

# Many-body Entanglement and Tensor Networks

course taught by Guifré Vidal (January 2017) - [PIRSA](#)

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## 1 Course Structure

These notes aim to be a complementary material for those interested in following the 2017 *Perimeter Scholars International* course on *Many-Body Entanglement and Tensor Networks*. To successfully follow the course, basic knowledge in Condensed Matter and Statistical Physics is expected. The theoretical contents of the course are complemented by computational tutorials, see Section 1.2.

### 1.1 Course Outline

#### Part 1: The Many-body Computational Challenge

- Quantum Ising model. Conformal data at criticality.
- Exact Diagonalisation and Lanczos method ( $N \sim 10, N \sim 20$ ).
- Free Fermions ( $N \sim 100$  or  $N \sim \infty$ ).
- Julia/Python Jupyter Notebooks.
- Free Majorana fermion formalism,  $SO(2N)$ .
  - \* Solving free Majorana fermion model (Julia). Conformal data. Jordan-Wigner transform.
- Free fermion formalism,  $U(N)$ .
  - \* Solving free fermion model (Julia). Conformal data. Jordan-Wigner transform.
- Ground state entanglement in the free fermion formalism (theory + Julia).
- Area law for entanglement entropy.

#### Part 2: Tensor Network (TN) States

- Basics.
- Matrix product states (MPS).
- Multi-scale entanglement renormalisation ansatz (MERA).
- Higher dimensional generalisations (PEPS, 2D MERA, branching MERA).
- Applications.

Some areas of impact of tensor networks:

- Condensed matter
- Statistical mechanics
- Quantum chemistry
- Error correction (quantum and classical)
- Image compression
- Machine learning
- Quantum gravity (AdS/CFT)

## 1.2 Python tutorials

All the Python tutorials associated with the course can be found in my personal [Github](#).

**Tutorial 1:** Python and linear algebra basics.

**Tutorial 2:** Solving the quantum Ising model ground-state energy and energy spectrum through exact diagonalisation for  $N = 3$  and  $N \leq 10$  for varying

**Tutorial 3:** Numerically obtaining universal CFT data from quantum Ising model for PBC and APBC for  $N \sim 10$ . We observe finite-size effects.

**Tutorial 4:** We implement the power and sparse multiplication method. We then use this to numerically obtain CFT data for the quantum Ising model for  $N \sim 20$ .

**Tutorial 5:** We calculate entanglement entropy and correlations for a random state and a critical ground-state  $N = 20$  and compare.

**Tutorial 6:** We work within the free Majorana fermions formalism. We compute the single particle and multi-particle energy and momenta for PBC and APBC. We then obtain conformal data to characterise this CFT. Finally, after observing the entanglement scaling we confirm that this is a  $c = 1/2$  theory and this is in the same class as the Ising model.

**Tutorial 7:** We work within the free fermion formalism. We will study the energy and ground-state entanglement for two free fermionic systems: one with two zero modes and one with more zero modes. We confirm our central charge value expectations.

## Part I

# The Many-Body Problem

## 2 Motivation

Consider a simple Hamiltonian on a  $D$ -dimensional lattice, e.g: the Transverse Field Ising Model (TFIM) for  $N$  quantum spins:

$$H_{TFIM} = - \sum_{\langle m,n \rangle} \sigma_m^x \sigma_n^x - h \sum_{m=1}^N \sigma_m^z, \quad (1)$$

where  $\sigma_i^{(x,z)}$  are the  $x, z$  Pauli matrices acting on site  $i$  defined such that:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2)$$

Following the rules of quantum mechanics, the Hilbert space  $\mathcal{H}$  for this system is defined by the tensor product of the Hilbert spaces of each individual spin:

$$\mathcal{H} = \bigotimes_{m=1}^N (\mathbb{C}_2) \quad \rightarrow \quad \dim(\mathcal{H}) = \dim(\mathbb{C}_2)^N = \exp(aN) \sim 2^N. \quad (3)$$

The dimension of  $\mathcal{H}$  is exponential in the number of spins, which quickly makes the problem intractable. Any state of our system is defined by a **wavefunction** which is written as a superposition of the  $2^N$  classical configurations defining the basis of our Hilbert space. We will be interested in understanding, in particular, the properties of the **ground-state** of the system:

$$H |\psi_0\rangle = E_0 |\psi_0\rangle, \quad (4)$$

where  $E_0$  is the lowest eigenvalue of  $H$ . In general we don't know how to solve for  $E_0$ .

Moreover,  $H$  is not really the Hamiltonian that we are after, it is an approximation in what we call **minimal model Hamiltonian**. This is a crude approximation to the degrees of freedom that we want and to the interactions of our spins, so (we hope) it captures the essence of our system. However, the interaction might be more complicated than the one given by  $H$ .

### 2.1 Approaches to finding the ground-state

1. **Exact diagonalisation**: get the matrix form of  $H$  and use matrix diagonalisation techniques to find the eigenvalues. The computational cost of this technique is exponential in  $N$ .
2. **Perturbation theory**: assumes we have an exact solution of another Hamiltonian  $H'$  nearby that differs from  $H$  by a small parameter. This technique fails for strongly interacting systems.
3. **Quantum Monte Carlo**: relies on sampling over a representative subset of spin configurations. Suffers from the sign problem (e.g: fermionic systems, frustrated antiferromagnets, ...).
4. **Variational approaches**: take the vector space  $\mathcal{H}$  where  $\dim(\mathcal{H}) \sim 2^N$  and consider a submanifold  $\mathbb{K} \subseteq \mathcal{H}$  with less-than-exponential dimension in  $N$ , e.g:  $\dim(\mathbb{K}) = \mathcal{O}(N)$  or  $\dim(\mathbb{K}) = \mathcal{O}(\text{poly}(N))$ . We therefore restrict our attention to a more tractable subset of  $\mathcal{H}$  in the hope that this is near our states of interest.

### 3 Quantum Ising Spin Chain

Consider the Hamiltonian in Equation 2. The  $h$ -term (magnetic transverse field) brings the *quantumness* since  $\sigma^x$  doesn't commute with  $\sigma^z$ . For a 1D chain at  $T = 0$  we have a **quantum critical point**<sup>1</sup> caused by quantum (not thermal) fluctuations.

We can describe the low-temperature low-distance behaviour of a quantum spin chain with a quantum field theory (QFT) which, at criticality ( $h = 1$ ), can be described by a special QFT, a conformal field theory (CFT).

#### 3.1 Some Conformal Field Theory notions

We focus on  $1 + 1$  dimensions (1 space 1 time). This is naturally parameterised using complex variables on the complex plane ( $z$ ). Consider the following transformations:

- **Scaling:**  $z \rightarrow \lambda z$ , where  $\lambda$  is the scale factor.
- **Rotation:**  $z \rightarrow e^{i\theta} z$ , where  $\theta$  is the rotation angle.

A **Scaling operators**,  $\phi_\alpha(z)$ <sup>2</sup> is one that transforms under scalings and rotations in the following manner:

$$\text{Scaling: } \phi_\alpha(0) \rightarrow \lambda^{\Delta_\alpha} \phi_\alpha(0), \quad (5)$$

$$\text{Rotation: } \phi_\alpha(0) \rightarrow e^{i\theta S_\alpha} \phi_\alpha(0), \quad (6)$$

where  $\Delta_\alpha$  is the **scaling dimension** of the field and  $S_\alpha$  is the **conformal spin** of the field. From these two parameters we could derive the **critical exponents** of the phase transition. That is,  $\phi_\alpha(0)$  is mapped to a proportional operator of themselves. We will be able to extract these two properties from our spin chain system.

##### 3.1.1 Example: Ising model CFT

Characterised by infinitely many scaling operators  $\phi_\alpha$ , but the three primary operators (also called primary fields) are:

- **Identity**,  $\mathbb{1}$ :  $\Delta_{\mathbb{1}} = 0$ ,  $S_{\mathbb{1}} = 0$ .
- **Spin**,  $\sigma$ :  $\Delta_\sigma = 1/8$ ,  $S_\sigma = 0$ .
- **Energy density**,  $\epsilon$ :  $\Delta_\epsilon = 1$ ,  $S_\epsilon = 0$ .

These primary operators can be used to define many other operators which we call descendants. See Figure 1 below for the Ising fields and descendants. It is also worth noting that in every CFT there exists a stress-energy tensor with  $\Delta_T = S_T = 2$ .

<sup>1</sup>NB: In 1D the Ising model has not classical critical point.

<sup>2</sup> $\alpha$  is the index for the different scaling operators.

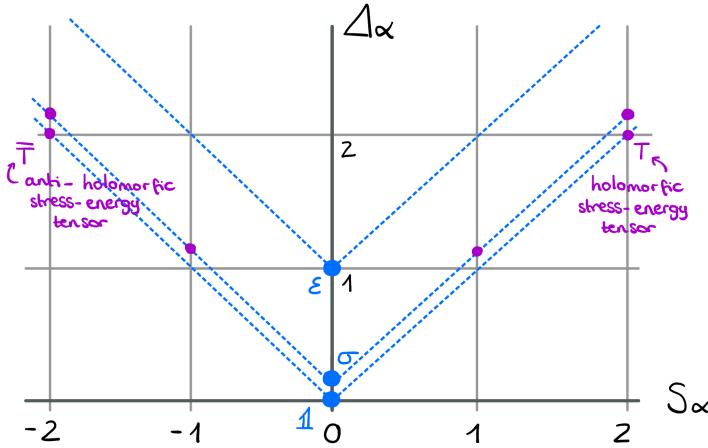


Figure 1: Ising CFT scaling operators (blue) and some descendent fields (purple).

### 3.1.2 Operator-State correspondence

For every scaling operator in a CFT we have a state in the Hilbert space:

$$\phi_\alpha \iff |\psi_\alpha\rangle. \quad (7)$$

All states in the theory can be created by operators which act locally in a small neighborhood of the origin. The entire Hilbert space of a CFT can be thought of as living at a single point.

This is related to a **universal finite size scaling**<sup>3</sup>:

Consider a finite  $N$  spin chain with periodic boundary conditions. The  $H_{TFIM}$  is invariant under translations  $T^4$  that map spin  $m \rightarrow m + 1$ . Therefore:

$$[H, T] = 0 \quad \text{and} \quad H |\psi_\alpha\rangle = E_\alpha |\psi_\alpha\rangle, \quad T |\psi_\alpha\rangle = e^{ik_\alpha} |\psi_\alpha\rangle, \quad (8)$$

and we have results that relate the energy to the scaling dimension, and the momentum to the conformal spin (which goes back to the operator-state correspondence):

$$E_\alpha = A + B \left( \Delta_\alpha + \frac{c}{12} \right) + \mathcal{O} \left( \frac{C_\alpha}{N^2} \right), \quad (9)$$

$$k_\alpha = \frac{2\pi}{N} S_\alpha. \quad (10)$$

These relations bring together a lattice calculation ( $E, k$ ) to a CFT calculation ( $\Delta, S$ ) from which you can extract **universal** information. Note, however, that we expect to observe **finite-size effects**.

<sup>3</sup>See work by John Cardy.

<sup>4</sup>We need  $T^N = \mathbb{1}$ , so  $T$  is unitary and its eigenvalues are given by phases.

## 4 Beyond Diagonalisation: Alternative Tricks

Other than the straight-forward but computationally costly Hamiltonian diagonalisation, there exist other methods for finding the energy eigenstates.

Method	Function	Based on	Time	Memory
full diagonalisation	numpy.linalg.eig()	matrix-matrix mult.	$\mathcal{O}(m^3) = (2^N)^3$	$\mathcal{O}(m^2) = (2^N)^2$
sparse diagonalisation (power method, Lanczos method)	scipy.sparse.linalg.eigs()	matrix-vector mult. sparse vector update	$\mathcal{O}(m^2) = (2^N)^2$ $\mathcal{O}(m) = N2^N$	$\mathcal{O}(m^2) = (2^N)^2$ $\mathcal{O}(m) = 2^N$

### 4.1 Power method

Given a Hamiltonian:  $H = \sum_{\alpha=0}^{m-1} E_\alpha |E_\alpha\rangle\langle E_\alpha|$  with  $|E_0| > |E_1| \geq |E_2| \dots$  (where  $E_\alpha \leq 0 \forall \alpha$ ). For an arbitrary state in the eigen-basis of the Hamiltonian:  $|\psi\rangle = \sum_\alpha c_\alpha |E_\alpha\rangle$ , consider the action applying  $H$  repeatedly:

$$\text{Once: } H|\psi\rangle = \sum_\alpha E_\alpha c_\alpha |E_\alpha\rangle \quad (11)$$

$$p \text{ times: } H^p |\psi\rangle = \sum_\alpha (E_\alpha)^p c_\alpha |E_\alpha\rangle = E_0^p \left[ c_0 |E_0\rangle + \left(\frac{E_1}{E_0}\right)^p c_1 |E_1\rangle + \dots \right] \quad (12)$$

where:

$$\left| \frac{E_1}{E_0} \right| < 1 \quad \text{and so} \quad \left( \frac{E_1}{E_0} \right)^p \ll 1 \quad (13)$$

and using this fact:

$$H^p |\psi\rangle = E_0^p [c_0 |E_0\rangle + \mathcal{O}(e^{-p})], \quad (14)$$

meaning that the second term is exponentially suppressed in  $p$ .

We can conclude that when acting with the Hamiltonian repeatedly on a state, we are converging towards the **ground-state**. This is useful since, from Appendix A, we know that matrix-vector multiplication is cheaper than matrix-matrix multiplication. Exact diagonalisation relies on the latter.

