

PHD THESIS

Entanglement in open quantum systems  
and many body simulations by tensor  
networks

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# Chapter 1

## Open Quantum Systems

In physics, the use of the so-called quantum theory becomes necessary when one wishes to investigate Nature's behaviour on submicroscopic scale. This is the case when we take observations on the atomic or sub atomic scale. It is generally believed that we should use quantum theory as the appropriate theory to understand the world of elementary particles such as atoms, molecules and the matter built from these. Although the scales where quantum mechanical effects become relevant ('quantum realm') is considered to be a few hundred nanometers, it may happen that some macroscopic effects can only be fully explained by using quantum mechanics, instead of classical one. While the classical theories (theories used before quantum mechanics) capture many relevant physics of the macroscopic world, they certainly fail in the quantum realm. Although, there are still debates on the interpretation or universality of the theory, it is widely believed that in principle any macroscopic effect can be described if we apply quantum mechanics to the elementary particles of which the objects of interest are made.

In practice, it turns out, however, that the quantum mechanical equations become intractable unless one has only a few particles. That's why people had to look for approximate techniques to study the behaviour of quantum many body systems.

In the following, a brief introduction of the mathematical foundations of quantum mechanics is given. It is not by any means exhaustive but only gives the essential ground for the forthcoming studies of finite dimensional open systems, entanglement detections and interacting spin systems.

## 1.1 Mathematical foundations of quantum mechanics

The theory of quantum mechanics associates a Hilbert space to a physical system being under investigation. The Hilbert space is a vector space endowed by a scalar (or inner) product.

**Definition 1.1.** A complex vector space endowed by a scalar or inner product  $\langle \cdot | \cdot \rangle$  is called a **Hilbert space**. It is also a complete metric space with respect to the distance induced by this scalar product. For example the vector space  $\mathbb{C}^n$  becomes a Hilbert space if we introduce the scalar product of  $x, y \in \mathbb{C}^n$  as

$$\langle x | y \rangle = \sum_{j=1}^n \overline{x_j} y_j.$$

We will later use the notation  $|x\rangle$  for the vector  $x$  (called "ket" by physicist) and  $\langle x|$  ("bra") for its Hermitian conjugate. Clearly,  $\overline{\langle x | y \rangle} = \langle y | x \rangle$ . Note that  $|x\rangle\langle y|$  defines an operator, namely the outer product of  $x$  and  $y$ :  $|x\rangle\langle y|_{ij} = x_i \overline{y_j}$ .

### Postulates of quantum mechanics

1. **System.** Every quantum mechanical systems is associated with a complex separable Hilbert space  $\mathcal{H}$ . The state of the system corresponds to the so-called statistical operator  $\rho$  (or density matrix in the finite dimensional case) acting on  $\mathcal{H}$ . We call  $\rho$  a statistical operator if it is a non-negative, self-adjoint, trace-class operator of trace 1 on  $\mathcal{H}$ . If  $\dim \mathcal{H} < \infty$ , we call  $\rho$  a density matrix if  $\rho \geq 0$  and  $\text{Tr} \rho = 1$ .
2. **Observables** is given by a self-adjoint operator  $A$  acting on  $\mathcal{H}$ . Given the spectral decomposition of  $A$  as

$$A = \int \lambda dE_\lambda,$$

where  $E$  is a projection valued measure (spectral measure) in the subset of  $\mathbb{R}$ . If we measure  $A$  in the state  $\rho$ , the outcome of the measurement fall into the subset  $\Delta \in \mathbb{R}$  with probability  $\text{Tr} E_A(\Delta) \rho$ . Here  $E_A(\Delta)$  denotes the spectral projection belonging to the set  $\Delta$ . This implies  $\langle A \rangle = \text{Tr} \rho A$  for the expectation of  $A$ .

If  $\mathcal{H}$  is finite dimensional then the spectral decomposition reads  $A = \sum_i \lambda_i P_i$ , where  $P_i$  are projectors,  $\lambda_i \in \mathbb{R}$ . Then, if we measure  $A$  in the state  $\phi$ , the outcome of the measurement occurs to be  $\lambda_i$  with probability  $\langle \phi | P_i | \phi \rangle$ . This implies that the expectation value of  $A$  in the state  $\phi$  is  $\langle A \rangle = \langle \phi | A | \phi \rangle = \text{Tr} | \phi \rangle \langle \phi | A$ .

3. **Measurement** is modelled by the set of operators  $V_x \in \mathcal{S}(\mathcal{H})$  for a finite set  $x \in \mathcal{X}$ , such that  $\sum_x V_x^\dagger V_x = \mathbb{1}$ . The possible outcomes corresponds to the set  $\mathcal{X}$ .

If this measurement is performed in a state  $\rho$  then the probability of the outcome  $x$  is  $\text{Tr}V_x\rho V_x^\dagger$ . After the measurement with outcome  $x$ , the state of the system switches to  $\rho_x = \frac{V_x\rho V_x^\dagger}{\text{Tr}V_x\rho V_x^\dagger}$ .

4. **Composite system** consisting of two subsystems corresponding to  $\mathcal{H}_1$  and  $\mathcal{H}_2$  is described by the tensor product Hilbert space  $\mathcal{H}_1 \otimes \mathcal{H}_2$ .

See [1], [2] for references.

### 1.1.1 Examples.

**Example 1.1.** *Hilbert spaces corresponding to physical systems.* A spin of a particle with spin quantum number  $s$  can be associated with the Hilbert space  $\mathcal{H} = \mathbb{C}^{2s+1}$ .

**Example 1.2.** *The position of an electron closed in a three dimensional "box"  $A \subset \mathbb{R}^3$  is written by the functions  $f \in L^2(A)$ , i.e. the functions  $f : A \rightarrow \mathbb{C}$  for which  $\int_{x \in A} |f(x)|^2 dx < \infty$ .*

**Example 1.3.** *Most of the times we use a simplified picture of a complicated system in order to understand some physical phenomena. For example, in the ethylen molecule ( $C_2H_6$ ) there are  $2 \cdot 6 + 6 = 18$  electrons, out of which 6 are valence electrons. Two of them make up the bond between the two carbon atoms. If one of them gets removed, the state of the remaining one can be described by a 2 dimensional Hilbert space  $\mathbb{C}^2$ , to a first, rough approximation. The 2 basis states correspond to the 2 simplified states of this electron: to which carbon atom it belongs to'. Considering its spin as well, we should use the Hilbert space  $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ . If both electrons are present in the bond then the corresponding Hilbert space becomes  $\mathcal{H} \otimes \mathcal{H}$ .*

*Despite the obvious coarseness of this picture, it can be used to explain some energy properties of the ionized ethylen molecule. [3]*

**Example 1.4.** *The dynamics of a system with  $\mathcal{H}$  is described by the self-adjoint Hamilton operator  $H = H^\dagger \in \mathcal{S}(\mathcal{H})$ . For the  $\beta \in \mathbb{R}_+$  inverse temperature one can define the so-called Gibbs state as*

$$\rho_\beta = \frac{\exp -\beta H}{\text{Tr} \exp -\beta H}.$$

*For fixed  $\beta$ , this particular state minimizes the free energy which is a functional of the form*

$$f(\rho_\beta) = \text{Tr} \rho H - \beta^{-1} S(\rho_\beta)$$

*where  $S$  is the von-Neumann entropy:  $S(\rho) = -\text{Tr} \rho \log \rho$ . [4]*

**Definition 1.2. Pure and mixed states** The finite dimensional state  $\rho$  is said to be pure if it is of rank 1, otherwise it is mixed.

This implies that  $\rho$  is pure if and only if  $\rho = \rho^2$ . In this case there exist a vector  $\phi$  for which  $\rho = |\phi\rangle\langle\phi|$ . Sometimes one can check purity by computing (or giving an upper bound for) the quantity  $\text{Tr}\rho^2$ .  $\rho$  is pure if and only if  $\text{Tr}\rho^2 = 1$ , otherwise mixed.

*Remark 1.3.* The set of densities form a convex subset of the complex matrices  $M_n(\mathbb{C})$ . The extremal points are the pure states.

*Remark 1.4.* With the help of the Riesz representation theorem, a quantum state  $\rho \in \mathcal{S}(\mathcal{H})$  can be associated with a positive linear functional of norm 1 on  $\mathcal{S}(\mathcal{H})$  as

$$f_\rho(A) = \text{Tr}\rho A.$$

This makes it possible to define it precisely in the infinite dimensional case. It uses the GelfandNaimark-Segal (GNS) construction in a C\*-algebraic context, see e.g. [http://en.wikipedia.org/wiki/Gelfand-Naimark-Segal\\_construction](http://en.wikipedia.org/wiki/Gelfand-Naimark-Segal_construction) as we will not work within this context.

### Definition 1.5. Partial trace and reduced densities

Consider the composite system  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ , consisting of possibly different Hilbert spaces, and an observable  $A = A^\dagger$  acting only on the first one. Let  $\rho$  be the density on  $\mathcal{H}$ . Then there exists a density operator  $\rho_1 \in \mathcal{S}(\mathcal{H}_1)$  such that

$$\text{Tr}(A \otimes \mathbb{1})\rho = \text{Tr}A\rho_1. \quad (1.1)$$

This is called the reduced density matrix of  $\rho$  into the first subsystem or also first marginal density.

### Proof.

We give a constructive proof. In the two subsystems let us denote the basis states as  $\{e_i\}_i$  and  $\{f_j\}_j$ , respectively. Make the following decompositions

$$\rho = \sum_{ii',jj'} \rho_{ij,i'j'} |e_i f_j\rangle\langle e_{i'} f_{j'}|$$

and

$$A = \sum_{ii'} A_{ii'} |i\rangle\langle i'|.$$

With this,  $(A \otimes \mathbb{1})_{ij,i'j'} = A_{ii'}\delta_{jj'}$  with which we can now write

$$\text{Tr}(A \otimes \mathbb{1})\rho = \sum_{ij} ((A \otimes \mathbb{1})\rho)_{ij,ij} \quad (1.2)$$

$$= \sum_{ij} \sum_{i'j'} A_{ii'}\delta_{jj'}\rho_{i'j',ij} \quad (1.3)$$

$$= \sum_{ii'} \sum_j A_{ii'}\rho_{i'j,ij} \quad (1.4)$$

$$= \sum_{ii'} A_{ii'} \sum_j \rho_{i'j,ij} \quad (1.5)$$

now it's plausible to define  $\rho_1 \in \mathcal{H}_1$  as

$$(\rho_1)_{i'i} = \sum_j \rho_{i'j,ij}.$$

in terms of matrix entries, or in other words

$$\rho_1 = \sum_j \langle f_j | \rho | f_j \rangle \quad (1.6)$$

In fact, plugging this into 1.5 we finally get

$$\text{Tr}(A \otimes \mathbb{1})\rho = \sum_{ii'} A_{ii'}(\rho_1)_{i'i} = \text{Tr} A \rho_1.$$

Note that considering the first reduced density is equivalent of discarding the second subsystem and its computation reduces to ‘tracing out’ the second subsystem. For this reason the operation 1.6 has got its own name: partial trace (over the second Hilbert space). We will simply write

$$\rho_1 = \text{Tr}_2 \rho.$$

This can be generalized straightforwardly for the case when  $\mathcal{H}$  consists of more than two (even countably many) Hilbert spaces.

Observe its similarity with partial integrals for multivariate functions where one ‘integrates out’ the discarded dimensions. Even more straightforward its relation to marginal probability distributions if one makes the analogy between Hilbert spaces and set of events, observables and random variables, probability measures and density matrices, then marginal densities correspond to marginal probabilities.

**Theorem 1.6. *Schmidt decomposition***

*Let  $H_1$  and  $H_2$  be Hilbert spaces of dimensions  $n$  and  $m$  respectively. For any vector  $\phi$  in the tensor product  $H_1 \otimes H_2$ , there exist orthonormal sets  $\{u_1, \dots, u_n\} \subset H_1$  and*

$\{v_1, \dots, v_m\} \subset H_2$  such that

$$\phi = \sum_{k=1}^{m \wedge n} \alpha_k u_k \otimes v_k$$

where the scalars  $\alpha_i$  are non-negative and, as a set, uniquely determined by  $\phi$ .

**Proof** Any vector  $\phi \in \mathcal{H}$  can be written as

$$|\phi\rangle = \sum_{i=1}^n \sum_{j=1}^m C_{ij} |e_i f_j\rangle$$

with the complex,  $n \times m$  matrix  $C$ . For any matrix there exists the singular value decomposition, i.e. can be written as

$$C = USV \tag{1.7}$$

where  $U : n \times n$ ,  $V : m \times m$  complex unitary matrices, and  $S : n \times m$  diagonal matrix with only non-negative entries and  $\text{rank}(S) \leq m \wedge n$ . This follows from the spectral decomposition of the Hermitian matrices  $CC^\dagger$  and  $C^\dagger C$ . Using 1.7 we get

$$|\phi\rangle = \sum_{ijk} (U_{ik} S_{kk} V_{kj}) |e_i, f_j\rangle = \sum_{k=1}^{m \wedge n} S_{kk} \sum_i U_{ik} |e_i\rangle \sum_j V_{kj} |f_j\rangle = \sum_{k=1}^{m \wedge n} S_{kk} |e'_k, f'_k\rangle.$$

Here  $\{e'_k\}$  and  $\{f'_k\}$  form orthonormal sets in  $\mathcal{H}_1$  and in  $\mathcal{H}_2$ , respectively, due to the unitarity of  $U$  and  $V$ .

This simple theorem turns out to be very useful in quantum information because of its role in checking entanglement (see later) and becomes even more crucial in describing ground states of many body systems. (See chapter 4-5.)

## 1.2 Dynamics: Reversibility and Irreversibility

### 1.2.1 Closed systems: Unitary Evolution

Consider a closed system and its density matrix as a function of time  $\rho_t \in \mathcal{D}_{\mathcal{H}}$ , where  $\mathcal{D}_{\mathcal{H}}$  denotes the set of densities on the Hilbert space  $\mathcal{H}$ . The dynamics is governed by the so-called Hamiltonian operator  $H = H^\dagger \in \mathcal{S}(\mathcal{H})$ . The equation of motion reads

$$\partial_t \rho_t = -\frac{i}{\hbar} [H, \rho_t]. \tag{1.8}$$

this is called the Liouville-von Neumann equation. From now on we will set the constant  $\hbar = 1$ .

If  $H$  does not depend on time and given the initial state  $\rho_0$ , it is easy to see that the solution is

$$\rho_t = U_t \rho_0 U_{-t}, \quad U_t = e^{-iHt}. \quad (1.9)$$

Defining the generator  $\mathbb{L}_H$ , the equation of motion reads:

$$\partial_t \rho_t = \mathbb{L}_H[\rho_t]. \quad (1.10)$$

$$\rho_t = e^{t\mathbb{L}_H}[\rho_0] = \mathbb{U}_t[\rho_0]. \quad (1.11)$$

Maps  $\mathbb{U}_t$  form a one parameter unitary group, i.e.  $U_t$  is a family of unitary operators such that  $U_0 = \mathbb{1}$  and

- (i)  $U_t U_s = U_{t+s}$
- (ii)  $t \mapsto U_t \in \mathcal{S}(\mathcal{H})$  is strongly continuous.

This time evolution is reversible since the  $U_t$  unitary operator has the inverse  $U_{-t}$ .

Note that if  $H$  is time dependent, then the evolution still remains unitary, but the unitary propagator is defined by a time ordered integral. If the propagator  $U(s, t)$  corresponds to the evolution of the system between times  $s$  and  $t$  then  $U(s, t)$  form a family of unitary operators such that

- (i)  $U(t, s)U(s, r) = U(t, r)$
- (ii)  $(s, t) \mapsto U(s, t) \in \mathcal{S}(\mathcal{H})$  is strongly continuous.

*Remark 1.7.* The above defined time evolution is called Schroedinger picture, where the observables do not change in time but only the states. Through the expectation values one can define the dual linear map of  $\mathbb{U}_t$  as

$$\text{Tr}[\mathbb{U}_t[\rho_0]X] = \text{Tr}[\rho_0 \mathbb{U}_t^*[X]].$$

Here  $\mathbb{U}_t^*$  makes the observables evolve in time. This evolution is just the backward time evolution of  $\mathbb{U}_t$

$$\mathbb{U}_t^*[X] = U_{-t} X U_t = e^{-t\mathbb{L}_H}[X].$$

This is called the Heisenberg time evolution. [5].

### 1.2.2 Quantum channels

Now suppose that our system of interest  $S$  is immersed into an environment  $E$ , in other words we have to take into account the interactions between them. In this setup, the

evolution of the total system will be unitary and that of our system can be obtained by tracing out the environment

$$\rho_S(t) = \text{Tr}_E(\mathbb{U}_t^{S+E}[\rho_{S+E}(0)]). \quad (1.12)$$

By taking a factorized initial state:  $\rho_{S+E}(0) = \rho_S(0) \otimes \rho_E(0)$

$$\rho_S(t) = \text{Tr}_E(\mathbb{U}_t^{S+E}[\rho_{S+E}(0)]) = \sum_{j,k} \lambda_k \langle j | \mathbb{U}_t^{S+E} | k \rangle \rho_S(0) \langle k | \mathbb{U}_{-t}^{S+E} | j \rangle = \sum_{\alpha} V_{\alpha}(t) \rho_S(0) V_{\alpha}^{\dagger}(t). \quad (1.13)$$

with compound indices  $\alpha$  and where  $|k\rangle$  form the orthonormal basis of eigenvectors of  $\rho_E(0)$  with  $\lambda_k$  being the corresponding eigenvalues. And by the normalization of the trace of a density one gets

$$\sum_{\alpha} V_{\alpha}(t)^{\dagger} V_{\alpha}(t) = \mathbb{1}. \quad (1.14)$$

(1.13) sends a positive matrix to another one, such a map is called positivity preserving or simply positive map, while (1.14) gives a further constraint.

A map satisfying both property is called completely positive which is a necessity of being a quantum channel.

### 1.3 Complete Positivity

**Definition 1.** A linear map  $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$  is completely positive, if and only if  $\Lambda \otimes \mathbb{1}$  is a positive map on  $M_n(\mathbb{C}) \otimes M_m(\mathbb{C})$  for all  $m \geq 1$ , that is for all possible statistical couplings with finite-dimensional ancillas.

**Theorem 1.3.1.** A linear, identity preserving (unital) map  $\Lambda : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$  is completely positive if it can be expressed in the form

$$\Lambda[X] = \sum_{\alpha} V_{\alpha}(t) X V_{\alpha}^{\dagger}(t)$$

and

$$\sum_{\alpha} V_{\alpha}(t)^{\dagger} V_{\alpha}(t) = \mathbb{1}. \quad (1.15)$$

Note that 1.15 is called the Kraus representation and it is not unique.

**Example 1.3.1.** The transposition map on the  $2 \times 2$  matrices is positive but not completely positive.

**Proof.**

Define the transposition operator using the basis  $|0\rangle, |1\rangle$  as

$$\Gamma(|i\rangle\langle j|) = |j\rangle\langle i|, \quad i, j = 0, 1.$$

$\Gamma$  leaves the matrix spectrum unchanged, so it is apparently positive. We choose the matrix  $|\psi\rangle\langle\psi|$ , with  $|\psi\rangle = |00\rangle + |11\rangle$  as a candidate for which  $\mathbb{1} \otimes \Gamma$  is not positive.

$$\mathbb{1} \otimes \Gamma(|\psi\rangle\langle\psi|) = \mathbb{1} \otimes \Gamma\left(\sum_{i,j} |ii\rangle\langle jj|\right) = \sum_{i,j} |ij\rangle\langle ji|.$$

Indeed, this latter matrix

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

is not positive, therefore  $\Gamma$  is not completely positive. This property of the partial transposition will be used to detect entanglement, see in the next Chapter.

### Example 1.3.2. Depolarizing channel

Define the following map  $\mathcal{E} : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ , for  $0 < p < 1$  as

$$\mathcal{E}(\rho) = p\rho + (1-p)\mathbb{1}_n/n$$

## 1.4 Markovian Approximation

With the assumption that initial state of the system and the environment has a tensor product form:  $\rho_S \otimes \rho_E$ , i.e. in  $t = 0$  it is completely decoupled from the environment, the general evolution is given by a completely positive, time depending map. The time evolution can be described by an integro-differential equation and contains memory effects: the noisy effect of  $E$  cannot be read off easily.

However, we can intuitively expect that sufficiently weak couplings between the environment and the system might result in a dynamics when these memory effects are weak enough to discard, and thus the evolution is approximated by a one-parameter semigroup. In fact, under some assumptions, one can derive a time evolution of the form

$$\partial\rho_S(t) = \mathbb{L}[\rho_S(t)] = (\mathbb{L}_H + \mathbb{D})[\rho_S(t)] \tag{1.16}$$

with linear operators where  $\mathbb{L}_H$  describes an effective Hamiltonian and  $\mathbb{D}$  describes the noise

$$\gamma_t = \exp[t(\mathbb{L}_H + \mathbb{D})]$$

### 1.4.1 Generators of the Markovian Dynamics

It turns out that the most general type of Markovian and time-homogeneous master equation describing non-unitary evolution of the density matrix  $\rho$  that is trace preserving and completely positive for any initial condition has the following form:

**Theorem 1.4.1.** Kossakowsky Lindblad equation

Let  $\gamma_t : M_n(\mathbb{C}) \mapsto M_n(\mathbb{C})$ ,  $t \geq 0$ , form a time-continuous semigroup of unital, completely positive linear maps. Then, the most general Markovian, completely positive, trace preserving semigroup has the form  $\gamma_t = \exp[t(\mathbb{L}_H + \mathbb{D})]$  with generators

$$\begin{aligned} \mathbb{L}_H[\rho] &= -i[H, \rho] \\ \mathbb{D}[\rho] &= \sum_{i,j=1}^{n^2-1} C_{ij} (F_i \rho F_j^\dagger - \frac{1}{2} \{F_i^\dagger F_j, \rho\}). \end{aligned}$$

with  $H = H^\dagger$  effective Hamiltonian, the so-called Kossakowski matrix  $C$  being positive definite, and the set of operators  $\{F_i\}_i^{n^2}$  such that  $F_{n^2} = \mathbb{1}_n/\sqrt{n}$  and  $\text{Tr}(F_j F_k^\dagger) = \delta_{jk}$  for  $0 \leq j, k \leq n^2$  and .

For the derivation of the Markovian generators in the weak coupling limit, and an exhaustive introduction to the open systems see e.g. [5] or [6].

## Chapter 2

# Entanglement Generation

### 2.1 Entanglement

#### Definition 2. Two party entanglement

Consider the set of densities on the tensor product Hilbert space:  $\mathcal{S}(S_1 \otimes S_2)$ . All the states  $\rho \in \mathcal{S}$  which can be written as a convex combination of product states, so

$$\rho = \sum_i \lambda_{ij} \rho_i^1 \otimes \rho_j^2 \quad \sum_{i,j} \lambda_{i,j} = 1 \quad \lambda_{ij} \geq 0 \quad (2.1)$$

are called separable, otherwise they are called entangled.

**Remark 2.1.1.** The definition of a fully separable state naturally arises from that of the two party case. If  $\rho \in \mathcal{S}(S_1 \otimes \dots \otimes S_n)$  is a state over an  $n \leq \infty$  fold tensor product (for example describes an  $n$  particle state) then we call it fully separable if it is a convex combination of  $n$  fold product states

$$\rho = \sum_{i_1 \dots i_n} \lambda_i \rho_{i_1}^1 \otimes \dots \otimes \rho_{i_n}^n$$
$$i = (i_1, i_2, \dots, i_n) \quad \sum_i \lambda_i = 1 \quad \lambda_i \geq 0.$$

If such a decomposition does not exist then  $\rho$  is entangled.

**Remark 2.1.2.** Having  $2 < n$  parties one has more possibilities regarding separability. We can select two subspaces of the state Hilbert space and consider the separability only between these subspaces. For example having three parties:  $\rho \in \mathcal{S}(S_1 \otimes S_2 \otimes S_3)$  we can group together the first two spaces. So if  $\rho_{12} \in \mathcal{S}(S_1 \otimes S_2)$ ,  $\rho_3 \in \mathcal{S}(S_3)$  and if  $\rho = \rho_{12} \otimes \rho_3$  then the first two parties are separable from the third one, however  $\rho_{12}$  can be entangled, so the whole state  $\rho$  is not fully separable over the three parties.

**Remark 2.1.3.** The set of separable states form a closed convex subset of the state-space.

**Example 2.1.1.** Bell states

On two subsystems  $A$  and  $B$  consider the states:

$$|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B + |1\rangle_A \otimes |1\rangle_B)$$

$$|\Phi^-\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |0\rangle_B - |1\rangle_A \otimes |1\rangle_B)$$

$$|\Psi^+\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B + |1\rangle_A \otimes |0\rangle_B)$$

$$|\Psi^-\rangle = \frac{1}{\sqrt{2}}(|0\rangle_A \otimes |1\rangle_B - |1\rangle_A \otimes |0\rangle_B).$$

Note that local unitary transformations preserves separability, hence entanglement is independent of the selection of the local basis, it's a real feature of a quantum state.

## 2.2 Entanglement Detection

One sufficient test to detect entanglement can be the use of a non positive map which however preserves the positivity of all the separable states. To construct one as an example for the space  $\mathcal{S}(S_1 \otimes S_1)$  consider the positive map  $\Lambda : \mathcal{S}(S_1) \mapsto \mathcal{S}(S_2)$ . If it does not remain positive when extending to  $\mathcal{S}$  so if  $\Lambda \otimes \mathbb{1}$  is not positive any more (implying that  $\Lambda$  is not completely positive) then we are done since it sends all separable states to positive ones

$$(\Lambda \otimes \mathbb{1})[\rho] = \sum_i \lambda_{ij} \Lambda[\rho_i^1] \otimes \rho_j^2 \geq 0$$

but since it's not completely positive there exists at least one state  $\rho$  for which we get a non positive output, meaning that the input was entangled. In this case  $\Lambda$  is called an entanglement detector for the state  $\rho$ . Note that the above method works for any parties but in general it's only a sufficient and not a necessary condition.

It happens that taking the map  $\Lambda$  the matrix transposition fulfills then the above statements. Horodecki has shown in which case it is also a necessary condition.

**Remark 2.2.1.** Entanglement detection for pure states is much more easier. Consider the pure state  $|\Psi\rangle\langle\Psi|$  and for a sake of simplicity assume a bipartite system, (however the idea works for any number of subsystems) and suppose we have a decomposition

$$|\Psi\rangle\langle\Psi| = \sum_i \lambda_i \rho_i^1 \otimes \rho_i^2$$

and use the spectral decomposition of the densities  $\rho_i^1, \rho_i^2$  to write it as a convex combination of projectors

$$|\Psi\rangle\langle\Psi| = \sum_i \alpha_i P_i^1 \otimes Q_i^2.$$

Since  $|\Psi\rangle\langle\Psi|$  has rank 1, the above sum has to be trivial so a pure state is either a product state itself or otherwise entangled.

**Example 2.2.1.** Entangled state remaining positive under partial transposition. See e.g. in the paper [7].

**Theorem 2.2.1.** Horodecki criterion for entanglement

Consider a bipartite system  $S_1 \otimes S_2$ , with  $S_1$  a 2-level system and  $S_2$  either a 2-level or a 3-level system; a state  $\rho \in \mathcal{S}(S_1 + S_2)$  is entangled if and only if  $T_2 \otimes \mathbb{1}_2[\rho]$ , respectively  $T_2 \otimes \mathbb{1}_3[\rho]$ , is not positive.

Concurrence.

Having a density  $\rho$  on a 2-dimensional bipartite system, define the following quantity

$$R \equiv \rho \sigma_2 \otimes \sigma_2 \bar{\rho} \sigma_2 \otimes \sigma_2 \quad (2.2)$$

this matrix turns out to be positive and let  $R_1, R_2, R_3, R_4$  are the square roots of its eigenvalues in decreasing order.

**Theorem 2.2.2.** A state  $\rho \in M_2(\mathbb{C}) \otimes M_2(\mathbb{C})$  is entangled if and only if its so-called concurrence

$$C(\rho) \equiv \max\{R_1 - R_2 - R_3 - R_4\}$$

is strictly positive.

## 2.3 Entanglement Generation in Noisy Environment

In this section we will consider a system  $S$  composed of two initially separable qubits immersed in a common external bath  $E$  with which they weakly interact, but not directly interacting between each other (Ref., pages 3124-3126); thus the total Hamiltonian is  $H = H_1 + H_2 + H_B + H_I$ , where  $H_1, H_2$  and  $H_B$  are Hamiltonians pertaining to the first and second qubit, respectively the bath within which they are immersed, while the interaction Hamiltonian is given by  $H_I = \sum_{i=1}^3 (\sigma_i \otimes \mathbb{1}) \otimes B_i^{(1)} + (\mathbb{1} \otimes \sigma_i) \otimes B_i^{(2)}$  with  $\mathbb{1}$  the identity  $2 \times 2$  matrix and  $B_i^{(a)}, a = 1, 2, i = 1, 2, 3$  bath operators that describe the interaction with the two qubits. In the following, we shall use the convenient notation  $\sigma_i^{(1)} := \sigma_i \otimes \mathbb{1}$  and  $\sigma_i^{(2)} := \mathbb{1} \otimes \sigma_i$ . By means of standard weak coupling limit techniques,

the reduced dynamics of  $S$  is given by the Master equation

$$\partial_t \rho_t = \mathbb{L}_H[\rho_t] + \mathbb{D}[\rho_t] = -i[H_{eff}, \rho(t)] + \mathbb{D}[\rho(t)] \quad (2.3)$$

where  $H_{eff} = H^{(1)} + H^{(2)} + H^{(12)}$  with  $H^{(a)} = \sum_{i=1}^3 h_i^{(a)} \sigma_i^{(a)}$ ,  $h_i^{(a)} \in \mathbb{R}$ ,  $a = 1, 2$  are the Hamiltonians acting on the two qubits independently and their bath mediated interaction is described by

$$H^{(12)} = \sum_{i,j=1}^3 h_{ij}^{(12)} (\sigma_i \otimes \sigma_j), \quad h_{ij}^{(12)} \in \mathbb{R}$$

while

$$\begin{aligned} \mathbb{D}[\rho] = & \sum_{i,j=1}^3 (A_{ij} [\sigma_j^{(1)} \rho \sigma_i^{(1)} - \frac{1}{2} \{\sigma_i^{(1)} \sigma_j^{(1)}, \rho\}] + \\ & C_{ij} [\sigma_j^{(2)} \rho \sigma_i^{(2)} - \frac{1}{2} \{\sigma_i^{(2)} \sigma_j^{(2)}, \rho\}] + \\ & B_{ij} [\sigma_j^{(1)} \rho \sigma_i^{(2)} - \frac{1}{2} \{\sigma_i^{(2)} \sigma_j^{(1)}, \rho\}] + \\ & \overline{B}_{ji} [\sigma_j^{(2)} \rho \sigma_i^{(1)} - \frac{1}{2} \{\sigma_i^{(1)} \sigma_j^{(2)}, \rho\}]) \end{aligned}$$

is a Kossakowski-Lindblad contribution describing dissipation and noise. The first two lines described the dissipative noise affecting separately the first and the second qubits, respectively, while the last two lines represent dissipation which can correlate the two subsystems if  $B \neq 0$ . The  $3 \times 3$  matrices of the coefficients  $A = A^\dagger$ ,  $C = C^\dagger$  and  $B$  form the so-called Kossakowski matrix

$$K = \begin{bmatrix} A & B \\ B^\dagger & C \end{bmatrix}. \quad (2.4)$$

**Theorem 2.1.** *The semigroup  $\{\gamma_t\}_{t \geq 0}$  consist of completely positive maps if and only if the Kossakowski matrix is positive definite.*

### 2.3.1 Condition for Entanglement Production

We are provided two qubits uniformly interacting with the bath:

$$K = \begin{bmatrix} A & B \\ B^\dagger & A \end{bmatrix}. \quad (2.5)$$

Assume that we prepare the system in a separable state :

$$\rho(0) = |\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi| \quad (2.6)$$

Now, we want to find a criterion for the entanglement creation of the dynamics. We can use Horodecki's criterion: If at any time  $t > 0$ , the partial transpose of  $\rho_t$  becomes non positive it implies that  $\rho_t$  is entangled. Perform a partial transposition on the second qubit and denote the result by  $\tilde{\rho}(t)$  as well as on both sides of the Lindblad equation

$$\partial\tilde{\rho}(t) = -i[\tilde{H}_{eff}, \tilde{\rho}(t)] + \tilde{\mathbb{D}}[\tilde{\rho}(t)] \quad (2.7)$$

where the structure of the equation remains unchanged but of course we get a new Hamiltonian and dissipative part, namely

$$\tilde{H}_{eff} = H_{eff}^{(1)} + \mathbb{1} \otimes (EH^{(2)}) \cdot \sigma + \sum_{i,j=1}^3 \mathbf{Im}(\mathbf{BE})_{ij} (\sigma_i \otimes \sigma_j) \quad (2.8)$$

where  $E = \text{diag}(-1, 1, -1)$ . The dissipative term has the same Lindbladian form but with new Kossakowsky matrix

$$\tilde{K} = \mathcal{E}K'\mathcal{E}^+ \quad (2.9)$$

$$\tilde{K} = \begin{bmatrix} A & \text{Re}(B) + iH^{(12)} \\ \text{Re}(B^T) - iH^{(12)T} & C^T \end{bmatrix}. \quad (2.10)$$

$$\mathcal{E} = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & E \end{bmatrix}. \quad (2.11)$$

Now we can for example state that if  $\tilde{K} \geq 0$  then the new dynamics is completely positive, implying that  $\tilde{\rho}(t)$  remains positive for all time so  $\rho(t)$  also remains surely separable at any time. In other words, entanglement production requires  $\tilde{K}$  not to be positive semi definite.

**Example 2.3.1.** Consider the Kossakowsky matrix

$$K = \begin{bmatrix} A & A \\ A & A \end{bmatrix}. \quad (2.12)$$

with

$$A = A^\dagger = \begin{bmatrix} 1 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & x \end{bmatrix} \quad (2.13)$$

with  $x \geq 1$  so that  $K \geq 0$ . The choice  $A = B = C$  describes for example a special case of collective resonance fluorescence. See Ref.

After performing partial transpose we substitute  $K$  with

$$\tilde{K} = \begin{bmatrix} A & -\text{Re}(A) \\ -\text{Re}(A^T) & A^T \end{bmatrix} \quad (2.14)$$

can be verified to be not positive thus proving that pure dissipation is in fact able to generate entanglement.

### 2.3.2 Necessary and sufficient condition

The above condition is clearly only sufficient for entanglement production, but not a necessary one. For a circumspect study one has to look at the positivity of  $\tilde{\rho}(t)$ . As soon as it is not positive any more the state gets entangled. If it happens there exist a vector  $\phi$  and a time  $t^* > 0$  for which the time dependent quantity

$$f_\phi(t) = \langle \phi | \tilde{\rho}(t) | \phi \rangle \quad (2.15)$$

gets negative. Assuming a separable initial state  $f_\phi(0) > 0$  so in case of entanglement creation, by the continuity of  $t \mapsto f_\phi(t)$  there should exist a state  $\phi$  and a time  $t^* > 0$  for which

$$f_\phi(t^*) = 0 \quad (2.16)$$

and

$$\partial_t f_\phi(t^*) < 0. \quad (2.17)$$

**Remark 2.3.1.** The above criterium is clearly a sufficient condition. In the case when the first is true but  $\partial_t f_\phi(t^*) = 0$  one has to investigate higher order derivatives as well.

