Notes de cours pour la minischool du GDR NBODY

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Contents

Introduction

These notes constitute a short introduction to the tensor train (TT) decomposition (also called matrix product state - MPS), with a particular focus on solving the many-body electronic Schrödinger equation. The beginning of TT can be tied to the density matrix renormalisation group [Whi92] (DMRG), although the connection with the TT/MPS ansatz has been made a few years later. Originally, DMRG has been applied to one-dimensional statistical physics systems with tremendous success, becoming the state-of-the-art numerical method to compute ground-state and low-excited states properties. It has then been tested for two-dimensional systems, where the question of the geometry of the tensor train, or the ordering of the sites has been difficult to overcome. It has also been successfully applied to quantum chemistry systems -with the name QC-DMRG (quantum chemistry-DMRG)-, where the question of the ordering of the sites is at first glance unclear.

The first part of the lecture notes is devoted to the electronic Schrödinger equation in the second quantisation and the introduction of the tensor to approximate.

The tensor train decomposition [OT09] is presented as a generalisation of the singular value decomposition for matrices, which is central in the characterisation of the low-rank approximation problem.

As quantum entropy is central in the ordering scheme for QC-DMRG [BLMR11], we introduce several notions of the quantum entropy as well as the connection with the TT/MPS approximation.

Finally, we address two points that explain the success of DMRG:

- Hastings area law [Has07] for one-dimensional system which proves that the TT/MPS approximation of a nearest neighbour Hamiltonian is at most *polynomial* in the system size;
- the DMRG algorithm and its polynomial scaling for electronic structure problems.

The content is inspired by the following texts on TT/MPS [Hac12, Hac14, Sch11, BSU16, UV20].

Chapter 1

Tensors in quantum chemistry

1.1 The many-body Schrödinger equation

1.1.1 The equation and its discretisation

Under the Born-Oppenheimer approximation, the ground-state of an electronic system with N electrons and N_{at} atoms with charges Z_K and located at the positions R_K, $1 \leq K \leq N_{\text{at}}$ is given by the lowest eigenvalue

$$H^N \Psi_0^N = E_0^N \Psi_0^N, \tag{1.1.1}$$

where the operator H^N is the many-body electronic Schrödinger operator

$$H^N = \sum_{i=1}^{N} \Big(-\frac{1}{2}\Delta_{r_i} - \sum_{K=1}^{N_{\text{at}}} \frac{Z_K}{|r_i - R_K|} \Big) + \sum_{1 \leq i < j \leq N} \frac{1}{|r_i - r_j|}, \tag{1.1.2}$$

and the wave function Ψ_0^N belongs to $\bigwedge^N L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$.

Using the Rayleigh-Ritz principle, the eigenvalue problem can be rephrased as an optimisation problem

$$E_0^N = \min_{\substack{\Psi \in \bigwedge^N L^2(\mathbb{R}^3 \times \mathbb{Z}_2) \\ \|\Psi\|_{L^2} = 1}} \langle \Psi, H^N \Psi \rangle. \tag{1.1.3}$$

A standard way to solve the eigenvalue problem (1.1.1) is to use a Galerkin scheme of the following form. Let $(\phi_i)_{1 \leq i \leq L}$ be an L^2-orthogonal family of $L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ and let

$$\mathcal{V}_N^L = \text{Span}\Big(\phi_{i_1} \wedge \cdots \wedge \phi_{i_N} = \frac{1}{\sqrt{N!}} \det\big(\phi_{i_j}(x_k)\big), 1 \leq i_1 \leq \cdots \leq i_N \leq L \Big), \tag{1.1.4}$$

then the problem to solve numerically becomes

$$E_{0,L}^N = \min_{\substack{\Psi \in \mathcal{V}_N^L \\ \|\Psi\|_{L^2} = 1}} \langle \Psi, H^N \Psi \rangle \geq E_0^N. \tag{1.1.5}$$

The approximate ground-state wave function is given by

$$\Psi_{0,L} = \sum_{1\le i_1<\cdots<i_N\le L} C_{i_1\dots i_N}\phi_{i_1}\wedge\cdots\wedge\phi_{i_N}. \tag{1.1.6}$$

The number of such coefficients is exponential in the number of electrons, hence a clever parametrisation of the coefficients as well as an insightful choice of the Galerkin basis is needed.

Several methods have been tried to sparsely parametrise the coefficients of the ground-state wave function:

- the configuration interaction (CI) method, which is a hierarchical truncation of the coefficients in (1.1.6);
- the coupled-cluster (CC) method, which relies on an intricate parametrisation of the wave function;
- the density matrix renormalisation group (DMRG) which is based on a tensor factorisation of the coefficients in the second quantisation.

1.1.2 Fock space

The discrete Fock space $\mathcal{F}_L$ is defined as the direct sum of the Galerkin spaces $\mathcal{V}_N^L$ given in Eq. (1.1.4)

$$\mathcal{F}_L = \mathcal{V}_0^L \oplus \mathcal{V}_1^L \oplus \cdots \oplus \mathcal{V}_L^L. \tag{1.1.7}$$

A general state $\mathbf{\Psi} \in \mathcal{F}_L$ is the collection $(\Psi^0, \Psi^1, \dots, \Psi^L)$ where each Ψ^k is a wave function belonging to $\mathcal{V}_k^L$.

To move from $\mathcal{V}_k^L$ to its neighbour, the creation operator $(c_j^\dagger)_{1\le j\le L}$ and the annihilation operator $(c_j)_{1\le j\le L}$ are used. The annihilation operator c_j is the map such that

$$c_j \;:\; \begin{cases} \mathcal{V}_{k+1}^L \to \mathcal{V}_k^L \\ \phi_{i_1}\wedge\cdots\wedge\phi_{i_{k+1}} \mapsto \begin{cases} 0 & \text{if } \forall\, 1\le \ell\le k+1, j\neq i_\ell \\ (-1)^{\ell-1}\phi_{i_1}\wedge\cdots\wedge\phi_{i_{\ell-1}}\wedge\phi_{i_{\ell+1}}\wedge\cdots\wedge\phi_{i_{k+1}}, & \text{if } j=i_\ell. \end{cases} \end{cases} \tag{1.1.8}$$

The annihilation operator c_j destroys a particle in the state ϕ_j if it exists and returns 0 otherwise. Likewise, the creation operator $c_j^\dagger$ is given by

$$c_j^\dagger \;:\; \begin{cases} \mathcal{V}_k^L \to \mathcal{V}_{k+1}^L \\ \phi_{i_1}\wedge\cdots\wedge\phi_{i_k} \mapsto (-1)^\ell \phi_{i_1}\wedge\cdots\wedge\phi_{i_\ell}\wedge\phi_j\wedge\phi_{i_{\ell+1}}\wedge\cdots\wedge\phi_{i_{k+1}}, \end{cases} \tag{1.1.9}$$

with $i_1<\cdots<i_\ell<j<i_{\ell+1}<\cdots<i_k$. Note that by antisymmetry, if $j=i_\ell$ for some ℓ, then $c_j^\dagger(\phi_{i_1}\wedge\cdots\wedge\phi_{i_k})=0$. For the creation operator $c_j^\dagger$, a particle is created in the state ϕ_j.

The creation and annihilation operators satisfy the following anticommutation rules

$$\{c_i^\dagger, c_j^\dagger\} = \{c_i, c_j\} = 0, \quad \text{and} \quad \{c_i, c_j^\dagger\} = \delta_{ij}. \tag{1.1.10}$$

The Hamiltonian is written (in the Mulliken convention)

$$\hat{H} = \sum_{i,j=1}^{L} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,\ell=1}^{L} V_{ijk\ell} c_i^\dagger c_j^\dagger c_\ell c_k, \tag{1.1.11}$$

where $c_i^\dagger$, c_j are the creation and annihilation operators, h is a Hermitian matrix and $(V_{ij,k\ell}) \in \mathbb{C}^{L^2 \times L^2}$ is also Hermitian.

In quantum chemistry, given an orthonormal basis $(\phi_i)_{i\in\mathbb{N}}$ of $L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$ the coefficients h_{ij} and $V_{ijk\ell}$ are given by [HJO14, Equation (1.4.40) and (1.4.41)]

$$\begin{cases} h_{ij} = \displaystyle\sum_{s\in\{0,1\}} \int_{\mathbb{R}^3} \phi_i(r,s)^* \big(-\tfrac{1}{2}\Delta + v_{\mathrm{ne}} \big) \phi_j(r,s)\, \mathrm{d}r \\ V_{ijk\ell} = \displaystyle\sum_{s,s'\in\{0,1\}} \int_{\mathbb{R}^3} \frac{\phi_i(r,s)^* \phi_j(r',s')^* \phi_k(r,s) \phi_\ell(r',s')}{|r-r'|}\, \mathrm{d}r\mathrm{d}r'. \end{cases} \tag{1.1.12}$$

The problem to solve is

$$\min \left\{ \langle \Psi, \hat{H}\Psi \rangle_{\mathcal{F}}, \Psi \in \mathcal{F}_L, \|\Psi\|_{\mathcal{F}_L} = 1, \hat{N}\Psi = N\Psi \right\}, \tag{1.1.13}$$

where $\hat{N}$ is the particle number operator

$$\hat{N} = \sum_{i=1}^{L} c_i^\dagger c_i. \tag{1.1.14}$$

Remark 1.1.1. *As the constraint on the number of particles can be cumbersome to take into account, the constraint is changed to a mean-value constraint*

$$\min \left\{ \langle \Psi, \hat{H}\Psi \rangle_{\mathcal{F}}, \Psi \in \mathcal{F}_L, \|\Psi\|_{\mathcal{F}_L} = 1, \langle \Psi, \hat{N}\Psi \rangle = N \right\}. \tag{1.1.15}$$

This quadratic constraint can be reformulated as a Lagrange multiplier where we solve

$$\min \left\{ \langle \Psi, (\hat{H} - \mu\hat{N})\Psi \rangle_{\mathcal{F}}, \Psi \in \mathcal{F}_L, \|\Psi\|_{\mathcal{F}_L} = 1, \right\}. \tag{1.1.16}$$

for a fixed value $\mu \in \mathbb{R}$. Both minimisation problem are not equivalent in general.

A minimiser of (1.1.15) or (1.1.16) is of the form

$$\Psi = \sum_{\mu_1,\dots,\mu_L} \Psi_{i_1\dots i_N} c(\phi_{i_1})^\dagger \cdots c(\phi_{i_N})^\dagger |\Omega\rangle. \tag{1.1.17}$$

Another way to parametrise the wave function Ψ is with respect to the occupation number representation where instead of only keeping track of the occupied orbitals, we look at the occupancy of each orbital. More precisely, we define

$$\Phi_{(\mu_1,\dots,\mu_L)} = c(\phi_{i_1})^\dagger \cdots c(\phi_{i_k})^\dagger |\Omega\rangle, \tag{1.1.18}$$

if $i_1 < \cdots < i_k$ and $(i_j)_{1\le j\le k}$ are precisely the indices such that $\mu_{i_j} = 1$. The wave function Ψ can then be written

$$\Psi = \sum_{\mu_1,\dots,\mu_L} \Psi_{\mu_1,\dots,\mu_L} \Phi_{(\mu_1,\dots,\mu_L)}. \tag{1.1.19}$$

In DMRG, the tensor $\Psi \in \mathbb{C}^{2^L}$ is expressed as a *matrix product state*, also called a *tensor train* in the mathematical community.

Chapter 2

The low-rank approximation problem for matrices and tensors

2.1 Singular value decomposition and generalisations for tensors

This chapter is devoted to the tensor train decomposition, as a generalisation of the singular value decomposition (SVD) for high-dimensional tensors. The SVD arises in the low-rank approximation of matrices, as such, it is natural to look for generalisation of the SVD for high-dimensional tensors. As it will be mentioned, the historical tensor formats, i.e. the CP decomposition and the Tucker decomposition suffer from drawbacks that the tensor train format does not have.

2.1.1 The low-rank approximation for matrices

The basis tool for the low-rank approximation of matrices is the singular value decomposition (SVD).

Theorem 2.1.1 (Singular value decomposition)**.** *Let $A \in \mathbb{C}^{m\times n}$ be a matrix. There exist unitary matrices $U \in \mathbb{C}^{m\times r_A}$ and $V \in \mathbb{C}^{n\times r_A}$, and a diagonal matrix $\Sigma = \mathrm{Diag}(s_1, \ldots, s_{r_A})$ with $s_1 \geq \cdots \geq s_{r_A} > 0$ such that $A = U\Sigma V^*$. The triplet of matrices (U, Σ, V^*) satisfying these properties is called a singular value decomposition (SVD) of A.*

The SVD given in the above theorem is sometimes called the *compact* SVD of A. Another common definition of the SVD is a decomposition of the matrix $A \in \mathbb{C}^{m\times n}$ is to write the SVD as $A = \mathcal{U}\mathcal{\Sigma}\mathcal{V}^*$ where $\mathcal{U} \in \mathbb{C}^{m\times m}$ and $\mathcal{V} \in \mathbb{C}^{n\times n}$ are unitary matrices and $\mathcal{\Sigma} \in \mathbb{C}^{m\times n}$ is diagonal. The relationship between this SVD and its compact version is the following

$$\mathcal{U} = \begin{bmatrix} U & 0 \end{bmatrix}, \quad \mathcal{\Sigma} = \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathcal{V} = \begin{bmatrix} V & 0 \end{bmatrix}.$$

The SVD of A can be derived from the eigenvalue decomposition of the matrices AA^* and AA^*. Indeed, if $A = \mathcal{U}\Sigma\mathcal{V}^*$ is the SVD of A, then $A^* = \mathcal{V}\Sigma\mathcal{U}^*$ so using that $\mathcal{U}$ and $\mathcal{V}$ are unitary matrices, we have

$$AA^* = \mathcal{U}\Sigma\Sigma^*\mathcal{U}^* = \mathcal{U}\begin{bmatrix} s_1^2 & & & & \\ & \ddots & & & \\ & & s_r^2 & & \\ & & & 0 & \\ & & & & \ddots \end{bmatrix}\mathcal{U}^*, \quad A^*A = \mathcal{V}\Sigma^*\Sigma\mathcal{V}^* = \mathcal{V}\begin{bmatrix} s_1^2 & & & & \\ & \ddots & & & \\ & & s_r^2 & & \\ & & & 0 & \\ & & & & \ddots \end{bmatrix}\mathcal{V}^*.$$

The singular values of A are simply the eigenvalues of the matrices AA^* and A^*A and the unitary matrices $\mathcal{U}$ and $\mathcal{V}$ the corresponding eigenvectors.

From the singular value decomposition -and its connection to the eigenvalue decomposition- it is possible to give another characterisation of the singular values:

$$s_k = \max_{\dim V_k = k} \min_{x \in V_k} \frac{\|Ax\|_2}{\|x\|_2}. \tag{2.1.1}$$

From the SVD, it is possible to directly read the rank of the matrix A. It is simply the number of nonzero singular values.