### 4.2 Sparse vector update

We have state  $|\psi\rangle$  and we want to compute  $|\psi'\rangle = H|\psi\rangle$  without building this  $2^N \times 2^N$  matrix  $H$  fully. We can exploit the **locality** of our Hamiltonian. A local Hamiltonian in one such that:  $H = \sum_l^N h_{l,l+1}$ . In the case of the Ising model this local structure is easy to see:

$$H_{TFIM} = \sum_m \left( -\sigma_m^x \sigma_{m+1}^x - h \frac{\sigma_m^z + \sigma_{m+1}^z}{2} \right) = \sum_m h_{m,m+1} \quad (15)$$

We write  $|\psi\rangle$  as an  $N$ -rank tensor:

$$|\psi\rangle = \sum_{\alpha_1, \alpha_2, \dots, \alpha_N=0}^1 \psi_{\alpha_1, \alpha_2, \dots, \alpha_N} |\alpha_1 \alpha_2 \cdots \alpha_N\rangle, \quad (16)$$

where  $|\alpha_1 \alpha_2 \cdots \alpha_N\rangle$  with  $\alpha_i = \{0, 1\}$  is a basis of the Hilbert space with  $2^N$  basis vectors.

Using the TN notation presented in Appendix B we represent the multiplication by local Hamiltonian

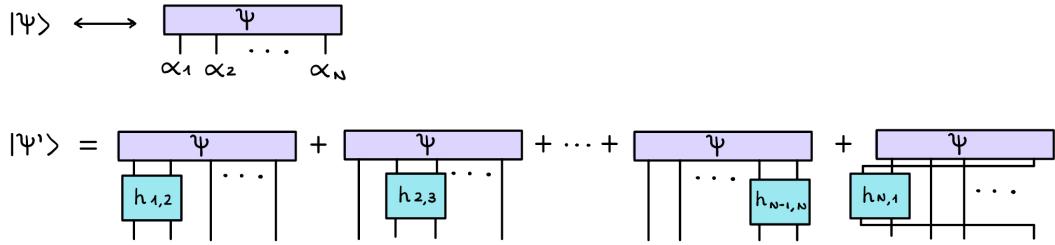


Figure 2: TN diagram representing the multiplication of  $|\psi\rangle$  by every single local Hamiltonian term.

terms graphically in Figure 1. As we can see from the diagram, at no point did we need to build a  $2^N \times 2^N$  matrix. We simply had to compute  $N$  vectors (each resulting from each  $|\psi\rangle h_{i,i+1} |\psi\rangle$  term) and then add them together. The cost of computing each of these  $N$  terms is the product of the dimensions of all the legs involved in each diagram, which is  $2^{N+2} \in \mathcal{O}(2^N)$ . This needs to be done  $\mathcal{O}(N)$  times, yielding a **total cost** of  $\mathcal{O}(N2^N)$ .

## 5 Structure of the ground-states

### 5.1 Basic Quantum Information Notions

#### 5.1.1 Composite systems

- **Single  $n$ -level quantum system:**

This is a single particle quantum system whose states  $|\psi\rangle \in \mathbb{C}$ . This space has an orthonormal basis  $\{|1\rangle, |2\rangle, \dots, |n\rangle\}$  where  $\langle \alpha | \alpha' \rangle = \delta_{\alpha\alpha'}$ . Therefore, any state can be expressed as:

$$|\psi\rangle = \sum_{\alpha=1}^N A_\alpha |\alpha\rangle. \quad (17)$$

- **Bipartite quantum system:**

States are described by  $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B = \mathcal{H}_{AB}$ . The basis of this space is  $\{|1\rangle_A, |1\rangle_A, \dots, |m\rangle_A\} \otimes \{|1\rangle_B, |1\rangle_B, \dots, |m\rangle_B\}$ . We can re-write these basis vectors using the notation  $|\alpha\beta\rangle = |\alpha\rangle_A \otimes |\beta\rangle_B$ , so that we get  $m \cdot n$  basis vectors:  $\{|11\rangle, |12\rangle, \dots, |1n\rangle, |21\rangle, \dots, |m1\rangle, \dots, |mn\rangle\}$ . A general state in  $\mathcal{H}_{AB}$  will be expressed as:

$$|\psi_{AB}\rangle = \sum_{\alpha}^m \sum_{\beta}^n M_{\alpha\beta} |\alpha\beta\rangle \quad (18)$$

- **Multipartite quantum system:**

The above logic can be generalised to an  $N$  particle composite system:

$$|\psi\rangle = \sum_{\alpha_1, \alpha_2, \dots, \alpha_N=0}^1 \psi_{\alpha_1, \alpha_2, \dots, \alpha_N} |\alpha_1 \alpha_2 \cdots \alpha_N\rangle. \quad (19)$$

More intuitively, the **wavefunction** is an assignment of an amplitude  $\psi_{\{\sigma_i\}} \in \mathbb{C}$  to every classical state that the particles in a many-body system can be in. The size of the wavefunction grows as  $p^N$  where  $p$  is the number of states one particle can be in (e.g spin systems:  $\{\uparrow, \downarrow\}$  means  $p = 2$ ) and  $N$  is the number of particles.

Mathematically the wavefunction is therefore a  $p^N$  dimensional vector.

#### 5.1.2 Pure and mixed states

We introduce the **density matrix** formalism to be able to deal with mixed states. We use it to express the statistical ensemble of pure quantum states that the system is in <sup>5</sup>. The density matrix is a positive semi-definite, Hermitian and trace-1 operator defined as:

$$\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i| \quad (20)$$

- **Pure states:** pure states are well defined and are not in a probabilistic mixture. Therefore:  $\rho = |\psi\rangle \langle \psi|$  and  $Tr(\rho^2) = 1$ .
- **Mixed states:** probabilistic mixture of pure states. Mixed states cannot be written with a ket state  $|\psi\rangle$ . For mixed states  $Tr(\rho^2) < 1$  and they are are vector with length  $0 \leq l < 1$  in the Bloch sphere.

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<sup>5</sup>Note that this *statistical* nature is purely classical.

### 5.1.3 Von Neumann Entropy

The von Neumann entropy<sup>6</sup> of a density matrix,  $S(\rho)$  provides a measure of **mixedness**. For pure states  $S(\rho) = 0$  while for mixed states  $0 < S(\rho) < \log(\dim(\mathcal{H}))$ , with maximum entropy is  $\rho = \mathbb{1}/\dim(\mathcal{H})$ . It's defined as:

$$S(\rho) = -Tr(\rho \log[\rho]) = -\sum_i p_i \log p_i \quad \text{where } p_i \text{ are the eigenvalues of } \rho \quad (21)$$

### 5.1.4 Reduced density matrix

Given a composite quantum state  $|\psi\rangle$  its **reduced density matrix** of one of the subsystems, say  $A$ , is obtain by tracing out over all the subsystems except for  $A$ :  $\rho_A = tr_{\text{All}-A}(\rho)$ . This is called **partial trace**. The order of performing partial traces does not matter. For example, for a bipartite system  $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ , with  $\dim(\mathcal{H}_A) = m$  and  $\dim(\mathcal{H}_B) = n$ , as defined in Equation 18, the reduced density matrix of system  $A$ :

$$\begin{aligned} \rho^A &= tr_B |\psi_{AB}\rangle \langle \psi_{AB}| = \sum_{\beta=1}^n \langle \beta|_B |\psi\rangle_{AB} \langle \psi|_{AB} |\beta\rangle_B \stackrel{*}{=} \sum_{\alpha\alpha'} \left( \sum_{\beta} M_{\alpha\beta} M_{\alpha'\beta}^* \right) |\alpha\rangle \langle \alpha'| \\ &= \sum_{\alpha\alpha'} \rho_{\alpha\alpha'}^A |\alpha\rangle \langle \alpha'| \quad \text{where} \quad \rho_{\alpha\alpha'}^A = (M \cdot M^\dagger)_{\alpha\alpha'}, \end{aligned} \quad (22)$$

where in (\*) we used, by definition:  $\langle \beta'|\alpha\beta\rangle = |\alpha\rangle \langle \beta'|\beta\rangle = \langle \alpha|\delta_{\beta\beta'}$ .

## 5.2 Entanglement

### 5.2.1 Definition

A composite quantum state which is not the tensor product of quantum states of individual Hilbert spaces is entangled. Otherwise, we say it is **separable** (or a product state). For an **entangled** bipartite state:

$$|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \neq |\phi_1\rangle \otimes |\phi_2\rangle \quad \text{with} \quad |\phi_1\rangle \in \mathcal{H}_1 \text{ and } |\phi_2\rangle \in \mathcal{H}_2 \quad (23)$$

*Examples:*

- \*  $|11\rangle + |12\rangle = |1\rangle \otimes (|1\rangle + |2\rangle)$  (not entangled)
- \*  $|11\rangle + |12\rangle + |21\rangle + |22\rangle = (|1\rangle + |2\rangle) \otimes (|1\rangle + |2\rangle)$  (not entangled)
- \*  $|11\rangle + |12\rangle + |21\rangle - |22\rangle$  (entangled)
- \*  $|11\rangle + |22\rangle$  (entangled)

However, we know the following consequences between reduced density matrices and the entanglement of our state  $\rho$ :

1. If  $\rho$  is not entangled partial traces of it ( $\rho^A$  or  $\rho^B$ ) lead to pure states in the reduced Hilbert space.
2. If  $\rho$  represents an entangled state, taking the partial trace ( $\rho^A$  or  $\rho^B$ ) will lead to a mixed state.

However, we also want to see the Point 1: if the reduced density matrix of a state is pure, the original state was necessarily entangled. For this we will introduced the **Schmidt decomposition**.

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<sup>6</sup>Equivalent form to classical Shannon entropy.

### 5.2.2 Schmidt decomposition

It is always possible to express a bipartite quantum system  $|\psi_{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  as:

$$|\psi_{AB}\rangle = \sum_{i=1}^{\chi} \sigma_i |a_i\rangle |b_i\rangle, \quad (24)$$

where  $\{|a_i\rangle\}$  and  $\{|b_i\rangle\}$  form an orthonormal basis for Hilbert spaces  $\mathcal{H}_A$  and  $\mathcal{H}_B$  respectively and are denoted **Schmidt vectors**;  $\sigma_i > 0$  are the **Schmidt coefficients**; and  $\chi \leq \min(d_A, d_B)$  is the **Schmidt rank**. This way of expressing the state of a bipartite system is in contrast to Equation 18, where the sum runs for  $m \cdot n$  terms.

The Schmidt coefficients are the eigenvalues of  $\rho_A$  and  $\rho_B$  so:  $\{p_i\} = \{\sigma_i^2\}$ . More explicitly:

$$\rho^A = \sum_{i=1}^{\chi} \sigma_i^2 |a_i\rangle \langle a_i| \quad \text{and} \quad \rho^B = \sum_{i=1}^{\chi} \sigma_i^2 |b_i\rangle \langle b_i| \quad (25)$$

The Schmidt decomposition is a direct consequence of the singular value decomposition used in standard linear algebra, see Appendix C.

→ **Theorem:**

Consider a bipartite system  $|\psi_{AB}\rangle = \sum_{\alpha\beta} M_{\alpha\beta} |\alpha\beta\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  with  $p_i = (p_1, p_2, \dots, p_\chi) = (\sigma_1^2, \sigma_2^2, \dots, \sigma_\chi^2)$  the eigenvalues of the reduced density matrices. If  $p_i = (1, 0, 0, \dots)$ , meaning  $\chi = 1$  then the state  $|\psi_{AB}\rangle$  is a product state. If  $\chi > 1$  then  $|\psi_{AB}\rangle$  is entangled.

In other words if  $\chi = 1$  the state corresponding to the reduced density matrix is pure, and so the original state must have been non-entangled.

### 5.2.3 Characterising entanglement

We can define many different measures of entanglement. They provide us with an idea of how mixed a state is after taking a partial trace of a subsystem.

- A complete characterisation of entanglement is using the **Schmidt coefficients**  $\sigma_i$  (or, equivalently, their square,  $p_i$ ). We consider all the coefficients:  $p_i = (p_1, p_2, \dots, p_\chi)$ . These coefficients  $p_i$  are invariant under local unitary transformations  $|\psi'^{AB}\rangle = U^A \otimes V^B |\psi^{AB}\rangle$ . For example, the state  $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$  is unitarily equivalent to  $|\psi\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$  and both have Schmidt coefficients  $p_i = (\frac{1}{2}, \frac{1}{2})$ .

We may also define the **entanglement spectrum**:

$$e_i = \log(p_i) \quad (26)$$

- The **entanglement entropy** is the von Neumann entropy of subsystem  $\rho_A$  or  $\rho_B$ . It is one of the most common entanglement measures. Given a bipartite (pure) system  $|\psi^{AB}\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$  with reduced density matrices  $\rho_A$  and  $\rho_B$ , the entanglement entropy between  $A$  and  $B$  is:

$$S(\rho_A) = S(\rho_B) = -\text{tr}(\rho_A \log \rho_A) = -\sum_{i=1}^{\chi} p_i \log p_i,$$

where  $\sigma_i^2$  are the eigenvalues of  $\rho_A$  or  $\rho_B$ . It is bounded such that:  $0 \leq S \leq \log \chi$ .

*Examples:*

\* Entanglement entropy of  $|\psi\rangle = |00\rangle$ :  $p_i = p_1 = 1$  and so  $S = -1 \log 1 = 0$ .

\* Entanglement entropy of  $|\psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ :

$$\rho = \frac{1}{2}(|00\rangle + |11\rangle)(\langle 00| + \langle 11|) \xrightarrow{\text{Tr}_B} \rho_A = \frac{1}{2}(|0\rangle \langle 0| + |1\rangle \langle 1|),$$

plugging in the entropy equation:  $S_A = -\text{tr}(\rho_A \log \rho_A) = -\text{tr}(\frac{1}{2} \log(1/2)\mathbb{1}) = \log 2$ .

\* Entanglement entropy of  $|\psi\rangle = \frac{3}{5}|0+\rangle + \frac{4}{5}|1-\rangle$ . This state is already in Schmidt form so:  $S_A = -(\frac{3}{5})^2 \log(\frac{3}{5})^2 - (\frac{4}{5})^2 \log(\frac{4}{5})^2 = 0.942$ .