Without loss of generality, one can set  $t^* = 0$  and, as already remarked, restrict the attention to factorized pure initial states.

**Proposition 2.2.** *The semigroup  $\gamma_t : M_4(\mathbb{C}) \mapsto M_4(\mathbb{C})$  is entangling if there exist a separable initial projector  $Q \in M_4(\mathbb{C})$  and a vector  $\phi \in \mathbb{C}^4$  such that:*

$$\langle \phi | \tilde{Q} | \phi \rangle = 0 \quad \text{and} \quad \langle \phi | \tilde{\mathbb{L}}[\tilde{Q}] | \phi \rangle < 0. \quad (2.18)$$

*Vice versa, the semigroup  $\gamma_t$  cannot be entangling if*

$$\langle \phi | \tilde{Q} | \phi \rangle = 0 \quad \text{and} \quad \langle \phi | \tilde{\mathbb{L}}[\tilde{Q}] | \phi \rangle > 0 \quad (2.19)$$

*for all  $\phi \in \mathbb{C}^4$  and projectors  $Q \in M_4(\mathbb{C})$ .*

**Proof.** It follows easily from the fact that as stated before,  $\gamma_t$  is entangling if and only if there exist  $Q$  and  $t > 0$  such that  $\langle \phi | \tilde{\mathbb{L}}[\tilde{Q}] | \phi \rangle < 0$ . For the details see [8].

Now we want to establish a concrete condition of entanglement production in terms of the sub matrices of the Kossakowsky matrix. So assume that we are given the two qubit

state (projector)

$$Q = |\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi|$$

$$|\psi\rangle, |\varphi\rangle \in \mathbb{C}^2.$$

Latter proposition tells us that we can concentrate on the mean values of  $\tilde{\mathbb{L}}[\tilde{Q}]$  with respect to  $\gamma_t : M_4(\mathbb{C})$  that belong to the subspace orthogonal to  $\tilde{Q}$ . Therefore, we can restrict our attention upon the matrix  $M = \tilde{Q}^\perp \tilde{\mathbb{L}}[\tilde{Q}] \tilde{Q}^\perp$ , where  $\tilde{Q}^\perp := I - \tilde{Q}$ , that we will represent with respect to the following orthogonal basis.

$$\begin{aligned} |\Psi_1\rangle &:= |\psi\rangle \otimes |\bar{\varphi}\rangle, & |\Psi_2\rangle &:= |\psi\rangle \otimes |\bar{\varphi}_\perp\rangle \\ |\Psi_3\rangle &:= |\psi_\perp\rangle \otimes |\bar{\varphi}\rangle, & |\Psi_4\rangle &:= |\psi_\perp\rangle \otimes |\bar{\varphi}_\perp\rangle. \end{aligned}$$

The conjugates of the second factor come from the partial transposition and  $\varphi_\perp$  is an orthogonal unit vector to  $\varphi$ . In this basis:  $M_{ij} = \langle\psi_i|\tilde{\mathbb{L}}[\tilde{Q}|\psi_j\rangle$ . It happens that only the following four entries are non-zeros

$$M_{22} = \langle v|C^T|v\rangle, \quad M_{23} = \overline{M_{32}} = \langle i|(h^{12})^T + \Re(B)|u\rangle, \quad M_{33} = \langle u|A|u\rangle.$$

with the definitions of the  $\mathbb{C}^3$  vectors

$$u_i := \langle\psi_i|\sigma_i|\psi_\perp\rangle, \quad v_i := \langle\varphi_i|\sigma_i|\varphi_\perp\rangle.$$

Then it suffices to study the positivity of the essentially  $2 \times 2$  matrix  $M$ .

1. If there exist  $\varphi, \psi$  such that  $\det(M) < 0$  then the semigroup is entangling.
2. If  $\det(M) > 0$  for all  $\varphi, \psi$  then the semigroup is non entangling.
3. If  $\det(M) = 0$ , one has to check higher than first order terms in the small  $t > 0$  expansion of  $f(t) = \langle\phi|\tilde{\gamma}_t[\tilde{Q}|\phi\rangle$ .

### 2.3.3 Adding more qubits enhances the entangling capacity of the bath

Assume we are provided 4 qubits immersed in a common bath and their states evolve according to a purely dissipative generator as follows

$$\mathbb{L}[\rho] = \sum_{p=1}^4 \sum_{i,j=1}^3 (A_{ij} [\sigma_j^{(p)} \rho \sigma_i^{(p)} - \frac{1}{2} \{\sigma_i^{(p)} \sigma_j^{(p)}, \rho\}]) \quad (2.20)$$

$$+ \sum_{p,q=1}^4 \sum_{i,j=1}^3 (C_{ij} [\sigma_j^{(p)} \rho \sigma_i^{(q)} - \frac{1}{2} \{\sigma_i^{(q)} \sigma_j^{(p)}, \rho\}]) + \quad (2.21)$$

$$(2.22)$$

This depicts a dissipative environment which acts uniformly on each qubit with the Kossakowsky matrix

$$K_4 = \begin{bmatrix} A & C & C & C \\ C & A & C & C \\ C & C & A & C \\ C & C & C & A \end{bmatrix}.$$

Now, if we put just , say 2 qubits to the same environment, the Kossakowsky matrix would be

$$K_2 = \begin{bmatrix} A & C \\ C & A \end{bmatrix}.$$

This can be verified for example by tracing out two qubits out of the original four. We will show that there exists an environment which does not generate entanglement if we immerse two qubits into it, however, by putting other two qubits into this bath there will be entanglement generation between pairs of qubits. We give a concrete example demonstrating that the conditions for a non-entangling semigroup is fulfilled but fail if we examine entanglement between pairs of qubits in case of four qubits in total. Set

$$A = \begin{bmatrix} 1 & iz & 0 \\ -iz & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad C = \begin{bmatrix} x & 0 & 0 \\ 0 & -x & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

with  $x, z \in \mathbb{R}$ ,  $0 \leq x, z \leq 1$ .

$K_4$  must be postive semi-definite which implies

$$z^2 + 9x^2 \leq 1 \quad (2.23)$$

as its non-zero eigenvalues are  $1 \pm \sqrt{x^2 + z^2}$  and  $1 \pm \sqrt{x^2 + 9z^2}$ . Clearly  $0 \leq K_4$  involves  $0 \leq K_2$ . The  $2 \times 2$  matrix to be verified happens to be

$$M_2 = 2 \begin{bmatrix} 1+z & x \\ x & 1+z \end{bmatrix}$$

if we have only 2 qubits. Therefore, entanglement generation does not occur if

$$(1+z)^2 > x^2 \tag{2.24}$$

If we have 4 qubits then the matrix of interest is 6 dimensional, but it reduces to the  $4 \times 4$  one

$$M_4 = \begin{bmatrix} 1+z & 0 & x & x \\ 0 & 1+z & x & x \\ x & x & 1+z & 0 \\ x & x & 0 & 1+z \end{bmatrix}.$$

It can be seen that under the conditions 3.29 and 2.24 there exist  $(x, z)$  such that  $M_4$  is not positive semi-definite. It is because the third principal minor of  $M_4$ , namely the determinant

$$\begin{vmatrix} 1+z & 0 & x \\ 0 & 1+z & x \\ x & x & 1+z \end{vmatrix} = 8(1+z)((1+z)^2 - 2x^2)$$

is negative if

$$(1+z)^2 \leq 2x^2. \tag{2.25}$$

In fact, there is a region in the plane where all the conditions 3.29 2.24 and 2.25 are fulfilled. Mathematically it is because the number of principal minors increases with the dimension of the parties, for more than two qubits a richer variety of noise-induced entanglement is available. As an example, we provided a purely dissipative time evolution that entangles two subsystems, each consisting of two qubits, without entangling any two single qubits.

For the original paper and other details of the calculations, see [8].

## Chapter 3

# Asymptotic States

In the following we shall study an open quantum system of three qubits in weak interaction with their environment  $E$ . We shall denote by  $M$  the algebra of  $8 \times 8$  matrices  $x \in M_8(\mathbb{C})$  and by  $\rho \in M$  the positive matrices of trace 1 that describe the states of  $S$  and by  $\mathcal{S}(M)$  the convex set of all states. For sake of simplicity, we shall sometimes write  $\rho(x)$  for the expectation values  $\text{Tr}(\rho x)$ ; further, by  $x^{(1)}, y^{(2)}, z^{(3)}$ , respectively  $\rho_1^{(1)}, \rho_2^{(2)}, \rho_3^{(3)}$ , we will denote the local one-qubit observables  $x \otimes \mathbb{1} \otimes \mathbb{1}$ ,  $\mathbb{1} \otimes y \otimes \mathbb{1}$ ,  $\mathbb{1} \otimes \mathbb{1} \otimes z$ , respectively the one-qubit states  $\rho_1 \otimes \mathbb{1} \otimes \mathbb{1}$ ,  $\mathbb{1} \otimes \rho_2 \otimes \mathbb{1}$  and  $\mathbb{1} \otimes \mathbb{1} \otimes \rho_3$ .

In the present case of three qubits, we shall concretely study the following time-evolution equation,

$$\partial_t \rho_t = -i \left[ \sum_{a=1}^3 \frac{\omega_a}{2} \sigma_3^{(a)}, \rho_t \right] + \sum_{\substack{a,b=1 \\ i,j=1}}^3 C_{ij}^{(ab)} \left( \sigma_i^{(a)} \rho_t \sigma_j^{(b)} - \frac{1}{2} \left\{ \sigma_j^{(b)} \sigma_i^{(a)}, \rho_t \right\} \right) = L[\rho_t], \quad (3.1)$$

where  $\sigma_i^{(a)}$  is the  $i$ -th Pauli matrix of the  $a$ -th qubit, and the coefficients  $C_{ij}^{(ab)}$  form a  $9 \times 9$  positive matrix, the so-called Kossakowski matrix:

$$0 \leq K = \begin{pmatrix} C^{(11)} & C^{(12)} & C^{(13)} \\ (C^{(12)})^\dagger & C^{(22)} & C^{(23)} \\ (C^{(13)})^\dagger & (C^{(23)})^\dagger & C^{(33)} \end{pmatrix}, \quad C^{(ab)} = [C_{ij}^{(ab)}]_{i,j=1}^3. \quad (3.2)$$

The analytic solution of (3.1) can in general be addressed only numerically; we shall instead consider a simpler class of master equations amenable to a partially analytic study. Notice that, by taking the trace of the generator  $L$  in (3.1) with respect to any single qubit, one gets the generator of a master equation relative to the other two qubits;

thus, by choosing  $\omega_1 = \omega_2 = \omega_3 = \omega$  and

$$C^{(11)} = C^{(22)} = C^{(33)} = A ; C^{(12)} = C^{(21)} = C^{(13)} = C^{(31)} = C^{(23)} = C^{(32)} = B ,$$

one obtains a highly symmetric generator with Kossakowski matrix

$$K = \begin{pmatrix} A & B & B \\ B^\dagger & A & B \\ B^\dagger & B^\dagger & A \end{pmatrix} , \quad (3.3)$$

such that any pair of qubits is affected in the same way by the presence of the environment. As apparent from (3.3), the matrix  $A$  governs the dissipative reduced dynamics of each one of the qubits, while  $B$  rules the dissipative statistical coupling of pairs of different qubits. However, in the following, we shall further restrict the case to master equations where one and two-qubit terms are the same and choose

$$A = B = \begin{pmatrix} a & ib & 0 \\ -ib & a & 0 \\ 0 & 0 & c \end{pmatrix} , \quad c \geq 0 , 0 \leq |b| < a . \quad (3.4)$$

Then, the Kossakowski matrix (3.2) reads  $K = 3A \otimes P$ , where  $P$  projects onto the vector  $(1, 1, 1)/\sqrt{3}$  and  $A \geq 0$ . The resulting master equation for the states (Schrödinger time-evolution) and its dual for the system operators (Heisenberg time-evolution) can conveniently be recast as

$$\partial_t \rho_t = -i \frac{\omega}{2} [S_3, \rho_t] + \sum_{i,j=1}^3 A_{ij} \left( S_i \rho_t S_j - \frac{1}{2} \{S_j S_i, \rho_t\} \right) = L[\rho_t] \quad (3.5)$$

$$\partial_t x_t = i \frac{\omega}{2} [S_3, x_t] + \sum_{i,j=1}^3 A_{ij} \left( S_j x_t S_i - \frac{1}{2} \{S_j S_i, x_t\} \right) = \hat{L}[x_t] , \quad (3.6)$$

in terms of global spin operators

$$S_{1,2,3} = \sum_{a=1}^3 \sigma_{1,2,3}^{(a)} = \sigma_{1,2,3}^{(1)} + \sigma_{1,2,3}^{(2)} + \sigma_{1,2,3}^{(3)} . \quad (3.7)$$

*Remark 3.1.* For three qubits ( $n = 3$ ), a master equation of the form

$$\begin{aligned} \partial_t \rho_t &= -i \frac{\omega}{2} [S_3, \rho_t] + \sum_{a=1}^n \sum_{i,j=1}^3 A_{ij} \left( \sigma_i^{(a)} \rho_t \sigma_j^{(a)} - \frac{1}{2} \left\{ \sigma_j^{(a)} \sigma_i^{(a)}, \rho_t \right\} \right) \\ &+ \sum_{a \neq b=1}^n \sum_{i,j=1}^3 B_{ij} \left( \sigma_i^{(a)} \rho_t \sigma_j^{(b)} - \frac{1}{2} \left\{ \sigma_j^{(b)} \sigma_i^{(a)}, \rho_t \right\} \right), \end{aligned}$$

may have direct experimental implication in certain realizations of the driven cavity array proposed in [10]. For  $n = 2$ , the above equation have been derived in a physical scenario where the qubits are at a distance from each and immersed in a scalar Bose field in thermal equilibrium [21], while a master equation of the form

$$\partial_t \rho_t = -i \frac{\omega}{2} [S_3, \rho_t] + \sum_{a,b=1}^3 \sum_{i,j=1}^3 A_{ij} \left( \sigma_i^{(a)} \rho_t \sigma_j^{(b)} - \frac{1}{2} \left\{ \sigma_j^{(b)} \sigma_i^{(a)}, \rho_t \right\} \right),$$

corresponds to two qubit immersed in an environment described by a thermal, scalar Bose field when the spatial distance among the qubits is negligible [12].

### 3.0.4 Identifying the asymptotic states

The forthcoming general observations lead essential results for the search of the asymptotic states of a completely positive dynamics.

Let  $\mathcal{S}_\gamma = \{\rho \in \mathcal{S}(M) : \gamma_t[\rho] = \rho \ \forall t \geq 0\}$  denote the set of stationary states of the quantum dynamical semigroup  $\{\gamma_t\}_{t \geq 0}$ , and by  $M_\gamma = \{x \in M : \hat{\gamma}_t[x] = x \ \forall t \geq 0\}$  the set of invariant operators.

From [14] one knows that, if a full-rank stationary state  $\rho_\infty$  exists, then

First of all, in finite dimension,  $\mathcal{S}_\gamma$  is never empty; indeed, from the subset of finite time-averages,

$$\mathcal{S}(M) \ni \rho_T = \frac{1}{T} \int_0^T dt \gamma_t[\rho], \quad T > 0, \quad \rho \in \mathcal{S}(M), \quad (3.8)$$

one can always extract convergent sequences  $\{\rho_{T_n}\}_{n \in \mathbb{N}}$ , for instance with respect to the trace-norm  $\|x\| = \text{Tr} \sqrt{x^\dagger x}$ . One can simply show that for any positive numbers  $S > 0$  and  $\epsilon > 0$  there exist a large enough  $T$  such that  $|\rho_{T+S} - \rho_T| < \epsilon$ , so the series of  $\rho_T$  is Cauchy. Then, any limit point  $\rho_\infty = \lim_{n \rightarrow +\infty} \rho_{T_n}$ , provides a stationary state.

Then, one starts by looking at the time-evolution of operators (Heisenberg picture) and to the Kraus form of the time-evolution equation (3.6):

$$\partial_t x_t = i \frac{\omega}{2} [S_3, x_t] + \sum_{i=1}^3 V_i^\dagger x_t V_i - \frac{1}{2} \{V_i^\dagger V_i, x_t\}. \quad (3.9)$$

This form can be obtained always, if all the submatrices of  $K$  are the same  $A$ . If we restrict ourselves to the special form 3.4 then the operators  $V_i$  are obtained by diagonalizing the  $2 \times 2$  matrix in the upper left corner of  $A$  in (3.4); concretely, in terms of the spin operators  $S_i$  in (3.7),

$$V_{1,2}^\dagger = \sqrt{2(a \mp b)} \frac{S_1 \mp i S_2}{2}, \quad V_3 = \sqrt{c} S_3. \quad (3.10)$$

The main point is that, if there exist a full-rank stationary state  $\rho_\infty$  for the master equation of a finite level system, then [13]

1. the subset of time-invariant matrices  $M_\gamma = \{x \in M : \hat{\gamma}_t[x] = x\}$  is a  $C^*$  sub-algebra of  $M$ , that is  $\hat{\gamma}_y[x^\dagger] = x^\dagger$  and also  $\hat{\gamma}[x^\dagger x] = x^\dagger x$ .
2. the time-average

$$\hat{\mathbb{E}}[x] = \lim_{T \rightarrow +\infty} \frac{1}{T} \int_0^T dt \hat{\gamma}_t[x] \quad (3.11)$$

defines a *conditional expectation* from  $M$  onto  $M_\gamma$ , that is a completely positive unital map such that

$$\hat{\mathbb{E}}[y_1 x y_2] = y_1 \hat{\mathbb{E}}[x] y_2 \quad \forall y_{1,2} \in M_\gamma, \quad \forall x \in M. \quad (3.12)$$

*Remark 3.2.* 1. The diagonal form (3.9) of the master equation (3.5) is independent of the number of qubits involved which only enter in the expression of the operators  $S_i$  given by (3.7).

2. The dual map of the conditional expectation  $\hat{E} : M \mapsto M_\gamma$ , defined by

$$\text{Tr}(\rho \hat{E}[x]) = \text{Tr}(E[\rho] x), \quad \forall \rho \in \mathcal{S}(M), \quad x \in M, \quad (3.13)$$

is a linear map on the state-space  $\mathcal{S}(M)$  which associates to each initial  $\rho$  its asymptotic state

$$E[\rho] = \lim_{t \rightarrow +\infty} \gamma_t[\rho]. \quad (3.14)$$

In particular, for any stationary state  $\rho_\infty \in \mathcal{S}(M)$ ,  $E[\rho_\infty] = \rho_\infty$ .

**Theorem 3.3.** *The stationary states  $M_\gamma$  of 3.9 are the elements of the commutant set of the operators  $V_i$*

$$\mathcal{M}(\gamma) = \{V_i\}' \equiv \mathcal{K} \quad (3.15)$$

**Proof.**

As in Frigerio's papers [13], [14] introduce the quantity:

$$D_t(A, B) = \hat{\gamma}_t(A^*B) - \hat{\gamma}_t(A^*)\hat{\gamma}_t(B)$$

and denote the null space of  $\{D_t : t \geq 0\}$ , i.e.

$$\mathcal{N}(\gamma) = \{A \in \mathcal{M} ; D_t(A, A) = 0 \ t \geq 0\}.$$

In general  $\mathcal{M}(\gamma) \subset \mathcal{N}(\gamma)$ . Now observe that:

$$\dot{D}_0 \equiv \frac{d}{dt}D(A, A) |_{t=0} = \hat{L}(A^*A) - \hat{L}(A^*)A - A^*\hat{L}(A).$$

Of course  $\mathcal{N}(\gamma) \subset Ker(\dot{D}_0)$ . Let us determine  $Ker(\dot{D}_0)$ . By using the form of  $\hat{L}$  one obtains:

$$\dot{D}_0 = \sum_i [A, V_i][V_i^*, A^*] = \sum_i [A, V_i][A, V_i]^* \geq 0$$

so  $\dot{D}_0 = 0$  if and only if:  $[A, V_i] = 0$  for all  $i$ , thus  $Ker \dot{D}_0 = \{V_i\}'$ . Denote the commutant of the operators in  $L$  by  $\mathcal{K} \equiv \{V_i\}'$ .

The commutant is a subalgebra which need not coincide with the time-invariant  $*$ -subalgebra  $M_\gamma$ . This is however the case if the operators [14] commuting with all  $V_i$  also commute with their adjoints and with the Hamiltonian  $H$ . Indeed, if  $\{V_i\}' = \{V_i, V_i^\dagger, H\}'$ , then  $M_\gamma \subseteq \mathcal{N}_\gamma \subseteq M_\gamma$  as (3.9) yields  $\{V_i, V_i^\dagger, H\}' \subseteq M_\gamma$ .

Moreover, the equality  $\{V_i\}' = \{V_i, V_i^\dagger, H\}'$  is also sufficient [14] to guarantee that  $\lim_{t \rightarrow +\infty} \hat{\gamma}_t[x] = \hat{\mathbb{E}}[x]$ , for all  $x \in M$ , whence (??) follows by duality.

So after all in the case at hand  $\mathcal{N}(\gamma) = \mathcal{M}(\gamma)$  also holds [13], yielding  $\mathcal{M}(\gamma) \subset \{V_i\}'$ ,

In our case every element of  $\{V_i\}'$  can be stationary so we even have

$$\mathcal{M}(\gamma) = \{V_i\}' \equiv \mathcal{K}. \quad (3.16)$$

**Remark 3.0.2.** In the special case when  $\mathcal{K} = \mathbb{C}\mathbb{1}$ , so the commutant contains only the identity implying that all the stationary state of  $\hat{\gamma}_t$  are proportional with  $\mathbb{1}$  and implying that  $\gamma_t$  has a unique stationary state too. We show that this is the case for an important class of dynamics.

**Theorem 3.4.** *If the dissipative part of  $\gamma_t$  has the Kossakowsky matrix of the form of 3.3 with  $A \neq B$ , then it has a unique stationary state.*

**Proof.**

Let us restructurize the master equation as a sum of two parts. The two parts has the same structure as that of the original equation, but the first one refers to a dynamics where all subsystem is affected uniformly, and the second one describes a noise which does not induce correlations between different subsystems. In other words, we split the coefficients into two parts as

$$K'_{A-B} = \begin{pmatrix} A-B & 0 & 0 \\ 0 & A-B & 0 \\ 0 & 0 & A-B \end{pmatrix} \quad K_B = \begin{pmatrix} B & B & B \\ B & B & B \\ B & B & B \end{pmatrix}.$$

Apparently  $K = K'_{A-B} + K_B$ . The last part has the Kraus operators discussed already in the previous theorem, and for the first part we have the form

$$L[\rho] = \sum_a \sum_{i,j=1}^3 C_{ij} \left( \sigma_i^{(a)} \rho_t \sigma_j^{(a)} - \frac{1}{2} \left\{ \sigma_j^{(a)} \sigma_i^{(a)}, \rho_t \right\} \right)$$

where  $C = A - B$ . Its Kraus form is obtained via diagonalizing  $C$ :  $C_{ij} = \sum_k U_{ik} \lambda_k \bar{U}_{jk}$ . And then we can define the Kraus operators

$$W_k^{(a)} = \sum_i \sqrt{\lambda_k} U_{ik} \sigma_i^{(a)}.$$

It is easy to see that (unless  $C = 0$ ) due to the structure of  $W_k^{(a)}$

$$\{W_k^{(a)}\}' \cap \{V_j\}' = \mathbb{C}1.$$

### 3.0.5 One qubit

In case of a simple qubit, a unique stationary state exists. The solution of the master equation

$$\partial_t \rho_t = -i \frac{\omega}{2} [\sigma_3, \rho_t] + \sum_{i,j=1}^3 A_{ij} \left( \sigma_i \rho_t \sigma_j - \frac{1}{2} \left\{ \sigma_j \sigma_i, \rho_t \right\} \right), \quad (3.17)$$

with  $A = [A_{ij}]$  as in (3.4), can easily be found by considering the corresponding time-evolution equation of the Bloch vector  $\vec{r}_t$  in  $\rho_t = \frac{1}{2}(1 + \vec{r}_t \cdot \vec{\sigma})$ ,  $\dot{\vec{r}}_t = \mathcal{L}\vec{r}_t - \vec{z}$ , where

$$\mathcal{L} = \begin{pmatrix} a+c & -\omega/2 & 0 \\ \omega/2 & a+c & 0 \\ 0 & 0 & 2a \end{pmatrix}, \quad \vec{z} = \begin{pmatrix} 0 \\ 0 \\ 2b \end{pmatrix}. \quad (3.18)$$

Setting  $\dot{\vec{r}}_t = 0$ , one finds a unique mixed stationary state:

$$\rho_\infty = \frac{1}{2}(1 + r_\infty \sigma_3), \quad \vec{r}_\infty = \begin{pmatrix} 0 \\ 0 \\ r_\infty \end{pmatrix} = \mathcal{L}^{-1}\vec{z} = \begin{pmatrix} 0 \\ 0 \\ b/a \end{pmatrix}. \quad (3.19)$$

**Remark 2.** Consider two qubits ( $a = 1, 2$  in (3.7)); and the generator specified by 3.4. One explicitly verifies (see also [12]) that  $\rho_\infty^{\otimes 2} = \rho_\infty^* \otimes \rho_\infty^*$  is a full-rank stationary state for (3.5):  $L[\rho_\infty^{\otimes 2}] = 0$ .

The generator of (3.5) can be extended to the case of  $n$  qubits by extending to  $n$  the summation index of single qubit Pauli matrices in (3.7); further, it can conveniently be recast as  $L = \sum_{a,b=1}^n L_{ab}$  where the sum is over generators (3.5) involving only the  $a$ th and  $b$ th qubit. Let  $\rho_\infty^{\otimes n} = \underbrace{\rho_\infty^* \otimes \rho_\infty^* \cdots \otimes \rho_\infty^*}_{n \text{ times}}$ ; then,

$$L^{(12)}[\rho_\infty^{\otimes n}] := (L_{11} + L_{22} + L_{12} + L_{21})[\rho_\infty^{\otimes n}] = L^{12}[\rho_\infty^{\otimes 2}] \otimes \rho_\infty^{\otimes (n-2)} = 0,$$

where  $L^{12}$  is the generator in (3.5) for two qubits and  $\rho_\infty^{\otimes 2}$  is a two qubit stationary state. This result clearly holds for all pairs  $(ab)$ , that is  $L^{(ab)}[\rho_\infty^{\otimes n}] = 0$ , whence  $L[\rho_\infty^{\otimes n}] = 0$  and  $\rho_\infty^{\otimes n}$  is an  $n$ -qubit full-rank stationary state.

Note that it is not always true that one can find a product stationary state according to this simple procedure. Nevertheless, for the sake of simplicity, we will assume it exists due to the form 3.4, but for the ideas of the forthcoming general observations one only needs a full-rank stationary state, not necessarily in a product form.

### 3.0.6 Two qubits

As previously observed,  $\{V_i\}' = \{V_i, V_i^\dagger, H\}' = \{S_i\}'$  independently of the number of qubits. In order to find the commutant  $\{S_i\}'$  for the case of two qubits, we use the Pauli

matrices and write

$$M \ni x = \lambda \mathbb{1} + \sum_{i=1}^3 \sum_{a=1}^2 \lambda_i^{(a)} \sigma_i^{(a)} + \sum_{i,j=1}^3 \lambda_{ij} \sigma_i \otimes \sigma_j .$$

Then, by imposing that  $[x, S_p] = 0$  for all  $p = 1, 2, 3$ ,  $\{V_i\}'$  amounts to being the linear span of the identity matrix  $\mathbb{1}$  and of the symmetric sum  $T = \sum_{i=1}^3 \sigma_i \otimes \sigma_i$ . It follows that  $M_\gamma = \{S_i\}'$  is a commutative algebra; it coincides with its center,  $M_\gamma = \mathcal{Z} = \{S_i\}' \cap \{S_i\}'' = M_\gamma \cap M_\gamma'$  and is generated by the two orthogonal projections

$$P = \frac{1}{4}(\mathbb{1} - T) , \quad Q = \mathbb{1} - P = \frac{1}{4}(3 + T) , \quad (3.20)$$

where the first one is 1-dimensional and projects onto the two-qubit singlet state

$$|\Psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle) , \quad (3.21)$$

with  $\sigma_3|0\rangle = |0\rangle$  and  $\sigma_3|1\rangle = -|1\rangle$ .

From Remark 2.,  $\rho_\infty^{\otimes 2} = \rho_\infty^* \otimes \rho_\infty^*$  is a full-rank stationary state; then, (??) ensures that the asymptotic state  $\rho_\infty$  corresponding to an initial  $\rho$  is obtained as  $\mathbb{E}[\rho]$ , by means of (3.13). In order to construct it, we first construct the conditional expectation  $\hat{\mathbb{E}}$  onto the sub-algebra of constant matrices;  $\hat{\mathbb{E}}$  must be such that  $\hat{\mathbb{E}}[x] = \lambda(x)P + \mu(x)Q$ . From the properties (3.12) of the conditional expectation,

$$\hat{\mathbb{E}}[PxP] = \lambda(x)P , \quad \hat{\mathbb{E}}[QxQ] = \mu(x)Q ,$$

where, with  $\rho(x) := \text{Tr}(\rho x)$ ,

$$\lambda(x) = \frac{\text{Tr}(P \rho_\infty^{\otimes 2} P x)}{\rho_\infty^{\otimes 2}(P)} , \quad \mu(x) = \frac{\text{Tr}(Q \rho_\infty^{\otimes 2} Q x)}{\rho_\infty^{\otimes 2}(Q)} .$$

Then, from (3.21) one gets

$$\rho_\infty^{\otimes 2} P = \frac{1 - r_\infty^2}{4} P , \quad r_\infty = \frac{b}{a} , \quad (3.22)$$

so that, given any initial state  $\rho$ , its asymptotic state  $\rho_\infty$  is given by (compare with [12])

$$\begin{aligned} \rho_\infty = \mathbb{E}[\rho] &= \frac{4\rho(P)}{1 - r_\infty^2} P \rho_\infty^{\otimes 2} P + \frac{4\rho(Q)}{3 + r_\infty^2} Q \rho_\infty^{\otimes 2} Q \\ &= \frac{4(1 - \rho(P))}{3 + r_\infty^2} \rho_\infty^{\otimes 2} + \frac{4\rho(P) - 1 + r_\infty^2}{3 + r_\infty^2} P . \end{aligned} \quad (3.23)$$

### Asymptotic entanglement

The entanglement content of any two-qubit state  $\rho$  is quantified by the concurrence  $C(\rho)$  [15]: consider the complex conjugate matrix  $\rho^*$ , construct  $\tilde{\rho} = \sigma_2 \otimes \sigma_2 \rho^* \sigma_2 \otimes \sigma_2$  and compute the (positive) eigenvalues  $\lambda_i^2$  of  $\rho\tilde{\rho}$ . Then,  $C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}$ . For all asymptotic states  $\rho_\infty$  in (3.23), one easily calculates

$$C(\rho_\infty) = \frac{1}{2(3+r_\infty^2)} \max\left\{0, 2|4\rho(P) - (1-r_\infty^2)| - 2(1-\rho(P))(1-r_\infty^2)\right\} \quad (3.24)$$

In [12] the entanglement capability of the environment has been studied by comparing the concurrence of certain initial states with that of their asymptotes; in the following, we shall focus upon the following one-parameter family of initial conditions

$$\rho(\alpha) = \alpha \mathbb{1} + (1-4\alpha)P, \quad 0 \leq \alpha \leq 1/3. \quad (3.25)$$

One easily finds that  $C(\rho(\alpha)) = \max\{0, 1-6\alpha\}$ . Furthermore, if

$$0 \leq \alpha < \alpha(r_\infty) = \frac{3+r_\infty^2}{6(3-r_\infty^2)}, \quad (3.26)$$

where  $\alpha(r_\infty)$  is an increasing function of  $r_\infty$ :  $1/6 \leq \alpha(r_\infty) \leq 1/3$ , the corresponding asymptotic states obtained, according to (??), as

$$\rho_\infty(\alpha) = \mathbb{E}[\rho(\alpha)] = \frac{12\alpha}{3+r_\infty^2} \rho_\infty^{\otimes 2} + \frac{3+r_\infty^2-12\alpha}{3+r_\infty^2} P \quad (3.27)$$

have concurrence

$$C(\rho_\infty(\alpha)) = \frac{1}{2} - 3\alpha \frac{3-r_\infty^2}{3+r_\infty^2} > 0. \quad (3.28)$$

Otherwise, namely for  $\alpha(r_\infty) \leq \alpha$ ,  $\rho_\infty(\alpha)$  is separable. One can then conclude:

1. both  $\rho(\alpha)$  and  $\rho_\infty(\alpha)$  are separable if

$$\frac{1}{6} \leq \alpha(r_\infty) \leq \alpha \leq \frac{1}{3}. \quad (3.29)$$

2.  $\rho(\alpha)$  is separable and  $\rho_\infty(\alpha)$  is entangled if

$$\frac{1}{6} \leq \alpha \leq \alpha(r_\infty). \quad (3.30)$$

3. Since  $\alpha(r_\infty) \geq 1/6$ , it follows that, when  $0 \leq \alpha < 1/6$ , the initial state  $\rho(\alpha)$  is entangled as well as  $\rho_\infty(\alpha)$ ; the entanglement difference

$$\Delta(\alpha) := C(\rho_\infty(\alpha)) - C(\rho(\alpha)) = 9\alpha \frac{1+r_\infty^2}{3+r_\infty^2} - \frac{1}{2} \quad (3.31)$$

becomes positive (entanglement gain) if

$$\alpha > \alpha^*(r_\infty) = \frac{3 + r_\infty^2}{18(1 + r_\infty^2)}, \quad (3.32)$$

where  $\alpha^*(r_\infty)$  is a monotonically decreasing function of  $r_\infty$ :  $1/6 \geq \alpha^*(r_\infty) \geq 1/9$ .

### 3.0.7 Three qubits

Differently from the two-qubit case, we are not able to fully characterize the set of asymptotic states  $M_\gamma$ , in that we could not find a complete characterization of the conditional expectation (3.11). However, we could explicitly find the action of its dual (3.13) on certain subsets of initial states containing among others the states  $\rho(\alpha)$  in (3.25).