Another important property of the singular value decomposition for the low-rank approximation problem is the following.

Theorem 2.1.2 (Best rank r approximation of a matrix [Sch08])**.** *Let $A \in \mathbb{C}^{m\times n}$ be a matrix and (U, Σ, V^*) an SVD of A. The best rank-r of A in the Frobenius norm is given by*

$$A_r = U_r\Sigma_r V_r^* = \sum_{k=1}^{r} s_k u_k v_k^*,$$

where $U_r \in \mathbb{C}^{m\times r}$, $\Sigma_r \in \mathbb{R}^{r\times r}$ and $V_r \in \mathbb{C}^{n\times r}$ are the respective truncations of U, Σ and V. The error is given by

$$\|A - A_r\|_F = \Big(\sum_{k\geq r+1} s_k^2\Big)^{1/2}. \tag{2.1.2}$$

The best approximation is unique if $s_r > s_{r+1}$.

Proof. An upper bound is obtained by a direct computation

$$\|A - A_r\|_F^2 = \Big\|\sum_{j\geq r+1} s_j u_j v_j^*\Big\|_F^2 = \Big\|\sum_{j\geq r+1} s_j u_j \otimes v_j\Big\|_2^2 = \sum_{j\geq r+1} s_j^2.$$

The lower bound is shown using a bound on the singular values: let $M, N \in \mathbb{R}^{p\times q}$

$$\forall\, 1 \leq i, j \leq \min(p, q), 0 \leq j \leq d - i, s_{i+j-1}(M + N) \leq s_i(M) + s_j(N), \tag{2.1.3}$$

where $(s_k(M))_k, (s_k(N))_k, (s_k(M+N))_k$ are the respective singular values of M, N and $M+N$. This singular value bounds are derived by considering the following subspaces (without loss of generality, we can assume that $q \leq p$):

$$V^{M+N} = \mathrm{Span}\big(v_1^{M+N}, \dots, v_{i+j-1}^{M+N}\big), \quad V^M = \mathrm{Span}\big(v_i^M, \dots, v_q^M\big)$$
$$V^N = \mathrm{Span}\big(v_j^N, \dots, v_q^N\big).$$

By estimating the dimension of the intersection (by using that $\dim V^M + \dim V^N + \dim V^{M+N} = (q-i+1) + (q-j+1) + i + j - 1 = 2q+1$), we deduce that there exists a normalised vector $x \in V^M \cap V^N \cap V^{M+N}$:

$$s_{i+j-1}(M+N) \leq \|(M+N)x\|_2 \leq \|Mx\|_2 + \|Nx\|_2 \leq s_i(M) + s_j(N).$$

We apply the inequality (2.1.3) with $M = A - \widetilde{A_r}$, $N = \widetilde{A}_r$ and $j = r+1$, where $\widetilde{A}_r$ is a matrix of rank r. Since $s_{r+1}(\widetilde{A}_r) = 0$, we have

$$\forall\, 1 \leq i \leq q, s_{k+i}(A) \leq s_i(A - \widetilde{A_r}).$$

Hence $\|A - \widetilde{A_r}\|_F^2 = \sum_{i=1}^q s_i(A - \widetilde{A_r})^2 \geq \sum_{i=k+1}^q s_i(A)^2$, which is the result. □

Remark 2.1.3. *A similar approximation result can be written in the matrix norm $\|\cdot\|_2$ subordinate to the vector $\|\cdot\|_2$. In that case, it is straightforward to check that $\|A - A_r\|_2 = \big\|\sum_{j\geq r+1} s_j u_j v_j^*\big\|_2 = s_{r+1}$. Moreover for a rank-$r$ matrix $\widetilde{A}_r$, by definition, there is a normalised vector $x \in \mathrm{Span}(v_1, \dots, v_{r+1})$ such that $\widetilde{A}_r x = 0$. Thus*

$$\|A - \widetilde{A}_r\|_2 \geq \|(A - \widetilde{A}_r)x\|_2 \geq \|Ax\|_2 \geq s_{r+1}.$$

Another way to phrase the best rank r approximation of a matrix is to take the subspace point of view. A matrix $A \in \mathbb{C}^{m\times n}$ can be viewed as a vector of the product space $\mathbb{C}^m \otimes \mathbb{C}^n$ which is isometrically isomorphic to $\mathbb{C}^{mn}$. The subspace problem is phrased as follows: find subspaces $\mathcal{U} \subset \mathbb{C}^m$ and $\mathcal{V} \subset \mathbb{C}^n$ both of dimension r such that it minimises the distance

$$\mathrm{dist}(A, \mathcal{U}\otimes\mathcal{V}) = \|A - \Pi_{\mathcal{U}\otimes\mathcal{V}} A\| = \min_{\substack{\widetilde{\mathcal{U}}\subset\mathbb{C}^m, \dim\widetilde{\mathcal{U}}=r \\ \widetilde{\mathcal{V}}\subset\mathbb{C}^n, \dim\widetilde{\mathcal{V}}=r}} \|A - \Pi_{\widetilde{\mathcal{U}}\otimes\widetilde{\mathcal{V}}} A\|, \tag{2.1.4}$$

where $\Pi_{\mathcal{W}}$ is the orthogonal projection onto the subspace $\mathcal{W} \subset \mathbb{C}^{mn}$. The SVD of the matrix (A_i^j) is also a representation of the vector $(A_{ij})_{1\leq i\leq m, 1\leq j\leq n}$ in the orthonormal basis $(u_i \otimes v_j)_{1\leq i\leq m, 1\leq j\leq n}$:

$$A = \sum_{k=1}^{r_A} s_k u_k \otimes v_k. \tag{2.1.5}$$

Proposition 2.1.4. *Let $A \in \mathbb{C}^{m\times n}$, (U,Σ,V^*) its SVD and $r \in \mathbb{N}$. Denote $(u_1,\dots,u_{r_A})$ and $(v_1,\dots,v_{r_A})$ the respective columns of U and V. A solution to the subspace minimisation problem (2.1.4) is given by*

$$\mathcal{U} = \mathrm{Span}(u_1,\dots,u_r), \quad \mathcal{V} = \mathrm{Span}(v_1,\dots,v_r). \tag{2.1.6}$$

The solution is unique if $s_r > s_{r+1}$.

Proof. Let $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$ be respectively subspaces of $\mathbb{C}^m$ and $\mathbb{C}^n$ of dimension r. Let $(\widetilde{u}_i)_{1\le i\le r}$ and $(\widetilde{v}_i)_{1\le i\le r}$ be ONB of respectively $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$. The minimisation problem (2.1.4) can be rewritten as

$$\min_{\substack{\widetilde{\mathcal{U}}\subset\mathbb{C}^m,\dim\widetilde{\mathcal{U}}=r\\ \widetilde{\mathcal{V}}\subset\mathbb{C}^n,\dim\widetilde{\mathcal{V}}=r}} \|A-\Pi_{\widetilde{\mathcal{U}}\otimes\widetilde{\mathcal{V}}}A\| = \min_{\substack{\widetilde{\mathcal{U}}\subset\mathbb{C}^m,\dim\widetilde{\mathcal{U}}=r\\ \widetilde{\mathcal{V}}\subset\mathbb{C}^n,\dim\widetilde{\mathcal{V}}=r}} \|A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\|_F^2,$$

where $P_{\widetilde{\mathcal{U}}}$ (resp. $P_{\widetilde{\mathcal{V}}}$) is the orthogonal projection onto $\widetilde{\mathcal{U}}$ (resp. $\widetilde{\mathcal{V}}$).

Let $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$ be respectively subspaces of $\mathbb{C}^m$ and $\mathbb{C}^n$ of dimension r. Let $(\widetilde{u}_i)_{1\le i\le r}$ and $(\widetilde{v}_i)_{1\le i\le r}$ be ONB of respectively $\widetilde{\mathcal{U}}$ and $\widetilde{\mathcal{V}}$. Then we have

$$\begin{aligned}\|A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\|_F^2 &= \mathrm{Tr}\big((A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}})^*(A-P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}})\big)\\ &= \mathrm{Tr}\big(A^*A - P_{\widetilde{\mathcal{V}}}A^*P_{\widetilde{\mathcal{U}}}A - A^*P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}} + P_{\widetilde{\mathcal{V}}}A^*P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big)\\ &= \mathrm{Tr}(A^*A) - \mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^*P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big),\end{aligned}$$

where we have used that since $P_{\widetilde{\mathcal{V}}}$ is an orthogonal projection, we have $\mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^*P_{\widetilde{\mathcal{U}}}A\big) = \mathrm{Tr}\big(A^*P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big) = \mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^*P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big)$. We realise that

$$\mathrm{Tr}\big(P_{\widetilde{\mathcal{V}}}A^*P_{\widetilde{\mathcal{U}}}AP_{\widetilde{\mathcal{V}}}\big) = \sum_{1\le i,j\le r}\langle\widetilde{u}_i, A\widetilde{v}_j\rangle^2.$$

Solving the minimisation problem (2.1.4) is equivalent to maximising $\sum_{1\le i,j\le r}\big(\langle\widetilde{u}_i, A\widetilde{v}_j\rangle\big)^2$ where $(\widetilde{u}_i)_{1\le i\le r}$ and $(\widetilde{v}_i)_{1\le i\le r}$ are orthonormal families. Using the SVD of A, the previous quantity is maximised for $\widetilde{\mathcal{U}} = \mathrm{Span}(u_1,\dots,u_r)$ and $\widetilde{\mathcal{V}} = \mathrm{Span}(v_1,\dots,v_r)$. □

2.1.2 Tensors and reshapes

A tensor C of order $L \in \mathbb{N}$ is a multidimensional array $C_{i_1\dots i_L} \in \mathbb{C}^{n_1\times\cdots\times n_L}$.

A convenient way to represent tensor and product of tensors is the graphical representation. Let $C \in \mathbb{C}^{n_1\times\cdots\times n_L}$ be a tensor. The graphical representation of C is given by Figure 2.1. It is a powerful tool to avoid writing cumbersome operations between tensors, using the dictionary in Figure 2.2.

Definition 2.1.5 (Reshape of a tensor)**.** *Let $C \in \mathbb{C}^{n_1\times\cdots\times n_L}$ be a tensor. Let $(j_1,\dots,j_\ell,k_1,\dots,k_n)$ be a permutation of $\{1,\dots,L\}$. We say that the matrix $C^{i_{k_1}\dots i_{k_n}}_{i_{j_1}\dots i_{j_\ell}} \in \mathbb{R}^{n_{j_1}\cdots n_{j_\ell}\times n_{k_1}\cdots n_{k_n}}$ is a reshape of C.*

The reshapes $C^{i_{\ell+1}\dots i_L}_{i_1\dots i_\ell}$ will be of particular interest for tensor trains.

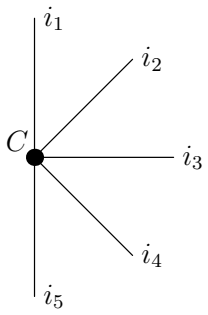
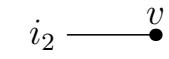
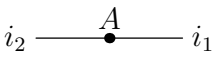


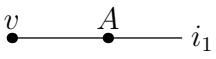
Figure 2.1: Graphical representation of C. The tensor C is represented by its vertex and its indices by the free edges.



(a) Vector v_{i_2}.



(b) Matrix $A^{i_2}_{i_1}$.



(c) Matrix-vector product $(Av)_{i_1} = \sum_{i_2} A^{i_2}_{i_1} v_{i_2}$.

Figure 2.2: Contraction of tensors. Every pair of connected edges is a summation over the shared index.

2.1.3 Generalisations of the SVD for tensors

For higher-order tensors, different schematic generalisations of the SVD are possible. With the previous discussion, there are two natural options that emerge:

- write the tensor as a sum of rank-1 tensors:

$$C = \sum_{k=1}^{r} u_k^{(1)} \otimes \cdots \otimes u_k^{(L)},$$

  where $u_k^{(j)} \in \mathbb{C}^{n_j}$. This is the *canonical polyadic decomposition* (CP decomposition);

- consider the subspace minimisation problem:

$$\operatorname{dist}(C, \mathcal{U}_1 \otimes \mathcal{U}_2 \otimes \cdots \otimes \mathcal{U}_L) = \min_{\widetilde{\mathcal{U}}_1 \subset \mathbb{C}^{n_1}, \dim \widetilde{\mathcal{U}}_1 = r_1, \ldots, \widetilde{\mathcal{U}}_L \subset \mathbb{C}^{n_L}, \dim \widetilde{\mathcal{U}}_L = r_L} \| C - \Pi_{\widetilde{\mathcal{U}}_1 \otimes \cdots \otimes \widetilde{\mathcal{U}}_L} C \|,$$

  where $\dim \mathcal{U}_k = r_k$ for all $1 \leq k \leq L$. This yields the Tucker decomposition.

The canonical decomposition looks the most appealing as it is the most sparse way to represent a tensor. It has however one major drawback, being that the best rank r approximation (in the sense of the CP decomposition) is *ill-posed!* [DSL08] Consider noncolinear vectors $a \in \mathbb{C}^n$, $b \in \mathbb{C}^n$ and the tensor

$$C = b \otimes a \otimes a + a \otimes b \otimes a + a \otimes a \otimes b.$$

which is a tensor of canonical rank 3. It can however be approximated as well as we wish by a tensor of canonical rank 2: let $\varepsilon > 0$, then we see that

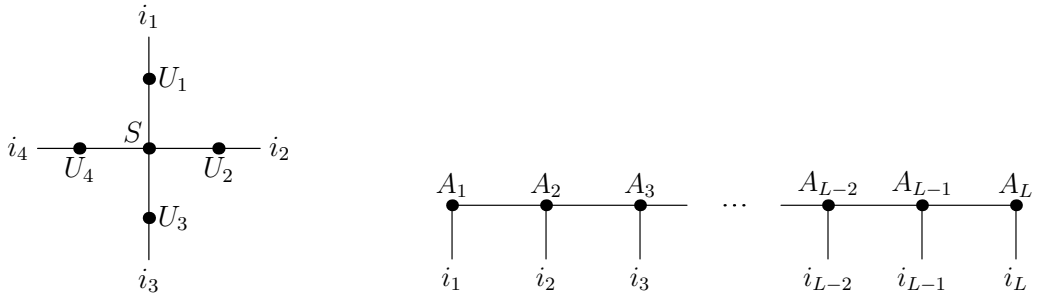
$$C - \Big(\frac{1}{\varepsilon}(a + \varepsilon b) \otimes (a + \varepsilon b) \otimes (a + \varepsilon b) - \frac{1}{\varepsilon} a \otimes a \otimes a\Big) = \mathcal{O}(\varepsilon). \tag{2.1.7}$$

Contrary to matrices, the set of tensors of canonical rank less than r is not closed.