#### 5.2.4 (Bipartite) entanglement in many-body states

Entanglement in many-body system is often analysed by consider two subsystems and studying bipartite entanglement as we have so far. Recall Equation 19 for a many-body wavefunction. Consider  $N = 5$  and divide the system into two subsystems with  $N_A = 2$  and  $N_B = 3$ . We can define two new indeces:  $\mu = (\alpha_1, \alpha_2)$  with dimension 4, and  $\nu = (\alpha_3, \alpha_4, \alpha_5)$  with dimension 8. The wavefunction reads:

$$|\psi\rangle = \sum_{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5=0}^1 \psi_{\alpha_1, \alpha_2, \alpha_3, \alpha_4, \alpha_5} \underbrace{|\alpha_1, \alpha_2\rangle}_{\text{A}}, \underbrace{|\alpha_3, \alpha_4, \alpha_5\rangle}_{\text{B}} = \sum_{\mu\nu} M_{\mu\nu} |\mu_A \nu_B\rangle, \quad (27)$$

so now we have a bipartite system and we can employ the techniques described above. The bi-partition of the system is not unique, and with different bi-partitions we may get different entanglement entropies between the resulting subsystems. The entanglement entropy as a function of bi-partition spin  $S(L)$  with  $1 \geq L \geq N - 1$  provides information about the entanglement structure of this wavefunction. Conformal field theory calculations predict the function of this entanglement entropy in the ground-state to be:

$$S(L) = \frac{c}{3} \log \left( \frac{N}{\pi} \sin \left( \frac{L\pi}{N} \right) \right) + c_1 \quad (28)$$

where  $c$  is a universal quantity called **central charge** and is also a properfy of the CFT.

### 5.3 Correlations

The **two-point correlator** of an operator  $\hat{Q}$  is defined to be:

$$\mathcal{C}(l, m) = \langle \psi | \hat{Q}_l \hat{Q}_m | \psi \rangle - \langle \psi | \hat{Q}_l | \psi \rangle \langle \psi | \hat{Q}_m | \psi \rangle. \quad (29)$$

The two-point correlatior decays as:  $\frac{1}{x^{2\Delta}}$ , recall that for Ising  $\Delta_\sigma = \frac{1}{8}$ .

## 6 Free Majorana Systems

So far we have employed the Hamiltonian formalism which involved dealing with a  $2^N \times 2^N$  sized matrix and a ground-state described by a vector that was also exponential in size ( $2^N$ ). We have been able to compute smaller quantities such as the reduced density matrix  $\rho^A$  of size  $2^L \times 2^L$  with  $L < N$  and the entanglement spectrum  $\{p_i\}$  of size  $2^L$ .

In this section we will introduce a new formalism, the **free particle formalism**. This will allow us to reduce the size of our problem from exponential to polynomial. This will be done by working with a  $2N \times 2N$  matrix  $C$  instead of our original Hamiltonian  $H$ , and a correlation matrix  $\Gamma$  also of size  $2N \times 2N$  that will contain all the information about the ground-state of our system. The Hilbert space remains exponentially large but, for this particular systems, we can generate this reduced complete description.

### 6.1 Simple case: $N = 1$ qubit system

We start simple and consider a  $N = 1$  two-level (qubit) system. We will present three equivalent ways of describing operators on this one qubit: Pauli matrices, fermionic creation/annihilation operators and a pair of Majorana operators. As a summary, the relation between the generators of their algebras is the following:

$$\begin{aligned} a &= \frac{1}{2}(\sigma^x + \sigma^y) = \frac{1}{\sqrt{2}}(\psi_1 + i\psi_2) \\ \psi_1 &= \frac{1}{\sqrt{2}}\sigma^x, \quad \psi_2 = \frac{1}{\sqrt{2}}\sigma^y \\ \psi_1 &= \frac{1}{\sqrt{2}}(a + a^\dagger), \quad \psi_2 = \frac{1}{i\sqrt{2}}(a + a^\dagger) \end{aligned} \tag{30}$$

#### 6.1.1 Pauli matrices: $\sigma^x, \sigma^y, \sigma^z$

The Pauli matrices  $\sigma^{(x,y,z)}$  obey the following commutation relations<sup>7</sup>:

$$[\sigma^i, \sigma^j] = 2i\varepsilon^{ijk}\sigma^k. \tag{31}$$

The Pauli matrices may take the following representation:

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{32}$$

We can construct a Hamiltonian to be:

$$H = -\frac{\epsilon}{2}\sigma^z = \begin{pmatrix} -\epsilon/2 & 0 \\ 0 & \epsilon/2 \end{pmatrix}, \tag{33}$$

---

<sup>7</sup>If we define  $X^i = -\frac{1}{2}\sigma^i$  the commutation relations in Equation 31 become the commutators of the infinitesimal generators of  $SO(3)$  and  $SU(2)$ . Therefore, the Pauli matrices are the infinitesimal generators of  $SO(3)$  and  $SU(2)$  and form a representation of its Lie algebra.

which therefore defines a ground-state  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  with energy  $E_0 = -\epsilon/2$ , and an excited state  $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$  with energy  $E_1 = \epsilon/2$ .

If we consider the following mixed state:

$$\rho = p|0\rangle\langle 0| + (1-p)|1\rangle\langle 1| \quad (34)$$

$$\text{with eigenvalues: } p, 1-p \longrightarrow S[\rho] = -p \log_2 p - (1-p) \log_2(1-p) \quad (35)$$

then the expectation values  $\langle \sigma^x \rangle = \text{tr}(\rho \sigma^x) = \langle \sigma^y \rangle = 0$ , and  $\langle \sigma^z \rangle = 2p - 1$ .

### 6.1.2 Fermionic annihilation and creation operators: $a, a^\dagger$

We present an equivalent picture by introducing the anhiliation,  $a$ , and creation,  $a^\dagger$  operators. These have anticommutation relations given by:

$$\{a, a^\dagger\} = \mathbb{1}, \quad \{a, a\} = \{a^\dagger, a^\dagger\} = 0. \quad (36)$$

We can represent these operators as matrices:

$$a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad a^\dagger = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad a^\dagger a = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad aa^\dagger = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}. \quad (37)$$

We can write the Hamiltonian as in Equation 33 now with these new operators:

$$H = \epsilon \left( a^\dagger a - \frac{1}{2} \right). \quad (38)$$

For the same state presented in Equation 34, the expectation values of these operators become  $\langle a \rangle = \langle a^\dagger \rangle = 0$ ,  $\langle a^\dagger a \rangle = 1 - p$  and  $\langle aa^\dagger \rangle = p$ .

### 6.1.3 Pair of Majorana operators: $\psi_1, \psi_2$

These two operators are hermitian and anticommute such that:

$$\psi_i = \psi_i^\dagger \quad \text{and} \quad \{\psi_i, \psi_j\} = \delta_{ij}. \quad (39)$$

A possible matrix representation is:

$$\psi_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \psi_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad -i(\psi_1\psi_2 - \psi_2\psi_1) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (40)$$

Once again, we can rewrite the same Hamiltonian:

$$H = \frac{i}{2}\epsilon(\psi_1\psi_2 - \psi_2\psi_1) \quad (41)$$

Similarly, using the state in Equation 34 we get that  $\langle \psi_1 \rangle = \langle \psi_2 \rangle = 0$  and  $-i\langle [\psi_1, \psi_2] \rangle = 2p - 1 \equiv \nu$ . We can also introduce the **correlation matrix**:

$$\Gamma = -i\langle [\psi_m, \psi_n] \rangle = \begin{pmatrix} 0 & \nu \\ -\nu & 0 \end{pmatrix}. \quad (42)$$

We can write our expression for the entropy as:

$$S[\rho] = - \left( \frac{1+\nu}{2} \right) \log_2 \left( \frac{1+\nu}{2} \right) - \left( \frac{1-\nu}{2} \right) \log_2 \left( \frac{1-\nu}{2} \right) \quad (43)$$

## 6.2 $N$ pairs of Majorana modes

This is a system of  $2N$  Majorana modes. The algebra is:

$$\psi_I, I \equiv (n, \alpha) \quad \text{with } n = 1, 2, \dots, N \text{ and } \alpha = 1, 2, \quad (44)$$

where  $n$  is used to denote the pair and  $\alpha$  to refer to the mode within each pair.

As for  $N = 1$ , these generic case operators also obey hermitianity and anticommutativity:

$$\psi_I^\dagger = \psi_I, \{ \psi_I, \psi_J \} = \delta_{IJ}. \quad (45)$$

A representation of these operators could be of the form of  $2^N \times 2^N$  matrices. However, we will be able to leverage their anticommutation relations and perform less costly calculations. The summary of the steps is:

1. Obtain  $2N \times 2N$  matrix  $C$  representing our Hamiltonian and diagonalise it such that  $C = O\tilde{C}O^T$ .
2. From this diagonalisation we obtain the ground state as a diagonal correlation matrix  $\tilde{\Gamma}$ , also of size  $2N \times 2N$ .
3. Go back to the original variables of the Majorana modes to obtain the ground state correlation matrix  $\tilde{\Gamma}$  (which will no longer be diagonal).

### 6.2.1 Quadratic Hamiltonian: matrix $C$

Consider a Hamiltonian which is quadratic in the Majorana operators. The sizes of each element are specified in the equation:

$$\underbrace{H}_{2^N \times 2^N} = \frac{i}{2} \sum_{I,J} \underbrace{\psi_I}_{2^N} \underbrace{C_{I,J}}_{2N \times 2N} \underbrace{\psi_J}_{2^N} = \frac{i}{2} \vec{\psi}^T C \vec{\psi}. \quad (46)$$

Since  $H^\dagger = H$  then we know  $C_{IJ}^* = C_{IJ}$  and  $C_{IJ} = -C_{JI}$ . This means that the matrix  $C$  is real and skew-symmetric. Recall that for  $N = 1 \rightarrow C = \begin{pmatrix} 0 & \epsilon \\ -\epsilon & 0 \end{pmatrix}$ .

→ Theorem [ref]:

Given a  $2N \times 2N$  real and skew-symmetric matrix  $C$ , then  $\exists O \in O(2N)$ <sup>8</sup> such that  $C$  can be written in terms of a block diagonal matrix  $\tilde{C}$  in the following way:

$$C = O\tilde{C}O^T \quad \text{with} \quad \tilde{C} = \begin{pmatrix} \begin{pmatrix} 0 & \epsilon_1 \\ -\epsilon_1 & 0 \end{pmatrix} & 0 & \cdots & 0 \\ 0 & \begin{pmatrix} 0 & \epsilon_2 \\ -\epsilon_2 & 0 \end{pmatrix} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \begin{pmatrix} 0 & \epsilon_N \\ -\epsilon_N & 0 \end{pmatrix} \end{pmatrix} = \bigoplus_{k=1}^N \begin{pmatrix} 0 & \epsilon_k \\ -\epsilon_k & 0 \end{pmatrix}, \quad (47)$$

where the entries can be chosen such that  $0 \leq \epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_N$ .

<sup>8</sup> $O(N)$  is the orthogonal group ( $OO^T = O^TO = \mathbb{1}$ ) of  $N \times N$  matrices.

We can use this theorem to bring  $H$  in Equation 46 into diagonal form:

$$H = \frac{i}{2} \vec{\psi}^T C \vec{\psi} = \frac{i}{2} \underbrace{\vec{\psi}^T O}_{\vec{\phi}^T} \tilde{C} \underbrace{O^T \vec{\psi}}_{\vec{\phi}} = \frac{i}{2} \vec{\phi}^T \tilde{C} \vec{\phi}. \quad (48)$$

These new vector  $\vec{\phi}$  introduces a new set of Majorana modes  $\vec{\phi} = (\phi_{1,1}, \phi_{1,2}, \phi_{2,1}, \dots, \phi_{N,2})$ . This is simply a change of basis to one such that the new modes are linear combinations of the original ones. Just as the original set, they are Majorana mode since they anticommute and are hermitian:

$$\{\phi_I, \phi_J\} = \delta_{IJ} \quad \text{and} \quad \phi_I^\dagger = \phi_I. \quad (49)$$

We can rewrite the Hamiltonian in Equation 48 as:

$$H = \frac{i}{2} \sum_{k=1}^N \epsilon_k (\phi_{k,1}\phi_{k,2} - \phi_{k,2}\phi_{k,1}) = \sum_{k=1}^N \epsilon_k (a_k^\dagger a_k - \frac{1}{2}) = - \sum_{k=1}^N \frac{\epsilon_k}{2} \sigma_k^z, \quad (50)$$

where, using Equation 30, we have defined  $a_k = \frac{1}{\sqrt{2}} (\phi_{k,1} + i\phi_{k,2})$  and  $\sigma_k^z = -i(\phi_{k,1}\phi_{k,2} - \phi_{k,2}\phi_{k,1})$ . This Hamiltonian now defines an  $N$  independent (decoupled) spins system.

### 6.2.2 Ground-state: correlation matrix $\Gamma$

The ground-state of this system is some state  $|\psi\rangle$  that satisfies:

$$\sigma_k^z |\psi\rangle = |\psi\rangle \quad \text{where } \sigma_k^z \text{ satisfies } \sigma_k^z |0\rangle_k = |0\rangle_k \quad \text{such that} \quad |\psi\rangle = |0\rangle |0\rangle \cdots |0\rangle, \quad (51)$$

while  $\langle \sigma_k^x \rangle = \langle \sigma_k^z \rangle = 0$ .