Essential tools will be the following facts:

1. Because of Remark 3, we know that the state  $\rho_\infty^{\otimes 3} = \rho_\infty \otimes \rho_\infty \otimes \rho_\infty$  with  $\rho_\infty$  as in (3.19), is a full-rank stationary state for (3.5).
2. Because the structure of the master equation (3.5) does not vary by addition of extra qubits in the global spin operators  $S_i$  (3.7), the algebra of time-invariant operators  $M_\gamma$  is still given the commutant set  $\{S_i\}'$ . In the appendix it is showed that  $M_\gamma$  is the linear span of the the  $3 \times 3$  identity matrix and of the following operators

$$S^{(ab)} = \sum_{i=1}^3 \sigma_i^{(a)} \sigma_i^{(b)}, \quad a, b = 1, 2, 3, \quad a < b; \quad S = \sum_{i,j,k=1}^3 \varepsilon_{ijk} \sigma_i \otimes \sigma_j \otimes \sigma_k. \quad (3.33)$$

3. The center  $\mathcal{Z} = \{S_i\}' \cap \{S_i\}'' = M_\gamma \cap M_\gamma'$  surely contains the operator

$$T = \sum_{a < b} S^{ab} = S^{(12)} + S^{(23)} + S^{(13)}. \quad (3.34)$$

**Remark 5** In Appendix A it is showed that, differently from the two-qubit case, the commutant  $M_\gamma$  is not commutative; thus  $\mathcal{Z} \neq M_\gamma$  and one cannot construct the conditional expectation (3.11) onto  $M_\gamma$  by simple use of the orthogonal projections that generate it. Furthermore, it also turns out that  $M_\gamma$  does not coincide with the commutant of its center,  $M_\gamma \neq \mathcal{Z}'$ , which is the other case where one would immediately know how to construct the conditional expectation [13, 14, 16].

Consider the projections  $P^{(ab)} = \frac{\mathbb{1} - S^{(ab)}}{4} \in M_\gamma$  given by (A.10); since  $[P^{(ab)}, S_i] = 0$  for all  $i = 1, 2, 3$ , using the form (3.9) of (3.5) and Remark 4.1, it turns out that, given

any  $\rho \in \mathcal{S}(M)$  the states  $\rho^{(ab)} = \frac{P^{(ab)} \rho P^{(ab)}}{\rho(P^{(ab)})}$  are such that

$$L[\rho^{(ab)}] = P^{(ab)} L[\rho] P^{(ab)} \implies \gamma_t[\rho^{(ab)}] = P^{(ab)} \gamma_t[\rho] P^{(ab)}. \quad (3.35)$$

Moreover, as  $P^{(ab)} = |\Psi_{ab}\rangle\langle\Psi_{ab}| \mathbb{1}_c$  projects onto the singlet vector state  $|\Psi_{ab}\rangle$  of the qubits  $a$  and  $b$ , it turns out that

$$\gamma_t[\rho_{ab}] = P^{(ab)} \rho_t^{(c)}, \quad (3.36)$$

where  $\rho_t^{(c)}$  is a density matrix of qubit  $c$ .

**Proposition 1** The state  $\rho_t^{(c)}$  evolves in time according to the master equation (3.5) for one qubit and  $E[\rho^{(ab)}] = P^{(ab)} \rho_\infty^{(c)}$ , where  $\rho_\infty^{(c)}$  is the stationary one-qubit state given by (3.19).

**Proof:** The time-evolution of  $\rho_t^{(c)}$  is obtained by tracing (3.36) with respect to  $P^{(ab)}$  over the qubits  $a$  and  $b$  and using (3.35):

$$\partial_t \rho_t^{(c)} = \text{Tr}_{ab} \left( P^{(ab)} L[P^{(ab)} \rho_t^{(c)}] \right).$$

By splitting the generator as  $L = \sum_{p,q=1}^3 L_{pq}$  (see Remark 3), one gets

$$\begin{aligned} L[P^{(ab)} \rho_t^{(c)}] &= \underbrace{\left( (L_{aa} + L_{bb} + L_{ab} + L_{ba}) [P^{(ab)}] \right)}_{L_I[P^{(ab)} \rho_t^{(c)}]} \otimes \rho_t^{(c)} \\ &+ \underbrace{\left( (L_{ac} + L_{ca} + L_{cb} + L_{bc}) [P^{(ab)}] \otimes \rho_t^{(c)} \right)}_{L_{II}[P^{(ab)} \rho_t^{(c)}]} \\ &+ P^{(ab)} \otimes L_{cc}[\rho_t^{(c)}]. \end{aligned}$$

The contribution  $L_I = 0$  for it consists of the generator of the master equation (3.5) for two qubits applied to the projection  $P^{(ab)}$  onto the singlet state; from (3.23) it follows that this latter state is time-invariant, whence the statement.

Since  $P^{(ab)} \in \{\mathcal{S}_i\}'$ , the trace over the qubits  $a$  and  $b$  of  $L_{II}$  multiplied by  $P^{(ab)}$  reads

$$\text{Tr} \left( P^{(ab)} L_{II}[P^{(ab)} \rho_t^{(c)}] \right) = \text{Tr} \left( P^{(ab)} L_{II}[\mathbb{1}^{(ab)} \rho_t^{(c)}] \right).$$

This piece vanishes, too; indeed, all Kraus operators contribute with terms of the form  $\text{Tr}(P^{(ab)} \sigma_i^{(a)})$  or  $\text{Tr}(P^{(ab)} \sigma_i^{(b)})$  which are both zero as the partial trace of  $P^{(ab)}$  is proportional to the  $2 \times 2$  identity matrix and the Pauli matrices are traceless. Therefore,  $\partial_t \rho_t^{(c)} = L_{cc}[\rho_t^{(c)}]$  whence the result follows from Section 2.1.

One can now fix the action on the projectors  $P^{(ab)} = \frac{\mathbb{1} - S^{(ab)}}{4}$  and  $P = \frac{2}{3} \sum_{a>b=1}^3 P^{(ab)}$  (see (A.11)) of the dual map introduced in (3.13) and (3.14) which associates to any initial condition its asymptote.

**Corollary 1**  $E[P^{(ab)}] = 2 P^{(ab)} \rho_\infty^{(c)}$  and  $E[P] = \frac{4}{3} \sum_{a>b=1}^3 P^{(ab)} \rho_\infty^{(c)}$ .

**Proof:** Set  $\rho = P^{(ab)}$  in (3.36); then,  $E[P^{(ab)}] = \lim_{t \rightarrow +\infty} \gamma_t[P^{(ab)}] = 2 P^{(ab)} \rho_\infty^{(c)}$ . The second relation follows by the linearity of the map  $E : \mathcal{S}(M) \mapsto \mathcal{S}(M)$ .

**Remark 5** Notice that while  $P^{(ab)} \in M_\gamma$  and thus  $\hat{E}[P^{(ab)}] = P^{(ab)}$ ,  $\frac{P^{(ab)}}{2}$  is not an invariant state:  $E\left[\frac{P^{(ab)}}{2}\right] \neq \frac{P^{(ab)}}{2}$ .

The last necessary tool for the applications to be discussed in the next section is the action of the map  $E$  on the projection  $Q = \mathbb{1} - P \in M_\gamma$ .

**Proposition 2**  $E[Q] = \frac{8}{1+r_\infty^2} \left( \rho^{\otimes 3} - \frac{1-r_\infty^2}{6} \sum_{a>b=1}^3 P^{(ab)} \rho_\infty^{(c)} \right)$ .

**Proof:** Since  $Q \in M_\gamma$ , the properties of the conditional expectation (3.12) and the algebraic relations (A.12) applied to  $E[x] = \lambda(x) \mathbb{1} + \sum_{a>b=1}^3 \lambda_{ab}(x) S^{(ab)} + \mu(x) S$ ,  $x \in M$ , give

$$\hat{E}[Q x Q] = Q E[x] Q = \beta(x) Q, \quad \beta(x) = \lambda(x) + \sum_{a,b=1}^3 \lambda_{ab}(x).$$

Using the time-invariant state  $\rho_\infty^{\otimes 3}$ ,  $E[\rho_\infty^{\otimes 3}] = \rho_\infty^{\otimes 3}$ , one obtains

$$\mathrm{Tr}\left(Q \rho_\infty^{\otimes 3} Q x\right) = \mathrm{Tr}\left(\rho_\infty^{\otimes 3} Q x Q\right) = \mathrm{Tr}\left(\rho_\infty^{\otimes 3} \hat{E}[Q x Q]\right) = \beta(x) \mathrm{Tr}\left(\rho_\infty^{\otimes 3} Q\right).$$

This gives  $\beta(x) = \frac{\mathrm{Tr}\left(Q \rho_\infty^{\otimes 3} Q x\right)}{\mathrm{Tr}\left(\rho_\infty^{\otimes 3} Q\right)}$ ; on the other hand, for all  $x \in M$ ,

$$\mathrm{Tr}\left(x E[Q]\right) = \mathrm{Tr}\left(\hat{E}[Q x Q]\right) = \frac{\mathrm{Tr}(Q)}{\mathrm{Tr}\left(\rho_\infty^{\otimes 3} Q\right)} \mathrm{Tr}\left(x Q \rho_\infty^{\otimes 3} Q\right).$$

Then, the result follows using that (see (3.22))

$$P \rho_\infty^{\otimes 3} = \frac{2}{3} \sum_{a>b=1}^3 P^{(ab)} \rho_\infty \otimes \rho_\infty \otimes \rho_\infty = \frac{1-r_\infty^2}{6} \sum_{a>b=1}^3 P^{(ab)} \rho_\infty^{(c)} = \rho_\infty^{\otimes 3} P.$$

### 3.0.8 Applications

We now apply the previous results to the study of the asymptotic entanglement properties of a class of three-qubit states obtained by the two-qubit states (3.25) by appending to them a third qubit in the completely depolarized state; we shall thus focus onto initial density matrices of the form

$$\rho^{123}(\alpha) = \rho(\alpha) \otimes \frac{\mathbb{1}}{2} = \frac{\alpha}{2} \mathbb{1} + \frac{1-4\alpha}{2} P^{(12)}, \quad 0 \leq \alpha \leq 1/3, \quad (3.37)$$

where, according to the notation of the previous section,  $P \otimes \mathbb{1} = P^{(12)}$ .

The corresponding asymptotic states are given by the map  $E : \mathcal{S}(M) \mapsto \mathcal{S}(M)$  whose action is given by Corollary 1 and Proposition 2; indeed, writing  $\mathbb{1} = P + Q$ ,

$$E[\mathbb{1}] = \frac{8}{1+r_\infty^2} \rho_\infty^{\otimes 3} + \frac{8r_\infty^2}{3(1+r_\infty^2)} \sum_{a>b=1}^3 P^{(ab)} \rho_\infty^{(c)} \quad (3.38)$$

$$\begin{aligned} \rho_\infty^{123}(\alpha) = E[\rho^{123}(\alpha)] &= \frac{4\alpha}{1+r_\infty^2} \rho_\infty^{\otimes 3} + \frac{4\alpha r_\infty^2}{3(1+r_\infty^2)} \sum_{a>b=1}^3 P^{(ab)} \rho_\infty^{(c)} \\ &+ (1-4\alpha) P^{(12)} \rho_\infty^{(3)}. \end{aligned} \quad (3.39)$$

The physical idea is to append the third qubit and to exploit the symmetric coupling to the environment described by the master equation (3.5) in order to improve the asymptotic entanglement generation between the first two qubits. In order to proceed, we thus trace the asymptotic states  $\rho_\infty^{123}(\alpha)$  with respect to the appended qubit:

$$\begin{aligned} \rho_\infty^{12}(\alpha) &= \text{Tr}_3(\rho_\infty^{123}(\alpha)) = \frac{4\alpha}{1+r_\infty^2} \rho_\infty \otimes \rho_\infty + \frac{4\alpha r_\infty^2 + 3(1-4\alpha)(1+r_\infty^2)}{3(1+r_\infty^2)} P \\ &+ \frac{2\alpha r_\infty^2}{3(1+r_\infty^2)} (\mathbb{1} \otimes \rho_\infty + \rho_\infty \otimes \mathbb{1}), \end{aligned} \quad (3.40)$$

where  $P$  projects onto the two-qubit singlet state. The concurrence  $C(\rho_\infty^{(12)}(\alpha))$  of this two-qubit state can be computed and compared with that of the asymptotic state  $\rho_\alpha^\infty$  in (3.32). The goal is to see whether the addition and final discarding of the ancillary third qubit may improve on the asymptotic entanglement of  $\rho_\alpha^\infty$  in (3.27). Though easy to calculate, the expression of  $C(\rho_\infty^{(12)}(\alpha))$  is not particularly inspiring and is discussed in Appendix B.

We start by considering the case when no separable two-qubit state  $\rho(\alpha)$  can get asymptotically entangled by the action of the master equation (3.5). According to (3.29), this occurs for  $\frac{1}{6} \leq \alpha(r_\infty) \leq \alpha \leq \frac{1}{3}$ .

Consider a third qubit prepared in the totally depolarized state and appended to the qubits 1 and 2 prepared in a state  $\rho(\alpha)$  with  $\alpha$  in the above range. According to Appendix B, by tracing the asymptotic 3-qubit state  $\rho_\infty^{123}(\alpha)$  over the appended qubit, the qubits 1 and 2 are entangled if either  $0 \leq \alpha \leq \alpha_+(r_\infty)$  or  $\alpha_-(r_\infty) \leq \alpha \leq \frac{1}{3}$ . One checks that  $\alpha_+(r_\infty) \leq \alpha(r_\infty)$ ; therefore, the first condition is incompatible with (3.29); however, the second one is not so.

Let  $r^* \leq r_\infty \leq 1$  as in Appendix B; if  $\alpha_-(r_\infty) \leq \alpha(r_\infty)$ , all initial states  $\rho(\alpha)$  with  $\alpha > \alpha(r_\infty)$  correspond to an asymptotic state  $\rho_\infty^\alpha$  separable, but to a reduced asymptotic state  $\rho_\infty^{12}(\alpha)$  entangled. The same occurs for  $\alpha_-(r_\infty) \geq \alpha(r_\infty)$  for initial states  $\rho(\alpha)$  with  $\alpha > \alpha_-(r_\infty)$ . Therefore, there are separable  $\rho(\alpha)$  which do not get asymptotically entangled by immersion in the environment described by (3.5), but do get entangled if a third depolarized qubit is appended to them initially.

### 3.0.9 Generation of strong entanglement by noise in practice

This subsection is devoted to the practical question: How can we profit from the environment in practice and generate strongly entangled qubits, or having a disentangling dissipation leading to a unique stationary state, what Hamiltonian should we choose to generate considerable entanglement?

As we have seen, three uniformly interacting qubits has the Kossakowsky matrix

$$K = \begin{bmatrix} A & B & B \\ B & A & B \\ B & B & A \end{bmatrix}. \quad (3.41)$$

In practice  $A \neq B$  but there exist important practical cases when they are proportional  $B = \gamma A$ ,  $\gamma \neq 1$ . Following by the previous theory in these cases the asymptotic state is unique so the only thing left is to determine this unique stationary state.

**Example 3.1.** *If  $B = \gamma A$ ,  $|\gamma| < 1$  where  $A$  has the form 3.4 then dissipation itself has a product state as the unique asymptotic state for any number of qubits, yet adding an appropriate Hamiltonian it gets entangled.*

*We have already shown in Remark 2 that if all the submatrices of the Kossakowsky  $K$  are the same,  $B = \gamma A$ , then for any number of qubits, there exists a product steady state, i.e.  $\mathbb{L}[\rho_\infty^{\otimes n}] = 0$ . Moreover, following from the proof of the previous statement, it is also a steady state of the dynamics corresponding to a block diagonal Kossakowsky  $K'$  with blocks  $(1 - \gamma)A$ . Thus it is also satisfies  $(\mathbb{L} + \mathbb{L}')[\rho_\infty^{\otimes n}] = 0$ . We also know that it is the unique solution if  $\gamma \neq 1$ .*

We can try for example the case with

$$A = \begin{bmatrix} 1 & -i & 0 \\ i & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (3.42)$$

$B = \gamma A$  and a simple (Ising) Hamiltonian on the two qubits  $H = \sigma_1 \otimes \sigma_1 + h(\sigma_3 \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_3)$ . Note that with this choice of a  $A$  the Lindbladian has the compact form as below

$$\mathbb{L}_D[\rho] = \sum_{a,b=1,2} C_{a,b}(\sigma_+^{(a)} \rho \sigma_-^{(b)} - \frac{1}{2}\{\sigma_-^{(b)} \sigma_+^{(a)}, \rho\})$$

with  $\sigma_{\pm} = \sigma_1 \pm i\sigma_2$  and

$$C = \begin{bmatrix} 1 & \gamma \\ \gamma & 1 \end{bmatrix}. \quad (3.43)$$

Indeed, we may get an entangled asymptotic states, however considerably less entangled than the eigenstate of  $H$ . For any  $|\gamma| < 1$ , the dissipation itself has the unique asymptotic state  $|00\rangle\langle 00|$ , but switching on the interaction with  $h = 0$  the unique asymptotic state becomes

$$\rho_{\infty} = \begin{pmatrix} 0.85 & 0 & 0 & -0.2i \\ 0 & 0.05 & 0 & 0 \\ 0 & 0 & 0.05 & 0 \\ 0.2i & 0 & 0 & 0.05 \end{pmatrix}$$

whose partial transpose has one negative eigenvalue which is equal to  $-0.15$ .

If  $A \neq \gamma B$  then we can have asymptotic entanglement even with a non entangling Hamiltonian as it will be also shown in the next Chapter, by perturbation theory.

## Chapter 4

# Perturbative Approach to Asymptotic States and Entanglement of Lindblad Dynamics

In the previous chapter we investigated certain classes of dynamics and obtain important results about the manifold of their invariant states. We did not give however a full characterization. In this chapter we present a perturbative approach and many examples for possible outcomes. We will focus on the following scenario: Given two finite level systems without a direct interaction, so the Hamiltonian is  $H = H_1 + H_2$  with the unitary generator  $\mathbb{L}_0[\rho] = -i[H, \rho]$ . Assume that they are weakly coupled to the same environment and undergo an open, dissipative dynamics generated by  $\mathbb{L} = \mathbb{L}_0 + \varepsilon\mathbb{L}_1$ , where the dissipative generator of Lindblad form is taken into account only in the order of  $\varepsilon \ll 1$ . Suppose the spectrum of the Hamiltonian  $H = H_1 + H_2$  be non-degenerate, then  $\mathbb{L}_0[\rho_0] = 0$  only if  $\rho$  is a separable state. Intuitively, if such states are well inside the closed convex subset of separable states, no dissipative perturbation  $\mathbb{L}_1$  could provide entangled states  $\rho_\varepsilon$  such that  $\mathbb{L}_\varepsilon[\rho_\varepsilon] = 0$ . Indeed, by continuity, such asymptotic states are perturbations of those of  $\mathbb{L}_0$ , namely  $\rho_\varepsilon = \rho_0 + \varepsilon\rho_1 + o(\varepsilon)$ , and thus remain separable if  $\rho_0$  is separable. On the contrary, for separable stationary states  $\rho_0$  on the boundary of the subset of separable states, it should be possible to construct entangled  $\rho_\varepsilon$  by suitably engineered, small dissipative perturbations.

In the following, we give mathematical ground to these expectations by developing a systematic perturbation expansion of the states  $\rho_\varepsilon$  that are invariant under generators of the form  $\mathbb{L}_\varepsilon = \mathbb{L}_0 + \varepsilon\mathbb{L}_1$  where  $\mathbb{L}_0$  and  $\mathbb{L}_1$  are generic Lindblad type generators.

So as before we have the master equations and dynamics as

$$\partial_t \rho(t) = \mathbb{L}[\rho(t)] = -i[H, \rho(t)] + \mathbb{D}[\rho(t)] , \quad (4.1)$$

where  $M_d(\mathbb{C}) \ni H = H^\dagger$ , while

$$\mathbb{D}[\rho] = \sum_{\alpha} \left( h_{\alpha} \rho h_{\alpha}^{\dagger} - \frac{1}{2} \{ h_{\alpha}^{\dagger} h_{\alpha}, \rho \} \right) , \quad (4.2)$$

where  $h_{\alpha}, \sum_{\alpha} h_{\alpha}^{\dagger} h_{\alpha} \in M_d(\mathbb{C})$ .

Concerning  $\gamma_t$ -invariant states, the following result was obtained in [18] (see also [17]).

*Proposition 1.* Let  $\mathbb{L}$  be the generator of a Lindblad-type dynamics  $\gamma_t$ ; one can always construct orthogonal stationary states  $\rho_j$  of  $\gamma_t$ :  $\mathbb{L}[\rho_j] = 0$  and  $\rho_j \rho_k = 0$  unless  $j = k$ .

**Example 4.0.2.** Let  $\mathbb{L}[\rho] = -i[H, \rho]$ , where the Hamiltonian  $H = \sum_{j=1}^d E_j |j\rangle\langle j|$  has a non-degenerate spectrum; then, the stationary states  $\rho_j$  of Proposition 1 are the orthogonal one-dimensional eigen-projectors  $|j\rangle\langle j|$ . For later application, we need extend the conditional expectation  $E$  to the whole matrix algebra  $M_d(\mathbb{C})$ ; in the present case it reads

$$\mathbb{E}[X] = \sum_{j=1}^d \langle j| X |j\rangle |j\rangle\langle j| . \quad (4.3)$$

Clearly, because of the oscillatory behavior, there is no tendency to equilibrium:  $\gamma_t[\rho]$  does not converge to  $\mathbb{E}[\rho]$  when  $t \rightarrow +\infty$ .

**Example 4.0.3.** Let  $H = 0$  in 4.1 and  $h_{\alpha} = |\psi\rangle\langle\alpha|$  in 4.2, where  $\{|\alpha\rangle\}$  is an orthonormal basis of  $\mathbb{C}^d$ . Then,

$$\mathbb{L}[\rho] = |\psi\rangle\langle\psi| - \rho \implies \gamma_t[\rho] = e^{-t} \rho + (1 - e^{-t}) |\psi\rangle\langle\psi| . \quad (4.4)$$

Hence,  $\rho = |\psi\rangle\langle\psi|$  is the only stationary state and all others converge to it asymptotically:  $\gamma_t[\rho] \mapsto |\psi\rangle\langle\psi|$ . The corresponding map  $\mathbb{E}$  is given by (on  $M_d(\mathbb{C})$ )

$$\mathbb{E}[X] = \text{Tr}(X) |\psi\rangle\langle\psi| . \quad (4.5)$$

Despite the abstract characterizations of [6, 19], the convex subset of stationary states is difficult to control in practice; we shall thus concentrate on understanding how the invariant states of a semigroup  $\gamma_t^{(0)}$  are modified by a perturbation  $\mathbb{L}_1$  of its Lindblad generator  $\mathbb{L}_0$ . Concretely, we will investigate the set  $\mathcal{S}_{\varepsilon}$  of stationary states of Lindblad-type dynamics  $\gamma_t^{(\varepsilon)}$  generated by  $\mathbb{L}_{\varepsilon} = \mathbb{L}_0 + \varepsilon \mathbb{L}_1$ ,  $0 < \varepsilon \ll 1$ . By switching on the perturbation, the dimension of  $\mathcal{S}_{\varepsilon}$  decreases, but it is guaranteed that there exists at least one stationary state.

*Lemma 1.* Consider the generator  $\mathbb{L}_\varepsilon = \mathbb{L}_0 + \varepsilon \mathbb{L}_1$ , where both  $\mathbb{L}_{0,1}$  are generators in Lindblad form and the semigroups  $\gamma_t^{(0)}$  and  $\gamma_t^{(\varepsilon)}$  generated by  $\mathbb{L}_0$  and  $\mathbb{L}_\varepsilon = \mathbb{L}_0 + \varepsilon \mathbb{L}_1$ . Let  $n(0)$  be the number of  $\gamma_t^{(0)}$ -invariant orthogonal density matrices and  $n(\varepsilon)$  that of  $\gamma_t^{(\varepsilon)}$ -invariant orthogonal density matrices for  $0 < \varepsilon \ll 1$ ; then  $n(0) \geq n(\varepsilon)$ .

**Proof:** From Proposition 1, one can always choose density matrices such that  $\mathbb{L}_\varepsilon[\rho_j(\varepsilon)] = 0$  and  $\text{Tr}(\rho_j(\varepsilon)\rho_k(\varepsilon)) = 0$  for  $j \neq k$ . In finite dimension, eigenvalues and eigen-projectors are continuous in  $\varepsilon$ ; therefore, should  $\rho_j(\varepsilon) \neq \rho_k(\varepsilon)$  merge as  $\varepsilon \rightarrow 0$ , the continuity of the Hilbert-Schmidt scalar product would be violated.

Because of finite dimensionality, the solutions can always be expressed as converging series in powers of  $\varepsilon$

$$\rho_\varepsilon = \sum_{n \geq 0} \varepsilon^n \rho_n, \quad (4.6)$$

where the operators  $\rho_n$  must solve the iterative procedure

$$\left( \mathbb{L}_0 + \varepsilon \mathbb{L}_1 \right) [\rho(\varepsilon)] = \mathbb{L}_0[\rho_0] + \sum_{n=1} \varepsilon^n \left( \mathbb{L}_0[\rho_n] + \mathbb{L}_1[\rho_{n-1}] \right) = 0, \quad \text{whence} \quad (4.7)$$

$$\mathbb{L}_0[\rho_0] = 0, \quad \mathbb{L}_0[\rho_n] = -\mathbb{L}_1[\rho_{n-1}] \quad n \geq 1, \quad (4.8)$$

where  $\rho_0$  is a stationary state of  $\gamma_t^{(0)}$ . Also, since  $\text{Tr}(\rho(\varepsilon)) = 1$ , it follows that  $\text{Tr}(\rho_n)$  must vanish at all orders. In the following, we discuss when  $\rho_n = -\mathbb{L}_0^{-1}[\mathbb{L}_1[\rho_{n-1}]]$  are acceptable solutions.

**Definition 3.** Let  $\mathbb{F} = \text{id} - \mathbb{E}$ , where  $\mathbb{E}$  is as in (3.13); since  $\mathbb{E}$  is trace-preserving, the image of  $M_d(\mathbb{C})$  by  $\mathbb{F}$  consists of traceless matrices:  $\text{Tr}(\mathbb{F}[X]) = 0$  for all  $X \in M_d(\mathbb{C})$ .

*Lemma 2.*  $\mathbb{L}^{-1}$  can be defined as a map from  $\mathbb{F}[M_d(\mathbb{C})]$  into itself.

**Proof:** Notice that  $\mathbb{E}$ , as a time-average, maps into the kernel of  $\mathbb{L}$  and leaves it invariant; thus, if  $\exists X'$  such that  $\mathbb{L}[X'] = X$  then applying  $\mathbb{E}$  to both sides gives  $\mathbb{E} \circ \mathbb{L}[X'] = \mathbb{L} \circ \mathbb{E}[X'] = 0 = \mathbb{E}[X]$ . So,  $\mathbb{L}^{-1}$  exists for  $M_d(\mathbb{C}) \ni X \neq 0$  only if  $\mathbb{E}[X] = 0$ .

In this case,  $X = \mathbb{E}[X] + \mathbb{F}[X] = \mathbb{F}[X]$  and  $\mathbb{L}^{-1}$  is constructed as a linear map from the range of  $\mathbb{F}$  into itself such that  $\mathbb{L} \circ \mathbb{L}^{-1} = \mathbb{L}^{-1} \circ \mathbb{L} = \text{id}$  on  $\mathbb{F}(M_d(\mathbb{C}))$ . This guarantees that  $\mathbb{L}^{-1}[0] = 0$ ; indeed, consider  $Z = \mathbb{L}^{-1}[X] - \mathbb{L}^{-1}[Y]$ , with  $X = \mathbb{L}[V] = Y = \mathbb{L}[V + W]$ ,  $W \neq 0$ ,  $\mathbb{L}[W] = 0$ ; then,  $\mathbb{F}[Z] = \mathbb{F} \circ \mathbb{L}^{-1}[X] - \mathbb{F} \circ \mathbb{L}^{-1}[Y] = 0$ .

In the following, the form of  $\mathbb{L}^{-1}$  is shown using the previous examples.

**Example 4.0.4.** In the case of Example 4.0.2, where  $\mathbb{L}[\rho] = -i[H, \rho]$  and  $H$  is non-degenerate,  $\mathbb{E}[X] = 0$  if and only if  $\langle j|X|j \rangle = 0$  for all  $j$ ; one thus gets

$$\mathbb{L}^{-1}[X] = i \sum_{j \neq k} \frac{\langle j|X|k \rangle}{E_j - E_k} |j \rangle \langle k| . \quad (4.9)$$

**Example 4.0.5.** In the case of Example 4.0.3,  $\mathbb{E}[X] = 0$  if and only if  $\text{Tr}(X) = 0$ ; one can verify that, on traceless matrices,

$$\mathbb{L}^{-1}[X] = -X . \quad (4.10)$$

*Lemma 3.* Given  $\mathbb{L}_\varepsilon = \mathbb{L}_0 + \varepsilon \mathbb{L}_1$ , if  $\mathbb{L}_0[\rho_0] = 0$  for a unique state  $\rho_0$  and  $\mathbb{L}_1[\rho_0] \neq 0$ , then  $\mathbb{L}_\varepsilon[\rho_\varepsilon] = 0$  for a unique  $\rho_\varepsilon$  given by

$$\rho_\varepsilon = \sum_{n=0}^{\infty} (-\varepsilon)^n \left( \mathbb{L}_0^{-1} \circ \mathbb{L}_1 \right)^n [\rho_0] = \frac{1}{1 + \varepsilon \mathbb{L}_0^{-1} \circ \mathbb{L}_1} [\rho_0] . \quad (4.11)$$

**Proof:** As  $\mathbb{E}_0$  maps into the kernel of  $\mathbb{L}_0$  and is trace preserving, from the hypothesis of the lemma it follows that  $\mathbb{E}_0 \circ \mathbb{L}_1[\rho_0] = \lambda \rho_0$ . Then,  $\lambda = \text{Tr}(\mathbb{E}_0 \circ \mathbb{L}_1[\rho_0]) = \text{Tr}(\mathbb{L}_1[\rho_0]) = 0$  implies  $\mathbb{E}_0 \circ \mathbb{L}_1[\rho_0] = 0$  so that  $\mathbb{L}_0$  can be inverted on  $\mathbb{L}_1[\rho_0]$  and one can solve the first recursive relation in 4.8. As  $\mathbb{L}_0^{-1}$  maps into  $\mathbb{F}_0[M_d(\mathbb{C})]$  where  $\mathbb{F}_0 = \mathbb{1} - \mathbb{E}_0$  and  $\mathbb{E}_0$  is the trace-preserving map in 3.13 corresponding to  $\mathbb{L}_0$ , then  $\text{Tr}(\rho_1) = 0$ . Iterating this argument yields the result.

**Example 4.0.6.** For  $\mathbb{L}_0$  as in Example 4.0.3, there is only one invariant state so that Lemma 3 applies. Furthermore, since  $\mathbb{L}_0^{-1}[X] = -X$ , 4.11 yields  $\rho_\varepsilon = \left( \mathbb{1} - \varepsilon \mathbb{L}_1 \right)^{-1} [\rho]$ . In such a case of a unique invariant state under  $\mathbb{L}_0$ , we can make some preliminary considerations about the entanglement of the unique state invariant under  $\mathbb{L}_0 + \varepsilon \mathbb{L}_1$ . Consider a separable pure state  $\rho = P \otimes Q \in M_d(\mathbb{C})$ , where  $P = |\phi \rangle \langle \phi|$  and  $Q = |\chi \rangle \langle \chi|$ ; then, suitable non-local perturbations,  $\mathbb{L}_1$  may entangle it. Indeed, by partial transposition[20],  $\rho_\varepsilon \mapsto \rho_\varepsilon^\Gamma$ , operated on the second party with respect to an orthonormal basis starting with  $|\chi \rangle$ , one gets

$$\rho_\varepsilon^\Gamma = P \otimes Q + \varepsilon \left( \mathbb{L}_1[P \otimes Q] \right)^\Gamma + o(\varepsilon) . \quad (4.12)$$

By projecting with  $\Pi_\perp$  onto a subspace orthogonal to  $P \otimes Q$ , it follows that

$$\text{Tr}(\rho_\varepsilon^\Gamma \Pi_\perp) = \varepsilon \text{Tr} \left( \Pi_\perp \left( \mathbb{L}_1[P \otimes Q] \right)^\Gamma \right) + o(\varepsilon) .$$

If  $\mathbb{L}_1[\rho] = -i[H_1 \otimes 1 + 1 \otimes H_2 + H_{12}, \rho]$ , where  $H_{12}$  is a non-local coupling of the two sub-systems, then the quantity

$$\mathrm{Tr}(\rho_\varepsilon \Pi_\perp) \simeq -i\varepsilon \mathrm{Tr}\left(\Pi_\perp\left([H_{12}, P \otimes Q]\right)^\Gamma\right)$$

can be made negative by suitably choosing  $H_{12}$ ; then, one violates the positivity of partial transposition at order  $\varepsilon$  and  $\rho_\varepsilon$  is entangled at that order.

Entanglement can also be obtained via a purely dissipative time-evolution as the one generated by  $\mathbb{L}_1$  as in Example 3 in [23]; indeed, choosing  $|1\rangle\langle 1| = P \otimes Q$  yields

$$\mathrm{Tr}(\rho_\varepsilon^\Gamma \Pi_\perp) \simeq \varepsilon \mathrm{Tr}\left(\Pi_\perp\left(|\psi\rangle\langle\psi|\right)^\Gamma\right),$$

which can become negative by a suitable choice of entangled  $|\psi\rangle$  and  $\Pi_\perp$ .

The possibility of generating entanglement in the above two cases comes from the fact that the 0-th order state  $P_1 \otimes P_2$  is on the border of the closed subset of separable states and can thus be moved into the open complementary subset of entangled states by suitable terms of order  $\varepsilon$ .

Notice that if the kernel of  $\mathbb{L}_0$  contains more than one stationary state, still one may seek a  $\rho_0$  such that  $\mathbb{L}_0[\rho_0] = 0$  and

$$\mathbb{E}_0 \circ \mathbb{E}_1[\rho_0] = \widehat{\mathbb{L}}_1[\rho_0] = 0, \quad \text{where} \quad \widehat{\mathbb{L}}_1 := \mathbb{E}_0 \circ \mathbb{L}_1 \circ \mathbb{E}_0, \quad (4.13)$$

so that the first order correction can be obtained as

$$\rho_1 = -\mathbb{L}_0^{-1} \circ \mathbb{L}_1[\rho_0].$$

In order to continue the iteration in (4.7) and get

$$\rho_2 = -\mathbb{L}_0^{-1} \circ \mathbb{L}_1[\rho_1],$$

again by inverting  $\mathbb{L}_0$ , one has first to ensure that

$$\mathbb{E}_0 \circ \mathbb{L}_1[\rho_1] = -\mathbb{E}_0 \circ \mathbb{L}_1 \circ \mathbb{L}_0^{-1} \circ \mathbb{L}_1[\rho_0] = 0, \quad (4.14)$$

and, analogously, for the higher order contributions to 4.6.

#### 4.0.10 Dissipative Perturbation of a Unitary Evolution

In the following, we restrict to a less general situation than the ones addressed in the previous section; namely, we will stick to purely dissipative perturbations  $\mathbb{L}_1 = \mathbb{D}$  as in 4.2 of a generator  $\mathbb{L}_0[\rho] = -i[H, \rho]$  as in Example 4.0.2:

$$\mathbb{L}_\varepsilon[\rho] = -i[H, \rho] + \varepsilon \mathbb{D}[\rho], \quad \mathbb{D}[\rho] = \sum_\alpha \left( h_\alpha \rho h_\alpha^\dagger - \frac{1}{2} \{ h_\alpha^\dagger h_\alpha, \rho \} \right). \quad (4.15)$$

*Lemma 4.* The map  $\widehat{\mathbb{D}} = \mathbb{E}_0 \circ \mathbb{D} \circ \mathbb{E}_0$ , with  $\mathbb{E}_0$  given by 4.3, generates a positive, trace preserving map on the  $\gamma_t^{(0)}$ -invariant states  $\rho$  that commute with  $H$ .