Regarding the Tucker decomposition, let $C \in \mathcal{U}_1 \otimes \cdots \otimes \mathcal{U}_L$. Then there is a core tensor $S \in \mathbb{C}^{r_1 \times \cdots \times r_L}$ and matrices $(U_k)_{1 \leq k \leq L} \in \bigotimes_{k=1}^{L} \mathbb{C}^{n_k \times r_k}$ such that

$$\forall\, 1 \leq i_k \leq n_k,\ C_{i_1 \ldots i_L} = \sum_{j_1=1}^{r_1} \cdots \sum_{j_L=1}^{r_L} S_{j_1 \ldots j_L} (U_1)_{i_1}^{j_1} \cdots (U_L)_{i_L}^{j_L}.$$

The storage cost of the tensor C is still exponential in the order L of the tensor (except if some r_k are equal to 1). As such it is a useful decomposition only for low order tensors. In the following, we will focus on the efficient representation of tensors of order up to a hundred, for which the Tucker decomposition is not suited.



(a) Tucker decomposition (b) Tensor train decomposition

Figure 2.3: Tucker and tensor train decompositions

Remark 2.1.6. *In the context of quantum chemistry, the previous tensor decompositions have been tried in a disguise form in the context of electronic structure. The Tucker decomposition corresponds to the MC-SCF ansatz whereas the CP decomposition is behind the CI methods.*

2.2 Tensor train decomposition

2.2.1 Definition

The tensor train (TT) decomposition [OT09], also called *matrix product state* [KSZ91] in the physics litterature is the simplest instance of a tensor network. The TT decomposition

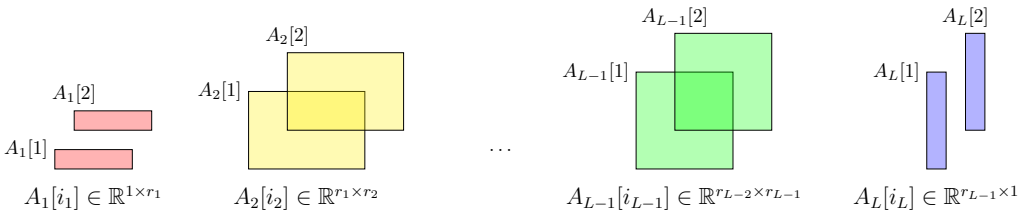


Figure 2.4: Schematic representation of the TT decomposition

is related to the density-matrix renormalisation group (DMRG) [Whi92] pioneered by White for the computation of properties of one-dimensional statistical physics systems. The connection between DMRG and TT has been realised later [OR95, DMNS98].

Definition 2.2.1 ([KSZ91, OT09]). *Let $C \in \mathbb{C}^{n_1\times\cdots\times n_L}$ be a tensor. We say that $(A_1, \ldots, A_L)$ is a tensor train decomposition of C if we have for all $1 \leq i_k \leq n_k$*

$$C_{i_1\ldots i_L} = A_1[i_1]A_2[i_2]\cdots A_L[i_L] \tag{2.2.1}$$

$$= \sum_{\alpha_1=1}^{r_1}\sum_{\alpha_2=1}^{r_2}\cdots\sum_{\alpha_{L-1}=1}^{r_{L-1}} A_1[i_1]_{\alpha_1}A_2[i_2]^{\alpha_1}_{\alpha_2}\cdots A_L[i_L]^{\alpha_{L-1}}, \tag{2.2.2}$$

where for each $1 \leq i_k \leq n_k$, $A_k[i_k] \in \mathbb{C}^{r_{k-1}\times r_k}$ ($r_0 = r_L = 1$). The tensor A_k are called the TT cores *and the sizes of the TT cores are the* TT ranks *of C.*

Such a representation has a storage cost of $\sum_{k=1}^{L} n_k r_{k-1} r_k$. Provided that the TT ranks do not increase exponentially with the order L of the tensor, the TT decomposition is a sparse representation of the tensor C. As it will be highlighted later, an exact TT representation of any tensor C can be derived using the hierarchical SVD. Generically, the TT ranks of the tensor will be exponential in L, however, good approximations for problems can be achieved for problems with some notion of sparsity [Has07, DDGS16].

Example 2.2.2.

- *a tensor product $C_{i_1\ldots i_L} = u^{(1)}_{i_1}\cdots u^{(L)}_{i_L}$ is a TT of TT rank 1, as the cores are $(u^{(k)}_{i_k})_{1\leq k\leq L, 1\leq i_k\leq n_k}$.*
- *the unnormalised Bell state $B \in \bigotimes_1^{2L}\mathbb{C}^2$*

$$B_{i_1\ldots i_{2L}} = \left(\delta_{1,i_1}\delta_{2,i_2} + \delta_{2,i_1}\delta_{1,i_2}\right)\left(\delta_{1,i_3}\delta_{2,i_4} + \delta_{2,i_3}\delta_{1,i_4}\right)\cdots \left(\delta_{1,i_{2L-1}}\delta_{2,i_{2L}} + \delta_{2,i_{2L-1}}\delta_{1,i_{2L}}\right),$$

is a TT of rank 2: let $(B_k)_{1\leq k\leq 2L}$ be defined by

$$B_{2k-1}[i_{2k-1}] = \begin{bmatrix}\delta_{1i_{2k-1}} & \delta_{2i_{2k-1}}\end{bmatrix}, \quad B_{2k}[i_{2k}] = \begin{bmatrix}\delta_{2i_{2k}} \\ \delta_{1i_{2k}}\end{bmatrix}, \quad k = 1, \ldots, L.$$

By a direct calculation, we can check that $B_{i_1\ldots i_{2L}} = B_1[i_1]\cdots B_{2L}[i_L]$.

- *for $L = 2$, the following reordering of the indices of the Bell state $\widetilde{B} \in \bigotimes_1^4 \mathbb{C}^2$*

$$\widetilde{B}_{i_1 \dots i_4} = \left(\delta_{1,i_1}\delta_{2,i_3} + \delta_{2,i_1}\delta_{1,i_3}\right)\left(\delta_{1,i_2}\delta_{2,i_4} + \delta_{2,i_3}\delta_{1,i_4}\right)$$

has a TT decomposition of rank 4:

i_k	$\widetilde{B}_1$	$\widetilde{B}_2$	$\widetilde{B}_3$	$\widetilde{B}_4$
1	$\begin{bmatrix}1 & 0\end{bmatrix}$	$\begin{bmatrix}0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\end{bmatrix}$	$\begin{bmatrix}0 & 0\\ 0 & 1\\ 0 & 0\\ 1 & 0\end{bmatrix}$	$\begin{bmatrix}1\\ 0\end{bmatrix}$
2	$\begin{bmatrix}0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\end{bmatrix}$	$\begin{bmatrix}1 & 0\\ 0 & 0\\ 0 & 1\\ 0 & 0\end{bmatrix}$	$\begin{bmatrix}0\\ 1\end{bmatrix}$

This elementary example highlights the importance of the ordering of the indices of the tensor for an efficient TT representation.

Remark 2.2.3. *The reordered Bell state example $\widetilde{B} \in \bigotimes_1^{2L} \mathbb{C}^2$*

$$\widetilde{B}_{i_1 \dots i_{2L}} = \prod_{k=1}^{L} \left(\delta_{1,i_k}\delta_{2,i_{k+L}} + \delta_{2,i_k}\delta_{1,i_{k+L}}\right)$$

has a TT decomposition of rank 2^L. The optimality of the ranks is proved by the characterisation of the TT ranks stated in Theorem 2.2.7.

It is clear that there is no uniqueness of the TT decomposition. Indeed for a tensor $C \in \mathbb{C}^{n_1 \times \cdots \times n_L}$ if $(A_1, \dots, A_L)$ is a tensor train decomposition, then for any invertible matrices $(G_k)_{1 \leq k \leq L-1} \in \bigotimes_{k=1}^{L-1} \mathrm{GL}_{r_k}(\mathbb{C})$, the TT cores $(\widetilde{A}_1, \dots, \widetilde{A}_L)$ defined by

$$\begin{cases} \widetilde{A}_1[i_1] = A_1[i_1]G_1, \ i_1 = 1, \dots, n_1, \quad \widetilde{A}_L[i_L] = G_{L-1}^{-1}A_L[i_L], \ i_L = 1, \dots, n_L \\ \widetilde{A}_k[i_k] = G_{k-1}^{-1}A_k[i_k]G_k, \ i_k = 1, \dots, n_k, \ k = 2, \dots, L-1, \end{cases}$$

is an equivalent TT representation.

As we are going to see later on, it is possible to partially lift this gauge freedom by imposing additional properties on the TT cores (A_k).

Proposition 2.2.4 (Algebraic properties of TT). *Let* $(A_1, \dots, A_L)$ *and* $(\widetilde{A}_1, \dots, \widetilde{A}_L)$ *be the respective TT decompositions of the tensors* $C, \widetilde{C} \in \mathbb{C}^{n_1 \times \cdots \times n_L}$. *Then*

$$\begin{aligned} B_1[i_1] &= \begin{pmatrix} A_1[i_1] & \widetilde{A}_1[i_1] \end{pmatrix}, \quad B_L[i_L] = \begin{bmatrix} A_L[i_L] \\ \widetilde{A}_L[i_L] \end{bmatrix} \\ B_k[i_k] &= \begin{bmatrix} A_k[i_k] & 0 \\ 0 & \widetilde{A}_k[i_k] \end{bmatrix}, k = 2, \dots, L-1 \end{aligned} \tag{2.2.3}$$

is a TT decomposition of the sum $C + \widetilde{C}$.

The proof consists in expanding the TT decomposition $(B_1, \dots, B_L)$. The TT decomposition (2.2.3) is in general not minimal and can be compressed as explained in Section 2.3.

Remark 2.2.5. *Since a tensor product* $u^{(1)} \otimes \cdots \otimes u^{(L)}$ *is a TT of rank 1, we deduce that a CP decomposition of rank* r *has at most a TT representation of rank* r. *The TT decomposition is a generalisation of the CP format, with advantageous algebraic and topologic properties.*

2.2.2 The hierarchical SVD

The hierarchical SVD (HSVD) is an algorithm [Vid03, OT09] to obtain a tensor train representation of any tensor. In the HSVD, we apply successive SVD to $C \in \mathbb{R}^{n_1 \times \cdots \times n_L}$:

$$\begin{aligned} C_{i_1 \dots i_L} &= (C_{i_1}^{i_2 \dots i_L}) && \text{(reshape of } C \text{ to } n_1 \times n_2 \cdots n_L) \\ &= (U_1)_{i_1}^{\alpha_1} (\Sigma_1 V_1)_{\alpha_1}^{i_2 \dots i_L} && \text{(SVD)} \\ &= (U_1)_{i_1}^{\alpha_1} (\Sigma_1 V_1)_{\alpha_1 i_2}^{i_3 \dots i_L} && \text{(reshape of } \Sigma_1 V_1) \\ &= (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} (\Sigma_2 V_2)_{\alpha_2}^{i_3 \dots i_L} && \text{(SVD of } \Sigma_1 V_1) \\ &= (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} (\Sigma_2 V_2)_{\alpha_2 i_3}^{i_4 \dots i_L} && \text{(reshape of } \Sigma_2 V_2), \end{aligned}$$

we repeat the process until we get

$$C_{i_1 \dots i_L} = (U_1)_{i_1}^{\alpha_1} (U_2)_{\alpha_1 i_2}^{\alpha_2} \cdots (U_{L-1})_{\alpha_{L-2} i_{L-1}}^{\alpha_{L-1}} (\Sigma_{L-1} V_{L-1})_{\alpha_{L-1}}^{i_L}.$$

The identification with the TT decomposition is clear, one simply needs to be careful with the switch in the role played by the virtual indices:

$$\begin{aligned} C_{i_1 \dots i_L} &= (U_1)_{i_1}^{\alpha_1} \quad (U_2)_{\alpha_1 i_2}^{\alpha_2} \quad \cdots \quad (U_{L-1})_{\alpha_{L-2} i_{L-1}}^{\alpha_{L-1}} (\Sigma_{L-1} V_{L-1})_{\alpha_{L-1}}^{i_L} \\ &= A_1[i_1]_{\alpha_1} \quad A_2[i_2]_{\alpha_2}^{\alpha_1} \quad \cdots \quad A_{L-1}[i_{L-1}]_{\alpha_{L-1}}^{\alpha_{L-2}} \quad A_L[i_L]^{\alpha_{L-1}}. \end{aligned}$$

There are a few immediate remarks:

(i). it is possible to start at the end, *i.e.* by first reshaping C into the matrix $C^{i_L}_{i_1\dots i_{L-1}} \in \mathbb{C}^{n_1\cdots n_{L-1}\times n_L}$, perform its SVD and carry on. Another TT representation is obtained this way;

(ii). from the HSVD algorithm, we guess that the singular values Σ_k are related to the singular values of the reshapes $C^{i_{k+1}\dots i_L}_{i_1\dots i_k} \in \mathbb{C}^{n_1\cdots n_k\times n_{k+1}\cdots n_L}$ and that they play a key role in the best approximation by a TT at fixed TT ranks. This is indeed the case and it will be treated in Section 2.3.

This algorithm is central in the theory of TT and more generally in the approximation theory by tensor networks. It is somewhat clear that such an algorithm extends to the decomposition into a tree tensor network. Indeed, in the HSVD algorithm, we simply partition $\{1,\dots,L\}$ into the sets $(\{1\},\{2,\dots,L\})$, then $(\{1\},\{2\},\{3,\dots,L\})$, and so on so forth. For trees, we choose different partition choices that does not have to reduce to a singleton right away. For tensor networks with loops, there is no equivalent of the HSVD for the construction of a tensor network directly from the tensor. This makes the analysis of such networks much more difficult.

2.2.3 Normalisation and gauge freedom

Definition 2.2.6. *We say that a TT decomposition $(A_1,\dots,A_L)$ is*

- left-orthogonal *if for all $1\le k\le L-1$ we have*

$$\sum_{i_k=1}^{n_k} A_k[i_k]^* A_k[i_k] = \mathrm{id}_{r_k}; \tag{2.2.4}$$

- right-orthogonal *if for all $2\le k\le L$ we have*

$$\sum_{i_k=1}^{n_k} A_k[i_k] A_k[i_k]^* = \mathrm{id}_{r_{k-1}}\,. \tag{2.2.5}$$

From the HSVD algorithm, we see that we obtain a left-orthogonal TT decomposition of the tensor C. By starting from the end, we would get a right-orthogonal TT representation of C.

