair State involves a sharp reduction of the complexity of the multi–dimensional many–body problem, since these states, as in the case of the Matrix Product States, fulfil an area law.

This means that the entanglement between any region and the environment, *i.e.* the rest of the system, is proportional to the area of the boundary, and not to the bulk of the region.

The results shown in this Chapter, especially in Section 5.3, are published in [PGSGG+10]. The organization of this Chapter is essentially the same as in Chapter 1, which allows us to make the differences between both systems more illustrative.

- In Section 5.2, we start by explicitly constructing the Projected Entangled Pair States' expression in a general framework [PGVCW08], *i.e.* without assuming a regular lattice or translational invariance. We focus afterwards on the three topologically non–equivalent two–dimensional regular lattices, since they might be eventually transformed into a one–dimensional problem.

- As already shown for Matrix Product States, there exists a freedom in the choice of the tensor representation [PGSGG+10]. We prove in Section 5.3 that, for regular injective lattices, this freedom is reduced to the multiplication by invertible matrices in the virtual level. This is precisely the key for the existence of a canonical form for Projected Entangled Pair States.

5.2 Constructing Projected Entangled Pair States

Projected Entangled Pair States (PEPS) are the natural extension of Matrix Product States beyond the one–dimensional case. Although we follow in this Section the very general construction proposed in [PGVCW08], we focus afterwards on some regular lattices and translational invariant states. However, in principle, the great majority of the results shown in the following chapters are extendable to arbitrary dimensions, provided that the lattice can be generalized (essentially, the square lattice).

Let us consider a quantum state $|\psi\rangle$ corresponding to a many–body system with its particles distributed in the vertex of a certain (arbitrary) lattice. Then, we proceed as in the case of MPS [VC04a]:

1. We assign to the physical spin sitting at vertex ν as many virtual spins (local Hilbert spaces) as the coordination number e_ν of the vertex ν, each of them with dimension D. In principle, they can have different dimensions and depend simultaneously on the vertex, but we can always take D as the maximum of these dimensions and call it **bond dimension**, as in MPS.

2. We assign an unnormalized maximally entangled state $|\Omega\rangle = \sum_{\alpha=1}^{D} |\alpha,\alpha\rangle$ to each bond. This is what we call here the **virtual substructure** of the PEPS.

3. We apply a map in each vertex ν,

$$\mathcal{A}_\nu : \mathcal{H}_1^{(D)} \otimes \cdots \otimes \mathcal{H}_{e_\nu}^{(D)} \to \mathcal{H}^{(d_\nu)} \qquad (5.1)$$

which maps the virtual spins to the physical one. By writing the map in a basis,

$$A^{(\nu)} = \sum_{i=1}^{d_\nu} \sum_{j_1,\ldots,j_{e_\nu}}^{D} (A_i^{[\nu]})_{j_1\ldots j_{e_\nu}} |i\rangle\langle j_1 \ldots j_{e_\nu}| \qquad (5.2)$$

where e_ν is the **number of edges** at vertex ν or its **coordination number**, as pointed out above. For the sake of simplicity in the notation, we consider that $d_\nu = d$, but it can be written in general without difficulty.

4. Finally, we have to contract the tensor network. As this process is not as simple as in MPS, where it is translated into products of matrices, we will stress that the virtual substructure is contracted by means of a **contracting operator** $\mathcal{C}$, which takes care of the lattice structure. This contraction can be performed with a vector in the boundaries, which leads to OBC, or with the other edges forming a torus (see Fig. 5.1), leading to PBC.

Therefore, we can now enunciate the following definitions.

Definition 21 (PEPS–OBC) Let us consider a lattice with N sites, in each of which a d–dimensional physical spin, and a virtual substructure with bond dimension D are sited. If the open boundary conditions are given by the vector $|\phi_{BC}\rangle$[1], any **Projected Entangled Pair State with Open Boundary Conditions** (PEPS–OBC) has the structure:

$$|\psi\rangle = \sum_{i_1,\ldots,i_N}^{d} \mathcal{C}_{|\phi_{BC}\rangle}\left[\{A_{i_\nu}^{[\nu]}\}_\nu\right] |i_1,\ldots,i_N\rangle \qquad (5.3)$$

where $\mathcal{C}$ implicitly depends on the lattice structure. □

The definition for periodic boundary conditions straightforwardly follows,

Definition 22 (PEPS–PBC) Let us consider a lattice with N sites, in each of which a d–dimensional physical spin, and a virtual substructure with bond dimension D are sited, as shown in Fig. 5.1. Then, any **Projected Entangled Pair State with Periodic Boundary Conditions** (PEPS–PBC) has the structure:

$$|\psi\rangle = \sum_{i_1,\ldots,i_N}^{d} \mathcal{C}\left[\{A_{i_\nu}^{[\nu]}\}_\nu\right] |i_1,\ldots,i_N\rangle \qquad (5.4)$$

where $\mathcal{C}$ implicitly depends on the lattice structure. □

[1]The boundary conditions are normally encoded in tensor which is contracted with all the open bonds of the lattice. However, as in the one–dimensional case, the tensor can be decomposed into a linear combination of vectors, which justifies our notation.

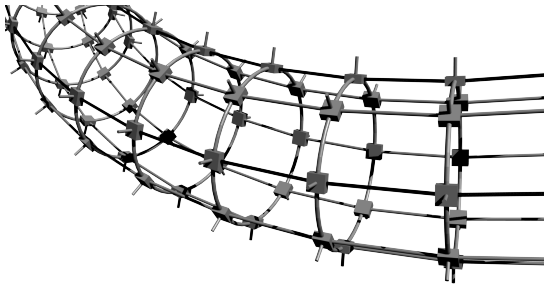


Figure 5.1: **PEPS-PBC**. A Projected Entangled Pair State with periodic boundary conditions on a square lattice is nothing but a tensor network with a toroidal topology.

5.2.1 Regular 2D lattices

In this Subsection, we focus on the regular 2D lattices, which are the simplest and, therefore, the most interesting ones (a significant number of materials in Nature correspond to these crystallographic structures). Additionally, the generalization to regular lattices in higher dimensions is often simple, like in the case of the cubic lattice.

It is well–known that there are five regular lattices in 2D [AM76, Chapter 1], known as Bravais lattices. These lattices are: oblique, rectangular, square, centered rectangular (triangular) and hexagonal (honeycomb). However, the PEPS construction is not based on distances between vertices or angles between bonds, but only on the coordination number of each vertex, as shown in Fig. 5.2. This means that the first three lattices are topologically equivalent, so the problem is reduced to the three following structures:

1. **Square lattice**, with coordination number 4. (See Fig. 5.2a)
2. **Hexagonal lattice**, with coordination number 3. (See Fig. 5.2b)
3. **Triangular lattice**, with coordination number 6. (See Fig. 5.2c)

We are particularly interested in the first case, the *square lattice*. Let us consider an $N \times M$ square lattice on a torus (PBC) and a PEPS–PBC defined there. Then, Eq. 5.4 is transformed into:

$$|\psi^{(N,M)}\rangle = \sum_{i_{1,1},\ldots,i_{N,M}} \mathcal{C}\left[\{A^{[j,k]}_{i_{j,k}}\}_{j,k}\right] |i_{1,1}\ldots i_{N,M}\rangle$$

It is clear that, if the tensors $\{A^{[j,k]}_{i_{j,k}}\}$ do not depend on the position $[i,j]$, then the state is translational invariant (in the sense of Definition 2, which is the definition that we assume in this Chapter). The converse is also true, as in MPS. For any translational invariant PEPS, there is always a representation (possibly with larger

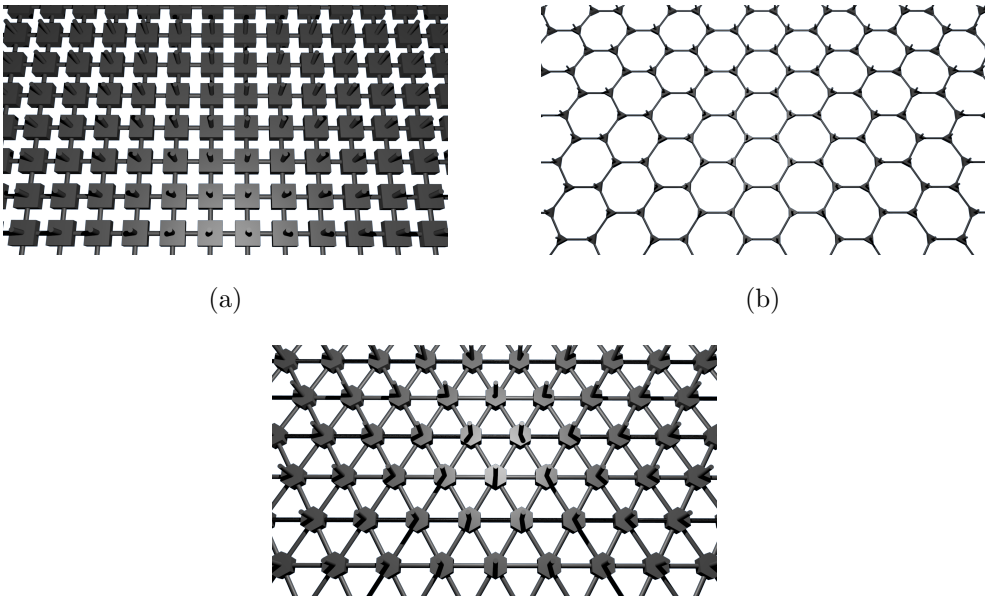


Figure 5.2: **Regular 2D lattices**. (a) Square lattice. (b) Hexagonal or honeycomb lattice. (c) Triangular lattice.

bond dimension, as in MPS) with site–independent tensors $A_i^{[j,k]} = A_i$. This was proven in [PGVCW08, Appendix] and it is summarized in the following Theorem:

Theorem 29 (Site–independent representation of TI–PEPS) *Let $|\psi^{(N,M)}\rangle$ be a translational invariant PEPS, in the sense of Definition 2, defined on an $N \times M$ square lattice by the site–dependent tensors $\{A_{i_{j,k}}^{[j,k]}\}$. Then, there exists a site–independent representation $\{B_{i_{j,k}}\}$ of this state with, in general, larger bond dimension.* □

Proof The proof is similar to the proof of Theorem 3. Let us write the tensor in a basis

$$A_i^{[j,k]} = \sum_{u,d,l,r=1}^{D} (A_i^{[j,k]})_{udlr} \, |l\rangle\langle r|_h \otimes |u\rangle\langle d|_v$$

where h (or v) indicate that we are alluding to the Hilbert spaces in the horizontal (or vertical) bonds. The horizontal contraction of two tensors leads to

$$A_{i_{jk}}^{[j,k]} — A_{i_{j+1k}}^{[j+1,k]} = \sum_{\substack{u_1,d_1,l_1 \\ u_2,d_2,r_2 \\ a}}^{D} (A_{i_{jk}}^{[j,k]})_{u_1 d_1 l_1 a} (A_{i_{j+1k}}^{[j+1,k]})_{u_2 d_2 a r_2} (|l_1\rangle\langle r_2|_h \otimes |u_1, u_2\rangle\langle d_1, d_2|_v)$$

By using this notation, let us define the new *site–independent tensors*:

$$B_i = \left(\frac{1}{NM}\right)^{\frac{1}{NM}} \sum_{\substack{u,d,l,r \\ j,k}} (A_{i_{jk}}^{[j,k]})_{udlr} \, |j,k,l\rangle\!\rangle j,k+1,r| \, {}_h \otimes \, |k,j,u\rangle\!\rangle k,j+1,d| \, {}_v \qquad (5.5)$$

It is trivial to see that the state can be written in terms of these tensors

$$|\psi^{(N,M)}\rangle = \sum_{i_{11},\ldots,i_{NM}} \mathcal{C}\left[\{B_{i_{j,k}}\}_{j,k}\right] \, |i_{11}\ldots i_{NM}\rangle$$

which proves the Theorem. ∎

Let us remark that one can do exactly the same in the triangular lattice, by adding a couple of extra virtual bonds.

The hexagonal lattice is slightly different, because the unit cell contains two (non–equivalent) sites so, in general, the translational invariance refers to the *unit cell* and not to the vertex itself. However, proving the existence of TI (for the unit cell) representation in the hexagonal lattice is trivial, since we only have to couple both of the sites which compose the unit cell to obtain the square lattice and then apply Theorem 29.

5.3 A canonical form for PEPS

This is undoubtedly the main section of this Chapter, since we provide here a sort of generalization for PEPS in a square lattice of the fruitful canonical form constructed for MPS in Theorem 4. We prove in this Section that, for injective states, two PEPS on a square lattice are equal iff they are related by invertible matrices in the virtual bond (see Fig. 5.3). Although the result for PEPS is not as strong as for MPS, due to the absence of a connection with completely positive maps, this allows us to prove, for instance, the results shown in Chapter 7.

5.3.1 Canonical form for MPS: improvement

Let us start by proving Theorem 5, *i.e.* the gauge freedom for MPS. It is shown in [PGVWC07, Theorem 7] that two injective representations of the same MPS must be related by an invertible matrix X as $A_i = XB_iX^{-1}$. This holds if the number of sites satisfies $N \geq 2L_0 + D^4$, where L_0 is the injectivity length and D is the bond dimension of the MPS. Since we are interested in applying this to a column of a PEPS (see the argument in Theorem 31 below), the exponential dependence on D would be critical. Therefore, in this Subsection, we modify the proof of [PGVWC07, Theorem 6] to make N depend only on L_0. In particular, we obtain that the result holds when $N \geq 4L_0 + 1$, as stated in Theorem 5.

Theorem 30 (Gauge freedom for TI–MPS) *Let*

$$|\psi_A^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[A_{i_1}\cdots A_{i_N}\right]|i_1\ldots i_N\rangle$$

and

$$|\psi_B^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} \mathrm{tr}\left[B_{i_1}\cdots B_{i_N}\right]|i_1\ldots i_N\rangle$$

be two injective TI–MPS representations with bond dimension D, and injectivity length L_0. If $|\psi_A^{(N)}\rangle = |\psi_B^{(N)}\rangle$ and $N \geq 4L_0+1$, then there exists an invertible matrix R such that $A_i = RB_iR^{-1}$, for all i. □

Proof We can obtain an OBC representation by observing that

$$|\psi_A^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} a_{i_1}^{[1]}(A_{i_2}\otimes\mathbb{1})\cdots(A_{i_{N-1}}\otimes\mathbb{1})a_{i_N}^{[N]}|i_1\ldots i_N\rangle$$

where $a_i^{[1]}$ is the vector that contains all the rows of A_i and $a_i^{[N]}$ is the vector that contains all the columns in A_i. By doing the same with the B's

$$|\psi_B^{(N)}\rangle = \sum_{i_1,\ldots,i_N=1}^{d} b_{i_1}^{[1]}(B_{i_2}\otimes\mathbb{1})\cdots(B_{i_{N-1}}\otimes\mathbb{1})b_{i_N}^{[N]}|i_1\ldots i_N\rangle$$

we obtain an OBC canonical representation (with C–matrices for the A's and D–matrices for the B's). By means of Theorem 2, we obtain Y_j, Z_j, R_j and S_j with $Y_jZ_j = \mathbb{1}$, $R_jS_j = \mathbb{1}$ such that:

$$\begin{aligned} C_i^{[1]} &= a_i^{[1]}Z_1, C_i^{[N]} = Y_{N-1}a_i^{[N]} \\ C_i^{[m]} &= Y_{m-1}(A_i\otimes\mathbb{1})Z_m \text{ for } 1<m<N \\ D_i^{[1]} &= b_i^{[1]}S_1, D_i^{[N]} = R_{N-1}b_i^{[N]} \\ D_i^{[m]} &= R_{m-1}(B_i\otimes\mathbb{1})S_m \text{ for } 1<m<N \end{aligned}$$

Additionally, by using [HJ91, Theorem 3.1.1'], we get that any two OBC canonical representations are related by unitary matrices, *i.e.* there exist $V_1,\ldots,V_{N-1}$ such that:

$$\begin{aligned} C_i^{[1]}V_1^\dagger = D_i^{[1]}, V_{N-1}C_i^{[N]} = D_i^{[N]} \\ V_{j-1}C_i^{[j]}V_j^\dagger = D_i^{[j]} \text{ for } 1<j<N \end{aligned}$$

By using injectivity now, we know that Y_s, Z_s, R_s, S_s are invertible for $L_0 \leq s \leq N-L_0$ and so are the matrices $W_k \in \mathcal{M}_{D^2}$ defined as:

$$W_k = S_{L_0+k} V_{L_0+k} Y_{L_0+k} \qquad k = 0, \ldots, 2L_0 + 1$$

It is easy to verify that

$$W_k (A_i \otimes \mathbb{1}) W_{k+1}^{-1} = (B_i \otimes \mathbb{1}) \text{ for } 0 \leq k \leq 2L_0,$$

for all i. In fact, by grouping and denoting $A_{I_l} = A_{i_1} \cdots A_{i_l}$, we have that

$$W_m (A_{I_{n-m}} \otimes \mathbb{1}) W_n^{-1} = B_{I_{n-m}} \otimes \mathbb{1} \tag{5.6}$$

for every $0 \leq m < n \leq 2L_0 + 1$ and every multi–index I_{n-m}. Then, for adequate values of m and n, we obtain

$$W_{k+1}^{-1} W_k (A_{I_{2L_0-k}} \otimes \mathbb{1}) W_{2L_0}^{-1} W_{2L_0+1} = A_{I_{2L_0-k}} \otimes \mathbb{1}$$

for every $0 \leq k \leq L_0$.

As we are in an injective region for every k, the matrix could be taken as the identity and then we get that

$$T \equiv W_{k+1}^{-1} W_k = W_{2L_0+1}^{-1} W_{2L_0} \tag{5.7}$$

for every $0 \leq k \leq L_0$.

Therefore, $T(X \otimes \mathbb{1})T^{-1} = (X \otimes \mathbb{1})$ for every X. Let us make use of the following Lemma, which is a consequence of [HJ91, Theorem 4.4.14].

Lemma 20 (Property of linear systems) *If $B, C \in \mathcal{M}_n$, the space of solutions of the matrix equation*

$$W(C \otimes \mathbb{1}) = (B \otimes \mathbb{1})W$$

is $S \otimes M_n$, where S is the space of solutions of the equation $XC = BX$. □

It is easy to deduce from this Lemma that $T = \mathbb{1} \otimes \tilde{T}$, so that

$$W_{L_0}^{-1} W_0 = W_{L_0}^{-1} W_{L_0-1} W_{L_0-1}^{-1} \cdots W_0 = (\mathbb{1} \otimes \tilde{T})^{L_0}$$

from where we obtain

$$W_{L_0}^{-1} = (\mathbb{1} \otimes \tilde{T}^{L_0}) W_0^{-1}$$

and, in the same way,

$$W_{L_0+1}^{-1} = (\mathbb{1} \otimes \tilde{T}^{L_0+1}) W_0^{-1}$$

By replacing these results in Eq. 5.6:

$$(B_{I_{L_0}} \otimes \mathbb{1}) = W_0 (A_{I_{L_0}} \otimes \mathbb{1}) W_{L_0}^{-1} = W_0 (A_{I_{L_0}} \otimes \tilde{T}^{L_0}) W_0^{-1}$$
$$(B_{I_{L_0+1}} \otimes \mathbb{1}) = W_0 (A_{I_{L_0+1}} \otimes \mathbb{1}) W_{L_0+1}^{-1} = W_0 (A_{I_{L_0+1}} \otimes \tilde{T}^{L_0+1}) W_0^{-1}$$

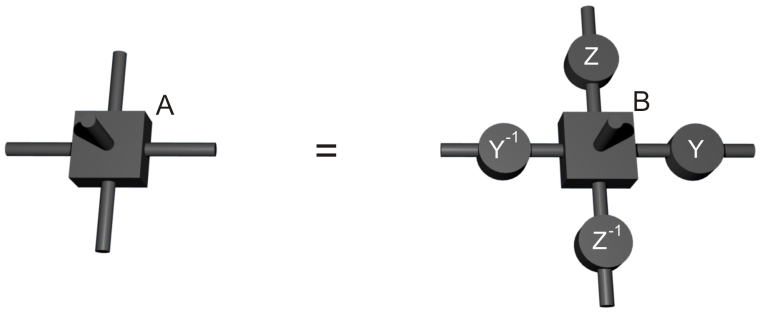


Figure 5.3: **Canonical form in square lattice**. Representation of the relationship which the tensors defining two TI–PEPS on a square lattice must fulfil in order to represent the same state.

By using the fact that $B_{I_{L_0}}$ and $B_{I_{L_0+1}}$ are injective, we can sum with appropriate coefficients to obtain $\mathbb{1}$ on the LHS. Then, we get that $\tilde{T}^{L_0} = \mathbb{1} = \tilde{T}^{L_0+1}$, which gives $\tilde{T} = \mathbb{1}$, and hence, $B_i \otimes \mathbb{1} = W_0(A_i \otimes \mathbb{1})W_0^{-1}$ for all i.

By means of Theorem 4 and Lemma 6, we can assume w.l.o.g. that $\sum_i A_i A_i^\dagger = \mathbb{1}$ and that $\sum_i B_i^\dagger \Lambda B_i = \Lambda$ for a full–rank diagonal matrix Λ. The proof follows straightforwardly, as in [PGVWC07, Theorem 7]. ∎

This Theorem gives the proof of Theorem 5, that we left unproven, due to the fact that injectivity was not defined at that moment.

5.3.2 Canonical form for PEPS

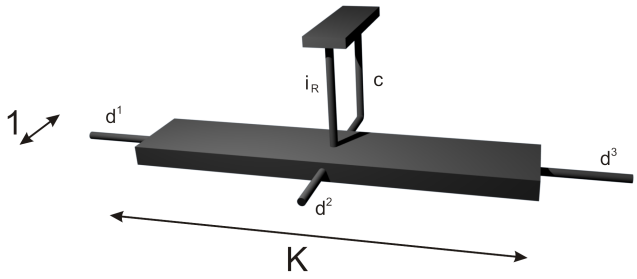
In this Subsection, we show that Theorem 30 holds in any spatial dimension: two injective representations of the same TI–PEPS are related by the trivial gauge freedom in the bonds, as shown in Fig. 5.3. In this Section, we make use of the extension to higher dimensions of the concept of injectivity defined in Chapter 2. Check Section 6.2 in general, and particularly Definition 23 for further details.

We prove the result in 2D by using the result in 1D proven in Theorem 30. This argumentation can be generalized to higher spatial dimensions by induction. We initially consider a square lattice, but we show at the end of the Section how to extend the result to other regular lattices.

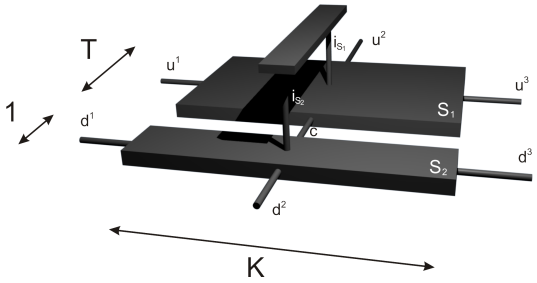
We need to prove several previous lemmas before proving the main result. The first one advances a result that should appear in Section 6.2, but that we require here in this proof.

Lemma 21 (Injectivity remains) *If a region of size $H \times K$ of a TI–PEPS is injective, then a region of size $(H+1) \times K$ (and $H \times (K+1)$) is also injective.* □

Proof Let us start by claiming the following: If a region with size $H \times K$ is injective, then a region with size $1 \times K$ is also injective when one of the sides of



(a)



(b)

Figure 5.4: Representation of the argument used to prove Lemma 21.

the square (for instance, the upper one), and the physical indices are considered as inputs (see Fig. 5.4a). To see this, we take an injective region S of dimension $H \times K$ and split it into two subregions S_1, S_2, as in Fig. 5.4b with $T = H - 1$. For simplicity, in the rest of the proof we gather the indices u_1, u_2, u_3 and d_1, d_2, d_3 which appear in Fig. 5.4, calling them u and d, respectively. We also gather all the physical indices of region S_1 into the index i_{S_1}, and all the physical indices of region S_2 into the index j_{S_2}.

By using the injectivity of the region S, there exists $\{\alpha_{i_{S_1},j_{S_2},u_0,d_0}\}_{i_{S_1},j_{S_2}}$ for any u_0, d_0 such that

$$\sum_{c,i_{S_1},j_{S_2}} \alpha_{i_{S_1},j_{S_2},u_0,d_0} (A^{[S_1]}_{i_{S_1}})_{u,c} (A^{[S_2]}_{j_{S_2}})_{c,d} = \delta_{u,u_0}\delta_{d,d_0}$$

By taking $u = u_0$, we get

$$\sum_{c,i_{S_1},j_{S_2}} \alpha_{i_{S_1},j_{S_2},u_0,d_0} (A^{[S_1]}_{i_{S_1}})_{u_0,c} (A^{[S_2]}_{j_{S_2}})_{c,d} = \delta_{d,d_0}$$

which proves the claim.

Now, if we take a new region S of size $(H+1) \times K$ and divide it into two parts

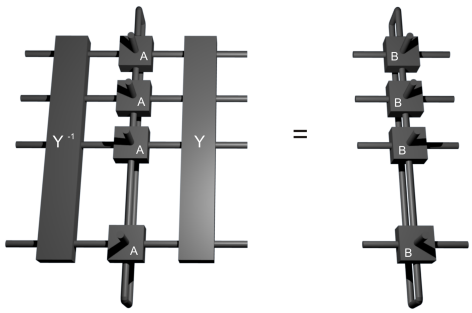


Figure 5.5: **Dimensional reduction**. Reduction from the 2D case to the 1D problem. This allows us to apply the results shown in Chapters 1 to 4.

S_1, S_2, as in Fig. 5.4b, with $T = H$ then, by applying the claim above, there exists $\{\beta_{j_{S_2},c,d_0}\}_{j_{S_2},c}$ for any d_0, such that

$$\sum_{j_{S_2},c} \beta_{j_{S_2},c,d_0} (A^{[S_2]}_{j_{S_2}})_{c,d} = \delta_{d,d_0}$$

By using the injectivity of a region of dimension $H \times K$, there exists $\{\alpha_{i_{S_1},j_{S_2},u_0,c_0,d_0}\}_{i_{S_1}}$ such that

$$\sum_{i_{S_1}} \alpha_{i_{S_1},j_{S_2},u_0,c_0,d_0} (A^{[S_1]}_{i_{S_1}})_{u,c} = \beta_{j_{S_2},c_0,d_0} \delta_{u,u_0} \delta_{c,c_0}$$

Gathering both equalities, we find

$$\begin{aligned}
\sum_{c,c_0,i_{S_1},j_{S_2}} \alpha_{i_{S_1},j_{S_2},u_0,c_0,d_0} (A^{[S_1]}_{i_{S_1}})_{u,c} (A^{[S_2]}_{j_{S_2}})_{c,d} &= \sum_{c,c_0,j_{S_2}} \beta_{j_{S_2},c_0,d_0} \delta_{u,u_0} \delta_{c,c_0} (A^{[S_2]}_{j_{S_2}})_{c,d} \\
&= \sum_{c_0 j_{S_2}} \beta_{j_{S_2},c_0,d_0} \delta_{u,u_0} (A^{[S_2]}_{j_{S_2}})_{c_0,d} \\
&= \delta_{u,u_0} \delta_{d,d_0}
\end{aligned}$$

Therefore, S is an injective region and the Lemma is proven. ∎

This allows us to reduce the 2D case with size $L \times N$ to the 1D case by grouping all the tensors from a column. The 1D case (Theorem 30) ensures that there is a global invertible matrix Y which verifies the equality in Fig. 5.5, provided that $L \geq 4L_0 + 1$ (hence, it can be taken $L \geq 5L_0$). Y acts on a column of virtual systems, so it maps $Y : (\mathbb{C}^D)^{\otimes L} \to (\mathbb{C}^D)^{\otimes L}$. The next step is to show that:

Lemma 22 (Y maps tensor states to product states) *Y maps product vectors into product vectors, i.e. $Y \bigotimes_{i=1}^{L} |x_i\rangle = \bigotimes_{j=1}^{L} |y_j\rangle$.* □

Proof In order to prove the Lemma, we prove that $Y \bigotimes_i |x_i\rangle$ is a vector with the following property:

(*) It is a product in *any* bipartition $R - S$, for compact regions (of consecutive sites) R and S with a size larger than or equal to $\frac{L}{5}$ (note that this condition comes from the fact that $L \geq 4L_0 + 1$).

Any vector with property (*) is obviously a product vector, which implies the result of the Lemma. We prove this by contradiction.

Let us take a product $\otimes_i |x_i\rangle$ and assume that this product is mapped by Y into a vector with Schmidt decomposition $Y(\bigotimes_i |x_i\rangle) = \sum_r \beta_r |v_r w_r\rangle$ in a partition $R - S$ for compact regions of consecutive sites and size larger than or equal to $\frac{L}{5}$. Due to the properties of the Schmidt decomposition, the vectors $\{|v_r\rangle \in (\mathbb{C}^D)^{\otimes R}\}$ and $\{|w_r\rangle \in (\mathbb{C}^D)^{\otimes S}\}$ are orthonormal. For the same bipartition, we denote $\bigotimes_i \langle x_i| Y^{-1} = \sum_r \alpha_r \langle v'_r w'_r|$, which could be a product. Let us now gather $\frac{N}{5}$ columns and sandwich both sides of the equality shown in Fig. 5.5 with the product state $\bigotimes_i |x_i\rangle$.

The goal is now to analyse the Schmidt rank between the two physical $R \times \frac{N}{5}$ and $S \times \frac{N}{5}$ regions in both the right and left part of the equality in Fig. 5.5, in order to find a contradiction in the initial hypothesis. The RHS clearly gives $D^{2\frac{N}{5}}$ by using injectivity as in Subsubsection 1.4.3.1. The Kraus operators (the state is now an MPS) have bond dimension $D^{\frac{N}{5}}$

$$\begin{aligned}
|\psi\rangle &= \sum_{i_1,\ldots,i_L} \mathrm{tr}\left[A^{[1]}_{i_1} \cdots A^{[L]}_{i_L}\right] |i_1 \ldots i_L\rangle \\
&= \sum_{i_1,\ldots,i_L} \sum_{\alpha,\beta} \langle\alpha| A^{[1]}_{i_1} \cdots A^{[R]}_{i_R} |\beta\rangle\langle\beta| A^{[R+1]}_{i_{R+1}} \cdots A^{[L]}_{i_L} |\alpha\rangle |i_1 \ldots i_L\rangle \\
&= \sum_{\alpha,\beta} |\psi_{\alpha\beta}\rangle \otimes |\tilde{\psi}_{\alpha\beta}\rangle
\end{aligned}$$

as both regions are injective, the Schmidt rank is indeed $D^{2\frac{N}{5}}$.

Let us focus now on the LHS. By performing the changes of bases $|r\rangle \mapsto |v_r\rangle$ and $|r\rangle \mapsto |w_r\rangle$ (and the same for the primes) to tensors $A^{[R\times\frac{N}{5}]}$ and $A^{[S\times\frac{N}{5}]}$ in the LHS, new tensors A' and A'' are obtained. We get from them that

$$|\psi\rangle = \sum_{abcd} \alpha_a \beta_c [\sum_i (A'_i)_{abcd} |i\rangle][\sum_j (A''_j)_{adcb} |j\rangle]$$

By means of injectivity, we know that the set $\{\sum_i (A'_i)_{abcd} |i\rangle\}_{abcd}$ is linearly independent (and the same for A''). This means that the Schmidt rank of the LHS is, at least, $2D^{2\frac{N}{5}}$, which is the desired contradiction. ∎

The following three lemmas specify the form of Y. The first one uses Lemma 22 to prove the tensor structure of Y.