*Lemma 5.* The map  $\widehat{\mathbb{D}} = \mathbb{E}_0 \circ \mathbb{D} \circ \mathbb{E}_0$ , with  $\mathbb{E}_0$  given by 4.3, generates a positive, trace preserving map on the  $\gamma_t^{(0)}$ -invariant states  $\rho$  that commute with  $H$ .

**Proof:** If  $\mathcal{S}_0 \ni \rho = \sum_{j=1}^d \rho_{jj} |j\rangle\langle j|$ ,

$$\widehat{\mathbb{D}}[\rho] = \sum_{i,j=1}^d \rho_{ii} \langle j | \mathbb{D} [|i\rangle\langle i|] |j\rangle\langle j| = \sum_{i,j=1}^d \rho_{ii} \sum_\alpha \left( |\langle j | h_\alpha | i \rangle|^2 - \delta_{ij} \langle j | h_\alpha^\dagger h_\alpha | j \rangle \right) |j\rangle\langle j|. \quad (4.16)$$

Then,

$$\dot{\rho}_{jj} = \sum_{i=1}^d \rho_{ii} \sum_\alpha \left( \left| \langle j | h_\alpha | i \rangle \right|^2 - \delta_{ij} \langle j | h_\alpha^\dagger h_\alpha | j \rangle \right) \geq -h \rho_{jj}, \quad (4.17)$$

where  $h = \left\| \sum_\alpha h_\alpha^\dagger h_\alpha \right\|^2$ . Therefore, the eigenvalues of any  $\rho \in \mathcal{S}_0$  remain positive while evolving with  $\exp(t\widehat{\mathbb{D}})$ .

#### 4.0.11 Entanglement production

In this section we shall study whether an appropriate, purely dissipative Lindblad dynamics can create entanglement even when it is a weak perturbation of a non-entangling unitary dynamics. The fact that a Lindblad dynamics that does not include a unitary part is able to create entanglement is shown in [21] in a very concrete example, and the fact that a unitary evolution can be added if the invariant state is an eigenstate of the unitary evolution is the result in [22]. Here we concentrate on the assumption that this is exactly not the case; instead, we tackle the situation where the states invariant under the unitary time evolution are all separable. First, we observe that

*Lemma 6.* Let the generator  $\mathbb{L}_0$  be given by a Hamiltonian of the form  $H = H_1 \otimes 1 + 1 \otimes H_2$  where  $H_1$  has eigenvalues  $E_{1,k}$  and  $H_2$  eigenvalues  $E_{2,l}$  where  $E_{1,k} \neq E_{2,l} \quad \forall l, k$ . Then, all  $\gamma_t^{(0)}$ -invariant states are separable. If the solutions of  $\widehat{\mathbb{D}}[\rho] = 0$ , where  $\widehat{\mathbb{D}}$  is as in 4.16,

are not on the border of the set of separable states, then there exists  $\varepsilon_0$  such that for all  $\varepsilon \leq \varepsilon_0$  the invariant state is unique and separable.

**Proof:** Let  $\varepsilon_0$  be smaller than the radius in which the perturbation expansion of  $\rho(\varepsilon)$  such that  $\mathbb{L}_\varepsilon[\rho(\varepsilon)] = 0$  converges. Because of Proposition 1, if all solutions of  $\widehat{\mathbb{D}}[\rho] = 0$  are invertible, then there can exist only one; as a consequence (see the proof of Lemma 3), there can be only one  $\rho(\varepsilon)$  within its convergence radius. Further, in a sufficiently small neighborhood of a state not on the border of the convex set of separable states, all states are separable.

The following result will instead provide instances of a contrary behavior, more along the lines of Example 4.0.6, showing the possibility of creating entanglement by weak dissipative perturbations.

*Proposition 2.* Consider the generator 4.15 with a non-entangling Hamiltonian as in Lemma 6 and a dissipative perturbation  $\mathbb{D}$  such that  $\widehat{\mathbb{D}}[\rho] = 0$  has only one solution. Then, there is a unique state in the kernel of  $\mathbb{L}_\varepsilon$ , given by the perturbation expansion  $\rho(\varepsilon) = \sum_n \varepsilon^n \rho_n$  where

$$\rho_n = (-)^n \left( (\text{id} - \widehat{\mathbb{D}}^{-1} \circ \mathbb{E}_0 \circ \mathbb{D}) \circ \mathbb{L}_0^{-1} \circ \mathbb{D} \right)^n [\rho_0]. \quad (4.18)$$

**Proof:** Given a zero-th order approximation  $\rho_0$  such that  $\mathbb{L}_0[\rho_0] = 0$  and  $\widehat{\mathbb{D}}[\rho_0] = 0$ , we put ourselves in the most general situation where  $\mathbb{E}_0 \circ \mathbb{D} \circ \mathbb{L}_0^{-1} \circ \mathbb{D}[\rho_0] \neq 0$ . We then add to  $\rho_1 = -\mathbb{L}_0^{-1} \circ \mathbb{D}[\rho_0]$  a matrix  $\sigma_1$  such that  $\mathbb{L}_0[\sigma_1] = 0$ ; the new matrix  $\tilde{\rho}_1 = \rho_1 + \sigma_1$  still solves  $\mathbb{L}_0[\tilde{\rho}_1] = -\mathbb{D}[\rho_0]$ . Since we want to solve  $\mathbb{L}_0[\rho_2] = -\mathbb{D}[\tilde{\rho}_1]$  by inverting  $\mathbb{L}_0$ , we seek  $\sigma_1$  such that

$$\mathbb{E}_0 \circ \mathbb{D}[\rho_1] + \widehat{\mathbb{D}}[\sigma_1] = 0. \quad (4.19)$$

Since we assumed that  $\widehat{\mathbb{D}}$  to have only one state in its kernel, it cannot vanish on  $\mathbb{E}_0 \circ \mathbb{D}[\rho_1]$ ; the latter is a traceless matrix and both its normalized positive and negative parts would be states in the kernel of  $\widehat{\mathbb{D}}$  (see the proof of Lemma 3). Therefore,

$$\tilde{\rho}_1 = \left( \text{id} - \widehat{\mathbb{D}}^{-1} \circ \mathbb{E}_0 \circ \mathbb{D} \right) [\rho_1] = - \left( \text{id} - \widehat{\mathbb{D}}^{-1} \circ \mathbb{E}_0 \circ \mathbb{D} \right) \circ \mathbb{L}_0^{-1} \circ \mathbb{D}[\rho_0].$$

Iterating this construction, one obtains the contributions to the perturbation expansion as in [? ].

**Remark 4.0.3.** In general, according to Lemma 2, in order to solve equation 4.19 for a generic  $\mathbb{L}_1$  in the place of  $\mathbb{D}$ , one has to consider the map  $\widehat{\mathbb{E}}_1$  that remains associated to it by the time-average, and check whether  $\widehat{\mathbb{E}}_1 \circ \mathbb{E}_0 \circ \mathbb{D}[\rho_1] = 0$ .

**Example 4.0.7.** The map  $\widehat{\mathbb{D}}$  in Example 4.0.3 has only one invariant state; according to 4.0.5 its inverse is given by  $\widehat{\mathbb{D}}^{-1}[X] = -X$  on  $X$  such that  $\text{Tr}(X) = 0$ . Therefore, by means of 4.19 equation 4.18 with  $n = 1$  and  $\rho_0 = \sum_{i=1}^d \rho_{ii} |i\rangle\langle i|$  yields

$$\rho_1 = -\left(\text{id} - \mathbb{E}_0 \circ \mathbb{D}\right) \circ \mathbb{L}_0^{-1} \circ \mathbb{D}[\rho_0] = \sum_{i=1}^d |\psi(i)|^2 |i\rangle\langle i| - i\varepsilon \sum_{j \neq k} \frac{\psi(j)\psi^*(k)}{E_j - E_k} |j\rangle\langle k| \quad (4.20)$$

$$\rho(\varepsilon) = (1 + \varepsilon) \sum_{i=1}^d |\psi(i)|^2 |i\rangle\langle i| - i\varepsilon \sum_{j \neq k} \frac{\psi(j)\psi^*(k)}{E_j - E_k} |j\rangle\langle k| + o(\varepsilon). \quad (4.21)$$

Consider the bipartite setting of Lemma 6 and set  $1 \leq \alpha, \beta \leq a$ ,  $a^2 = d$ ,

$$|j\rangle = |\alpha\beta\rangle = |\alpha\rangle \otimes |\beta\rangle \quad \text{where} \quad H|\alpha\beta\rangle = E_{\alpha\beta}|\alpha\beta\rangle, \quad E_{\alpha\beta} = E_{1,\alpha} + E_{2,\beta}.$$

By transposing the first party with respect to the orthonormal basis  $\{|\alpha\rangle\}_{\alpha=1}^a$ , as in Example 4.0.6, one obtains

$$\rho^\Gamma(\varepsilon) = (1 + \varepsilon) \sum_{\alpha,\beta=1}^a |\psi_{\alpha\beta}|^2 |\alpha\rangle\langle\alpha| \otimes |\beta\rangle\langle\beta| - i\varepsilon \sum_{(\alpha,\beta) \neq (\gamma,\delta)} \frac{\psi_{\alpha\beta}\psi_{\gamma\delta}^*}{E_{\alpha\beta} - E_{\gamma\delta}} |\gamma\rangle\langle\alpha| \otimes |\beta\rangle\langle\delta| + o(\varepsilon).$$

Suppose  $\psi_{\alpha_1\beta_1} = \psi_{\alpha_2\beta_2} = 0$  for  $\alpha_1 \neq \alpha_2$  and  $\beta_1 \neq \beta_2$ ; then, choosing an entangled state  $|\phi\rangle$  supported only in the subspace spanned by  $|\alpha_1\beta_1\rangle$  and  $|\alpha_2\beta_2\rangle$ , one calculates

$$\langle\phi|\rho^\Gamma(\varepsilon)|\phi\rangle = \varepsilon \frac{\Im\left(\phi_{\alpha_1\beta_1}\psi_{\alpha_2\beta_1}\phi_{\alpha_2\beta_2}^*\psi_{\alpha_1\beta_2}^*\right)}{E_{1,\alpha_1} + E_{2,\beta_2} - (E_{1,\alpha_2} + E_{2,\beta_1})} + o(\varepsilon).$$

This expectation can always be made negative and thus, by applying the partial transposition criterion,  $\rho(\varepsilon)$  results entangled to order  $\varepsilon$ . Notice that the assumptions on the coefficients ensure that the projection of  $|\psi\rangle$  onto the subspace spanned by  $|\alpha_2\beta_1\rangle$  and  $|\alpha_1\beta_2\rangle$  is entangled; furthermore, Example 11 in [23] ensures that  $\rho(\varepsilon)$  is an asymptotic state for the given time-evolution.

## Chapter 5

# Matrix Product States and Classical Simulation of Spin Systems

The second part of this Thesis is devoted to novel algorithms for simulating ground states of locally interacting spin chains on a lattice. How is it related to quantum information?

Well, the concept of entanglement lies at the core of these methods.

These recently developed methods use a certain class of states which has only a limited amount of entanglement but yet being a very good ansatz to approximate ground states of the systems mentioned above.

The essential difficulty that arises when calculating quantities in many body problem is the exponentially scaling number of the required parameters as a function of the system size (number of interacting particles). Thus, lacking of an explicit solution, one has to find some description of the state which has only polynomially many parameters and an algorithm with polynomial computational cost.

It turned out, that a non critical ground state of local Hamiltonians on a spin chain has the very important property that the entropy of a selected block saturates as the block size grows, while diverges logarithmically at critical points.

It also turned out that in 1D these kind of ('finitely correlated' [24]) states has a computationally very beneficial characterization, the so-called MPS (matrix product states) for which efficient algorithms have been constructed and achieved decent success.

It can be shown that the celebrated DMRG method by S.White [25] also uses the class of MPS, but important enhancements over the DMRG method have been given, not to

mention the extension for higher dimensional geometries. The matrix product states description gives us an accurate approximation of the ground states of gapped Hamiltonians on a spin chain, but it can also be applied to detect phase transitions. Various numerical methods have been proposed to carry out these simulations and have achieved decent success. Their higher dimensional generalizations also appeared the PEPS [26], [29] and its extension to infinite lattices, the iPEPS [30] and [31], tree tensor networks [32], [59], MERA [34] and other approaches are promising, but their extensive use is hampered by their large (but nevertheless polynomial) computational costs.

In one branch of these methods, that uses MPS description in one spatial dimension and more generally tensor networks in higher dimensions, one describes the state of a spin system in a lattice by placing tensors to each vertex. These tensors has one ‘physical’ index corresponding to the local spin basis vectors, and ‘virtual indices’ for each bond coming out from the vertex. The dimension of this index, the ‘bond dimension’ is a parameter. The quantum mechanical amplitude of a given spin configuration is obtained by fixing the physical indices and contracting all the virtual ones. In one dimension, the computation of the expectation of a local operator  $O$  i.e.  $\langle \psi | O | \psi \rangle$  can be interpreted as the contraction of the chain since we have to sum over all the virtual indices. This can be computed exactly for a fixed bond dimension in 1D, but for higher dimensional lattices this does not hold any more. To see this, consider a subset of the lattice and contract all the indices belonging to the ‘inner’ bonds. Clearly the resulting tensor has a number of indices proportional to the length of the boundary of the subset. Several approximative techniques have been developed (see e.g. [26], [51]) to overcome this and carry out the contraction in polynomial time.

The construction of efficient algorithms for higher dimensional case is still a very challenging task.

Without completeness let us list some leading researchers with major contributions to this field: S. R. White, U. Schollwöck (DMRG method), G. Vidal, J. I. Cirac, F. Verstraete (MPS and PEPS methods), M. B. Hastings (essential mathematical proofs).

The next chapters are organized as follows. In Chapter 5 we give a brief introduction to MPS (with references) and give the main ideas of constructing algorithms for a 1D lattice and their possible extension for square lattices. In Chapter 6, a so-called finite entanglement-scaling method is presented, which is an effective tool to study phase transitions, a concrete interesting model is also discussed here. Chapter 7 gives a brief introduction to the generalizations for higher dimensions: Tensor network states and their use. Only a very short insight is given to this mathematically extremely challenging, fruitful topic which still offers many hard open problems. Lastly, in Chapter 8, we present an algorithm for simulating locally interacting translational symmetric spin systems on

infinite trees. Probing this for the Ising model on the Bethe lattice we find similarities between the physics of the 1D model and this model with one striking difference.

## 5.1 Matrix Product States

Assume we have  $N$  spins along a chain. As usual, introduce local basis states for each spin, e.g. for the  $i$ th spin  $|s_i\rangle \in \{|0\rangle, |1\rangle\}$ . The state  $|\Psi\rangle$  of the whole system can be written as

$$|\Psi\rangle = \sum_{s_1 \dots s_N} c_{s_1 \dots s_N} |s_1\rangle \dots |s_N\rangle.$$

Obviously for a chain of half spins we have  $2^N$  coefficients. This description is not pretty useful if one has many qubits, because the number of the coefficients grows exponentially in  $N$  and it's not straightforward to read out translation invariance either, which is often the case if for example  $|\Psi\rangle$  is an eigenstate of a translation-invariant Hamiltonian. Now we apply the Schmidt decomposition to rewrite the coefficients as follows.

As introduced in [37], split the state  $\Psi$  of  $n$  qubits on a  $n$  site lattice  $(1, 2, \dots, n)$  into two parts by cutting between the site  $i-1$  and site  $i$

$$|\Psi\rangle = \sum_{a=1}^{D_{i-1}} \lambda_a^{(i-1)} |e_a^{(1..i-1)}\rangle |f_a^{(i..N)}\rangle \quad (5.1)$$

where  $\{e_a^{(1..i-1)}\}_{a=1}^{D_{i-1}}$  stands for the  $D_{i-1}$  dimensional basis on the first sublattice up to the site  $i-1$ , and  $\{f_a^{(i..N)}\}_{a=1}^{D_{i-1}}$  denotes the basis on the rest of the chain, while  $\lambda_a^{(i-1)} > 0$ ,  $a = 1, 2, \dots, D_{i-1}$  are the Schmidt coefficients across the cut between site  $(i-1)$  and site  $i$ . Clearly  $D_{i-1} \leq 2^{i-1} \wedge 2^{N-i+1}$ . In the same fashion let us do the cut after the site  $i$

$$|\Psi\rangle = \sum_{b=1}^{D_i} \lambda_b^{(i)} |g_b^{(1..i)}\rangle |h_b^{(i+1..N)}\rangle. \quad (5.2)$$

We can combine the two decompositions, expressing  $f_a^{(i..N)}$  by the basis  $\{h_b^{(i+1..N)}\}$  and the local basis  $s_i$

$$|f_a^{(i..N)}\rangle = \sum_{s_i=0}^1 \sum_{b=1}^{D_i} \Gamma_{a,b}^{(i)s_i} \lambda_b^{(i)} |s_i\rangle |h_b^{(i+1..N)}\rangle.$$

In this way we have got the tensors  $\Gamma_{a,b}^{(i)s_i}$ , we inserted  $\lambda_b^{(i)}$  only for convenience. The indices  $a, b$  are called virtual and  $s_i$  is called physical index. In the general case, these tensors vary from site to site.

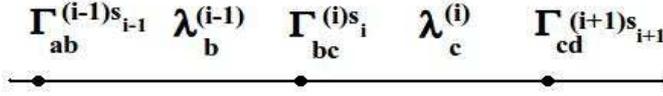


FIGURE 5.1: MPS tensors and Schmidt vectors

Plug this into (5.1) to get

$$|\Psi\rangle = \sum_{s_i=0}^1 \sum_{a=1}^{D_{i-1}} \sum_{b=1}^{D_i} \lambda_a^{(i-1)} \Gamma_{a,b}^{(i)s_i} \lambda_b^{(i)} |e_a^{(1..i-1)}\rangle |s_i\rangle |h_b^{(i+1..N)}\rangle \quad (5.3)$$

The use of orthonormal basis in the Schmidt theorem implies some normalization conditions for the Schmidt vectors and the  $\Gamma$  tensors. For later purposes we list them.

$$\text{Tr} \lambda^{(i)2} = 1 \quad (5.4)$$

$$\sum_s (\Gamma^{(i)s} \lambda^{(i)})^\dagger \Gamma^{(i)s} \lambda^{(i)} = \mathbb{1} \quad (5.5)$$

$$\sum_s (\lambda^{(i-1)} \Gamma^{(i)s})^\dagger \lambda^{(i-1)} \Gamma^{(i)s} = \mathbb{1}. \quad (5.6)$$

If we introduce  $A_i^s = \Gamma^{(i)s} \lambda^{(i)}$  we obtain the form

$$|\Psi\rangle = \sum_{a,b,s_i} A_{a,b}^{s_i} |e_a^{(1..i-1)}\rangle |s_i\rangle |h_b^{(i+1..N)}\rangle. \quad (5.7)$$

Recapitulating the coefficients of the tensor  $A_{a,b}^{(s_i)}$ . This procedure gives rise to the form of

$$|\Psi\rangle = \sum_{s_1, \dots, s_N=1}^d \text{Tr}[A_1^{s_1} \dots A_N^{s_N}] |s_1\rangle \dots |s_N\rangle. \quad (5.8)$$

with the  $N$  pieces of matrices  $A_i^{s_i}$  of dimension  $D_i$  (usually called the bond dimension) each of them associated with a lattice site and having a physical index  $s_i$  (e.g. spin). This decomposition of a state is called MPS, short for matrix product state for apparent reason, because the coefficients are expressed as a trace of a product of matrices. For open boundary conditions  $A_1^{s_1}$  must be a row and  $A_N^{s_N}$  must be a column vector. Translation invariance manifests itself in the use of the same square matrices for each site i.e.  $A_i^{s_i} = A^{s_i}$  independently from the position. This also enables the extension to an infinite chain when the iMPS name is used: We describe the state by only a set of matrices moreover we can also forget about boundary conditions.

**Remark 5.1.1.** Why it may be useful? An  $N$ -particle quantum state can be fully characterized by  $O(d^N)$  parameters, in the worst case. The MPS description are described by a number of parameters that does not grow exponentially with the number of particles. For instance, for  $N$  pieces of  $d$ -level systems it is  $O(NdD^2)$  and in case of full translation invariance and an infinite chain is described by only  $d$  MPS matrices, so the number of the required parameters scales like  $O(dD^2)$ . As will be pointed out later, certain important classes of states, namely those with bounded entanglement entropy can be well described by means of MPS. These include ground states of local Hamiltonians, or even low lying excited states.

**Remark 5.1.2.** The special case  $D = 1$  corresponds to the product state as one can readily see. E.g. in case of a spin chain with  $d = 2$  one place the state

$$|\varphi\rangle_i = A_i^0|0\rangle_i + A_i^1|1\rangle_i$$

to site  $i$  with  $A_i^0, A_i^1 \in \mathbb{C}$ ,  $|(A_i^0)^2| + |(A_i^1)^2| = 1$  and the state vector reads

$$\begin{aligned} |\Psi\rangle &= |\varphi\rangle_1 \otimes |\varphi\rangle_2 \otimes \dots \otimes |\varphi\rangle_N \\ &= \sum_{s_1} A_1^{s_1} |s_1\rangle \otimes \sum_{s_2} A_2^{s_2} |s_2\rangle \otimes \dots \otimes \sum_{s_N} A_N^{s_N} |s_N\rangle \\ &= \sum_{s_1 \dots s_N} A_1^{s_1} A_2^{s_2} \dots A_N^{s_N} |s_1, s_2 \dots s_N\rangle \end{aligned}$$

This is indeed an MPS but with complex numbers instead of matrices (therefore the  $\text{Tr}$  can be omitted).

**Remark 5.1.3.** Any state has an MPS description, however not unique, e.g. if  $A_i^{s_i}$  and  $T$  has the same size and  $\exists T^{-1}$  then the new MPS matrices

$$A_i^{s_i} \mapsto T A_i^{s_i} T^{-1}$$

describe the same state [26].

**Remark 5.1.4.** Translational invariance manifests itself in placing the same set of matrices to each vertex. As we will point out later it also implies that MPS are well suited for local transformations and computation of the expectations of local operators.

**Remark 5.1.5. Valence bond construction.** There exist an other useful way of looking at the construction of the MPS which help us to generalize such kind of states to higher dimensions [26].

Start by introducing a virtual substructure: Assign two virtual particles to each physical constituent (e.g. spins) with virtual (or bond) dimension  $D$  and let the neighbouring

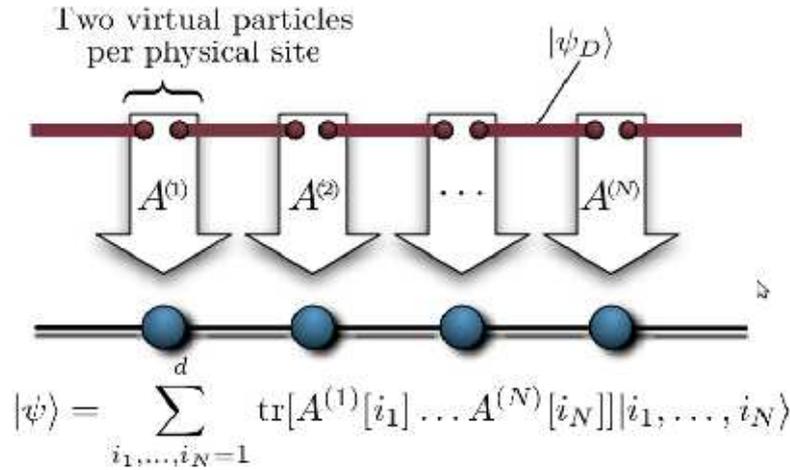


FIGURE 5.2: Valence bond construction of MPS

states be in the maximally entangled state as follows

$$|\Psi_D\rangle = \frac{1}{\sqrt{D}} \sum_{k=1}^D |k\rangle|k\rangle. \quad (5.9)$$

So now one associates a virtual state  $|\Psi_D\rangle^{\otimes N}$  on the Hilbert space  $(\mathbb{C}^D \otimes \mathbb{C}^D)^{\otimes N}$  to the real state.

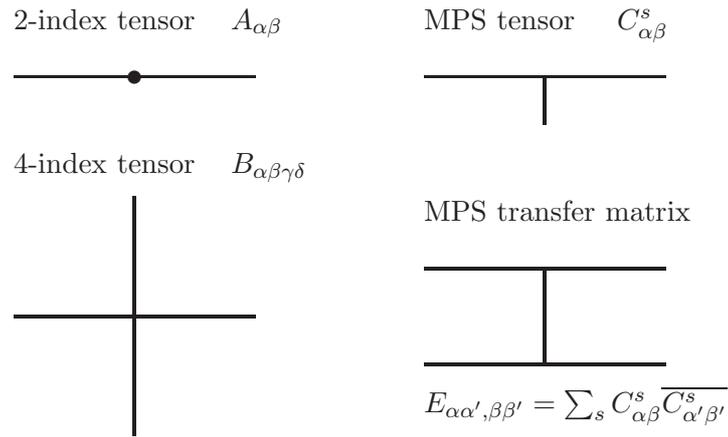
Then introduce local linear maps  $A^{(s_k)} : \mathbb{C}^D \otimes \mathbb{C}^D \mapsto \mathbb{C}^d$  for each of these pairs to construct the real state vector

$$A^{(s_k)} = \sum_{s_k=1}^d \sum_{a,b=1}^D A_{a,b}^{(s_k)} |s_k\rangle \langle a, b|.$$

In other words this means that we associate  $d$  pieces of  $D$  by  $D$  matrices (a tensor with 3 indices) to each site. So in this picture, one prepares a virtual systems with duplicated number of particles with virtual dimension  $D$ , every neighbour being in a maximally entangled state. Then, one applies local maps to all pairs in order to obtain our real physical state with the parameters of these local maps, see figure (5.2).

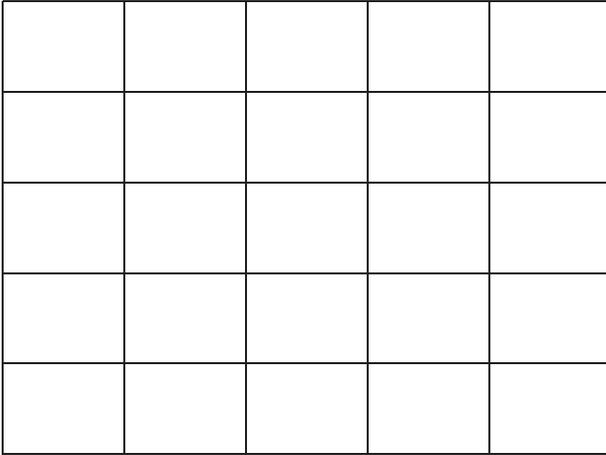
### Diagrammatic representations of tensors

One can make useful diagrams about the tensor network which shows its structure and the contractions to be performed. So we draw a graph, each vertex corresponds to a tensor, each bond represents an index. If a bond connects two vertices then summation takes place over the bond index, an open edge denotes a free index.



### 2D tensor network

Tensor network of PEPS with OBC in a  $6 \times 6$  square lattice. Each vertex represents a tensor, every bond corresponds to an index.



#### 5.1.1 Correlations

For example take the two operators  $T^{(i)}$  and  $T^{(j)}$  acting on the sites  $i$  and  $j$  of the spin chain. The expectation of their products can be expressed as

$$\langle T^{(i)} T^{(j)} \rangle = \text{Tr}(E_1^{(1)} \dots E_1^{(i-1)} E_T^{(i)} E_1^{(i+1)} \dots E_1^{(j-1)} E_T^{(j)} E_1^{(j+1)} \dots E_1^{(N)}) \quad (5.10)$$

where the so-called transfer operators are defined as follows

$$E_T^i = \sum_{j,k=1}^d \langle j|T|k\rangle (A_k^{(i)} \otimes \overline{A_j^{(i)}}).$$

From now on, assume translational invariance i.e. site independent set of MPS matrices i.e.  $A_k^{(i)} = A_k$ , moreover denote  $E_{\mathbb{1}}$  simply by  $E$ . With these assumptions one uses the expansion  $E^{n-1} = |L\rangle\langle R| + \lambda_2^{n-1}|L'\rangle\langle R'| + \dots$  using the eigenvectors of  $E$ ,  $\lambda_2$  the second largest eigenvalue (assumed to be unique here for simplicity) and assuming that  $E$  is normalized such that  $\langle R|L\rangle = 1$ . Let us plug this into (5.10) to get

$$\begin{aligned} \langle T^{(i)}T^{(i+n)}\rangle &= \langle R|T^{(i)}E^{n-1}T^{(i+n)}|L\rangle \\ &= \langle R|T^{(i)}|L\rangle\langle R|T^{(i+n)}|L\rangle + \lambda_2^{n-1}\langle R|T^{(i)}|L'\rangle\langle R'|T^{(i+n)}|L\rangle \\ &= \langle T^{(i)}\rangle\langle T^{(i+n)}\rangle + \lambda_2^{n-1}\langle R|T^{(i)}|L'\rangle\langle R'|T^{(i+n)}|L\rangle \end{aligned}$$

which gives rise to the relation

$$C_T(n) = \langle T^{(i)}T^{(i+n)}\rangle - \langle T^{(i)}\rangle\langle T^{(i+n)}\rangle \propto \lambda_2^{n-1}.$$

This shows the necessarily exponential falling of the correlation function and the implication of the relation

$$\xi = -1/\log |\lambda_2| \tag{5.11}$$

for the correlation length, given  $\lambda_1 = 1$ . Mind that these concrete formulas are valid as long as the largest eigenvalue is unique and normalized to one, and  $\lambda_2 < 1$  is also unique, but (5.11) remains valid in case of degeneracy, however the degenerate leading eigenvalues can cause problems in the algorithms based on finding the leading eigenvectors. Hereinafter this question will be investigated as well.

### Example 5.1. AKLT model

*Interestingly, MPS have already been appeared in the work of Affleck, Kennedy, Lieb and Tasaki [38]. They pointed out that the ground state of the following Hamiltonian on a spin-1 chain had got an exact MPS description with bond dimension 2*

$$H_{AKLT} = \sum_i \left( \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2 + \frac{2}{3} \right) = \sum_i P_{i,i+1}$$

*so the Hamiltonian can be also written as a sum of projectors:  $P_{i,i+1}$  projects onto onto the 5-dimensional spin 2 subspace of 2 spin 1s on the site  $i$  and  $i + 1$ . See also in [26].*

One can show that its ground state is

$$|\Psi\rangle_{AKLT} = \sum_{s_1, \dots, s_N=1}^3 \text{Tr}[A^{(s_1)} \dots A^{(s_N)}] |s_1\rangle \dots |s_N\rangle$$

with matrices  $A^1 = \sigma_3$ ,  $A^2 = \mathbb{1}$ ,  $A^3 = -\sigma_1$  therefore the bond dimension 2 and due to translational invariance, we have got the same set of matrices for all sites. Notice that as can be concluded from forthcoming facts about MPS, finite bond dimensions imply finite entanglement entropy and finite correlation lengths.

### 5.1.2 Matrix Product Operators

Take the matrices  $Q^{k_i}$  associated to each lattice site and the spin operators  $Z^{k_i}$  in the basis of the site  $i$ . The operator  $M$  of the form

$$M = \sum_{k_1 \dots k_N} \text{Tr}(Q_1^{k_1} Q_2^{k_2} \dots Q_N^{k_N}) Z^{k_1} \otimes \dots \otimes Z^{k_N}. \quad (5.12)$$

is called MPO, short for matrix product operator. Accordingly we call the dimensions of  $Q^{k_i}$  the bond dimensions of the MPO [36].

Applying this to  $|\Psi\rangle$  the updated MPS matrices are easy to compute site by site from the corresponding terms of  $M$ . In brief, taking the  $i$ th spin, the related set of the MPS matrices  $A_i^{s_i}$  then the updated ones can be obtained by manipulating on them with the related MPO matrices  $Q_i^{s_i}$ . In fact

$$M|\Psi\rangle = \sum_{s_1, \dots, s_N=1}^d \sum_{k_1 \dots k_N=1}^D \text{Tr}[(Q_1^{k_1} \otimes A_1^{s_1}) \dots (Q_N^{k_N} \otimes A_N^{s_N})] |Z^{k_1} s_1\rangle \dots |Z^{k_N} s_N\rangle$$

from which one can read the required transformations for the new MPS matrices (from now on we omit the site indices)

$$A^{s'} \longrightarrow \sum_{s,k} Q^k \langle s' | Z^k | s \rangle \otimes A^s. \quad (5.13)$$

We can write it even more compactly as

$$A^{s'} \longrightarrow \sum_s \hat{Q}^{s's} \otimes A^s \quad (5.14)$$

by defining the ‘local transfer tensors’ as  $\hat{Q}^{s's} = \sum_k Q^k \langle s' | Z^k | s \rangle$ . As it resembles the usual matrix product, we could even define the operation  $\hat{\otimes}$  between two block matrices

as follows

$$(B\hat{\otimes}C)_{ij} = \sum_k B_{ik}\hat{\otimes}C_{kj}.$$

Making use of this, (5.21) reads

$$\hat{A} \longrightarrow \hat{Q}\hat{\otimes}\hat{A}$$

where the block vector  $\hat{A} = (A^1 \dots A^d)$  consists of the MPS matrices.

### 5.1.3 Area laws in one dimension

Given a state  $\psi$  in a Hilbert space which consists of local Hilbert spaces associated to the vertices of the graph  $G$ , the so-called entanglement entropy of the contiguous set  $I \subset G$  with reduced density  $\rho_I$

$$S(\rho_I) = -\text{Tr}\rho_I \log \rho_I \tag{5.15}$$

turns out to play the key role in the validity and the accuracy of all the simulations based on MPS (and their higher dimensional generalizations).

The first crucial observation is the maximal entanglement entropy content of the MPS. The definition of the MPS gives us a clear upper bound for the entropy content

$$S(\rho_I) \leq 2 \log(D).$$

This very important relation shows that the maximal entropy content scales logarithmically with the bond dimension. Its crucial importance lies in the fact that non critical ground states has a finite entropy which thus can be described by MPS with a high enough but finite bond dimension. In general an ‘area law for the entropy’ means that the entanglement entropy is bounded by the boundary surface area of a distinguished region  $I$  of the lattice

$$S(\rho_I) = O(s(I)).$$

### General 1-D gapped local spin Hamiltonians

An area law exists for non critical ground states. Its proof was given by Hastings based on Lieb-Robinson bounds which is also essential in the proof of exponential damping correlations in gapped local models.

$$H = \sum_j H_{j,j+1}$$

Impose finite interaction strength:  $\|H_{j,j+1}\| < \infty$ .

**Theorem 5.1. Area law for spin chains with energy gap** *Let  $H$  a local Hamiltonian on a spin chain having a unique ground state with a finite energy gap  $\Delta E$  to the first excited state. Consider the block  $I = \{1, \dots, N\}$ . Then,*

$$S(\rho_I) \leq c_0 \xi \log(6\xi) \log(d) 2^{6\xi \log(d)}$$

for some constant  $c_0 > 0$  of order unity,  $\xi = \max(2v/\Delta E, \xi_C)$ ,  $v$  is the velocity of sound and  $\xi_C$  is defined by the Lieb-Robinson theorem.