We now introduce a correlation matrix  $\tilde{\Gamma} = O^T \Gamma O = -i\langle \psi | [\phi_I, \phi_J] | \psi \rangle$ , which more explicitly takes the form:

$$\tilde{\Gamma} = \begin{pmatrix} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & 0 & \cdots & 0 \\ 0 & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \end{pmatrix} = \bigoplus_{k=1}^N \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (52)$$

It does not come as a surprise that this correlation matrix has no off-diagonal terms, meaning there are no correlations between pairs of Majorana modes, as expected from the Hamiltonian in Equation 50. Consider one of these  $2 \times 2$  blocks in Equation 52:

$$\begin{pmatrix} -i\langle \psi | [\phi_1, \phi_1] | \psi \rangle = 0 & -i\langle \psi | [\phi_1, \phi_2] | \psi \rangle = \langle \psi | \sigma^z | \psi \rangle = 1 \\ \langle \psi | [\phi_2, \phi_1] | \psi \rangle = -\langle \psi | \sigma^z | \psi \rangle = -1 & -i\langle \psi | [\phi_2, \phi_2] | \psi \rangle = 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (53)$$

We now want to revert back to our original Majorana operators  $\psi_I$ , whose original form for the correlation matrix  $\Gamma$  of the ground-state is:

$$\Gamma_{IJ} = -i\langle [\Psi_I, \Psi_J] \rangle, \quad (54)$$

which forms a complete characterisation of the ground-state. This means that any expectation value  $\langle \psi | O | \psi \rangle$  can be calculated from the correlation function<sup>9</sup>  $\Gamma$ . For example, for four Majorana operators  $\langle \psi_I \psi_J \psi_K \psi_L \rangle = \langle \psi_I \psi_J \rangle \langle \psi_K \psi_L \rangle + \dots$ .

### 6.2.3 Reduced density matrix

We consider the correlation matrix for a subsection  $L$  of all the Majorana pairs in our system, we denote the reduced correlation matrix corresponding of this subsystem as  $\Gamma^A$ . This is a  $2L \times 2L$  matrix which is also real and skew-symmetric.

We can therefore diagonalise this matrix  $\Gamma^A = R \tilde{\Gamma}^A R^T$  with  $R \in O(2L)$ . More explicitly:

$$\tilde{\Gamma}^A = \begin{pmatrix} \begin{pmatrix} 0 & \nu_1 \\ -\nu_1 & 0 \end{pmatrix} & 0 & \cdots & 0 \\ 0 & \begin{pmatrix} 0 & \nu_2 \\ -\nu_2 & 0 \end{pmatrix} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \begin{pmatrix} 0 & \nu_N \\ -\nu_N & 0 \end{pmatrix} \end{pmatrix} = \bigoplus_{k=1}^L \begin{pmatrix} 0 & \nu_k \\ -\nu_k & 0 \end{pmatrix}. \quad (55)$$

Where, once again  $\tilde{\Gamma}^A$  is block diagonal meaning there are no correlations between different pairs. We now have a new set of Majorana modes associated with part  $A$ :  $\tilde{\eta} = R^T(\vec{\psi}|_A) = (\eta_{1,1} \eta_{1,2}, \eta_{2,1} \dots, \eta_{L,2})$ . These are also Majorana operators since they anticommute and are hermitian:

$$\{\nu_I, \nu_J\} = \delta_{IJ} \quad \text{and} \quad \nu_I^\dagger = \nu_I. \quad (56)$$

There also exists a unitary transformation  $U \in U(2^L)$  such that:

$$U \rho^A U^\dagger = \rho_1 \otimes \rho_2 \otimes \cdots \otimes \rho_L = \bigotimes_{k=1}^L \rho_k, \quad (57)$$

where each  $\rho_k$  is a one-qubit density matrix:

$$\rho_k = \begin{pmatrix} \frac{1+\nu_k}{2} & 0 \\ 0 & \frac{1-\nu_k}{2} \end{pmatrix} \quad (58)$$

### 6.2.4 Entanglement spectrum

The  $2^L$  eigenvalues  $(p_1, p_2, \dots, p_{2^L})$  of the reduced density matrix are given by the product of each eigenvalue of  $\rho_k$ :

$$p_\alpha = \left( \frac{1+\nu_1}{2} \right) \times \left( \frac{1+\nu_2}{2} \right) \times \cdots \times \left( \frac{1+\nu_L}{2} \right). \quad (59)$$

This therefore makes a total of  $2^L$  combinations. More formally:

$$\rho^A \xrightarrow{\text{eigenvals.}} p_\alpha = p_{s_1 s_2, \dots, s_L} = \prod_{k=1}^L \frac{1 + (-1)^{s_k} \nu_k}{2}. \quad (60)$$

---

<sup>9</sup>This procedure is essentially Wick's theorem: when working with a free theory it is enough to have knowledge of just the two-point correlators.

We then exploit the fact that the entanglement entropy is additive:

$$S[\rho^A] = S \left[ \bigotimes_{k=1}^L \rho_k^A \right] = \sum_{k=1}^L S[\rho_k^A], \quad (61)$$

and we get an expression for the entanglement entropy:

$$S[\rho^A] = \sum_{k=1}^L S[\rho_k] = - \sum_{k=1}^L \left[ \left( \frac{1 + \nu_k}{2} \right) \log_2 \left( \frac{1 + \nu_k}{2} \right) + \left( \frac{1 - \nu_k}{2} \right) \log_2 \left( \frac{1 - \nu_k}{2} \right) \right], \quad (62)$$

which we were able to write as a sum since the reduced density matrix originated from the tensor product of one-qubit density matrices and is therefore additive.

## 7 Free Fermionic System

### 7.1 Operator algebra

We have  $N$  fermionic annihilation operators  $a_i$  with  $i = 1, 2, 3, \dots, N$  that obey the anticommutation relations:

$$\{a_i, a_j^\dagger\} = \delta_{ij}, \quad \{a_i, a_j\} = 0. \quad (63)$$

The smallest non-trivial matrices that would fulfill these relations are of size  $2^N \times 2^N$ .

We consider canonical transformations into a new set of modes  $\vec{b}$  that would still fulfill these relations:

$$\vec{a} = (a_1, a_2, \dots, a_N) \rightarrow \vec{b} = U\vec{a} = (b_1, b_2, \dots, b_N) \quad \text{such that} \quad \{b_i, b_j^\dagger\} = \delta_{ij}, \quad \{b_i, b_j\} = 0 \quad (64)$$

with  $U \in U(N)$ ,  $UU^\dagger = \mathbb{1}$ .

### 7.2 $N$ independent fermionic modes

#### 7.2.1 Hamiltonian: decoupled modes

For  $N$  independent fermionic modes we start with a Hamiltonian that is a sum over  $N$  single decoupled modes:

$$H = \sum_{k=1}^N \epsilon_k b_k^\dagger b_k = -\frac{1}{2} \sum_{k=1}^N \epsilon_k \sigma_k^z + \frac{1}{2} \sum_{k=1}^N \epsilon_k \quad (65)$$

where in the second equality we have brought it into spin operators by using  $b_k^\dagger b_k = \frac{1}{2}(1 - \sigma_k^z)$ . Using this last expression we can see that our system consists of  $N$  spin degrees of freedom each associated with some energy  $\epsilon_k$ .

#### 7.2.2 Ground-state: correlation matrix $\tilde{M}$

The form of the ground-state will be:

$$|\psi_0\rangle = |s_1, s_2, \dots, s_N\rangle \quad \text{where} \quad s_k = \begin{cases} 0 & \text{if } \epsilon_k > 0 \\ 1 & \text{if } \epsilon_k < 0 \end{cases} = \frac{1}{2}(1 - \text{sign}(\epsilon_k)). \quad (66)$$

The correlation matrix for the ground-state will take the form:

$$\tilde{M}_{kk'} = \langle \psi_0 | b_k^\dagger b_k | \psi_0 \rangle = \delta_{kk'} - 2\langle b_{kk'} \rangle = \delta_{kk'} \text{sign}(\epsilon_k) \quad (67)$$

### 7.3 $N$ correlated fermionic modes

#### 7.3.1 Quadratic Hamiltonian: matrix $A$

For an correlated system, the Hamiltonian will not be diagonal in the modes. We consider a general quadratic Hamiltonian:

$$H = \sum_{i,j=1}^N A_{ij} a_i^\dagger a_j \quad \text{where} \quad \underbrace{A_{ij}}_{N \times N} \in \mathbb{C} \text{ and } A^\dagger = A. \quad (68)$$

By considering the particle number operator:

$$\hat{N} = \sum_i a_i^\dagger a_i \quad \text{such that} \quad [\hat{N}, H] = 0 \quad \text{and} \quad [\hat{N}, a_j] = -a_j, \quad (69)$$

we can show that the Hamiltonian has a  $U(1)$  symmetry:

$$a'_i = e^{i\phi} a_i, \quad a'_i{}^\dagger = e^{-i\phi} a_i{}^\dagger \quad \rightarrow_i^\dagger a_j = a'_i{}^\dagger a'_j. \quad (70)$$

This is a special case of what we saw in the Majorana formalism. It is the fact that there is particle number conservation that our matrices will now be  $N \times N$  instead of  $2N \times 2N$ .

### 7.3.2 Ground-state: correlation matrix $M$

We may express the ground-state of our system as a correlation matrix  $M$  that we can obtain from diagonalising the matrix of coefficients  $A$  from our Hamiltonian.

→ **Theorem:**

Given a  $N$  hermitian matrix  $A$  such that  $A^\dagger = A$ , then  $\exists U \in U(N)^{10}$  such that  $A$  can be written as

$$A = UDU^\dagger \quad \text{where} \quad D = \text{diag}(e_1, e_2, \dots, e_m) \quad (71)$$

We can leverage the above theory and apply a canonical transformation to define new modes  $\vec{b} = U^\dagger \vec{a}$  such that the Hamiltonian is now  $H = \sum_k e_k b_k^\dagger b_k$ .

Recall that in Equation 67 we defined the correlation matrix for the  $b$ -modes. We may rewrite this as  $\tilde{M}_{kk'} = \delta_{kk'} \text{sign}(\epsilon_k) = \text{sign}(D)$ . Then use  $M_{mn} = (U\tilde{M}U^\dagger)_{mn}$  to get an expression for the correlation matrix of the  $a$  modes:

$$M = U \text{sign}(D) U^\dagger \quad \text{where} \quad D = U^\dagger A U. \quad (72)$$

### 7.3.3 Reduced density matrix

We have our ground-state expressed by an  $N \times N$  matrix  $M$ . We are interested in a sub-region containing  $L$  modes. We use  $M^A$  to denote the  $L \times L$  correlation matrix for this sub-system. By construction this matrix is hermitian<sup>11</sup>. We can therefore diagonalise  $M^A$  such that:

$$M^A = V \begin{pmatrix} \mu_1 & & & \\ & \mu_2 & & \\ & & \ddots & \\ & & & \mu_N \end{pmatrix} V^\dagger = V \tilde{M}^A V^\dagger. \quad (73)$$

There also exist a set of  $L$  modes  $\vec{c} = V^\dagger \vec{a}^A$  (where  $\vec{a}^A$  denotes the modes corresponding to the  $L$  sub-region modes) such that:

$$\langle c_m^\dagger c_n \rangle = \delta_{mn} \langle c_m^\dagger c_m \rangle = \frac{1 - \mu_m}{2} \delta_{mn}. \quad (74)$$

<sup>10</sup> $U(N)$  is the unitary group ( $U^\dagger U = UU^\dagger = \mathbb{1}$ ) of  $N \times N$  matrices.

<sup>11</sup>This is due to the fact that it is a sub-matrix of a hermitian matrix,  $M$ .

We see that when we work in the modes that diagonalise the correlation matrix  $M^A$  there are no correlations between said modes.

We now consider the reduced density matrix of those  $L$  uncorrelated spins:

$$\tilde{\rho}^A = \bigotimes_{k=1}^L \begin{pmatrix} \frac{1+\mu_k}{2} & 0 \\ 0 & \frac{1-\mu_k}{2} \end{pmatrix}. \quad (75)$$

The  $2^L$  eigenvalues of this density matrix, as in Equation 59, are given by:

$$p_\alpha = p_{s_1 s_2, \dots s_L} = \prod_{k=1}^L \frac{1 + (-1)^{s_k} \mu_k}{2}. \quad (76)$$

We then again exploit the fact that the entanglement entropy is additive in order to get:

$$S[\rho^A] = \sum_{k=1}^L S[\tilde{\rho}_k^A] = - \sum_{k=1}^L \left[ \left( \frac{1 + \mu_k}{2} \right) \log_2 \left( \frac{1 + \mu_k}{2} \right) + \left( \frac{1 - \mu_k}{2} \right) \log_2 \left( \frac{1 - \mu_k}{2} \right) \right], \quad (77)$$

where we have avoided building exponentially many eigenvalues of  $\tilde{\rho}^A$ .

## 8 Scaling of Entanglement in Ground-States

In this section we will study the entanglement in ground-states of local Hamiltonians (generally of free fermions), which we have learnt how to compute in the preceding sections.

We will consider systems of size  $N$  with  $N \rightarrow \infty$ . The only finite distance is  $L$ , used to define measures such as correlations or entanglement entropy:

$$\text{correlator : } c(L) = \langle \psi | \mathcal{O}(0)\mathcal{O}(L) | \psi \rangle \quad (78)$$

$$\text{entanglement entropy : } S(L) = -\text{tr}(\rho^A \log \rho^A) \quad (79)$$

The summary of the scaling of the entanglement entropy is the following:

$D + 1$ dimension	gapped	gapless				
$D = 1$	$S(L) \sim \text{const}$	$S(L) \sim \log L$				
$D = 2$	$S(L) \sim L$	<table style="margin-left: auto; margin-right: auto;"> <tr> <td style="text-align: center;">type I</td> <td style="text-align: center;">type II</td> </tr> <tr> <td style="text-align: center;"><math>S(L) \sim L</math></td> <td style="text-align: center;"><math>S(L) \sim L \log L</math></td> </tr> </table>	type I	type II	$S(L) \sim L$	$S(L) \sim L \log L$
type I	type II					
$S(L) \sim L$	$S(L) \sim L \log L$					
$D = 2$	$S(L) \sim L^2$	$S(L) \sim L^2 \quad S(L) \sim L^2 \log L$				

Table 1: Scaling of entanglement entropy for systems depending on their energy gap. Gapless *special* in  $D = 2, 3$  refers to Fermi surfaces with co-dimension greater than 1.