Such a normalisation turns out to be convenient for the computation of the norm a tensor. Suppose that $(A_1,\dots,A_L)$ is a left-orthogonal TT decomposition. The norm of

the corresponding tensor C remarkably simplifies

$$\begin{aligned}
\|C\|_F^2 &= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} \big(A_1[i_1] \cdots A_L[i_L]\big)^2 \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} A_L[i_L]^* \cdots A_1[i_1]^* A_1[i_1] \cdots A_L[i_L] \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} A_L[i_L]^* \cdots A_1[i_1]^* A_1[i_1] \cdots A_L[i_L] \\
&= \sum_{i_2=1}^{n_2} \cdots \sum_{i_L=1}^{n_L} A_L[i_L]^* \cdots \Big(\sum_{i_1=1}^{n_1} A_1[i_1]^* A_1[i_1]\Big) \cdots A_L[i_L] \\
&= \sum_{i_2=1}^{n_2} \cdots \sum_{i_L=1}^{n_L} A_L[i_L]^* \cdots A_2[i_2]^* A_2[i_2] \cdots A_L[i_L],
\end{aligned}$$

where the left-orthogonality of A_1 has been used. Hence by iterating this argument, the norm of C is simply the norm of the last TT core A_L.

Another instance where the choice of the normalisation is crucial is in solving eigenvalue problems in DMRG (see Chapter 5).

It is also possible to mix both normalisations, in the sense that for some $2 \leq n \leq L-1$, we have

- the first $n-1$ TT cores are left-orthogonal: for $1 \leq k \leq n-1$

$$\sum_{i_k=1}^{n_k} A_k[i_k]^* A_k[i_k] = \mathrm{id}_{r_k};$$

- the last $L-n+1$ TT cores are right-orthogonal: for $n+1 \leq k \leq L$

$$\sum_{i_k=1}^{n_k} A_k[i_k] A_k[i_k]^* = \mathrm{id}_{r_{k-1}}\,. \tag{2.2.6}$$

In that case, the norm of the tensor is carried by the TT core that is not normalised,

using the following trick:

$$\begin{aligned}
\|C\|_F^2 &= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} A_L[i_L]^* \cdots A_1[i_1]^* A_1[i_1] \cdots A_L[i_L] \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} \operatorname{Tr}\left(A_L[i_L]^* \cdots A_1[i_1]^* A_1[i_1] \cdots A_L[i_L]\right) \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} \operatorname{Tr}\left(A_{k+1}[i_{k+1}] \cdots A_L[i_L] A_L[i_L]^* \cdots A_1[i_1]^* A_1[i_1] \cdots A_k[i_k]\right) \\
&= \sum_{i_k=1}^{n_k} \operatorname{Tr}\left(A_k[i_k]^* A_k[i_k]\right).
\end{aligned}$$

Conversion between left and right orthogonal TT representations

By successive LQ decompositions, it is possible to transform a left-orthogonal to a right orthogonal TT decomposition. Let $(A_1, \ldots, A_L)$ be a left-orthogonal TT decomposition of $C \in \mathbb{C}^{n_1 \times \cdots \times n_L}$. Then we have

$$\begin{aligned}
C_{i_1 \ldots i_L} &= A_1[i_1] \cdots A_L[i_L] \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{L-1}[i_{L-1}]^{\alpha_{L-1}}_{\alpha_{L-2}} \left(A_L\right)^{i_L}_{\alpha_{L-1}} \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{L-1}[i_{L-1}]^{\alpha_{L-1}}_{\alpha_{L-2}} \left(L_L\right)^{\beta_{L-1}}_{\alpha_{L-1}} \left(Q_L\right)^{i_L}_{\beta_{L-1}} \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{L-2}[i_{L-2}]^{\alpha_{L-2}}_{\alpha_{L-3}} \left(A_{L-1} L_L\right)^{i_{L-1}\beta_{L-1}}_{\alpha_{L-2}} \left(Q_L\right)^{i_L}_{\beta_{L-1}} \\
&= A_1[i_1]^{\alpha_1} A_2[i_2]^{\alpha_2}_{\alpha_1} \cdots A_{L-2}[i_{L-2}]^{\alpha_{L-2}}_{\alpha_{L-3}} \left(L_{L-1}\right)^{\beta_{L-2}}_{\alpha_{L-2}} \left(Q_{L-1}\right)^{i_{L-1}\beta_{L-1}}_{\beta_{L-2}} \left(Q_L\right)^{i_L}_{\beta_{L-1}},
\end{aligned}$$

we repeat this process until we reach

$$\begin{aligned}
C_{i_1 \ldots i_L} &= \left(A_1 L_2\right)^{i_1 \beta_1} \quad \left(Q_2\right)^{i_2 \beta_2}_{\beta_1} \quad \cdots \quad \left(Q_{L-1}\right)^{i_{L-1}\beta_{L-1}}_{\beta_{L-2}} \quad \left(Q_L\right)^{i_L}_{\beta_{L-1}} \\
&= \quad B_1[i_1]_{\beta_1} \quad B_2[i_2]^{\beta_1}_{\beta_2} \quad \cdots \quad B_{L-1}[i_{L-1}]^{\beta_{L-2}}_{\beta_{L-1}} \quad B_L[i_L]^{\beta_{L-1}}.
\end{aligned}$$

We simply need to check that the TT cores $B_2, \ldots, B_L$ are right-orthogonal:

$$\sum_{i_k=1}^{n_k} B_k[i_k] B_k[i_k]^* = \mathrm{id}_{r_{k-1}}.$$

Theorem 2.2.7 (Characterisation of the TT ranks [HRS12b])**.** *Let $C \in \mathbb{C}^{n_1 \times \cdots \times n_L}$ be a tensor. Then the following assertions are true:*

(i). the HSVD algorithm given in Section 2.2.2 gives a TT decomposition of minimal TT rank;

(ii). the minimal TT rank $(r_1, \dots, r_{L-1})$ *is equal to the rank of the reshapes of* C, i.e.

$$r_k = \operatorname{Rank} C^{i_{k+1}\dots i_L}_{i_1\dots i_k}. \tag{2.2.7}$$

Proof. Let $(A_1, \dots, A_L)$ be the TT cores given by the HSVD algorithm. The proof of item (ii) follows from the following identity

$$C^{i_{k+1}\dots i_L}_{i_1\dots i_k} = \big(A_1[i_1]A_2[i_2]\cdots A_k[i_k]\big)\big(A_{k+1}[i_{k+1}] \ \cdots \ A_L[i_L]\big),$$

where $\big(A_1[i_1]A_2[i_2]\cdots A_k[i_k]\big) \in \mathbb{C}^{n_1\cdots n_k \times r_k}$ and $\big(A_{k+1}[i_{k+1}] \ \cdots \ A_L[i_L]\big) \in \mathbb{C}^{r_k \times n_{k+1}\cdots n_L}$. By construction and by the property of the SVD, both matrices are full rank, hence $r_k = \operatorname{Rank} C^{i_{k+1}\dots i_L}_{i_1\dots i_k}$. □

These normalisations have the advantage of reducing the gauge freedom in the TT representation.

Proposition 2.2.8 (Gauge freedom of left-orthogonal TT decompositions [HRS12b])**.** *A left-orthogonal TT representation of minimal TT rank* $(r_1, \dots, r_{L-1})$ *is unique up to the insertion of unitary matrices,* i.e. *if* $(A_1, \dots, A_L)$ *and* $(B_1, \dots, B_L)$ *are left-orthogonal TT representations of the same tensor* C*, then there are unitary matrices* $(Q_k)_{1\le k\le L-1}$*,* $Q_k \in \mathbb{C}^{r_k \times r_k}$ *such that for all* $1 \le i_k \le n_k$ *we have*

$$\begin{aligned} A_1[i_1]Q_1 = B_1[i_1], \quad Q^*_{L-1}A_L[i_L] = B_L[i_L] \\ Q^*_{k-1}A_k[i_k]Q_k = B_k[i_k], \ \text{for } k = 2, \dots, L-1. \end{aligned} \tag{2.2.8}$$

Proof. The proof relies on the following observation: let $M_1, N_1 \in \mathbb{C}^{p\times r}$ and $M_2, N_2 \in \mathbb{C}^{r\times q}$ be matrices of rank r such that

$$M_1M_2 = N_1N_2 \quad \text{and} \quad M_1^*M_1 = N_1^*N_1 = \mathrm{id}_r,$$

there is a unitary matrix $Q \in \mathbb{C}^{r\times r}$ such that

$$M_1 = N_1Q \quad \text{and} \quad M_2 = Q^*N_2.$$

The proof of this lemma is straightforward:

$$N_2 = N_1^*M_1M_2 = N_1^*M_1M_1^*N_1N_2,$$

which shows that $N_1^*M_1$ is a unitary matrix. Denote this matrix Q. Hence $N_2 = QM_2$ and $M_1N_1^*N_1 = M_1$ thus, $N_1 = M_1Q^*$.

The proof then goes by iteration. We have

$$\begin{aligned} \big(A_1[i_1]\big)\big(A_2[i_2]\cdots A_L[i_L]\big) &= \big(B_1[i_1]\big)\big(B_2[i_2]\cdots B_L[i_L]\big) \\ \sum_{i_1=1}^{n_1} A_1[i_1]^*A_1[i_1] &= \sum_{i_1=1}^{n_1} B_1[i_1]^*B_1[i_1] = \mathrm{id}_{r_1}. \end{aligned}$$

Since $\big(A_1[i_1]\big), \big(A_2[i_2]\cdots A_L[i_L]\big), \big(B_1[i_1]\big)$ and $\big(B_2[i_2]\cdots B_L[i_L]\big)$ have rank r_1, by the lemma there is a unitary matrix $Q_1 \in \mathbb{C}^{r_1\times r_1}$ such that

$$\begin{aligned} A_1[i_1]Q_1 &= B_1[i_1] \\ Q_1^*\big(A_2[i_2]\cdots A_L[i_L]\big) &= \big(B_2[i_2]\cdots B_L[i_L]\big). \end{aligned}$$

For the next iteration, we have

$$\begin{aligned} \big(Q_1^*A_2[i_2]\big)\big(A_3[i_3]\cdots A_L[i_L]\big) &= \big(B_2[i_2]\big)\big(B_3[i_3]\cdots B_L[i_L]\big) \\ \sum_{i_2=1}^{n_2} A_2[i_2]^*Q_1Q_1^*A_2[i_2] &= \sum_{i_2=1}^{n_2} B_2[i_2]^*B_2[i_2] = \mathrm{id}_{r_1}. \end{aligned}$$

Applying again the lemma, we have

$$\begin{aligned} Q_1^*A_2[i_2]Q_2 &= B_2[i_2] \\ Q_2^*\big(A_3[i_3]\cdots A_L[i_L]\big) &= \big(B_3[i_3]\cdots B_L[i_L]\big). \end{aligned}$$

By iteration, we prove the proposition. □

The Vidal representation

A convenient - albeit numerically unstable - way to convert easily between left-orthogonal and right-orthogonal TT representations is to use the Vidal representation [Vid03].

Definition 2.2.9 (Vidal representation [Vid03])**.** *Let $C \in \mathbb{C}^{n_1\times\cdots\times n_L}$ be a tensor. We say that $(\Gamma_k)_{1\le k\le L}$, $(\Sigma_k)_{1\le k\le L-1}$ is a Vidal representation if Σ_k are diagonal matrices with positive entries,*

$$C_{i_1,\ldots,i_L} = \Gamma_1[i_1]\Sigma_1\Gamma_2[i_2]\Sigma_2\cdots\Sigma_{L-1}\Gamma_L[i_L], \tag{2.2.9}$$

and the matrices $\Gamma_k[i_k] \in \mathbb{C}^{r_{k-1}\times r_k}$ satisfy

$$\sum_{i_1=1}^{n_1}\Gamma_1[i_1]^*\Gamma_1[i_1] = \mathrm{id}_{r_1}, \quad \sum_{i_L=1}^{n_L}\Gamma_L[i_L]\Gamma_L[i_L]^* = \mathrm{id}_{r_{L-1}} \tag{2.2.10}$$

$$\forall\, k=2,\ldots,L-1,\ \sum_{i_k=1}^{n_k}\Gamma_k[i_k]^*\Sigma_{k-1}^2\Gamma_k[i_k] = \mathrm{id}_{r_k}, \quad \sum_{i_k=1}^{n_k}\Gamma_k[i_k]\Sigma_k^2\Gamma_k[i_k]^* = \mathrm{id}_{r_{k-1}}. \tag{2.2.11}$$

The Vidal representation directly gives left and right orthogonal TT decompositions:

(i). $(A_1,\ldots,A_L)$ left-orthogonal TT representation

$$\begin{aligned} A_1[i_1] &= \Gamma_1[i_1], \quad A_L[i_L] = \Sigma_{L-1}\Gamma_L[i_L] \\ A_k[i_k] &= \Sigma_{k-1}\Gamma_k[i_k], \quad k=2,\ldots,L-1; \end{aligned}$$

(ii). $(B_1, \dots, B_L)$ right-orthogonal TT representation

$$\begin{aligned} B_1[i_1] &= \Gamma_1[i_1]\Sigma_1, \quad & B_L[i_L] &= \Gamma_L[i_L] \\ B_k[i_k] &= \Gamma_k[i_k]\Sigma_k, \quad & k &= 2, \dots, L-1. \end{aligned}$$

The conversion from left (or right) orthogonal decomposition to a Vidal representation is more involved [Sch11, Section 4.6]. Let A_k be the TT components of a left-orthogonal TT representation. Notice that for all k, let Σ_k be the singular values of the tensor reshape $C^{i_{k+1}\dots i_d}_{i_1\dots i_k}$. Then we have

$$C^{i_{k+1}\dots i_L}_{i_1\dots i_k} = \underbrace{\begin{bmatrix} A_1[1]A_2[1]\cdots A_k[1] \\ \vdots \\ A_1[n_1]A_2[n_2]\cdots A_k[n_k] \end{bmatrix}}_{=:M_k \in \mathbb{R}^{n_1\cdots n_k \times r_k}} \underbrace{\begin{bmatrix} A_{k+1}[i_{k+1}] & \cdots & A_L[i_L] \end{bmatrix}}_{\in \mathbb{R}^{r_k \times n_{k+1}\cdots n_L}}$$

Because A_k are left-orthogonal, then $M_k^* M_k = \mathrm{id}_{r_k}$, hence the singular values of the reshaped tensor is exactly the singular values of the right matrix.

With this remark, we can now write the iterative algorithm to get the Vidal representation of the tensor.