For the complicated proof of Hastings, see his paper itself [39]. The essential, profound theorem is as follows [40]

**Theorem 5.2. Lieb-Robinson-Theorem**

*Let  $H$  a local Hamiltonian as above. Then there exists a velocity of sound  $v > 0$  and  $\mu, c > 0$  such that for any two operators  $A$  and  $B$  with support on disjoint sets  $X$  and  $Y$  we have the following upper bound for the norm of the time dependent commutator*

$$\|[A(t), B]\| \leq c \|A\| \|B\| \exp(-\mu l_{XY} - v|t|), \quad (5.16)$$

where the distance between the sets is  $l_{XY} = \text{dist}(X, Y) = \min_{i \in X, j \in Y} (|i - j|)$ , moreover

$$A(t) = e^{iHt} A e^{-iHt}.$$

*The velocity  $v$  is of order of the maximal strength of the pair interactions in the Hamiltonian.*

To highlight the intuitive essence of this statement imagine the following. If we have two operators,  $A$  and  $B$  acting on disjoint sets of the chain, so far away from each other, then they commute:  $[A, B] = 0$ . As soon as  $A$  gets evolved by the Hamiltonian, its support gets larger and larger, so the commutator becomes nonzero, but bounded. However, after some time its norm decays at least exponentially and tends to zero in time, according to the theorem above.

This extremely important theorem can also be used to give a bound for the group velocity of a large class of discrete quantum systems which can be used to prove that a non-vanishing spectral gap implies exponential clustering in the ground state of such systems [27].

See [28] for a review on area laws.

**Example 5.2.** *1D Ising model asymptotic entropy, sketch of the proof with references [28].*

### 5.1.4 Phase Transitions and The Goal of the Simulations

The aim of the simulations is to find the ground state  $\psi$  and compute some relevant physical quantities [41]. This means expectations of local observables like  $\langle \psi | O | \psi \rangle$ , spatial correlations like  $\langle \psi | O^i O^j | \psi \rangle$  or even simulate real time evolution of states and compute time depending quantities such as correlations in time. Computing the ground state corresponds to study the system at zero temperature. Note that sometimes the study of the low lying energy levels can also be very important.

An other issue, the computation of thermal averages will also be addressed later.

Usually one can view the Hamiltonian as the function of parameters such as the coupling strength or external magnetic field, so we have the form, say  $H(\lambda)$  is a one or more parameter family of Hamiltonians. Very often, the study of complex systems reveals that the macroscopic behavior of the system, characterized by the physical quantity  $O(\lambda)$  can show drastic changes when tuning a parameter  $\lambda$  of the model. From a mathematical point of view, we say that a phase transition happens when  $O(\lambda)$  is not an analytic function of  $\lambda$  in the thermodynamical limit. The physics and mathematics of phase transitions are extremely extensive.

Usually, when trying to give a rigorous solution for the underlying model (i.e. explicitly compute the underlying quantities) one encounters massive mathematical difficulties. What is even more, it is proven that for many (relevant!) models such an explicit exact solution does not exist in the sense that one cannot find the exact answer in polynomial time (when the number of the operations grows polynomially with the size of the system). For example it is shown that the partition function of classical Ising models cannot be computed efficiently on non planar lattices [47].

In fact, one can solve explicitly only some classes of one dimensional quantum models, no general method for the 2D case exists. This disappointing fact also justifies the need for efficient, versatile numerical methods.

The existing exact solutions has a very extensive literature, without the sake of completeness, we just mention the main approaches and the essential tools. The 1D quantum Ising model can be solved by the famous Jordan-Wigner transformation ([44], see also in Appendix A), which can be applied to the XX model as well. The 1D Heisenberg model can be solved by the Bethe ansatz [42], which was later applied to the 1D Hubbard model [43] by Lieb and Wu.

A famous exactly solvable two-dimensional model by Kitaev [45] has special symmetries and the Jordan-Wigner transformation can be easily applied.

For the case of the non planar classical models see [47], while the standard book for exactly solvable models is written by Baxter [46].

## 5.2 Algorithms in 1D

### 5.2.1 Effective ground state energy minimization

A system of interacting particles is described by  $H$  consists of the sum of terms, each describing the interactions between a smaller subset of particles. The computational difficulty arises because these terms usually do not commute with each other therefore one cannot factorize  $\exp(-\beta H)$  straightforwardly and the dimension of  $H$  grows exponentially in the size of the system. Two usual approaches are the imaginary time evolution which is essentially the power method for finding the eigenvector for the highest eigenvalue of  $\exp(-\beta H)$ , and the minimization of the expectation of the energy, i.e. for a fixed bond dimension, find the MPS  $\psi$  which makes the functional

$$\hat{E}_H(\psi) = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}$$

minimal [26].

#### Mean field theories

Notice that one dimensional ( $D = 1$ ) MPS describe a product state, which offers a solution for non-interacting particles. Let us assume that within some mean field theory, we approximate the system Hamiltonian by an effective, non-interacting Hamiltonian  $\tilde{H}$ , and look for its ground state  $\tilde{\Psi}$ . Apparently  $\tilde{\Psi}$  will be a product state, in other words, an MPS with  $D = 1$ .

### 5.2.2 Imaginary Time Evolution Using MPS

Taking the initial state  $|\Psi_0\rangle$ , its imaginary time evolution induced by the Hamiltonian  $H = H^\dagger$  reads

$$|\Psi_t\rangle = e^{-Ht}|\Psi_0\rangle = \sum e^{-E_k t} |\chi_k\rangle \langle \chi_k | \Psi_0 \rangle \quad (5.17)$$

expanded in the energy eigenstates basis  $|\chi_k\rangle$  of  $H$ .

With the normalization it converges to the ground state assuming its uniqueness

$$\lim_{t \rightarrow \infty} \frac{|\Psi_t\rangle}{\| |\Psi_t\rangle \|} = |\chi_0\rangle.$$

The speed of the convergence is exponential in time and quantified by the energy gap  $\Delta E = E_1 - E_0$ . Assuming  $H = H_1 + H_2$  with non commuting terms:  $[H_1, H_2] \neq 0$ . According to the Trotter-Suzuki formula

$$\exp -(H_1 + H_2)t = \lim_{n \rightarrow \infty} \left( \exp -\frac{H_1 t}{n} \exp -\frac{H_2 t}{n} \right)^n$$

allowing us to split the time  $t$  into small pieces e.g.  $\delta t = \frac{t}{n}$  to perform the multiplications piece by piece, by the terms close to the identity operator:  $e^{-\delta t H_1}$  and  $e^{-\delta t H_2}$ , respectively.

Notice that the applicability of the Trotter formula requires  $n \rightarrow \infty$  besides  $\frac{t}{n} \rightarrow 0$ , whereas the convergence to the ground state requires  $t \rightarrow \infty$  at the same time, as well. In practice one can set a  $t$  and small  $\delta t$  and apply the operators  $n$  times consecutively. Then a big enough  $n$  ensures a good convergence for example regarding the energy or other quantity. Lowering the time step  $\delta t$  and at the same time increasing the number of steps to control the convergence we get a more precise estimate. Then one should check that the results don't change significantly by increasing  $t$ .

### 5.2.3 TEBD and iTEBD

First of all, one can take finite or infinite number of lattice sites. In the finite case one should choose some boundary condition like periodic or open boundary condition and then in every time step the MPS matrices are modified. In the finite case the number of these modifications is proportional with the system size as it can be performed site by site from one end to the other.

However, taking an infinite chain and a translational invariant Hamiltonian, one can argue that the MPS description reflects that translational symmetry if one places the same set of matrices to each site. This enables us to modify only a small number of matrices (depending on the length of the period and the physical dimension). Guifré Vidal introduced such a method [48] using a representation containing the Schmidt coefficients explicitly as

$$|\Psi\rangle = \sum_{s_i, s_{i+1} \dots}^d \text{Tr}[\dots \lambda^{(i-1)} \Gamma_i^{s_i} \lambda^{(i)} \Gamma_{i+1}^{s_{i+1}} \dots] \dots |s_i\rangle |s_{i+1}\rangle \dots \quad (5.18)$$

with  $\lambda^{(i)}$  being the diagonal matrices containing the Schmidt coefficients. If for example we wish to apply a 1-local unitary  $U$  acting only on the site  $i$  then we simply need to change only(!)  $\Gamma_i^{(s_i)}$  as

$$\Gamma_i^{s_i} \longrightarrow \sum_{s'_i} U_{s_i, s'_i} \Gamma_i^{s'_i}.$$

Note that the Schmidt vector has remained unchanged meaning no variation in the entropy. No better illustration is needed to highlight the fact that the entanglement entropy (and thus the quantum correlation) between two parts of the chain can only be increased if they interact.

In fact, a 2-local operator requires a more complicated update rule involving the MPS matrices of the affected sites (and only them) and leading to a larger Schmidt number in general, yielding more entropy as well. Then we also need to neglect the small Schmidt coefficients to keep the bond dimension fixed, otherwise it grows exponentially with the number of update steps.

In order to obtain the update rule for a 2-local unitary  $O$  acting on site  $i$  and  $i+1$ , one build a larger tensor as follows

$$T^{s,t} = \lambda^{(i-1)} \Gamma^{(i)s} \lambda^{(i)} \Gamma^{(i+1)t} \lambda^{(i+1)} \quad (5.19)$$

where we signed the physical indices only and a summation is meant over the virtual ones. Our state looks like

$$|\psi\rangle = \sum_{s,t=1}^d \sum_{a=1}^{D_{i-1}} \sum_{c=1}^{D_{i+1}} T_{a,c}^{s,t} |e_a\rangle |s,t\rangle |f_c\rangle$$

with some basis  $|e_a\rangle$  and  $|f_a\rangle$ . Acting by  $O$  we should replace the tensor  $T$  by  $\tilde{T}$  according to

$$\tilde{T}_{a,c}^{s',t'} = \sum_{s,t} O_{s,t}^{s',t'} T_{a,c}^{s,t}. \quad (5.20)$$

Now, the trick is to build a matrix from  $\tilde{T}$  and perform its SVD to obtain the new tensors and Schmidt vector between the two affected sites [37]. Define the  $dD_{i-1} \times dD_{i+1}$  matrix

$$M_{(as),(ct)} = \tilde{T}_{a,c}^{s,t}$$

and decompose as

$$M_{(as),(ct)} = \sum_{b=1}^{\tilde{D}} U_{(as),b} \Lambda_{b,b} V_{b,(ct)} = \sum_{b=1}^{\tilde{D}} \lambda_a^{(i-1)} \tilde{\Gamma}_{a,b}^{(i)s} \tilde{\lambda}_b^{(i)} \tilde{\Gamma}_{b,c}^{(i+1)t} \lambda_c^{(i+1)}$$

from where the new  $\tilde{\Gamma}^{(i)}$ ,  $\tilde{\lambda}^{(i)}$  and  $\tilde{\Gamma}^{(i+1)}$  can be read out, and observe that  $\tilde{D} = \min\{dD_{i-1}, dD_{i+1}\}$ .

It is easy to see that without truncation the bond dimensions grow exponentially due to the factor  $d$ . Here comes the crucial cut: In order to keep the bond dimension fixed, we keep only the largest  $\min\{\tilde{D}, D_{cut}\}$  singular values and discard the others, where  $D_{cut}$

is a preset constant. After the truncation, a renormalization of the new Schmidt vector is needed to meet (5.4), the normalization condition (5.6) will be satisfied exactly, while there will be a small error in (5.5). In [37] they corrected this numerically by performing a 2-local update and truncation with the identity operator  $O = \mathbb{1}$  in each step.

Note that the validity of the whole algorithm is based on the fact that non-critical ground states of local Hamiltonians can actually be described by finite dimensional MPS. The case of the critical systems will be discussed later. Vidal has introduced his method to perform these steps and has called it Time Evolving Block Decimation (TEBD), or infinite TEBD (iTEBD) for the infinite case. Check out [48], [49], [50] for the original papers or see [37] for an other nice and comprehensive review by D. Nagaj, E. Farhi et al. where they extended these methods for a tree geometry as well.

#### 5.2.4 Translational Invariant Matrix Product Operators

In this paper only some of the branches of these algorithms are reviewed which are afterwards used for the study of a non trivial system possessing a complex phase diagram. In this case we use an iMPS and iMPO to perform the time evolution step. So imagine that  $H_1$  is a fully translation-invariant piece of the Hamiltonian and we could rewrite  $O_\epsilon = \exp(\epsilon H_1)$  as an iMPO with  $\epsilon = t/n$  being the time step.

$$M = \sum_{k_1, k_2, \dots} \text{Tr}(Q_1^{k_1} Q_1^{k_2} \dots) Z^{k_1} \otimes Z^{k_2} \dots$$

In this case the ground state can also assumed to have a translational invariant MPS. The MPS matrices for the product  $M|\Psi\rangle$  can be obtained by the rule

$$C^{s'} = \sum_{s, k} Q^k \langle s' | Z^k | s \rangle \otimes A^s = \sum_s Q^{\hat{s}'s} \otimes A^s. \quad (5.21)$$

Now if the bond dimension of the original MPS is  $D$  while that of the MPO is  $d$  then we have got a  $dD$  dimensional MPS and a Schmidt coefficient vector  $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_{dD})$ . In order to keep the fixed  $D$  bond dimension we have to cut these new matrices somehow optimally such that the Schmidt coefficients after the cut are close to the first  $D$  larger pieces of the Schmidt vector before the cut:  $(\lambda_1^{cut}, \dots, \lambda_D^{cut}) \sim (\lambda_1, \dots, \lambda_D)$ . In other words the state vector after the cut should be the best approximation of the updated one

$$\Psi_D^{cut} = \{\Psi_D : \|\Psi_{dD} - \Psi_D\| = \min\}.$$

One possible process is based on the observation that we can obtain the Schmidt vector as singular values of a given matrix constructed by the leading eigenvectors of the transfer

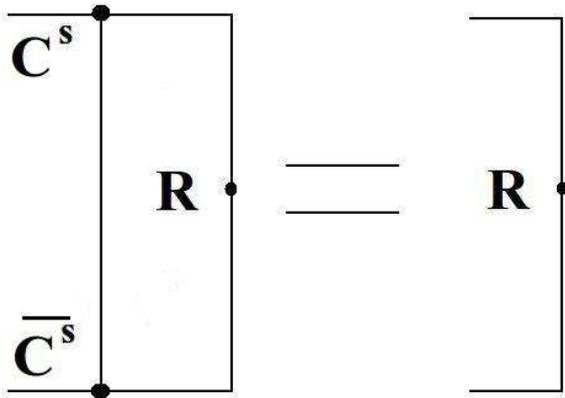


FIGURE 5.3: Right leading eigenvector equation in diagram

matrix. So denote  $r$  and  $l$  the  $d^2D^2$  dimensional right and left eigenvectors belonging to the maximal eigenvalue of  $E = \sum_s C^s \otimes \overline{C^s}$ . Assume here that this is unique and equals one in accordance with  $\langle \Psi | \Psi \rangle = 1$ .

Recast the entries of  $r$  in the  $dD \times dD$  matrix  $R$  as

$$|r\rangle = \sum_{ij} R_{ij} |ij\rangle, \quad \|r\|^2 = \text{Tr} R R^+ = 1.$$

Now we show that  $0 \leq R$  and due to the structure of  $E$  it can be computed in a more beneficial way than a leading eigenvector of a general matrix. Multiplying by  $E$  one gets

$$E|r\rangle = \sum_s C^s \otimes \overline{C^s} \sum_{ij} R_{ij} |ij\rangle = \sum_{ijk} R_{ij} C^s |i\rangle \otimes \overline{C^s} |j\rangle$$

implying

$$R'_{i'j'} = \langle i'j' | E|r\rangle = \sum_{ijs} \langle i' | C^s |i\rangle R_{ij} \langle j' | \overline{C^s} |j\rangle = \sum_k (C^s R C^{s+})_{i'j'}.$$

So the multiplication of a vector by  $E$  of this structure in the means of the matrix  $R$  is a positivity preserving map

$$R \mapsto \sum_s C^s R C^{s+}. \quad (5.22)$$

This corresponding to the power iteration and determines a positivity preserving map on the matrices (See figure (5.3)).

Assuming a unique right leading eigenvector one sees that the matrix  $R$  describing the right leading eigenvector is the fix point of this transformation, it must also be

positive, since being the unique fix point of a positive map. Same story for  $L$  with  $L = \sum_s C^{s+} L C^s$ .

Furthermore note that the computational cost of the application of  $E$  in this way scales like  $O(d^3 D^3)$  instead of  $O(d^4 D^4)$ .

The desired Schmidt vector is provided through a singular value decomposition of the product

$$\overline{\sqrt{L}} \sqrt{R} = U \lambda V'.$$

**Proof.**

Having a translation-invariant iMPS in the so-called ‘canonical form’, i.e. the Schmidt coefficients are explicitly written like in (5.18)

$$|\Psi\rangle = \sum_{s_i, s_{i+1} \dots}^d \text{Tr}[\dots \lambda \Gamma^{(s_i)} \lambda \Gamma^{(s_{i+1})} \dots] \dots |s_i\rangle |s_{i+1}\rangle \dots$$

then this obeys some normalization conditions coming from the Schmidt theorem for the decomposition, namely:

$$\sum_{a=1}^D \lambda_a^2 = 1 \quad (5.23)$$

and

$$\sum_s \sum_{b=1}^D \overline{\Gamma_{a',b}^s} \Gamma_{a,b}^s \lambda_b^2 = \delta_{a,a'}. \quad (5.24)$$

It also has a consequence for the leading eigenvector of the transfer matrix  $E = \sum_s \Gamma^s \lambda \otimes \overline{\Gamma^s} \lambda = \sum_s A^s \otimes \overline{A^s}$  with the matrices  $A^s = \Gamma^s \lambda$ . Note that we can rewrite (5.24) as  $\sum_s A^s A^{s\dagger} = \mathbb{1}$  like in (5.5). This means that the map (5.22) is completely positive and unital if the MPS matrices are normalized properly. Observe also that one can also write (5.24) as the eigenvalue equation

$$\sum_{scc'} \Gamma_{b,c}^s \overline{\Gamma_{b',c'}^s} \lambda_c \lambda_{c'} \delta_{cc'} = \sum_{cc'} E_{bb',cc'} \delta_{cc'} = \delta_{bb'}$$

so  $\delta_{bb'}$  (which can be regarded as combined index  $(bb')$ ) is a right eigenvector with eigenvalue 1, which is also the largest one. For the sake of simplicity let us simply write  $\mathbb{1}$  the  $D \times D$  unit matrix but which now can also be regarded as a  $D^2$  dimensional vector obtained by the concatenation of the rows of  $\mathbb{1}$ .

Now, imagine that after performing some operations the iMPS described by  $\Gamma^s$ ,  $\lambda$  is not in the canonical form any more, so  $E$  does not have the right leading eigenvector of the above form but some  $R_{bb'}$  with eigenvalue 1 (after normalization). Considering  $R$  as a

matrix it can be chosen to be positive (as we have seen in the last section) and written as  $R = XX^\dagger$ . E.g.  $X = X^\dagger = \sqrt{R}$ .

Now one has to find the transformation  $\Gamma^s \rightarrow \Gamma'^s$  and  $\lambda \rightarrow \lambda'$  which brings the iMPS into canonical form. The idea is to rewrite  $ER = R$  such that we arrive at the new form  $E'\mathbb{1} = \mathbb{1}$  where  $E'$  contains the new tensors  $\Gamma'^s$  and Schmidt vectors  $\lambda'$ . Let us write  $L = Y^\dagger Y$  for the left eigenvector and compute the SVD:

$$Y^T \lambda X = U \lambda' V \quad (5.25)$$

then the assertion is as follows

$$\Gamma' = VX^{-1} \Gamma(Y^T)^{-1} U. \quad (5.26)$$

For its proof, first consider the identity containing the unitary  $V$ :

$$\sum_{\gamma} V_{\beta\gamma} V_{\gamma\beta'}^\dagger = \sum_{\gamma} V_{\beta\gamma} \overline{V_{\beta'\gamma}} = \sum_{\gamma\gamma'} (V \otimes \overline{V})_{(\beta\beta', \gamma\gamma')} \delta_{\gamma\gamma'} = \delta_{\beta\beta'}.$$

This can be summarized as  $V \otimes \overline{V} \mathbb{1} = \mathbb{1}$ . Now define  $E' = \sum_s \Gamma'^s \lambda' \otimes \overline{\Gamma'^s} \lambda'$  plugging in the assertion (5.26) and consider

$$E' \mathbb{1} = E' V \otimes \overline{V} \mathbb{1} = VX^{-1} \otimes \overline{VX^{-1}} \sum_s \Gamma^s \lambda \otimes \overline{\Gamma^s} \lambda X \otimes \overline{X} \mathbb{1} = VX^{-1} \otimes \overline{VX^{-1}} EX \otimes \overline{X} \mathbb{1}.$$

We have also utilized (5.25). Now using  $X \otimes \overline{X} \mathbb{1} = XX^\dagger = R$  and exploiting the fact that

$$ER = R \iff EX \otimes \overline{X} \mathbb{1} = X \otimes \overline{X} \mathbb{1}$$

rewrite the right hand side, which leads to

$$VX^{-1} \otimes \overline{VX^{-1}} EX \otimes \overline{X} \mathbb{1} = V \otimes \overline{V} \mathbb{1} = \mathbb{1}.$$

This proves that in fact  $E' \mathbb{1} = \mathbb{1}$ .

The only thing remained is to use  $A^s = \Gamma^s \lambda$  to verify that indeed  $\sqrt{L} \sqrt{R} = Y^T \lambda X$ .  $\square$

### 5.2.5 MPO for the 1D Ising model

Let us compute the translational invariant MPO representation of the Ising Hamiltonian with periodic boundary conditions on a spin chain which has been discussed in [36].

$$H_{Ising} = - \sum_i (J_1 \sigma_i^Z \sigma_{i+1}^Z + h \sigma_i^X) = H_Z + H_X.$$

Here  $H_Z$  and  $H_X$  contain all the terms with  $\sigma^Z$  and  $\sigma^X$  operators, respectively. All sub-terms in  $H_Z$  and in  $H_X$  commute and we can calculate  $O_Z = O_{NN} = \exp\left(\epsilon \sum_i Z_i Z_{i+1}\right)$  and  $O_X$  exactly. (The subscript  $NN$  refers to nearest neighbour interaction.) After performing the computations one finds

$$O_Z(\epsilon) = \exp\left(\epsilon \sum_i Z_i Z_{i+1}\right) = \sum_{k_1, k_2, \dots} \text{Tr}(C^{k_1}(\epsilon) C^{k_2}(\epsilon) \dots) Z^{k_1} \otimes Z^{k_2} \dots \quad (5.27)$$

with 2 dimensional MPO matrices  $C^k(\epsilon)$  given by

$$C^0(\epsilon) = \begin{pmatrix} \cosh(\epsilon) & 0 \\ 0 & \sinh(\epsilon) \end{pmatrix} \quad (5.28)$$

$$C^1(\epsilon) = \begin{pmatrix} 0 & \sqrt{\cosh(\epsilon) \sinh(\epsilon)} \\ \sqrt{\cosh(\epsilon) \sinh(\epsilon)} & 0 \end{pmatrix}. \quad (5.29)$$

And the spin operators are  $Z^0 = \mathbb{1}$ ,  $Z^1 = \sigma^z$ .

#### Proof.

As in [36] let us begin with the identity

$$\exp\left(\epsilon Z \otimes Z\right) = \cosh(\epsilon) \mathbb{1} \otimes \mathbb{1} + \sinh(\epsilon) Z \otimes Z = \sum_{i,j} (B_i^T B_j) Z^i \otimes Z^j \quad (5.30)$$

with the vectors  $B_0^T = (\sqrt{\cosh(\epsilon)} \ 0)$  and  $B_1^T = (0 \ \sqrt{\sinh(\epsilon)})$ . Now if we take  $N$  spins with periodic boundary conditions and we just need to regroup the corresponding vectors as follows

$$\begin{aligned} \exp\left(\epsilon \sum_i Z_i Z_{i+1}\right) &= \prod_i \exp(\epsilon Z_i Z_{i+1}) \\ &= \sum_{i_1, i_2, \dots} \left( B_{i_1}^T B_{i_2} B_{i_2}^T B_{i_3} \dots B_{i_N}^T B_{i_1} \right) Z_1^{i_1+i_1} \otimes Z_2^{i_2+i_2} \otimes \dots \\ &= \sum \text{Tr}\left( B_{i_1} B_{i_1}^T B_{i_2} B_{i_2}^T \dots \right) Z_1^{i_1+i_1} \otimes Z_2^{i_2+i_2} \otimes \dots \end{aligned}$$

we used that  $Z^i Z^j = Z^{i+j}$  where the sum  $i+j$  is taken modulo 2. Introduce the matrices

$$\begin{aligned} C^0(\epsilon) &= \sum_i B_i B_i^T = \begin{pmatrix} \cosh(\epsilon) & 0 \\ 0 & \sinh(\epsilon) \end{pmatrix} \\ C^1(\epsilon) &= \sum_i B_{i\oplus 1} B_i^T = \begin{pmatrix} 0 & \sqrt{\cosh(\epsilon) \sinh(\epsilon)} \\ \sqrt{\cosh(\epsilon) \sinh(\epsilon)} & 0 \end{pmatrix}. \end{aligned}$$

From numerical reasons it is beneficial to use the symmetrized form

$$O = O_X(\delta/2) O_Z(\epsilon) O_X(\delta/2) = e^{\frac{\delta}{2} H_X} e^{\epsilon H_Z} e^{\frac{\delta}{2} H_X}.$$

Trivially

$$O_X(\delta/2) = \prod_i \exp(\delta \sigma_i^X / 2)$$

which can be used to show that  $O$  has an MPO description with the same matrices  $C^k$  and  $Z^1$  but  $Z^0 = I$  is replaced by

$$Z^0 = e^{\delta \sigma^X / 2} I e^{\delta \sigma^X / 2} = e^{\delta \sigma^X} = \begin{pmatrix} \cosh(\delta) & \sinh(\delta) \\ \sinh(\delta) & \cosh(\delta) \end{pmatrix}.$$

One arrives to the final form

$$O = \sum_{k_1, k_2, k_3, \dots} \text{Tr}(C^{k_1} C^{k_2} C^{k_3} \dots) Z^{k_1} \otimes Z^{k_2} \otimes Z^{k_3} \otimes \dots \quad (5.31)$$

There are several advantages of this description. Besides its full translational invariance it is valid for all  $\epsilon$  since no approximation has been used, moreover it can be used as a basis to construct further MPO forms of exponentials of other similar Hamiltonians.

Trivially, taking  $\exp\left(\epsilon \sum_i Y_i Y_{i+1}\right)$  does not change the matrices  $C^k$  but only the spin operators to  $Y^k$ . This provides us the MPO description of the XYZ Heisenberg model. An other example is the next nearest neighbor interaction.

### Next nearest neighbor (NNN) interactions

Let us do the split  $H_{NNN} = \sum_i Z_i Z_{i+2} = H_{\text{even}} + H_{\text{odd}}$  according to the even or odd sublattices to write

$$O_{\text{even}} = \exp\left(\epsilon \sum_{i:\text{even}} Z_i Z_{i+2}\right) = \sum_{k_2, k_4, \dots} \text{Tr}(I C^{k_2} I C^{k_4} I \dots) I \otimes Z^{k_2} \otimes I \otimes Z^{k_4} \otimes \dots \quad (5.32)$$

So all the matrices are the same as in  $O_{NN}$  with the difference that they are assigned to the even sublattice only, and we put identities associated to the odd sublattice. Accordingly

$$O_{odd} = \exp\left(\epsilon \sum_{i:odd} Z_i Z_{i+2}\right) = \sum_{k_1, k_3, \dots} \text{Tr}(C^{k_1} I C^{k_3} I \dots) Z^{k_1} \otimes I \otimes Z^{k_3} \otimes I \otimes \dots \quad (5.33)$$

Now take the product of the two (5.33) and (5.32) in order to obtain  $O_{NNN} = O_{odd} O_{even}$

$$O_{NNN} = \exp\left(\epsilon \sum_i Z_i Z_{i+2}\right) = \sum_{k_1, k_2, k_3, \dots} \text{Tr}\left((C^{k_1} \otimes C^{k_2})(C^{k_3} \otimes C^{k_4}) \dots\right) Z^{k_1} \otimes Z^{k_2} \otimes Z^{k_3} \otimes Z^{k_4} \dots \quad (5.34)$$

Note that one needs to regroup neighboring pairs of spins to get a 2-site translational invariant MPO with bond dimension 4.

Using the above procedures it is clear how to obtain MPO for longer but finite range Hamiltonians or NN Hamiltonians with alternating couplings for example.

### Alternating couplings

Consider the Hamiltonian with nearest neighbor couplings alternating in sign as

$$H = +JZ_1Z_2 - JZ_2Z_3 + JZ_3Z_4 - JZ_4Z_5 + \dots$$

Quite clearly one has to repeat the derivation for the NN case taking care about the alternating signs of the  $\epsilon$ -s. Changing the sign of  $\epsilon$  in every second pair results in replacing the vector  $B_1^T$  in (5.30) with  $B_1^{T-} = (0 \quad i\sqrt{\sinh|\epsilon|})$ . After regrouping the appropriate terms turns out that the  $C^k$  matrices are

$$C_e^0(\epsilon) = \begin{pmatrix} \cosh|\epsilon| & 0 \\ 0 & i \sinh|\epsilon| \end{pmatrix}$$

$$C_e^1(\epsilon) = \begin{pmatrix} 0 & i\sqrt{\cosh|\epsilon| \sinh|\epsilon|} \\ \sqrt{\cosh|\epsilon| \sinh|\epsilon|} & 0 \end{pmatrix}$$

for the even sites and

$$C_o^0 = C_e^0$$

$$C_o^1 = (C_e^1)^T$$

for the odd ones, reflecting the periodicity of 2 lattice sites.

## 5.2.6 PEPS and algorithms

In this subsection I introduce the Projected Entangled Pair States (PEPS) and try to summarize the basic facts about them. Naturally, being aware of the success of the MPS in describing efficiently the ground states of local Hamiltonians the question arises about its possible generalizations for higher dimensions and different types of lattices, as well as possible algorithms of the simulations.

### 5.2.6.1 Bethe lattice

The Bethe lattice (Cayley tree) is a translationally invariant infinite tree: Every lattice site has  $q$  neighbors and the tree it looks the same from every vertex. One can then associate a tensor to each vertex point with a physical index and three bond indices corresponding to each bond. The same idea, by using the Schmidt theorem can also be applied as cutting the tree between two sites results in two separate graphs. Thus, basically all the iTEBD algorithm can be applied with these  $D^3d$  dimensional tensors and making use of the symmetry, but one has got more update steps coming from the 3 neighbors. The Ising model on the Bethe lattice has been successfully discussed in [37] together with the appropriate modification of the iTEBD algorithm. One crucial fact is the time costs: In case of  $q = 3$  each update step runs to  $O(D^8)$ , significantly higher than the  $O(D^3)$  of the 1D case. Notice that using infinite, translation-invariant operators this can be reduced to  $O(D^{q+1})$ . (See the chapter about this.)

### 5.2.7 Square lattice and PEPS

In the general case, consider a connected graph  $G$  where each vertex is adjacent to at most  $K$  other vertices. We assign a tensor to vertex  $i$  with one physical index and  $k_i$  bond indices, if  $i$  is adjacent to  $k_i$  other vertices. Now, when computing expectation values one has to sum over all adjacent bond indices (see further). This structure is called a tensor network, and its contraction the tensor trace. Now take the 2D square lattice of high importance. Here we can think of a tensor  $A_{lrud}^s$ , with four bond indices  $\{l, r, u, d\}$  of dimension  $D$ , corresponding to the bonds on the left, right, up and down, respectively and one physical index  $s$  of dimension  $S$ . Clearly this idea works for different type of lattices such as triangular, honeycomb, Kagomè etc. or even in higher dimensions, but for the sake of concreteness let us discuss the 2D square lattice case. Unfortunately, splitting only one bond between two vertex does not cut the lattice into two separate halves, one cannot apply the Schmidt theorem simply between two vertices, to this end one would cut the whole lattice at a cost of exponentially many indices. Nevertheless, the

construction from maximally entangled pairs between neighboring sites is still effective. So place auxiliary systems to each bond such that each of these systems is in a maximally entangled state  $\sum_{j=1}^D |jj\rangle$ . The so-called PEPS  $|\Psi\rangle$  is then obtained by applying an operator  $Q_i$  to every single site which maps the auxiliary systems onto the physical ones, just as in the 1D case. In this way the coefficients of the tensors are given by

$$A_{lrud}^s = \langle k|Q_i|l, r, u, d\rangle.$$

In a square lattice of  $N \times N$  sites,  $|\Psi\rangle$  is characterized by  $O(SN^2D^4)$  parameters. Of course one then needs to calculate expectation values of local or two point operators etc. and update the state after the action of some local operator. In the case of PEPS, e.g. the expectation of a one-local operator  $O$  could be handled by computing the product of transfer matrices and one other operator  $E_O$ , constructed from  $O$  and summing over the bond indices. This operation is the ‘contraction’ of the tensor network or it can be called as ‘tensor trace’.

Here comes the major difference contrast to MPS: The cost of contraction of such a tensor network is exponential in  $N$ . The reason is sketched below, as well as some approximative methods yielding efficient computation.

**Corollary 5.3.** *Consider a translational invariant system and in analogy to the 1D-case define transfer operator of site  $i$  as*

$$[E_i]_{ll',rr'}^{uu',dd'} = \sum_{s=1}^S [A_i]_{lrud}^s \overline{[A_i]_{l'r'u'd'}^s}$$

with four indices running from 1 to  $D^2$ , each. (E.g.  $ll' \in \{1, 2, \dots, D^2\}$  is a compound index.) More simply:  $E_i = \sum_s [A_i]^s \otimes \overline{[A_i]^s}$ .

Let  $O^i$  be a local operator acting on site  $i$ . Define

$$E_{O_i} = \sum_{s,s'=1}^S \langle s|O_i|s'\rangle [A_i]^s \otimes \overline{[A_i]^{s'}}.$$

The exact computational costs of  $\langle \Psi|\Psi\rangle$ ,  $\langle \Psi|O^i|\Psi\rangle$ ,  $\langle \Psi|O^i O^j|\Psi\rangle$  scale exponentially in  $N$ .