We say we have an **area-law** scaling of the entanglement entropy if

$$S(L) \sim L^{D-1}, \quad (80)$$

which is what we observe in ground-states of gapped local Hamiltonians. On the other hand, we say we have **volume-law** entanglement if  $S(L) \sim L^D$ , which is observed for random states

We show more explicitly the scaling for  $1 + 1$  and  $2 + 1$  dimensions in the subsections below.

## 8.1 $1+1$ Space-time dimensions

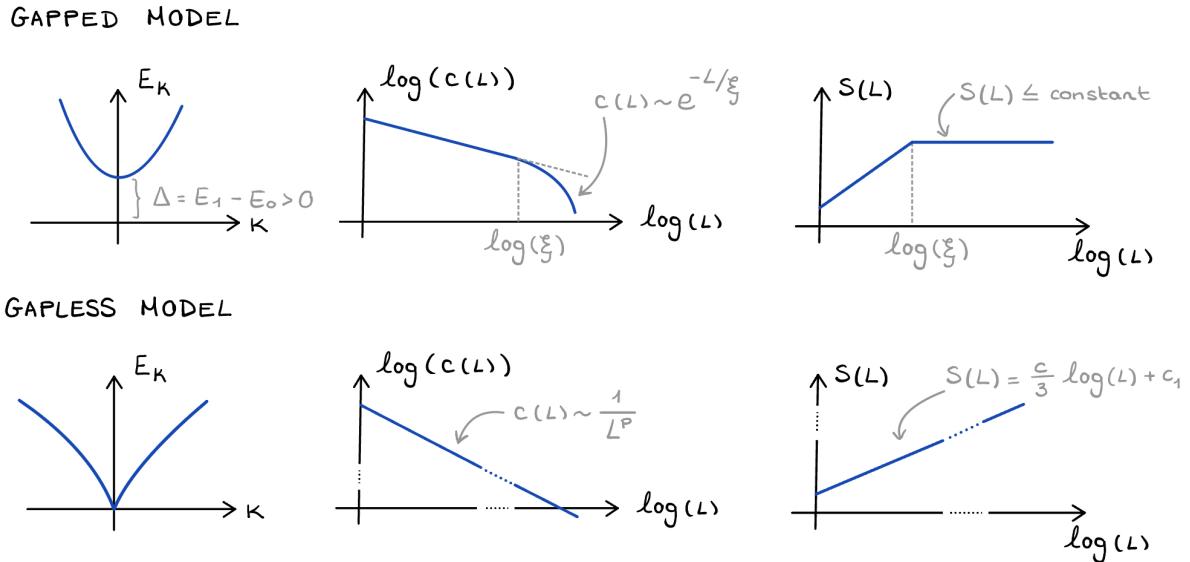


Figure 3: Energy, correlator and entanglement entropy comparison for gapped and gapless systems.

### 8.1.1 Gapped system

An example of such system might be, for example, the Ising model off criticality ( $h \neq J$ ). When observing correlations, there will be a regime for which correlations are compatible with power-law decay, but this then switches to an exponential decay in correlations. This means that correlations may be more or less intense at short distances but, as we go above a certain correlation length  $\xi$  these correlations decay exponentially fast.

Regarding the entanglement entropy, we will see that it initially grows with the size of the reduced density matrix,  $L$ , and it then saturates to a constant.

### 8.1.2 Gapless system

An example could be the Ising model at criticality ( $h = J$ ). We find that the correlations grow as a power law indefinitely. the entropy also grows indefinitely. This means the correlation length for this gapless systems is infinity. The power  $P$  and central charge  $c$  in the scaling of the correlator and entanglement entropy are model-specific (for critical Ising  $c = 1/2$ ). The central charge is larger for a larger number of zero modes ( $c = 1/2 \times \# \text{zero modes}$ ).

### 8.1.3 Computational Implications

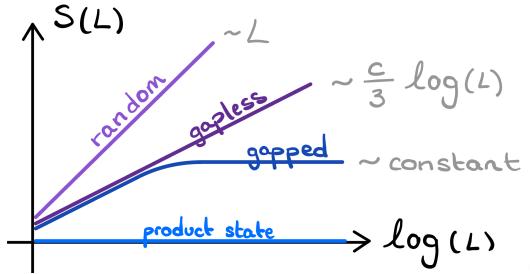


Figure 4: Scaling of entanglement entropy for different systems. For a random state we have almost maximum entropy (volume law entanglement), while a product state has zero entropy.

We see that the entanglement entropy for gapped ground-states is low. We may be able to leverage this property in order to economise the memory cost required to store the information about these systems. The memory cost required to specify each system is:

- Product state  $\equiv \mathcal{O}(N)$
- Random state  $\equiv \mathcal{O}(2^N)$
- Gapped ground-state  $\stackrel{?}{\equiv} \mathcal{O}(2^N)$

## 8.2 $2 + 1$ Space-time dimensions

Below we present the entropy scaling for different gaps in our system. For comparison purposes, for a  $2 + 1D$  random system we expect the entanglement entropy to be  $S(L) \sim L^2$ .

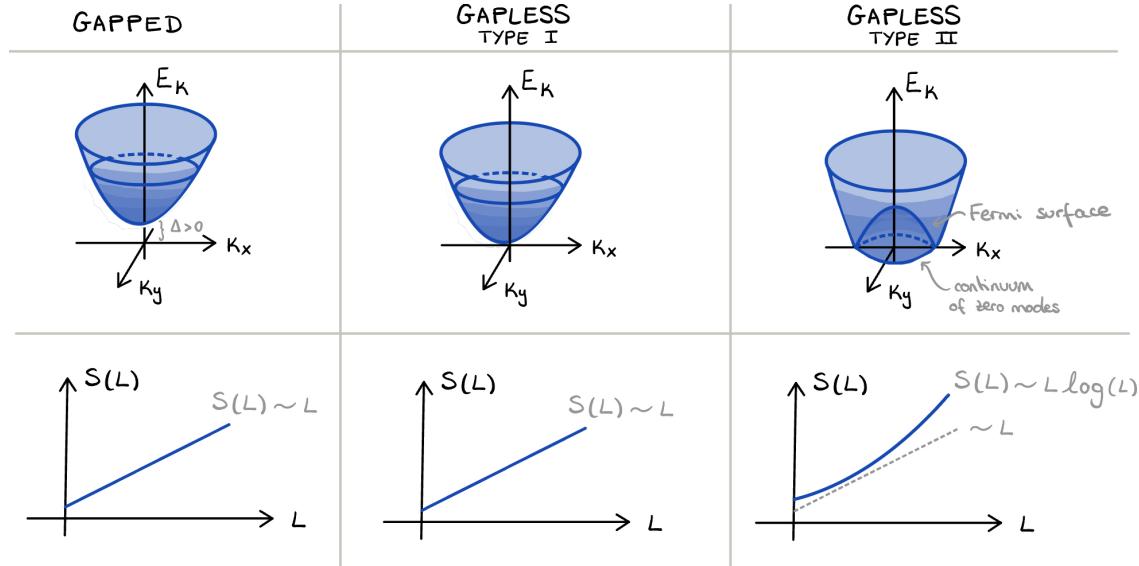


Figure 5: Energy and entanglement entropy scaling comparison for gapped and gapless systems in  $2 + 1D$ .

## 8.3 Simple Entanglement Toy Models

### 8.3.1 Area-law Entanglement

We build a very simple toy model that will motivate the construction of tensor networks. We can measure the entanglement of a subsystem by counting how many bonds are being broken when doing the partition.

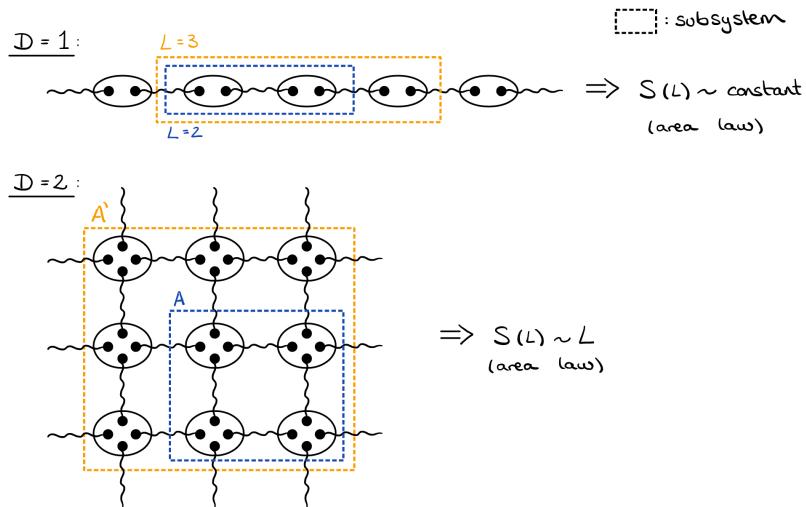


Figure 6: Simple model that captures area-law entanglement properties.

### 8.3.2 Logarithmic Corrections

We can account for logarithmic scaling in 1 spatial dimension by considering contributions at different length scales by coarse-graining. If we ignore the contributions from a given length scale we will get finite correlation length  $\xi$  and logarithmic contributions will be capped at  $\log(\xi)$ . However, in 2 spatial dimensions with the architecture presented in Figure 6 this is not possible. These results are presented in the diagrams below.

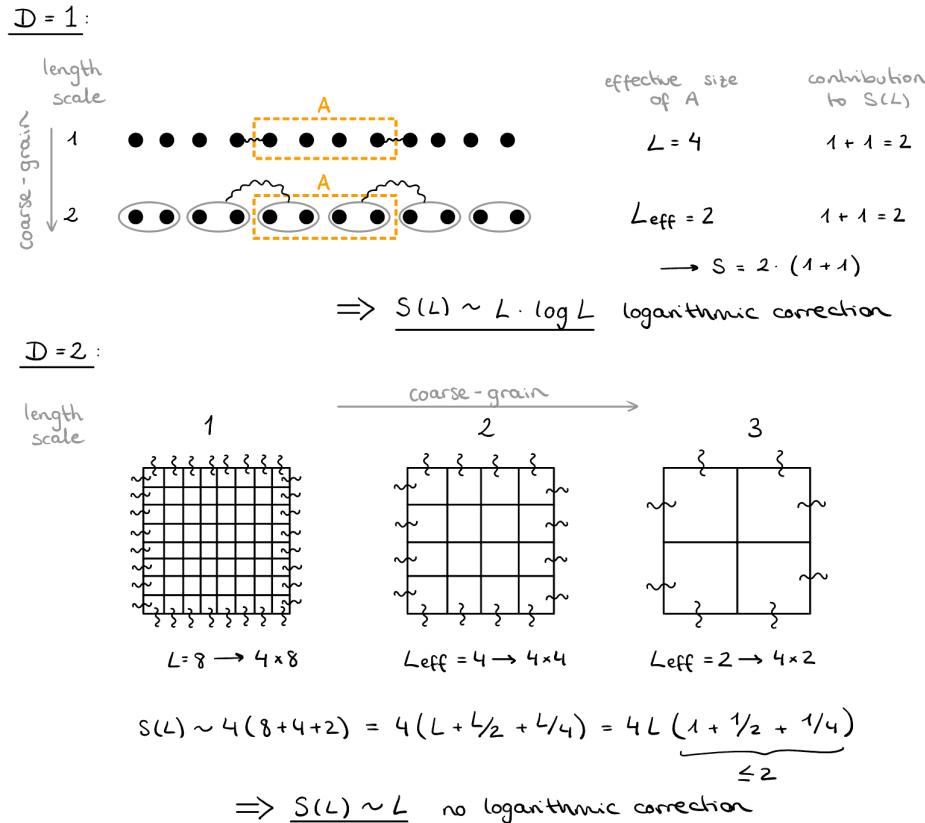


Figure 7: Toy model in 1D that captures the logarithmic scaling of entropy for galpess systems. In 2D this logarithmic behaviour is not possible using this architecture.

We are able to obtain logarithmic scaling for the 2D system if at every step of the coarse-graining we double the number of copies of the system we have, so that even though each scale contributes less, we have more copies of it to account for this.

## 9 Entanglement as a Theoretical Tool

We have seen that if we have a local Hamiltonian in  $D$  space dimensions we observe area-law entanglement (up to a logarithmic correction):  $S(L) \sim L^{D-1}$  (or  $S \sim L^{D-1} \log(L)$ ). The majority of states that live in the exponentially large Hilbert space of a system are not *relevant*. In this sense, this picture is a redundant description of the physics that we see in nature. We truly only need a number of parameters linear in the system size.

Entanglement also provides quantitative information about the universality class of the renormalisation group (RG) fixed points. We extract this information using the entanglement behaviour. There two fixed points that we will discuss:

1. Gapped phases fixed points: these are stable fixed points. These are understood within the framework of topological quantum field theories (TQFTs).
2. Phase transitions fixed points: the entanglement entropy provides information about the conformal field theories (CFT) at these points.