Lemma 23 (Tensor structure of Y) *If Y is invertible and maps products to products, then it presents a tensor structure, i.e. it is of the form $P_\pi(Y_1 \otimes \cdots \otimes Y_L)$ where P_π implements a permutation π among the Hilbert spaces.* □

PROOF We reason in the bipartite case for the sake of simplicity, since the argument can be straightforwardly generalized to the general case by induction. Let $Y : \mathbb{C}^D \otimes \mathbb{C}^D \longrightarrow \mathbb{C}^D \otimes \mathbb{C}^D$ be an invertible matrix which maps products to products and let $\{|i,j\rangle\}_{i,j=1}^D$ be the product basis. Then, we can denote $Y|i,1\rangle = |\alpha_i, \beta_i\rangle$. If we take $i_0 \neq i_1 \in \{1,...,D\}$, then $Y(|i_0,1\rangle + |i_1,1\rangle) = |\alpha_{i_0},\beta_{i_0}\rangle + |\alpha_{i_1},\beta_{i_1}\rangle$ is a product because the initial state is a product state. Then, at least one of the vectors indexed by i_0 must be proportional to its counterpart indexed by i_1:

(I) either $|\alpha_{i_0}\rangle \propto |\alpha_{i_1}\rangle$ and $|\beta_{i_0}\rangle \not\propto |\beta_{i_1}\rangle$,

(II) or $|\alpha_{i_0}\rangle \not\propto |\alpha_{i_1}\rangle$ and $|\beta_{i_0}\rangle \propto |\beta_{i_1}\rangle$.

The case where both are proportional is discarded, since Y is invertible and it cannot map two orthogonal vectors to the same vector. However, let us prove that we are always in the same case:

1. If $D = 2$, then (I) and (II) are equal, so there is only one case.

2. Otherwise, if $D > 2$, then we can always take three different $i_0, i_1, i_2 \in \{1,...,D\}$ such that $|\alpha_{i_0}\rangle \not\propto |\alpha_{i_1}\rangle$ and $|\beta_{i_1}\rangle \not\propto |\beta_{i_2}\rangle$. Therefore, we reach a contradiction from the fact that $Y(|i_0,1\rangle + |i_2,1\rangle)$ is a product.

The same argumentation can be carried out for the second tensor. Therefore, we can assume w.l.o.g. that

$$Y|i,1\rangle = |\alpha_i, \beta_1\rangle$$

which means that the second subspace does not depend on the first one and

$$Y|1,j\rangle = |\alpha_1, \beta_j\rangle$$

In the other case, we just permute the indices by means of the swap operator P_π.

Let us consider $Y|i,j\rangle = |a_{i,j}, b_{i,j}\rangle$. Now, due to the fact that:

$$Y(|i,j\rangle + |i,1\rangle) = |a_{i,j}, b_{i,j}\rangle + |\alpha_i, \beta_1\rangle$$

is a product, we obtain that $\alpha_i \propto a_{i,j}$ or $\beta_1 \propto b_{i,j}$. However, the second case is only possible if $j = 1$, because of the invertibility of Y, so $a_{i,j} \propto \alpha_i$. A similar argumentation on the second tensor gives $Y|i,j\rangle = c_{i,j}|\alpha_i, \beta_j\rangle$. By making now $Y(\sum_{i,j=1}^d |ij\rangle) = \sum_{i,j=1}^D c_{i,j}|\alpha_i,\beta_j\rangle$, and by using the fact that the *Schmidt rank* of the resulting vector must be 1, we conclude that matrix $(c_{i,j})_{i,j}$ has rank 1 and, therefore, is of the form $c_{i,j} = r_i s_j$, giving $Y|i,j\rangle = |r_i\alpha_i, s_j\beta_j\rangle$, which is the desired result. ∎

Let us now show that P_π is the trivial permutation:

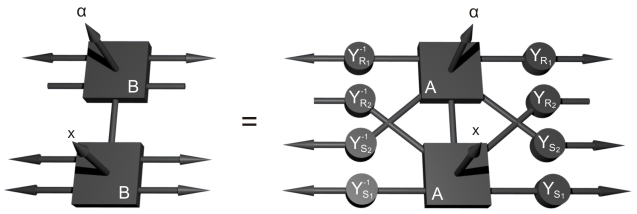


Figure 5.6: **Proof of Lemma 24**. The upper squares correspond to $B^{[R\times\frac{N}{5}]}$, $A^{[R\times\frac{N}{5}]}$ and the lower ones to $B^{[S\times\frac{N}{5}]}$, $A^{[S\times\frac{N}{5}]}$. The cones represent vectors multiplying the legs of the tensor. In the virtual space, these vectors are $|0\rangle$, while the vectors in the leg corresponding to the physical space are $|x\rangle$ and $|\alpha\rangle$ respectively.

Lemma 24 (P_π is the trivial permutation) *The permutation operator P_π which appears in Lemma 23 is trivial, i.e. $P_\pi = \mathbb{1}$.* □

Proof Let us prove the Lemma by contradiction and assume that P_π is not the identity. By taking a $R-S$ bipartition (with sizes larger than or equal to $\frac{L}{5}$) such that P_π maps one Hilbert space of R into one of S. We block again $\frac{N}{5}$ columns to get two injective regions with sizes $R\times\frac{N}{5}$ and $S\times\frac{N}{5}$, respectively. Let us denote by R_1 and S_1 the subregions which stay within the regions, and by R_2, S_2 the ones that are mapped to the other side. Then, we can decompose Y as in Fig. 5.6.

Let us consider now Fig. 5.6. We contract all virtual indices (except the pair in the second row) with $|0\rangle$ and the physical indices with $|\alpha\rangle$ and $|x\rangle$, where the latter is chosen in such a way that $A^{[S\times\frac{N}{5}]}|x\rangle = |0\rangle|0\rangle|0\rangle|0\rangle|0\rangle$. Since the dimensions corresponding to the five virtual systems arising in the decomposition of $A^{[S\times\frac{N}{5}]}$ are different, $|0\rangle$ can be taken as any *fixed* vector in each one of these systems (the same occurs for $A^{[R\times\frac{N}{5}]}$). Let V be the linear space spanned in the remaining two virtual indices under the variation of $|\alpha\rangle$. It is clear that, in the LHS of Fig. 5.6, $\dim V = \dim(\mathrm{supp}(Y_{R_2}))$, whereas $\dim V = 1$ in the RHS, which leads to a contradiction unless R_2 and S_2 are empty. ■

By using both the injectivity and the translational invariance of the RHS term in Fig. 5.5, we observe that:

Lemma 25 (Y is translational invariant) *From Lemma 23 and 24, we know that $Y = \bigotimes_k Y_k$. Moreover, $Y_i = Y_1$ for all i.* □

Proof The proof follows straightforwardly from the translational invariance. ■

Let us now study the orthogonal direction. Then, we can prove the following Lemma:

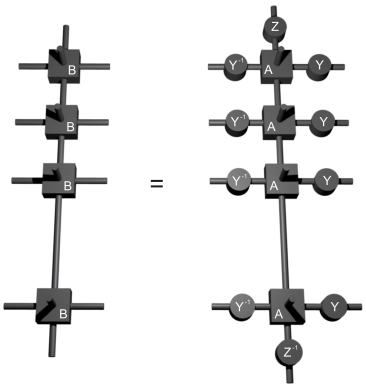


Figure 5.7: **Proof of Lemma 26 (a)**. Under the conditions of Theorem 31, rows of K spins are related by invertible matrices as in the figure as long as $K \geq \frac{N}{5}$. The analogue property holds for columns of H spins as long as $H \geq \frac{L}{5}$.

Lemma 26 (Orthogonal direction) *Let K be any length for which one gets injectivity in the orthogonal direction, then we obtain the structure shown in Fig. 5.7. The case where vertical is interchanged with horizontal is equivalent.* □

PROOF We redefine now A_i as $\sum_{abcd}(A_i)_{abcd}(Y_1^{-1}\otimes\mathbb{1})\,|ab\rangle\langle cd|\,(Y_1\otimes\mathbb{1})$, *i.e.* we incorporate Y_1 and Y_1^{-1} into tensor A. Then, we block $\frac{N}{5}$ columns together and sandwich them with $|n\rangle^{\otimes L}$ and $\langle m|^{\otimes L}$ in Fig. 5.5. By defining $\tilde{A}^{(mn)}$ as

$$\sum_{bd}(\tilde{A}_i^{(mn)})_{bd}\,|b\rangle\langle d| \;=\sum_{bd}\langle m|\,A_i^{[1\times\frac{N}{5}]}\,|n\rangle\;|b\rangle\langle d|$$

and doing the analogue for $\tilde{B}^{(mn)}$, we have two injective representations of the same MPS (with bond dimension $D^{\frac{N}{5}}$). By means of the results for the 1D case shown in Theorem 30, we obtain invertible matrices Z_{nm} acting on $(\mathbb{C}^D)^{\otimes\frac{N}{5}}$ such that $Z_{mn}^{-1}\tilde{A}_i^{(mn)}Z_{mn}=\tilde{B}_i^{(mn)}$ for all i.

The next step is to show that Z_{mn} does not depend on m and n. We sandwich Fig. 5.5 with $\langle m'|^{\otimes\frac{L}{2}}\langle m|^{\otimes\frac{L}{2}}$ and $|n'\rangle^{\otimes\frac{L}{2}}\,|n\rangle^{\otimes\frac{L}{2}}$, getting Fig. 5.8. By summing with appropriate coefficients in order to obtain Kronecker deltas, we get that $\langle l|\,Z_{mn}Z_{m'n'}^{-1}\,|k\rangle\langle r|\,Z_{mn}^{-1}Z_{m'n'}\,|s\rangle=\delta_{kl}\delta_{rs}$, so $Z_{mn}=Z$ is indeed independent of m and n. By reasoning as above, but in the opposite direction, one can prove that $Z=Z'^{\otimes\frac{N}{5}}$. ■

We proceed now to the proof of the main Theorem:

Theorem 31 (Canonical form for TI–PEPS) *Let $|\psi_A^{(L,N)}\rangle$ and $|\psi_B^{(L,N)}\rangle$ be two PEPS in an $L\times N$ square lattice, defined by tensors $A_i=\sum_{abcd}(A_i)_{abcd}\,|ab\rangle\langle cd|$ and $B_i=\sum_{abcd}(B_i)_{abcd}\,|ab\rangle\langle cd|$, with the property that for a region of size smaller than $\frac{L}{5}\times\frac{N}{5}$ both PEPS are injective. Then, the states are equal $|\psi_A^{(L,N)}\rangle=|\psi_B^{(L,N)}\rangle$ iff there exist invertible matrices Y,Z such that $A_i=(Y^{-1}\otimes Z^{-1})B_i(Y\otimes Z)$ for all i (Fig. 5.3). Moreover, Y and Z are unique.* □

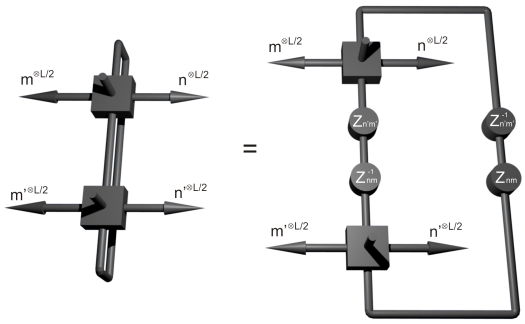


Figure 5.8: **Proof of Lemma 26 (b)**. All squares in the figure correspond to the gathered tensor $A^{[\frac{L}{2}\times\frac{N}{5}]}$. The cones in the boundary represent tensor products of $\frac{L}{2}$ local vectors in the virtual space.

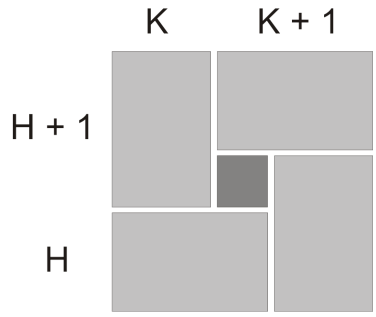


Figure 5.9: **Regions of Theorem 31**. Representation of the injectivity regions for the proof of Theorem 31.

PROOF Uniqueness is a straightforward consequence of injectivity. Let us now prove the existence part.

Let us consider a $H \times K$ injective region, for instance $H = \frac{L}{5}$, $K = \frac{N}{5}$. From Lemma 21, the larger regions in Fig. 5.9 are also injective. If we replace Fig. 5.7, first in each subregion (not the center), and then in the whole region, we get the desired result by using injectivity in the four subregions. ∎

5.3.2.1 Hexagonal lattice

As we said in the introduction of this Section, we can generalize Theorem 31 to the honeycomb lattice. However, we need to prove first the following Lemma.

Lemma 27 (Splitting tensors) *Let $A \in \mathcal{M}_{d_1,d_2}$, $B \in \mathcal{M}_{d_2,d_1}$, $C \in \mathcal{M}_{d_1,d_2'}$ and $D \in \mathcal{M}_{d_2',d_1}$, and let us assume that* $\mathrm{rank}\,(AB) = d_2$. *Then, if $AB = CD$, there exist matrices W and U such that $A = CW$ and $B = UD$, with $UW = \mathbb{1}_{d_2}$.* □

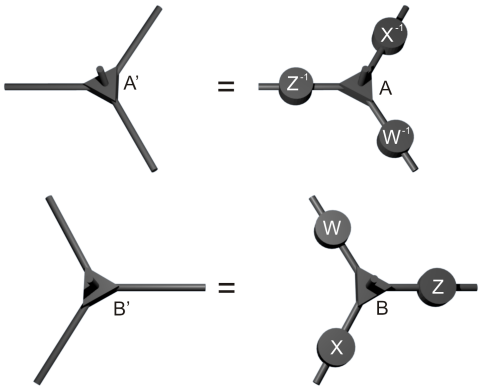


Figure 5.10: **Canonical form for hexagonal lattices**. These are the relationships which the tensors defining two TI–PEPS on a honeycomb lattice must fulfil in order to represent the same state.

Proof It is straightforward to see that:

$$d_2 = \text{rank}\,(AB) \leq \min\left(\text{rank}\,(A), \text{rank}\,(B)\right) \leq \min(d_1, d_2)$$

This proves that $d_1 \geq d_2$ and that $\text{rank}\,(A) = \text{rank}\,(B) = d_2$, so they are both full rank. By using now that $AB = CD$, we get that $d_2 \leq \min\left(\text{rank}\,(C), \text{rank}\,(D)\right) \leq \min(d_1, d_2')$, which implies that $d_2 \leq d_2'$. Since B is full–rank and $\min(d_1, d_2) = d_2$, there exists a matrix that we can call $B^{-1} \in \mathcal{M}_{d_1,d_2}$ such that $BB^{-1} = \mathbb{1}_{d_2}$. Therefore, $A = C(DB^{-1})$ and we can symbolize $W = DB^{-1} \in \mathcal{M}_{d_2',d_2}$. Similarly, $B = A^{-1}CD$ and we can denote $U = A^{-1}C \in \mathcal{M}_{d_2,d_2'}$. Since $UW = A^{-1}CDB^{-1} = A^{-1}ABB^{-1} = \mathbb{1}_{d_2}$, the lemma follows. Note that the case $d_2' > d_2$ is nothing but padding the matrix with zeros, since $\text{rank}\,(WU) = d_2$. This turns relevant below, when the Lemma is applied to the honeycomb lattice, because this case is discarded by injectivity. ∎

We can now prove the theorem for the honeycomb lattice. Let us remark that the unit cell of this lattice contains two sites and that the lattice associated to the unit cells is a square lattice. Translational invariance is not site by site, but unit cell by unit cell.

Theorem 32 (The hexagonal lattice) *Let $|\psi\rangle$ and $|\psi'\rangle$ be two PEPS defined in an hexagonal lattice and such, that the square lattice constituted by the unit cells fulfils the conditions of Theorem 31. Then, $|\psi\rangle = |\psi'\rangle$ iff the conditions shown in Fig. 5.10 hold.* □

Proof Let us apply Theorem 31 to the square lattice formed by the unit cell. Then, we obtain the equality shown in Fig. 5.11. Lemma 27 completes the proof

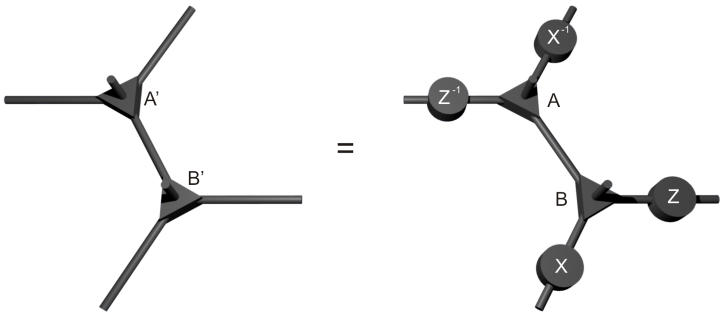


Figure 5.11: **Hexagonal lattice → square lattice**. The possibility of transforming the honeycomb lattice into a square lattice by blocking tensors enables us to apply the result to equivalent TI–PEPS representations for the square lattice.

of the Theorem, but we have to previously invoke injectivity in order to discard the case $d_2' > d_2$. As we already mentioned in the proof of the Lemma, this case is nothing but padding the tensor with zeros, which increases the bond dimension. This subspace is not going to be expanded, so injectivity is not possible. Thus, in our case $d_2' = d_2$ and $U = W^{-1}$. ∎

5.3.2.2 Triangular lattice

The generalization to the triangular lattice is slightly more complicated than the hexagonal one, since we cannot gather different sites to construct the square lattice. However, we can apply a singular value decomposition (SVD) to the tensor in order to transform the triangular lattice into a square lattice (Fig. 5.12) composed of two sublattices:

$$\begin{aligned} T^{i}_{\alpha_1\alpha_2\alpha_3\alpha_4\alpha_5\alpha_6} &= T^{i\alpha_1\alpha_2\alpha_3}_{\alpha_4\alpha_5\alpha_6} \\ &= \sum_{\beta,\gamma=1}^{D^3} A^{i\alpha_1\alpha_2\alpha_3}_{\beta} D^{\beta}_{\gamma} B'^{\gamma}_{\alpha_4\alpha_5\alpha_6} \end{aligned} \qquad (5.8)$$

where $D^{\beta}_{\gamma} = d_{\beta}\delta^{\beta}_{\gamma}$ is a diagonal matrix $D \in \mathcal{M}_{D^3}$, and $A^{i}_{\alpha_1\alpha_2\alpha_3\beta}$ and $B_{\beta\alpha_4\alpha_5\alpha_6} = \sum_{\gamma} D_{\beta\gamma} B'^{\gamma}_{\alpha_4\alpha_5\alpha_6}$. Note that the notation is not related with covariance. Rather, it is a resource to stress which indices are collected together. Then, the associated square lattice of the triangular lattice is an AB–lattice where sublattice A has the physical spin of the original triangular lattice, while sublattice B has physical spin 0, *i.e.* a one–dimensional Hilbert space, as shown in Fig. 5.13.

Theorem 33 (The triangular lattice) *Let $|\psi\rangle$ and $|\psi'\rangle$ be two injective PEPS defined in a triangular lattice and such, that the associated square lattice fulfils the*

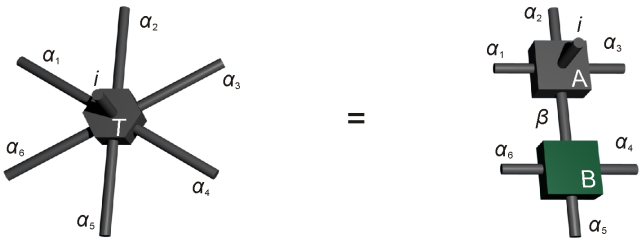


Figure 5.12: **SVD**. Singular value decomposition (SVD) of the triangular lattice which transforms it into an AB square lattice.

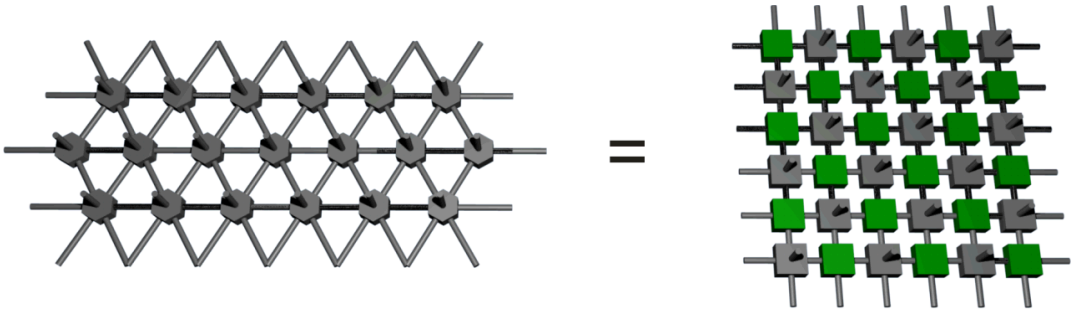


Figure 5.13: **Triangular lattice → square lattice**. The possibility of transforming the triangular lattice into a square lattice with an AB–substructure by performing an SVD on the tensors enables us to apply the result for the square lattice with only slight modifications.

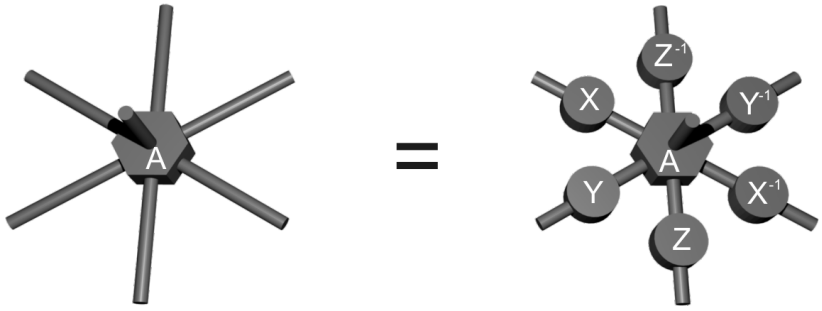


Figure 5.14: **Canonical form in triangular lattice**. Relationship which the tensors defining two TI–PEPS on a triangular lattice must fulfil in order to represent the same state.

conditions of Theorem 31. Then, $|\psi\rangle = |\psi'\rangle$ *iff the conditions shown in Fig. 5.14 hold.* □

PROOF We just have to generalize the results shown in this Section to an AB–square lattice. As Theorem 30 holds also for this case, because one of the sites has spin 0 ($d = 1$), then Lemmas 21 to 24 hold as well. However, Lemma 25 is no longer true, since the translational invariance is partially broken, and we have two invertible matrices Y_A and Y_B corresponding to the A–tensors and B–tensors respectively. We can work as in Lemma 26, except the last step, where we cannot apply translational invariance either, so we obtain again a couple of matrices Z_A and a Z_B. However, by grouping until reaching injectivity, one can straightforwardly prove that $Z_A = Z_B$. This proves the relationship shown in Fig. 5.14. ■

Sólo el que ensaya lo absurdo es capaz de conquistar lo imposible.

Miguel de Unamuno
(1864-1936)

6 Injectivity and parent Hamiltonians in PEPS

6.1 Introduction

In this Chapter, we study the generalization to higher dimensions of the very fruitful concept of injectivity proposed in Chapter 2 as well as the construction method for parent Hamiltonians proposed in Chapter 3.

Injectivity was defined in Chapter 2 as a property which relates different boundary conditions of a MPS–OBC to linearly independent states. In this Chapter, we were able to prove the equivalence of this property with a local characterization based on the eigenvalues and eigenvectors of the transfer matrix called strong irreducibility. Even though the idea of injectivity is straightforwardly generalizable to higher dimensions, unfortunately there is no equivalent extension for strong irreducibility. The reason lies on the fact that the two–dimensional lattice can no longer be understood as a trivial coupling of quantum channels.

Afterwards, we explain the extension to higher dimensions of the technique to construct parent Hamiltonians, connecting it subsequently with injectivity, as done in Chapter 3. In the case of MPS, injectivity turned out to be a relevant property, since it is a necessary and sufficient condition for the uniqueness of the parent Hamiltonian's ground state, as well as for the existence of a gap above it. In the case of PEPS, *injectivity* is only a sufficient condition for the uniqueness of the parent Hamiltonian's ground state and does not imply any gap above it, as shown in Section 6.3. However, the fact of being a sufficient condition for uniqueness is already relevant, and as it was already advanced in Section 5.3, a very useful property for simplifying proofs.

The organization of this Chapter is essentially the same as in Chapters 2 and 3, which allows us to better illustrate the differences between one–dimensional and higher–dimensional systems:

- In Section 6.2, we extend the physical one–dimensional definition of injectivity, and show some of its properties as well. Nevertheless, the non–existence of a property equivalent to strong irreducibility in Matrix Product States, which locally determines from the tensor when an injective state will arise out of it, notably complicates the proof of results as strong as the ones in Chapter 2.
- We extend in Section 6.3 the definition of parent Hamiltonian to higher dimensions and show that injectivity is, in the case of Projected Entangled Pair States, a sufficient but not necessary condition for uniqueness of the parent Hamiltonian's ground state [PGVCW08]. Furthermore, it does not imply the existence of a spectral gap either. In order to show that, we make use of Projected Entangled Pair States coming from classical spin models [VWPGC06], which provide counter–examples for both the necessity of injectivity for uniqueness, and injective examples with a unique but gapless ground state [PGVCW08].

6.2 Injectivity

We discuss in this Section the generalization to PEPS of the useful concept of injectivity shown in Chapter 2. Let us start by extending Definition 8 to the case of PEPS.

Definition 23 (Injectivity for PEPS) Let us consider a PEPS $|\psi\rangle$ defined by the tensor $(A_i)_{\boldsymbol{a}} \in (\mathbb{C}^d \otimes (\mathbb{C}^D)^{\otimes e_\nu})$ (e_ν is the *coordination number* of the vertex and D the *bond dimension*, as defined in Section 5.2), and a region R containing $|R|$ sites and e_R bonds connecting R to the rest of the lattice (along the boundary ∂R). Let us consider the D^{e_R} vectors $|\phi_\alpha^{\partial R}\rangle$ composing a basis of $(\mathbb{C}^D)^{\otimes e_R}$ which define D^{e_R} states by

$$|\psi_\alpha\rangle = \sum_{i_1,\ldots,i_{|R|}=1}^{d} \mathcal{C}_{|\phi_\alpha^{\partial R}\rangle}\left[\{(A_i)_{\boldsymbol{a}}\}_{\boldsymbol{a}}\right] |i_1,\ldots,i_{|R|}\rangle \tag{6.1}$$

Then, we say that the PEPS is **injective**, as shown in Fig. 6.1, if there exists a finite region R, such that the vector space spanned by the vectors in Eq. 6.1 has dimension D^{e_R}, *i.e.* if $\dim \operatorname{span}[\{|\psi_\alpha\rangle\}] = D^{e_R}$. □

In general, the properties of the bulk are determined by the behaviour in the boundary ∂R, which is a remarkable property of PEPS and the reason why they fulfil an area law. This relationship is even stronger for injective PEPS.

It is clear that we can also connect this definition to the injectivity of a certain linear map, by following the same construction as in Section 2.2.

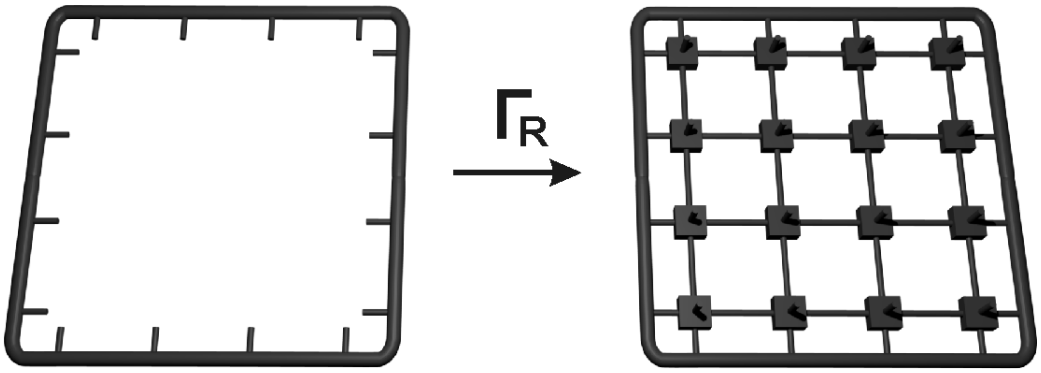


Figure 6.1: **Injectivity (PEPS)**. A Projected Entangled Pair State is injective in a region R if, for the PEPS–OBC constructed in R, different (linearly independent) boundary conditions, represented by the frame in the figure, give rise to different (linearly independent) states.

Lemma 28 (Injectivity of $\Gamma_R(X)$) *A PEPS $|\psi\rangle$ defined by tensor $(A_i)_{\boldsymbol{a}} \in (\mathbb{C}^d \otimes (\mathbb{C}^D)^{\otimes e_R})$ (where e_R is the coordination number of the vertex and D the bond dimension) is injective in a region R iff the linear map $\Gamma_R : (\mathbb{C}^D)^{\otimes e_R} \to (\mathbb{C}^d)^{\otimes |R|}$ defined by*

$$\Gamma_R(X) = \sum_{i_1,\ldots,i_{|R|}=1}^{d} \mathcal{C}\left[\{(A_i)_{\boldsymbol{a}} X\}_{\boldsymbol{a}}\right] |i_1,\ldots,i_{|R|}\rangle \tag{6.2}$$

*is **injective**, where X is a tensor which represents the boundary conditions coupled to the free bonds in the boundary ∂R.* □

Proof The proof is a straightforward generalization of Lemma 4, which does not assume any lattice structure or translational invariance. ■

Let us now enunciate a generalization of Lemma 21:

Lemma 29 (The union of injective regions is injective) *If R and S are two disjoint injective regions, then $R \cup S$ (assumed connected) is also injective.* □

Proof The proof of this Lemma can originally be found in [PGVCW08, Lemma 1]. ■

Let us stress again that this Lemma is notably general, since it does not assume any lattice structure or translational invariance.

Let us denote by $\mathcal{G}_R = \text{span}\left[\Gamma_R(X)\right]$ the subspace of the vector space generated by Γ_R, as in the case of MPS. Obviously, the vector space $\mathcal{S}_R = \text{supp}[\rho^{(R)}]$, where $\rho^{(R)}$ is the reduced density matrix in region R, is a subspace $\mathcal{S}_R \subseteq \mathcal{G}_R$, where the equality holds if the PEPS is injective in the region R.

We now enunciate a result which extends Theorem 23 to higher dimensions:

Theorem 34 (Intersection property for PEPS) *Let R_1, R_2 and R_3 be three disjoint regions and let us denote the Hilbert space corresponding to a region R by $\mathcal{H}_R = \mathbb{C}^{d^{|R|}}$. Then,*

1. $\mathcal{G}_{R_1\cup R_2\cup R_3} \subseteq (\mathcal{G}_{R_1\cup R_2}\otimes\mathcal{H}_{R_3})\cap(\mathcal{H}_{R_1}\otimes\mathcal{G}_{R_2\cup R_3})$.
2. *If R_1 and R_3 are not connected and both R_2 and R_3 are injective, then the equality $\mathcal{G}_{R_1\cup R_2\cup R_3} = (\mathcal{G}_{R_1\cup R_2}\otimes\mathcal{H}_{R_3})\cap(\mathcal{H}_{R_1}\otimes\mathcal{G}_{R_2\cup R_3})$ holds.*
3. *If all three regions are injective, then $\mathcal{G}_{R_1\cup R_2\cup R_3} = (\mathcal{G}_{R_1\cup R_2}\otimes\mathcal{H}_{R_3})\cap(\mathcal{H}_{R_1}\otimes\mathcal{G}_{R_2\cup R_3})\cap(\mathcal{G}_{R_1\cup R_3}\otimes\mathcal{H}_{R_2})$.* □

Proof The proof of this Theorem can be found in [PGVCW08, Lemma 2]. ■

Unfortunately, no necessary and sufficient local characterization which ensures the injectivity for PEPS just by analysing the tensor, such as strong irreducibility for MPS, is known. Furthermore, we cannot take advantage of connections with completely positive maps, and all the associated mathematical machinery, since the coupling of tensors generating the two–dimensional lattice can no longer be considered a trivial coupling of quantum channels. This has as a consequence that proofs with PEPS are much more difficult and less fruitful.

However, we can make a clever use of the results for MPS in the framework of PEPS in some specific cases, such as the square lattice. Section 5.3 is a very good example of this idea. It would be very interesting to obtain a generalization of the Wielandt–type result to higher dimensions, understood as an upper bound, independent of the tensors, for the size of a region in which the injectivity of the PEPS is ensured. However, this is a very complex problem in an arbitrary lattice.