**Proof.** Let us compute just  $\langle \Psi|\Psi\rangle$ , and PBC, as the simplest case. In the first row, denote the indices of the horizontal bonds as  $\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_N$  and the vertical ones by  $\beta_1, \beta'_1, \beta_2, \beta'_2, \dots$ , yielding tensors like  $E_{\alpha_1, \alpha_2}^{\beta_1, \beta'_1}$  as it can be seen in the figure (Fig...). If we consider the first row and sums up over the row indices we get a tensor with exponential

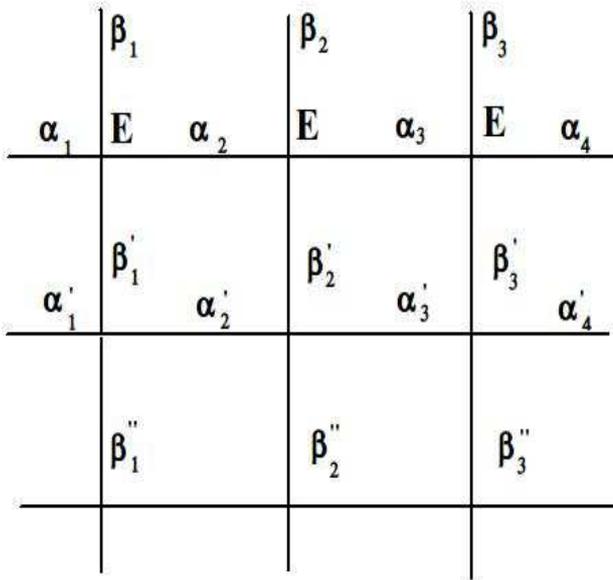


FIGURE 5.4: Local transfer operators and indexing in the two-dimensional square lattice

number of indices in  $N$ :  $\widehat{E}^{\beta, \beta'}$  with combined index  $\beta = (\beta_1, \beta_2 \dots \beta_N)$ ,  $\widehat{E}$  can be regarded as a  $D^{2N} \times D^{2N}$  matrix.

After summing over the horizontal indices in the second row we end up with :  $\widehat{E}^{\beta', \beta''}$ , and so on. After all  $\langle \Psi | \Psi \rangle = \sum_{\beta, \beta', \dots, \beta^{(N)}} \widehat{E}^{\beta, \beta'} \widehat{E}^{\beta', \beta''} \dots \widehat{E}^{\beta^{(N)}, \beta} = \text{Tr} \widehat{E}^N$  running to a computational cost of  $O(D^{6N})$ .

*Remark 5.4.* Interpretation of the contraction of the tensor network. Define the matrix  $(M^{\beta_1 \beta'_1})_{\alpha_1 \alpha_2} = T_{\alpha_1, \alpha_2}^{\beta_1, \beta'_1}$ . Summing up the horizontal indices in the first row, we end up with:  $\text{Tr} M^{\beta_1 \beta'_1} M^{\beta_2 \beta'_2} \dots M^{\beta_n \beta'_n}$ , similarly in the second row we get:  $\text{Tr} M^{\beta_1 \beta'_1} M^{\beta_2 \beta'_2} \dots M^{\beta_n \beta'_n}$  etc. For ease let us take a  $3 \times 3$  lattice. Here

$$\langle \Psi | \Psi \rangle = \sum_{\beta_1 \dots \beta_3''} \text{Tr}(M^{\beta_1 \beta'_1} M^{\beta_2 \beta'_2} M^{\beta_3 \beta'_3}) \text{Tr}(M^{\beta_1 \beta''_1} M^{\beta_2 \beta''_2} M^{\beta_3 \beta''_3}) \text{Tr}(M^{\beta''_1 \beta_1} M^{\beta''_2 \beta_2} M^{\beta''_3 \beta_3})$$

whose terms remind us of MPS, moreover looking at a given column, the appropriate vertical neighboring matrix indices have to be the same.

Evidently, one has to develop an algorithm to carry out this calculation efficiently. Several methods have been used to achieve this, using some approximation while computing the contraction.

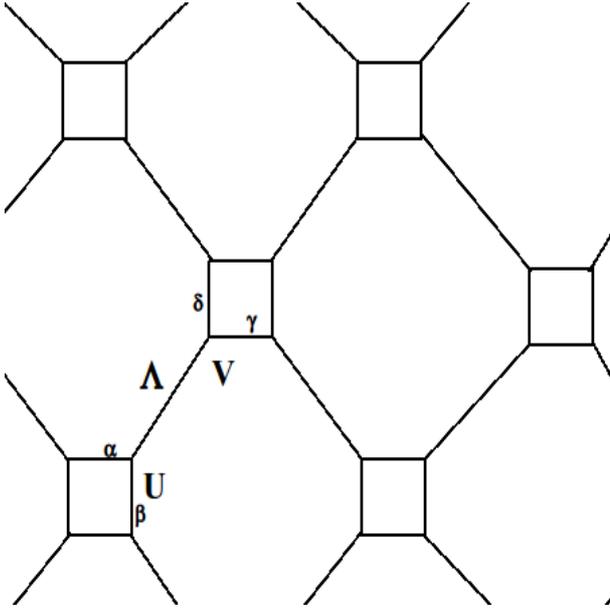


FIGURE 5.5: SVD decomposition of the local transfer tensors on the square lattice and the ‘inner squares’

### 5.2.8 TERG

First, the so-called Tensor Entanglement Renormalization Group Method (TERG) method is presented. This has been proposed by Zheng-Cheng Gu, Michael Levin and Xiao-Gang Wen [51].

Consider an  $L \times L$  square lattice. Label those sites which form the smallest possible square by  $i \in \{1, 2, 3, 4\}$  and at each vertex take the SVD of the local tensor; i.e.  $E^i = U^i \Lambda^i V^i$  (Figure 5.5). Now the idea is to sum over the indices on the inner squares coming from four unitaries and keep the four indices coming from the diagonal matrices in the SVDs. In this way we halve the number of the tensors associated to the lattice, and the new tensors will sit on vertices of a rotated square lattice of halved size. These new tensors however will have a bond dimension squared, so as usual one needs to neglect the small ones in order to keep the bond dimension fixed. If the discarded weight is not small enough we increase the bond dimension. We repeat the procedure for the coarse gained lattices until only a few tensor left which can be now contracted explicitly.

TERG is based on a nice idea but has obvious defects such as time evolution cannot be applied readily and the minimization of the energy is problematic because one can stuck to local minima of a highly non linear and multivariate function.

## Chapter 6

# Entanglement Scaling

As we have seen the MPS describe state vectors with finite entanglement entropy. As the entanglement entropy of a finite 1D system remains also finite we can therefore write its ground state as an exact MPS with a suitable finite bond dimension. Now, if the system's size is sent to infinity, its entanglement entropy still can remain finite in some cases like having a Hamiltonian with local or fast decaying interactions and if the gap in the energy spectrum remains nonzero, as Hastings has proven. There exist interesting situations however, when the gap of the infinite systems is zero. In these 'critical points' the entropy of entanglement is infinite implying straightforwardly that no exact finite dimensional MPS description exist. So yet what can we learn from simulating critical systems by MPS?

First of all, even if the entanglement diverges, other relevant quantities like the energy per site remain finite and can eventually be well approximated by that of the MPS state.

Secondly, concerning a quantity which becomes infinite (like entanglement entropy, correlation length) in the exact infinite model at a critical point, performing its simulation by MPS it should diverge as the function of the applied bond dimension yielding some 'scaling' from which one can exploit some features of the critical point. It turns out that these 'finite-entanglement' scalings have a different origin as opposed to the finite-size scalings, and governed by the 'central charge' of the critical point.

In this subsection we summarize the crucial facts about finite-entanglement scaling of local Hamiltonians in a spin chain and present the result of [52].

We have two goals: Find a suitable efficient algorithm based on MPS to simulate Hamiltonians with second neighbor interactions and frustration, as well as demonstrate the use of universal tools, especially finite-entanglement scaling to study different types of

phase transitions. Its validity arises from general facts about critical points and the definition of the MPS, hence it can be applied quite universally. As opposed to the usual finite-size scaling it may also have a better scaling for the computational costs if using the same maximal bond dimensions for both cases (see below). Here the 1-dimensional version of the transverse axial next nearest neighbor Ising (ANNNI) model has been chosen which is non-integrable and possesses a quite complex phase diagram, despite being the simplest model with NNN interactions. This model is notable due to several facts. As earlier studies have shown, unlike the Ising model, it has a critical region, i.e. a 2D parameter region where it is critical. A probably infinite order phase transition also takes place (besides second order phase transitions). As mentioned earlier, the detection of an infinite (e.g. Kosterlitz-Thouless) transition is a notoriously hard computational challenge, that's why a computationally beneficial method is needed. The same holds for exploring the physics of a critical region.

In order to study such a model one can choose a finite chain of length  $L$  with periodic (PBC) or open boundary conditions (OBC) and then look at the scaling of some physical quantities depending on  $L$  and the bond dimension  $D$ . It is known that the overall computational costs scales  $O(D^3)$  in the best case. The latter happens for example when the correlations are very small  $\xi \ll L$  as it is discussed in Ref. [9], however when  $\xi \approx L$  e.g. it can be as large as  $O(D^5)$  and the precise behaviour of the scaling as a function of  $D$  and  $L$  is unclear.

Note that in this paper, iMPS and imaginary time evolution are used, hence one works directly on the infinite lattice and the only scaling parameter is  $D$ . In this case the computational cost in every small time step  $\Delta t$  scales as  $O(D^3)$ . Roughly speaking, convergence can be reached if:  $\exp(t\Delta E) = \exp(n\Delta t\Delta E) \ll 1$  with the  $\Delta E$  energy gap and  $n$  the number of time steps. Approaching to a critical point,  $\Delta E$  vanishes as a function of the effective correlation length  $\xi_D$ , and at the same time we also have a scaling relation like  $\xi_D \propto D^k$  (see below). With this in mind, it can be estimated how the overall computational time scales as a function of  $D$  and one sees why it is slower than  $O(D^3)$  near to a critical point. For instance, if  $\Delta E \propto \xi_D^{-\alpha} \propto D^{-\alpha k}$ ,  $\alpha > 0$  then  $n$  should scale as  $O(D^{\alpha k})$  that makes the overall scaling  $O(D^{3+\alpha k})$ . Previous work about finite-D scaling can be found e.g. in [55].

Now the idea is to study the scaling of physical quantities not as a function of the system size, but simply as a function of the bond dimension  $D$ . Instead of finite-size scaling this can be called as 'finite-D' or 'finite-entanglement' scaling as a MPS with a given  $D$  can contain a finite amount of entanglement. As it will be argued in Section IV. the overall computation cost of finite-D scaling can be considerably reduced compared to that of the usual finite-size scaling. In fact, this turns out to be the case for the

presented model as well as for the Ising and Heisenberg models, and essentially this depends on the central charge. The key point to this computational cost reduction is our off critical scaling ansatz for the correlation length as a function of  $D$  which turns out to be computationally more beneficial than that of used in Ref. [57] for the entanglement entropy.

Clearly, our methods can be applied straightforwardly to any other 1D model with NN and NNN interactions, such as the  $J_1 - J_2$  Heisenberg model, but can also be adapted for the 2D version using PEPS. Despite the polynomial computational time scaling, unfortunately its exponent is so high in the 2D case that in practice one can apply only very small bond dimensions providing only a few and ambiguous results that are not yet sufficient for numerical analysis.

### 6.0.9 MPS scalings

Suppose we are working with iMPS so no finite-size effects emerge, the scaling relations come from the finite entanglement only. Let us use a subindex for the quantities computed by the iMPS with bond dimension  $D$ , e.g.  $\xi_D$  and  $S_D$ .

First we bring into focus the entropy of entanglement of the iMPS state  $S_D$ : How does it behave as a function of the bond dimension? If the corresponding exact model has a gap and possesses finite entanglement entropy  $S < \infty$  then  $S_D$  saturates to  $S$  as  $D \rightarrow \infty$  in a non universal way depending on the model and its parameters [54].

At a critical point however, if the correlation length of the iMPS  $\xi_D \gg a$  ( $a$  is the lattice spacing) then the scaling for the entropy is found to be

$$S_D = \alpha \log D \tag{6.1}$$

with corrections of  $O(\frac{1}{\log D})$ , and  $\xi_D$  scales as

$$\xi_D \propto D^\kappa \tag{6.2}$$

again with corrections of  $O(\frac{1}{\log D})$ . Moreover the constants  $c$  and  $\kappa$  depend only on the central charge characterizing the underlying critical point. It is possible to show that for large  $D$

$$\kappa = \frac{6}{c\sqrt{12/c+1}}, \quad \alpha = \frac{1}{\sqrt{12/c+1}}. \tag{6.3}$$

Note that the maximal entanglement that can be stored by an MPS of bond dimension  $D$  is  $\log D$ , but  $\alpha$  arises less than unity. I ignore here the details of their derivations which can be found in [54] and in [55], just scetch the main ideas.

One crucial observation of Calabrese et al [56] refers to the eigenvalue distribution of the reduced density matrix  $\rho_A$  of one half of a gapped 1D system with long correlation. It turns out that it does not matter if we take the iMPS approximation of a critical system with large  $D$  and  $\xi_D \gg 1$  or take the exact ground state of a non-critical one but close to the critical point and possessing a large  $\xi$ , the eigenvalue distributions will be the same in the large  $\xi$  limit! It can be interpreted such that simulating a critical system with large  $D$  reflects the information about the same systems near to that critical point. In the latter case one can compute the entropy as a limit of  $\text{Tr} \rho_A^n$  which scales like  $c_n \exp(-b(n - 1/n))$  and turns out to be model independent as  $b > 0$  depends on the characteristic length of the system and on the central charge only. After performing the limit one finds  $S_A = -\log \lambda_{\max}$ . Being aware of this universal distribution, the entropy at the critical point using  $D$  dimensional MPS is given by the largest eigenvalue of  $\rho_A$  as

$$S_D = 2b = -2 \log \lambda_{\max}$$

Taking into account other considerations from thermodynamics ....REF here Pollmann....and using the fact that  $\xi^{-1}$  is small it can also be shown that  $\lambda_{\max} \propto D$  for large enough  $D$ , yielding  $S_D = \alpha \log D$ .

On the other hand, from conformal field theory follows that the entropy of entanglement of a system in the vicinity of the critical point grows also logarithmically with the correlation length

$$S = \frac{c}{6} \log \frac{\xi}{a}$$

with  $c$  being the "central charge" of the critical point counting its universal degrees of freedom [54]. Then the universality of the distribution implies

$$\alpha \log D = \frac{c}{6} \log \frac{\xi}{a}$$

so  $\xi \propto D^{\kappa}$  as well (we set  $a = 1$ ).

These relations make the MPS based methods capable of apprehending the essential informations about critical systems. One can have a chance to decide whether a given point is critical or not by testing the scaling laws above, in addition can obtain an estimate for the central charge. Knowing the existence of a critical point in advance one can localize it as well as characterize it with high precision depending on the bond dimension and the Trotter and convergence errors. In case of critical intervals and infinite order transitions however these tasks get more involved as one cannot be sure about a large  $\xi$  if it should diverge or saturate to a high value. For example a study of Kosterlitz-Thouless transition offers notoriously hard challenge for numerical simulations as it will be presented later also in this paper.

Usually in practice one should go in the other way round: As our goal is to explore the phase diagram we do not know the critical points so first looking at the scaling relations one should decide whether a phase transition takes place and if so, characterize that. Let us denote the limit values by  $\xi = \xi_\infty = \lim_{D \rightarrow \infty} \xi_D$  and  $S = S_\infty = \lim_{D \rightarrow \infty} S_D$  which converge to the exact values if other errors of the applied algorithm tend to zero (e.g. the Trotter errors in the imaginary time evolution). Nevertheless, if one stays in the vicinity of a critical point so that  $1 \ll \xi$  still holds then the scaling relations (6.1) and (6.2) still hold approximately for smaller  $D$  too, but break down and converge to a large but finite value as  $D$  is increased. Assume that the deviation has the form of

$$\log \xi_D = \kappa \log D + f(x) \quad (6.4)$$

with  $x = \frac{D^\kappa}{\xi_\infty}$  inspired by (6.2). Clearly  $f$  has to fulfil the conditions:  $f(x) \rightarrow 0$  as  $x \rightarrow 0$  and  $\frac{f(x)}{\log(x)} \rightarrow -1$  as  $x \rightarrow \infty$ . One should use some scaling ansatz at this point and for example the following simple ansatz meets these requirements

$$f(x) = -\log(x + e^{-\alpha x}), \quad \alpha > 0. \quad (6.5)$$

Plugging  $x = \frac{D^\kappa}{\xi_\infty}$  one can see that for a fixed  $\xi_\infty$  and small enough  $D$  the first term will dominate in (6.5). It turns out that (6.5) fits well to the data and therefore one can give an estimation for the correlation length.

Let us compare this approach to the usual finite-size scaling. When using PBC and a chain of length  $L$  the computational cost scales like  $O(LD^3)$  in every small time step, in contrast to the  $O(D^3)$  scaling of the iMPS method. The other very important issue is the number of the necessary time steps  $n$ , required to achieve a convergence within some given, small error. This also depends on the correlation length of the system and through (6.2), also on  $D$ , and for a finite chain also on  $L$ . It is not clear how to determine these relations. In the finite-size case however, one can investigate the scaling of the entropy by a relation similar to (6.5)

$$S_L \propto \log D + f(L/\xi). \quad (6.6)$$

This approach has been used e.g. in [57] with the same ansatz for  $f$ . Now we have the analogy  $L \rightarrow D$  and  $S \rightarrow \log \xi_D$ , but instead of  $L/\xi$  we have to plug in  $D^\kappa/\xi_D$ . This is a good news for  $\kappa > 1$  since one needs a smaller  $D$  compared to  $L$  for the same  $\xi$  to indicate the off-critical scaling.

Having the same  $\xi_\infty$  for the infinite system, for the same accuracy one has considerably smaller computational cost if the scaling exponent  $k > 1$ . (This will turn out to be the case in the present model as the central charges are found to be  $c = 1$  implying  $k \approx 1.34$ )

and  $c = 1/2$  implies  $k \approx 2.03$ .) In any case, the time cost of one update step scales as  $O(LD^3)$  in the finite size case as opposed to  $O(D^3)$  for the infinite case. Now, if one takes the same maximal bond dimension  $D$  for both cases, then for the finite- $D$  scaling one also needs to apply somewhat smaller  $D$ -s which makes the overall time costs scale as  $O(D^4)$  (at most, if one passes along  $1, 2, \dots, D-1, D$ ). On the other hand in case of finite-size scaling the time costs  $\propto O(L^2 D^3)$ . In order to detect off critical scaling with the same accuracy one expects the necessary maximal length  $L$  in the finite-size case must be bigger than the maximal  $D$  in the finite- $D$  case, if  $k > 1$ . Nevertheless, this can be estimated by studying the scaling ansatz (6.4) and (6.6). In terms of  $D$  this would result in an overall effective scaling higher than  $O(D^5)$ , in the finite-size case, obtained by the assumption  $L \propto D$ .

### 6.0.10 1D ANNNI model

The Axial Next Nearest Neighbor Interaction model is originally defined on a square lattice but its alternative on a spin chain is the following Hamiltonian

$$H = - \sum_i (J_1 \sigma_i^z \sigma_{i+1}^z + J_2 \sigma_i^z \sigma_{i+2}^z + h \sigma_i^x) = H_{Ising} + H_{NNN}. \quad (6.7)$$

Here we consider interactions between the  $z$  components only and add a transverse external magnetic field. Now we have all the ingredients to construct its MPO description, as well as the time evolution algorithm. One has simply take the MPO for the Ising part and for the NNN part, respectively and take their product.

Before discussing the details let us summarize briefly its ground states and their degeneracy in the special cases, also because of their important role in the proper choice of the applied algorithm. Clearly the Hamiltonian has the symmetry

$$U H U^\dagger = H$$

under the rotations of all the spins around the axis  $x$ :  $U = \bigotimes_i X_i$ .

Instead of three, it is enough to study two parameters  $\kappa = J_2/J_1$  and  $h/J_1$ . Setting  $\kappa = 0$  the model yields the Ising model while  $h/J_1 = 0$  is a classical one. It is easy to see that the most interesting case is the one with  $J_2 < 0$  when the system gets 'frustrated' as no spin configurations can fulfill simultaneously the energy constraints of the two interaction terms. There is no rotation existing to cease this 'frustration'. So now on we take  $J_2 < 0$  and we can simply take  $J_1 > 0$ . The phase diagram of this model is shown in figure as it has been reported by earlier studies. What is important is the fact that along the line  $h = 0$  there is a critical point at  $|\kappa| = 1/2$  under which the

ground state has a doubly degenerated ferromagnetic order like  $\uparrow\uparrow\uparrow\uparrow$  or  $\downarrow\downarrow\downarrow\downarrow$  and above which there is a doubly degenerated antiferromagnetic order like  $\uparrow\uparrow\downarrow\downarrow$  or  $\downarrow\downarrow\uparrow\uparrow$  with the periodicity of 2 lattice sites. The  $\kappa = -1/2$  point is infinitely degenerated and all the basis states are ground states with domains larger than 2 spins. Excluding this distinct point, the problem for our algorithm is the periodicity of the antiferromagnetic order as it can be fully translationally invariant as a superposition of the two. Unfortunately, the state like  $\Psi = c_0 \uparrow\uparrow\downarrow\downarrow + c_1 \downarrow\downarrow\uparrow\uparrow$  has a transfer matrix with degenerate dominant eigenvalue which makes our algorithm break down. Thus, this case needs a special care. One possible cure can be the rotations of the basis of every second neighboring pair of spins leading to a ferromagnetic ordering in the ground state causing no problems in the algorithm. These rotations lead to all ferromagnetic NNN couplings ( $J_2 > 0$ ) and alternating ( $+J_1, -J_1, +J_1, -J_1..$ ) NN couplings whose MPO description has been given in the previous section. Note that no rotations needed for  $\kappa > -1/2$  as the ground state is expected to be ferromagnetic for small magnetic fields. Besides the validity of the algorithm, this rotation also allows us to analyze the magnetization as a simple order parameter. In this picture here, both the transverse magnetic field and the remittent NN couplings are trying to destroy the ferromagnetic order forced by the (flipped) NNN interactions.

### 6.0.11 Exploring phase transition in the 1D ANNNI model by MPS-scaling

## 6.1 Results

Figure [8.1] shows the phase diagram as it has been found in earlier studies by simulations Ref.[57] and perturbative analysis Ref.[58]. We try to explore the phase boundaries by looking at the correlation lengths as a function of the parameters and the second derivative of the energy. A Kosterlitz-Thouless type transition is conjectured between the floating and the paramagnetic(PM) phase where the derivatives of the energy are useless indicators so the expected divergence of the correlation length is checked only. In the critical points we also check the finite entanglement scaling laws and find very good agreement with the theoretical results. Moreover, in some special points we calculate the critical charges as well as the correlation scaling exponents.

We intend to determine some points of the line of phase transitions between the distinct phases and check these relations as well as the finite-entanglement scaling and compute the central charge. There are three lines of phase transitions, two of them are of second order while an infinite order transition is expected for the third one which needs a

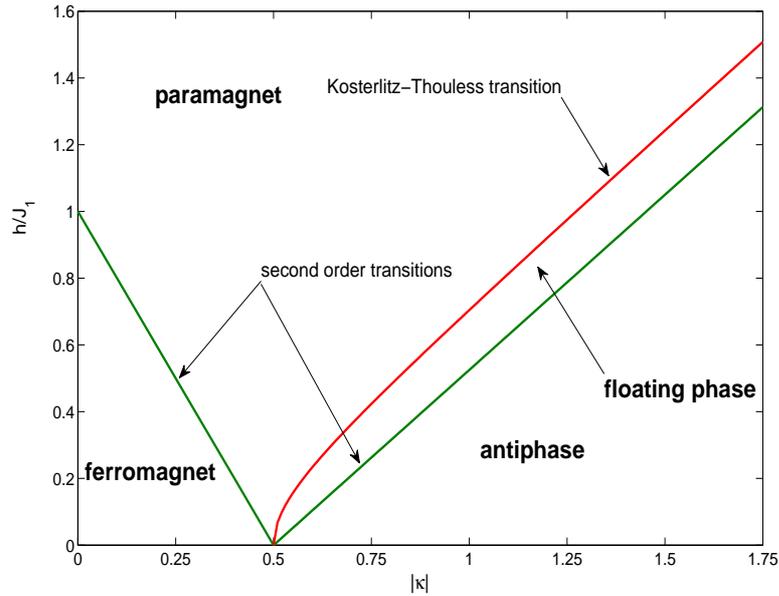


FIGURE 6.1: Schematic phase diagram

special care. We also try to detect the floating phase when  $\kappa < 0$  and  $|\kappa|$  is large, since its existence for arbitrary large  $|\kappa|$  is still an open question.

### 6.1.1 FM-PM transition

In case of the Ising model, in the vicinity of the critical point as a function of the magnetic field, the correlation length and the magnetization diverges as

$$\xi \propto |h - h_c|^{-\nu}, \quad M \propto |h - h_c|^\beta$$

and the energy and its first derivative are continuous but its second derivative diverges at  $h = h_c$ . Using  $D = 40$  we get  $0.535 < h_c < 0.538$  by looking at the extrema of the finite derivative  $\partial^2 E / \partial h^2$ . At the transition corresponding to  $\kappa = -0.25$  we find the same behaviour for the energy as a function of  $h$  and a very good agreement with  $\nu = 1$  as in the simple Ising case:  $\nu = 1.02$  comes from the linear fit on the figure below.

### 6.1.2 Antiphase-floating phase transition

Again a second order phase transition is suggested by the numerics but with a central charge  $c = 1$  of the floating phase as opposed to the Ising case with  $c = 1/2$ . See figure (8.4).

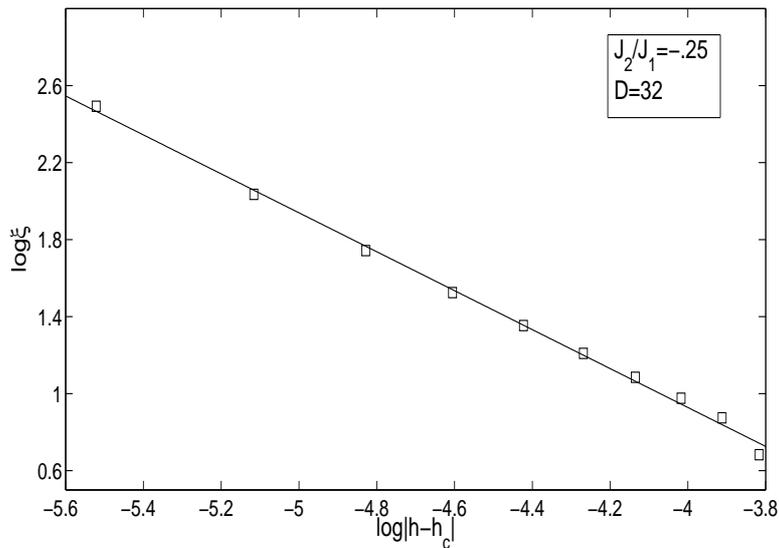


FIGURE 6.2: Estimation of the scaling exponent at  $\kappa = -0.25$  paramagnetic-ferromagnetic transition

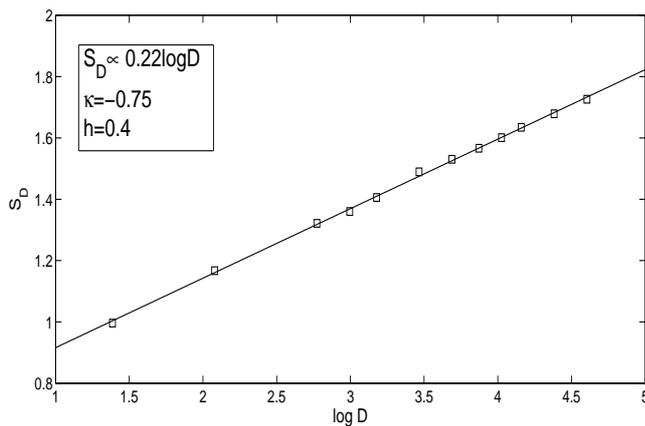


FIGURE 6.3: Entanglement entropy scaling inside the floating phase at  $\kappa = -0.75$ ,  $h = 0.4$  up to  $D = 100$ .

Central charge  $c = 1$  is suggested according to (6.1) and (6.3).

### 6.1.3 Floating phase-paramagnetic phase transition

First, we check the power-law scaling of  $\xi$  assumed for critical points as in (6.2). If this power-law scaling can be rejected statistically, then for a given  $h$  and  $\kappa$ ,  $\xi_\infty$  is computed by the best fit using (6.4) and finite- $D$  scaling. (See the inset in FIG.8.5.) We observe that (6.4) fits well using the ansatz function (6.5) with weak dependence of the parameter  $\alpha$  which can be set to 1.

In fact, the numerics indicate a higher order transition here, with continuous derivatives of the energy. Probably a Thouless-Kosterlitz type transition takes place as suggested

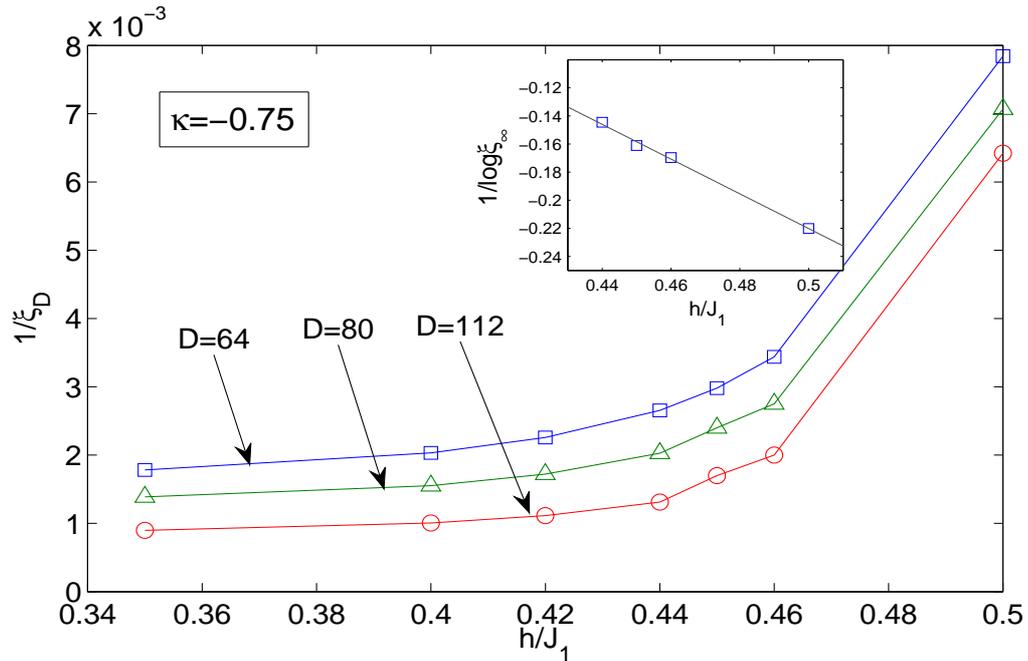


FIGURE 6.4: Floating phase-paramagnetic phase transition illustrated with the inverse correlations plotted for three different bond dimensions. The inner plot shows  $1/\log(\xi_\infty)$  vs  $h$ . Here, for a fixed  $h$ ,  $\xi_\infty$  is computed by fitting (6.4).

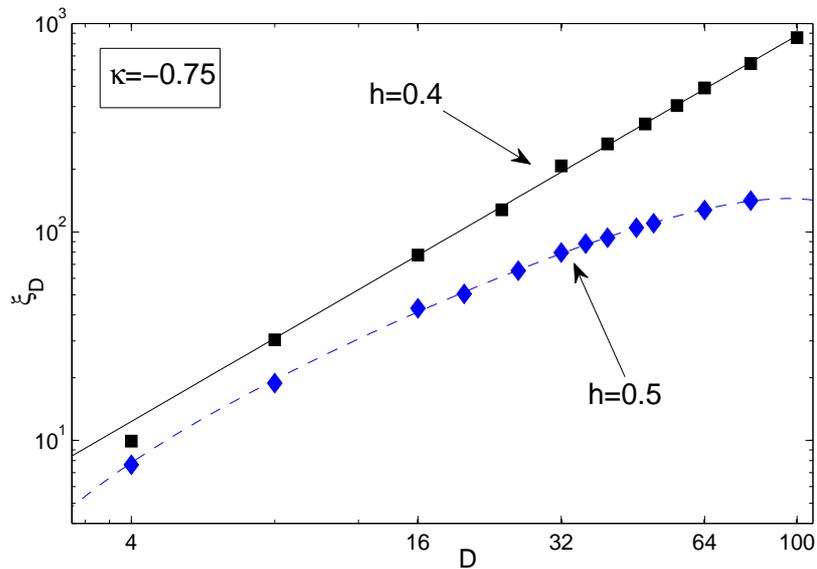


FIGURE 6.5:  $\xi_D$  against  $D$  in the two sides of the floating-paramagnetic transition. It can be seen in the log-log scale how it bends down from the straight line for higher  $D$ , implying a non critical point at  $h = 0.5$ . On the other hand, at  $h = 0.4$  the critical scaling hypothesis (6.2) cannot be rejected with the applied maximal bond dimension

by the plot  $\xi^{-1}$  vs  $h$  since  $\xi(h)^{-1} \propto \exp(\frac{\alpha}{h_c-h})$  could be fitted if  $h > h_c$ ,  $\alpha > 0$ . At the point  $\kappa = -0.75$  around  $h = 0.45$  very close to the floating/PM transition we need about  $D > 80$  to point out the non power-law scaling (see. FIG. 8.7). Otherwise, where we cannot reject the power-law scaling hypothesis, even though a finite value for

$\xi_\infty$  obtained by fitting (6.4) is rejected. In these cases one cannot rule out the critical scaling statistically. We have got anyway quite ambiguous results for  $\xi_\infty$  which –in this case– can be regarded as a consequence of the errors of the simulation. As in Ref. [57], in FIG. 8.5 we plot the inverse correlation length along the line  $\kappa = -0.75$  near to the supposed Kosterlitz-Thouless transition and find similar results with those calculated by finite DMRG and studying domain wall energies. Having our division for the magnetic field, the critical value can be estimated roughly as  $0.42 < h_c < 0.44$ . Note that here, the study of model specific quantities have been avoided.

#### 6.1.4 Large frustration

At  $\kappa = -10$  up to the the applied maximal bond dimension  $D_{max} = 80$  and the division for the magnetic field, the numerics do not seem to indicate the presence of the floating phase because one sees a sharp peak plotting  $\xi$  against  $h$ . See Fig.6.6.

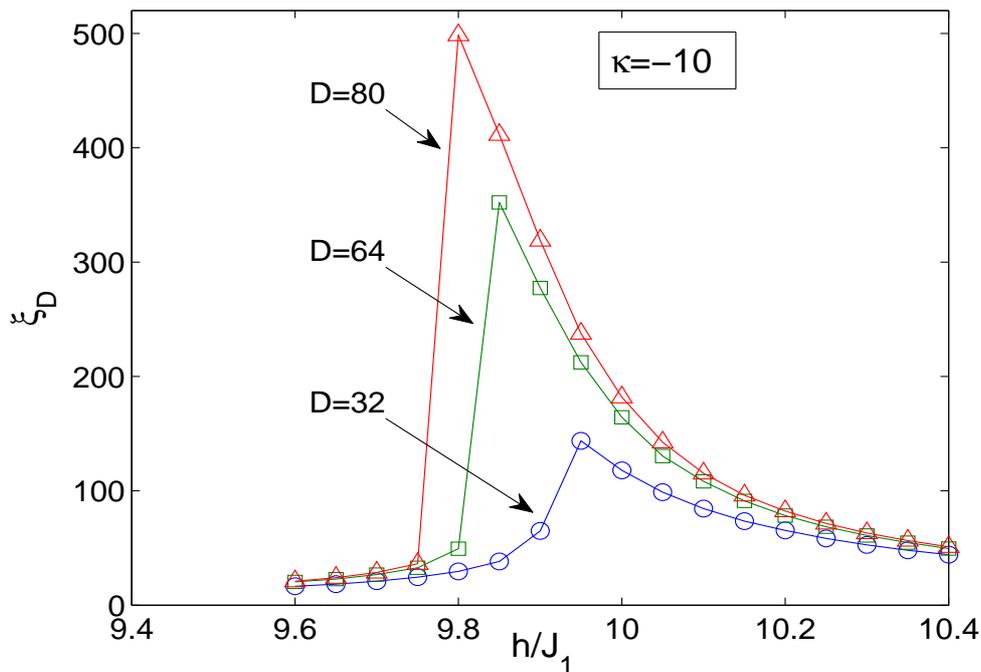


FIGURE 6.6: Sharp peaks of the correlation length against the magnetic field using different bond dimensions at  $\kappa = -10$  around the phase transition.