### 9.1 Entanglement Entropy in Quantum Critical Systems

We think of the CFT as describing a universality class. In short, a universality class refers to a group of models which may have very different microscopic properties but behave the same way at criticality. The CFT is described by some conformal data, which we have calculated numerous times in this course for different systems. This conformal data includes: primary fields ( $\phi_\alpha$ ), scaling dimensions ( $\Delta_\alpha$ ), conformal spins, etc. In  $1+1$  dimensions, conformal data includes the central charge  $c$ . As presented initially in Equation 28, this central charge can be extracted from the scaling of the entanglement entropy:  $S(L) \sim \frac{c}{3} \log(L)$ . Even though this may not fully characterise the CFT in  $1+1$  dimensions, it does provide some very useful information:

- $c = 1 - \frac{6}{m(m+1)} < 1$ : discrete set of unitary minimal modes. Fully characterises the CFT.
  - $c = \frac{1}{2}$  : Ising
  - $c = \frac{7}{10}$  : tricritical Ising
  - $c = \frac{4}{5}$  : 3-level Potts model
- $c = 1$ : there are infinitely many CFTs with this central charge. Therefore, entanglement entropy only partially characterises the CFT. We observe two continuous families of CFTs (compactified bosons):
  - Circle/Coulomb models, characterised by  $R_{circle}$ . For each value of this parameter we have a different CFT, and each scaling dimension depends continuously on this parameter.
  - Orbifold models: characterised by  $R_{orbifold}$

#### 9.1.1 $C$ -theorem

(See Zamoldchikov, 1986). In quantum field theory the  $C$ -theorem establishes that there exists a positive real function  $C(g_i, \mu) \geq 0$ , depending on the coupling constants of the QFT considered, the  $g_i$ , and on the energy scale,  $\mu$  which has the following properties:

- $C$  decreases monotonically under the renormalization group (RG) flow. This means that the RG flow is irreversible.
- At the fixed points of the RG flow the function is a constant, therefore independent of the energy scale.

A function fulfilling these requirements is<sup>12</sup>:  $C(L) = 3L \frac{dS(L)}{dL}$ . For a CFT, this is:

$$C(L) = 3L \frac{dS(L)}{dL} = 3L \frac{\frac{c}{3} \log(L)}{dL} = c \quad (81)$$

This allows us to go from one CFT to another monotonically, remaining critical at all points. For example, we may go from  $c = 1$  (XX model CFT) to  $c = \frac{1}{2}$  (Ising model CFT) by interpolating with the XY Hamiltonian:

$$H_{XY} = - \sum_{i=1}^{N-1} \left( \left( \frac{1+\gamma}{2} \right) \sigma_i^x \sigma_{i+1}^x + \left( \frac{1-\gamma}{2} \right) \sigma_i^y \sigma_{i+1}^y \right) \quad (82)$$

The  $\gamma$  anisotropy parameter will act as a perturbation to flow between the models.

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<sup>12</sup>Casini & Huerta, 2006.

## Part II

# Tensor Networks

### 10 Introduction and Basics

#### 10.1 Motivation

Tensor networks (TN) provide an efficient formalism to describe ground states of local Hamiltonians on a lattice. They constitute an order  $\mathcal{O}(N)$  description instead of the  $\mathcal{O}(\exp(N))$  full characterisation of the Hilbert space. This formalism was initially motivated as a variational wave-function ansatz for non-perturbative numerical many-body lattice problems. Much of its usefulness relies on the fact that TN descriptions are local in real space<sup>13</sup>, meaning we can attach a tensor for every position in the lattice. They also directly capture the structure of entanglement and correlations in many-body ground states. Tensor networks have been used to numerically study quantum critical phenomena, topological order, frustrated quantum magnets, interacting fermions, etc. They have also enabled the classification of symmetry protected topological (SPT) phases of matter, the reformulation of the renormalisation group (RG), provided new insights into holography. Its use has spread from condensed matter to quantum chemistry, statistical mechanics, quantum error correction, image compression, machine learning and quantum gravity.

#### 10.2 Tensor Networks Usefulness

We have three main conditions that make a tensor network useful.

1. Tensor networks should constitute an **efficient representation** of wavefunctions. The number of parameters of the tensor network should scale linearly in the system size,  $\mathcal{O}(N)$ , whereas with the original wavefunction tensor it was exponential in the system,  $\mathcal{O}(d^N)$ .
2. The polynomial efficiency of these architectures is not free and tensor networks are only an approximation. Tensor networks only define a subset of states within the full Hilbert space. We hope this is an **accurate approximation**. We assess this accuracy by studying whether the TN displays the right ground-state properties that we expect, for example: entanglement and correlations.
3. **Efficient manipulation** of tensor networks. We should be able to extract properties from this wavefunction such us expectation values. We should also be able to efficiently produce wavefunctions from Hamiltonians of interest.

#### 10.3 Definition and Graphical Notation

Recall that given a lattice of  $N$  sites each with  $d$  levels we define the lattice's vector space as:  $\mathbb{V}^{(N)} = (\mathbb{C}_d)^{\otimes N}$ . This space has exponential size in  $N$ , namely  $d^N$ . A quantum state  $|\psi\rangle \in \mathbb{V}^{(N)}$  takes the form:

$$|\psi\rangle = \sum_{\alpha_1, \alpha_2, \dots, \alpha_N=1}^d \psi_{\alpha_1, \alpha_2, \dots, \alpha_N} |\alpha_1 \alpha_2 \cdots \alpha_N\rangle \quad \text{and} \quad \langle \psi | \psi \rangle = 1. \quad (83)$$

<sup>13</sup>For the MERA ansatz we will also have an idea of locality with respects to scale

Following the TN notation presented in Appendix B this wavefunction may be represented as a big tensor with  $N$  open indeces, where each of these indeces has dimension  $d$ . This object (Figure 8a) would have size  $d^N$ . Alternatively we may choose to represent the original wavefunction information with a network of different rank interconnected subtensors as long as this new structure has  $N$  number of open unconnected legs as per Figure 8b. This new characterisation of the wavefunction will have a different size than the original  $d^N$  object, but could also have lower accuracy to the original wavefunction. This will become more explicit once more concrete tensor network architectures are explored.

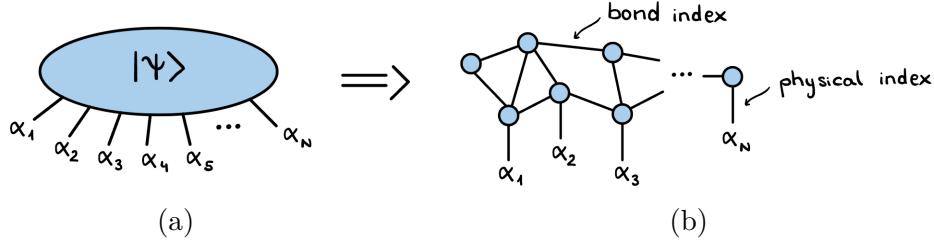


Figure 8: Representation of a wavefunction as an arbitrary tensor network. This depiction indicates the distinction between bond and physical indeces.

Some useful tensor network definitions are presented below:

- **Rank:** number of indeces sticking out of a tensor. E.g: matrices are rank-2 tensors, vectors are rank-1, etc.
- **Factor tensor or subtensor:** each tensor making up the tensor network.
- **Physical index/leg:** open index. They represent the original degrees of freedom of the wavefunction.
- **Bond index/leg:** index connecting two factor tensors in a tensor network. They enable for correlations in the tensor network.
- **Dimension:** size of an index, namely the number of values the index spans.
  - **Physical dimension:** size of the space of each site or element of the physical system. Usually denoted with  $d$ , such that  $\alpha_i = 1, 2, \dots, d$ . For example, for a spin-1/2 system  $d = 2$ .
  - **Bond dimension:** usually denoted with  $\chi$ , is the dimension of a bond index. This will determine the number of parameters needed to store the tensor network.

Tensor networks are also direct representations of quantum circuits, which can be used to represent the preparation of a wavefunction from a product state as depicted in Figure 9.

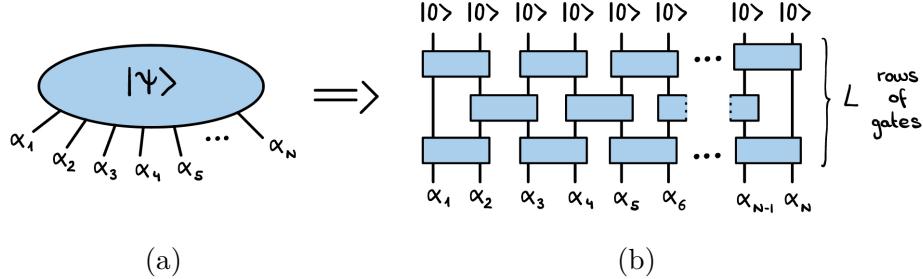


Figure 9: Preparation of a wavefunction (a) as a quantum circuit tensor network (b). The tensor network state begins as a product state of  $|0\rangle$  single qubit states.

For a circuit with  $N$  qubits and  $T$  rows of gates, we require order  $TNd^4$  parameters to specify the circuit. If  $T = \text{poly}(N)$  then this is a cheaper representation for our initially exponential wavefunction.

## 10.4 Cost of Contractions

A very common operation when manipulating tensor networks is contracting two (or a group of) tensors together. This means summing over all the bond indeces shared between these tensors. The cost of this operation follows from that of the standard multiplication algorithm, as presented in Appendix A. For two tensors  $A$  and  $B$  the cost of contracting them is:

$$\text{cost}(A \times B) = \frac{\|A\| \|B\|}{\|A \cap B\|}, \quad (84)$$

where  $\|A\|, \|B\|$  are the total dimension of each tensor (product of the dimensions of all their indeces), and  $\|A \cap B\|$  is the total dimension of the indices shared between the two tensors. Some examples of this cost are presented in Figure 10.

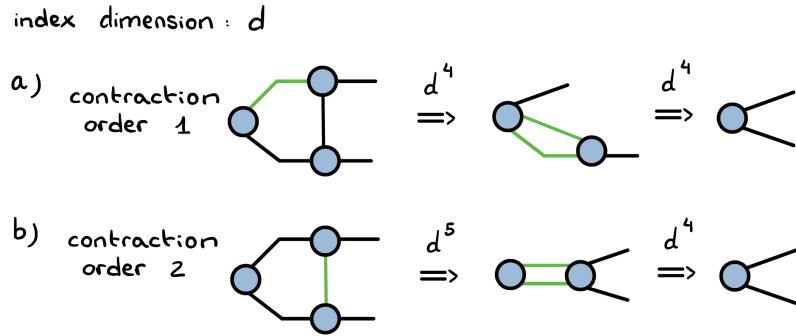


Figure 10: Different contraction orders for the same initial tensor network. Even though the resulting contracted tensor is the same in both scenarios, the leading order computational cost is greater in contraction order 2.

## 10.5 Gauge Freedom, Isometries and Centre of Orthogonality

Consider a tensor network that, after contraction of its bond indices, evaluates to a tensor  $T$ . This tensor network is not unique since we have a gauge freedom on the bonds and we are able to insert resolutions of the identity, namely two invertible matrices  $G^{-1}G = \mathbb{1}$ , see Figure 11a. Upon contraction of the bond indices we will obtain the same resulting tensor  $T$ .

This gauge freedom is a very powerful tool that we may leverage, for example, to create isometries. We define isometries to be tensors (or branches of tensors) that when contracted with their complex conjugate through their open indices result in the identity (see Figure 11b).

Generating isometries in a tensor network through gauge transformations can help us create a centre of orthogonality. A tensor  $O$  in our tensor network is a center of orthogonality if, for every branch of the network attached to  $O$ , the branch forms an isometry between its open indices and the index connected to tensor  $O$ . An example is presented in Figure 11c). This centre of orthogonality need not be a tensor with an open leg, it could be set to be a matrix (rank-2 tensor) at a bond.

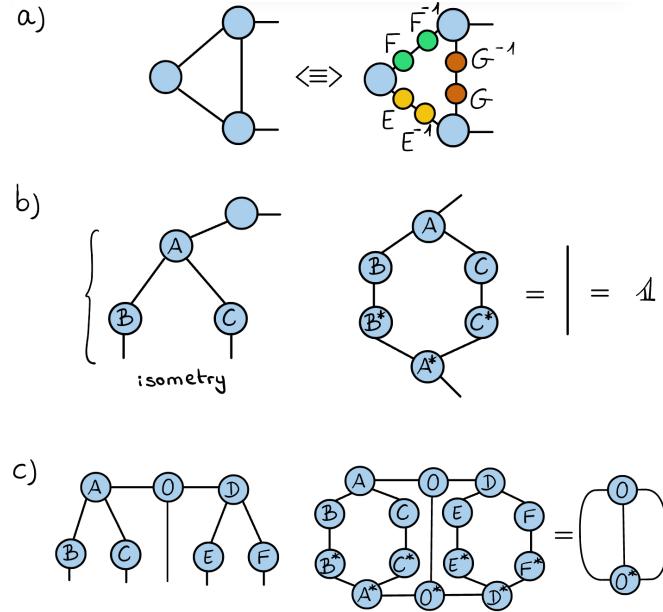


Figure 11: (a) Exploiting gauge freedom in a tensor network. (b) Isometry condition for the branch of tensors containing  $A, B, C$ . (c) Tensor  $O$  is a centre of orthogonality in the tensor network (left) if the isometry constraints (right) are satisfied.

## 11 Matrix Product States (MPS)

### 11.1 Definition

A matrix product state (MPS) is a tensor network architecture resulting from the factorisation of a tensor with  $N$  indeces into a chain-like product of rank-3 tensors. Each tensor  $A$  (which might be different at each site) in the MPS represents one site in the many-body system we aim to represent, therefore having one physical index while the remaining two are bond indeces.

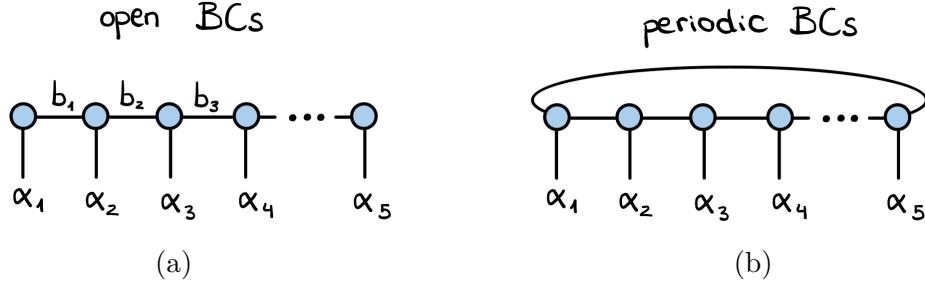


Figure 12: Graphical representation of a matrix products state with open boundary conditions (a) and periodic boundary conditions (b). The indeces  $\alpha_i$  represent the physical indeces and  $b_i$  the bond indeces. (c)

More explicitly, the coefficients of a wavefunction (as in Equation 85) can be obtained by contracting (summing over) the MPS bond indeces. For an MPS with open boundary conditions this is:

$$\psi_{\alpha_1, \alpha_2, \dots, \alpha_N} = \sum_{\{b_1, b_2, \dots, b_N\}} A_{\alpha_1}^{b_1} A_{\alpha_2}^{b_1 b_2} A_{\alpha_3}^{b_2 b_3} \dots A_{\alpha_N}^{b_{N-1} b_N}, \quad (85)$$

where  $A$  is each of the factor tensors.