6.3 Parent Hamiltonian

We start by exposing a general definition of parent Hamiltonian in the context of higher–dimensional tensor networks, generalizing the results shown in Chapter 3 for MPS. After that, we try to relate the injectivity to the uniqueness of the parent Hamiltonian's ground state and to the existence of a gap above it, following the outline of Chapter 3. However, we show here that injectivity in the context of PEPS is not such a strong condition as in the one–dimensional framework. Injectivity turns out to be a sufficient condition for the uniqueness of the ground state [PGVCW08, Theorem 3], but it is not actually necessary [PGVCW08, Section VI.B]. Furthermore, it is possible to construct injective PEPS whose parent Hamiltonian is gapless [PGVCW08, Section VI.A], so injectivity does not imply the existence of a spectral gap either.

6.3.1 Definition of parent Hamiltonian

In this Subsection, we provide a generalization for PEPS of the definition of parent Hamiltonian. In Section 3.2, we gave two definitions of parent Hamiltonian, which turn out to be equivalent when the MPS is injective, and we proceed similarly here.

Let us consider a PEPS $|\psi\rangle$ (assumed TI, but a general definition is also possible) and a region R of the lattice. Let us denote the reduced density operator by $\rho^{(R)} = \mathrm{tr}_{R^C}[\,|\psi\rangle\langle\psi|\,]$ and its support by $\mathcal{S}_R$, *i.e.* $\mathcal{S}_R = \mathrm{supp}[\rho^{(R)}]$. Then, we can provide the generalization of Definition 16:

Definition 24 (Parent Hamiltonian 1 (PEPS)) Let us consider a positive operator $h \geq 0$ such that $\mathrm{supp}[h] = \ker[\rho^{(R)}]$. Then, if τ_ν is the translation operator by a lattice vector ν, we call

$$H = \sum_\nu \tau_\nu (h \otimes \mathbb{1}_{\mathrm{rest}}) \tag{6.3}$$

parent Hamiltonian of $|\psi\rangle$. Obviously, $H \geq 0$ and $\langle\psi| H |\psi\rangle = \sum_\nu \mathrm{tr}\left[h\rho^{(R)}\right] = 0$, so $|\psi\rangle$ is a ground state of H. □

Let us now extend Definition 17 to PEPS. This is straightforwardly generalizable by replacing $\Gamma_n \hookrightarrow \Gamma_R$.

Definition 25 (Parent Hamiltonian 2 (PEPS)) Let us denote now the image space of $\Gamma_R(X)$ by $\mathcal{G}_R = \langle \Gamma_R(X) \rangle_X$, with Γ_R defined in Eq. 6.2. Let us consider a positive operator $h \geq 0$ with support on the orthogonal subspace $\mathcal{G}_R^\perp$. Then, we call the TI Hamiltonian constructed as in Eq. 6.3 **parent Hamiltonian**. □

As in the one–dimensional case, $\mathcal{S}_R \subseteq \mathcal{G}_R$, and they are equal iff the state is injective in R. Therefore, both definitions of parent Hamiltonians are again equivalent only in this case.

The parent Hamiltonian is obviously not uniquely defined, the only existing constraint is the support, so there are internal degrees of freedom. For instance, if h is a local term fulfilling the conditions above, then $\tilde{h} = h + hQh$ also defines a parent Hamiltonian for every $Q \geq 0$. However, in specialized literature it is common to specifically designate it as the case which corresponds to the *sum of projectors with the same weight*.

The parent Hamiltonian is also **frustration–free**, in the sense of Definition 18, since the energy is also locally minimized, and has the properties shown in Lemma 13. In fact, one can also extend the definition of **strongly frustration–free** Hamiltonians to higher dimensions. Then, the parent Hamiltonians associated to PEPS are evidently also strongly frustration–free.

6.3.2 Uniqueness of the ground state

The aim of this Subsection is to prove that every injective PEPS $|\psi\rangle$ is the only ground state of the parent Hamiltonian with structure given by Eq. 6.3.

Let us assume that the lattice can be covered by disjoint injective regions and gather the spins in each region in such a way that we form a super–lattice where every site is injective. Let us now construct a Hamiltonian on the super–lattice with the structure given in Eq. 6.3, by taking $\ker h^{(i,j)} = \mathcal{G}_{R_i \cup R_j}$, where i, j denote the sites in the super–lattice (*i.e.* the injective regions in the lattice).

Let us enunciate the Theorem which ensures the uniqueness of the ground state [PGVCW08, Theorem 3]:

Theorem 35 (Injectivity ⇒ Uniqueness (PEPS)) *For every injective PEPS $|\psi\rangle$ on an arbitrary lattice, there is a local frustration–free parent Hamiltonian H, given by Eq. 6.3, such that the $|\psi\rangle$ is the unique ground state of H.* □

Proof This proof was originally published in [PGVCW08, Theorem 3]. Slightly abusing the notation, let us denote the space $\mathcal{G}_R \otimes \mathcal{H}_{R^\perp}$ by $\mathcal{G}_R$. Then, the goal is to prove that, when the state is injective,

$$\bigcap_{i,j} \mathcal{G}_{R_i \cup R_j} = \mathcal{G}_{\cup_k R_k} \tag{6.4}$$

The LHS is nothing but the ground level of H (because this is local and frustration–free, so the ground state subspace coincides with the intersection of the local ground state subspaces). The RHS is the one–dimensional subspace generated by the PEPS. If they are equal, then $|\psi\rangle$ is the only ground state of H.

$\boxed{\supseteq}$

This inclusion follows from point 1. of Theorem 34. The subspace generated by the PEPS is always, by construction, in the ground subspace of its parent Hamiltonian.

$\boxed{\subseteq}$

Let us prove this inclusion by induction. Therefore, we start by proving a general inclusion that we can use in the induction step. Let us consider a set of disjoint injective regions $\{T_i\}_{i=0}^N$ and denote $T = \bigcup_{i=0}^N T_i$. Let us assume that every region in the subset $\{T_i\}_{i=1}^N$ is connected to another injective region S. Then,

$$\Big(\bigcap_{i=1}^N \mathcal{G}_{T_i \cup S}\Big) \cap \mathcal{G}_T \subseteq \bigcap_{i=1}^N \Big(\mathcal{G}_{T_0 \cup T_i} \cap \mathcal{G}_{T_i \cup S}\Big) = \bigcap_{i=1}^N \mathcal{G}_{T_0 \cup T_i \cup S}$$

where the first inclusion uses the fact that $\mathcal{G}_T \subseteq \mathcal{G}_{T_0 \cup T_i}$ (which can be easily proven from point 1 of Theorem 34), and the equality comes from point 2 of Theorem 34.

By using again the fact that $\mathcal{G}_T \subseteq \mathcal{G}_{\cup_{i\in\mathcal{I}} T_i}$, for any subset $\mathcal{I} \subseteq \{0,\ldots,N\}$ and point 3 of Theorem 34, one can obtain that

$$\Big(\bigcap_{i=1}^{N} \mathcal{G}_{T_i\cup S}\Big) \cap \mathcal{G}_T \subseteq \mathcal{G}_{T\cap S}$$

The proof of the inclusion can be obtained by using this result in an inductive process over the regions. ∎

This Theorem proves that injectivity of PEPS is a *sufficient* condition for the uniqueness of the parent Hamiltonian's ground state. Subsequently, we will see that injectivity is, however, not a *necessary* condition for that.

6.3.2.1 PEPS from classical spin models

Let us now recall the construction in [VWPGC06] of PEPS coming from classical spin models with nearest–neighbour interactions. We consider classical *spins* with d possible configurations and temperature $\beta = \frac{1}{k_B T}$.

Let us consider a classical two–body interacting Hamiltonian for N particles $H(x_1,\ldots,x_N) = \sum_{(i,j)} h(x_i,x_j)$, with $x_i = 1,\ldots,d$ and its corresponding partition function $Z = \sum_{\boldsymbol{x}} \exp[-\beta H(\boldsymbol{x})]$. Then, we construct the associated PEPS as

$$|\psi_{H,\beta}\rangle = \frac{1}{\sqrt{Z}} \sum_{\boldsymbol{x}} e^{-\frac{\beta}{2}H(\boldsymbol{x})} |\boldsymbol{x}\rangle \tag{6.5}$$

where $\boldsymbol{x} = x_1,\ldots,x_N$ and the superposition coefficients are nothing but the *Boltzmann weights*.

Theorem 36 (Properties of PEPS coming from classical systems)
These states have the following properties:

1. *The expectation values and correlations of state 6.5 with respect to operators diagonal in the basis $|\boldsymbol{x}\rangle$ are the same as those of the classical state, so the PEPS reproduces the correlation functions of the classical thermal states.*

2. *State 6.5 has a PEPS representation with bond dimension $D = d$.*

3. *State 6.5 is the ground state of a local quantum Hamiltonian.*

4. *The block entropy asymptotically obeys a strict area law.* □

Proof Let us prove these properties:

1.

This is a direct consequence of the construction given by Eq. 6.5. If we consider only diagonal operators $D^{(i)}$, the correlation function or expectation values are given by

$$\begin{aligned}\langle\psi_{H,\beta}|\, D^{(i)}D^{(j)}\,|\psi_{H,\beta}\rangle &= \frac{1}{Z}\sum_{\boldsymbol{x}} D^{(i)}_{\boldsymbol{x}} D^{(j)}_{\boldsymbol{x}} e^{-\frac{1}{\beta}H(\boldsymbol{x})} \\ &= \langle (D^{(i)} - \langle D^{(i)}\rangle)(D^{(j)} - \langle D^{(j)}\rangle)\rangle\end{aligned}$$

which is the classical correlation function.

2.

Let us construct the tensors explicitly. By applying an SVD, one obtains the vectors $|\phi^i_{x_i}\rangle$ verifying:

$$e^{-\frac{\beta}{2}h(x_i,x_j)} = \sum_k \langle\phi^i_{x_i}|k\rangle\langle k|\phi^j_{x_j}\rangle$$

Then, the tensors defining the PEPS are:

$$(A^i_{x_i})_{\alpha_1\ldots\alpha_\chi} = \prod_e \langle\phi^e_{x_i}|\alpha_e\rangle \quad \alpha_e = 1,\ldots,d \tag{6.6}$$

where $|\phi^e_{x_i}\rangle$ may be different for each lattice site i, and the product is taken over all edges connected with this site (see the explicit construction for the $2D$ Ising model in the example below). Therefore, these are the tensors describing state 6.5.

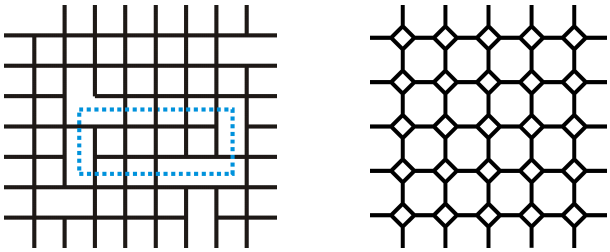
3. and 4.

Both are consequences of point 2., *i.e.* of the PEPS structure of the state. The existence of such a structure implies that there exists an upper bound for the block entropy between a region R and the rest of the lattice, given by $\mathcal{O}(e_R \log D)$, where e_R is the number of outgoing bonds which connect R to the lattice. Moreover, there is always a parent Hamiltonian for this PEPS, as shown in Subsection 6.3.1. ■

Example 8 (2*D* Ising model) Let us consider the classical 2D Ising model on a square lattice, whose Hamiltonian is given by $H = -\sum_{(i,j)} x_i x_j$, with $x_i = \pm 1$. Then,

$$|\phi_1\rangle = \begin{pmatrix}\sqrt{\sinh\frac{\beta}{2}} \\ \sqrt{\cosh\frac{\beta}{2}}\end{pmatrix} \qquad |\phi_{-1}\rangle = \begin{pmatrix}-\sqrt{\sinh\frac{\beta}{2}} \\ \sqrt{\cosh\frac{\beta}{2}}\end{pmatrix}$$

and from here one can easily construct the tensors which define the PEPS. □



(a) (b)

Figure 6.2: **Lattice–dependent injectivity**. A PEPS derived from a classical model in a square lattice is not injective, but (a) if some defects on the lattice bonds are allowed, or (b) if the square lattice has a substructure, then it can be injective.

In the case of PEPS coming from classical models, injectivity does not depend on the type of interaction, but only on the lattice geometry (see Fig. 6.2), which coincides with the interaction pattern of the classical model. Let us enunciate this statement properly [PGVCW08, Section VI.A]:

Theorem 37 (Conditions for injectivity) *A PEPS $|\psi\rangle$ coming from a classical spin system is **injective** iff there exists a finite subregion of the lattice, such that every spin in the boundary of the region has at most one outgoing bond.* □

Proof Let us consider a region R of the lattice and let e_R be the number of outgoing bonds E in the boundary $\partial R \subseteq R$, which connect R with the rest of the lattice. Then, we have to study the injectivity of the operator $\Gamma_R : (\mathbb{C}^D)^{\otimes e_r} \to (\mathbb{C}^d)^{\otimes |R|}$ (so we see Γ_R now as a matrix). Then, the matrix elements are (see [MVC09])

$$\langle x|\,\Gamma_R\,|\bar{\alpha}\rangle = C(x)\,\langle \bar{x}|\,F\,|\bar{\alpha}\rangle \qquad (6.7)$$

The bar means here that the vectors are *at the boundary*, *i.e.* they are a basis of the tensor product of the Hilbert spaces corresponding to the spins in the boundary ∂R (the information about the boundary is summarized in the operator F). Function $C(x)$ is the result of the contraction of the bounds $e \notin E$. We have two cases:

$e_R = |\partial R|$

Vectors $\bar{x}$ and $\bar{\alpha}$ have the same dimension and $F = \bigotimes_{e\in E} \phi^e$, where ϕ^e is an invertible matrix constructed from the $\langle \phi^e|$ defined in the proof of point 2. of Eq. 6.5 via $\langle x_i| \mapsto \langle \phi^e_{x_i}|$. Therefore, F is invertible and hence, Γ_R is injective. Let us remark that this is true if, for each $\bar{x} \in \partial R$, there is at least one configuration x such that $C(x) = 0$.

$e_R > |\partial R|$

In this case, F is rectangular and non–invertible. Hence, Γ_R cannot be injective. ■

From this proof, one can easily see that we cannot have injectivity for the square lattice, but one can have it for the hexagonal lattice. However, the 2D square lattice can also lead to injectivity in case of defects or a substructure (see Fig. 6.2).

These models allow us to prove that, although injectivity is a sufficient condition for uniqueness of the parent Hamiltonian's ground state, this is *not necessary*. This is shown with a particular case in [PGVCW08, Section VI.B]. In this paper, the steps of the proof of Theorem 35 are followed, but without actually using injectivity.

6.3.3 Gap

In Section 3.4 we proved that injectivity is the necessary and sufficient condition for the existence of a one–dimensional gapped parent Hamiltonian. In this Subsection, we show that, although injectivity is still a very powerful condition to ensure uniqueness, it is not sufficient to ensure the existence of a gap over the ground state of the parent Hamiltonian. We use the PEPS constructed from classical spin systems described in Subsection 6.3.2 to show a counter–example to that.

Let us consider the 2D classical isotropic Ising model on the honeycomb lattice. On the one hand, we have that the hexagonal structure ensures injectivity, as shown in Theorem 37, which at the same time ensures the existence of a parent Hamiltonian which has this state as a unique ground state. On the other hand, the hexagonal Ising model is critical for the inverse temperature $\beta = \frac{1}{2}\ln(2+\sqrt{3})$ [PF84, KS50]. This means that the correlation functions decay polynomially, which implies, by means of Theorem 36, that the correlation functions of the PEPS also decay polynomially. However, this means that the parent Hamiltonian is gapless as well [HK06, NS07].

Therefore, injectivity is not a sufficiently strong condition to ensure the existence of a non–trivial uniform (independent of system size) gap over the ground state. The question is now how one can guarantee the existence of such a gap without making use of a tensorial (local) characterization, such as injectivity. The question is relevant, since the detection of either criticality or the existence of a spectral gap is an important problem both in condensed matter and quantum information. Let us enunciate a computable sufficient condition for the existence of a uniform gap, whose proof is based on the one–dimensional case (see [FNW92]) and can be found in [PGVCW08, Proposition 4].

Lemma 30 (Sufficient condition for a gap (PEPS)) *Let us denote the parent Hamiltonian of an injective TI–PEPS in a square lattice by* $H = \sum_{(i,j)} \tau_{(i,j)}(h \otimes \mathbb{1}_{rest})$. *Hereafter,* h_{ij} *stands for* $\tau_{(i,j)}(h \otimes \mathbb{1}_{rest})$. *Since* H *is local, there exists a small* $\mathcal{I} \subset \{1,\dots,M\} \times \{1,\dots,N\}$ *such that* $hh_{ij} \geq 0$ *whenever* $(i,j) \notin \mathcal{I}$. *If*

$$\sum_{(i,j)\in\mathcal{I}} hh_{ij} + h_{ij}h > -\frac{1}{|\mathcal{I}|+1}\Big(h + \sum_{(i,j)\in\mathcal{I}} h_{ij}\Big) \qquad (6.8)$$

then, there exists an $\epsilon > 0$ *such that* $H^2 > \epsilon H$ *and hence, there is a* ***uniform*** *(independent of the system size)* ***spectral gap*** *over the ground state of* H. □

The mathematical sciences particularly exhibit order, symmetry, and limitation; and these are the greatest forms of the beautiful.

Aristotle (384 BC-322 BC)

7 Symmetries in PEPS

7.1 Introduction

In this Chapter, we extend the results obtained in Chapter 4 to the case of PEPS, as a consequence of the canonical form shown in Section 5.3. The reasons which justify the study of symmetric states are extensively explained in the one–dimensional case, so it would be redundant to repeat them here.

However, let us introduce an additional justification for this. *String order* is an order parameter widely employed in the detection and understanding of quantum phase transitions, which we will study in depth in Section 9.3. However, as pointed out in [AR07a], there could exist some limitations in its employability, and its application might not go beyond one–dimensional systems. In [PGWS$^+$08], it has been shown with the aid of MPS that the existence of a string order parameter is intimately related to the existence of a symmetry (see Section 9.3), which allows us to design an appropriate 2D extension: the existence of a local symmetry when we consider increasing sizes of the system. A trivial sufficient condition for this to hold in PEPS is proposed there (see Fig. 7.1) and further analysed in [SPV10] in the more general context of tensor network states.

The organization of this Chapter is similar to Chapter 4, which allows us, as usual, to remark the differences more illustratively:

- In Section 7.2, we make use of the results shown in Section 5.3 to provide the necessary and sufficient conditions that an *injective* tensor must fulfil in order to generate a symmetric state [PGSGG$^+$10]. The result is firstly proven for continuous groups, focusing afterwards on spatial symmetries: reflection symmetry, $\frac{\pi}{2}$–rotations and π–rotations. In Chapter 9, these results are ap-

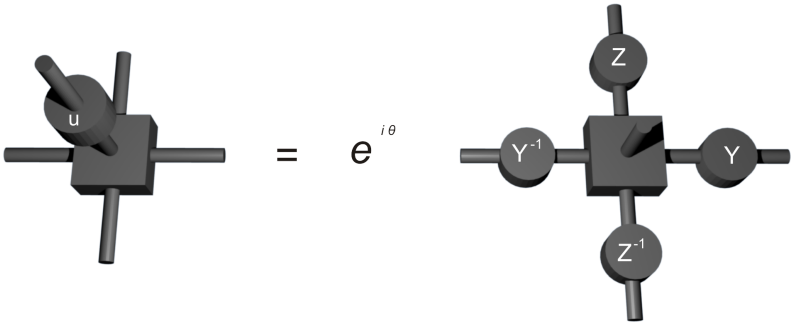


Figure 7.1: **Symmetries in a square lattice**. Graphical representation of the equation fulfilled by a PEPS if it is invariant under a representation u_g of a group G. Then, the symmetry is inherited by the virtual indices, which transform according to two representations of G, called Y_g and Z_g, up to a phase $e^{i\theta_g}$.

plied in order to generalize the concept of *string order* to higher dimensions, prove a generalization of the *Oshikawa–Yamanaka–Affleck Theorem*, and a relationship between the existence of *Wilson loops* (a topological property of the quantum state) with the absence of injectivity.

- In Section 7.3, we transform the tensor into a matrix and apply the results shown in Section 4.3 to the uniqueness of the symmetric–MPS construction, in order to extend the result to PEPS.

7.2 Characterization of symmetric states

The aim of this Section is to prove the necessary and sufficient conditions for an injective PEPS to be invariant under a symmetry group [PGSGG+10, Theorems 13–16], *i.e.* the extension of the results proven in Chapter 4 to injective PEPS. We focus on the case of the square lattice, but this can be generalised to other regular lattices by an argumentation similar to the one shown in Section 5.3, since this is a straightforward consequence of the canonical form.

We prove first the Theorem for continuous groups, focusing later on the spatial discrete symmetries: reflection symmetry, $\frac{\pi}{2}$–rotations and π–rotations.

Theorem 38 (Local symmetry) *If a PEPS defined on an $L \times N$ lattice has a symmetry u, i.e. $u^{\otimes NL}|\psi_A\rangle = e^{i\theta'}|\psi_A\rangle$, and is injective in regions of size $\frac{L}{5} \times \frac{N}{5}$, then the tensors defining the PEPS satisfy the relation shown in Fig. 7.1 with $e^{i\theta NL} = e^{i\theta'}$. Moreover, if u_g is a representation of a group G, then Y_g, Z_g and $e^{i\theta_g}$ are also representations of G.* □

Proof Notice that, when acting with u and $e^{-i\theta}$ on the tensor A which defines the PEPS (see Fig 7.1), we get a new tensor B that is also injective in regions of size $\frac{L}{5} \times \frac{N}{5}$ and such that $|\psi_A\rangle = |\psi_B\rangle$. Theorem 31 then gives the result. In order to

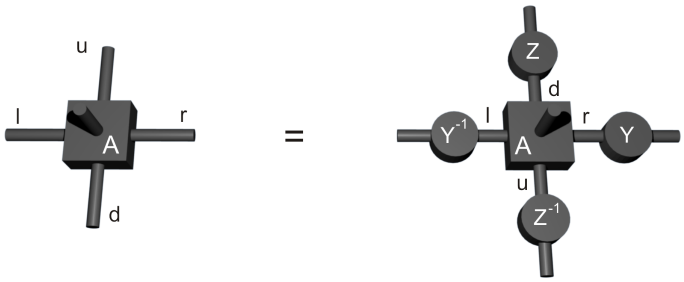


Figure 7.2: **Reflection symmetry**. This figure represents the condition which must be fulfilled by a PEPS in order to generate a state invariant under reflections (in this case with respect to the horizontal plane).

prove that the invertible matrices Y_g and Z_g are representations of G, we only need to follow the arguments used in Theorem 26. ∎

With exactly the same reasoning, we can characterize the spatial symmetries, *i.e.* the symmetries corresponding to the point group of the square lattice: reflection, $\frac{\pi}{2}$–rotations and π–rotations:

Theorem 39 (Reflection symmetry) *Let us consider an $L \times N$ PEPS with the property that it is injective for a region of size smaller than $\frac{L}{5} \times \frac{N}{5}$. If this TI–PEPS is invariant under a reflection with respect to a horizontal axis, then there exist invertible matrices Y and Z such that the tensors defining the PEPS verify Fig. 7.2.* □

Moreover, it is easy to see that Y and Z must satisfy $Y^T = Y$, $Z^2 = \mathbb{1}$. The characterization of the reflection with respect to the vertical axis follows straightforwardly by interchanging the roles of the horizontal/vertical directions.

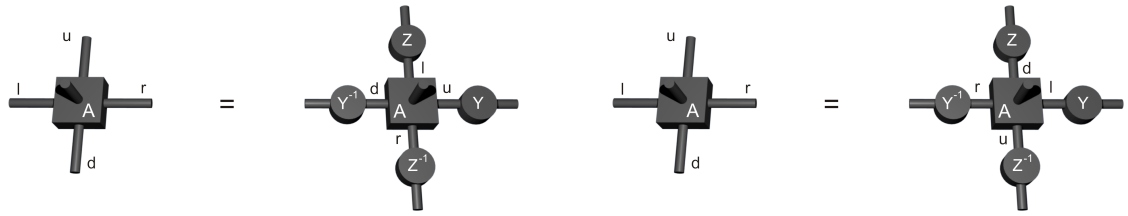
Theorem 40 (Spatial $\frac{\pi}{2}$–rotation symmetry) *If an $L \times N$ PEPS with the property that it is injective for a region of size smaller than $\frac{L}{5} \times \frac{N}{5}$ is generated by a tensor with a spatial $\frac{\pi}{2}$–rotation invariance, then there exist invertible matrices Y and Z such that the tensors A^i defining the PEPS verify Fig. 7.4a.* □

In this case, one can see that Y and Z must satisfy the additional constraints $(YZ)^T = YZ$, $(ZY)^T = ZY$.

Finally, we characterize the PEPS which are symmetric respect to a π–rotation.

Theorem 41 (Spatial π–rotation symmetry) *Let us consider an $L \times N$ PEPS with the property that it is injective for a region of size smaller than $\frac{L}{5} \times \frac{N}{5}$ and generated by a tensor invariant under a π–rotation, then there exist invertible matrices Y and Z such that the tensors defining the PEPS verify Fig. 7.4d.* □

Now the constraints are $Z^T = Z$ and $Y^T = Y$.



(a) (b)

Figure 7.3: **Rotational symmetry**. This figure represents the condition which must be fulfilled by a PEPS in order to generate a state invariant under (a) $\frac{\pi}{2}$–rotations (in this case a clockwise rotation) and (b) π–rotations.

7.3 Uniqueness of the construction method

In this Section, we show that constraints similar to the ones shown for MPS determine the construction of invariant injective PEPS, so the entries of the tensor are essentially Clebsch–Gordan coefficients. In fact, the proof is just an application of the results proven in Section 4.3.

Let us enunciate the Theorem which ensures the uniqueness of the construction of the PEPS which fulfil the equation shown in Fig. 7.1.

Theorem 42 (Piecewise construction (PEPS)) *Let us consider a finite or compact group G and three representations of this group: u_g (d–dimensional and irrep), $Z_g \in \mathcal{M}_{D_1}$ and $Y_g \in \mathcal{M}_{D_2}$. Then, all the solutions of the equality shown in Fig. 7.1 have the structure of Eq. 4.10.* □

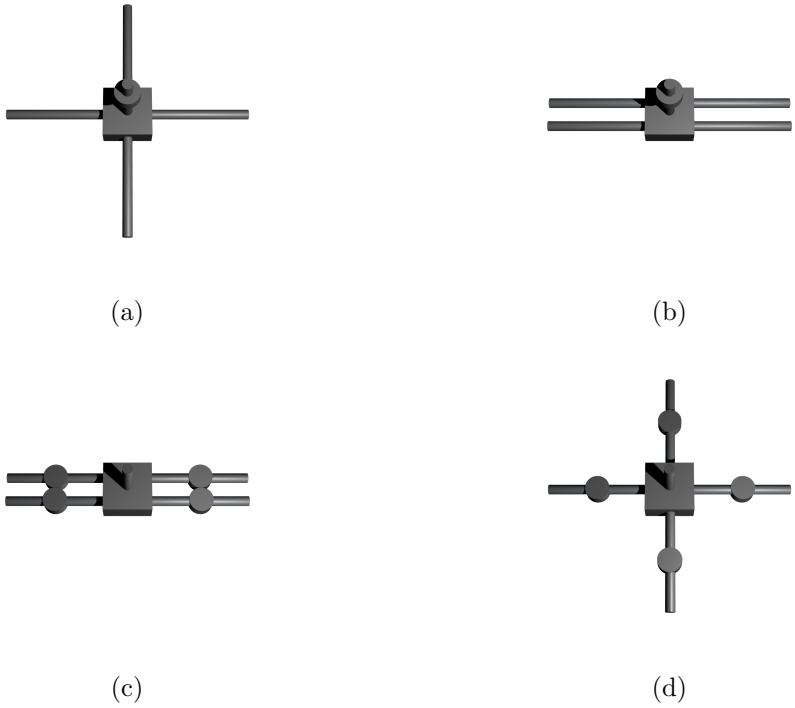
Proof The first step is to transform the tensor into a Kraus operator, but this can be done by gathering the orthogonal legs together, so the equation shown in Fig. 7.1 transforms into:

$$\sum_{j=1}^{d} u_{ij}^{(g)} A_j = e^{i\theta_g} (Y_g \otimes Z_g) A_i (Y_g^{-1} \otimes Z_g^{-1})$$

Y and Z, however, can be considered w.l.o.g. unitary representations, since the group is compact or finite. Obviously, $A_i \in \mathcal{M}_{D_1 D_2}$. Therefore, by applying the Clebsch–Gordan decomposition theorem, there is a global unitary W such that

$$U_g = W(Y_g \otimes Z_g)W^\dagger = \bigoplus_r U_g^{D_r}$$

with $U_g^{D_r}$ being D_r–dimensional irreps of G. We assume that any additional labels which could be required to determine the representation are included, but we do not write them explicitly, for the sake of clarity in the notation. The transformation of the Kraus operators into the isometry is performed by means of Eq. **??**.



(a) (b)

(c) (d)

Figure 7.4: **Transformation into an MPS**. This figure illustrates how to deal with the construction of invariant PEPS by transforming the tensor into s set of Kraus operators. Thus, the techniques and results shown in Chapter 4 are available by taking into account that the virtual representation is now always a tensor product of representations. (a) Physical unitary acting on the tensor, (b) the symmetry is inherited by the virtual spins, (c) the virtual legs can be gathered, and (d) the unitaries of the virtual spins of the PEPS can be understood as a tensor product representation in an invariant a MPS.

Therefore, we can now apply Theorem 27. This construction is unique, and all the transformations are invertible, so the Theorem follows. ∎

We have seen in the previous three Chapters that, although MPS and PEPS share a common framework and some properties, their physical behaviour differs remarkably, with the higher–dimensional case presenting much more richness. However, when we restrict ourselves to the set of invariant states (for sufficiently complex groups), the similarities become more relevant, as we attempted to show in this Chapter.

Les vieillards aiment à donner de bons préceptes, pour se consoler de n'être plus en état de donner de mauvais exemples.

François de la Rochefoucauld (1613-1680)

8

Quasi–solvable 1D Hamiltonians

8.1 Introduction

Due to their inherent complexity, many–body system Hamiltonians are, in general, not spectrally solvable. The ability to provide quasi–solvable examples is paramount in condensed matter. For instance, as already explained in the Introduction, the publication by I. Affleck *et al.* of their model [AKLT88] was an important support for the Haldane hypothesis, which had been received with incredulity by part of the scientific community at that moment.

However, among the uncountable possible quasi–solvable Hamiltonians, only a few contain physical relevance. Of particular interest are *two–body Hamiltonians*; that is, Hamiltonians consisting only of interactions with, at most, two non–trivial (different from the identity) local operators. And within those, the ones which are invariant under a large symmetry group, such as $SU(2)$, especially deserve our attention, since this kind of interactions is the one which naturally appears in spin systems. Two prominent examples are the already mentioned AKLT state [AKLT88], and the Majumdar–Ghosh state [MG69], which have two–body parent Hamiltonians with $SU(2)$ symmetry. They have served as toy models to understand certain physical behaviours in real physical systems, such as the existence of a Haldane gap in spin chains with integer spin [Hal83a, Hal83b], or the phenomenon of dimerization [MG69], respectively. In spite of the key role played by these states in the understanding of the physical properties of spin chains, there are very few other examples of TI–MPS with $SU(2)$ symmetry and a two–body parent Hamiltonian [FNW92, KM08].

The organization of this Chapter is as follows:

- In Section 8.2, we concentrate on MPS that are eigenstates (not necessarily ground states) of a kinsfolk Hamiltonian showing $SU(2)$ symmetry and containing only two–body interactions. We find other families of Hamiltonians with those features, beyond the well–known AKLT and Majumdar–Ghosh. Furthermore, we provide the first examples of MPS that correspond to excited states of $SU(2)$–invariant Hamiltonians. There is a new example of a state with spin 1, which is never the ground state of any frustration–free $SU(2)$–invariant two–body Hamiltonian. In order to perform a systematic search of all those MPS we developed a simple technique, easily generalizable to other groups or interactions. The results shown in this Section are taken from [SWPGC09].