Note that in Ref. [57] the existence of the floating phase up to  $\kappa = -5$  has been indicated but the DMRG method has become imprecise for higher frustrations, however with our new method, the floating phase can be suspected even with  $D_{max} = 50$  as shown in FIG. 6.7.

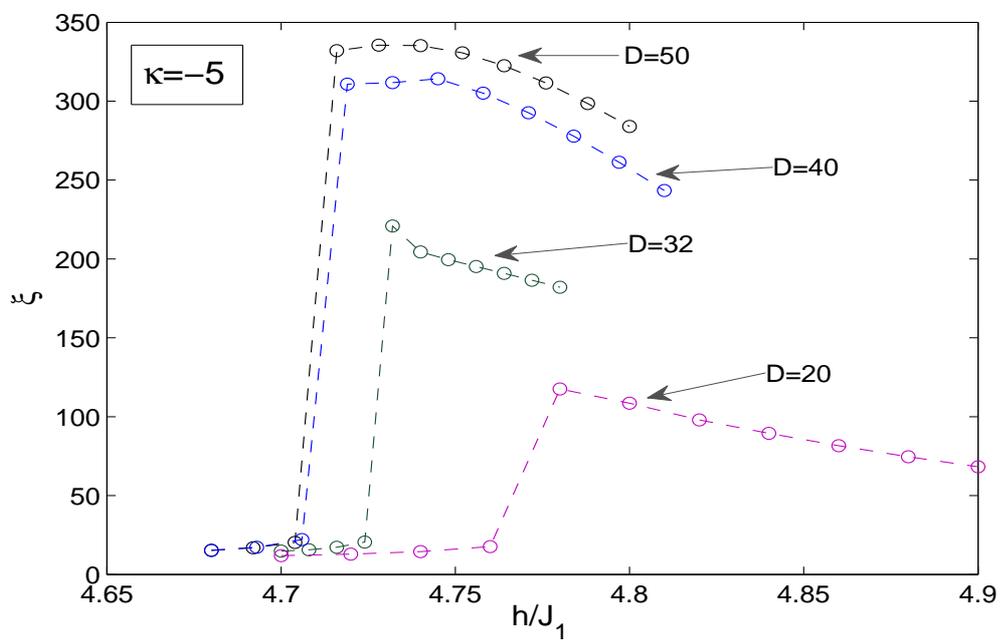


FIGURE 6.7: The correlation length against the magnetic field using different bond dimensions at  $\kappa = -5$  indicates an extended critical interval.

## Chapter 7

# Simulation in higher dimensions: Tensor Networks

As in the previous chapter recall the idea of the imaginary time evolution with the help of the Trotter decomposition. Now we will not restrict ourselves to one dimension and will investigate time evolution in an arbitrary lattice of spins or particles in any spatial dimension with local interactions.

Again by the Trotter decomposition we divide the time  $T$  into time slices  $\Delta t = T/n$  and write

$$\exp(-tH) \approx [\exp(-H_1\Delta t) \exp(-H_2\Delta t)]^n.$$

We can define the (time independent) transfer matrix as

$$\langle s' | T_{\Delta t} | s \rangle = \langle s' | \exp(-H_1\Delta t) \exp(-H_2\Delta t) | s \rangle.$$

We can write  $\exp(-H_1\Delta t) \exp(-H_2\Delta t)$  as an MPO using local tensors and for fixed  $s$  and  $s'$  one can compute  $\langle s' | T | s \rangle$  by contracting the spatial indices. In case of a system in  $d$  spatial dimension this leads to a tensor network of dimension  $d + 1$ : For each time  $t_k = k\Delta t, k = 0, 1 \dots n$  we have a  $d$  dimensional network with local transfer tensors in the vertices. These local tensors has  $p + 2$  indices, where  $p$  denotes the adjacency number of the given vertex. Contracting a layer in a given time step  $t$  gives the transfer matrix  $T_t$ .  $T_t(s, s')$  gives the amplitude of the event that the spin configuration  $s$  of time  $t$  is transferred to  $s'$  at the time  $t + \Delta t$ . Computing  $\langle \Psi_0 | \exp(-HT) A | \Psi_0 \rangle$  requires the complete contraction of this network.

If we lack of a method providing exact contraction then we can pursue various approaches to perform a numerical approximation. One method is to begin with some initial state which is updated in each time step. The state is described by PEPS tensors which must

be updated in each time step accordingly. If the dimension is higher than one, we have to contract the PEPS tensor network in order to evaluate a physical quantity and obtain a scalar. Moreover, in many algorithms we also need to contract the network in each time step to compute the updated PEPS tensors. This is problematic because of the exponential operation costs of the contraction for any (larger than one) bond dimension. So again approximative techniques are used to tackle this.

Another possibility might be the approximation of the transfer matrix and its leading eigenvector. In fact, when a model is exactly solvable, one is able to derive the leading eigenvalue of the transfer matrix—like for the 2D classical Ising model. In the latter case (or in a 1D quantum chain), the transfer matrix is given as a contraction of a 1D chain of local transfer tensors. In a  $d$  dimensional quantum model, this contraction must be performed on a  $d$  dimensional lattice. This can be done exactly for  $d = 1$  otherwise only numerically. A possible advantage of this approach could be the fact that in this tensor network (which is one layer in the spatial dimension of the 'path summation') the bond dimension is usually small (e.g. two) and the local tensors are known exactly.

### 7.0.5 Contraction of tensor networks of the time evolution

#### Ising model as an example

$$H = - \sum_{i \sim j} (J X_i X_j - h Z_i)$$

Define the vectors:

$$v_0 = \sqrt{\cosh(J\Delta t)} \quad v_1 = \sqrt{\sinh(J\Delta t)}$$

and

$$u_0 = \exp(h\Delta t/2) \quad u_1 = \exp(-h\Delta t/2).$$

In 1D, the MPO-s has the form

$$C_{\alpha\beta}^k = v_\alpha v_\beta \mathbb{1}\{k = \alpha + \beta\}$$

$\alpha, \beta$  corresponding to the  $x$  direction, and  $\mathbb{1}\{A\}$  being the indicator function of the event  $A$ . The translational invariant local transfer tensors read

$$Q_{\alpha\beta}^{s s'} = v_\alpha v_\beta u_s u_{s'} \mathbb{1}\{s + s' = \alpha + \beta\}.$$

very similarly, in 2D, the MPO-s has the form

$$C_{\alpha\beta\gamma\delta}^k = v_\alpha v_\beta v_\gamma v_\delta \mathbb{1}\{\alpha + \beta + \gamma + \delta = k\}$$

$\alpha, \beta$  corresponding to the  $x$  direction,  $\gamma, \delta$  to the  $y$  direction. The translational invariant local transfer tensors read

$$Q_{\alpha\beta\gamma\delta}^{ss'} = v_\alpha v_\beta v_\gamma v_\delta u_s u_{s'} \mathbb{1}\{s + s' = \alpha + \beta + \gamma + \delta\}.$$

This resembles the decomposition of a one-rank tensor, but the entry vanishes if the parity of the sum of the spatial bonds and that of the time bond is not equal.

This implies that each vertical and horizontal bond has some weight (amplitude). The total weight of a given configuration is the sum of them. The contraction of the network can be seen as the sum of all total weights, taking into account only the allowed configurations.

If these tensors were rank-one tensors e.g. in a factorized form, the contraction would be done exactly since the network would factorize: We would need to sum over each bond separately, and then take the product of these sums.

One possible way to the solution: Decompose the local tensors to sum of rank-one tensors! If this way is amenable then it makes the contraction equivalent to a classical spin system where the 'spins' have as many values as the number of terms in the rank one decomposition. Either in this case or in other approaches one need to use approximative techniques in performing the contraction.

This can be done easily for a NN interaction  $\sigma_i \otimes \sigma_j$ ,  $i \sim j$ , with the help of the sort of 'complementer' of  $Q$ . To see this, in the 2D case, define the tensor

$$(Q^-)_{\alpha\beta\gamma\delta}^{ss'} = v_\alpha v_\beta v_\gamma v_\delta u_s u_{s'} (1 - \mathbb{1}\{s + s' = \alpha + \beta + \gamma + \delta\})$$

and use the fact that  $1 - \mathbb{1}\{s + s' = \alpha + \beta + \gamma + \delta\} = (-1)^{s+s'+\alpha+\beta+\gamma+\delta}$  if all the indices are binary numbers and the sum is taken modulo 2. So straightforwardly  $Q^-$  factorizes as

$$(Q^-)_{\alpha\beta\gamma\delta}^{ss'} = \tilde{v}_\alpha \tilde{v}_\beta \tilde{v}_\gamma \tilde{v}_\delta \tilde{u}_s \tilde{u}_{s'}$$

if we define  $\tilde{u}_s = (-1)^s u_s$  and  $\tilde{v}_\alpha = (-1)^\alpha v_\alpha$ . Define also simply

$$(Q^+)_{\alpha\beta\gamma\delta}^{ss'} = v_\alpha v_\beta v_\gamma v_\delta u_s u_{s'}.$$

Then clearly  $2Q = Q^+ + Q^-$ . It means that  $t\text{Tr}\{Q\} = t\text{Tr}\{(Q^+ + Q^-)/2\}$ . Now observe that we can compute the contraction exactly if we place  $Q^+$  or  $Q^-$  to each vertex, thanks to its factorized form, but the problem seems to remain as we have  $2^N$  possibilities, with  $N$  being the total number of vertices. We can get rescued by Monte Carlo simulations however, if all weights can be made positive.

### 7.0.6 Contraction along time: Exact local PEPS tensors

Without loss of generality let us work with 3 leg local tensors, corresponding to the honeycomb lattice. The idea is to pick a vertex in the lattice and compute the corresponding tensor by contracting only along the time direction. This results in the PEPS tensor for this given site. To this end recall and rewrite the local tensors

$$Q_{\alpha\beta\gamma}^{ss'} = (Q^+)_{\alpha\beta\gamma}^{ss'} + (Q^-)_{\alpha\beta\gamma}^{ss'} \quad (7.1)$$

$$= v_\alpha v_\beta v_\gamma u_s u_{s'} (1 + (-1)^{s+s'+\alpha+\beta+\gamma}) \quad (7.2)$$

$$= v_\alpha v_\beta v_\gamma u_s u_{s'} \sum_{p=0,1} (-1)^{p(s+s'+\alpha+\beta+\gamma)}. \quad (7.3)$$

This form renders the sum over the spin values manageable since if we take the sum

$$\sum_{s_2} Q_{\alpha_1\beta_1\gamma_1}^{s_1 s_2} Q_{\alpha_2\beta_2\gamma_2}^{s_2 s_3}$$

then what we need to perform is simply

$$\sum_{s_2} u_{s_2}^2 (-1)^{(p_1+p_2)s_2} = u_0^2 + (-1)^{p_1+p_2} u_1^2.$$

So after all

$$Q_{\alpha\beta\gamma}^{s_0 s_N} = u_{s_0} \sum_{p_1 \dots p_N} \prod_{i=1}^N (-1)^{p_i(\alpha_i+\beta_i+\gamma_i)} v_{\alpha_i} v_{\beta_i} v_{\gamma_i} \prod_{j=1}^N (u_0^2 + (-1)^{p_j+p_{j+1}} u_1^2) (-1)^{p_N s_N} u_{s_N}$$

where  $\alpha = (\alpha_1 \dots \alpha_N)$  etc. Now make a simplification  $u_0^2 + (-1)^{p_j+p_{j+1}} u_1^2 = c e^{K p_j p_{j+1}}$ , for some constant  $c$  and  $q_j = 2p_j - 1$ . The product part can be compressed as

$$Q_{\alpha\beta\gamma}^{s_0 s_N} = \text{const} \times u_{s_0} \sum_{q, p_N} v_\alpha^q v_\beta^q v_\gamma^q e^{H(q)} (-1)^{p_N s_N} u_{s_N}$$

with  $H(q) = K \sum_{j=1}^{N-1} q_j q_{j+1}$  and  $v_\alpha^q = v_{\alpha_1} (-1)^{p_1 \alpha_1} \dots v_{\alpha_N} (-1)^{p_N \alpha_N}$ . Note that  $H(q)$  is just the energy of a classical Ising chain with spins  $q$ . Assuming that having started with all spins up, i.e.  $s_j = 0$ , one obtains the two PEPS tensors after  $N$  time steps

$$A_{\alpha\beta\gamma}^0 = \text{const} \times u_0 \sum_q v_\alpha^q v_\beta^q v_\gamma^q e^{H(q)} u_0$$

$$A_{\alpha\beta\gamma}^1 = \text{const} \times u_0 \sum_q v_\alpha^q v_\beta^q v_\gamma^q e^{H(q)} u_1 (-1)^{q_N}.$$

Now as before, define  $E = \sum_{s=0,1} A^s \otimes \overline{A^s}$  and use the above formulas to write

$$E_{\alpha\alpha',\beta\beta',\gamma\gamma'} = \text{const} \times \sum_{q,q'} e^{H(q)+H(q')} e^{Kq_N q'_N} v_\alpha^q v_{\alpha'}^{q'} v_\beta^q v_{\beta'}^{q'} v_\gamma^q v_{\gamma'}^{q'}$$

Observe its direct relation to  $A^0$  since

$$E(N) = \text{const} \times A^0(2N).$$

Note that using the tensor notation, the expressions above can be written in a more compact form. For each site  $i$ , introduce the local, rank one tensors  $V^{q_i}$  as

$$V_{\alpha_i\beta_i\gamma_i}^{q_i} = v_{\alpha_i}^{q_i} v_{\beta_i}^{q_i} v_{\gamma_i}^{q_i}$$

then

$$A^0 = \text{const} \times \sum_{q_1 \dots q_N} e^{H(q)} V^{q_1} \otimes V^{q_2} \otimes \dots \otimes V^{q_N}. \quad (7.4)$$

**Remark 7.0.1.** Notice the analogy between computing the partition function of the 3D classical Ising model and the contraction of the tensor network above: The set of  $\{p_i\}$  (or  $\{q_i\}$ , respectively) plays the role of the classical Ising spins with interaction Hamiltonian  $H(\{p\})$  and one has a 3D lattice, two spatial and one time dimension.

**Remark 7.0.2.** Performing the contractions only in the time direction up to time  $N$  we get classical ‘superspins’ of  $2^N$  different values, interacting on the original lattice.

### 7.0.7 Contraction in spatial dimension: Transfer matrix

To sum over the spatial indices only we will write the local PEPS tensors in one layer in the form of 7.3. Then in complete analogy with the contraction along the time dimension the summation over the spatial bond between the vertices having say  $p_i$  and  $p_j$  yields

$$\sum_{\alpha} v_{\alpha}^2 (-1)^{p_i+p_j} = v_0^2 + (-1)^{p_i+p_j} v_1^2.$$

Performing all the summations we obtain

$$T_{s'}^s = \sum_{\{q\}} e^{H(q)} \prod_i u_{s_i}^{q_i} u_{s'_i}^{q_i} = \sum_{\{q\}} e^{H(q)} u_s^q u_{s'}^q \quad (7.5)$$

where  $H(q)$  is the classical Ising energy on the lattice, defined as  $v_0^2 + (-1)^{p_i+p_j} v_1^2 = c \exp(Kq_i q_j)$ . Note that the formula 7.5 remains valid for the quantum Ising model on an arbitrary lattice in any dimension as well as the idea of computing in case of other Hamiltonians.

By defining the (local) rank one matrix  $L^{q_i} = |\overline{u^{q_i}}\rangle\langle u^{q_i}|$ , we can express  $T$  as a weighted sum of rank one tensor products as follows

$$T = \sum_{\{q\}} e^{H(q)} L^{q_1} \otimes \dots \otimes L^{q_N}. \quad (7.6)$$

**Remark 7.0.3.** This enables us to check the very fact on which the validity of all the MPS methods depends. Given a spin chain one considers the exact MPS matrices after  $N$  time steps, this gives us a virtual dimension of  $2^N$ . Then we take the MPS transfer matrix and computes its dominant eigenvector and the Schmidt coefficients explicitly, using the local transfer tensors of the 1D quantum Ising model. We should see that the singular values fall off rapidly.

### 7.0.8 Outlook: Higher order tensor approximation

We note that the SVD for matrices can be extended for tensors directly: The higher order tensor singular value decomposition (HOSVD) enables us to find the best low rank approximation of a high rank tensor.

#### Tensors

Consider a tensor  $A$ . The number of indices is sometimes called the order or degree of  $A$ . Although misleading, it is sometimes even called the rank. For example  $A_{\alpha\beta\gamma}$  is a 3rd order tensor (or sometimes a 3-way tensor), a 2nd order tensor is a matrix, a first order tensor is a vector.

We will say that  $A$  is fully symmetric, if  $A_{\alpha_1\alpha_2\dots\alpha_n} = A_{\alpha_{\pi(1)}\alpha_{\pi(2)}\dots\alpha_{\pi(n)}}$  for any permutation  $\pi$  of the set  $\{1, 2, \dots, n\}$ .

Multiplications of tensors make sense if we specify the indices to be contracted. For instance we can define the  $j$ -mode multiplication of the tensor  $A \in \mathbb{C}^{\{I_1 \times I_2 \times \dots \times I_n\}}$  by the vector  $v \in \mathbb{C}^{I_j}$  as follows

$$(A \times_j v)_{\alpha_1 \dots \alpha_j \dots \alpha_n} := \sum_{\alpha'_j} A_{\alpha_1 \dots \alpha'_j \dots \alpha_n} v_{\alpha'_j}$$

where we also introduced the symbol  $\times_j$ . Similarly one can multiply  $A$  by the matrix  $M \in \mathbb{C}^{I_j \times J_j}$ , as

$$(A \times_j M)_{\alpha_1 \dots \alpha_j \dots \alpha_n} := \sum_{\alpha'_j} A_{\alpha_1 \dots \alpha'_j \dots \alpha_n} M_{\alpha'_j \alpha_j}.$$

We will also make use of the outer product, i.e. one can make a 3rd order tensor  $A$  out of vectors  $u, v, w$  as

$$A_{\alpha\beta\gamma} = (u \circ v \circ w)_{\alpha\beta\gamma} := u_{\alpha}v_{\beta}w_{\gamma}.$$

### HOSVD

For example given a 3 order (3 way) tensor  $A_{\alpha\beta\gamma}$  of dimension  $d_1 \times d_2 \times d_3$  we require the 3 way tensor  $\tilde{A}$  of dimension  $r_1 \times r_2 \times r_3$  with  $r_i \leq d_i$ , respectively. Let us build three different matrices out of  $A$  as

$$\begin{aligned} A_{\alpha,\beta\gamma}^{(1)} &:= A_{\alpha,\beta\gamma} & A^{(1)} &: d_1 \times d_2d_3 \\ A_{\beta,\alpha\gamma}^{(2)} &:= A_{\beta,\alpha\gamma} & A^{(2)} &: d_2 \times d_1d_3 \\ A_{\gamma,\alpha\beta}^{(3)} &:= A_{\gamma,\alpha\beta} & A^{(3)} &: d_3 \times d_1d_2 \end{aligned}$$

The above defined matrices (2 way tensors) are called matrix unfoldings of the original tensor  $A$ . Clearly, the number of the unfoldings equals the order of  $A$ . Now performing the usual SVD for these matrices one gets

$$A^{(j)} = U^{(j)} S^{(j)} V^{(j)} \quad j = 1, 2, 3. \quad (7.7)$$

$U^{(j)}$  has size of  $d_j \times d_j$  and for example  $V^{(1)}$  has size of  $d_2d_3 \times d_2d_3$  and  $S^{(1)}$  is diagonal  $d_1 \times d_2d_3$  matrix but has only  $\min(d_1, d_2d_3)$  positive entries.

**Definition 7.1.** *Tensor matrix multiplication.*

For a tensor  $A$  of size  $d_1 \times d_2 \times d_3$  we define the multiplication by a matrix  $M$  of size  $d_1 \times d$  along the first mode as

$$B_{\alpha'\beta\gamma} = \sum_{\alpha} A_{\alpha\beta\gamma} M_{\alpha\alpha'}$$

and simply write

$$B = A \times_1 M.$$

**Definition 7.2.** *Scalar product of tensors.*

Given tensors  $A$  and  $B$  of the same order and dimensions their scalar product is

$$\langle A, B \rangle = \sum_{\alpha_1 \dots \alpha_n} \bar{A}_{\alpha_1 \dots \alpha_n} B_{\alpha_1 \dots \alpha_n}.$$

**Definition 7.3.** *All-orthogonality.*

Given tensors  $A$  and  $B$  construct subtensors by fixing one entry of the same modes, respectively. They are all-orthogonals is for each possibilities of  $i, \beta, \gamma$  subject to  $\beta \neq \gamma$

$$\langle A_{\alpha_i=\beta}, B_{\alpha_i=\gamma} \rangle = 0 \quad \text{when} \quad \beta \neq \gamma.$$

**Theorem 7.4.** *HOSVD.*

Given the 3 way tensor  $A_{\alpha\beta\gamma}$  of dimension  $d_1 \times d_2 \times d_3$  its higher order singular value decomposition is of the form

$$A_{\alpha\beta\gamma} = \sum_{\alpha'\beta'\gamma'} S_{\alpha'\beta'\gamma'} U_{\alpha\alpha'}^{(1)} U_{\beta\beta'}^{(2)} U_{\gamma\gamma'}^{(3)} \quad (7.8)$$

with the unitaries defined in 7.7. More simply

$$A = S \times_1 U^{(1)} \times_2 U^{(2)} \times_3 U^{(3)}.$$

The tensor  $S$  of size  $d_1 \times d_2 \times d_3$  is all orthogonal.

## Chapter 8

# Simulation of the quantum Ising model on Bethe lattices

We construct an algorithm to simulate imaginary time evolution of translationally invariant spin systems with local interactions on an infinite, symmetric tree. We describe the state by symmetric infinite-Tree Tensor Network (iTNN) and use translation-invariant operators for the updates at each time step. The contraction of this tree tensor network can be computed efficiently by recursion without approximations and one can then truncate all the iTNN tensors at the same time. The translational symmetry is preserved at each time step that makes the algorithm very well conditioned and stable. The computational cost scales like  $O(D^{q+1})$  with the bond dimension  $D$  and coordination number  $q$ , much favourable than that of the iTEBD on trees [D. Nagaj et al. Phys. Rev. B **77**, 214431 (2008)]. Studying the transverse-field Ising model on the Bethe lattice, the numerics indicate a ferromagnetic-paramagnetic phase transition, with a finite correlation length even at the transition point.

### 8.1 Contraction of Tree Tensor Networks

#### 8.1.1 Tensors

Consider a tensor  $A$ . The number of indices is sometimes called the order or degree of  $A$ . Although misleading, it is sometimes even called the rank, for example  $A_{\alpha\beta\gamma}$  is a 3rd order tensor (or sometimes a 3-way tensor), a 2nd order tensor is a matrix, a first order tensor is a vector.

We will say that  $A$  is fully symmetric, if  $A_{\alpha_1\alpha_2\dots\alpha_n} = A_{\alpha_{\pi(1)}\alpha_{\pi(2)}\dots\alpha_{\pi(n)}}$  for any permutation  $\pi$  of the set  $\{1, 2, \dots, n\}$ .

Multiplications of tensors make sense if we specify the indices to be contracted. For instance we can define the  $j$ -mode multiplication of the tensor  $A \in \mathbb{C}^{\{I_1 \otimes \dots \otimes I_j \otimes \dots \otimes I_n\}}$  by the vector  $v \in \mathbb{C}^{I_j}$  producing a tensor  $A \otimes_j v \in \mathbb{C}^{\{I_1 \otimes \dots \otimes I_{j-1}, I_{j+1}, \dots \otimes I_n\}}$  as follows

$$(A \otimes_j v)_{\alpha_1 \dots \alpha_{j-1}, \alpha_{j+1} \dots \alpha_n} := \sum_{\alpha_j} A_{\alpha_1 \dots \alpha_j \dots \alpha_n} v_{\alpha_j}$$

where we also introduced the symbol  $\otimes_j$  as in [60]. Similarly one can multiply  $A$  by the matrix  $M \in \mathbb{C}^{I_j \otimes J_j}$ , as

$$(A \otimes_j M)_{\alpha_1 \dots \alpha_j \dots \alpha_n} := \sum_{\alpha'_j} A_{\alpha_1 \dots \alpha'_j \dots \alpha_n} M_{\alpha_j \alpha'_j}.$$

We will also make use of the outer product, i.e. one can make a 3rd order tensor  $A$  out of vectors  $u, v, w$  as

$$A_{\alpha\beta\gamma} = (u \circ v \circ w)_{\alpha\beta\gamma} := u_\alpha v_\beta w_\gamma.$$

### 8.1.2 Contraction, expectation values and correlations

Consider the Bethe lattice (Fig. 8.1) with coordination number  $q$  and place fully symmetric TTN tensors  $A^s$  to each node. This describes the translation-invariant state  $\psi$ ; from each node, the tree looks the same.

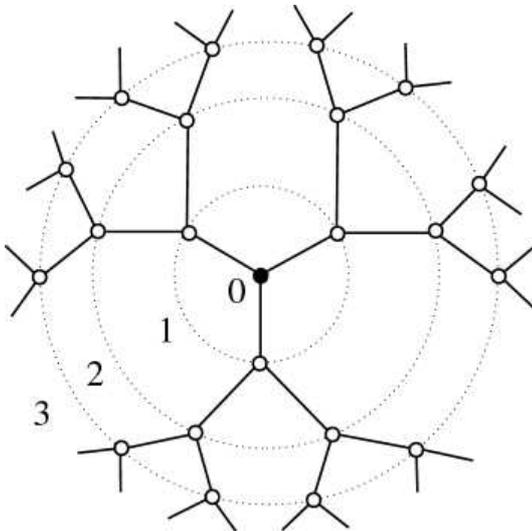


FIGURE 8.1: Three layers of the Bethe lattice with coordination number  $q = 3$

Observe that the computation of the norm square  $\langle \psi | \psi \rangle$  on trees essentially reduces to the computation of the leading vector  $r$  of the transfer matrix  $E = \sum_s A^s \otimes \overline{A^s}$ , and it can be done efficiently by recursion. This statement is well known and easy to see in 1D, but similarly simple also for trees. Without loss of generality take  $q = 3$  and use

tensor notations for simplicity. Begin with the 3-way, fully symmetric,  $d \otimes d \otimes d$  tensor  $E$  and a random vector  $r^{(0)}$  of dimension  $d$ . For  $n = 0, 1, 2, \dots$  define the series

$$r^{(n+1)} = E \otimes_1 r^{(n)} \otimes_2 r^{(n)}. \quad (8.1)$$

The normalized series converges to the so-called leading vector of  $E$ , i.e.  $r^{(n)}/\|r^{(n)}\| \rightarrow r$ , given  $\langle r|r_0 \rangle \neq 0$  so the leading vector  $r$  is a fix point of the recursion (8.1)

$$r = E \otimes_1 r \otimes_2 r.$$

Notice that this is just the extension of the power iteration, which is originally an algorithm for finding the dominant eigenvector of a matrix. Its generalization for the case where  $E$  is not symmetric and has different leading vectors for each mode is straightforward. Notice also, that for a generic 3rd order tensor  $T$ , its leading vectors  $u, v, w$  give the best rank-one decomposition [61], i.e. minimize

$$\|T - \lambda u \circ v \circ w\|$$

and  $\lambda = T \otimes_1 u \otimes_2 v \otimes_3 w$ , assuming  $\|u\| = \|v\| = \|w\| = 1$ .

Using the leading vector  $r$  one gets

$$\langle \psi|\psi \rangle = \langle \bar{r}|r \rangle = \sum_{\alpha} r_{\alpha}^2.$$

The expectation of a local operator  $O$  in the state  $\psi$  reads

$$\langle O \rangle = \frac{\langle \bar{r}|E_O|r \rangle}{\langle \bar{r}|E|r \rangle}$$

with  $E_O = \sum_{s,s'} \langle s|O|s' \rangle A^s \otimes \overline{A^{s'}}$ , and the correlation between two sites of distance  $n$  reduces to the computation of the second largest eigenvalue of the matrix

$$M = E \otimes_1 r.$$

This is in accordance with the findings of [37] but written in a much more compact form.

### 8.1.3 Computational costs

Clearly, the direct computational cost of each iteration step scales as  $O(d^q)$  for arbitrary  $q \in \mathbb{N}$ . As for the convergence, we can state the followings. If the fully symmetric  $E$  can

be decomposed such that

$$E = \sum_i \lambda_i v_i \circ v_i \circ v_i$$

where  $\langle v_i | v_j \rangle = 0$  for  $i \neq j$  and  $|\lambda_1| > |\lambda_2| \geq |\lambda_3| \geq \dots$  then the convergence is surely geometric with ratio  $|\lambda_2/\lambda_1|$ . This corresponds to the matrix case when the matrix is diagonalizable. In any case, given a concrete  $E$ , the convergence should be checked by doing the numerics. Let us mention that since  $|\lambda_2/\lambda_1|$  is related to the correlation length of the system, one can expect an exponentially fast convergence only if the correlation length is finite. Otherwise, if the correlation length diverges as the function of the bond dimension, the algorithm slows down.

However, we can exploit the symmetries of  $E$  to get a much better scaling. To this end, simply exploit the structure of  $E = \sum_s A^s \otimes \overline{A^s}$ . Rewrite (8.1) explicitly

$$r_{\gamma\gamma'}^{(n+1)} = \sum_{s=0}^1 \sum_{\alpha\alpha'\beta\beta'} A_{\alpha\beta\gamma}^s \overline{A_{\alpha'\beta'\gamma'}^s} r_{\alpha\alpha'}^{(n)} v_{\beta\beta'}^{(n)} \quad (8.2)$$

where all the Greek indices run from 1 to  $D$ . Now break the sum into four parts. First let us sum over  $\alpha$ , then over  $\beta$ . When regarding  $r_{\alpha\alpha'}$  as a matrix, we will write  $R$ , i.e. define the tensor  $\mathcal{B}^s = A^s \otimes_1 R^{(n)}$ , explicitly written

$$\mathcal{B}_{\alpha'\beta\gamma}^s := \sum_{\alpha=1}^D A_{\alpha\beta\gamma}^s r_{\alpha\alpha'}^{(n)}.$$

This requires  $O(D^4)$  steps because we fix  $s, \alpha', \beta, \gamma$  and sum over  $\alpha$ . In the same way perform

$$\mathcal{C}_{\alpha'\beta'\gamma}^s := \sum_{\beta=1}^D \mathcal{B}_{\alpha'\beta\gamma}^s r_{\beta\beta'}^{(n)}.$$

Finally we arrive at

$$r_{\gamma\gamma'}^{(n+1)} = \sum_{s=0}^1 \sum_{\alpha'\beta'=1}^D \mathcal{C}_{\alpha'\beta'\gamma}^s \overline{A_{\alpha'\beta'\gamma'}^s}.$$

again at a cost of  $O(D^4)$ . Performing the recursion as described above requires  $O(D^4)$  computational steps. Its easy to see that the idea works for arbitrary  $q$  and its cost scales like  $O(D^{q+1})$ .

Note that, the above argument still holds for the computation of the expectation value  $\langle O \rangle$ .

In order to compute the correlation length one has to find the second largest eigenvalue of the  $D^2 \otimes D^2$  matrix  $M$  at a cost of  $O(D^4)$  steps.

### 8.1.4 Tensor updates

Let us consider a time evolution induced by a translationally invariant Hamiltonian on the tree lattice. If one starts with a translation-invariant state, then the symmetry of the Hamiltonian guarantees that it is never broken in time. Assume we have a TTN description with bond dimension  $D$  for this translation-invariant state  $\psi$ . Obviously each site has the same TTN tensors  $A^s$ . Now we update these tensors in every time step and obtain the updated state  $\psi'$  with new TTN tensors and bond dimension  $2D$ . Then we need to truncate them in an optimal way, i.e. we should find TTN tensors  $\widetilde{A}^s$  with bond dimension  $D$  describing a state  $\widetilde{\psi}$  which minimizes the distance from  $\psi'$ , i.e. for which

$$\|\psi' - \widetilde{\psi}\|$$

is minimal.

In order to carry out the optimal cut express the norm square by the leading vector  $r'$  of the updated  $E'$  as

$$\langle \psi' | \psi' \rangle = E' \otimes_1 r' \otimes_2 r' \otimes_3 r' = r' \otimes r' = \sum_{\gamma\gamma'=1}^{2D} r'_{\gamma\gamma'} r'_{\gamma\gamma'} = \langle \overline{r'} | r' \rangle.$$

One can look at  $r'_{\gamma\gamma'}$  as a symmetric  $2D \otimes 2D$ , complex matrix which we will denote by  $R' = R'^{\dagger}$ . Perform its singular value decomposition:  $R' = U\Lambda U^{\dagger}$  and introduce the  $D \otimes 2D$  matrix  $\widetilde{U}$  consisting of the first  $D$  rows of  $U$  and  $\widetilde{\Lambda}$  is a  $D \otimes D$  diagonal matrix made up of the  $D$  largest singular values. Define the self adjoint projection  $P = \widetilde{U}^{\dagger} \widetilde{U}$ , indeed  $P = P^{\dagger} = P^2$  since  $\widetilde{U} \widetilde{U}^{\dagger} = \mathbb{1}_D$ . We can project to the subspace of the highest  $D$  singular values as  $A^s \otimes_1 P \otimes_2 P \otimes_3 P$ , implying that the appropriate cut is then given by the transformation

$$A^s \longrightarrow \widetilde{A}^s = A^s \otimes_1 \widetilde{U} \otimes_2 \widetilde{U} \otimes_3 \widetilde{U}.$$

These new tensors will have the right size  $D \otimes D \otimes D$  and describe the state  $\widetilde{\psi}$ . This is nothing else than the extension of the 1D algorithm to the tree geometry. Recall that in one dimension the truncation step looks like [36]

$$A^s \longrightarrow \widetilde{A}^s = \widetilde{U} A^s \widetilde{U}^{\dagger} = A^s \otimes_1 \widetilde{U} \otimes_2 \widetilde{U}.$$

As always, the lower the discarded weight relatively, the higher the accuracy of the approximation. If the former is not small enough, one should increase the bond dimension.