Algorithm 1 Left-orthogonal to Vidal representation

Input: $(A_1, \dots, A_L)$ left-orthogonal TT representation
Output: $(\Gamma_1, \dots, \Gamma_L), (\Sigma_1, \dots, \Sigma_{L-1})$ Vidal representation

function LeftToVidal($(A_1, ..., A_L)$)
  $U_{L-1}, \Sigma_{L-1}, V_L^* = \texttt{svd}\big(\begin{bmatrix} A_L[1] & A_L[2] & \cdots & A_L[n_L] \end{bmatrix} \big)$
  $\begin{bmatrix} \Gamma_L[1] & \cdots & \Gamma_L[n_L] \end{bmatrix} = V_L^*$
  for $k = L-1, \dots, 1$ **do**
    $U_{k-1}, \Sigma_{k-1}, V_k^* = \texttt{svd}\big(\begin{bmatrix} A_k[1]U_k\Sigma_k & \cdots & A_k[n_k]U_k\Sigma_k \end{bmatrix} \big)$.
    Γ_k solution to $V_k^* = \begin{bmatrix} \Gamma_k[1]\Sigma_k & \cdots & \Gamma_k[n_k]\Sigma_k \end{bmatrix}$
  end for
  return $(\Gamma_1, \dots, \Gamma_L), (\Sigma_1, \dots, \Sigma_{L-1})$.
end function

By induction, one can show that the singular values of the successive SVD in the previous algorithm are indeed the singular values of the tensor reshape.

Proposition 2.2.10. *Let $(\Gamma_k)_{1\le k\le L}$, $(\Sigma_k)_{1\le k\le L-1}$ be a Vidal representation of $C \in \mathbb{C}^{n_1\times\cdots\times n_L}$. Then Σ_k is the matrix of the singular values of the reshape $C^{i_{k+1}\dots i_L}_{i_1\dots i_k} \in \mathbb{C}^{n_1\cdots n_k \times n_{k+1}\cdots n_L}$.*

Proof. By definition of the SVD, the Vidal TT components Γ_k satisfy

$$\sum_{i_k=1}^{n_k} \Gamma_k[i_k]\Sigma_k^2\Gamma_k[i_k]^* = \mathrm{id}_{r_{k-1}}\,.$$

We also have

$$\begin{bmatrix} A_k[1]U_k & \cdots A_k[n_k]U_k \end{bmatrix} = \begin{bmatrix} U_{k-1}\Sigma_{k-1}\Gamma_k[1] & \cdots & U_{k-1}\Sigma_{k-1}\Gamma_k[n_k] \end{bmatrix}.$$

Thus

$$\begin{aligned}\sum_{i_k}^{n_k} \Gamma_k[i_k]^*\Sigma_{k-1}^2\Gamma_k[i_k] &= \sum_{i_k}^{n_k} \Gamma_k[i_k]^*\Sigma_{k-1}U_{k-1}^*U_{k-1}\Sigma_{k-1}\Gamma_k[i_k] \\ &= \sum_{i_k}^{n_k} U_k^*A_k[i_k]^*A_k[i_k]U_k \\ &= \mathrm{id}_{r_k}\,.\end{aligned}$$

□

2.3 Approximation by tensor trains

A natural way to reduce the TT ranks of the TT representation of a tensor is to truncate the SVD at each step of the HSVD algorithm to a tolerance ε:

$$\begin{aligned} C_{i_1\dots i_L} = \; & C_{i_1}^{i_2\dots i_L} && \text{(reshape of } C \text{ to } n_1 \times n_2\cdots n_L) \\ \simeq \; & \big(U_1\big)_{i_1}^{\alpha_1}\big(\Sigma_1^\varepsilon V_1^*\big)_{\alpha_1}^{i_2\dots i_L} && \text{(truncated SVD)} \\ \simeq \; & \big(U_1\big)_{i_1}^{\alpha_1}\big(\Sigma_1^\varepsilon V_1^*\big)_{\alpha_1 i_2}^{i_3\dots i_L} && \text{(reshape of } \Sigma_1^\varepsilon V_1^*) \\ \simeq \; & \big(U_1\big)_{i_1}^{\alpha_1}\big(U_2\big)_{\alpha_1 i_2}^{\alpha_2}\big(\Sigma_2^\varepsilon V_2^*\big)_{\alpha_2}^{i_3\dots i_L} && \text{(truncated SVD of } \Sigma_1^\varepsilon V_1^*) \\ \simeq \; & \big(U_1\big)_{i_1}^{\alpha_1}\big(U_2\big)_{\alpha_1 i_2}^{\alpha_2}\big(\Sigma_2^\varepsilon V_2^*\big)_{\alpha_2 i_3}^{i_4\dots i_L} && \text{(reshape of } \Sigma_2^\varepsilon V_2^*), \end{aligned}$$

we repeat the process until we get

$$C_{i_1\dots i_L} \simeq \big(U_1\big)_{i_1}^{\alpha_1}\big(U_2\big)_{\alpha_1 i_2}^{\alpha_2}\cdots\big(U_{L-1}\big)_{\alpha_{L-2} i_{L-1}}^{\alpha_{L-1}}\big(\Sigma_{L-1}^\varepsilon V_{L-1}\big)_{\alpha_{L-1}}^{i_L}.$$

This algorithm is often called a *TT rounding* [Ose11] or *TT compression*. Truncating the successive SVDs gives an estimate on the best approximation by a tensor train of fixed TT ranks.

Theorem 2.3.1 ([Gra10, Ose11, Hac12, Hac14]). *Let $C \in \mathbb{C}^{n_1 \times \cdots \times n_L}$, $(\tilde{r}_1, \ldots, \tilde{r}_{L-1}) \in \mathbb{N}^{L-1}$ and $\mathcal{M}_{\tilde{\mathbf{r}}}$ be the space of tensor trains of ranks bounded by $(\tilde{r}_1, \ldots, \tilde{r}_{L-1})$. Then we have*

$$\min_{V \in \mathcal{M}_{\tilde{\mathbf{r}}}} \|C - V\| \leq \sqrt{\sum_{k=1}^{L-1} \sum_{j > \tilde{r}_k} {\sigma_j^{(k)}}^2} \leq \sqrt{L-1} \min_{V \in \mathcal{M}_{\tilde{\mathbf{r}}}} \|C - V\|,$$

where for $1 \leq k \leq L-1$, $(\sigma_j^{(k)})_{1 \leq j \leq r_k}$ are the singular values of the reshape $(\Psi^{\mu_1 \cdots \mu_k}_{\mu_{k+1} \cdots \mu_L})$.

Proof. The proof of the left-hand side inequality follows from the HSVD algorithm. Let $\Pi_k : \mathbb{C}^{n_1 \cdots n_k \times n_{k+1} \cdots n_L} \to \mathbb{C}^{n_1 \cdots n_k \times n_{k+1} \cdots n_L}$ be the SVD truncation of rank $\tilde{r}_k$. This operator is an orthogonal projection in the Hilbert space $\mathbb{C}^{n_1 \cdots n_k \times n_{k+1} \cdots n_L}$ equipped with the Frobenius norm. The HSVD algorithm with truncation at each step is the tensor $\Pi_{L-1} \cdots \Pi_1 C$. We thus have using the property of the SVD truncation:

$$\begin{aligned} \|C - \Pi_{L-1} \cdots \Pi_1 C\|_F^2 &\leq \|\Pi_{L-1}^{\perp} C\|^2 + \|\Pi_{L-1} C - \Pi_{L-1} \cdots \Pi_1 C\|_F^2 \\ &\leq \sum_{j > \tilde{r}_k} {\sigma_j^{(k)}}^2 + \|C - \Pi_{L-2} \cdots \Pi_1 C\|_F^2, \end{aligned}$$

hence by iteration

$$\|C - \Pi_{L-1} \cdots \Pi_1 C\|_F^2 \leq \sum_{k=1}^{L-1} \sum_{j > \tilde{r}_k} {\sigma_j^{(k)}}^2.$$

This provides a bound on the best approximation by a tensor train in $\mathcal{M}_{\tilde{\mathbf{r}}}$.

For the lower bound on the best approximation C_{best}, we have for each k by definition of the SVD truncation

$$\|C - \Pi_k C\|_F^2 = \sum_{j > \tilde{r}_k} {\sigma_j^{(k)}}^2 \leq \|C - C_{\text{best}}\|_F^2,$$

hence by summing over k we get the lower bound. □

A drawback of the HSVD algorithm or its truncated version is that it requires to handle the full tensor. If the tensor is already in a TT format, it is possible to reduce the cost of this truncation. Let $(A_1, \ldots, A_L)$ be a right-orthogonal TT representation of the tensor $C \in \mathbb{C}^{n_1 \times \cdots \times n_L}$. The first reshape is

$$C_{i_1}^{i_2 \ldots i_L} = \begin{bmatrix} A_1[1] \\ \vdots \\ A_1[n_1] \end{bmatrix} \begin{bmatrix} A_2[1] \cdots A_L[1] & \cdots & A_2[n_2] \cdots A_L[n_L] \end{bmatrix},$$

and since the TT cores $(A_2, \ldots, A_L)$ are right-orthogonal, the matrix $V_2 = \begin{bmatrix} A_2[1] \cdots A_L[1] & \cdots & A_2[n_2] \cdots A_L[n_k] \end{bmatrix}$ satisfies $V_2 V_2^* = \mathrm{id}_{r_1}$. Hence the first step

of the HSVD truncation can be reduced to the SVD of the reshape of A_1. The same would hold for the next step of the HSVD truncation, hence the total cost of the TT compression of C in a TT format is reduced to $\mathcal{O}(Lr^3)$ where $r = \max(r_k)$.

The algorithm is summarised in Algorithm 2.

Algorithm 2 TT rounding algorithm

Input: $(A_1, \dots, A_L)$ right-orthogonal TT representation, $\varepsilon > 0$ tolerance
Output: $(A_1^\varepsilon, \dots, A_L^\varepsilon)$ TT representation such that $\|\mathrm{TT}(A_i^\varepsilon) - \mathrm{TT}(A_i)\|_F \leq \sqrt{L-1}\,\varepsilon$

function HSVD($(A_1, \dots, A_L), \varepsilon$)
  for $k = 1, \dots, L-1$ **do**
    $U_k, \Sigma_k, V_k^* = \mathtt{svd}\Big(\begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}\Big)$
    $r_k = \arg\max_r \|\Sigma_k[1:r] - \Sigma_k\| \leq \varepsilon$
    $(A_k^\varepsilon)^{\alpha_k}_{i_k \alpha_{k-1}} = (U_k)^{\alpha_k}_{i_k \alpha_{k-1}}, \quad i_k = 1, \dots, n_k, \alpha_{k-1} = 1, \dots, r_{k-1}, \alpha_k = 1, \dots, r_k$
    $A_{k+1}[i_{k+1}] = \Sigma_k[1:r] V_k^*[1:r, :] A_{k+1}[i_{k+1}], \quad i_{k+1} = 1, \dots, n_{k+1}$
  end for
  $A_L^\varepsilon = A_L$
  return $(A_1^\varepsilon, \dots, A_L^\varepsilon)$
end function

2.4 Manifold of tensor trains

Even in finite-dimensions, the example exhibited in eq. (2.1.7) shows that the set

$$\mathcal{M}_{\mathrm{CP}_{\leq r}} = \Big\{ C = \sum_{i=1}^{r} v_1^{(i)} \otimes \cdots \otimes v_L^{(i)}, \forall\, 1 \leq i \leq r, 1 \leq j \leq L, v_j^{(i)} \in \mathbb{C}^{n_j} \Big\},$$

is not closed if $L \geq 3$.

For tensor trains, the question of the closedness has a clear answer, as the characterisation of the TT rank relies on the matricisation of the tensor.

Proposition 2.4.1. *The set of tensor trains with TT rank less that r*

$$\mathcal{M}_{\mathrm{TT}_{\leq r}} = \Big\{ C \mid \forall\, 1 \leq i_k \leq n_k,\ C_{i_1 \dots i_L} = A_1[i_1] \cdots A_L[i_L],\ A_k[i_k] \in \mathbb{C}^{r_{k-1} \times r_k}, r_k \leq r \Big\},$$

is a closed set.

Proof. The proof follows from the characterisation of the TT ranks given by Theorem 2.2.7: given a tensor C, for $1 \leq k \leq L-1$, the minimal TT rank r_k is equal to the rank of the matrix $C^{i_{k+1}\dots i_L}_{i_1\dots i_k}$. We conclude by recalling that the set of matrices with rank less than r is a closed set. □

Proposition 2.4.2. *The set of tensor trains with TT rank* $\mathbf{r} = (r_1, \dots, r_{L-1})$

$$\mathcal{M}_{\mathrm{TT}_\mathbf{r}} = \left\{C \mid \forall\, 1 \leq i_k \leq n_k,\ C_{i_1\dots i_L} = A_1[i_1]\cdots A_L[i_L],\ A_k[i_k] \in \mathbb{C}^{r_{k-1}\times r_k}\right\},$$

is of dimension

$$\dim \mathcal{M}_{\mathrm{TT}_\mathbf{r}} = \sum_{i=1}^{L} r_{i-1} n_i r_i - \sum_{i=1}^{L-1} r_i^2. \tag{2.4.1}$$

Proof. Two TT representations $(A_1, \dots, A_L)$ and $(\tilde{A}_1, \dots, \tilde{A}_L)$ of a same tensor are related by a gauge $(G_1, \dots, G_{L-1}) \in \mathrm{GL}_{r_1}(\mathbb{C}) \times \cdots \mathrm{GL}_{r_{L-1}}(\mathbb{C})$

$$\forall\, 1 \leq i_k \leq n_k, A_k[i_k] = G_{k-1}\tilde{A}_k[i_k]G_k, \quad k = 1, \dots, L, \quad (G_0 = G_L = 1).$$

The dimension of $\mathrm{GL}_{r_k}(\mathbb{C})$ is r_k^2, hence the dimension of $\mathcal{M}_{\mathrm{TT}_\mathbf{r}}$ is

$$\dim \mathcal{M}_{\mathrm{TT}_\mathbf{r}} = \sum_{i=1}^{L} r_{i-1} n_i r_i - \sum_{i=1}^{L-1} r_i^2.$$

□

Proposition 2.4.3 (Tangent space of $\mathcal{M}_{\mathrm{TT}_\mathbf{r}}$ [HRS12b])**.** *Let* $A \in \mathcal{M}_{\mathrm{TT}_\mathbf{r}}$ *and* $(A_1, \dots, A_L)$ *be a left-orthogonal TT representation of* A*. Let* $\delta A \in \mathcal{T}_A\mathcal{M}_{\mathrm{TT}_\mathbf{r}}$*.*

There are unique components $(W_k)_{1\leq k\leq L} \in \bigotimes_{k=1}^{L} \mathbb{C}^{r_{k-1}\times n_k\times r_k}$ *such that*

$$\delta A = \sum_{k=1}^{L} \delta A^{(k)}, \tag{2.4.2}$$

with

$$\delta A^{(k)}_{i_1\dots i_L} = A_1[i_1]\cdots A_{k-1}[i_{k-1}]W_k[i_k]A_{k+1}[i_{k+1}]\cdots A_L[i_L], \tag{2.4.3}$$

and where for $k = 1, \dots, L-1$ *we have*

$$\sum_{i_k=1}^{n_k} A_k[i_k]^* W_k[i_k] = \mathbf{0}_{r_k\times r_k}. \tag{2.4.4}$$

Proof. By definition of the tangent space $\mathcal{T}_A\mathcal{M}_{\mathrm{TT}_\mathbf{r}}$, the tangent vectors are given by the derivatives $\dot{\Gamma}$ of the differentiable curves $\Gamma : \mathbb{R} \to \mathscr{M}_{\mathrm{TT}_\mathbf{r}}$ such that $\Gamma(0) = A$.