- In Section 8.3, we introduce a real–space exact renormalization group method to find exactly–solvable quantum spin chains and their ground states. This method allows us to provide a complete list of exact solutions within $SU(2)$–symmetric quantum spin chains with $S \leq 4$ and nearest–neighbour interactions, as well as new examples with $S = 5$. We obtain two classes of solutions: In the first class the renormalization group converges toward a fixed point and the ground state of the Hamiltonian is an MPS. The other class does not present any renormalization fixed point and the ground state is a partially ferromagnetic state. The results shown in this Section arise from [TS10].

8.2 $SU(2)$ two–body kinsfolk Hamiltonians

We have seen in Section 3.2 a method, called *parent Hamiltonian*, to construct local Hamiltonians with Matrix Product States (MPS) as ground states. In Section 3.5, we proposed the definition of *kinsfolk Hamiltonian* as a generalization of the parent Hamiltonian (see Definition 20), and we proposed a method to compute this class of Hamiltonians by means of Eq. 3.8, which we left unproven. In this Section, we first prove that this method is the most general one for finding Hamiltonians with a given MPS as a *local eigenstate*, *i.e.* as eigenstate of each local term in the Hamiltonian.

In Chapter 4, we provide the necessary and sufficient conditions for an MPS to be invariant under a given group, so in this Section we make use of these results in order to construct examples with $SU(2)$ invariance, a symmetry of particular relevance in spin systems.

Then, we show examples (including the AKLT and Majumdar–Ghosh states) of MPS which are *excited* eigenstates of local two–body $SU(2)$–symmetric TI–Hamiltonians. In fact, we analyse the subfamilies of kinsfolk Hamiltonians which have the state as a ground state, providing a numerical proof of the existence of subfamilies for which the state is excited. This is proven by constructing states with less energy. Finally, we present a detailed list of kinsfolk Hamiltonians for the smallest spin values.

8.2.1 Completeness of the method

The aim of this Subsection is to provide a proof of the completeness of the method for computing kinsfolk Hamiltonians proposed in Section 3.5. Therefore, let us prove the following Theorem:

Theorem 43 (Local structure of kinsfolk Hamiltonians) *Let $|\psi\rangle$ be an MPS, local eigenstate of its kinsfolk Hamiltonian $H = \sum_i \tau_i(h \otimes \mathbb{1}_{rest})$ in the sense of Definition 20. Then, the structure of the local term is $h = \sum_{P_\mu \in \mathcal{C}^\perp} \alpha_\mu P_\mu + \lambda \mathbb{1}$, where $\mathcal{C}^\perp$ is a set of projectors onto the kernel of the reduced density matrix $\rho = \sum_{P_\nu \in \mathcal{C}} b_\nu P_\nu$ and α_μ, $\lambda \in \mathbb{R}$.* □

Proof Let us call h the local Hamiltonian. By the hypothesis of *local eigenstate*,

$$h\rho = \lambda\rho \tag{8.1}$$

for certain $\lambda \in \mathbb{R}$. This is equivalent to $[\rho, h] = 0$ and hence one can find a set of projectors $\mathcal{P} = \{P_\mu, \mu = 1, \ldots, r \mid \sum_\nu P_\nu = \mathbb{1}\}$ such that we can decompose both ρ and h by means of them, *i.e.* $h = \sum_\nu a_\nu P_\nu$ and $\rho = \sum_{P_\mu \in \mathcal{C}} b_\mu P_\mu$, where $\mathcal{C}$ represents the set of projectors which describe the support of ρ. By using Eq. 8.1 together with this decomposition, we obtain that $a_\nu = \lambda$ for all $\nu \in \mathcal{C}$ and hence:

$$h = \sum_{P_\mu \in \mathcal{C}^\perp} a_\mu P_\mu + \lambda \sum_{P_\nu \in \mathcal{C}} P_\nu = \sum_{P_\mu \in \mathcal{C}^\perp} (a_\mu - \lambda) P_\mu + \lambda \mathbb{1}$$

Then, the translational invariant kinsfolk Hamiltonian is $H = \sum_i \tau_i(h \otimes \mathbb{1}_{\text{rest}})$, where τ is the translation operator, which proves the Theorem. ■

One may wonder about the reason why the condition of being local eigenstate is imposed. It is for practical purposes, since we can capture with this method all possible frustration–free Hamiltonians, it keeps a manageable local structure (we work with h and not with H), and it allows us to go further than parent Hamiltonians, entering into the world of frustrated Hamiltonians and excited states. This Theorem shows that, given an MPS $|\psi\rangle$, looking for all possible parent Hamiltonians of *interaction length* n is equivalent to looking for all possible solutions to the equation

$$h\rho^{(n)} = \lambda\rho^{(n)} \tag{8.2}$$

with $\lambda = \text{tr}\left[h\rho^{(n)}\right]$. The next Lemma gives yet another equivalent formulation, which is the one we will use below, which finally proves the statement about Eq. 3.8.

Lemma 31 (Proof of the completeness of Eq. 3.8) *Given a hermitian matrix h and a density matrix ρ, $h\rho = \lambda\rho$ iff*

$$\text{tr}\left[h^2\rho\right] - \text{tr}\left[h\rho\right]^2 = 0 \tag{8.3}$$

□

PROOF Let us prove both implications:

$\boxed{\Rightarrow}$

This implication is clear, since one only needs to substitute the equality $h\rho = \lambda\rho$ in Eq. 8.3 and to check that the equality holds.

$\boxed{\Leftarrow}$

Let us denote $\langle h \rangle = \mathrm{tr}\,[h\rho]\,\mathbb{1}$. By assumption,

$$\mathrm{tr}\left[(h - \langle h \rangle)^2 \rho\right] = \mathrm{tr}\left[h^2 \rho\right] - \mathrm{tr}\,[h\rho]^2 = 0$$

So $\rho^{\frac{1}{2}}(h - \langle h \rangle)^2 \rho^{\frac{1}{2}} = 0$, since it is a positive operator with trace 0. This implies that $(h - \langle h \rangle)\rho = 0$ and hence $h\rho = \lambda\rho$. ∎

With this at hand, we can systematically search for MPS which are excited *local eigenstates* of $SU(2)$–invariant Hamiltonians with two–body interactions. We will proceed as follows: we start with a given $SU(2)$–symmetric MPS $|\psi\rangle$ and fix the interaction length n; then, we look for possible solutions to Eq. 8.3 of the form

$$h = \sum_{i<j\leq n} \sum_{\alpha=1}^{2J} a_{ij}^{(\alpha)} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j)^\alpha + a_0 \mathbb{1} \qquad \boxed{8.4}$$

where $\boldsymbol{S}_i$ are the generators of $SU(2)$ in the representation of spin J, sitting at site i. To ensure $SU(2)$ symmetry and two–body interactions in the Hamiltonian. Note that the Hamiltonian written in Eq. 8.4 is the most general local two–body Hamiltonian which is invariant under the group $SU(2)$.

Finally, in order to guarantee that the MPS $|\psi\rangle$ is an *excited state*, we find another $SU(2)$–symmetric MPS with less energy which acts as a **witness**. In the next section, we illustrate this procedure by starting with $|\psi\rangle$ being either the AKLT, the Majumdar–Ghosh state, or generalizations thereof. Throughout this work we consider spin chains in the *thermodynamic limit* $N \to \infty$. Let us summarize the idea in the following table:

Local GS	$\Longrightarrow$	global GS	(FF)	
Local ES	$\nearrow$	global ES	$\longmapsto$	Find state with less energy $\hookrightarrow$ easy to check
	$\searrow$	global GS	$\longmapsto$	Hard calculation

8.2.2 Examples of $SU(2)$ two–body Hamiltonians

In this Subsection, we make use of the results provided in the previous Subsection to construct kinsfolk Hamiltonians and illustrate the method which allows us to test that the states are sometimes excited. The Subsection is split into several Subsubsections. The first two correspond to the well–known AKLT and Majumdar–Ghosh states, which are used to illustrate the method. The third one is a new example of state which is always an excited state of the kinsfolk Hamiltonian. We finally provide a detailed list of kinsfolk Hamiltonians corresponding to the lowest spins.

8.2.2.1 Models with spin 1

Let us consider the AKLT state [AKLT88] as a first example. Its Kraus operators are $A_{-1} = -\sqrt{2}\sigma^-$, $A_0 = \sigma^z$, $A_1 = \sqrt{2}\sigma^+$.

In the case when the number of spins is $n = 2$, the only solution to Eq. 8.3 is the AKLT Hamiltonian. In case $n = 3$, the solutions are given by

$$h = (-3v_1 + v_2 + 3v_3)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2) + v_3(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2)^2 + \frac{1}{2}(-3v_1 + v_2)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_3) - \frac{1}{2}(-3v_1 + v_2)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_3)^2 + v_2(\boldsymbol{S}_2 \cdot \boldsymbol{S}_3) + v_1(\boldsymbol{S}_2 \cdot \boldsymbol{S}_3)^2$$

where the eigenvalue corresponding to the AKLT state is $7v_1 - 3v_2 - 2v_3$. The total translational invariant Hamiltonian is then

$$H = \sum_i (-3v_1 + 2v_2 + 3v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + (v_1 + v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 + \frac{1}{2}(-3v_1 + v_2)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) - \frac{1}{2}(-3v_1 + v_2)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2$$

which contains the usual AKLT model. It is not difficult to check that there is a region in the parameter space where the AKLT state is still the ground state of this Hamiltonian. For instance, while $h \geq 0$, it is ensured that the state is the ground state. However, let us remark that the Hamiltonian in this case is not the parent Hamiltonian proper since, as we are imposing a two–body structure and perhaps $\mathrm{supp}[h] \subset \ker \rho$, so the results on uniqueness are not necessarily true.

To find regions where it is an **excited eigenstate** we will use the $SU(2)$–symmetric MPS associated to the virtual representation $\frac{3}{2} \oplus \frac{1}{2}$ as a witness (see Chapter 4 to check how to perform the construction). The result is plotted in Fig. 8.1, where one sees the existence of points in this family of spin–1 Hamiltonians for which the AKLT state is excited.

Note that it is possible to perform a change of variables in the total Hamiltonian, for instance $a \to \frac{1}{2}(-3v_1 + v_2)$ and $b \to v_1 + v_3$, such that it depends only on two parameters. However, the number of parameters that the local Hamiltonian h

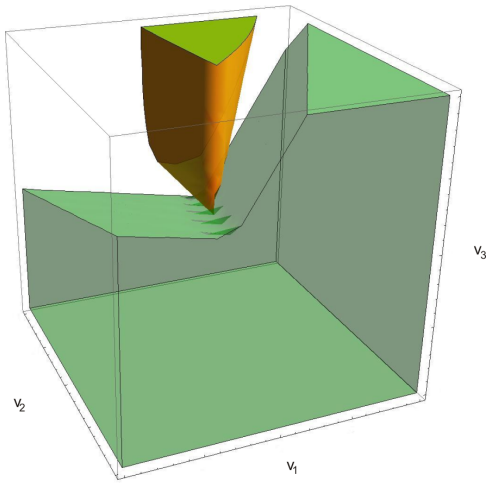


Figure 8.1: **Kinsfolk Hamiltonian of AKLT**. Space of parameters of the local Hamiltonian h for the AKLT state and $n = 3$. The orange volume represents the points where the state is the local (and hence the global) ground state. The green volume represents points corresponding to excited states detected with the witness $\frac{3}{2} \oplus \frac{1}{2}$.

depends on cannot be reduced, which means that there are non–physical parameters in it. In Fig. 8.2, we have represented the problem above ($n = 3$ and AKLT state) in terms of the physical parameters. The positive axis b corresponds there to the usual AKLT Hamiltonian.

Concerning FNW states [FNW92], that is, integer spin J and virtual irrep j, we have performed an exhaustive search whose main results are gathered in Table 8.1. The study has been carried out by increasing n and studying the number of parameters which the family of Hamiltonians depends on (notice that the case of interaction length n contains the case of interaction length $n-1$). We have increased n until the number of parameters stops growing. In all the cases considered in the Table, a saturation occurs when $n > 3$, *i.e.* considering more than 3 particles apparently does not add new Hamiltonians.

Let us also introduce a new state with spin 1, which is never the ground state of any frustration–free $SU(2)$–invariant two–body Hamiltonian. The state has both physical and virtual spin 1, and it is described by the Kraus operators

$$A_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad A_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$A_{-1} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}$$

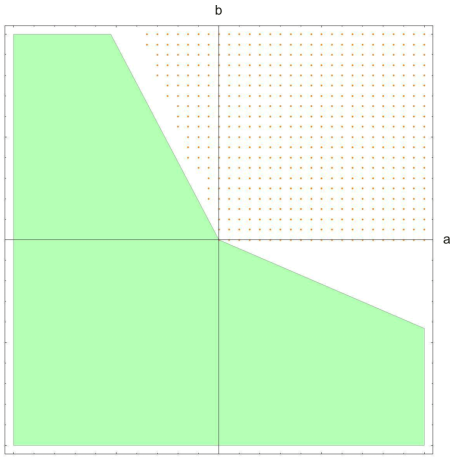


Figure 8.2: **Kinsfolk Hamiltonian of AKLT (2D)**. Space of physical parameters of the Hamiltonian H corresponding to $n = 3$ and the AKLT state. The dots (orange) represent where the state is the local (and hence the global) ground state. The surface (green) represents points corresponding to excited states detected by means of the witness $\frac{3}{2} \oplus \frac{1}{2}$. The blank wedges correspond to cases which cannot be detected by the method.

The translational invariant Hamiltonian which has this state as an eigenstate is:

$$H = \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 - (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) - (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2$$

This state is injective and a local excited state. The fact that this state is an excited state of the total Hamiltonian can be verified as above by means of the witness $1 \oplus 0$.

J \ j	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$
1	2	1	■	■	■	■	■
2	—	5	3	■	■	■	■
3	—	—	4	2	2	1	■

Table 8.1: Table of results for FNW states with physical spin J and virtual spin j. The numbers in the table are the number of parameters the obtained families of Hamiltonians depend on. The ■ represent the cases for which no solution was found.

8.2.2.2 Model with spin $\frac{1}{2}$

Let us consider now the Majumdar–Ghosh state as an example with semi–integer spin. The Kraus operators are now:

$$A_{-\frac{1}{2}} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix} \qquad A_{\frac{1}{2}} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

As in the previous case, we do not find any solution for $n = 2$ and only the Majumdar–Ghosh Hamiltonian for cases $n = 3$ and $n = 4$. For $n = 5$, the solutions to Eq. 8.3 are given by:

$$\begin{gathered} h = (v_1 - v_2 + v_4)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2) + (v_1 - v_2 + v_4)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_3) + v_3(\boldsymbol{S}_1 \cdot \boldsymbol{S}_4) \\ + v_3(\boldsymbol{S}_1 \cdot \boldsymbol{S}_5) + v_4(\boldsymbol{S}_2 \cdot \boldsymbol{S}_3) + (-v_1 + v_2 + v_3)(\boldsymbol{S}_2 \cdot \boldsymbol{S}_4) + v_3(\boldsymbol{S}_2 \cdot \boldsymbol{S}_5) \\ + v_2(\boldsymbol{S}_3 \cdot \boldsymbol{S}_4) + v_1(\boldsymbol{S}_3 \cdot \boldsymbol{S}_5) + v_1(\boldsymbol{S}_4 \cdot \boldsymbol{S}_5) \end{gathered}$$

and the energy associated to the state is $-\frac{3}{4}(v_1 + v_4)$. The total Hamiltonian $H = \sum_i \tau_i(h)$ is given by:

$$H = \sum_i 2(v_1 + v_4)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + (v_1 + v_3 + v_4)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) + 2v_3(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+3}) + v_3(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+4}) \quad (8.5)$$

As in the AKLT case, by means of a change of variables $a \to v_3$ and $b \to v_1 + v_4$, the number of physical parameters in the total Hamiltonian is 2, compared with the four parameters the local Hamiltonian depends on. The Majumdar–Ghosh state is an excited local eigenstate for a region in the space of parameters, which in this case is detected by the witness $\frac{1}{2} \oplus 1 \oplus 0$, as shown in Fig. 8.3. The usual Majumdar-Ghosh Hamiltonian[1] corresponds to the positive axis b.

8.2.2.3 Model with spin $\frac{3}{2}$

Let us consider as a final example the $SU(2)$–symmetric MPS corresponding to spin $\frac{3}{2}$ and virtual representation $\frac{3}{2} \oplus 0$. For $n = 3$, the solutions to Eq. 8.3 are given by:

$$\begin{gathered} h = v_3(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2) + v_2(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2)^2 + v_1(\boldsymbol{S}_1 \cdot \boldsymbol{S}_2)^3 \\ + (2v_1 - v_2 + v_3)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_3) + (4v_1 - v_2)(\boldsymbol{S}_1 \cdot \boldsymbol{S}_3)^2 + v_1(\boldsymbol{S}_1 \cdot \boldsymbol{S}_3)^3 \\ + v_3(\boldsymbol{S}_2 \cdot \boldsymbol{S}_3) + v_2(\boldsymbol{S}_2 \cdot \boldsymbol{S}_3)^2 + v_1(\boldsymbol{S}_2 \cdot \boldsymbol{S}_3)^3 \end{gathered}$$

[1] The family of Hamiltonians constructed in [Kum02] is quite remarkable. In this paper, the ground state of the Hamiltonian which corresponds to $b = 2a$ is calculated, and fits our results perfectly.

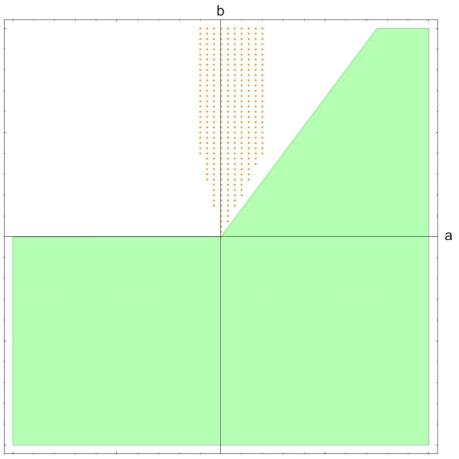


Figure 8.3: **Kinsfolk Hamiltonian of Majumdar–Ghosh**. Space of physical parameters of the total Hamiltonian for $n = 5$ associated to the Majumdar–Ghosh state. The dots (orange) represent where the state is the local (and hence the global) ground state. The surface (green) represents points corresponding to excited states detected by means of the witness $\frac{1}{2} \oplus 1 \oplus 0$.

and the energy associated to the MPS is in this case $-\frac{15}{64}(165v_1 - 60v_2 + 16v_3)$. The total Hamiltonian now reads:

$$H = \sum_i 2v_3(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + 2v_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 + 2v_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^3$$
$$+(2v_1 - v_2 + v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) + (4v_1 - v_2)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2 + v_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^3$$

It is remarkable that in this case there are no spurious parameters in the local Hamiltonian h. Considering the family of states whose virtual representation is $\frac{3}{2} \oplus 1 \oplus 0$ as a witness, it is possible to prove that there is a region in the space of parameters of the Hamiltonian for which the MPS is an excited eigenstate, as shown in Fig. 8.4.

8.2.2.4 List of kinsfolk Hamiltonians

The following lists $SU(2)$–invariant two–body Hamiltonians for which the MPS with physical spin J (irrep) and virtual spin j is an exact eigenstate with energy ϵ.

Spin $J = \frac{1}{2}$

- $j = \frac{1}{2} \oplus 0$, $\epsilon = -\frac{3}{4}v_1$:

$$H = \sum_i 2v_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + (v_1 + v_2)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})$$
$$+2v_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+3}) + v_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+4})$$

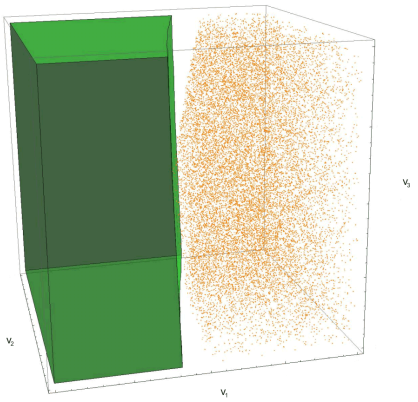


Figure 8.4: **Kinsfolk Hamiltonian of the spin–$\frac{3}{2}$ model**. Space of parameters of the spin–$\frac{3}{2}$ model. The dots (orange) are obtained numerically and they represent values of the parameters where the MPS state is the ground state. The volume (green) represents points corresponding to excited states detected with the witness $\frac{3}{2} \oplus 1 \oplus 0$.

- No solutions found (with $n \leq 6$) for $j = \frac{1}{2} \oplus 1$, $\frac{3}{2} \oplus 1$, $\frac{3}{2} \oplus 2$, $\frac{5}{2} \oplus 2$.

Spin $J = 1$

- $j = \frac{1}{2}$, $\epsilon = -2v_1 - 3v_2$:

$$H = \sum_i (3v_1 + 2v_2)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + v_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 + \frac{1}{2}v_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) - \frac{1}{2}v_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2$$

- $j = 1$, $\epsilon = 1$:

$$H = \sum_i (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 - (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) - (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2$$

- No solutions found (with $n \leq 4$) for $j = \frac{3}{2}, 2, \frac{5}{2}, 3$.

Spin $J = \frac{3}{2}$

- $j = \frac{3}{2} \oplus 0$, $\epsilon = -\frac{15}{64}(165v_1 - 60v_2 + 16v_3)$:

$$H = \sum_i 2v_3(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + 2v_2(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$$
$$+2v_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^3 + (2v_1 - v_2 + v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})$$
$$+(4v_1 - v_2)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2 + v_1(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^3$$

- $j = \frac{1}{2} \oplus 1$, $\epsilon = -\frac{495}{64}$:

$$H = \sum_i \frac{243}{16}(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}) + \frac{29}{4}(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 + (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^3$$

- No solutions found (with $n \leq 4$) for $j = \frac{3}{2} \oplus 1, \frac{5}{2} \oplus 1, \frac{1}{2} \oplus 2, \frac{3}{2} \oplus 2$.

Spin $J = 2$

- $j = 1$, $\epsilon = (-6986v_1 + 778v_2 - 62v_3 + 1260v_4 - 90v_5)$:

$$H = \sum_i (2400v_1 - 63v_2 + 24v_3 - 792v_4 + 63v_5)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})$$
$$+(133v_1 - 14v_2 + 2v_3 - 133v_4 + 14v_5)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$$
$$+(v_2 + v_5)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^3 + (v_1 + v_4)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^4$$
$$+(\frac{1729}{2}v_1 - 91v_2 + \frac{13}{2}v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})$$
$$+(\frac{5719}{36}v_1 - \frac{301}{18}v_2 + \frac{43}{36}v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2$$
$$+(-\frac{665}{18}v_1 + \frac{35}{9}v_2 - \frac{5}{16}v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^3$$
$$+(-\frac{133}{12}v_1 + \frac{7}{6}v_2 - \frac{1}{12}v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^4$$

- $j = \frac{3}{2}$, $\epsilon = 0$:

$$H = \sum_i (580v_1 - 80v_2 + 10v_3 - 330v_4 + 30v_5)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})$$
$$+(91v_1 - 11v_2 2v_3 - 91v_4 11v_5)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2$$
$$+(v_2 + v_5)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^3 + (v_1 + v_4)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^4$$
$$+\frac{1}{6}(2275v_1 - 275v_2 + 25v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})$$
$$+\frac{1}{36}(455v_1 - 55v_2 + 5v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^2$$
$$+\frac{1}{18}(-455v_1 + 55v_2 - 5v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^3$$
$$+\frac{1}{36}(-91v_1 + 11v_2 - v_3)(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2})^4$$

• No solutions found (with $n \leq 4$) for $j = 2, \frac{5}{2}$.

Spin $J = 3$

Solutions (mostly cumbersome ones) were found for $j = \frac{3}{2}$ ($n = 3$) (FNW state), $j = 2$ ($n = 2$) and $j = \frac{5}{2}$ ($n = 2$).

8.3 Exact renormalization construction

The purpose of this Section is to investigate a real–space renormalization group and its applications in a systematic search for exactly solvable quantum spin chains. The present approach complements the parent Hamiltonian method shown in Section 8.2, such that one can start from the Hamiltonians and search for exactly solvable ones. We first briefly review the basics of real–space renormalization and its extension to systems with $SU(2)$ symmetry. The presence of symmetry allows us to design a simple exact renormalization scheme. By using this method, we study quantum spin chains with $SU(2)$ symmetry and nearest–neighbour interactions. For $S \leq 4$, we provide complete solutions for the models which are frustration–free for two neighbouring spins. Moreover, we provide new examples of $S = 5$ which were not previously known. We discuss these exact solutions by dividing them into two different classes, whose ground states are MPS and partially ferromagnetic states, respectively.

8.3.1 Real–space exact renormalization process

Let us consider a chain with N local d-dimensional Hilbert spaces $\mathcal{H}$, that we can assume as local spins. We denote by $|M\rangle \in \mathcal{H}$ an orthonormal basis in $\mathcal{H}$. And let us also consider a translational invariant local Hamiltonian $H = \sum_i \tau_i(h^{(L)} \otimes \mathbb{1}_{\text{rest}})$, where τ_i is the translation operator, containing local interaction terms acting on L contiguous sites. We can assume w.l.o.g. positive semidefinite interactions $h \geq 0$, since they can always be achieved by shifting their energy level.

Let us now briefly explain the real–space renormalization process. We start by coupling the first two spins, whose Hilbert space $\mathcal{H}\otimes\mathcal{H}$ is mapped into a Hilbert space $\mathcal{H}_2$, which has in general a dimension $D_2 < d^2$. The criterion followed to perform this reduction $\mathcal{H}\otimes\mathcal{H} \to \mathcal{H}_2$ is to conserve only the low–energy states of the Hamiltonian. In general, the method works by finding mappings $\mathcal{A}^{[i]} : \mathcal{H}_{i-1}\otimes\mathcal{H} \to \mathcal{H}_i$ which iterate this process. We continue this renormalization procedure until reaching the end of the chain and getting an orthonormal basis $\{|\chi\rangle\}_{\chi=1}^{D_N}$ of the Hilbert space $\mathcal{H}_N$.

Let us show the real–space renormalization process from the $(i-1)$-th spin to the i-th spin, which can be written in a basis as [ÖR95]

$$|\beta[i]\rangle = \sum_{\alpha,M} A_{\alpha,\beta}^{[M]} |\alpha[i-1]\rangle \otimes |M[i]\rangle \qquad (8.6)$$

where the input state $|\alpha[i-1]\rangle \in \mathcal{H}_{i-1}$, the output state $|\beta[i]\rangle \in \mathcal{H}_i$, and the Kraus operators $A^{[M_i]}$ are $D_{i-1} \times D_i$ matrices satisfying gauge condition $\sum_M A^{[M]} A^{[M]\dagger} = \mathbb{1}$. Here, we define $D_0 = 1$ so that the Kraus operator $A^{[M_1]}$ for the first spin can be viewed as a row vector.

Eq. 8.6 shows that the real–space renormalization results in an orthonormal basis $|\chi\rangle$ with a matrix product form (Fig. 8.5a)

$$|\chi\rangle = \sum_{M_1 \ldots M_N} (A^{[M_1]} A^{[M_2]} \cdots A^{[M_N]})_\chi \, |M_1 M_2 \ldots M_N\rangle \qquad \boxed{8.7}$$

$\chi = 1, \ldots, D$ with $D = \max_i D_i$ called the *bond dimension* of the matrix product, as explained in Chapter 1.

In the Density Matrix Renormalization Group (DMRG) algorithm, these MPS are used variationally to find the best approximation for the low energy sector of 1D systems.

In this Section, we are interested in special models, such that the states $|\chi\rangle$ *exactly* span the ground state subspace in the thermodynamic limit. The specification concerning the thermodynamic limit comes from the fact that, otherwise, every N–site state can be written by means of a matrix product Ansatz (given in Eq. 8.7) by taking $D > d^{\lfloor \frac{N}{2} \rfloor}$. However, we seek models for which an exact renormalization can be performed for arbitrarily long chains. In other words, the ground states of these models can be solved rigorously through real–space renormalization, and the truncation induced by the Kraus operators does no harm.

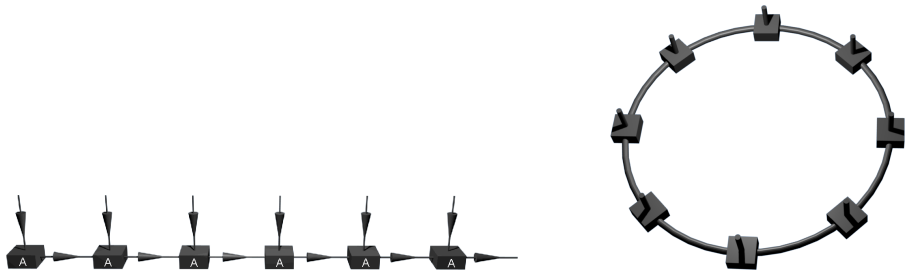
Practically, since $h_i \geq 0$, this search can be accomplished if the Kraus operators for each spin can be adjusted step by step in the renormalization group to fulfil

$$\mathrm{tr}\,[\rho_i^\chi h_i] = 0, \qquad \forall i = 1, \ldots, N \text{ and } \forall \chi = 1, \ldots, D_N \qquad \boxed{8.8}$$

where $\rho_i^\chi = \mathrm{tr}_{\mathrm{inv}}[\,|\chi\rangle\langle\chi|\,]$ is the reduced density matrix for L spins. The above condition leads to $H\,|\chi\rangle = 0$, which means that the vectors $|\chi\rangle$ are the ground states of H, because $H \geq 0$. Such Hamiltonians are called *frustration–free Hamiltonians* because their ground states locally minimize energy (see Definition 18). For instance, it is well–known that the ferromagnetic Heisenberg chain is a typical frustration–free model in which all the spins tend to align in parallel to gain energy. Recently, the frustration–free Hamiltonians have been reformulated as quantum k–SAT problems and attract considerable interests in quantum information community [Bra06, MFG$^+$10, dBOOE10, LMSS10, LLM$^+$10].

For generic models, this renormalization procedure will terminate after blocking a number of spins due to intrinsic frustrations. To find the exactly quasi–solvable model, the first possibility is that the renormalization group reaches a fixed point. Then, the ground state of the Hamiltonian in PBC can be written as a translational invariant MPS (see Fig. 8.5)

$$|\psi\rangle = \sum_{M_1, \ldots, M_N} \mathrm{tr}\left[A^{[M_1]} A^{[M_2]} \cdots A^{[M_N]}\right] \, |M_1 M_2 \ldots M_N\rangle$$



(a) (b)

Figure 8.5: **Real–space renormalization**. (a) The real–space renormalization group yields MPS. (b) In PBC, the TI–MPS are constructed from the fixed–point Kraus operators.

where the Kraus operators $A^{[M]}$ are the converged $D \times D$ matrices at the fixed point. We discuss these fixed–point MPS solutions in Subsubsection 8.3.2.2. Another possibility is that, for some models, the number of states $\dim \mathcal{H}_k$ we should keep increases when gathering more spins. Even though there is no renormalization fixed point, we find that it is still possible to obtain the ground states exactly if $\dim \mathcal{H}_k$ increases in a *controllable* way. We illustrate this point in Subsubsection 8.3.2.3, when discussing partially ferromagnetic states.

8.3.2 Quantum spin chains with $SU(2)$ symmetry

In this Subsection, we adapt the real–space exact renormalization method to $SU(2)$–symmetric quantum spin chains with nearest–neighbour interactions. Therefore, let us start by explaining some details about $SU(2)$–symmetric Hamiltonians. The most general $SU(2)$–symmetric spin–S TI–Hamiltonian with nearest–neighbour interactions can be expressed as

$$H = \sum_i \sum_{n=1}^{2S} a_n (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^n + a_0 \mathbb{1}. \tag{8.9}$$

which is a particular case of the Hamiltonian shown in Eq. 8.4. The study of these $SU(2)$–symmetric models has a long history in condensed matter physics. It was already known that some of these models can be solved by the Bethe Ansatz method and such models are fully classified by solutions of Yang–Baxter equations [Ken92].