In this course we will mostly cover finite size MPS and their main related algorithms. However, there also exist MPS algorithms for dealing with systems in the thermodynamic limit<sup>14</sup>.

### 11.2 Number of Parameters

The number of parameters needed to specify an  $N$  tensor MPS of physical index dimension  $d$  and (largest) bond dimension  $\chi$  is:

$$\mathcal{O}(Nd\chi^2) \quad (86)$$

An MPS may represent any 1D system if we allow for the bond dimension  $\chi$  to be large enough<sup>15</sup>, in particular  $\chi = d^{N/2}$ . However, our aim is to efficiently restrict the size of the bond dimension in order to make MPS useful.

### 11.3 Decomposition of a Wavefunction into an MPS

We will explore how to decompose a  $d^N$  sized tensor (i.e. the tensor encoding our  $N$  site wavefunction where each site has dimension  $d$ ) into an MPS. Note that this decomposition is not unique due to the

<sup>14</sup>Additional material in process.

<sup>15</sup>We note that for open boundary conditions the bond dimension at a given bond site should not exceed  $d^\Delta$  where  $\Delta$  is the bond's separation away from the boundary. Otherwise we would be overparametrising the tensor network.

gauge freedom of tensor networks 10.5. In order to do this, we repeat the following algorithm  $N - 1$  times. See Figure 13 for supplemental diagrams. At each iteration  $i$ :

1. First iteration,  $i = 1$ :

Reshape the  $N$  index tensor into a rank-2 tensor  $M_i$  (legs  $A$  and  $B$ ) of dimensions  $d_A = d$  and  $d_B = d^{N-1}$ .

After first iteration,  $i > 1$ :

Reshape the tensor  $Q_{i-1}$  (obtained from the previous iteration as a result of  $S'_{i-1}R'_{i-1}$ ) into a rank-2 tensor  $M_i$  (legs  $A$  and  $B$ ) of dimensions  $d_A = d\chi$  and  $d_B = d^{N-i}$ .

2. Perform a singular value decomposition (Appendix C) of this matrix  $M_i$  to obtain  $M_i = L_i S_i R_i$ .
3. The diagonal singular value matrix  $S_i$  contains the  $r$  Schmidt coefficients (Equation 24) in descending size order, namely  $S_i = \text{diag}(\sigma_1, \dots, \sigma_r)$  with  $\sigma_j \geq \sigma_{j+1}$ . The Schmidt coefficients are the square-rooted eigenvalues of the reduced density matrices of the subsystems represented by the reshaped indices  $A$  and  $B$  and therefore the singular value matrix  $\Sigma_i$  contains the information about the entanglement between them. At this stage we can choose to truncate the size of the resulting objects  $M_i = L_i \Sigma_i R_i \approx L'_i \Sigma'_i R'_i$  and keep only the  $\chi$  largest Schmidt coefficients. Note that here is the stage at which the approximation is introduced.
4. We redefine our right side tensor to be  $Q_i = S'_i R'_i$  of shape  $(\chi, d^{N-i})$  and repeat the algorithm to continue decomposing it. We reshape the left side matrix  $L'_i$  into a 3-index MPS like tensor of dimensions  $(\chi, d, \chi)$ . If  $i = 1$  then  $L_1$  is left as a dimension  $(d, \chi)$  rank-2 tensor. If  $i = N - 1$  then  $R_{N-1}$  is left as a dimension  $(\chi, d)$  rank-2 tensor.

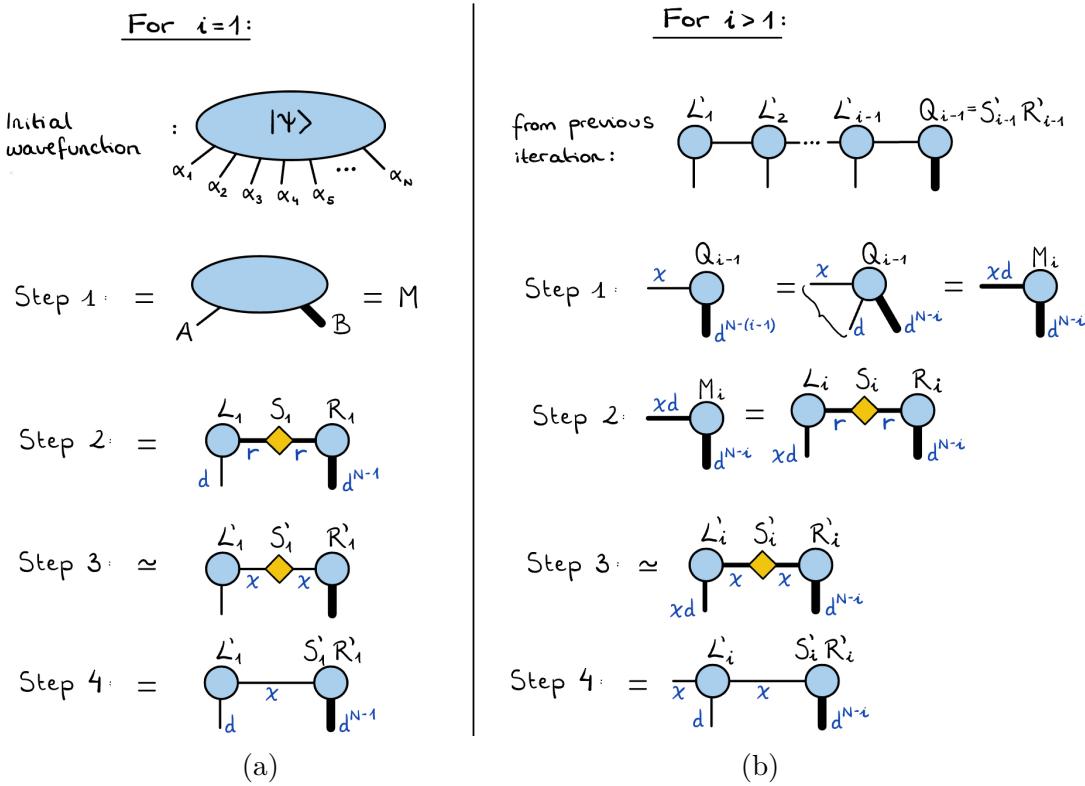


Figure 13: Steps of the iterative algorithm for the decomposition of a wavefunction into an open boundary condition MPS. First iteration detailed in (a) and rest of iterations in (b). The dimensions of each index are labelled in blue.

The procedure described above involved decomposing a wavefunction into an MPS from left to right and therefore produces an MPS whose tensors  $\{L_i\}$  are unitaries when contracted from the left. In other words, the MPS is in its left canonical form (see Section 11.4). We may choose to do this from right to left in a similar manner in order to produce a right canonical MPS, or leave the diagonal matrices in the bonds in what is known as Vidal's form.

When applying this decomposition, we have gone from a  $\mathcal{O}(d^N)$  sized object to an  $\mathcal{O}(Nd\chi^2)$  (Equation 86). This reduction in size was done at the expense of the approximation introduced in Step 3. The MPS representation will be more accurate (meaning the MPS representation of the wavefunction will have high fidelity with the original wavefunction  $|\psi\rangle$ ) if the entanglement of that wavefunction was low<sup>16</sup>.

## 11.4 Canonical Form of an MPS

### 11.4.1 Generating Isometries and Centres of Orthogonality in an MPS

In Section 10.5 we explored the idea of gauge freedom, isometries and centres of orthogonality. Applying this idea to an MPS is straightforward. Given an MPS representation of a wavefunction we may generate a centre of orthogonality on a site (rank-3 MPS tensor) or a bond  $n$  by generating left and right isometries to the left and right of the centre of orthogonality respectively:

- **Left Isometries** (Figure 14a): from left to right replace each tensor  $A_i$  for  $i < n$  find the (semi-

<sup>16</sup>G. Vidal, *Efficient Classical Simulation of Slightly Entangled Quantum Computations*, Phys. Rev. Lett 91, 14, 2003.

orthogonal) matrix  $V$  with its singular value decomposition of  $A_i = U_i S_i V_i^\dagger$  (after proper reshape of  $A_i$  into a rank-2 tensor). Absorb the bond matrices  $S_i$  and  $V_i^\dagger$  into the next tensor to the right  $A_{i+1}$ . The left isometries will be the SVD semi-orthogonal matrices  $U_i$ .

- **Right Isometries** (Figure 14b): similarly to the procedure above, replace each tensor  $A_i$  for  $n < i < N$  with its singular value decomposition and absorb  $U_i S_i$  to  $A_{i-1}$ . The right isometries will be the SVD semi-orthogonal matrices  $V_i^\dagger$ .

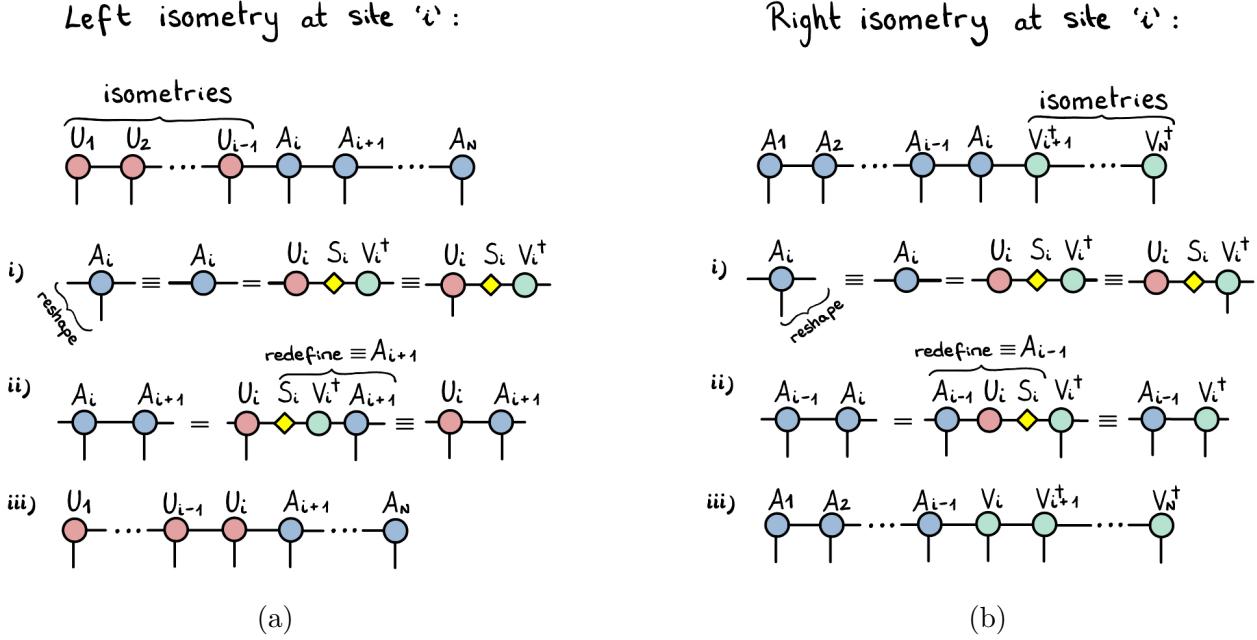


Figure 14: Generating left (a) and right (b) isometries at site  $i$  in an MPS. (i) We first obtain the singular value decomposition of the tensor  $A_i$  after reshaping and then reshape the isometry ( $U_i$  or  $V_i^\dagger$ ) into a rank-3 tensor. (ii) Substitute  $A_i$  for  $U_i S_i V_i^\dagger$  in the MPS and redefine  $A_{i+1}$  or  $A_{i-1}$  (left and right isometries respectively) by absorbing the remaining SVD terms. (iii) The MPS has one more isometry from the left or right respectively.

To set a bond  $b$  to be the centre of orthogonality of the MPS simply involves generating left and right isometries as detailed above up to that bond and leaving the resulting diagonal matrix on the bond. This diagonal matrix contains the density matrix eigenvalues (Schmidt values) of the subsystems  $\alpha, \beta$  given by  $\alpha = \{A_j | 1 \leq j < b\}$  and  $\beta = \{A_j | b < j \leq N\}$ .

By defining a site to be the centre of orthogonality of a MPS the calculation of expectation values of local operators is simplified, see Figure 15.

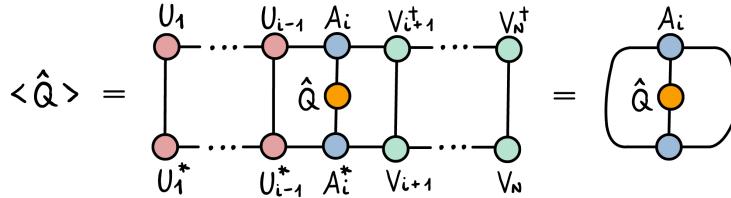


Figure 15: Evaluation of expectation value of one-site local operator  $\hat{Q}$  at site  $i$  once  $A_i$  has been set to be a centre of orthogonality. Here we have assumed that the MPS is normalised.

Applying the procedure in Figure 14 for generating left and right isometries to the entirety of the MPS define the **left and right canonical form** of the MPS.