For all $t \in \mathbb{R}$, since $\Gamma(t) \in \mathcal{M}_{\mathrm{TT_r}}$, we can choose a left-orthogonal TT representation of $\Gamma(t)$ such that

$$\Gamma(t)_{i_1 \ldots i_L} = \Gamma_1^{(t)}[i_1] \cdots \Gamma_L^{(t)}[i_L],$$

where for all $1 \leq k \leq L$, $t \mapsto \Gamma_k^{(t)} \in \mathbb{C}^{n_k \times r_{k-1} \times r_k}$ is differentiable and $\Gamma_k^{(0)} = A_k$.

Since for $1 \leq k \leq L-1$, $\sum_{i_k=1}^{n_k} \Gamma_k^{(t)}[i_k]^* \Gamma_k^{(t)}[i_k] = \mathrm{id}_{r_k}$, there is a differentiable function $t \mapsto U_k(t) \in \mathcal{O}_{n_k r_{k-1}}(\mathbb{C})$ such that

$$\begin{bmatrix} \Gamma_k^{(t)}[1] \\ \vdots \\ \Gamma_k^{(t)}[n_k] \end{bmatrix} = U_k(t) \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}.$$

This implies that $\begin{bmatrix} \dot{\Gamma}_k^{(0)}[1] \\ \vdots \\ \dot{\Gamma}_k^{(0)}[n_k] \end{bmatrix} = S_k \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}$ for some antisymmetric matrix $S_k \in \mathbb{C}^{n_k r_{k-1} \times n_k r_{k-1}}$.

Let

$$\begin{bmatrix} W_k[1] \\ \vdots \\ W_k[n_k] \end{bmatrix} = S_k \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix}.$$

Then

$$\sum_{i_k=1}^{n_k} A_k[i_k]^* W_k[i_k] = \begin{bmatrix} A_k[1]^* & \ldots & A_k[n_k]^* \end{bmatrix} S_k \begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix},$$

which is a symmetric and an antisymmetric matrix, hence it is zero.

The tangent vectors are hence necessarily of the form given by eq. (2.4.2)-(2.4.4). Dimension counting and invoking Proposition 2.4.2 show the uniqueness of the representation. □

Chapter 3

Reduced density matrix, block entropy and tensor trains

3.1 Reduced density matrix and the quantum entropy

The main idea of the Fiedler order is to minimise a proxy of the decay of the singular values, which is the block entropy. There are several possible choices of the entropy that can be minimised. In the litterature, the two main choices have been the von Neumann entropy and the Rényi entropy. We will first shortly review both concepts of entropy. A good reference on this topic is Carlen's notes [CL14] and for other discussions on matrix identities and inequalities, refer to Tropp's book [T+15].

3.1.1 Reduced density matrix

For a given normalised tensor $\Psi \in \mathbb{C}^{2^L \times 2^L}$, we define the *$k$-orbital reduced density matrix* (k-RDM) $\rho_{1:k} \in \mathbb{C}^{2^k \times 2^k}$ the matrix

$$\left(\rho_{1:k}\right)_{\mu_1 \dots \mu_k}^{\nu_1 \dots \nu_k} = \sum_{\mu_{k+1} \dots \mu_L} \left(\Psi_{\mu_1 \dots \mu_k}^{\mu_{k+1} \dots \mu_L}\right)^* \Psi_{\mu_{k+1} \dots \mu_L}^{\nu_1 \dots \nu_k}. \tag{3.1.1}$$

Note that the eigenvalues of the k-RDM are squares of the singular values of the reshaped tensor $(\Psi_{\mu_1 \dots \mu_k}^{\mu_{k+1} \dots \mu_L})$ which monitor the approximability of Ψ by TT.

More generally, for a subset $A \subset \{1, \dots, L\}$, we define the RDM $\rho_A \in \mathbb{C}^{2^{|A|} \times 2^{|A|}}$ by

$$\left(\rho_A\right)_{\mu_i, i \in A}^{\nu_i, i \in A} = \sum_{\mu_j, j \notin A} \left(\Psi_{\mu_i}^{\mu_j}\right)^* \Psi_{\mu_j}^{\nu_i}. \tag{3.1.2}$$

Note that since Ψ is normalised, we have

$$\operatorname{Tr} \rho_A = 1. \tag{3.1.3}$$

By definition, RDM are Hermitian and semi-positive definite matrices.

3.1.2 Quantum entropy

Definition 3.1.1 (Von Neumann and Rényi entropies)**.** *Let $\rho \in \mathbb{C}^{n\times n}$ be a Hermitian, semi-positive definite matrix such that $\operatorname{Tr}\rho = 1$. The von Neumann entropy is defined by*

$$S(\rho) = -\operatorname{Tr}(\rho \log \rho). \tag{3.1.4}$$

The Rényi entropy of parameter $\alpha \in (0,\infty)$, $\alpha \neq 1$ is defined by

$$S_\alpha(\rho) = \frac{1}{1-\alpha}\log(\operatorname{Tr}(\rho^\alpha)). \tag{3.1.5}$$

For pure states, *i.e.* when ρ is up to a scalar factor a projector, one can check that the entropy of ρ is 0. As pure states can be written as TT of TT rank 1, this motivates the further investigation of the entropy as a proxy for the approximability of Ψ by TT. This suggests that states with a low quantum entropy are easily approximable by TT. As we are going to highlight, although in practice the quantum entropy is a fair indicator for the approximation problem, there are counter-examples of states that have an exponentially complex TT representation but a low quantum entropy [SWVC08].

Another desirable property of the entropy is the additivity - also sometimes called the extensivity - and the subadditivity:

- additivity: we say that an entropy S is additive if for all RDM ρ_A and ρ_B we have
$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B); \tag{3.1.6}$$
- subadditivity: we say that an entropy S is subadditive if for all RDM ρ_{AB} defined on a tensor space $\mathcal{H}_A \otimes \mathcal{H}_B$, $\rho_A = \operatorname{Tr}_{\mathcal{H}_B}\rho_{AB}$ and $\rho_B = \operatorname{Tr}_{\mathcal{H}_A}\rho_{AB}$, we have
$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B). \tag{3.1.7}$$

We are going to review few important properties of the von Neumann and Rényi entropies.

Remark 3.1.2. *The Rényi and von Neumann entropies are closely related as*

$$\lim_{\alpha\to 1} S_\alpha(\rho) = S(\rho). \tag{3.1.8}$$

Proposition 3.1.3 (Schur concavity)**.** *The von Neumann and the Rényi entropies are Schur concave,* i.e. *if ρ_α and ρ_β are RDM with respective eigenvalues $(\alpha_i)_{1\leq i\leq n}$ and $(\beta_i)_{1\leq i\leq n}$ such that for all $1 \leq k \leq n$*

$$\sum_{i=1}^{k}\alpha_i \leq \sum_{i=1}^{k}\beta_i, \tag{3.1.9}$$

then $S(\rho_\alpha) \geq S(\rho_\beta)$.

From the Schur concavity, we deduce that

- a pure state ρ with eigenvalues $(1, 0, \dots, 0)$ majorises any sequence, hence for any $\tilde{\rho}$, $S(\tilde{\rho}) \geq S(\rho) = 0$;
- a state with maximal entanglement *i.e.* with eigenvalues $(\frac{1}{n}, \dots, \frac{1}{n})$ is majorised by any sequence, hence it is the state with maximal entropy.

Proof. We simply need to use the concavity of the map $g : x \mapsto -x \log x$ or $g : x \mapsto \frac{x^\alpha}{1-\alpha}$. Let us prove the result for $n = 2$. By assumption on the eigenvalues of ρ_1 and ρ_2, we have

$$\begin{cases} \alpha_1 \geq \beta_1 \\ \alpha_1 + \alpha_2 = \beta_1 + \beta_2, \end{cases} \tag{3.1.10}$$

hence there exists $\lambda \in [0, 1]$ such that

$$\begin{cases} \beta_1 = \lambda\alpha_1 + (1-\lambda)\alpha_2 \\ \beta_2 = (1-\lambda)\alpha_1 + \lambda\alpha_2. \end{cases} \tag{3.1.11}$$

We have then

$$\begin{aligned} S(\rho_\beta) &= g(\beta_1) + g(\beta_2) \\ &= g(\lambda\alpha_1 + (1-\lambda)\alpha_2) + g((1-\lambda)\alpha_1 + \lambda\alpha_2) \\ &\geq \lambda g(\alpha_1) + (1-\lambda)g(\alpha_2) + (1-\lambda)g(\alpha_1) + \lambda g(\alpha_2) = g(\alpha_1) + g(\alpha_2) = S(\rho_\alpha). \end{aligned}$$

□

It turns out that additivity holds for the von Neumann and the Rényi entropies but subadditivity - and strong subadditivity that is introduced further down - only holds for the von Neumann entropy [LMW13].

Proposition 3.1.4 (Additivity of the Rényi and von Neumann entropies)**.** *The von Neumann and the Rényi entropies are additive,* i.e. *for all RDM ρ_A, ρ_B respectively defined on $\mathcal{H}_A$ and $\mathcal{H}_B$, then we have*

$$S(\rho_A \otimes \rho_B) = S(\rho_A) + S(\rho_B). \tag{3.1.12}$$

Proof. The proof follows from a direct calculation of $S(\rho_A \otimes \rho_B)$. Let (λ_i) and (μ_j) be the eigenvalues of ρ_A and ρ_B, then we have

$$\begin{aligned} S_\alpha(\rho_A \otimes \rho_B) &= \frac{1}{1-\alpha} \log\big(\operatorname{Tr}(\rho^\alpha)\big) \\ &= \frac{1}{1-\alpha} \log\Big(\sum_{ij} \lambda_i^\alpha \mu_j^\alpha\Big) \\ &= \frac{1}{1-\alpha} \log\Big(\sum_i \lambda_i^\alpha \sum_j \mu_j^\alpha\Big) \\ &= S_\alpha(\rho_A) + S_\alpha(\rho_B). \end{aligned}$$

The proof is the same with the von Neumann entropy. □

Proposition 3.1.5 (Subadditivity of the von Neumann entropy)**.** *The von Neumann entropy is subadditive,* i.e.*for all RDM ρ_{AB} defined on a tensor space $\mathcal{H}_A \otimes \mathcal{H}_B$, $\rho_A = \mathrm{Tr}_{\mathcal{H}_B} \rho_{AB}$ and $\rho_B = \mathrm{Tr}_{\mathcal{H}_A} \rho_{AB}$, we have*

$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B). \tag{3.1.13}$$

Before giving the proof, we state the Klein's inequality.

Lemma 3.1.6 (Klein's inequality)**.** *Let f be a convex function, A and B be Hermitian matrices such that $f(A)$ and $f(B)$ are well-defined. Then the following inequality holds*

$$\mathrm{Tr}(f(A) - f(B) - (A - B)f'(B)) \geq 0. \tag{3.1.14}$$

If f is strictly convex, we have equality if and only if $A = B$.

Proof. We first write the spectral decomposition of A and B

$$\begin{cases} A = \sum_{i=1}^{n} \alpha_i |a_i\rangle\langle a_i| \\ B = \sum_{i=1}^{n} \beta_i |b_i\rangle\langle b_i|. \end{cases} \tag{3.1.15}$$

Then we have

$$\begin{aligned} \mathrm{Tr}(f(A) - f(B) - (A - B)f'(B)) &= \sum_{i=1}^{n} f(\alpha_i) - f(\beta_i) - \sum_{j=1}^{n} |\langle a_i, \beta_j\rangle|^2 \alpha_i f'(\beta_j) \\ &= \sum_{i,j=1}^{n} |\langle a_i, \beta_j\rangle|^2 \big(f(\alpha_i) - f(\beta_j) + (\beta_j - \alpha_i) f'(\beta_j)\big), \end{aligned}$$

where we have used that $\sum_{i=1}^{n} |\langle a_i, \beta_j\rangle|^2 = \sum_{j=1}^{n} |\langle a_i, \beta_j\rangle|^2 = 1$. We conclude using the convexity of f.

The equality case follows from the strict convexity and the properties of the scalar product. □

We can now prove the subadditivity of the von Neumann entropy.

Proof of Proposition 3.1.5. By additivity, we have

$$\begin{aligned} S(\rho_A) + S(\rho_B) - S(\rho_{AB}) &= \mathrm{Tr}(\rho_{AB} \log(\rho_{AB})) - \mathrm{Tr}(\rho_A \otimes \mathrm{id}_B \log(\rho_A \otimes \mathrm{id}_B)) \\ &\quad - \mathrm{Tr}(\mathrm{id}_A \otimes \rho_B \log(\mathrm{id}_A \otimes \rho_B)) \\ &= \mathrm{Tr}(\rho_{AB}(\log(\rho_{AB}) - \log(\rho_A \otimes \mathrm{id}_B) - \log(\mathrm{id}_A \otimes \rho_B))) \\ &= \mathrm{Tr}(\rho_{AB}(\log(\rho_{AB}) - \log(\rho_A \otimes \mathrm{id}_B + \mathrm{id}_A \otimes \rho_B))) \end{aligned}$$

where we have used that $\mathrm{Tr}(\rho_{AB}\log(\rho_A\otimes \mathrm{id}_B)) = \mathrm{Tr}(\rho_A\otimes \mathrm{id}_B \log(\rho_A\otimes \mathrm{id}_B))$. It remains to show that for positive semi-definite matrices M, N such that $\mathrm{Tr}\, M = \mathrm{Tr}\, N$, we have

$$\mathrm{Tr}(M(\log(M)-\log(N))) \geq 0. \tag{3.1.16}$$

The map $x \mapsto x\log x$ is convex hence by Klein's inequality 3.1.6, we have

$$\mathrm{Tr}(M\log(M) - N\log N) \geq \mathrm{Tr}(M-N+(M-N)\log(N)) \geq \mathrm{Tr}((M-N)\log(N)),$$

by simplifying $\mathrm{Tr}(N\log N)$ on both sides, we get (3.1.16) and this finishes the proof. □

Remark 3.1.7. *Note that we have proved that the relative entropy - also called the Kullback-Leibler divergence -*

$$d(\rho_1,\rho_2) = \mathrm{Tr}(\rho_1(\log(\rho_1)-\log(\rho_2))), \tag{3.1.17}$$

is always non negative for RDM.