We want to identify the frustration–free models in Eq. 8.9 and find their ground states through real-space exact renormalization. However, it is convenient to use projectors instead of spin operators, so we use the transformation

$$(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^n = \sum_{S_T=0}^{2S} [\frac{1}{2} S_T(S_T+1) - S(S+1)]^n P_{S_T}(i, i+1)$$

where P_{S_T} is a projector onto the total spin–S_T states of the two spins. By shifting the local energy levels, we can always rewrite Hamiltonian 8.9 as a sum of projectors

$$H = \sum_i \sum_{S_T \in \mathcal{K}} J_{S_T} P_{S_T}(i, i+1) \tag{8.10}$$

with coupling constants $J_{S_T} > 0$, and $\mathcal{K} \subseteq [0, 2S]$ is a set specifying the choice of projector(s) as local interactions. Since the local interactions in Eq. 8.10 are a sum of projectors, we have $H \geq 0$.

Let us remark that, as the physical representation is irreducible and we restrict ourselves to nearest–neighbour interactions, the exact value of J_{S_T} is not important, as long as the Hamiltonian is frustration–free.

From Hamiltonian 8.10, it is still not clear how to properly choose, if possible, the set $\mathcal{K}$ that makes the Hamiltonian frustration–free. However, as we restrict ourselves to frustration–free models with two neighbouring spins, we can provide a complete list by taking advantage of the renormalization group.

8.3.2.1 Exact renormalization with $SU(2)$ symmetry

In this Subsubsection, we explain how to make use of the $SU(2)$ symmetry in the exact renormalization scheme. This particularizes the real–space renormalization in Eq. 8.6 such that both the input and output states form representations of the symmetry group, which ensures that the symmetry is preserved in each renormalization step. The method shown here is a three–step process.

Eq. 8.6 can be promoted to an $SU(2)$–adapted basis [DMDNS98, SPV10]

$$|j_b t_b m_b\rangle = \sum_{j_a t_a m_a} \sum_M A^{[S,M]}_{j_a t_a m_a, j_b t_b m_b} |j_a t_a m_a\rangle |SM\rangle \tag{8.11}$$

where the j's denote the $SU(2)$ representations (total–spin quantum number), the t's make the degenerate states within the same j distinguishable, and the m's are the magnetic quantum numbers associated with j.

The first step of the process consists in splitting the Kraus operators into two terms by means of the **Wigner–Eckart Theorem** (see Fig. 8.6a) as

$$A^{[S,M]}_{j_a t_a m_a, j_b t_b m_b} = T_{j_a t_a, j_b t_b} \langle j_a m_a, SM | j_b m_b \rangle \tag{8.12}$$

where the indices $j_a t_a, j_b t_b$ keep track of the representations of the input and output states. The first term is a real matrix T denoting the weights of different input states in each output state. We call this matrix **weight matrix**. Let us remark that the weight matrix does not depend on the magnetic quantum numbers. The second term is the Clebsch–Gordan coefficient $\langle j_a m_a, SM | j_b m_b \rangle$, corresponding to the representation fusion $j_a \otimes S \hookrightarrow j_b$. To ensure that the output states always form an orthonormal basis, the weight matrix must fulfil the *triangle inequality*

$$T_{j_a t_a, j_b t_b} = 0 \quad \text{unless} \quad |j_a - S| \leq j_b \leq j_a + S \tag{8.13}$$

and

$$\sum_{j_a t_a} T_{j_a t_a, j_b t_b} T_{j_a t_a, j_b t'_b} = \delta_{t_b, t'_b} \tag{8.14}$$

for every j_b. The first constraint is related to $SU(2)$ fusion rules. The second constraint means that the columns of $T_{j_a t_a, j_b t_b}$ corresponding to the same j_b but different t_b, are orthonormal vectors, which guarantees the isometry condition for the Kraus operators, *i.e.* $\sum_M A^{[S,M]} A^{[S,M]\dagger} = \mathbb{1}$.

The advantage of this representation for Kraus operators is that it allows us to design an elegant way to perform the exact renormalization group, which is the second step of the method. Let us consider two neighbouring spins (see Fig. 8.6b). The renormalization process consists of two sequential representation fusions $j_a \otimes S \hookrightarrow j_b$ and $j_b \otimes S \hookrightarrow j_c$. As a result, we obtain the orthonormal basis

$$\begin{aligned} |j_c t_c m_c\rangle \;\; = \;\; & \sum_{M_1 M_2} \sum_{j_a t_a m_a} \sum_{j_b t_b m_b} T_{j_a t_a, j_b t_b} \langle j_a m_a, S M_1 | j_b m_b \rangle \langle j_b m_b, S M_2 | j_c m_c \rangle \\ & \times T'_{j_b t_b, j_c t_c} \, |j_a t_a m_a\rangle \, |M_1 M_2\rangle \end{aligned} \tag{8.15}$$

where the weight matrices T and T' for these two spins can be different in general. Alternately, the renormalization process in Eq. 8.15 can be first done by fusion of the two physical spins to their coupled representations $S \otimes S \hookrightarrow S_T$ and then $j_a \otimes S_T \hookrightarrow j_c$. In the latter fusion sequence, we obtain the same basis

$$\begin{aligned} |j_c t_c m_c\rangle \;\; = \;\; & \sum_{j_a t_a m_a} \sum_{S_T M_T} R^{S_T}_{j_a t_a, j_c t_c} \langle j_a m_a, S_T M_T | j_c m_c \rangle \\ & \times |j_a t_a m_a\rangle \, |S_T M_T\rangle \end{aligned} \tag{8.16}$$

where $|S_T M_T\rangle$ is the coupled basis of two physical spins. The two different fusion channels are unitarily related by the recoupling F–symbol (see Fig. 8.6c) defined by $F^{j_a S j_b}_{S S_T j_c} = \langle j_b(j_a S), S; j_c m_c | j_a, S_T(SS); j_c m_c \rangle$. By using Wigner's 6–$j$ symbol, this F–symbol can be expressed as [BS94]:

$$F^{j_a S j_b}_{S S_T j_c} = (-1)^{j_a + j_c} \sqrt{(2j_b+1)(2S_T+1)} \begin{Bmatrix} j_a & S & j_b \\ S & j_c & S_T \end{Bmatrix}$$

By substituting this in Eq. 8.15 and comparing with Eq. 8.16, we obtain:

$$R^{S_T}_{j_a t_a, j_c t_c} = \sum_{j_b t_b} T_{j_a t_a, j_b t_b} F^{j_a S j_b}_{S S_T j_c} T'_{j_b t_b, j_c t_c} \tag{8.17}$$

According to Eq. 8.16, the output states $|j_c t_c m_c\rangle$ only keep the local ground states of the Hamiltonian 8.10 if

$$R^{S_T}_{j_a t_a, j_c t_c} = 0 \tag{8.18}$$

holds for all j_a, t_a and $S_T \in \mathcal{K}$. This equation relates the weight matrices of two spins in Eq. 8.17 and plays an important role in our exact renormalization group method.

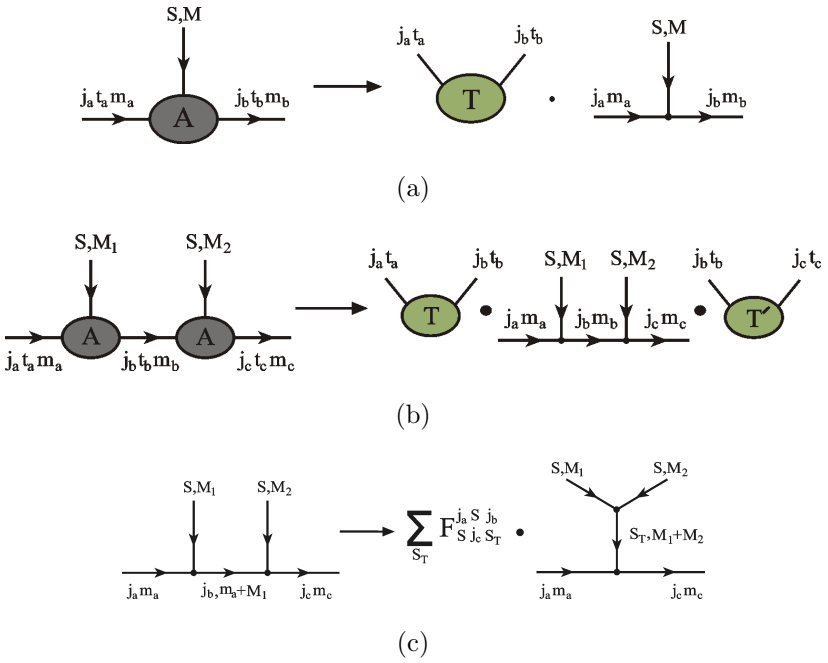


Figure 8.6: **Real space renormalization with** $SU(2)$. (a) An isometry $A^{[S,M]}$ is decomposed as a matrix T and a fusion of angular momenta. (b) The renormalization of two spins can be done in two successive steps. (c) The same input and output states with different intermediate fusion channels for two spins can be related by the F-symbol.

The third step of our method is to use Eq. 8.18 to carry out the renormalization group process for the whole spin chain. Hereafter we use $T^{[i]}$ to denote the weight matrix at site i. Let us start the renormalization from the first two spins. By taking the first physical spin S as the input representation, we have the initial condition $T^{[1]}_{j_1} = 1$ with $j_1 = S$. According to Eq. 8.17 and Eq. 8.18, we obtain $T^{[2]}_{j_1,j_2} = 1$. The output representation $j_2 \in \bar{\mathcal{K}}$, where $\bar{\mathcal{K}}$ is the orthogonal complement of $\mathcal{K}$. This simple test verifies that the output states are the zero–energy local ground states of the projector Hamiltonian 8.10.

The renormalization group follows naturally as $T^{[2]} \to T^{[3]} \to \cdots$ under renormalization condition 8.18 and constraints 8.13 and 8.14. Let us describe how to deal with these requirements simultaneously. Let us suppose we already know the weight matrix $T^{[i-1]}$, so the goal is to calculate $T^{[i]}$. After taking the square of Eq. 8.18 and summing over j_a, t_a and $S_T \in \mathcal{K}$, we obtain:

$$\sum_{j'_b t'_b} \sum_{j_b t_b} T^{[i]}_{j'_b t'_b, j_c t_c} \mathcal{M}^{[i] j_c}_{j'_b t'_b, j_b t_b} T^{[i]}_{j_b t_b, j_c t_c} = 0$$

where the positive semidefinite real hermitian matrix $\mathcal{M}^{[i] j_c}$ is given by:

$$\mathcal{M}^{[i] j_c}_{j'_b t'_b, j_b t_b} = \sum_{S_T \in \mathcal{K}} \sum_{j_a t_a} T^{[i-1]}_{j_a t_a, j'_b t'_b} F^{j_a S j'_b}_{S S_T j_c} F^{j_a S j_b}_{S S_T j_c} T^{[i-1]}_{j_a t_a, j_b t_b}$$

For every possible j_c from $j_b \otimes S$, we calculate the kernel of $\mathcal{M}^{[i] j_c}$, which gives us the weight matrix $T^{[i]}$. If $\mathcal{M}^{[i] j_c}$ does not have kernel vectors which satisfy Eq. 8.13, the corresponding output representation j_c must be discarded. If the kernel of $\mathcal{M}^{[i] j_c}$ has dimension larger than 1, the index t_c is used to tag the orthonormal kernel vectors for such j_c. Thus, the kernel vectors of $\mathcal{M}^{[i] j_c}$ constitute the columns of $T^{[i]}$ and the column indices j_c, t_c of $T^{[i]}_{j_b t_b, j_c t_c}$ denote the output representations. One can straightforwardly show that the resulting weight matrix $T^{[i]}$ satisfies the renormalization condition 8.18 and the orthonormal constraint 8.14, since $\mathcal{M}^{[i] j_c}$ is positive semidefinite and hermitian.

8.3.2.2 A fixed point: Matrix Product States

In this Subsubsection, we discuss models which have a renormalization fixed point and therefore, MPS as ground states.

Let us first recall the known results on the MPS solutions for Hamiltonian 8.10. The best–known models belong to the AKLT family [AKLT88], which are defined by $\mathcal{K} = \{S+1, S+2, \ldots, 2S\}$ with integer spin S. The MPS of spin–S AKLT models have a *Valence Bond Solid* (VBS) picture with irreducible virtual spin–$\frac{S}{2}$ representation.

The other family of models also has integer spin and the Hamiltonians are defined by $\mathcal{K} = \{2, 4, \ldots, 2S\}$ [TZX08, TZX$^+$09], which we call $SO(2S+1)$–symmetric family. For the $S = 2$ model of this family, the MPS have irreducible virtual spin–$\frac{3}{2}$

representations [TZX08], which is equivalent to the $SO(5)$–symmetric MPS in a two–leg electronic ladder [SZH98]. For $S \geq 3$ cases, the properties of the corresponding MPS are less clear, even though their explicit wave functions were found.

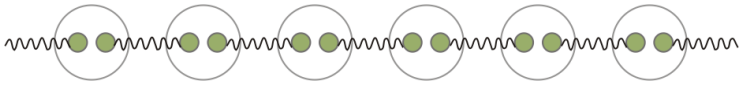
Now we turn to our results obtained by means of the exact renormalization group. For Hamiltonian 8.10, we check[2] all possible $\mathcal{K}$ and then provide a complete list of fixed point MPS solutions for $S \leq 4$, and a new solution for $S = 5$. All these solutions are integer–spin models[3], which are summarized in Table 8.2. For $S \leq 4$, we conclude that there is no solution other than the above two families. For $S = 5$, we find a new model, whose Hamiltonian is given by $\mathcal{K} = \{3, 7, 8, 9, 10\}$ and the ground state has a VBS picture with irreducible virtual spin–3 representations. For the $SO(2S+1)$ family with $S \geq 3$, the exact renormalization group provides us with a more comprehensible physical picture, which can be viewed as generalized VBS with *reducible* virtual spin representations. In Table 8.2, we also listed the minimum number of necessary blocked spins to reach the fixed–point representations. Since all these MPS are injective, this length scale is actually the injectivity length $i(A)$ [SPGWC10] (see Definition 9).

Let us explain these results with an explicit example in the $SO(2S+1)$ family: the spin–3 model with $\mathcal{K} = \{2, 4, 6\}$. Through the exact renormalization group, we can observe that the output states reach the fixed–point representation $0 \oplus 0 \oplus 1 \oplus 2 \oplus 3 \oplus 3 \oplus 3 \oplus 4 \oplus 5 \oplus 6$ after blocking 6 spins. To obtain the MPS, we do not really need to calculate the fixed–point Kraus operators by the renormalization group. The fixed–point representation allows us to construct this MPS directly [SWPGC09]. For the present example, the fixed–point representation gives an important hint that the MPS has a VBS picture (see Fig. 8.7a) with $SU(2)$ *reducible* virtual spin representation $0 \oplus 3$, which is quite different from the traditional VBS states with irreducible virtual spin representations, like the AKLT states [AKLT88] or their extensions [FNW92].

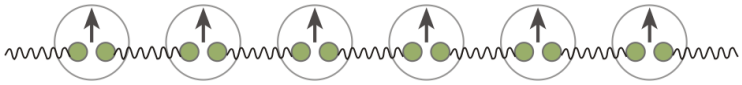
With a chain beyond the injectivity length $i(A) = 6$, the tensor product of two $0 \oplus 3$ representations at the two boundaries yields the observed fixed–point representation in the renormalization group. For OBC, in the thermodynamic limit, the unpaired representations $0 \oplus 3$ at the two edges are asymptotically free and become well–defined **edge states**. For PBC, all virtual spin representations are contracted into $SU(2)$ singlets with neighbouring sites and therefore the MPS is a

[2]In practice, one can rule out some models to simplify the calculation. For example, the element $2S$ is always included in $\mathcal{K}$, otherwise the model has (at least) a fully polarized ferromagnetic ground state. We also use the sets $\mathcal{K}'$ for AKLT models and SO$(2S+1)$ models. Since these known models have unique ground states, there is no need to check the sets $\mathcal{K}$ satisfying $\mathcal{K} \subset \mathcal{K}'$ or $\mathcal{K} \supset \mathcal{K}'$.

[3]For semi–integer spin chains, it is not possible to have a translationally invariant MPS as a unique ground state. According to the Lieb–Schultz–Mattis theorem, SU(2)–symmetric spin chains with semi–integer spins are critical if the ground state is unique. On the contrary, a fixed point MPS should have an energy gap and exponentially decaying correlations. However, the possibility of the MPS solution with breaking translation in symmetry cannot be ruled out. Although these models are within the scope of exact renormalization method, we do not obtain any such solution for $S \leq \frac{7}{2}$.



(a)



(b)

Figure 8.7: **Results of the technique**. (a) The fixed-point type MPS solutions have a VBS picture. The fixed–point representations come from the tensor product of two–edge states. (b) The partially ferromagnetic states have a magnetization plateau.

Spin	**Set $\mathcal{K}$**	**Virtual spin**	$i(A)$
1	$\{2\}$	$1/2$	2
2	$\{3,4\}$	1	2
2	$\{2,4\}$	$3/2$	4
3	$\{4,5,6\}$	$3/2$	2
3	$\{2,4,6\}$	$0\oplus 3$	6
4	$\{5,6,7,8\}$	2	2
4	$\{2,4,6,8\}$	$2\oplus 5$	8
5	$\{6,7,8,9,10\}$	$5/2$	2
5	$\{2,4,6,8,10\}$	$5/2\oplus 9/2\oplus 15/2$	10
5	$\{3,7,8,9,10\}$	3	4

Table 8.2: Models with $SU(2)$–invariance, nearest–neighbour interactions and matrix product ground states.

global spin singlet.

The renormalization group analysis has also been carried out for other models in the $SO(2S+1)$ family. From Table 8.2, one can see that, for $S \geq 3$, their matrix product ground states have reducible virtual spin representations, which directly correspond to the edge states in an open chain. This provides a more complete understanding of these systems. For all MPS in Table 8.2, we present their explicit Kraus operators below.

Let us make a remark about these exactly solvable models. All their fixed point MPS ground states have exponentially decaying correlations and there is an energy gap above the ground states, since they are injective. However, the different virtual spin representations (edge states) show that these MPS belong to different quantum phases of matter. Therefore, once a new Hamiltonian $H = (1-x)H_1 + xH_2$ is

constructed from two solvable models H_1 and H_2 in Table 8.2 with the same spin S, at least one quantum phase transition is expected to occur when tuning x from 0 to 1. Since both MPS ground states for H_1 and H_2 preserve SU(2) symmetry, the local order parameter description breaks down and unconventional quantum phase transitions may emerge. Very recently, this idea has been exploited to study the possibility of a topological quantum phase transition in an $S = 2$ chain [ZZXL11, ZJWZ10].

Let us explicitly present the Kraus operators needed for the definition of the MPS in Table 8.2. As we mentioned, the Kraus operators with $SU(2)$ symmetry are parametrized by Eq. 8.12, which requires both the set $\mathcal{V}$ containing the $SU(2)$ virtual spin representations and the weight matrix T.

For irreducible virtual spin representations, the set $\mathcal{V}$ contains a single representation j_a and therefore $T = 1$. In this case, the Kraus operators are simply the Clebsch–Gordan coefficients

$$A^{[S,M]}_{j_a m_a, j_a m_b} = \langle j_a m_a, SM | j_a m_b \rangle$$

For reducible virtual spin representations, the set $\mathcal{V}$ has multiple $SU(2)$ representations and the weight matrix T is necessary. The Kraus operators are given by

$$A^{[S,M]}_{j_a m_a, j_b m_b} = T_{j_a, j_b} \langle j_a m_a, SM | j_b m_b \rangle$$

where the index t is suppressed because no degeneracy occurs in $\mathcal{V}$ for our models. We use a convention to define matrix T such that the row and the column indices j_a, j_b are arranged in an incremental order. For instance, the $S = 3$ model with $\mathcal{K} = \{2, 4, 6\}$ has virtual representation $0 \oplus 3$ and

$$T = \begin{pmatrix} T_{0,0} & T_{0,3} \\ T_{3,0} & T_{3,3} \end{pmatrix} = \begin{pmatrix} 0 & \frac{-1}{\sqrt{7}} \\ 1 & \sqrt{\frac{6}{7}} \end{pmatrix}$$

For the $S = 4$ model with $\mathcal{K} = \{2, 4, 6, 8\}$, we have virtual representation $2 \oplus 5$ and

$$T = \begin{pmatrix} \frac{1}{3}\sqrt{\frac{7}{2}} & \frac{1}{3}\sqrt{\frac{5}{2}} \\ \frac{-1}{3}\sqrt{\frac{11}{2}} & \frac{1}{3}\sqrt{\frac{13}{2}} \end{pmatrix}$$

For the $S = 5$ model with $\mathcal{K} = \{2, 4, 6, 8, 10\}$, we have virtual representation $\frac{5}{2} \oplus \frac{9}{2} \oplus \frac{15}{2}$ and

$$T = \begin{pmatrix} \frac{1}{11}\sqrt{\frac{21}{2}} & \frac{-3}{\sqrt{22}} & \frac{-1}{11}\sqrt{\frac{21}{2}} \\ -\sqrt{\frac{15}{22}} & \sqrt{\frac{3}{26}} & -\sqrt{\frac{85}{286}} \\ \frac{2\sqrt{7}}{11} & 2\sqrt{\frac{17}{143}} & \frac{1}{11}\sqrt{\frac{969}{13}} \end{pmatrix}$$

It is straightforward to show that these solutions satisfy Eq. 8.13, Eq. 8.14 and Eq. 8.18.

8.3.2.3 Partially ferromagnetic states

In this Subsubsection, we discuss another class of models which do not have an exact renormalization fixed point but can still be solved exactly. The ground states of these models are partially ferromagnetic states.

This family includes both semi–integer–spin models and integer–spin models. The Hamiltonian is defined by $\mathcal{K} = \{0, 1, \ldots 2S-4, 2S\}$ and the physical spin $S \geq \frac{5}{2}$. Their ground states are partially ferromagnetic states with a magnetization plateau $\langle S_i^z \rangle = S - 1$. We have also found a physical picture (see Fig. 8.7b) for these states with partial magnetization: we prepare a spin–1 AKLT–type VBS state with virtual spin $\frac{1}{2}$ and a spin–$(S-1)$ maximally–polarized ferromagnetic state. In each site, we recover the physical spin–S Hilbert space by $(S-1) \otimes 1 \hookrightarrow S$, which is achieved by applying local projections.

Let us consider a typical example — the spin–$\frac{5}{2}$ model with $\mathcal{K} = \{0, 1, 5\}$. For a block of L_0 spins, the AKLT part contributes representations $0 \oplus 1$ and the polarized ferromagnetic part contributes representation $\frac{3L_0}{2}$. Thus, the total spin of the L_0–spin block is given by the tensor product of representations from these two parts

$$(0 \oplus 1) \otimes \frac{3L_0}{2} = (\frac{3L_0}{2} - 1) \oplus \frac{3L_0}{2} \oplus \frac{3L_0}{2} \oplus (\frac{3L_0}{2} + 1) \qquad (8.19)$$

For two spins ($L_0 = 2$), the allowed representations are $2 \oplus 3 \oplus 3 \oplus 4$ and cannot reach $\mathcal{K} = \{0, 1, 5\}$, which means that the partially ferromagnetic state is the zero–energy ground state of the projector Hamiltonian. In the exact renormalization process, we found that the four output representations in Eq. (8.19) are the only output representations for $L_0 \geq 6$. By adding one additional spin, the total spin of the four representations is increased by $\frac{3}{2}$. These observations actually strongly suggest the partially ferromagnetic picture of the ground state.

One may ask why this class starts with $S = \frac{5}{2}$ rather than $S = 2$. The reason is the following: for spin–2 model $\mathcal{K} = \{0, 4\}$, the renormalization group shows that the number of output representations does not saturate, which means that the partially ferromagnetic state is not the only ground state of the Hamiltonian.

Compared to the fixed–point MPS solutions in Subsubsection 8.3.2.2, the partially ferromagnetic states have a long range order and thus break the $SU(2)$ symmetry. According to *Goldstone's theorem*, we expect gapless spin wave excitations above the ground state, which is quite different from the fixed–point MPS with an energy gap and exponentially decaying spin correlations.

Die Mathematiker sind eine Art Franzosen: Redet man zu ihnen, so übersetzen sie es in ihre Sprache, und dann ist es alsobald ganz etwas anders.

J. W. von Goethe
(1749-1832)

9

MPS and PEPS as a laboratory for Condensed Matter

9.1 Introduction

After reading the first two Chapters, one may wonder why no one has already employed the results obtained for tensor networks to advance in the mathematical foundations of quantum magnetism with spin systems. This question was already advanced in the Introduction and, after three decades of employing Matrix Product States and Projected Entangled Pair States as a source of examples and counterexamples to support some hypotheses and discard others, the mathematical machinery is already sufficiently developed as to allow an attempt on providing a positive answer to this question. This is the aim we pursue in this Chapter.

The Chapter is essentially a collection of applications in condensed matter of the previously shown results:

- In Section 9.2, we prove a dichotomy theorem for frustration–free Hamiltonians. This is an application of quantum Wielandt's inequality (see Chapter 2) which was firstly proposed in [PGVWC07] and finally proven in [SPGWC10], and where it is shown that the ground state of a local strongly frustration–free Hamiltonian is either a Matrix Product State of bounded bond dimension, or the bond dimension grows faster than $N^{\frac{1}{5}}$, N being the length of the chain.

- In Section 9.3, we define *string order* in spin systems and provide its complete characterization in the framework of tensor networks. We find under which conditions the string order appears, for which kind of perturbations it is robust, or when it can be used to detect phase transitions. In addition, we propose a generalization of the string order parameter for higher dimensions keeping the desirable features of one–dimensional systems. The results shown in this Section are published in [PGWS+08].

- Kitaev's toric code [Kit03] is undoubtedly in the grounds of topological quantum computation. Despite of its simplicity, it shows very nontrivial features. One of these properties is the invariance of the state when a string of σ_X operators is applied along a line, which, as we will see in this Section, can be understood as a kind of Wilson loop. We prove in Section 9.4 that no state invariant under a Wilson loop can be injective, establishing a connection between injectivity and topological properties [PGSGG+10].

- The Lieb–Schultz–Mattis Theorem can be considered a macroscopic reflex of the quantum properties associated with Fermi–Dirac or Bose–Einstein statistics. We provide a tensor network–based proof of such Theorem and even its most important generalization: the Oshikawa–Yamanaka–Affleck Theorem. In the latter case, we provide a two–dimensional generalization of the Theorem [PGSGG+10]. As the proofs are restricted to a special class of states, they cannot be considered general proofs. However, they present several advantages: their simplicity allows us to get a great control over the conditions of the Theorem; they permit searching for counter–examples to conjectures; they allow for extensions to higher dimensions and the generalization to other symmetry groups; etc.

- Sections 9.6 and 9.7 are probably the best examples of the use of tensor networks as a laboratory for condensed matter. In the first case, we show the relationship between the fractionalization of a state's magnetization and the entanglement between two disjoint regions of such a state: the more fractional the magnetization, the larger the expected entanglement. In the second case, we firstly improve the bound provided in [VC06] for the approximation of a general state by a Matrix Product State. Then, we use this to provide a lower bound for the block entropy of a long–range interacting Hamiltonian's ground state. Both results are work in progress at the moment of publishing this Thesis [PGSC+], so we cannot provide specific examples that illustrate the statement.

9.2 Frustration–free Hamiltonians and MPS

Matrix Product States have proven to be a useful family of quantum states for explaining the low–energy sectors of locally–interacting one–dimensional systems. They constitute a suitable variational Ansatz to compute, for instance, ground state energies to high accuracy [VMC08] which can be explained by the fact that MPS approximate ground states of local one–dimensional Hamiltonians well [VC06, Has07a]. Similarly, as shown, they are used to understand effects on one–dimensional systems on analytic grounds, such as string orders [PGWS$^+$08], symmetries [SWPGC09], renormalization flows [VCL$^+$05] or sequential interactions [SSV$^+$05, LLPG$^+$08].

As already explained in Chapter 3, associated to each translational invariant MPS $|\psi_A\rangle$ there is a parent Hamiltonian H_A which is frustration–free and has $|\psi_A\rangle$ as ground state. Let us start by recalling the concept of frustration–free Hamiltonian explained in Definition 18. Consider a local translational invariant Hamiltonian in a spin chain $H = \sum_i \tau^i(h \otimes \mathbb{1}_{\text{rest}})$ where h denotes the local interaction term and τ the translation operator. Then, the Hamiltonian is called *frustration free* if its ground state $|\psi_0\rangle$ minimizes the energy *locally*, that is, if Eq. 3.4 is fulfilled. We assume w.l.o.g. that Eq. 3.4 is equal to 0. Such Hamiltonians include classical Hamiltonians, where the terms commute, as well as all *parent Hamiltonians* appearing in the Matrix Product State Theory [AKLT88, FNW92, SWPGC09, TS10, SCPG10].

The corresponding local interaction term h above is constructed as the projector onto the orthogonal complement of the image of

$$X \in M_{D\times D} \mapsto \sum_{i_1,\ldots,i_L} \operatorname{tr}\left[X A_{i_1} \cdots A_{i_L}\right] |i_1 \cdots i_L\rangle$$

as already shown in Definition 17 for some sufficiently large *interaction range* L. Note that the map in Eq. 2.2 is *injective* for sufficiently large L iff the map $\mathcal{E}_A(X) = \sum_i A_i X A_i^\dagger$ is primitive[1], as was proven in Section 2.2, and that injectivity holds for all $L \geq i(A)$, where $i(A)$ is the injectivity length which appears in Definition 9.

It was proven in Theorems 21 and 22 that injectivity is a necessary and sufficient condition for the uniqueness of the ground state of a frustration–free Hamiltonian, and this provides another application for the quantum Wielandt's inequalities shown in Theorem 19 for $i(A)$. We know from Theorems 22 and 24 that, if the interaction range L of the parent Hamiltonian H_A satisfies $L > i(A)$, then $|\psi_A\rangle$ is the unique ground state of H_A with a spectral gap above it (Theorem 24).

Hence, the quantum Wielandt's inequality provides a bound for the interaction length required to get a *good* parent Hamiltonian for an MPS. Indeed, the existence of such an inequality was already conjectured in the context of MPS [PGVWC07, Conjectures 1 and 2], and some results obtained so far about MPS do directly depend on the validity of that conjecture. In particular, a dichotomy results for ground states of frustration–free Hamiltonians (sketched in [PGVWC07] and for which we give a

[1] $\mathcal{E}_A$ may be assumed to be trace–preserving w.l.o.g. [PGVWC07].

complete proof below), and the characterization of global symmetries in arbitrary MPS given in [SWPGC09] and described in Section 4.2.

One might conjecture that the ground state of every frustration–free Hamiltonian (with non–degenerate ground state) is an MPS. In fact, the quantum Wielandt's inequality allows us to get a dichotomy theorem in this direction:

Theorem 44 (Dichotomy of frustration–free Hamiltonians' GS) *Let us take a local term h with interaction length L and assume that $H_N = \sum_{i=1}^{N} \tau^i(h \otimes \mathbb{1}_{rest})$ is strongly frustration–free and has a unique ground state for every N. Its ground state can be represented as an MPS with matrix size $D \times D$, where D is:*

(i) either independent of N,

(ii) or $D > \Omega(N^{\frac{1}{5}})$ for all prime numbers N. □

Proof Let us recall from Theorem 4 that each MPS with $D < N$ and prime N can be mapped into a *canonical* decomposition where all matrices are block diagonal $A_i = \oplus_{j=1}^{b} A_i^j$ and each block satisfies injectivity.

Moreover, Theorem 22 states that if $b \geq 2$, $L_0 = \max_j i(A^j)$ and L is the interaction length of any frustration–free translational invariant Hamiltonian H on N spins, having $|\psi_A\rangle$ as ground state; the condition $N \geq 3(b-1)(L_0+1)+L$ given by Lemma 14 implies that $|\psi_{A^j}\rangle$ is also a ground state of H for all j.