## 11.5 Efficiency of MPS contractions

One of the requisites we stated in Section 10.2 to define the ‘usefulness’ of tensor networks as a wavefunction ansatz was the efficiency of computing properties from them. Calculations involving MPS (such as the norm, expectations values of local operators, sampling wave-function amplitudes, overlaps of states, etc) are computationally efficient. To see this let us consider the inner product between two states represented by two MPS given by the set of  $N$  tensors  $\{A_i\}$  and  $\{B_i\}$  respectively. As seen in the contraction order in Figure 16, this procedure has a cost  $\mathcal{O}(N\chi^3d)$ , which is linear in the size of the system. The generalisation of this efficiency to other MPS calculations follows. For a tensor network with periodic boundary conditions (Figure 12b) we find that the cost of this operation increases to  $\mathcal{O}(N\chi^5d)$ .

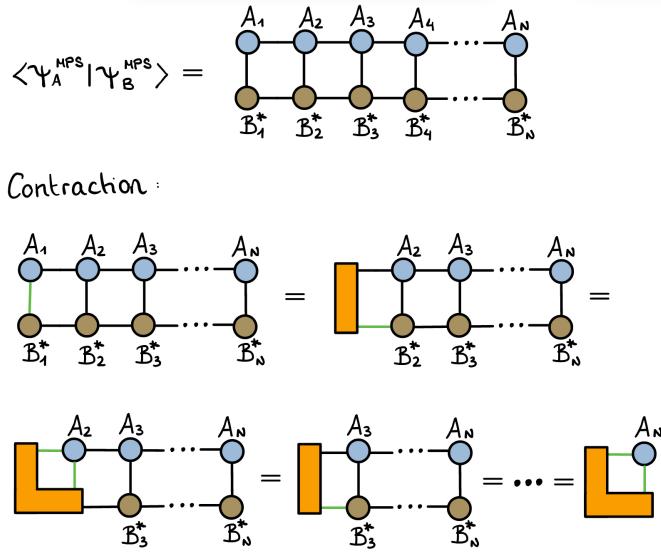


Figure 16: Contraction of the object representing the inner product of two states parametrised by two MPS. At each step we contract the index highlighted in green and we repeat this iteratively until we obtain the scalar value of the inner product.

## 11.6 Transfer Matrix

A key object ubiquitous in tensor networks algorithms is the **transfer matrix**. For a translationally invariant MPS with unit-cell tensor  $A$  and bond dimension  $\chi$ , the transfer matrix  $\hat{T}$  is a rank-4 tensor resulting from the physical index contraction between  $A$  and  $A^\dagger$  as depicted in Figure 17. This tensor has eigenvalue decomposition

$$\hat{T} = \sum_{\alpha=1}^{\chi^2} \lambda_\alpha |r_\alpha\rangle \langle l_\alpha| \quad (87)$$

where  $|r_\alpha\rangle$  and  $\langle l_\alpha|$  are two bi-orthogonal basis of right and left eigenvectors of  $\hat{T}$ , with  $\langle l_\alpha | r_\alpha \rangle = \delta_{\alpha,\beta}$ .

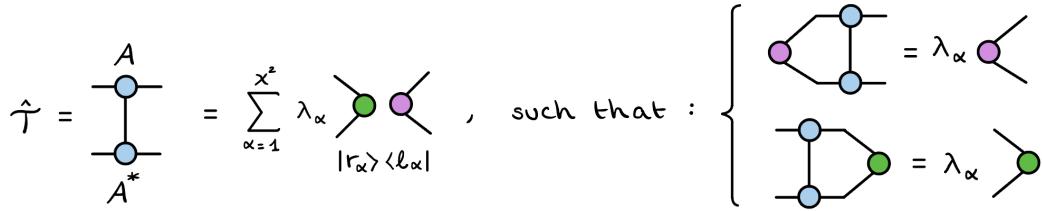


Figure 17: Tensor network representation of the transfer matrix for a translationally invariant MPS and its eigenvalue decomposition.

We assume  $\lambda_1 > \lambda_2 \geq \lambda_3 \geq \lambda_4 \dots$ . To normalise our MPS we redefine tensor  $A$  such that  $\lambda_1 = 1$ . The left and right eigenvectors  $|r_1\rangle$  and  $\langle l_1|$ , associated with  $\lambda_1 = 1$ , are called dominant eigenvectors. The  $p^{th}$  power of  $\hat{T}$  can then be approximated by  $|r_1\rangle\langle l_1|$  up to corrections that are exponentially suppressed in  $p$ , explicitly:

$$(\hat{T})^p = |r_1\rangle\langle l_1| + \mathcal{O}(\lambda_2^p + \lambda_3^p + \dots), \quad (88)$$

which is shown diagrammatically in Figure 18.

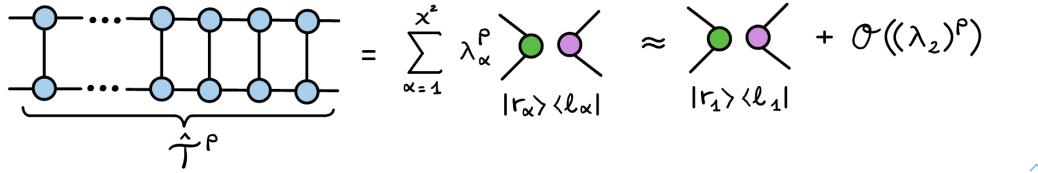


Figure 18: Taking the  $p^{th}$  power of the transfer matrix.

In the thermodynamic limit,  $N \rightarrow \infty$ , these contributions get suppressed and only the dominant eigenvalues remain. If  $\lambda_1 = 1$  the MPS is normalised,  $\langle \psi | \psi \rangle = 1$ , as depicted in Figure 19 a. Similarly, this transfer matrix formalism allows us to easily calculate expectation values, Figure 19 b.

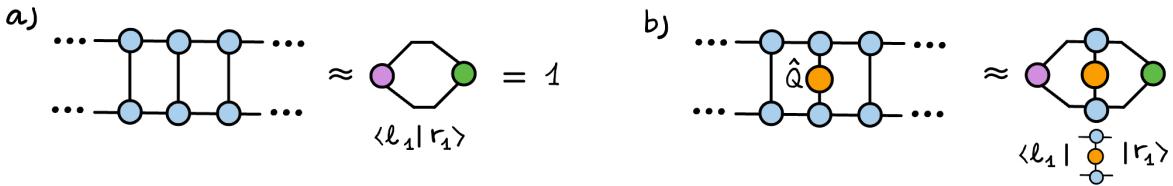


Figure 19: Norm (a) and expectation value of operator  $\hat{Q}$  for an infinite MPS.

## 11.7 Correlations in MPS

The two-point correlator of an operator  $\hat{Q}$  is defined as:

$$c(L) = \langle \hat{Q}_i \hat{Q}_{i+L} \rangle - \langle \hat{Q}_i \rangle \langle \hat{Q}_{i+L} \rangle \quad (89)$$

In an MPS always decays **exponentially** at large distances:

$$c(L) \sim e^{-L/\xi}, \quad (90)$$

where  $\xi$  is the correlation length. To see this, we consider the first and second terms of Equation 89 independently in tensor network notation for a large- $N$  translationally invariant MPS. We assume the MPS is normalised, meaning the largest eigenvalue of the transfer matrix is  $\lambda_1 = 1$ . As depicted in Figure 20a we notice that the first term breaks up into the second term plus an exponentially decaying correction. When put together, the terms cancel and the exponentially decaying term remains. The correlation length  $\xi$  is therefore defined as  $\xi = -1/\log(\lambda_\alpha)$ .

Figure 20: Diagrammatical calculation of the correlation length as  $|i - j| \gg 1$ . In (a) we observe the first term of the correlator becomes the square of the single site expectation value at sites  $i$  and  $j$  plus an exponentially decaying term. In the final expression for  $c(L)$  we are left with an exponential decay dictated by the correlation length  $\xi$  (b).

The correlation length in an MPS is always finite, and therefore MPS can not reproduce the properties of critical or scale-invariant systems, where the correlation length is known to diverge

## 12 Projected Entangled Pair States (PEPS)

### 12.1 Definition

## 13 Multi-scale Entanglement Renormalisation Ansatz (MERA)

### 13.1 Definition

# Appendices

## A Computational cost

Given a problem of size  $m$  we ask:

- how much space (memory) is required?
- how much time is required?

We are interested in the scaling of memory and time with  $m$ , this could be:  $\mathcal{O}(e^m)$ ,  $\mathcal{O}(m^n)$ , etc.

Examples of computations and their cost (all  $\alpha, \beta, \gamma = 1, \dots, m$ ):

Operation	Expression	Time	Memory
vector-vector multiplication	$s = \sum_{\alpha=1}^m v_\alpha^* w_\alpha$	$\mathcal{O}(m)$	$\mathcal{O}(m)$
matrix-vector multiplication	$w_\alpha = \sum_{\beta=1}^m M_{\alpha\beta} v_\beta$	$\mathcal{O}(m^2)$	$\mathcal{O}(m^2)$
matrix-matrix multiplication	$C_{\alpha\gamma} = \sum_{\beta=1}^m M_{\alpha\beta} B_{\beta\gamma}$	$\mathcal{O}(m^3)$	$\mathcal{O}(m^2)$

## B Tensor Networks Graphical Notation

The diagrams below introduce the tensor network notation we will use throughout the course:

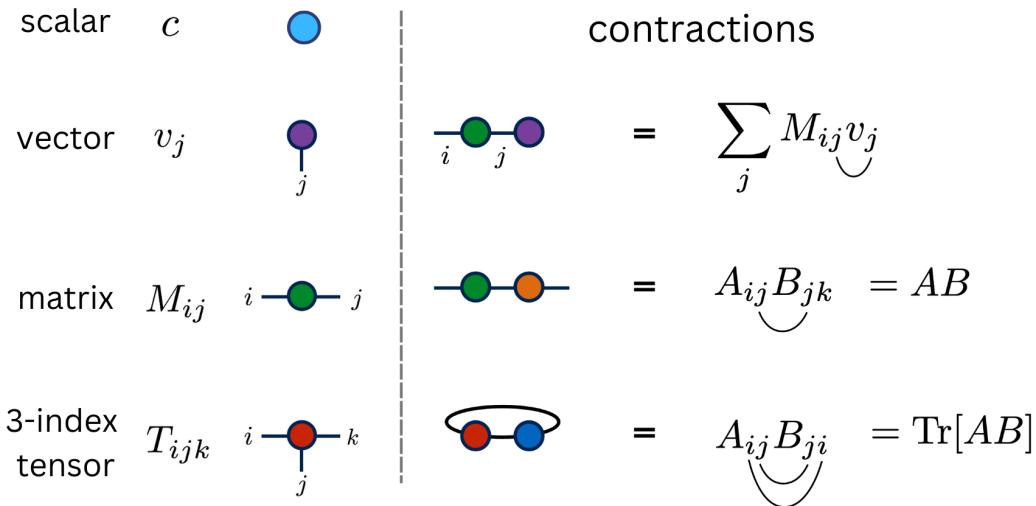


Figure 21: Tensor network (TN) objects and contraction notation. The components of the TN objects are  $z \in \mathbb{C}$ . Partial credits to [TensorNetwork.org](#).

## C Singular Value Decomposition

The singular value decomposition (SVD) states that any (square or rectangular)  $m \times n$  complex matrix  $M$  (which therefore acts as a linear transformation from  $\mathbb{R}^n \rightarrow \mathbb{R}^m$ ) can be factorised such that:

$$M = U \Sigma V^\dagger, \quad (91)$$

where  $U$  is an  $m \times m$  complex unitary (orthogonal if real) matrix,  $\Sigma$  is an  $m \times n$  positive rectangular diagonal matrix, and  $V^\dagger$  is the conjugate transpose of an  $n \times n$  complex unitary matrix  $V$ . If  $M_{ij} \in \mathbb{R} \rightarrow M = U\Sigma V^T$ . The diagonal entries of  $\Sigma$  are the singular values of  $M$ . The number of non-zero  $\Sigma_{ii}$  is the rank,  $r$ , of  $M$ .

We can also write the above expression as:

$$M_{ij} = \sum_{i=1}^r \sigma_i \mathbf{u}_i \otimes \mathbf{v}_i,$$

where  $\{\mathbf{u}_i\}, \{\mathbf{v}_i\}$  and the sets of orthogonal vectors that make up  $V, U$  and  $r \leq \min\{m, n\}$  is the rank of  $M$ .

We can see the connection to the Schmidt decomposition by considering  $M^\dagger M = V\Sigma^2V^\dagger$  and  $MM^\dagger = U\Sigma^2U^\dagger$  where  $MM^\dagger$  and  $M^\dagger M$  are both hermitian matrices.  $|\psi_{AB}\rangle$  would be  $M$ , and, in this sense,  $M^\dagger M = \rho^A$  while  $MM^\dagger = \rho^B$ .

## D Jordan-Wigner Transform

The Jordan–Wigner transformation is a transformation that maps spin operators onto fermionic creation and annihilation operators. Consequently, there is no distinction between spin–1/2 particles and fermions. Consider  $N$  different anhiliation modes. One can show that if we construct our annihilation operators such that:

$$a_m = \sigma_1^z \sigma_2^z \cdots \sigma_{m-1}^z \left( \frac{\sigma_m^x + i\sigma_m^y}{2} \right), \quad (92)$$

these will fulfil the required anticommutation relations:

$$\{a_m^\dagger, a_n\} = \delta_{mn} \quad , \quad \{a_m, a_n\} = 0. \quad (93)$$

Note that the expression in 92 is not local in the spin variables. This Jordan-Wigner transformation allows us to map a fermionic term to a spin term, for example:

$$-\sum_m (a_m^\dagger a_{m+1} + a_{m+1}^\dagger a_m) = -\frac{1}{2} \sum_m (\sigma_m^x \sigma_{m+1}^x + \sigma_m^y \sigma_{m+1}^y). \quad (94)$$

In the expression above we now see that our previously non-local spin operators take a local form in this term.