The von Neumann has an additional property that is useful to have better bounds of the entropy of a larger blocks. This property is the *strong subadditivity.*

Proposition 3.1.8 (Strong subadditivity of the von Neumann entropy)**.** *The von Neumann entropy is strongly subadditive,* i.e. *for all RDM ρ_{ABC} on the tensor space $\mathcal{H}_A\otimes\mathcal{H}_B\otimes\mathcal{H}_C$, ρ_{AB},ρ_{BC} and ρ_B the corresponding partial traces, we have*

$$S(\rho_{ABC}) \leq S(\rho_{AB}) + S(\rho_{BC}) - S(\rho_B). \tag{3.1.18}$$

The proof of the strong subadditivity follows the line of the subadditivity of the von Neumann entropy [AL70].

A summary of the properties satisfied by the Von Neumann and the Rényi entropies is provided in Table 3.1.

	Additivity	Schur concavity	Subadditivity	Strong subadditivity
Von Neumann entropy	YES	YES	YES	YES
Rényi entropy	YES	YES	NO	NO

Table 3.1: Properties of the Von Neumann and Rényi entropies

3.1.3 Relationship between TT approximability and entropy scaling

For the Rényi entropy, for $\alpha < 1$ a bound on the entropy is sufficient to bound the TT error.

Proposition 3.1.9 ([VC06]). *Let $\Psi \in \mathbb{C}^{2^L}$ be a normalised state and $\epsilon_j(r)$ the L^2 local error by its TT approximation of TT rank r. Then the error is bounded by*

$$\log_2(\epsilon_j(r)^2) \leq \frac{1-\alpha}{\alpha}(S_\alpha(\rho_{1:j}) - \log_2(\tfrac{r}{1-\alpha})). \tag{3.1.19}$$

These results are tied to the concept of *area laws* that states that the entropy is bounded regarless of the system size L. This is proved for 1D Hamiltonian with nearest neighbour interaction [Has07] under the assumption that the system is gapped. Indeed, if the entropy $S_\alpha(\rho_{1:j})$ for $\alpha < 1$ is bounded independently of j and L, then the local error is polynomial in the truncation rank r.

Numerous extensions of this result have been shown to include interactions with longer interactions. For higher dimensions, area laws have not been proved although it is generally accepted that the same statements should be true, in which case, the best tensor network to approximate the ground-state of such systems will not be TT but projected entangled pair states (PEPS).

Proof. We use the Schur convexity of the entropy and find a sequence that majorises the singular values of Ψ. □

For $\alpha > 1$, the Rényi entropy provides a lower bound of the TT error. This gives a sufficient condition for nonapproximability results.

Proposition 3.1.10 ([SWVC08]). *Let $\Psi \in \mathbb{C}^{2^L}$ be a normalised state and $\epsilon_j(r)$ the L^2 local error by its TT approximation of TT rank r. Then the error is bounded by*

$$S_\alpha(\rho_{1:j}) \geq \frac{1-\alpha}{\alpha}\log_2(1-\epsilon_j(r)^2) + \log_2(r). \tag{3.1.20}$$

Proof. We use the Schur convexity of the entropy and find a sequence that majorises the singular values of Ψ. □

For the von Neumann entropy, we have the same result in the nonapproximable case.

However, counterexamples of states exist where the von Neumann entropy is bounded but the state is not approximable by TT.

Proposition 3.1.11 ([SWVC08]). *Let $\Psi_{2N} \in \mathbb{C}^{3^{2N}}$ be the state defined by*

$$\Psi_{2N} = \sqrt{1-p_N}|2\rangle^{\otimes 2N} + \sqrt{\tfrac{p_N}{2^N}} \sum_{x\in\{0,1\}^N} |x\rangle \otimes |x\rangle, \tag{3.1.21}$$

with p_N and

$$|\chi_M\rangle = |\Psi_{2N}\rangle^{\otimes N^2}. \tag{3.1.22}$$

Proof. For the TT truncation error, for $r < 2^N$ the truncation error on Ψ_{2N} is bounded by

$$\|\Psi_{2N} - \mathrm{TT}_r\Psi_{2N}\| \leq p_N, \tag{3.1.23}$$

thus the truncation error on χ_M is bounded by

$$\|\chi_M - \mathrm{TT}_r\chi_M\| \leq N^2\|\Psi_{2N} - \mathrm{TT}_r\Psi_{2N}\| \leq N^2 p_N. \tag{3.1.24}$$

For the entropy, let $L \leq 2N^3$ then the L-orbital RDM of χ_M is bounded by the ℓ-orbital RDM of Ψ_{2N} where $\ell = L \mod 2N$

$$\begin{aligned} S(\rho_L(|\chi_M\rangle)) &\leq S(\rho_\ell(\Psi_{2N})) \\ &\leq S(\rho_{2N}^{(\ell)}) + p_N, \end{aligned}$$

with $\rho_{2N}^{\ell} = (1-p_N)|2\rangle^{\otimes\ell}\langle 2|^{\otimes\ell} + \frac{p_N}{2^\ell}\sum_{x\in\{0,1\}^\ell}$. The von Neumann entropy of $\rho_{2N}^{(\ell)}$ is explicit

$$\begin{aligned} S(\rho_{2N}^{(\ell)}) &= -(1-p_N)\log(1-p_N) - p_N\log\left(\tfrac{p_N}{2^\ell}\right) \\ &= -(1-p_N)\log(1-p_N) - p_N\log(p_N) + \ell p_N. \end{aligned} \tag{3.1.25}$$

We want the state to have a bounded entropy and not being approximable by a TT, hence we need to pick p_N such that

- ℓp_N bounded ;
- $N^2 p_N \to \infty$

thus $p_N = \mathcal{O}(\frac{1}{N^\beta})$, with $1 \leq \beta < 1$ will do. □

The different results regarding the boundedness of the entropy and the TT approximability are gathered in Table 3.2.

	Bounded entropy	Unbounded entropy
Rényi $\alpha < 1$	TT approximable	?
von Neumann	?	Non TT approximable
Rényi $\alpha > 1$	?	Non TT approximable

Table 3.2: TT approximability and entropy. Question marks mean that both can happen.

Although this counterexample seems to indicate that the von Neumann entropy is not suited to assess the TT approximability of a state, results that are obtained using the Fiedler order are generally satisfactory.

A heuristic argument relying on the strong subadditivity of the von Neumann entropy suggests that the Fiedler order is a first order optimiser of the block entropy. However as shown by the counterexample, it is not sufficient to argue that the state is easier to approximate by a TT. This suggests that such counterexamples are scarce.

3.2 Mutual information and the Fiedler order

The Fiedler order has been introduced in [LRH03] inspired by the notions of quantum entanglement in quantum information theory. It is the default ordering method in the major DMRG codes [LRH03, CHG02, RNW06, FKK+18].

For a quantum state $\Psi \in \mathbb{C}^{2^L}$, we introduce the *quantum mutual information matrix* (QMI) $I_{ij} \in \mathbb{R}^{L\times L}$ by

$$I_{ij} = \begin{cases} S(\rho_i) + S(\rho_j) - S(\rho_{i,j}), i \neq j \\ 0, i = j \end{cases} \tag{3.2.1}$$

The QMI is exactly the Kullback-Leibler divergence between ρ_{ij} and $\rho_i \otimes \rho_j$. As such, by Equation (3.1.17), the QMI has nonnegative entries.

The motivation of the Fiedler order scheme relies on the following proposition.

Proposition 3.2.1 ([Ali21])**.** *Let $\Psi \in \mathbb{C}^{2^L}$ be a normalised state. Let $1 \leq j \leq L-1$ and $1 \leq \delta \leq \frac{j}{2}$. Then we have*

$$S(\rho_{1:j}) \leq \sum_{k=1}^{j} S(\rho_k) - I_{k,k+\delta}. \tag{3.2.2}$$

To minimise the block entropy $S(\rho_{1:j})$, assuming that the one-site entropies are all of the same order, it is reasonable to maximise the QMI of neighbouring sites. This is the main idea of the Fiedler order. Before sketching the algorithm, we will prove the previous proposition.

Proof. By the strong subadditivity of the von Neumann entropy 3.1.8, for all $1 \leq k \leq j-\delta$ we have

$$S(\rho_{k:j}) + S(\rho_{k+\delta}) \leq S(\rho_{k,k+\delta}) + S(\rho_{k+1:j}). \tag{3.2.3}$$

Summing these equations, we obtain

$$\begin{aligned} S(\rho_{1:j}) + \sum_{k=1}^{j-\delta} S(\rho_{k+\delta}) &\leq \sum_{k=1}^{j-\delta} S(\rho_{k,k+\delta}) + S(\rho_{j-\delta+1:j}) \\ S(\rho_{1:j}) &\leq \sum_{k=1}^{j-\delta} S(\rho_k) - \sum_{k=1}^{j-\delta} I_{k,k+\delta} + S(\rho_{j-\delta+1:j}) \\ &\leq \sum_{k=1}^{j} S(\rho_k) - I_{k,k+\delta}, \end{aligned}$$

where we have used the definition of the QMI and the additivity of the entropy. □

For the Fiedler order [LRH03, BLMR11], the function that is minimised is the total entanglement

$$I_{\text{dist}}(\pi) = \sum_{i,j=1}^{L} I_{i,j}|\pi(i) - \pi(j)|^2, \tag{3.2.4}$$

over the set of permutations $\pi \in \mathcal{P}_N$.

As it is a combinatorial problem, it is necessary to resort to an approximation in practice. In that case, the problem that is solved is the minimisation of

$$\tilde{I}_{\text{dist}}(x) = \sum_{i,j=1}^{L} I_{i,j}|x_i - x_j|^2, \tag{3.2.5}$$

with $x \in \mathbb{R}^L$ under the constraint that $\sum_i x_i = 0$ and $\|x\|_2 = 1$. Introducing the graph Laplacian $L_{ij} = D_{ij} - I_{ij}$ where D is the diagonal matrix with diagonal entries $D_{ii} = \sum_{j=1}^{L} I_{ij}$, we see that

$$x^T L x = \sum_{i,j=1}^{L} I_{i,j}|x_i - x_j|^2. \tag{3.2.6}$$

The solution to this minimisation problem under the constraint that $\sum_i x_i = 0$ and $\|x\|_2 = 1$ is given by the second eigenvector of L (the lowest eigenvalue is 0 by construction of L), which is called the *Fiedler vector* . The Fiedler order consists in ordering the sites according to the magnitude of the entries of the Fiedler vector.

Indeed the Fiedler vector is related to the problem of *graph partitioning* or in our case the *min-cut* of the graph. The QMI matrix can be seen as a weight on the graph with L vertices, for which we need to determine a partition of the vertices into two distinct sets A and $\{1, \ldots, L\} \setminus A$ such that it minimises

$$\sum_{i \in A, j \notin A} I_{ij}. \tag{3.2.7}$$

For simple cases, it can be proved that the Fiedler vector solves this problem by considering $A = \{i \mid x_i > 0\}$. It is generally believed that for weighted graphs, the Fiedler vector is a good approximation to the min-cut problem.

3.3 An example: minimal-basis H_2

To illustrate the different ordering methods, we now apply them to the minimal-basis H_2 wavefunction

$$\Psi = \Big| (c\varphi_A + s\varphi_B)\uparrow, (c'\varphi_A + s'\varphi_B)\downarrow \Big\rangle, \tag{3.3.1}$$

where φ_A and φ_B are respectively the bonding and antibonding orbitals. In the occupation representation, the state Ψ has the following form

$$\Psi = cc'\Phi_{(1100)} + cs'\Phi_{(1001)} - sc'\Phi_{(0110)} + ss'\Phi_{(0011)} \in \bigotimes_{i=1}^{4} \mathbb{C}^2. \tag{3.3.2}$$

We will compute the singular values of the matrix reshape $\Psi^{\mu_1\mu_2}_{\mu_3\mu_4} \in \mathbb{R}^{2^2\times 2^2}$, for the different orderings of the basis set delivered by all the above ordering schemes. To avoid degenerate cases we assume that all coefficients c, s, c', s' in (3.3.1) are nonzero.

Canonical order. We abbreviate the single-particle basis states as $\{A\uparrow, A\downarrow, B\uparrow, B\downarrow\}$. Directly from (3.3.2) we see that with respect to the canonical order in which the bonding orbital with either spin comes first,

$$A\uparrow\ A\downarrow\ B\uparrow\ B\downarrow, \tag{3.3.3}$$

the reshape $\Psi^{\mu_1\mu_2}_{\mu_3\mu_4}$ is

$\mu_1\,\mu_2$ \ $\mu_3\,\mu_4$	00	01	10	11
00				ss'
01			$-sc$	
10		cs'		
11	cc'			

The singular values are

$$(cc')^2,\ (cs')^2,\ (sc')^2,\ (ss')^2$$

and the rank of the matrix reshape is 4.

Fiedler order. We begin by working out the one- and two-orbital density matrices and the corresponding entropies. The one-orbital quantities are elementary to compute, they are

$$\rho^{(1)}_{A\uparrow} = \begin{pmatrix} s^2 & 0 \\ 0 & c^2 \end{pmatrix}, \quad \rho^{(1)}_{A\downarrow} = \begin{pmatrix} s'^2 & 0 \\ 0 & c'^2 \end{pmatrix}, \quad \rho^{(1)}_{B\uparrow} = \begin{pmatrix} c^2 & 0 \\ 0 & s^2 \end{pmatrix}, \quad \rho^{(1)}_{B\uparrow} = \begin{pmatrix} c'^2 & 0 \\ 0 & s'^2 \end{pmatrix}.$$

It follows that

$$\begin{aligned} s^{(1)}_{A\uparrow} = s^{(1)}_{B\uparrow} &= -c^2\log c^2 - s^2\log s^2 =: s_\uparrow \in (0,1], \\ s^{(1)}_{A\downarrow} = s^{(1)}_{B\downarrow} &= -c'^2\log c'^2 - s'^2\log s'^2 =: s_\downarrow \in (0,1]. \end{aligned}$$

As regards the two-orbital density matrices, we find after some calculation that

$$\rho^{(2)}_{A\uparrow A\downarrow} = \begin{pmatrix} s^2s'^2 & & & \\ & s^2c'^2 & & \\ & & c^2s'^2 & \\ & & & c^2c'^2 \end{pmatrix}, \ \rho^{(2)}_{B\uparrow B\downarrow} = \begin{pmatrix} c^2c'^2 & & & \\ & c^2s'^2 & & \\ & & s^2c'^2 & \\ & & & s^2s'^2 \end{pmatrix}, \ \rho^{(2)}_{A\uparrow B\downarrow} = \begin{pmatrix} s^2c'^2 & & & \\ & s^2s'^2 & & \\ & & c^2c'^2 & \\ & & & c^2s'^2 \end{pmatrix}, \ \rho^{(2)}_{A\downarrow B\uparrow} = \begin{pmatrix} c^2c'^2 & & & \\ & c^2s'^2 & & \\ & & s^2s'^2 & \\ & & & s^2c'^2 \end{pmatrix}.$$