Since the quantum Wielandt's inequality allows us to bound $L_0 \leq O(D^4)$ and trivially $b \leq D$, we get that either (ii), *i.e.* $D \geq \Omega(N^{\frac{1}{5}})$, or $b = 1$ and $\ker(h) \ni \sum_{i_1,\cdots,i_L} \mathrm{tr}\left[X A_{i_1} \cdots A_{i_L}\right] |i_1 \cdots i_L\rangle$ where $X \in S_{N-L}(A)$. Since, by the quantum Wielandt's inequality, we have again that $N - L \geq i(A)$, we get for h that $\ker(h) \supseteq \{\sum_{i_1,\cdots,i_L} \mathrm{tr}\left[X A_{i_1} \cdots A_{i_L}\right] |i_1 \cdots i_L\rangle : X \in \mathcal{M}_D\}$. This trivially implies that $|\psi_A\rangle$ is also a ground state for $H_{N'}$ when $N' > N$ and therefore the only ground state, so we obtain (i). ■

Regarding the restriction to prime N note that, by the Prime Number Theorem, the number of primes less than or equal to a given N is asymptotically $\frac{N}{\log N}$. Therefore, in (ii) there are *many* lengths for which there is no MPS representation of the ground state with *small* matrices.

9.3 String order

Order parameters play a crucial role in describing the different phases of matter. However, there exist some phases which, despite displaying very intriguing features, are not amenable to a description by a local order parameter. In some cases it is nevertheless possible to introduce more sophisticated quantities that are able to characterize those phases. A paradigmatic example is given by the string order parameter (SOP), which reveals the appearance of a hidden order (so–called string

order, SO) in certain spin systems [dNR89, DBA06, AR07a, KFSS00, TMYT01]. This quantity can be expressed as an expectation value of a non–local operator, and the appearance of SO is signalled by a non–vanishing SOP value in the thermodynamic limit. Despite the importance of SOP, we still do not have a systematic characterization of its properties. It is not clear under which conditions SO appears in a one–dimensional system, with respect to which kind of small perturbations respecting the gap it is robust [AR07b], or when it can be used to detect a quantum phase transition. Apart from that, it seems that the SO loses some of its desirable properties beyond strictly one–dimensional systems [KFSS00, TMYT01, AR07b].

In this Section, we clarify all those questions for finitely correlated states [FNW92], *i.e.* MPS on infinite chains (see Subsection 1.4.2). The relevance of these states relies on the fact that every quantum state of a finite system has an exact MPS representation [PGVWC07, Vid03], and that ground states of one–dimensional short–range interactions can be efficiently approximated — with bond dimension $D \propto \mathrm{poly}N$ within this class [VC06, Has07b]. In this framework, we will show that the appearance of SO is intimately related to the existence of symmetries, which explains how it can be used to detect quantum phase transitions.

We propose another parameter, which better recognizes the appearance of string order, since it does not have some of the shortcomings of the SOP. We also provide a natural generalization of SO to higher–dimensional lattices (that we call *membrane order*), which retains all the desired properties. Finally, we give several examples displaying a large variety of phenomena.

9.3.1 Definition of string order in spin chains

We mostly consider infinite chains of identical spin–S particles in a translational invariant state $|\psi\rangle$. Then, we can define the string order as follows.

Definition 26 (String order) We say that the state $|\psi\rangle$ has string order if there exist a local unitary $u \neq \mathbb{1}$ and local operators x and y (which can be taken hermitian), such that

$$\lim_{L\to\infty} |S_L(x, y, u, |\psi\rangle)| > 0 \tag{9.1}$$

$$S_L(x, y, u, |\psi\rangle) \equiv \langle\psi|\, x \otimes u^{\otimes(L-2)} \otimes y \otimes \mathbb{1}_{\mathrm{rest}}\, |\psi\rangle \tag{9.2}$$

□

Later on, we introduce alternative quantities which extend this Definition.

Let us consider a TI–MPS $|\psi^{(N)}\rangle$ for N particles generated by the Kraus operators $\{A_i \in \mathcal{M}_D\}_{i=1}^d$. As usual,

$$|\psi^{(N)}\rangle = \sum_{i_1\ldots i_N=-S}^{S} \mathrm{tr}\left[A_{i_1}\cdots A_{i_N}\right] |i_1 \ldots i_N\rangle \tag{9.3}$$

We use the notation $|\psi_\infty\rangle$ for the thermodynamic limit, with the convention that the limit $N \to \infty$ is to be taken after the computation of expectation values. In this limit, the states are known as finitely correlated states (FCS) — the subject of our studies. As shown in Subsection 1.4.2, most of the properties of these states are encoded in a linear map defined as

$$\mathcal{E}(X) = \sum_{i=-S}^{S} A_i X A_i^\dagger \tag{9.4}$$

The matrices A_i can always be chosen in the canonical form (see Theorem 4), so that

$$\mathcal{E}(\mathbb{1}) = \mathbb{1}, \quad \mathcal{E}^*(\Lambda) = \Lambda \tag{9.5}$$

where $\mathcal{E}^*$ denotes the dual channel (see Definition 5), a map which is obtained by interchanging $A_i \leftrightarrow A_i^\dagger$ in Eq. 9.4, $\Lambda \geq 0$ and $\mathrm{tr}\,[\Lambda] = 1$. Thus, $\mathcal{E}$ and $\mathcal{E}^*$ are unital (trace–preserving) completely positive maps, *i.e. quantum channels*, each possessing an eigenvalue equal to 1.

A FCS is pure (in the sense of Definition 6) iff $\Lambda > 0$ and $\mathcal{E}$ has only one eigenvalue of modulus 1. Then, we have the following Lemma:

Lemma 32 (Restriction to pure FCS) *A general FCS has SO iff one of its pure components has it.* □

Proof The proof is trivial, since there is a unique decomposition of mixed FCS into pure ones. ■

We will restrict ourselves to *pure FCS* from now onwards. Note that all of them are unique ground states of gapped finite–range interactions.

9.3.2 String order and FCS

For any unitary u, the SOP given by Eq. 9.2 of a FCS is most easily expressed by introducing a map

$$\mathcal{E}_u(X) \equiv \sum_{i,i'} \langle i'|\, u\, |i\rangle A_i X A_{i'}^\dagger = \sum_j e^{i\theta_j} \tilde{A}_j X \tilde{A}_j^\dagger \tag{9.6}$$

where $\tilde{A}_j = \sum_i \langle \tilde{j}|i\rangle A_i$, and $u = \sum_j e^{i\theta_j} |\tilde{j}\rangle\langle\tilde{j}|$. Then,

$$S_L(x, y, u, |\psi_\infty\rangle) = \mathrm{tr}\left[\Lambda \mathcal{E}_x \mathcal{E}_u^{L-2} \mathcal{E}_y(\mathbb{1})\right] \tag{9.7}$$

where $\mathcal{E}_{x,y}$ are defined analogously to $\mathcal{E}_u$ in Eq. 9.6.

The following Lemma studies the *spectral radius* σ of $\mathcal{E}_u$, which is crucial for Eq. 9.7 due to the limit $L \to \infty$.

Lemma 33 (Spectral radius of $\mathcal{E}_u$) *$\sigma(\mathcal{E}_u) \leq 1$, with equality iff there exists a unitary V and $\theta \in [0, 2\pi)$ such that*

$$V^\dagger \tilde{A}_j = e^{i(\theta-\theta_j)} \tilde{A}_j V^\dagger. \tag{9.8}$$

$\mathcal{E}_u$ has at most one eigenvalue of modulus 1. □

Proof We will proceed as in the proof of Theorem 13 in order to show that $\sigma(\mathcal{E}_u) \leq 1$. Let us consider an eigenvector V of $\mathcal{E}_u$, with eigenvalue λ, *i.e.* $\mathcal{E}_u(V) = \lambda V$. By multiplying from the right by $\Lambda V^\dagger$ and by taking the absolute value of the trace, we obtain:

$$\begin{aligned} |\lambda| \mathrm{tr}\left[V\Lambda V^\dagger\right] &= \left|\mathrm{tr}\left[\mathcal{E}_u(V)\,\Lambda V^\dagger\right]\right| = \left|\sum_j e^{i\theta_j} \mathrm{tr}\left[\tilde{A}_j V \tilde{A}_j^\dagger \Lambda V^\dagger\right]\right| \\ &\leq \left[\sum_j \mathrm{tr}\left[V\tilde{A}_j^\dagger \Lambda \tilde{A}_j V^\dagger\right]\right]^{\frac{1}{2}} \left[\sum_j \mathrm{tr}\left[\tilde{A}_j^\dagger V \Lambda V^\dagger \tilde{A}_j\right]\right]^{\frac{1}{2}} \\ &= \mathrm{tr}\left[V\Lambda V^\dagger\right] \end{aligned} \tag{9.9}$$

where we have used the Cauchy–Schwarz inequality given in Eq. 9.22 together with Eq. 9.5. Since $\Lambda > 0$, $\mathrm{tr}\left[V\Lambda V^\dagger\right] > 0$ and thus $|\lambda| \leq 1$ as stated. Let us now show the implication $\boxed{\Leftarrow}$, if the condition given by Eq. 9.8 is fulfilled, one can readily see that $e^{i\theta}$ is an eigenvalue of $\mathcal{E}_u$ by using Eq. 9.6, and thus $\sigma(\mathcal{E}_u) = 1$.

To show the reverse implication $\boxed{\Rightarrow}$, if $|\lambda| = 1$, then the inequality in Eq. 9.9 has to become an equality, and thus $\alpha e^{i\theta_j} \Lambda^{\frac{1}{2}} V^\dagger \tilde{A}_j = \Lambda^{\frac{1}{2}} \tilde{A}_j V^\dagger$. By multiplying by the adjoint expression, taking traces, summing in j, and using again Eq. 9.5 one obtains that $|\alpha| = 1$, *i.e.* $\alpha = e^{-i\theta}$. Since Λ is invertible we obtain Eq. 9.8. This also implies that

$$\mathcal{E}(V^\dagger V) = V^\dagger \sum_j \tilde{A}^j \tilde{A}^{j\dagger} V = V^\dagger V, \tag{9.10}$$

where we have used Eq. 9.5. Since $\mathbb{1}$ is the only fixed point of $\mathcal{E}$, we get $V^\dagger V = \mathbb{1}$.

Moreover, suppose that $\mathcal{E}_u$ has two eigenvectors, V and V' with eigenvalues $e^{i\theta}$ and $e^{i\theta'}$, respectively. Then, by using Eq. 9.9, we have

$$\mathcal{E}(V^\dagger V') = \sum_j \tilde{A}_j V^\dagger V' \tilde{A}_j^\dagger = e^{i(\theta'-\theta)} V^\dagger V'$$

such that the same argument gives $V = V'$ and $\theta = \theta'$. ■

Now we can specify the conditions required for SO. First, $\sigma(\mathcal{E}_u) = 1$ since, otherwise, S_L will decay exponentially with L. By using Lemma 33, we know that the eigenvalue λ of magnitude 1 is not degenerate, so let us denote by V and Y the corresponding right and left eigenvectors, *i.e.* $\mathcal{E}_u(V) = \lambda V$, $\mathcal{E}_u^*(Y) = \lambda Y$, where $\mathcal{E}_u^*$ is again

the dual channel. We have $\lim_{L\to\infty} S_L(x,y,u,|\psi_\infty\rangle) = \mathrm{tr}\left[Y^\dagger \mathcal{E}_y(\mathbb{1})\right] \mathrm{tr}\left[\Lambda \mathcal{E}_x(V)\right]$. Writing $\mathcal{E}_u^*(Y)V = \lambda YV$ and by means of Eq. 9.8, we arrive at the conclusion that $Y = \Lambda V^\dagger$. Thus, the conditions for the SOP not to vanish are:

(i) $\sigma(\mathcal{E}_u) = 1$;

(ii) $\mathrm{tr}\left[\Lambda V^\dagger \mathcal{E}_y(\mathbb{1})\right], \mathrm{tr}\left[\Lambda \mathcal{E}_x(V)\right] \neq 0$

We may wonder whether the condition $\sigma(\mathcal{E}_u) = 1$ is sufficient to have SO, *i.e.* if there are always two operators x and y such that the other conditions are fulfilled. In order to answer this question, we notice that $\mathrm{tr}\left[\Lambda V^\dagger \mathcal{E}_y(\mathbb{1})\right]^* = \mathrm{tr}\left[\Lambda \mathcal{E}_z(V)\right]$, where $z = \tilde{u}y^\dagger$ and $\tilde{u} = \sum_j e^{i(\theta_j-\theta)} |\tilde{j}\rangle\langle\tilde{j}|$. Thus, we can always choose $y = x^\dagger \tilde{u}$ so that Condition (ii) above is simplified to $\mathrm{tr}\left[\Lambda \mathcal{E}_x(V)\right] \neq 0$. It is clear that it suffices that $\mathrm{tr}\left[V\Lambda A_i A_j^\dagger\right] \neq 0$ for some i,j, since we can then simply choose $x = |i\rangle\langle j|$. We conclude that:

Theorem 45 (Necessary and sufficient conditions for SO) *For a pure FCS there exists SO iff there exist a unitary $\tilde{u} \neq \mathbb{1}$, V, and i,j such that*

$$\mathcal{E}_{\tilde{u}}(V) = V, \quad \mathrm{tr}\left[V\Lambda A_i A_j^\dagger\right] \neq 0. \tag{9.11}$$

□

Now, we show that the second condition can be dropped in two situations.

Case 1

When x and y in Eq. 9.2 are products of observables acting on D^2 spins. The reason is that the set

$$S_D \equiv \mathrm{span}\left[A_{i_1}\cdots A_{i_D} A_{j_D}^\dagger \cdots A_{j_1}^\dagger\right]$$

spans the set of $D\times D$ matrices, so that there is always a linear combination X of these matrices for which $\mathrm{tr}\left[V\Lambda X\right] \neq 0$. To see that this set is complete, note first that $S_{m-1} \subseteq S_m$ since

$$\sum_{i_m} A_{i_1}\cdots A_{i_m} A_{j_m}^\dagger \cdots A_{j_1}^\dagger = A_{i_1}\ldots A_{i_{m-1}} A_{j_{m-1}}^\dagger \cdots A_{j_1}^\dagger$$

This inclusion must be strict unless $m > D^2$ since $S_{m-1} = S_m$ implies $S_m = S_{m+1}$, and for a sufficiently large L, the set $\{A_{i_1}\cdots A_{i_L}\}$ must span the entire space of matrices, *i.e.* it reaches full Kraus rank (see Section 2.2).

Case 2

There exists a continuous group of unitaries V fulfilling the first condition, i.e. we can parametrize $V = e^{i\phi\cdot vec H}$. Thus, as $\Lambda > 0$, we can always choose a sufficiently small ϕ such that $\mathrm{tr}\left[V\Lambda\right] \neq 0$ and this suffices, since we have Eq. 9.5. The necessary and sufficient conditions to obtain invariant MPS are given in Subsection 4.2.

The first case can be discarded when considering local observables. Therefore, the existence of a symmetry groups is essentially the necessary and sufficient condition for the emergence of string order in a pure FCS. Nonetheless, this is only sufficient in a quantum state or even in a general FCS. To see this, one only has to consider a FCS with two pure components: one with a symmetry and hence string order and the other without them. The combination has string order but is not invariant.

9.3.3 Alternative definition and generalizations

In this Subsection, we provide an alternative definition of the string order parameters based on the results on MPS shown above. We illustrate the idea with a couple of relevant examples: the AKLT state and the cluster state.

We employ the results shown in Chapter 7 to suggest a natural generalization of the concept of string order to higher dimensions, what we call *membrane order*. This generalization keeps the most relevant features of the one–dimensional definition. The idea is also illustrated with several examples.

9.3.3.1 Alternative definitions

One can understand the importance of the SOP in detecting quantum phase transition in terms of its relationship to local symmetries. If we have a Hamiltonian with a certain local symmetry and its ground state is unique, then there may exist SO. If we change the parameters of the Hamiltonian but keep the symmetry until the gap closes, then the ground state will be degenerate and the symmetry may be broken[2].

Thus, the SO may disappear at that point, indicating the presence of a phase transition. Note that, due to the possible choices of the operators x and y in the definition 9.2, it may happen that the SOP for a particular choice vanishes even if there still is a symmetry. In order to avoid this, one may look at the quantity

$$R_L(u) \equiv \langle \psi^{(L)} |\, u^{\otimes L} \, | \psi^{(L)} \rangle \tag{9.12}$$

where $|\psi^{(L)}\rangle$ is the ground state of the Hamiltonian acting on L sites with periodic boundary conditions, which is indeed directly related to the existence of a symmetry. In fact, $R_\infty(u) = \lim_L R_L(u)$ can only vanish if the gap is closed, and thus it is ideally suited to study the presence of transitions. Note also that it can be straightforwardly determined from numerical algorithms based on MPS [VPC04].

Example 9 It is instructive to revise the appearance of SO in the ground state of the AKLT model [AKLT88]. For that state, we have $S = 1$, $A_0 = \frac{1}{\sqrt{3}}\sigma_z$ and $A_{1,-1} = \sqrt{\frac{2}{3}}\sigma_\pm$ where the sigmas denote Pauli matrices. We find $\Lambda = \mathbb{1}$, and

[2]If one perturbs the Hamiltonian without keeping the symmetry, it is clear from our picture that the SO will vanish, even if the gap does not close. This explains the fragility of the SO (cf. [AR07a])

by taking $u = e^{i\pi S_z}$ we obtain $V = \sigma_z$, and we can take $x = y = S_z$, so that $S_L(x, y, u, |\psi\rangle_\infty) = -\frac{4}{9}$ [dNR89]. Note that the AKLT state has $SU(2)$ symmetry so, obviously, $R_L(u) = 1$, for all L. □

Example 10 Let us analyse the cluster state. The Kraus operators describing the state [PGVWC07] are:

$$A_0 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix} \qquad A_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix}$$

This has the symmetry induced by $u = -\sigma_x$. We have $V = \sigma_y$, and one can readily see that $\mathrm{tr}\left[V \Lambda A_i A_j^\dagger\right] = 0$. Thus, there is no SO. However, if we take two particles, we can choose $x = \sigma_z \otimes \sigma_y$ and $y = \sigma_y \otimes \sigma_z$, so that the SOP is 1. In general, we have $R_L(u) = 1$ as expected. □

9.3.3.2 Membrane order

The existence of a local symmetry allowed us to introduce the quantity R_L defined in Eq. 9.12. This quantity seems to be an appropriate definition of SO in one–dimensional systems, so we will now extend it to two dimensions. In this case, there is more freedom in the choice of locations for the local unitaries u. First we can let these unitaries act on the whole lattice. If the state remains invariant (or the respective R_L does not vanish) we will say that we have *membrane order* (MO). We can also allocate the unitaries as a string of operators, in which case we will strictly talk about SO[3] — or they can be distributed in even more sophisticated configurations, such as a *band of operators* (BO). Note that the so defined MO shares all the desired properties for the SO in one dimension, and thus provides a natural generalization to higher dimensions. In particular, it should not exhibit spontaneous breakdown when switching couplings on in the second dimension as pointed out in [AR07a] for the SO.

To gain more insight, we consider Projected Entangled Pair States (PEPS), defined in Section 5.2, where Kraus operators are replaced by tensors B_k whose coordination number depends on the geometry of the lattice. For these states, local symmetries can arise in a similar way as in the one–dimensional case, as shown in Section 7.2. We interpret each tensor as an operator $B = \sum_s |s\rangle\langle\phi_s| : (\mathcal{H}_D)^{\otimes 4} \to \mathcal{H}_S$, where $\mathcal{H}_S$ ($\mathcal{H}_D$) is the Hilbert space corresponding to the physical (virtual) spins. As shown in Chapter 7, the PEPS on a square lattice exhibits a local symmetry if there exist unitaries V_k and $U \neq \mathbb{1}$ with

$$UB = BV_1 \otimes \cdots \otimes V_4 \tag{9.13}$$

such that, when contracting the indices of B to create the state $|\psi\rangle$, the V's cancel each other. Thus, we will have $\langle\psi| U^{\otimes N} |\psi\rangle = |\psi\rangle$ and, therefore, MO. Note that

[3] In this case one can obtain again the equivalence with the *classical* definition of string order. In order to see this, it is enough to invoke the injectivity condition presented in Definition 23.

we have the possibility of having different V's, in contrast to what happens in one dimension. This structure also allows us to understand the (dis-)appearance of SO or BO. However, in the $2D$ case, the connection between the existence of a local symmetry and Eq. 9.13 is less straight, but was already solved in Chapter 7 for the case of injective PEPS. Let us now illustrate this point with some examples:

Example 11 Let us come back to the AKLT state but in two dimensions [AKLT88]. In this case $S = 2$, $|\phi_s\rangle = (\sigma_y \otimes \sigma_y \otimes \mathbb{1} \otimes \mathbb{1})\,|\bar{\phi}_s\rangle$, and $|\phi_s\rangle$ is an orthonormal basis of the symmetric subspace of $(\mathbb{C}^2)^{\otimes 4}$. U and V correspond to a 5– and 2–dimensional representation of $SU(2)$, respectively, and thus this fulfils the condition of MO. One can prove that there is no SO even for a simple ladder formed by two chains. □

Example 12 Let us consider the cluster state [RB01, VC04a]. Here, $S = \frac{1}{2}$ and $|\phi_{-\frac{1}{2}}\rangle = |++00\rangle$, $|\phi_{\frac{1}{2}}\rangle = |--11\rangle$ with $|\pm\rangle = |0\rangle \pm |1\rangle$. One can take $U = \sigma_x$, $V_u = V_r = \sigma_x$ and $V_d = V_l = \sigma_z$. But one can also take $U = \sigma_z$, three of the V's equal to $\mathbb{1}$ and decide either $V_u = \sigma_z$, $V_r = \sigma_z$, $V_d = \sigma_x$ or $V_l = \sigma_x$. As a consequence, there is MO. One can readily show that there is no SO. However, there is still a BO, in the sense that this state is an eigenstate of the operator obtained by applying unitaries to three consecutive lines (σ_z to the first and the third and σ_x to the one in the middle). □

Example 13 Let us consider Kitaev's toric code [Kit03], which we will study with further details in Section 9.4. This is a state which has spin $S = \frac{1}{2}$ and alternative tensors in the A and B sublattices. In this case, we have alternating projectors $B = |0\rangle\langle\phi_+\phi_+|_{uldr} + |1\rangle\langle\phi_-\phi_-|_{uldr}$ and $B' = |0\rangle\langle\phi_+\phi_+|_{urld} + |1\rangle\langle\phi_-\phi_-|_{urld}$, respectively. One can take $U = \sigma_x$, $V_l = V_r = \sigma_z$ and $V_u = V_d = \mathbb{1}$. Since there is no unitary to be cancelled in the up and down positions, it has SO (and also MO). □

9.4 Wilson loops

It is well known that decoherence makes quantum information fragile when we try to implement it in a laboratory. Topological quantum information was developed as an attempt to avoid this handicap. Its topological properties make the system (or the encoded information) insensitive to continuous deformations, resistant to local perturbations, and allow for quantum error–correction schemes which, all in all, makes topological quantum computation a good candidate for quantum information encoding and operations.

The very simplest model to implement topological quantum information is the Kitaev's well–known *toric code* [Kit03], already introduced in Example 13. This consists of a two–dimensional square lattice with qubits at its edges and a Hamiltonian which introduces two constraints.

Plaquette Even parity (in the computational basis):

$$\prod_{i\in\square} Z_i \,|\psi\rangle = |\psi\rangle, \qquad \forall\square$$

Vertex Spin flip invariance:

$$\prod_{i\in+} X_i \,|\psi\rangle = |\psi\rangle, \qquad \forall+$$

The ground state is unique in the sphere, but four–fold degenerate in the torus.

It has been observed in [VWPGC06] that the equal superposition of the four logical states of the toric code $|\psi\rangle$ has a PEPS representation with bond dimension 2. Since the logical X in the first (respectively second) logical qubit is implemented by a non–contractible cut of σ_X operators along the vertical (respectively horizontal) direction [Kit03], $|\psi\rangle$ remains invariant under these two *Wilson loops* (see Fig. 9.1).

We see in this Section how the existence of this kind of Wilson loops implies again that the PEPS cannot be injective.

Theorem 46 (Wilson loops ⇒ no injectivity) *Let $|\psi_A\rangle$ be a PEPS in a $L\times N$ square lattice with local Hilbert space dimension d such that there exists a $u\in U(d)$ with the properties:*

(i) $u^{\otimes L}\otimes \mathbb{1}_{rest}\,|\psi_A\rangle = |\psi_A\rangle$ *for a loop in the vertical direction.*

(ii) $u^{\otimes N}\otimes \mathbb{1}_{rest}\,|\psi_A\rangle = |\psi_A\rangle$ *for a loop in the horizontal direction.*

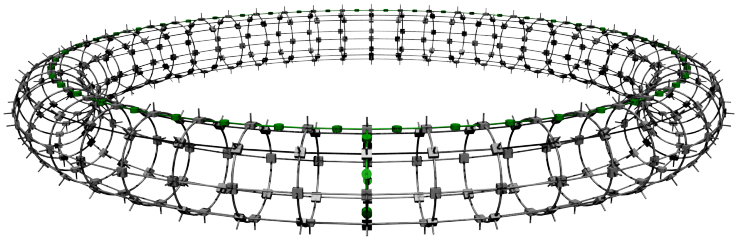
(iii) $u\otimes \mathbb{1}_{rest}\,|\psi_A\rangle \neq |\psi_A\rangle$ *for u acting on a single site.*

Then $|\psi_A\rangle$ cannot be injective for any region of size smaller than or equal to $\frac{L}{5}\times\frac{N}{5}$.□

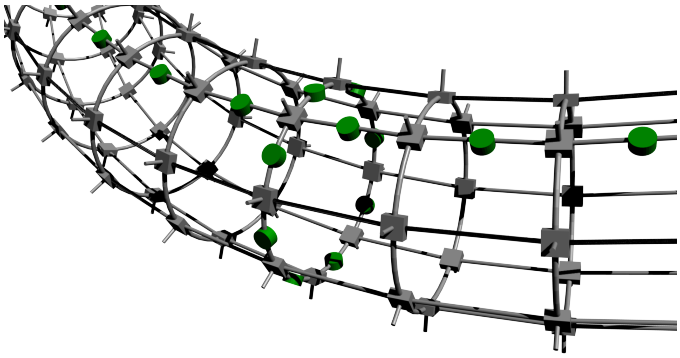
Proof We assume injectivity for a region of size $\frac{L}{5}\times\frac{N}{5}$, (i) and (ii), and will show that (iii) does not hold. By applying (i) to all columns, together with Theorem 38, we obtain that there exist unique Y and Z, such that Fig. 7.1 holds. By applying now (i) to $\frac{N}{5}$ columns together with injectivity, we obtain that $Y=\mathbb{1}$, and by applying (ii) to $\frac{L}{5}$ rows together with injectivity we obtain that $Z=\mathbb{1}$. Therefore, $u\otimes \mathbb{1}_{\rm rest}\,|\psi_A\rangle = |\psi_A\rangle$ for u acting on a single site. ∎

9.5 Lieb–Schultz–Mattis–type theorems

It is well known that particles with semi–integer spin, such as electrons, have fermionic statistics and their wave function acquires a minus sign under the interchange of identical particles. In general, this is a quantum behaviour which is hardly visible in the macroscopic world. However, in low dimensions, where the wave



(a)



(b)

Figure 9.1: **Wilson loops**. These are the Wilson loops which keep the PEPS associated to the toric code invariant.

functions are quite localized, the zero–point fluctuations are large and, consequently, the interference effects due to statistics become important [Aue98].

In this Section, we firstly show that low–dimensional $SU(2)$–invariant Hamiltonians present qualitatively different spectra when the spin is integer (bosonic statistic) than when it is semi–integer (fermionic). This qualitatively different behaviour was proposed by Haldane [Hal83a, Hal83b, CH05] and proven for one–dimensional spin–$\frac{1}{2}$ systems by E.H. Lieb, T.D. Schultz, and D.C. Mattis in 1961 [LSM61] and generalized to larger semi–integer spins by I. Affleck and E.H. Lieb in [AL86]. This Theorem has recently been extended and generalized. For instance, it was extended to two–dimensional systems [Has04, NS07] and, still for the one–dimensional case, generalizations relaxing the condition on $SU(2)$ symmetry [OYA97].

These theorems require a difficult machinery when attempting to prove them in complete generality. However, we will show in this Section that they can be easily proven in the framework of MPS and PEPS, by using the properties shown in Chapters 1–7. As the proofs are restricted to a special class of states, these are not general. However, they present several advantages that we already pointed out in the Introduction 9.1, and that will be studied in detail in Subsubsection 9.5.1.1.

9.5.1 Lieb–Schultz–Mattis theorem

The one–dimensional spin–$\frac{1}{2}$ Heisenberg Hamiltonian with antiferromagnetic interactions is exactly solvable by the Bethe Ansatz. This presents a power–law decay in the correlation functions and is gapless, *i.e.* there are local excitations with arbitrarily low energy. One could expect the same behaviour for larger values of the spin, independently of whether they are integer or semi–integer. However, F.D.M. Haldane argued [Hal83a, Hal83b, CH05], by means of quantum field theory techniques, that one should expect a different behaviour when the spin is integer: exponential decay in the correlation functions and a non–trivial gap above the ground state (often called *Haldane gap*). Let us remark that the existence of a gap in the spectrum and exponential clustering in the correlation functions is quite surprising in a model with continuous symmetry [LM66]. Let us now enunciate the Theorem strictly:

Theorem 47 (1*D* Lieb–Schultz–Mattis) *Let us consider a one–dimensional semi–integer antiferromagnetic translational invariant and $SU(2)$–invariant Hamiltonian describing a spin chain with (even) length L and periodic boundary conditions. Then, the gap above the (unique) ground state ϵ_L is upper bounded by*

$$\epsilon_L \leq C\frac{1}{L}$$

where C is a constant independent of L, as shown in Fig. 9.2. This implies either gapless excitations or ground level spontaneously broken translational symmetry in the thermodynamic limit $L \to \infty$. □

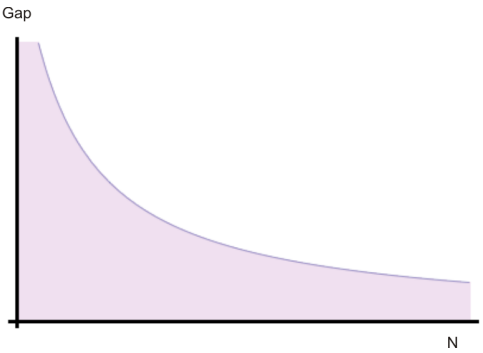


Figure 9.2: **Lieb–Schultz–Mattis Theorem**. Behaviour of the spectral gap over the ground state in the thermodynamic limit for a semi–integer spin $SU(2)$–invariant Hamiltonian, by the Lieb–Schultz–Mattis Theorem. It predicts that the gap vanishes proportionally to $\frac{1}{L}$ (or faster) in the thermodynamic limit.

Proof This Theorem was firstly proven for spin $\frac{1}{2}$ in [LSM61] and later extended to larger semi–integer spins in [AL86], but there is a simpler proof for the Heisenberg Hamiltonian in [Aue98]. ∎

The proof of this Theorem fails for integer spins, which leads to the existence of the Haldane phase without breaking the translational symmetry and the Haldane gap above the ground state.

The opposite behaviours, in precisely the thermodynamic limit, of integer and semi–integer spins results in a macroscopic manifestation of quantum properties. This is not, however, just a mathematical artefact, because this behaviour is supported by many experiments performed since the Haldane hypothesis was proposed.

The extension of this Theorem to higher dimensions was obtained by M. Hastings in [Has04], and rewritten afterwards in [NS07]. The difficulty in obtaining the generalization consists in the following:

(a) If the correlation functions are short–ranged, the ground state can be well–described by short–range resonating valence bond states. This leads to a similar construction for the excited state which appears in the original one–dimensional proof.

(b) If the correlation functions are long–ranged, the excited state constructed as above does not correspond to the low–energy sector. In lieu of this state, there exist low–energy spin wave excitations.

Therefore, in the higher–dimensional case, there exist two different means of obtaining the lowest–energy excitation, significantly complicating the construction.