### Translation-invariant iTEBD on the Bethe lattice

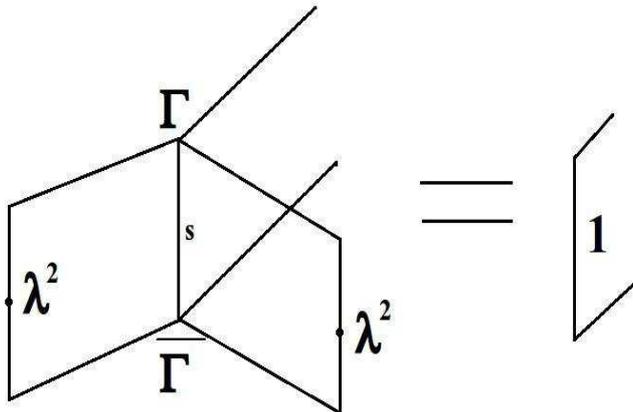


FIGURE 8.2: The norm condition (8.4) in diagram

We also show that the one dimensional iTEBD algorithm [62] which uses the so-called canonical representation of infinite-MPS (iMPS, see e.g. the review [26]) can also be extended to the Bethe lattice. Note that here one updates all the tensors at once therefore translation invariance is kept at each step, given that the infinite-MPO (iMPO) and the starting state have been so. Hence this update method differs from the one in [37] where instead of iMPO, the interaction between only two adjacent sites has been considered at each step, leading to the breaking of the translational symmetry during the process.

### Canonical iTTN

This representation contains the tensors  $\Gamma$ , placing to the sites and the explicit Schmidt coefficients  $\lambda$  (sitting on the bonds) that one gets if cutting the tree between two neighbouring sites [37]

$$|\psi\rangle = \prod_{k \in \text{bonds}} \sum_{\alpha_k} \lambda_{\alpha_k}^{(k)} \prod_{i \in \text{sites}} \sum_{s_i, \alpha_l \dots} \Gamma_{\alpha_l, \alpha_m, \alpha_n}^{(i), s_i} |s_i\rangle |.. \rangle$$

each index  $\alpha_l$  appears in two  $\Gamma$  tensors and one  $\lambda$ . The normalization conditions for the canonical iTTN on the Bethe lattice look like

$$\sum_{\alpha} \lambda_{\alpha}^2 = 1, \quad (8.3)$$

$$\sum_s \sum_{\alpha_k} \sum_{\alpha_l} \overline{\Gamma_{\alpha_k, \alpha_l, \alpha_m}^{(i), s_i}} \lambda_{\alpha_k}^{(k)2} \lambda_{\alpha_l}^{(l)2} \Gamma_{\alpha_k, \alpha_l, \alpha_m}^{(i), s_i} = \delta_{\alpha_m, \alpha_m'} \quad (8.4)$$

this latter relation becomes much more unambiguous if represented in diagram, see Fig.8.2. There are two conditions like this if  $q = 3$ , interchanging the legs of the tensor  $\Gamma$ , i.e. we have two layers due to the tensor product, and we leave two open legs (indices) in one direction and close the other legs by placing  $\lambda^2$  and sum over the corresponding

bonds. The directional symmetry manifests itself in a fully symmetric  $\Gamma^s$ . Now applying the iMPO to this iTTN results in higher bond dimension and the violation of these norm conditions: The new leading vector will be different from the identity. According to the procedure in [62], we have to bring this back to the canonical form (orthogonalization) and then truncate all bond indices by retaining the  $D$  highest Schmidt coefficients. We can naturally extend this by performing the same operations on each leg as in the one dimensional case, noting that we can define the dominant eigenvector by (8.1) and in case of directional symmetry, this will be the same for all legs. After computing this leading vector  $R$  (which is interpreted as a matrix because of the two layers), we perform the same manipulations as in Fig. 3 in [62], but now we have open legs in one direction and ‘closed legs’ in the other  $q - 1$  directions.

## 8.2 Imaginary Time Evolution

Consider the Hamiltonian on the Bethe tree  $G = (V, E)$  with coordination number  $q$

$$H = - \sum_{i,j \in V, i \sim j} J \sigma_i^x \sigma_j^x - \sum_{i \in V} h \sigma_i^z \quad (8.5)$$

As shown in [36] one can derive an elegant MPO representation for  $e^{-\varepsilon H}$  with  $H$  being the Ising Hamiltonian on a one-dimensional infinite chain.

$$\exp(-\varepsilon H) = \sum_{k_1, k_2, \dots} \text{Tr}(C^{k_1}(\varepsilon) C^{k_2}(\varepsilon) \dots) Z^{k_1} \otimes Z^{k_2} \dots \quad (8.6)$$

with 2 dimensional MPO matrices  $C^k(\varepsilon)$  given by

$$\begin{aligned} C^0(\varepsilon) &= \sum_i B_i B_i^T = \begin{pmatrix} \cosh \varepsilon & 0 \\ 0 & \sinh \varepsilon \end{pmatrix} \\ C^1(\varepsilon) &= \sum_i B_{i \oplus 1} B_i^T = \begin{pmatrix} 0 & \sqrt{\cosh \varepsilon \sinh \varepsilon} \\ \sqrt{\cosh \varepsilon \sinh \varepsilon} & 0 \end{pmatrix}. \end{aligned}$$

And the spin operators are  $X^0 = e^{\delta \sigma^z}$ ,  $X^1 = \sigma^x$ ,  $\delta = h \Delta t / 2$  for the second order Suzuki-Trotter formula [36]. We would like to determine the local ‘transfer tensors’  $Q_{\alpha\beta\gamma}^{s's}$  that makes the TTN tensors evolve as

$$A_{\alpha\beta\gamma}^s \longrightarrow \sum_{s'} A_{\alpha\beta\gamma}^{s'} Q_{\alpha'\beta'\gamma'}^{s's},$$

or using tensor notation

$$A^s \longrightarrow \sum_{s'} A^{s'} \otimes Q^{s's}.$$

We can express the MPO matrices by the sum of outer product of vectors. First define the vectors

$$v = (\sqrt{\cosh(J\Delta t)}, \sqrt{\sinh(J\Delta t)})$$

and

$$u = (\exp(h\Delta t/2), \exp(-h\Delta t/2)).$$

Then observe that in 1D, the MPO-s has the compact form

$$C_{\alpha\beta}^k = v_\alpha v_\beta \mathbb{1}\{k = \alpha + \beta\}$$

$\alpha, \beta$  corresponding to the  $x$  direction, and  $\mathbb{1}\{A\}$  being the indicator function of the event  $A$ .

The translationally invariant local transfer tensors read

$$Q_{\alpha\beta}^{ss'} = v_\alpha v_\beta u_s u_{s'} \mathbb{1}\{s + s' = \alpha + \beta\}.$$

analogously, if there are three spatial indices, the MPO-s has the form

$$C_{\alpha\beta\gamma}^k = v_\alpha v_\beta v_\gamma \mathbb{1}\{\alpha + \beta + \gamma = k\}$$

and the translationally invariant local transfer tensors read

$$Q_{\alpha\beta\gamma}^{ss'} = v_\alpha v_\beta v_\gamma u_s u_{s'} \mathbb{1}\{s + s' = \alpha + \beta + \gamma\}.$$

this can be written as a sum of two rank-one tensors as can be verified

$$Q = u \circ u \circ v \circ v \circ v + \tilde{u} \circ \tilde{u} \circ \tilde{v} \circ \tilde{v} \circ \tilde{v}$$

using tensor notation and  $\tilde{u} = \sigma^z u$ ,  $\tilde{v} = \sigma^z v$ .

Note that the above derivation for the local interactions like  $\sigma_x \otimes \sigma_x$  with a transverse-field can be repeated for  $\sigma_y \otimes \sigma_y$  or  $\sigma_z \otimes \sigma_z$ .

### 8.3 Results and discussion

We set  $J = 1$  making interactions ferromagnetic and vary  $h$ .

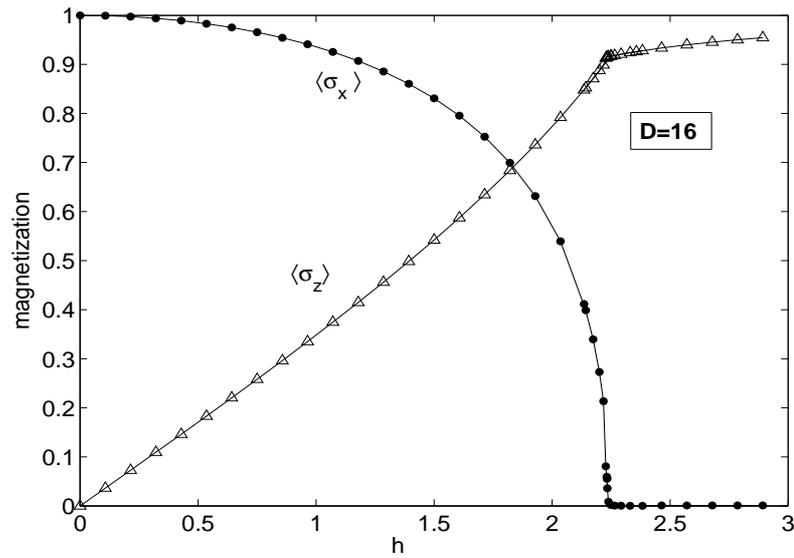


FIGURE 8.3: Longitudinal and transverse magnetization of the Ising model on the  $q = 3$  Bethe lattice.

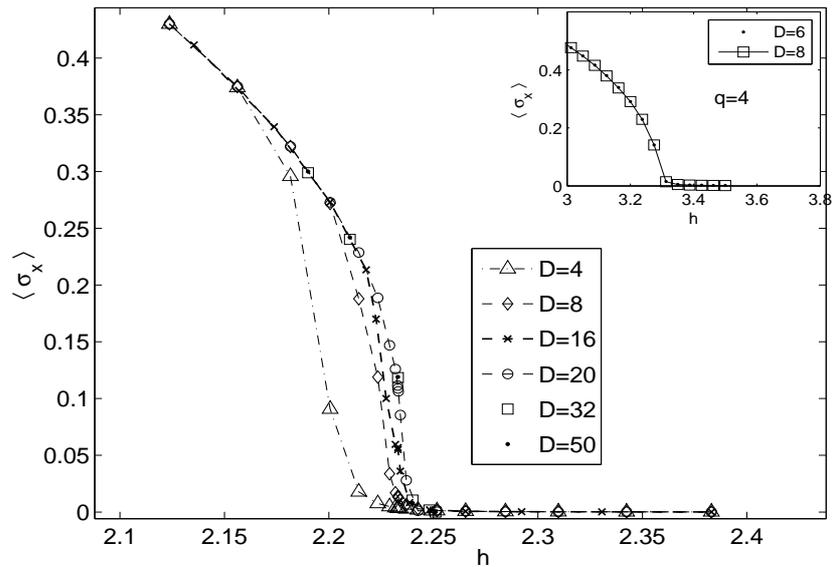


FIGURE 8.4: Longitudinal magnetization of the Ising model on the  $q = 3$  and  $q = 4$  (subplot) Bethe lattice around the transition point. Notice that even for small bond dimensions, the results are barely different.

Using the present algorithm I found very good agreement with the results reported earlier. Namely, the transverse and parallel magnetization as the function of the magnetic field behave similarly to that of the Ising model on an infinite line, but the critical point is shifted, and estimated to be in the interval  $2.23 < h/J < 2.25$ .

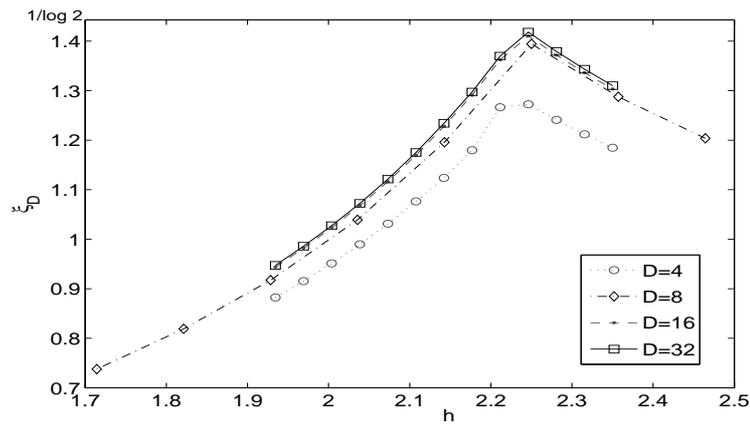


FIGURE 8.5: Correlation length around the transition point for different bond dimensions,  $q = 3$

One can also check whether the longitudinal magnetization obeys the scaling law

$$\langle \sigma_x \rangle \propto (h_c - h)^\beta$$

in the ferromagnetic phase, near to the transition point. Fitting a line in the log-log plot, we obtain  $\beta \approx 0.46$ . In [37] they reported  $\beta = 0.41$ , while the so-called ‘cavity method’ prediction  $\beta = 1/2$  equals the mean-field result, see [64].

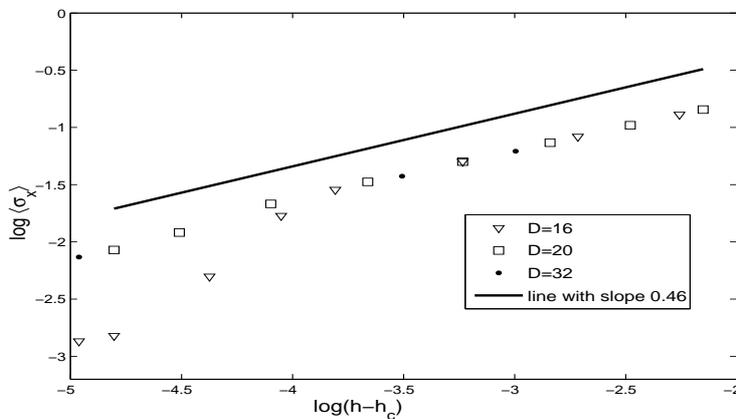


FIGURE 8.6: Log-log plot of the parallel magnetization vs  $h - h_c$

Surprisingly, the correlation length  $\xi$  at the transition point does not seem to diverge as  $D \rightarrow \infty$ , since the second largest eigenvalue  $\lambda_2$  of  $B$  never exceeds  $1/2$ , in complete agreement with the findings of [37]. This is a strong numerical evidence of a finite correlation length even in a presence of a (supposed) phase transition. Also, plotting the first derivative of the energy per site with respect to the magnetic field, we see a non analytic breaking-point at the suspected critical field, while the plot suggest a discontinuous second derivative with a finite jump at the same point, see Fig. 8.7.

Qualitatively the ground state energy behaves very similarly to that of the exactly solvable quantum Curie-Weiss model [64].

Note that in [37] they used a different parametrization of the Hamiltonian with the parameter  $s$  for which  $h/J = 3(1 - s)/s$ .

I also considered the Bethe lattice with coordination number  $q = 4$  and found similar phase diagrams, but with transition point at  $h/J \approx 3.3$  and the results suggest that  $\lambda_2 \leq 1/3$ .

### Previous results and theoretical considerations

In [63] the authors extended the cavity method to quantum spin-1/2 models making it applicable to Bethe lattices, too. In [64], by using Monte Carlo simulations, it is applied to the present model. They computed the magnetization for different temperatures, and their zero temperature extrapolations (e.g. for the ground state) agree very well with the present findings and with [37].

We would like to draw the reader's attention to the last section of [37], where the two point correlation is calculated. Given a translation-invariant Hamiltonian with nearest neighbour interactions on the Bethe lattice, it is shown that the two point correlations always fall off exponentially, and the correlation length is upper bounded by  $1/\log(q - 1)$ , confirming our numerical findings. According to this brief argument, it is a model-independent and computational method independent consequence of assuming that the translational independent ground state is the stable limit of a sequence of ground states as the size of the tree grows.

Notice that the argument also holds for the classical Ising model defined on the Bethe lattice which is exactly solvable and exhibits phase transition [46].

Note also, that in [64], the correlation length was not computed, but (mistakenly) supposed to be infinite at the critical point.

### Errors

Concerning the errors one can distinguish two sources: using the Trotter-Suzuki formula and the truncation. The former has the order of  $N(\Delta t)^3 = t^3/N^2$ , as the second order Trotter formula is used, i.e.  $e^{-tH} \approx \left( e^{-\frac{t}{2N}H_z} e^{-\frac{t}{N}H_x} e^{-\frac{t}{2N}H_z} \right)^N$ . So we need  $t \rightarrow \infty$  to obtain the ground state properties and  $N \rightarrow \infty$  together with  $\Delta t = t/N \rightarrow 0$  and  $N(\Delta t)^3 = t^3/N^2 \rightarrow 0$  to make the Trotter error go to zero. This can be achieved e.g. by setting  $N(t) = ct^2$  for some constant  $c$  and then increasing  $t$  until the results do not change significantly.

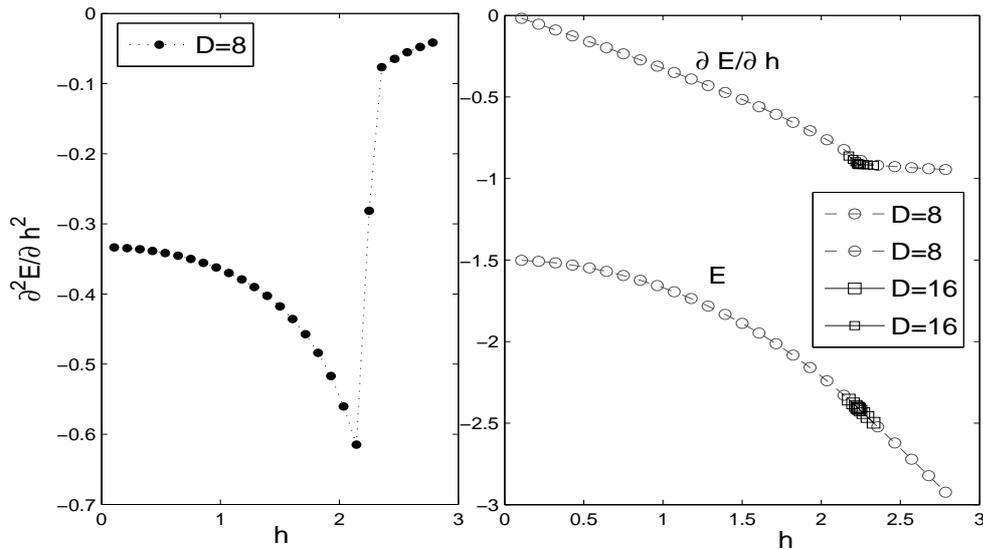


FIGURE 8.7: Ground state energy and its first and second derivatives with respect to  $h$  for  $q = 3$ . Notice that the results for  $D = 8$  and  $D = 16$  are indistinguishable in the figure.

In Fig. 8.8 we plot the longitudinal magnetization  $m_x = \langle \sigma_x \rangle$  computed as a function of time. Here we fix the maximum time  $T$  and run the algorithm five times with different number of time steps  $N$ . One can see that higher the  $N$  the slower the convergence to the limiting value  $m_x(T, N)$ , but as a function of  $N$  (or  $\Delta t = T/N$ ) the convergence to the limit  $m_x(T) = \lim_{N \rightarrow \infty} m_x(T, N)$  is very fast. Then increasing the time  $m_x(T) \rightarrow m_x$ , in the present case we can choose  $N(T) = 2T^2$ . In general, if the system is gapless, this convergence is exponential in  $T$ .

Note that one has to be cautious about the convergence of different quantities, usually the convergence of the energy is much faster than that of the magnetization, so it is not sufficient to check only the convergence of the energy.

## 8.4 Summary

We have derived an algorithm to simulate the imaginary time evolution induced by certain translationally invariant local Hamiltonians on the Bethe lattice. During the time evolution we have used a translationally invariant iTTN description of the evolving state and have given the optimal updates which retain the symmetry at every step. The presented method has much lower computational costs than that of the slightly modified version of the iTTEBD method for trees, reported in [37]. That scaled like  $O(D^8)$ , and the translational symmetry was broken during the algorithm. Investigated specifically the Ising model on trees, we have found very good agreement with previous numerical

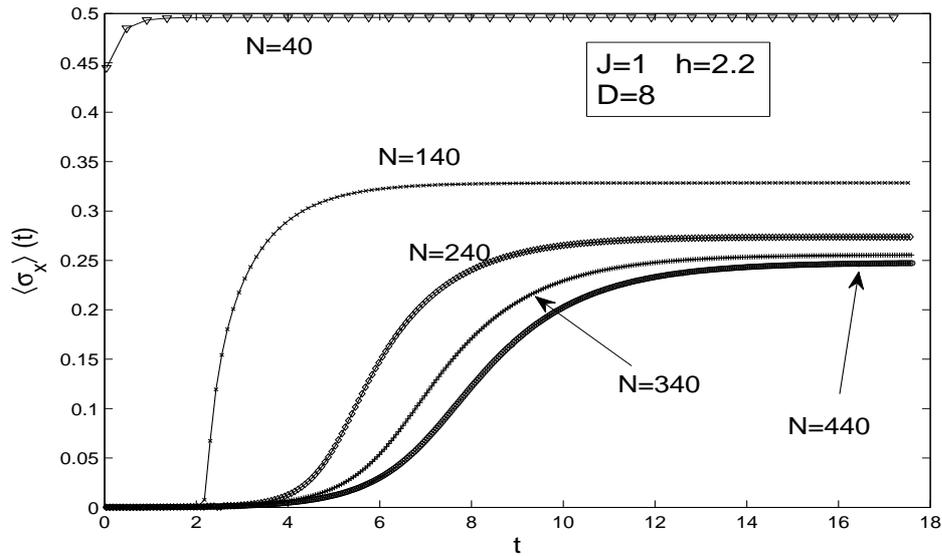


FIGURE 8.8: Typical behaviour of a computed physical quantity during the time evolution. The maximum time  $T$  is fixed, and the time steps  $N$  are increased linearly. Starting from the same initial state, we get different curves due to the Trotter errors.

results, namely a phase transition between a ferromagnetic and a paramagnetic phase but with finite correlation length even at the transition point. At this critical point, the second derivative of the energy with respect to the magnetic field has a finite jump, while the energy and its first derivative is continuous. Considering the results for  $q = 2, 3, 4$  suggests that increasing the coordination number  $q$ , at fixed  $J$ , the critical magnetic field increases, and the maximal correlation length decreases.

**Remark 8.4.1.** The striking fact that one has a phase transition (non analytic functions) but yet exponentially decaying correlations can be understood by applying the Lieb Robinson bound which gives conditions for the exponential clustering as mentioned earlier [27].

Taking a Cayley tree of radius  $N$ , it turns out that it is indeed possible to have a vanishing gap (as  $N$  goes to infinity) but still exponential correlations in the thermodynamical limit. (Private communications between A.Nagy and Jens Eisert.) It depends on the bizarre structure of the tree lattice: The number of sites grows exponentially with the radius of the tree, but usually never happens in case of square, triangulare, honeycomb etc. lattices which are topologically very different (and containing loops which bans the application of this simple algorithm for the contractions). On these lattices the vanishing gap accompanies with diverging correlation lengths. This helps us to resolve the puzzle.

## Appendix A

# Commutant set for the three qubit case

Given the operators  $S_i = \sum_{a=1}^3 \sigma_i^{(a)}$ ,  $i = 1, 2, 3$ , the commutant set  $M_\gamma = \{S_i\}'$  is found by expanding a generic  $x \in M$  by means of tensor products of the Pauli matrices:

$$x = \lambda_0 \mathbb{1} + \sum_{a=1, i=1}^3 \lambda_{ai}^{(1)} \sigma_i^{(a)} + \sum_{a < b=1, i, j=1}^3 \lambda_{ai, bj}^{(2)} \sigma_i^{(a)} \sigma_j^{(b)} + \sum_{i, j, k=1}^3 \lambda_{ijk}^{(3)} \sigma_i^{(1)} \sigma_j^{(2)} \sigma_k^{(3)}, \quad (\text{A.1})$$

and then imposing  $[x, S_i] = 0$  for all  $i = 1, 2, 3$ . By using the Pauli algebraic relations one finds the following equalities

$$\sum_{\ell=1}^3 \lambda_{a\ell}^{(1)} \varepsilon_{\ell pi} = 0 \quad \forall i, p = 1, 2, 3 \quad (\text{A.2})$$

$$\sum_{\ell=1}^3 \left( \lambda_{ai, b\ell}^{(2)} \varepsilon_{\ell pj} + \lambda_{a\ell, bj}^{(2)} \varepsilon_{\ell pi} \right) = 0 \quad \forall a < b, i, j, p = 1, 2, 3 \quad (\text{A.3})$$

$$\sum_{\ell=1}^3 \left( \lambda_{ij\ell}^{(3)} \varepsilon_{\ell pk} + \lambda_{i\ell k}^{(3)} \varepsilon_{\ell pj} + \lambda_{\ell jk}^{(3)} \varepsilon_{\ell pi} \right) = 0 \quad \forall i, j, k, p = 1, 2, 3, \quad (\text{A.4})$$

whence  $\lambda_{ai}^{(1)} = 0$  for all  $a, i = 1, 2, 3$ ,  $\lambda_{ai, bi}^{(2)} = \lambda_{aj, bj}^{(2)}$  for all  $a < b = 1, 2, 3$  and  $i, j = 1, 2, 3$ , while  $\lambda_{ijk}^{(3)} = \lambda \varepsilon_{ijk}$ . It thus follows that the commutant set is  $\{S_i\}' = \{\mathbb{1}, S^{(ab)}, S\}$ ,  $a, b = 1, 2, 3$ , namely the linear span of  $\mathbb{1}$  and

$$S^{(ab)} = \sum_{i=1}^3 \sigma_i^{(a)} \sigma_i^{(b)} \quad a < b = 1, 2, 3; \quad S = \sum_{i, j, k=1}^3 \varepsilon_{ijk} \sigma_i^{(1)} \sigma_j^{(2)} \sigma_k^{(3)}. \quad (\text{A.5})$$

Unlike for two qubits, the commutant set is not commutative; indeed, with  $a, b, c$  different indices,

$$\left[ S^{(ab)}, S^{(ac)} \right] = 2i\varepsilon_{abc} S^{(bc)}, \quad \left\{ S^{(ab)}, S^{(ac)} \right\} = 2 S^{(bc)} \quad (\text{A.6})$$

$$\left[ S^{(ab)}, S \right] = 4i \left( S^{(bc)} - S^{(ac)} \right), \quad a < b, \quad (\text{A.7})$$

whence

$$T = \sum_{a < b=1}^3 S^{ab} = S^{(12)} + S^{(23)} + S^{(13)} \Rightarrow [T, S^{(ab)}] = [T, S] = 0, \quad (\text{A.8})$$

so that  $T$  belongs to the center  $\mathcal{Z} = \{S_i\}' \cap \{S_i\}'' = M_\gamma \cap M_\gamma'$ . Other useful algebraic relations are as follows

$$(S^{(ab)})^2 = 3 - 2 S^{(ab)}, \quad a, b = 1, 2, 3; \quad S^2 = 2(3 - T). \quad (\text{A.9})$$

From the first relations it follows that

$$P^{(ab)} = \frac{\mathbb{1} - S^{(ab)}}{4} \in M_\gamma = \{S_i\}' = \{\mathbb{1}, S^{(ab)}, S\} \quad (\text{A.10})$$

$$P = \frac{2}{3} \sum_{a < b=1}^3 P^{(ab)} = \frac{1}{2} \left( \mathbb{1} - \frac{1}{3} T \right) \in M_\gamma \cap M_\gamma' \quad (\text{A.11})$$

are two-dimensional, respectively four-dimensional projections. In particular,  $P^{(ab)}$  is the tensor product of the projection onto the singlet state of the qubits  $a$  and  $b$  with the identity matrix for the qubit  $c$ . Furthermore, the projection  $Q = \mathbb{1} - P \in M_\gamma \cap M_\gamma'$  fulfils

$$Q S^{(ab)} = Q \quad \forall a < b; \quad Q S = 0. \quad (\text{A.12})$$

Other projections commuting with  $M_\gamma$ , that is in the commutant  $M_\gamma'$  are thus all sub-projections  $q \leq Q$  for which  $qQ = Q = Qq$ , whence

$$q S^{(ab)} = q Q S^{(ab)} = q Q = q, \quad q S = q Q S = 0.$$

However, unless  $q = Q$ , these projections  $q$  cannot belong also to  $M_\gamma$ ; this is proved by writing  $q = \lambda \mathbb{1} + \sum_{a < b=1}^3 \lambda_{ab} S^{(ab)} + \mu S$  and by imposing the previous conditions. It thus follows that, for the three-qubit case discussed in this work, neither  $\mathcal{Z} = M_\gamma$  as this would imply  $M_\gamma$  commutative, or  $\mathcal{Z}' = M_\gamma$  as this would imply  $M_\gamma' \subseteq M_\gamma$ . These are the two conditions for which a conditional expectation onto  $M_\gamma$  could easily be written analytically [13?, 14].

## Appendix B

# Exact Solution of the 1D Quantum Ising Model

I summarize briefly the widely used technique to determine the energy spectrum of some simple models like the Ising and the XY and XX models. For an exhaustive discussion see e.g. Subir Sachdev's book on phase transitions [41]. As the simplest case consider the quantum Ising model on a spin chain of  $N$  lattice sites (assuming e.g. periodic boundary conditions), so let

$$H = - \sum_{i=1 \dots N} \left( \sigma_i^Z \sigma_{i+1}^Z + h \sigma_i^X \right). \quad (\text{B.1})$$

First of all, one can make some qualitative statements of the ground states as follows. Taking  $h = 0$  (zero magnetic field) the ground state is simply  $\dots|0\rangle|0\rangle\dots$  so only spins up, while sending  $h$  to infinity, the pair interaction terms could be neglected and the spins get uncoupled so the ground state is again a tensor product  $\dots \frac{|0\rangle+|1\rangle}{\sqrt{2}} \otimes \frac{|0\rangle+|1\rangle}{\sqrt{2}} \dots$ . In the latter case the average magnetization along the  $z$ -axis vanishes, while it is 1 in the first case. One thus may conclude some phase transition for some intermediate value of  $h$ . Note that further perturbative considerations can give useful qualitative pictures as well as approximate energies for the first excited states for small but non zero  $h$  or similarly for  $1 \ll h$ .

In order to determine the exact spectrum we apply the so-called Jordan-Wigner transformation. This is a mapping between spin-1/2 models and spinless fermions based on the possibility of a correspondance between a spin up/down state and an empty/occupied fermionic state. Let us introduce the fermionic annihilation and creation operators  $c_i, c_i^\dagger$  associated to the site  $i$  and relate to the spin operator as

$$\sigma_i^Z = 1 - 2c_i^\dagger c_i.$$

Also introduce the well-known spin lowering and rising operators as  $\sigma^- = (\sigma_X - i\sigma_Y)/2$  and  $\sigma^+ = (\sigma_X + i\sigma_Y)/2$  to formulate the essence of the whole transformation

$$\begin{aligned}\sigma_i^+ &= \prod_{j<i} (1 - 2c_j^\dagger c_j) c_i \\ \sigma_i^- &= \prod_{j<i} (1 - 2c_j^\dagger c_j) c_i^\dagger.\end{aligned}\tag{B.2}$$

Their inverses are

$$\begin{aligned}c_i &= \left( \prod_{j<i} \sigma_j^Z \right) \sigma_i^+ \\ c_i^\dagger &= \left( \prod_{j<i} \sigma_j^Z \right) \sigma_i^-.\end{aligned}\tag{B.3}$$

Furthermore, they fulfill the following commutation and anticommutation relations

$$\begin{aligned}\{c_i, c_j^\dagger\} &= \delta_{ij}, & \{c_i, c_j\} &= \{c_i^\dagger, c_j^\dagger\} = 0 \\ [\sigma_i^+, \sigma_j^-] &= \delta_{ij} \sigma_i^Z, & [\sigma_i^Z, \sigma_j^\pm] &= \pm 2\delta_{ij} \sigma_i^\pm.\end{aligned}$$

In case of the Ising model it is convenient to rotate spin axes by 90 degrees about the y axis, which means the replacements

$$\sigma^Z \rightarrow \sigma^X, \quad \sigma^X \rightarrow -\sigma^Z.$$

Now, we have all the tools in hand to express the final mapping between the spin and our fermionic operators as

$$\begin{aligned}\sigma_i^X &= 1 - 2c_i^\dagger c_i \\ \sigma_i^Z &= - \prod_{j<i} (1 - 2c_j^\dagger c_j) (c_i + c_i^\dagger).\end{aligned}\tag{B.4}$$

Inserting this (B.4) to the Hamiltonian (B.1) we get a quadratic form in the Fermi operators

$$H = - \sum_i \left( c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}^\dagger + c_{i+1} c_i - 2hc_i^\dagger c_i + h \right).$$

Despite being quadratic it is not diagonal and the fermion number is not conserved because of the presence of terms such as  $c^\dagger c^\dagger$ . As in usual introduce the Fourier transforms

$$c_k = \frac{1}{N} \sum_j c_j e^{-ikaj}$$

where  $N$  is the number of lattice sites,  $a$  is the lattice spacing and  $k = \pm \frac{\pi}{Na}, \pm \frac{2\pi}{Na}, \dots, \pm(\frac{\pi}{a} - \frac{\pi}{Na})$ . As a final tool use the Bogoliubov transformation to map  $c_k$  and  $c_k^\dagger$  to new ones

for which the fermion number is conserved. Define

$$\gamma_k = u_k c_k - i v_k c_{-k}^\dagger.$$

One can verify that the  $u_k$  and  $v_k$  coefficients can be always found in order to cancel the terms like  $\gamma^\dagger \gamma^\dagger$  violating the conservation of the ' $\gamma$  fermions'. The final, diagonal form of  $H$  is

$$H = \sum_k \varepsilon_k \left( \gamma_k^\dagger \gamma_k - 1/2 \right)$$

with the energies

$$\varepsilon_k = (1 + h^2 - 2h \cos(ka))^{1/2}.$$

Expressed in this form, the ground state  $|0\rangle_{GS}$  is the vacuum state of  $\gamma_k$  that is  $\gamma_k |0\rangle_{GS} = 0$ . The full ground state energy is thus

$$E_0 = \langle 0_{GS} | H | 0_{GS} \rangle = -\frac{1}{2} \sum_k \varepsilon_k.$$

It is instructive to study how the energy per one lattice site depend on the magnetic field.

$$\widehat{\varepsilon}_N(h) = \frac{E_0}{N} = \frac{1}{\pi} \sum_{j=1}^N \left( 1 + h^2 - 2h \cos(ja\Delta k) \right)^{\frac{1}{2}} \Delta k$$

where  $\Delta k = \frac{\pi}{Na}$ . Sending  $N$  to infinity in the thermodynamic limit it becomes an elliptic integral

$$\widehat{\varepsilon}(h) = \frac{1}{\pi} \int_{x=0}^{\pi} \left( 1 + h^2 - 2h \cos(x) \right)^{\frac{1}{2}} dx.$$

When evaluating this integral it turns out that it is continuous in  $h$  such as its first derivative, unlike its second derivative exhibiting discontinuity at  $h = 1$ . (For instance, the energy at the critical point can be computed explicitly:  $\widehat{\varepsilon}(1) = 4/\pi$ .) Thus, studying  $h \mapsto d^2\widehat{\varepsilon}/dh^2$  provides a very flashy evidence of a second order quantum phase transition.

This significant behavior of the Ising model can be very well captured by the MPS based simulations providing very precise results for the ground state energy.

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