9.5.1.1 Lieb–Schultz–Mattis in the tensor network framework

As shown above, the Lieb–Schultz–Mattis Theorem states that, for semi–integer spins, an $SU(2)$–invariant one–dimensional *Hamiltonian* cannot have a uniform (system size–independent) energy gap above a unique ground state. That is, the symmetry imposes strong restrictions on the possible behaviours of a system. In this Subsubsection, we want to go a step further and analyse which implications one can obtain from having a *single* symmetric *state* in a semi–integer spin chain. By restricting our attention to the class of MPS, we will show:

Theorem 48 (Lieb–Schultz–Mattis with MPS) *Any $SU(2)$–invariant MPS in the sense of Eq. 4.1, i.e. $u_g^{\otimes N}|\psi\rangle = e^{i\theta_g}|\psi\rangle$, with $u_g^{(d)}$ an irrep and even physical dimension d (semi–integer spin) cannot be injective. In particular, by Theorem 22, this implies that it cannot be the unique ground state of any frustration–free Hamiltonian.* □

Proof Let us assume that the MPS is injective and prove the Theorem by contradiction. Theorems 25 and 26 guarantee that

$$\sum_j u_{jk}^g A_j = U_g A_k U_g^\dagger \tag{9.14}$$

We consider $u = e^{iJ_z}$ with $(J_z)_{j,k} = \delta_{j,k}\big(k - \frac{d+1}{2}\big)$, $k = 1, \ldots, d$. Then, Eq. 9.14 gives

$$e^{i\,\varphi_k} A_k = U A_k U^\dagger \tag{9.15}$$

for a unitary U and half–integer φ_k. We finish by proving that if N is odd, $\mathrm{tr}\,[A_{k_1}\cdots A_{k_N}] = 0$, and hence, by Lemma 5, the MPS cannot be injective for any N. From Eq. 9.15, we get $\mathrm{tr}\,[A_{k_1}\cdots A_{k_N}] = 0$, unless $\sum_{i=1}^N \varphi_{k_i} = 0$. However, the latter is impossible for odd N, because in this case the LHS is integer, whereas the RHS is half–integer. ■

From the proof, one may get the impression that only $U(1)$ symmetry is required, and this is indeed the case if the generator of such symmetry has eigenvalues $-\frac{m}{2}, \ldots, \frac{m}{2}$, as above. However, the next example shows that this is not true for *all* $U(1)$ representations, which in turn shows that a larger symmetry like $SU(2)$ is required for the Lieb–Schultz–Mattis Theorem.

Example 14 Let us consider a local symmetry G represented by $u_\beta = e^{i\beta H}$, for a hermitian matrix H. Let us choose the physical dimension $d = D^2 - D$, which is always even, and the set of Kraus operators $\mathcal{K} = \{A_{(i,j)} = |i\rangle\langle j|\,,\ i \neq j\}$. We select $\alpha_1, \ldots, \alpha_D \in \mathbb{R}$ such that $\alpha_i - \alpha_j \neq 0$ if $i \neq j$ and H with the diagonal form given by $H = \sum_{i\neq j}(\alpha_i - \alpha_j)\,|(i,j)\rangle\langle(i,j)|$ (which in addition has only non–zero eigenvalues). With $U_\beta = e^{i\beta\Omega}$, where $\Omega = \mathrm{diag}[\alpha_1 \ldots \alpha_D]$, it is clear that

$$e^{i\beta(\alpha_i - \alpha_j)} A_{(i,j)} = U_\beta A_{(i,j)} U_\beta^\dagger$$

so the MPS generated by means of the Kraus operators $\mathcal{K}$ has the local symmetry G. Moreover, the MPS is trivially injective when $D \geq 3$. We can prove this by choosing arbitrary k and k'. Since $D \geq 3$, we can always find an l such that $k' \neq l \neq k$, and then $|k\rangle\langle k'| = |k\rangle\langle l|\ |l\rangle\langle k'| = A_{(k,l)}A_{(l,k')}$. □

Let us remark that this counter–example is applicable to spin $\geq \frac{5}{2}$. Indeed, one can prove Theorem 48 for $U(1)$ and spin $\frac{1}{2}$, which is the content of the following Lemma. For the lowest values of the physical spin, the case of spin $\frac{3}{2}$ remains an open question.

Lemma 34 (Lieb–Schultz–Mattis for $U(1)$ and spin $\frac{1}{2}$) *Let $|\psi\rangle$ be an MPS with physical dimension $d = 2$ and $U(1)$–invariant, then $|\psi\rangle$ cannot be injective.* □

Proof Let us show this by contradiction. By choosing a basis where the physical unitary u is diagonal, the condition on the Kraus operators becomes

$$e^{i\lambda_n\phi}A_n = e^{iH\phi}A_n e^{-iH\phi}$$

where H is the hermitian generator of the symmetry. Let us expand the expression for infinitesimal angles

$$[H, A_n] = \lambda_n A_n$$

which is the equation of eigenvalues for the operator $L(\bullet) = [H, \bullet]$. This can be transformed into an ordinary eigenvalue equation for the matrix operator $L = H \otimes \mathbb{1} - \mathbb{1} \otimes \bar{H}$, where the bar indicates complex conjugation. The diagonalization can be easily performed by taking the spectral decomposition of $H = \sum_i \mu_i P_i$, where P_i are orthogonal projectors. It straightforwardly follows that the eigenvalues of L are $\lambda_{ij} = \mu_i - \mu_j$ and the corresponding eigenoperators fulfil $A_{ij} = P_i A_{ij} P_j$.

Let us focus now on the case $d = 2$. Then, we have that $A_1 = P_1 A_1 P_\alpha$ and $A_2 = P_\beta A_2 P_\gamma$ for some α, β, γ. If $\beta = 1$, $P_1 X = X$ for all $X \in \text{span}\,[A_{i_1} \cdots A_{i_n}]$, and the MPS cannot be injective. The same happens if $\alpha = \gamma$. So let us assume that $\beta \neq 1$ and $\gamma \neq \alpha$. Now, if $\alpha = 1$, we have $A_1 = P_1 A_1 P_1$, $A_2 = (\mathbb{1} - P_1)A_2(\mathbb{1} - P_1)$ and the MPS is block diagonal and hence non–injective. The same happens if $\beta = \gamma$. So $\alpha \neq 1$ and $\beta \neq \gamma$, and this gives $A_1^2 = 0 = A_2^2$, which implies that $\text{span}\,[A_{i_1} \cdots A_{i_n}] = \text{span}\,[A_1 A_2 A_1 A_2 \cdots, A_2 A_1 A_2 A_1 \cdots]$ has dimension smaller than or equal to 2. ■

We have proven the Lieb–Schultz–Mattis Theorem for one–dimensional systems, but the proof is equivalent for higher–dimensional cases whenever Theorem 38 holds, *i.e.* when there exists a local description of the invariant PEPS. We will see in the following Subsection a higher–dimensional generalization of the Oshikawa–Yamanaka–Affleck Theorem, which has the Lieb–Schultz–Mattis Theorem as a particular case.

The approach by means of local tensors has some advantages and one main disadvantage, which is that the proof is not general. The advantages are:

1. A simpler proof which allows a greater control over the conditions of the Theorem and permits slightly changing them in order to determine which ones are really necessary.

2. It allows for an easy proof of counter–examples.

3. Although the proof is less general, since we are restricting ourselves to a small (but very relevant) subclass of states, this transforms the enunciation of the Theorem from symmetric Hamiltonians to symmetric states. This leads to a generalization of the Theorem since, for a symmetric Hamiltonian, there is always a unitary combination of ground states such that it keeps the symmetry (in particular, if the ground state is unique, then the state itself has the symmetry). However, the symmetry of the ground state can be larger than the symmetry of the Hamiltonian (phenomenon known as *emergent symmetries* in condensed matter).

4. The Theorem can be proven for any dimension with essentially the same proof, by using the results from Chapter 2.

9.5.2 $2D$ Oshikawa–Yamanaka–Affleck theorem

By investigating the conditions which a weaker symmetry such as $U(1)$ can impose on the ground state, a very natural extension of the Lieb–Schultz–Mattis theorem emerges from the relaxation of the restrictions on the local symmetry. This was proposed by M. Oshikawa, M. Yamanaka and I. Affleck in the seminal paper [OYA97]. They observe that the original Lieb–Schultz–Mattis Theorem holds when a magnetic field hJ_z is added except when $J - m \in \mathbb{Z}$, where J is the physical spin and m is the magnetization per particle. Therefore, a massive phase without spontaneously broken translational symmetry is only possible when this relation holds.

Let us enunciate the Theorem explicitly:

Theorem 49 (1*D* Oshikawa–Yamanaka–Affleck) *Let H be a $U(1)$-invariant (with generator J_z corresponding to the third component of an irrep of $SU(2)$) one–dimensional Hamiltonian on a spin chain with physical spin J and L particles. Then, the gap above the ground state is upper bounded by $C\frac{1}{L}$ if $J - m \notin \mathbb{Z}$.* □

Proof This Theorem was firstly proven in [OYA97]. The proof is very close to the original proof of the Lieb–Schultz–Mattis Theorem. ■

This Theorem was originally used to predict the existence of magnetization plateaus when tuning the magnetic field h for the magnetization values in which $J - m \in \mathbb{Z}$ holds. Moreover, the possibility of translational symmetry breaking is exploited to forecast that this magnetization could be fractional, in a way similar to fractional quantization of the charge in the *quantum Hall effect*. The idea is that, if the ground state is p–fold degenerate, then the relationship $p(J-m) \in \mathbb{Z}$ must hold for a gap to

exist above the ground state manifold. It is stated in [OYA97] that the result can be generalized to Hamiltonians with spatial structures, *i.e.* which present translational invariance with a certain period.

9.5.2.1 $2D$ Oshikawa–Yamanaka–Affleck in tensor network framework

In [SWPGC09], it was shown how the original Lieb–Schultz–Mattis Theorem can be understood at the level of states, an idea which has already been explained in Subsubsection 9.5.1.1. More precisely, we showed that no $SU(2)$–invariant MPS with semi–integer spin can be injective. In this Subsubsection, we give a $2D$ version of the Oshikawa–Yamanaka–Affleck Theorem, by showing that a $U(1)$–symmetric PEPS for which $J - m$ is not an integer cannot be injective.

As was stated above, Oshikawa *et al.* [OYA97] proved the theorem by allowing for a breaking of the translational symmetry. The proof given here for larger dimensions is for strictly translational invariant states (eigenstates of the translation operator with eigenvalue $+1$), since we still do not have enough control over the periodic components in PEPS. However, in Section 9.6, we provide the complete proof for MPS, where we have full control.

Let us start with a PEPS $|\psi_A\rangle$ of spin–J particles with a $U(1)$ symmetry in the z direction, that is

$$u_g^{\otimes N} |\psi_A\rangle = e^{i\theta_g} |\psi_A\rangle$$

with $u_g = e^{igJ_z}$. Since $g \mapsto e^{i\theta_g}$ is clearly a representation, there exists θ such that $\theta_g = Ng\theta$. We will show that:

Lemma 35 (Physical meaning of $\boldsymbol{\theta}$) *Let $|\psi^{(N)}\rangle \in (\mathbb{C}^d)^{\otimes N}$ be an N–particle state, such that $u_g^{\otimes N} |\psi^{(N)}\rangle = e^{N\boldsymbol{g}\cdot\boldsymbol{\theta}} |\psi^{(N)}\rangle$, where $u_g = \exp(i\boldsymbol{g}\cdot\boldsymbol{J})$ is a representation of a compact Lie group with generators J_α. Then $\theta_\alpha = \frac{1}{N}\langle\psi^{(N)}| \sum_k J_\alpha^{(k)} |\psi\rangle$. In the particular case of $U(1)$, θ coincides with the magnetization per particle, m.* □

Proof To see this, it is enough to use the fact that the group is a compact Lie group to expand both sides of the expression $u_g^{\otimes N} |\psi^{(N)}\rangle = e^{iN\boldsymbol{g}\cdot\boldsymbol{\theta}} |\psi^{(N)}\rangle$ around the identity: from the LHS we get $u_g^{\otimes N} |\psi^{(N)}\rangle \simeq (\mathbb{1} + i\boldsymbol{g}\cdot\sum_k \boldsymbol{J}^{(k)}) |\psi^{(N)}\rangle$, while the RHS gives $e^{iN\boldsymbol{g}\cdot\boldsymbol{\theta}} |\psi^{(N)}\rangle \simeq (1 + iN\boldsymbol{g}\cdot\boldsymbol{\theta}) |\psi^{(N)}\rangle$. Computing the overlap with $|\psi^{(N)}\rangle$ we get $\boldsymbol{\theta} = \langle\psi^{(N)}| \sum_j \boldsymbol{J}^{(j)} |\psi^{(N)}\rangle$, the desired result. ■

Let us remark that, in the case of $SU(2)$ or larger groups for which the magnetization per particle is zero, $m = 0$, because of the rotational symmetry, the fact that no phase can appear in the symmetry condition is immediately apparent.

Now we can prove the Oshikawa–Yamanaka–Affleck Theorem for PEPS, as previously announced:

Theorem 50 (Oshikawa–Yamanaka–Affleck for PEPS) *Let $|\psi_A\rangle$ be a PEPS in a $L \times N$ square lattice which is injective in regions of size $\frac{L}{5} \times \frac{N}{5}$. If $|\psi_A\rangle$ is*

invariant under a representation of $U(1)$ with the usual generator of spin J given by $J_z^{(J)}$, then the magnetization per particle m fulfils that $(J-m)$ is an integer. Obviously, if the state has full $SU(2)$ symmetry, then $m=0$ and the usual Lieb–Schultz–Mattis Theorem emerges for PEPS. □

PROOF Let us choose $R \geq \frac{L}{5}$ and $S \geq \frac{N}{5}$, and consider the PEPS–PBC associated to the region $R \times S$, $|\psi_A^{(R\times S)}\rangle$. By means of injectivity, it is clear that $|\psi_A^{(R\times S)}\rangle \neq 0$.

By applying $e^{igJ_z^{(J)}}$ to all spins, and by using Theorem 38, there must exist a choice of indices $k_1, \ldots, k_{RS} \in \{-J, -J+1, \ldots, J-1, J\}$ such that $k_1 + \cdots + k_{RS} = SR\theta$.

We apply the same argument for regions of size $R \times (S+1), (R+1) \times S, (R+1) \times (S+1)$, getting indices k', k'' and k''' respectively. Therefore,

$$\begin{aligned}\theta &= (R+1)(S+1)\theta - (R+1)S\theta - R(S+1)\theta + RS\theta \\ &= \sum_{r=1}^{RS} k_r + \sum_{r=1}^{(R+1)S} k'_r + \sum_{r=1}^{R(S+1)} k''_r + \sum_{r=1}^{(R+1)(S+1)} k'''_r\end{aligned}$$

The RHS has the same character as J, that is, it is integer if J is integer and semi–integer otherwise. Therefore, $\theta - J \in \mathbb{Z}$. Since θ is the magnetization per particle by Lemma 35, the Theorem follows. ■

As in the Lieb–Schultz–Mattis case shown in Subsubsection 9.5.1.1, there are also several advantages and mainly one disadvantage in this approach. The disadvantage is again working in a framework which is not completely general, but restricted to a subset of states.

The advantages are essentially the same, but adding a very relevant one: there is no general higher–dimensional proof of this Theorem, so the result shown here is non–trivial.

Moreover, this construction allows us to better understand the physical meaning of the plateaus in one–dimensional systems. When $J - m \in \mathbb{Z}$, the state is injective and by the properties shown in Section 3.4, this ensures the existence of a gap. If we introduce a $U(1)$ symmetry–preserving magnetic term, then we ensure that the magnetization per particle remains unchanged for a non–trivial interval of the magnetic field (at least, while the energy introduced by the magnetic field is smaller than the the spectral gap divided by the total number of particles, $\epsilon > \|hJ_z\|$).

Example 15 Let us consider a very simple case: the Majumdar–Ghosh Hamiltonian given by

$$H = \sum_i \frac{2}{3}(2\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+2}) + \frac{1}{2}\mathbb{1}$$

where $\boldsymbol{S}$ are the three Pauli matrices. The MPS description of the ground states was already explained in Examples 2 and 4. In the thermodynamic limit, this

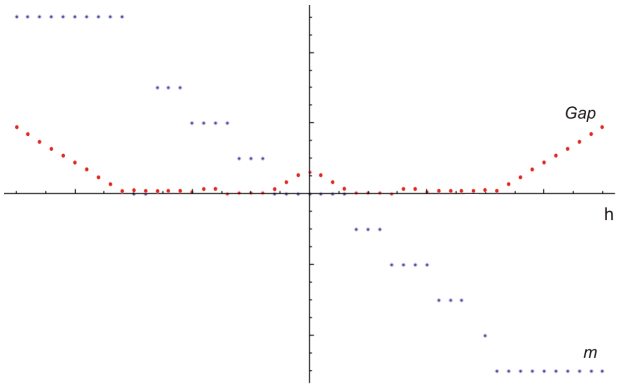


Figure 9.3: **Oshikawa–Yamanaka–Affleck Theorem**. The Oshikawa–Yamanaka–Affleck Theorem predicts the existence of plateaus with a magnetization fulfilling $p(J-m) \in \mathbb{Z}$. This example has been numerically obtained for 12 particles and the Majumdar–Ghosh Hamiltonian.

Hamiltonian has a two–fold degenerate ground state which breaks the translation invariance in the sense of Definition 2. This Hamiltonian has a gap above the ground state manifold, as proven in [AKLT88, Theorem 5.3].

Therefore, if we add a magnetic term hS_z to the Hamiltonian, then a plateau around $h = 0$ should appear, as shown in Fig. 9.3. Although this example does not present a plateau with fractional magnetization, it is a very simple way of illustrating the reason why plateaus emerge. □

9.6 Fractional magnetization vs. entanglement

Fractionalization of quantum numbers has attracted a lot of attention in the last years, since it has shown to be connected to most of the fundamental concepts in condensed matter physics, as conductivity, topological order, degeneracy or criticality [JR76, SSH80, FT81, TSG82, Lau83]. In this Section, we will relate fractionalization to entanglement, strengthening in this way the already close connections between quantum information ideas and strongly correlated systems.

Most of these connections have been made in the MPS framework [PGWS+08, SWPGC09, SPGWC10], which can then be justified by the fact that MPS faithfully approximate ground states of local one–dimensional Hamiltonians [VC06, Has07a]. This last result has opened the avenue of a new way of thinking. If MPS are essentially all one–dimensional quantum states and they have such a simple expression, one should be able to understand in this language all one–dimensional quantum effects, as it is already the case for string orders [PGWS+08], renormalization flows [Whi92, Whi93] or sequential interactions [LLPG+08]. The results which appear in this Section will be available in [PGSC+].

9.6.1 Inverse Oshikawa–Yamanaka–Affleck theorem

In this Subsection, we will first prove the Oshikawa–Yamanaka–Affleck Theorem in one–dimensional systems allowing for translational symmetry breaking. We show that only magnetizations fulfilling $J - m = \frac{q}{p}$ are allowed, and that some kind of periodicity is necessary in order to get such fractional magnetizations, which implies an inverse version of the Oshikawa–Yamanaka–Affleck Theorem.

Let us start by proving that, given a period p, only blocks which are multiples of p are permitted. We assume that we have a TI–MPS $|\psi^{(N)}\rangle$ with spin J and a $U(1)$ symmetry in the z–direction with generator J_z, *i.e.* this fulfils $u_g^{\otimes N}|\psi^{(N)}\rangle = e^{igNm}|\psi^{(N)}\rangle$ with $u_g = \exp(igJ_z)$. Then, we have the following Lemma:

Lemma 36 (Blocks of period multiple of p are permitted) *Let m be any rational number and $p \in \mathbb{N}$ such that there exist two spin–J states with sizes pN and $p(N+1)$, N being a given integer, and showing both of them magnetization per particle m. Then, $p(J-m) \in \mathbb{Z}$ holds.* □

Proof The proof is a one–dimensional version of the proof of Theorem 50. By expanding equation $u_g^{\otimes N}|\psi^{(N)}\rangle = e^{igNm}|\psi^{(N)}\rangle$ in the canonical basis, we get

$$\sum_{k_1,\ldots,k_{pN}} c_{k_1\ldots k_{pN}} e^{ig\sum_j k_j}|k_1\ldots k_{pN}\rangle = \sum_{k_1,\ldots,k_{pN}} e^{igpNm} c_{k_1\cdots k_{pN}}|k_1\ldots k_{pN}\rangle.$$

Since it is a basis and the state is not zero, there exist $k_1,\ldots,k_{pN} \in \{-J,-J+1,\ldots,J-1,J\}$ such that the condition $\sum_j k_j = Npm$ holds. By the same reason, there exist $k'_1,\ldots,k'_{pN+p} \in \{-J,-J+1,\ldots,J-1,J\}$ such that $\sum_j k'_j = (Np+p)m$. Subtracting them, we get that $mp = \sum_{j=1}^{pN+p} k'_j - \sum_{j=1}^{pN} k_j$ which has the same character (integer or semi–integer) as pJ, as summarized in the table below. ■

J **integer**			$\Longrightarrow$	mp integer	$\leftrightarrows$	pJ integer
J **semi–integer**	$\nearrow$	p even	$\Longrightarrow$	mp integer	$\leftrightarrows$	pJ integer
	$\searrow$	p odd	$\Longrightarrow$	mp semi–integer	$\leftrightarrows$	pJ semi–integer

With this at hand, if we consider a spin–J MPS $|\psi\rangle$ with a $U(1)$ symmetry generated by the canonical generator of spin J_z, we have the following Theorem:

Theorem 51 (Oshikawa–Yamanaka–Affleck with broken TI) *Let $|\psi^{(N)}\rangle$ be a TI–MPS, and p the smallest integer such that, after blocking p spins together, the MPS representation has a block–diagonal structure with injective blocks. Let us assume that $|\psi^{(N)}\rangle$ is $U(1)$–invariant in the sense defined above. Then, the magnetization per particle fulfils*

$$p(J-m)=q \tag{9.16}$$

q being an integer such that $0\leq q\leq 2pJ$. □

Proof We call $A_{k_1\ldots k_p}$ the Kraus operators after blocking p sites. By means of Theorem 26, the $U(1)$–invariance is translated into

$$\sum_{j_1,\ldots,j_p}(u_g^{\otimes p})_{j_1\ldots j_p,k_1\ldots k_p}A_{j_1\ldots j_p}=e^{ig\theta}U_gA_{k_1\ldots k_p}U_g^\dagger$$

where $\theta=pm$, as proven in Lemma 35. By using the structure of the generators, $(J_z)_{ik}=\delta_{ik}(k-\frac{d+1}{2})\equiv\phi_k$, with $d=2J+1$ the physical dimension, we obtain

$$A_{k_1\ldots k_p}=e^{ig(\theta-\sum_{j=1}^p\phi_{k_j})}U_gA_{k_1\ldots k_p}U_g^\dagger \tag{9.17}$$

Therefore, the coefficients of the state are

$$\mathrm{tr}\left[A_{k_1\ldots k_p}A_{k_{p+1}\ldots k_{2p}}\cdots A_{k_{(N-p)+1}\ldots k_N}\right]=$$
$$e^{ig(\frac{N\theta}{p}-\sum_{j=1}^N\phi_{i_j})}\mathrm{tr}\left[A_{k_1\ldots k_p}A_{k_{p+1}\ldots k_{2p}}\cdots A_{k_{(N-p)+1}\ldots k_N}\right]$$

By using that $\theta=mp$, in order to have a non–trivial state, we need the fact that there exists at least one combination of $k_1,\ldots,k_N$ for which the trace in the LHS of the previous equality is non–zero, so it is necessary to have solutions for the equation $Nm-\sum_{j=1}^N\phi_{i_j}=0$ (note that any other $2\pi n$ case is discarded, since the RHS is rational, while the LHS is irrational). As we are assuming that the symmetry is independent of N, then there particularly exist solutions for N and $N+p$, so by subtracting them, we get

$$pm-\left(\sum_{j=1}^{p(r+1)}\phi_j-\sum_j^{pr}\phi_j\right)\in\mathbb{Z}$$

Notice that the quantity between brackets has the same character as pJ, *i.e.* it is integer (semi–integer) if pJ is integer (semi–integer). Therefore, $p(J-m)\in\mathbb{Z}$. ■

Let us now prove a reciprocal Theorem, which ensures that periodicity is necessary to have fractional magnetization:

Theorem 52 (Inverse Oshikawa–Yamanaka–Affleck) *Let us assume that $J-m=\frac{q}{p}$, with $\gcd(p,q)=1$ for all large enough N in a $U(1)$–invariant TI–MPS. Then, the MPS has only $\tilde{p}$–periodic blocks, with $\tilde{p}$ a multiple of p. Moreover, states belonging to blocks of different periods are different.* □

PROOF By the characterization of the symmetries in Theorem 26, every block is an injective $U(1)$–invariant TI–MPS. By means of Lemma 35, all of them have the same magnetization. Moreover, from Lemma 36 follows that only blocks of period multiple of p are permitted. Additionally, a direct consequence of Theorem 13 is that states belonging to blocks of different periods are different. ∎

9.6.2 Fractional magnetization *vs.* entanglement

In this Subsection, we show the main result of this Section: a non–trivial relationship between magnetization and entanglement. In fact, the objective is to show that, in the framework of MPS, one can easily prove that large fractionalization in the magnetization of a given state requires large entanglement among the parts of the state (block entropy).

Let us summarize the idea in the following Theorem:

Theorem 53 (Fractional magnetization ⇒ large entanglement) *Let $|\psi_A\rangle$ be a spin J, $U(1)$–invariant TI–MPS (in the sense of Definition 2) with magnetization per particle verifying $J - m = \frac{q}{p}$ (with $\gcd(p,q) = 1$). Then, there exists a multiple of p, denoted by $\tilde{p}$, such that the entropy of the reduced density matrix for any region of size $L = k\tilde{p}, \forall k$ verifies*

$$S(\rho^{(L)}) \geq \log(p) \tag{9.18}$$

up to an exponentially small correction in $N - L$ (N is the length of the chain, which can be taken in the thermodynamic limit). □

PROOF Let $|\psi_A^{(N)}\rangle$ be a $U(1)$–invariant TI–MPS with physical spin J and magnetization per particle m. Then, by means of Theorem 52, there is a multiple of p, called $\tilde{p}$, such that all the blocks of $|\psi_A^{(N)}\rangle$ have period $\tilde{p}$. Let us consider a length $L = k\tilde{p}$. Then, by Lemma 7, the reduced density matrix of size L verifies $\rho^{(L)} = \bigoplus_{i=1}^{n} \lambda_i \rho_i$, up to a correction $\mathcal{O}(e^{-c(N-L)})$, where the reduced density matrices $\{\rho_i\}$ correspond to blocks giving rise to different states (repeated blocks are reflected in the λ_i).

Now, we only need to apply Lemma 7, together with Theorem 11, to show that $S(\rho_i) \geq \log p$, for all i, and hence, that $S(\rho^{(L)}) \geq \log(p)$ up to an exponentially small correction in $(N - L)$. ∎

Let us illustrate the idea with an example:

Example 16 Let us take $J = \frac{1}{2}$ and a p–particle state $|\mu\rangle = |\uparrow\uparrow \cdots \uparrow\downarrow \cdots \downarrow\rangle$. Then, by means of Eq. 9.16, q is the number of down spins. Let us construct the TI state $|\psi\rangle = \sum_{k=1}^{q} \tau^k(|\mu\rangle^{\otimes n})$. Defining the Kraus operators $A_\downarrow, A_\uparrow \in \mathcal{M}_q$ as follows

$$A_\downarrow = \sum_{i=1}^{p} |i\rangle\langle i+1| \qquad A_\uparrow = \sum_{i=p+1}^{q} |i\rangle\langle i+1| \tag{9.19}$$

the generated TI–MPS is $U(1)$–invariant and fulfils Eq. 9.16. Thus, we can construct states with arbitrarily fractional magnetization by tuning the values of p and q. □

A relevant question emerges: how should we understand this Theorem? If we go to a laboratory with a spin system which we previously know has a degenerate ground state and try to measure the magnetization or any other ground state property, we will never measure it in the translational invariant state, since a spontaneous symmetry breaking process would emerge and the probability of obtaining such state is zero. Therefore, the manner in which this Theorem has to be understood is that, if we measure a very fractional magnetization in a translational invariant state, then we can ensure that this state has long–range entanglement.

9.7 Long–range Hamiltonians vs entanglement

Locality, a property of quantum many–body systems arising from local interactions, has attracted a lot of attention in the last years motivated by a quantum information perspective. A great effort has been devoted to understanding the complexity that these systems can generate by showing, on the one hand, that such systems are simple enough to obey an area law [ECP10], but, on the other hand, that they still keep enough complexity to make their study intractable [GI09, AGIK09, KSV02].

Quantum information and, in particular, the concept of entanglement, has produced a considerable impact in the understanding of strongly correlated quantum systems, shedding new light in the behaviour of quantum phase transitions, topological order, or renormalization. Many of these contributions have been made by means of Matrix Product States and Projected Entangled Pair States, which have proven to be the exact family of quantum states needed to explain low energy sectors of locally interacting quantum systems, as already discussed in the previous chapters.

In this Section, we provide two interesting results: a sharply improved upper bound for the approximation of states by means of MPS, and a physical application of such result which illustrates the physical intuition that, if there are long–range forces which cannot be faithfully approximated by short–range ones, then long–range entanglement between disjoint regions of the system should exist.

The first result is an improvement of the upper bound for the distance in the trace norm provided by F. Verstraete *et al.* in [VC06, Lemma 3] between a general state (represented by an MPS with very large bound dimension) and a low–dimensional MPS. The result of that work is given for two–body reduced density matrices, and a straightforward generalization for L–body reduced density matrices leads to an exponential bound d^L, with d being the dimension of the local physical degrees of freedom, and L the interaction length of the Hamiltonian. As we are interested in long–range interactions, this exponential dependence is critical and must be improved. We provide here a linear–dependent bound on L, which is additionally independent from the physical dimension d. This last feature could turn out to be relevant for the study of bosonic systems.

In Subsection 9.7.3, we provide a fascinating application of the previous result.

We prove a theorem which makes use of the MPS formalism to illustrate that, if we have a long–range interacting Hamiltonian which cannot be faithfully approximated by a short–range interacting Hamiltonian, then the ground state of the former presents long–range entanglement between separate regions of the system. This Theorem is a perfect exemplification of the power of the MPS as a laboratory where one can *play* in order to obtain results in condensed matter.

The results shown in this Section are work in progress, so they are still unpublished, but they will be available in [PGSC$^+$].

9.7.1 Bounding distances between MPS

The objective in this Subsection is to improve the bound obtained in [VC06, Lemma 3] for the approximation of general states by means of MPS. In this pioneering work, the authors find an upper bound for the minimum distance between the 2–site reduced density matrix of an arbitrary state and that of an MPS of a given bond dimension. However, if one tries to straightforwardly extend this result to blocks of L particles, an exponential term d^L appears, making it useless for our purposes. We provide here a bound which depends linearly on L and does not depend on the physical dimension d, which significantly improves the previous result.

Let $A_i \in \mathcal{M}_D$ be the Kraus operators defining an MPS $|\psi\rangle$ in the thermodynamic limit, such that $\sum_{i=1}^d A_i A_i^\dagger = \mathbb{1}$ and $\sum_{i=1}^d A_i^\dagger \Lambda A_i = \Lambda$. Then, the normalized reduced density matrix for L particles $\rho_A^{(L)}(\Lambda)$ is written as in Eq. 1.17 by

$$\rho_A^{(L)}(\Lambda) = \sum_{\substack{i_1,\ldots,i_L \\ j_1,\ldots,j_L}} \mathrm{tr}\left[A_{j_L}^\dagger \cdots A_{i_1}^\dagger \Lambda A_{j_1} \cdots A_{j_L}\right] |i_1 \ldots i_L\rangle\langle j_1 \ldots j_L|$$

Our goal is to compute an upper bound for the norm $\|\rho_A^{(L)}(\Lambda) - \rho_{\tilde{A}}^{(L)}(\tilde{\Lambda})\|_2$, which is the normalized density matrix resulting from projecting the Kraus operators (and the fixed point) into a subspace of dimension $\tilde{D} \leq D$, *i.e.*. $\tilde{A}_i = PA_iP$ and $\tilde{\Lambda} = P\Lambda P$. To simplify the notation, as the reduced density matrix is later on for L particles, we will refer to this simply as ρ_A instead of $\rho_A^{(L)}$.

In order to do this, let us prove some previous lemmas. Let us call $\mathcal{E}$ the completely positive map associated to the Kraus operators A_i and $\tilde{\mathcal{E}}$ the one associated to $\tilde{A}$.

Lemma 37 (Bound for tr $\left[\tilde{\boldsymbol{\mathcal{E}}}^{\boldsymbol{L}}(\boldsymbol{\Lambda})\right]$) *$\|\tilde{\mathcal{E}}^L(\Lambda) - \Lambda\|_1 \leq 2L\delta$, where $\delta = \|\Lambda - \tilde{\Lambda}\|_1$. In particular,* $\mathrm{tr}\left[\tilde{\mathcal{E}}^L(\Lambda)\right] \geq 1 - 2L\delta$. □

Proof By means of the definition of δ, we get that $\|\Lambda - \mathcal{E}(P\Lambda P)\|_1 \leq \delta$, because $\mathcal{E}$ is contractible for the 1–norm. The map $P \cdot P$ is also contractible for the 1–norm, so

$$\|\Lambda - P\mathcal{E}(P\Lambda P)P\|_1 \leq \|\Lambda - P\Lambda P\|_1 + \|P\Lambda P - P\mathcal{E}(P\Lambda P)P\|_1 \leq 2\delta$$

This means that $\|\Lambda - \tilde{\mathcal{E}}(\Lambda)\|_1 \leq 2\delta$. However, $\tilde{\mathcal{E}}$ is also contractible respect to the 1–norm, so

$$\|\Lambda - \tilde{\mathcal{E}}^2(\Lambda)\|_1 \leq \|\Lambda - \tilde{\mathcal{E}}(\Lambda)\|_1 + \|\tilde{\mathcal{E}}(\Lambda) - \tilde{\mathcal{E}}^2(\Lambda)\|_1 \leq 4\delta$$

The result can be obtained by induction. ∎

From now on, we denote the normalized density matrix by ρ, while σ is reserved for its unnormalized counterpart, *i.e.* $\rho = \frac{\sigma}{\mathrm{tr}[\sigma]}$.

Lemma 38 (Distance for unnormalized rdm) *The distance may be bounded by* $\|\rho_A(\Lambda) - \rho_{\tilde{A}}(\Lambda)\|_2 \leq \|\sigma_{A,P}(\tilde{\Lambda}) - \sigma_{\tilde{A}}(\tilde{\Lambda})\|_2 + (2L+3)\delta$, *where the unnormalized density matrix* $\sigma_{\tilde{A}}(\Lambda) = \mathrm{tr}\left[\tilde{\mathcal{E}}^L(\Lambda)\right] \rho_{\tilde{A}}(\Lambda)$ *is generated by* $\tilde{A}_i$ *and*

$$\sigma_{A,P}(\tilde{\Lambda}) = \sum_{\substack{i_1,\ldots,i_L \\ j_1,\ldots,j_L}} \mathrm{tr}\left[P A^\dagger_{j_L} \cdots A^\dagger_{i_1} \tilde{\Lambda} A_{j_1} \cdots A_{j_L} P\right] |i_1 \cdots i_L\rangle\langle j_1 \cdots j_L|$$

is a positive operator. □

Proof By using the triangle inequality and the fact that $\|\cdot\|_1 \leq \|\cdot\|_2$,

$$\begin{aligned}\|\rho_A(\Lambda) - \rho_{\tilde{A}}(\Lambda)\|_2 \leq \|\rho_A(\Lambda) - \sigma_A(\tilde{\Lambda})\|_1 + \\ \|\sigma_A(\tilde{\Lambda}) - \sigma_{A,P}(\tilde{\Lambda})\|_1 + \|\sigma_{A,P}(\tilde{\Lambda}) - \sigma_{\tilde{A}}(\tilde{\Lambda})\|_2 + \|\sigma_{\tilde{A}}(\tilde{\Lambda}) - \rho_{\tilde{A}}(\tilde{\Lambda})\|_1\end{aligned}$$

The first term can be calculated exactly

$$\|\rho_A(\Lambda) - \sigma_A(\tilde{\Lambda})\|_1 = \sum_{i_1,\ldots,i_L} \mathrm{tr}\left[A^\dagger_{i_L} \cdots A^\dagger_{i_1} (\Lambda - \tilde{\Lambda}) A_{i_1} \cdots A_{i_L}\right] = \delta \qquad (9.20)$$

The first equality occurs since the operator is positive and the 1–norm can be replaced by a trace, while the second one takes place because the map is trace–preserving. The second term can be bounded in a similar way, since it is also a positive operator

$$\begin{aligned}\|\sigma_A(\Lambda) - \sigma_{A,P}(\tilde{\Lambda})\|_1 &= \mathrm{tr}\left[P^\perp \sum_{i_1,\ldots,i_L} A^\dagger_{i_L} \cdots A^\dagger_{i_1} \tilde{\Lambda} A_{i_1} \cdots A_{i_L} P^\perp\right] \\ &\leq \delta + \mathrm{tr}\left[P^\perp \sum_{i_2,\ldots,i_L} A^\dagger_{i_L} \cdots A^\dagger_{i_2} \Lambda A_{i_2} \cdots A_{i_L}\right]\end{aligned}$$

This is because $\|\Lambda - \mathcal{E}(\tilde{\Lambda})\|_1 = \|\mathcal{E}(\Lambda - \tilde{\Lambda})\|_1 = \delta$, where it is used that $\mathcal{E}$ is trace–preserving and $\mathcal{E}(\Lambda) = \Lambda$. Therefore, $\|\sigma_A(\Lambda) - \sigma_{A,P}(\tilde{\Lambda})\|_1 \leq \delta + \mathrm{tr}\left[P^\perp \Lambda\right] = 2\delta$.

Finally, the last term can be bounded by using Lemma 37 because

$$\|\sigma_{\tilde{A}}(\tilde{\Lambda}) - \rho_{\tilde{A}}(\tilde{\Lambda})\|_1 = -1 + \mathrm{tr}\left[\tilde{\mathcal{E}}^L(\Lambda)\right] \leq 2\delta L$$

We obtain the result by collecting all the bounds above. ∎

Let us remark that one can easily write

$$\|\sigma_{A,P}(\tilde{\Lambda}) - \sigma_{\tilde{A}}(\tilde{\Lambda})\|_2^2 \leq \Big[\Big(\mathrm{tr}\left[Q(\mathbb{E}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\mathbb{E}^L Q\right] - \mathrm{tr}\left[Q(\mathbb{F}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\mathbb{F}^L Q\right]\Big) + \Big(\mathrm{tr}\left[Q(\tilde{\mathbb{E}}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\tilde{\mathbb{E}}^L Q\right] - \mathrm{tr}\left[Q(\mathbb{F}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\mathbb{F}^L Q\right]\Big)\Big] \quad (9.21)$$

where $Q = P\otimes P$, $\mathbb{E} = \sum_i A_i\otimes\bar{A}_i$, and $\mathbb{F} = (\mathbb{1}\otimes P)\mathbb{E}(\mathbb{1}\otimes P)$.

We have now all the necessary tools to prove the main Theorem which provides the bound for the norm.

Theorem 54 (Upper bound for the distance) *The distance is upper bounded by* $\|\rho_A(\Lambda) - \rho_{\tilde{A}}(\Lambda)\|_2 \leq 2\mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]\sqrt{L}\delta^{1/4} + (2L+3)\delta$. *To obtain an upper–bound for the* 1*–norm, on only has to multiply the RHS by* $\tilde{D}$. □

Proof In order to prove this Theorem, let us start by bounding the term $\mu = \left|\mathrm{tr}\left[Q(\mathbb{E}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\mathbb{E}^L Q\right] - \mathrm{tr}\left[Q(\mathbb{F}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\mathbb{F}^L Q\right]\right|$. This can be done by adding and subtracting terms such that they differ by one projector, *i.e.*

$$\mu \leq \sum_r \left|\mathrm{tr}\left[\mathbb{F}^L Q(\mathbb{F}^\dagger)^r(\mathbb{1}\otimes P^\perp)(\mathbb{E}^\dagger)^{L-r}(\tilde{\Lambda}\otimes\tilde{\Lambda})\right]\right| + \sum_s \left|\mathrm{tr}\left[\mathbb{E}^s(\mathbb{1}\otimes P^\perp)\mathbb{F}^{L-s}Q(\mathbb{E}^\dagger)^L(\tilde{\Lambda}\otimes\tilde{\Lambda})\right]\right| = \sum_r \mu_r + \sum_s \nu_s$$

Let us bound the first family of terms

$$\mu_r = \left|\mathrm{tr}\left[\mathbb{F}^L Q(\mathbb{F}^\dagger)^r(\mathbb{1}\otimes P^\perp)(\mathbb{E}^\dagger)^{L-r}(\tilde{\Lambda}\otimes\tilde{\Lambda})\right]\right|$$

By applying the Cauchy–Schwarz inequality

$$\left|\mathrm{tr}\left[\sum_i A_i B_i\right]\right| \leq \mathrm{tr}\left[\sum_i A_i^\dagger A_i\right]^{\frac{1}{2}} \mathrm{tr}\left[\sum_i B_i B_i^\dagger\right]^{\frac{1}{2}} \quad (9.22)$$

which can be found in [Bha97], and by writing it down explicitly one obtains

$$\mu_r = \Big|\mathrm{tr}\Big[\sum_{\substack{k_1,\ldots,k_L\\ i_1,\ldots,i_r\\ j_1,\ldots,j_{L-r}}} \left(\sqrt{\tilde{\Lambda}}A_{k_1}\cdots A_{k_L}PA_{i_1}^\dagger\cdots A_{i_r}^\dagger A_{j_1}^\dagger\cdots A_{j_{L-r}}^\dagger\tilde{\Lambda}^{1/4}\otimes\tilde{\Lambda}^{1/4}\right) \times \left(\tilde{\Lambda}^{1/4}\otimes\tilde{\Lambda}^{1/4}\tilde{A}_{k_1}\cdots\tilde{A}_{k_L}\tilde{A}_{i_1}^\dagger\cdots\tilde{A}_{i_r}^\dagger P^\perp A_{j_1}^\dagger\cdots A_{j_{L-r}}^\dagger\sqrt{\tilde{\Lambda}}\right)^*\Big]\Big|$$

$$\leq \mathrm{tr}\Big[\sum_{\substack{k_1,\ldots,k_L \\ i_1,\ldots,i_r \\ j_1,\ldots,j_{L-r}}} \tilde{\Lambda}^{1/4} A_{j_{L-r}} \cdots A_{j_1} A_{i_r} \cdots A_{i_1} P A^\dagger_{k_L} \cdots A^\dagger_{k_1} \tilde{\Lambda} \cdot$$

$$\cdot A_{k_1} \cdots A_{k_L} P A^\dagger_{i_1} \cdots A^\dagger_{i_r} A^\dagger_{j_1} \cdots A^\dagger_{j_{L-r}} \tilde{\Lambda}^{1/4} \otimes \tilde{\Lambda}^{1/2} \Big]^{\frac{1}{2}} \times$$

$$\times \mathrm{tr}\Big[\sum_{\substack{k_1,\ldots,k_L \\ i_1,\ldots,i_r \\ j_1,\ldots,j_{L-r}}} \tilde{\Lambda}^{1/2} \otimes \tilde{\Lambda}^{1/4} \tilde{A}_{k_1} \cdots \tilde{A}_{k_L} \tilde{A}^\dagger_{i_1} \cdots \tilde{A}^\dagger_{i_r} P^\perp A^\dagger_{j_1} \cdots A^\dagger_{j_{L-r}} \tilde{\Lambda}$$

$$A_{j_{L-r}} \cdots A_{j_1} P^\perp \tilde{A}_{i_r} \cdots \tilde{A}_{i_1} \tilde{A}^\dagger_{k_L} \cdots \tilde{A}^\dagger_{k_1} \tilde{\Lambda}^{1/4} \Big]^{\frac{1}{2}} .$$

The first term is equal to

$$\mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]^{1/2} \mathrm{tr}\left[P\mathcal{E}^L(\tilde{\Lambda}) P \tilde{\mathcal{E}}^L(\tilde{\Lambda}^{1/2})\right]^{1/2} \leq \mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]$$

The second term is equal to

$$\mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]^{1/2} \mathrm{tr}\left[\tilde{\mathcal{E}}^r\left(P^\perp \mathcal{E}^{L-r}(\tilde{\Lambda}) P^\perp\right) \tilde{\mathcal{E}}^L(\tilde{\Lambda}^{1/2})\right]^{1/2} \leq \delta^{1/2} \mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]$$

where we have used that $\tilde{\Lambda} \leq \Lambda$ and therefore $\mathrm{tr}\left[P^\perp \mathcal{E}^{L-r}(\tilde{\Lambda}) P^\perp\right] \leq \delta$ and that both $\mathcal{E}$ and $\tilde{\mathcal{E}}$ are contractible for the trace norm. Therefore, $\mu_r \leq \mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]^2 \sqrt{\delta}$. The result for ν_s is exactly the same. Therefore, it follows that $\mu \leq 2L \mathrm{tr}\left[\tilde{\Lambda}^{1/2}\right]^2 \sqrt{\delta}$.

The other term can be calculated in the same way, but by replacing $\mathbb{E} \to \mathbb{F}$ and $\mathbb{F} \to \tilde{\mathbb{E}}$, and it gives exactly the same estimate. ∎

Let us remark that the physical dimension does not appear in the bound shown in Theorem 54. Moreover, the dependence on L is linear, instead of exponential, which will turn out to be very relevant in Subsection 9.7.3. We must remark that Theorem 54 provides an upper bound for Schatten's 2–norm, instead of the 1–norm (*cf.* [VC06, Lemma 3]). Obviously, the result for the 1–norm is stronger, but these norms are related by the rank of the operator, that is, in the first term of the inequality in the Theorem 54 one must add a $\tilde{D}^2$ factor. However, for the applications which we consider in the next Subsection, the 2–norm is adequate.

9.7.2 Generic Matrix Product States

We require an additional result about the injectivity length of a random MPS which, together with the bound obtained in the previous Subsection, allows us to prove the relationship between entanglement and long–range interacting Hamiltonians in the following Subsection. Let us start by defining what a *generic* MPS is:

Definition 27 (Generic MPS) We call an MPS **generic** when it is injective, and reaches injectivity in the minimum possible number of steps, *i.e.* $\lfloor \frac{2\log D}{\log d} \rfloor + 1$, where $\lfloor x \rfloor$ denotes the integer part of x. □

The goal in this Subsection is to prove a theorem which ensures that almost every MPS is generic. We provide two proofs, because the first one, even thought it is simpler, requires a background on algebraic geometry, while the second one is based on quantum expanders.

Theorem 55 (Generic interaction length) *Every MPS (with the exception of a zero–measure set) reaches injectivity in the minimal possible region, i.e. it is generic.* □

Proof Since the set of MPS failing this property is clearly a (projective) algebraic manifold in $\mathbb{C}^D \otimes \mathbb{C}^D \otimes \mathbb{C}^d$, standard algebraic geometry [Mum95] guarantees that, either this set is the complete set of MPS or it has a measure zero. It is therefore enough to find *a single* example of an MPS reaching injectivity as fast as possible. This fact has been numerically verified by computing the injectivity length of randomly chosen MPS with several bond dimensions. ■

We next provide a result, based on quantum expanders which is slightly less general than Theorem 55. It is proven in [Has07c] that, for all $d \geq 4$, there exists an hermitian trace–preserving completely positive map

$$\mathcal{E}(X) = \sum_{i=1}^{d} A_i^\dagger X A_i$$

where $A_i \in \mathcal{M}_D$, such that the second largest eigenvalue in absolute value fulfils that $|\lambda_2| \leq \left(\frac{2\sqrt{d-1}}{d}\right)\left(1 + \mathcal{O}\left(\log(D) D^{\frac{-2}{15}}\right)\right)$. By taking the MPS $|\psi\rangle$ generated by the matrices A_i and considering the map

$$\Gamma_n(X) = \sum_{i_1 \cdots i_n} \mathrm{tr}\left[X A_{i_1} \cdots A_{i_n}\right] |i_1 \ldots i_n\rangle$$

we want to show the following modification of Theorem 55:

Theorem 56 (Generic interaction length with QE) *Assuming D sufficiently large, Γ_n is an injective map for*[4]*:*

$$n \geq \left\lceil \frac{8\log(D)}{\log(d)} \right\rceil + 1$$

with $d > 16$. □

This Theorem is a consequence of the following Lemma:

[4] In fact, 8 can be made arbitrarily close to 4 by enlarging d

Lemma 39 (Bound for the second eigenvalue)

$$\sup_{\mathrm{tr}\left[X^\dagger X\right]=1} \left|\Gamma_n(X)^\dagger \Gamma_n(X) - \frac{1}{D}\mathrm{tr}\left[X^\dagger X\right]\right| \leq D|\lambda_2|^n \qquad \square$$

Proof Let us assume $\mathcal{M}_D$ with the usual Hilbert–Schmidt structure, it is easy to see that the LHS is equal to

$$\left\|\Gamma_n^*\Gamma_n - \frac{1}{D}\mathbb{1}\right\|_{\mathrm{op}}$$

for the usual operator norm on the Hilbert space $\mathcal{M}_D$.

Let us denote as usual $\mathbb{E} = \sum_i A_i \otimes \bar{A}_i$ and write the expression in coordinates:

$$\Gamma_n^*\Gamma_n - \frac{1}{D}\mathbb{1} = \sum_{abcd}\left(\langle cd|\,\mathbb{E}^n\,|ab\rangle - \frac{1}{D}\delta_{ab}\delta_{cd}\right)\,|bd\rangle\langle ac|$$

where we have just identified $\mathcal{M}_D = \mathbb{C}^D \otimes \mathbb{C}^D$, and used to the canonical (matrix) basis $|ij\rangle$ there.

As $\|\cdot\|_{op} \leq \|\cdot\|_2 \leq \sqrt{m}\|\cdot\|_{op}$ holds for every operator on an m–dimensional Hilbert space, $\|\cdot\|_2$ being the Hilbert–Schmidt norm, by using the fact that the Hilbert–Schmidt norm is invariant under arbitrary rearrangements of the coordinates, we get that:

$$\left\|\Gamma_n^*\Gamma_n - \frac{1}{D}\mathbb{1}\right\|_{\mathrm{op}} \leq D\left\|\sum_{abcd}\left(\langle cd|\,\mathbb{E}^n\,|ab\rangle - \frac{1}{D}\delta_{ab}\delta_{cd}\right)\,|ab\rangle\langle cd|\right\|_{op} =$$

$$D\|\mathbb{E}^n - \frac{1}{D}\,|\mathbb{1}\rangle\langle\mathbb{1}|\,\|_{op} = D\|\mathbb{E}^n - \mathbb{E}^\infty\|_{op} = D\|\mathcal{E}^n - \mathcal{E}^\infty\|_{op} = D|\lambda_2|^n$$

where, in the last step, the hermiticity of $\mathcal{E}$ has been used, and $|\mathbb{1}\rangle$ denotes the unnormalized vector $\sum_{i=1}^D |ii\rangle$. Now we are in a position to prove the following Theorem: ∎

Proof (Theorem 56) Γ_n must be injective as long as

$$|\lambda_2|^n < \frac{1}{D^2} \qquad (9.23)$$

Otherwise, by taking a (normalized) X such that $\Gamma_n(X) = 0$, we would get a contradiction to Lemma 39. By using the upper bound for $|\lambda_2|$ that we know from [Has07c], $|\lambda_2| \leq \left(\frac{2\sqrt{d-1}}{d}\right)\left(1 + \mathcal{O}\left(\log(D)D^{\frac{-2}{15}}\right)\right)$, it suffices to take n such that:

$$\left(\frac{2\sqrt{d-1}}{d}\right)^n \left(1 + \mathcal{O}\left(\log(D)D^{\frac{-2}{15}}\right)\right)^n < \frac{1}{D^2}$$

By taking logarithms,

$$2\log(D) + n\log\left[\left(\frac{2\sqrt{d-1}}{d}\right)\left(1+\mathcal{O}\left(\log(D)D^{\frac{-2}{15}}\right)\right)\right] < 0$$

which is equivalent to

$$n > \frac{2\log(D)}{\log\left[\left(\frac{d}{2\sqrt{d-1}}\right)\right] - \log\left(1+\mathcal{O}\left(\log(D)D^{\frac{-2}{15}}\right)\right)}$$

It is clear that, by taking D sufficiently large, we can upper–bound the RHS by:

$$\left\lfloor \frac{2\log(D)}{\log\left(\frac{d}{2\sqrt{d-1}}\right)} \right\rfloor + 1$$

which means that:

$$\begin{aligned}\frac{2\log(D)}{\log\left(\frac{d}{2\sqrt{d-1}}\right)} &= \frac{4\log(D)}{2\log(d) - \log(4) - \log(d-1)} \\ &\leq \frac{4K\log(D)}{\log(d)}\end{aligned}$$

as long as $\frac{1}{K} \leq 1 - \frac{2}{\log d}$, which finishes the proof of the Theorem. ∎

9.7.3 Long–range Hamiltonians *vs* entanglement

We show in this Subsection a relationship between the interaction length of a spin Hamiltonian and the entanglement of its ground state, by using the result shown in Theorem 54, which provides an upper–bound for the distance between any state and an MPS of a given bond dimension. The theorem which we prove here states that, if an MPS has small Rényi entropy (a measure of the entanglement in the state), then one cannot find a long–interacting parent Hamiltonian for such state. Let us enunciate it formally.

Theorem 57 (Large–range interaction ⇒ large entanglement) *Let $|\psi_A\rangle$ be a TI–MPS such that, for $\alpha = \frac{1}{6}$, the Rényi entropy of order α [Ŕ61] can be upper–bounded by*

$$S_\alpha(\rho_A^R) \leq \frac{4}{5}\log\epsilon + \frac{1}{10}(L\log d - \log L) - \log\frac{d}{4} \qquad (9.24)$$

where ρ_A^R is the reduced density matrix for a sufficiently large region R. Then, there exists another TI–MPS $|\psi_{\tilde{A}}\rangle$, with bond dimension $\tilde{D}$, showing the following properties:

(i) $|\psi_{\tilde{A}}\rangle$ is the unique ground state of a (gapped frustration–free) Hamiltonian with interaction length L,

(ii) $\|\rho_A^L - \rho_{\tilde{A}}^L\|_1 \leq \epsilon$.

Note that, up to constants, the bound on the Renyi entropy is of the form $L + \log \epsilon$.$_\square$

PROOF Let us call λ_i to the (ordered from the larger to the smaller modulus) eigenvalues of ρ_A^R (which, by Lemma 14, can be taken as close as wanted to $\Lambda \otimes \Lambda$). It is not difficult to see that if we call μ_i to the ordered elements of Λ, then $\sum_{i=\tilde{D}+1}^{\infty} \mu_i \leq \sum_{i=\tilde{D}+1}^{\infty} \lambda_i =: \delta$. By Theorem 54, there exist an MPS with bond dimension $\tilde{D} \leq d^{(L-1)/2}$ such that

$$\begin{aligned}\|\rho_A^L - \rho_{\tilde{A}}^L\|_1 \leq & 2\sqrt{2} d^{L/2} \sqrt{L} \delta^{1/4} + (2L+3)\delta \\ \leq & 4\sqrt{2} d^{L/2} \sqrt{L} \delta^{1/4} =: \epsilon'\end{aligned}$$

since the first term in the sum is clearly larger than the second. Moreover, by using Theorem 55, we can assume that the MPS has already reached injectivity in $L-1$ sites (otherwise, there is other arbitrarily close to it which does it) and it is, therefore, the unique ground state of a (frustration–free gapped) Hamiltonian with interaction length L [PGVWC07]. It only remains to show that $\epsilon' \leq \epsilon$, or equivalently, that $\delta \leq \frac{\epsilon^4}{2^{10} d^{2L} \sqrt{L}}$. In [VC06, Lemma 2], it is shown that:

$$\log(\delta) \leq \frac{1-\alpha}{\alpha} \left(S_\alpha(\rho_A^R) - \log \frac{\tilde{D}}{1-\alpha} \right)$$

By using this together with the fact that $\tilde{D} \geq d^{\frac{(L-2)}{2}}$, it is enough to show that:

$$\begin{aligned}S_\alpha(\rho_A^R) \leq & \frac{4\alpha}{1-\alpha} \log \epsilon + \frac{\log d}{2} \left(1 - \frac{4\alpha}{1-\alpha} \right) L - \\ & - \frac{\alpha}{(1-\alpha)} (10 + \frac{1}{2} \log L) - \log(1-\alpha) - \log d \\ = & \frac{4}{5} \log \epsilon + \frac{1}{10} (L \log d - \log L) - \log \frac{5}{6} - \log \frac{d}{4}\end{aligned}$$

where in the last step we have just replaced $\alpha = \frac{1}{6}$. This is true by the hypothesis on $S_\alpha(\rho_A^R)$. ∎

The Theorem illustrates the physical intuition which states that, if we have a long–range interaction which cannot be faithfully approximated by other short–range interactions, then this should lead to the existence of entanglement among separate regions of the system.

This Section, and especially this very last Subsection, is work in progress, so it could suffer several modifications in its final version. For instance, we could require the existence of a gap of the eigenvalues of the completely positive map in order for this Theorem to be applicable. Thus, we want to give a glimpse of the forthcoming work.

Conclusions and Outlook

We have come to the end of a long journey that has taken us from the local description of one–dimensional quantum states to relevant applications of tensor networks in condensed matter. In this Thesis we have given an overview of the state of the art in the theoretical aspects of tensor networks, especially Matrix Product States and Projected Entangled Pair States.

We have striven to present the new results in a self–contained framework, albeit the space constraints made us skip the proof of some theorems. This is motivated by the observation, while working on the topic, of the lack of literature providing a *panoramic view* on tensor networks. In fact, the interested reader must dive into a pile of articles with totally different —sometimes overtly incompatible— notations, even when they are written by the same authors (the choice of the gauge condition could be an example of this). They must also face up to the challenge of distinguishing between different concepts with the same name, as shown in examples like parent Hamiltonian or translation invariance; or conversely, identical concepts named in several different manners, as happens with the transfer matrix, which is nothing but the matrix representation of the dual channel in quantum information. Last but not least, they must swim in an ocean of vague ideas extracted from condensed matter without a clear and strict definition which is consistent among different works, for which a paradigmatic example is the notion of frustration freeness.

The inconsistencies listed above are a handicap for the communication between the quantum information and condensed matter communities working on tensor networks, even though they are interested in intimately related questions. For instance, the seminal work [FNW92], with a high content of algebra and analysis, is hardly understandable by someone without a certain sophisticated mathematical training. This has as a consequence that the lion's share of the research effort performed by the tensor network community is dedicated to numerical calculations, putting aside any attempt at answering mathematical questions in condensed matter.

Therefore, our overarching ambition in this Thesis has been to collect the most up–to–date fundamental results which make the theory of complete positive maps accessible to the condensed matter community. We additionally attempted to be consistent with the notation inasmuch as possible —as a counterexample, the injectivity length was denoted by $i(A)$ in the definition, but replaced by L_0 when we found it essential for the sake of clarity in the notation— which we hope helps the reader to come into the topic with the least possible effort.

The Thesis may be split into two blocks, the first one —the longest— being devoted to the study of the mathematical properties of tensor networks. One may distinguish there a subsequent subdivision into a first part dedicated to Matrix Product States (MPS) and a second one devoted to Projected Entangled Pair States (PEPS). The former contains new results such as a quantum Wielandt's inequality [SPGWC10], the introduction of kinsfolk Hamiltonians, and the characterization of local symmetries [SWPGC09], among others. The latter includes the proof of the existence of a canonical form for PEPS, the characterization of symmetries for injective PEPS [PGSGG$^+$10], and the extension of several concepts in MPS theory to higher dimensions.

This work, while admittedly abstract and mathematical, has addressed many questions about condensed matter. Therefore, in the second block, we introduce several applications of the theory explained in the first part: in Chapter 8, we focused on finding novel examples of quasi–solvable Hamiltonians showing special features, such as two–body interactions and $SU(2)$ invariance [SWPGC09, TS10]. In Chapter 9, we use the theory of tensor networks to allow for a better grasp of the order parameters for phase transition detection, in particular, string order [PGWS$^+$08]; to relate local properties of the tensor to some of the topological features of the state [PGSGG$^+$10]; to generalize the Lieb–Schultz–Mattis Theorem in several different manners [SWPGC09, PGSGG$^+$10]; to establish a relationship between fractionalization of the magnetization per particle of a quantum state and its entanglement [PGSC$^+$]; and to explain the natural intuition which suggests that Hamiltonians with long–range interactions should yield a ground state with high entanglement [PGSC$^+$], improving, in the process, the upper bound obtained in [VC06] for the distance between any quantum state and an MPS with a given bond dimension.

Our journey through tensor networks has brought us to the cutting edge of this field, and now that it has come to an end, let us foresee the time to come —or at least take a chance at it. However, as Niels Bohr once said, prediction is very difficult, especially about the future, so the following proposals should be understood as collection of ideas whose solution *we* would find particularly interesting.

Let us start with a question which was already pointed out in Section 3.2: the characterization of Hamiltonians which have a ground state with a size–independent MPS representation. We already emphasized that every MPS is the ground state of a strongly frustration–free Hamiltonian (a parent Hamiltonian), so it would only be natural to expect that the converse also holds. Nonetheless, we showed in that Section what seems to be a counter–example to this statement. However, one could possibly relax the conditions for strong frustration freeness, for instance, by asking the system to be frustration–free for an infinite subset of system sizes —with an even number of particles in our example— instead of for every N larger than or equal to a given constant N_0. A better understanding of this question could enlighten us as to the reason why MPS represent so many relevant states in Nature with such a great accuracy [VC06, Has06].

One of the most relevant outstanding questions is the extension of the tensor network theory to infinite bond dimensions, which one might call Operator Product Fields (OPF). The problems arising from this extension are challenging, since the local tensors are no longer matrices, but operators, and the straightforward construction of states by matrix multiplication turns out to be troublesome. A first attempt at solving this issue was made in the pioneering paper [CS10], where the authors replace the Kraus operators with chiral vertex operators of a Conformal Field Theory. Still, this was just the first step and the main question is now which properties of the finite bond–dimensional MPS representations are retained by OPF. One may wonder why this extension is relevant beyond the numerical applications shown in [CS10]. The straightforward answer is that, in case the properties of the MPS were preserved, then the results shown in Chapter 9 would be totally general, which would notably increase the power of the techniques explored in this Thesis.

We already pointed up in this work how injectivity simplifies proofs: when one tries to extend theorems to non–injective states, the complexity of the proofs increases sharply. We already showed that injective MPS are dense in the set of MPS, so it is expectable that many of the properties exhibited by the former, would also be manifested by any MPS. The development of functional analysis– and topology–based techniques which would allow us to extend proofs to any MPS, as well as the determination of their applicability —obviously, not every feature is extendible, merely because there are properties which are *exclusive* to injective MPS, like the existence of a parent Hamiltonian which has such MPS as its only ground state—, would be extremely worthwhile.

If MPS are complex, then PEPS are even more so. Consequently, a relevant issue we must delve into is the characterization of global features in the local tensors which define the PEPS, in a way resembling MPS. In this Thesis we already reviewed the up–to–date advances in this problem, but they are often quite limited: injectivity is only a sufficient condition for the uniqueness of the ground state and it is not related to the existence of a spectral gap; the provided characterization of local symmetries is lattice–dependent and only applies for injective PEPS, etc.

Last but not least, in [VGRC04] Matrix Product Operators were employed in the study of locally describable quantum states at finite temperature. The obstacle which must be tackled is, again, how to implement global properties in the local tensor. Nonetheless, an answer to this question would open a new branch in the study by means of tensor networks of quantum magnetism at non–zero temperature, of the theory of phase transitions, or of statistical mechanics.

One can see that a great deal of research work still remains to be done indeed, on both MPS and PEPS. The questions are undoubtedly very difficult, and perhaps some of the answers to them even unattainable. In any case, they are undeniably interesting and the research effort, which will certainly require an intensive collaborative work between the quantum information and the condensed matter communities, is well worth it.

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