It follows that $S^{(2)} = -\mathrm{tr}\,\rho^{(2)} \log \rho^{(2)} =: S_{\uparrow\downarrow}$ is the same for all four matrices. Moreover writing out the above trace and using $c^2 + s^2 = c'^2 + s'^2 = 1$ we find that

$$S_{\uparrow\downarrow} = s_\uparrow + s_\downarrow. \tag{3.3.4}$$

The two remaining two-orbital RDMs contain off-diagonal terms

$$\rho^{(2)}_{A\uparrow B\uparrow} = \begin{pmatrix} 0 & & & \\ & s^2 & -cs(c'^2 - s'^2) & \\ & -cs(c'^2 - s'^2) & c^2 & \\ & & & 0 \end{pmatrix}, \quad \rho^{(2)}_{A\downarrow B\downarrow} = \begin{pmatrix} 0 & & & \\ & s'^2 & c's'(c^2 - s^2) & \\ & c's'(c^2 - s^2) & c'^2 & \\ & & & 0 \end{pmatrix}.$$

We denote the associated entropies by $S^{(2)}_{A\uparrow B\uparrow} =: S_{\uparrow\uparrow}$, $S^{(2)}_{A\downarrow B\downarrow} =: S_{\downarrow\downarrow}$. The mutual information matrix and graph Laplacian are thus, using the vanishing of all nearest-neighbour elements of I by (3.3.4) and denoting $a := 2s_\uparrow - S_{\uparrow\uparrow}$, $b := 2s_\downarrow - S_{\downarrow\downarrow}$,

$I =$

	$A\uparrow$	$A\downarrow$	$B\uparrow$	$B\downarrow$
$A\uparrow$	0	0	a	0
$A\downarrow$	0	0	0	b
$B\uparrow$	a	0	0	0
$B\downarrow$	0	b	0	0

$L =$

	$A\uparrow$	$A\downarrow$	$B\uparrow$	$B\downarrow$
$A\uparrow$	a	0	-a	0
$A\downarrow$	0	b	0	-b
$B\uparrow$	-a	0	a	0
$B\downarrow$	0	-b	0	b

To determine the Fiedler ordering we need to find the second eigenvector of the graph Laplacian, alias Fiedler vector. The first eigenvector is always, by construction, the constant vector, with eigenvalue 0. For the above L, by inspection the remaining eigenvalues are 0, $2a > 0$, $2b > 0$, with eigenvectors $(1,-1,1,-1)$, $(1,0,-1,0)$, $(0,1,0,-1)$. The second eigenvector is thus $(1,-1,1,-1)$. It follows that the Fiedler ordering is

$$A\uparrow\ B\uparrow\ A\downarrow\ B\downarrow \tag{3.3.5}$$

(up to re-ordering the orbitals in the left block, re-ordering the orbitals in the right block, and flipping the two blocks; none of this affects the singular values). The matrix reshape $\Psi^{\mu_1\mu_2}_{\mu_3\mu_4}$ with respect to this ordering is

$\mu_1\,\mu_2$ \ $\mu_3\,\mu_4$	00	01	10	11
00	0			
01		ss'	sc'	
10		cs'	cc'	
11				0

Since the middle block is the rank-1 matrix $\begin{pmatrix} c \\ s \end{pmatrix} \begin{pmatrix} c' & s' \end{pmatrix}$, the singular values are

$$1,\ 0,\ 0,\ 0$$

and the rank of the matrix reshape is 1. We see that the Fiedler order has dramatically improved the decay of the singular values.

Chapter 4

Area laws for one-dimensional systems

Area laws have first been stated rigorously for ground-state of one-dimensional gapped systems with nearest neighbour interactions (NNI) by Hastings [Has07]. Later on, another proof using approximate ground-state projector has been discovered yielding better bounds [AKLV13]. For both proofs, the goal is to bound the Rényi entropy of the RDM $\rho_{j:j+\ell-1}$ by a constant S independent of ℓ and of the size of the system

$$S_\alpha(\rho_{j:j+\ell-1}) \leq S. \tag{4.0.1}$$

By Proposition 3.1.9, this implies that there is a TT approximation of the ground-state with TT ranks bounded by $2^{\frac{1-\alpha}{\alpha}S}$.

4.1 Hamiltonian with nearest neighbour interactions

The NNI Hamiltonian considered is of the form

$$H = \sum_{j=1}^{d-1} h_j, \tag{4.1.1}$$

where H is an operator acting on $\bigotimes_{j=1}^d \mathcal{H}_j$, with $\dim \mathcal{H}_j = n$ and h_j is a two-body operator of the form $\mathrm{id}_{1:j-1} \otimes \widetilde{h}_j \otimes \mathrm{id}_{j+2:d}$.

Assumption 4.1.1. *We are going to make the following assumptions on H*

- *the operators $\widetilde{h}_j$ are uniformly bounded, i.e. there is a constant C such that for all $1 \leq j \leq d-1, \|\widetilde{h}_j\| \leq \|h\|$;*
- *the commutators are uniformly bounded, i.e. there is a constant J such that for all $1 \leq j \leq d-2$, $\|[\widetilde{h}_j, \widetilde{h}_{j+1}]\| \leq J$;*

- *the many-body Hamiltonian H has a unique ground-state Ψ_0 with eigenvalue 0 and a spectral gap $\gamma > 0$ independent of d.*

The first assumption can actually be lifted and is taken for simplicity. As long as the commutators $[\widetilde{h}_j, \widetilde{h}_{j+1}]$ are uniformly bounded, the proof can be adapted to unbounded operators (see [Ali21]). If the gap closes not too fast, it is possible to still get a polynomial bound on the TT approximation of the ground-state instead of an exponential one.

4.2 Hastings area law

4.2.1 Lieb-Robinson bounds

An essential ingredient of the area law by Hastings is the repeated use of the Lieb-Robinson bound for NNI Hamiltonians. This bound describes how the correlation evolves for local operators.

Proposition 4.2.1 (Lieb-Robinson bound [NS06])**.** *Let $A \in \mathcal{L}(\mathcal{H}_X)$ and $B \in \mathcal{L}(\mathcal{H}_Y)$ be two operators with $X \cap Y = \varnothing$. Let $A(t) = e^{\mathrm{i}Ht} A \otimes \mathrm{id}_Y e^{-\mathrm{i}Ht}$ with H given by (4.1.1). Then there are constants $c, a, v > 0$ independent of A, B or d such that*

$$\|[A(t), \mathrm{id}_X \otimes B]\| \leq c|X||Y|\|A\|\|B\| \exp(-a(d(X,Y) - v|t|)), \tag{4.2.1}$$

where $d(X,Y) = \min_{x \in X, y \in Y} |x - y|$.

The Lieb-Robinson bound is stated here in the special case of a one-dimensional NNI Hamiltonian but it holds for more general local interactions types [NS06]. In that case, the distance d is replaced by the natural distance of the interaction picture.

The Lieb-Robinson bound enables to state that the evolution of a local operator remains local by the next lemma.

Lemma 4.2.2. *Let $A \in \mathcal{L}(\mathcal{H}_1 \otimes \mathcal{H}_2)$. We assume that $\mathcal{H}_2$ is finite-dimensional. Suppose there is $\varepsilon > 0$ such that for all $B \in \mathcal{H}_2$, we have*

$$\|[A, \mathrm{id} \otimes B]\| \leq \varepsilon \|B\|. \tag{4.2.2}$$

Then there is an operator $A_1 \in \mathcal{L}(\mathcal{H}_1)$ such that

$$\|A - A_1 \otimes \mathrm{id}\| \leq \varepsilon. \tag{4.2.3}$$

Moreover, if A is self-adjoint, then A_1 can also be chosen self-adjoint.

Proof of Lemma 4.2.2. The operator A_1 is explicitely constructed: take $A_1 = \frac{1}{\dim \mathcal{H}_2} \operatorname{Tr}_{\mathcal{H}_2} A = \int_{U(\mathcal{H}_2)} \mathrm{id} \otimes U^* A \, \mathrm{id} \otimes U \, \mathrm{d}U$ where $\mathrm{d}U$ is the uniform Haar measure on the unitary matrices of $\mathcal{H}_2$. Then we have

$$\|A - A_1 \otimes \mathrm{id}\| = \left\| \int_{U(\mathcal{H}_2)} \mathrm{id} \otimes U^* [A, \mathrm{id} \otimes U] \, \mathrm{d}U \right\| \leq \varepsilon.$$

□

Corollary 4.2.3. *Let $A \in \mathcal{L}(\mathcal{H}_X)$, $\ell > 0$ and $\widetilde{X} = \{\tilde{x} \mid \exists x \in X, |x - \tilde{x}| \leq \ell\}$. Let $A(t) = e^{\mathrm{i}Ht} A \otimes \mathrm{id}_{X^c} e^{-\mathrm{i}Ht}$ with H given by (4.1.1). Then for all $t \in \mathbb{R}$, there is an operator $A_\ell(t) \in \mathcal{L}(\mathcal{H}_{\widetilde{X}})$ such that*

$$\|A(t) - A_\ell(t) \otimes \mathrm{id}_{\widetilde{X}^c}\| \leq d|X|\|A\| \exp(-a(\ell - v|t|)). \tag{4.2.4}$$

If A is self-adjoint, then $A_\ell(t)$ is self-adjoint for all t.

Proof. Combining Lemma 4.2.2 with the Lieb-Robinson bonud (4.2.1), we directly get the result. □

4.2.2 Main theorem and Hastings area law

The main result in Hastings seminal paper states that the ground-state projector can be exponentially well approximated using an almost tensor product of operators with an overlapping domain of size ℓ independent of the size of the system.

Theorem 4.2.4. *Let H be the Hamiltonian defined in (4.1.1) satisfying the assumptions 4.1.1. For any $1 \leq j \leq d$ and any $\ell \geq 0$, there are operators $O_L \in \mathcal{L}(\mathcal{H}_{1:j})$, $O_M \in \mathcal{L}(\mathcal{H}_{j-\ell:j+\ell})$ and $O_R \in \mathcal{L}(\mathcal{H}_{j+1:d})$ with $\|O_M\|, \|O_L\|, \|O_R\| \leq 1$ and there is $\beta > 0$ independent of ℓ and d and $C > 0$ depending polynomially on d such that*

$$\left\|(\mathrm{id}_{1:j-\ell-1} \otimes O_M \otimes \mathrm{id}_{j+\ell+1:d})(O_L \otimes \mathrm{id}_{j+1:d})(\mathrm{id}_{1:j} \otimes O_R) - |\Psi_0\rangle\langle\Psi_0|\right\| \leq C \exp(-\beta\ell). \tag{4.2.5}$$

From eq. (4.2.5), the area law and the TT approximation of the ground-state follows.

Corollary 4.2.5. *Let Ψ_0 be the ground-state projection of H given by (4.1.1). Then the following assertions are true:*

(i). there is a constant S independent of L such that $S_\alpha(|\Psi_0\rangle\langle\Psi_0|) \leq S$;

(ii). for any $\varepsilon > 0$, there is a TT approximation $\mathrm{TT}_r\Psi_0$ with TT rank r independent of d of Ψ_0 such that

$$\|\mathrm{TT}_r\Psi_0 - \Psi_0\| \leq \varepsilon.$$

Remark 4.2.6. *It is possible to choose the operators O_L, O_M and O_R to be nonnegative. By construction, O_L and O_R are nonnegative and by a little trick, O_M can also be chosen nonnegative [Has07].*

Sketch of an almost-proof of Theorem 4.2.4 The proof of the theorem relies on the following approximation of the ground-state projection

$$\rho_q = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}Ht} e^{-\frac{t^2}{2q}} \,\mathrm{d}t, \tag{4.2.6}$$

where $q > 0$ is fixed later on. Using the spectral gap assumption, we see that

$$\|\rho_q - |\Psi_0\rangle\langle\Psi_0|\| \leq e^{-\frac{1}{2}\gamma^2 q}, \tag{4.2.7}$$

where γ is the spectral gap.

Using the NNI structure of the Hamiltonian, we can write

$$H = H_{L+R} + H_M,$$

with $H_M = \sum_{k=j-\frac{\ell}{2}}^{j+\frac{\ell}{2}} h_k$ and $H_{L+R} = \sum_{k<j-\frac{\ell}{2}} h_k + \sum_{k>j+\frac{\ell}{2}} h_k$. The evolution $e^{\mathrm{i}Ht}$ can be written

$$e^{\mathrm{i}Ht} = e^{\mathrm{i}H_{L+R}t + \mathrm{i}H_M t} e^{-\mathrm{i}H_{L+R}t} e^{\mathrm{i}H_{L+R}t}.$$

The trick is to realise that $e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t}$ is the solution to

$$\begin{cases} \mathrm{i}U'(t) = U(t)e^{\mathrm{i}H_{L+R}t} H_M e^{-\mathrm{i}H_{L+R}t} \\ U(0) = \mathrm{id}\,. \end{cases}$$

Since $H_M = \mathrm{id}_{1:j-\frac{\ell}{2}} \otimes \tilde{H}_M \otimes \mathrm{id}_{j+\frac{\ell}{2}+1:d}$, using Corollary 4.2.3, then for all $t \in \mathbb{R}$, there is $H_M^{(\ell)}(t) \in \mathcal{L}(\mathcal{H}_{j-\ell:j+\ell})$ such that

$$\left\| e^{\mathrm{i}H_{L+R}t} H_M e^{-\mathrm{i}H_{L+R}t} - \mathrm{id}_{1:j-\ell-1} \otimes H_M^{(\ell)}(t) \otimes \mathrm{id}_{j+\ell+1:d} \right\| \leq 2d\ell \|H_M\| \exp\bigl(-a(\tfrac{\ell}{2} - v|t|)\bigr).$$

Thus the operator $e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t}$ can be approximated by

$$e^{\mathrm{i}H_{L+R}t+\mathrm{i}H_M t}e^{-\mathrm{i}H_{L+R}t} = \mathcal{T}\exp\Bigl(\int_0^t \mathrm{id}_{1:j-\ell-1} \otimes H_M^{(\ell)}(\tau) \otimes \mathrm{id}_{j+\ell+1:d} \,\mathrm{d}\tau\Bigr)^*,$$

where for an operator $A(t)$, $\mathcal{T}\exp\bigl(\int_0^t A(\tau)\,\mathrm{d}\tau\bigr)$ is the time-ordered exponential defined by [RS75, Chapter X.12]

$$\mathcal{T}\exp\Bigl(\int_0^t A(\tau)\,\mathrm{d}\tau\Bigr) = \lim_{N\to\infty} e^{A(t_N)\Delta t} e^{A(t_{N-1})\Delta t} \cdots e^{A(t_1)\Delta t}, \quad t_k = k\Delta t, \quad \Delta t = \frac{t}{N}.$$

Using a Duhamel formula, the approximation of the ground-state projector is

$$\begin{aligned}|\Psi_0\rangle\langle\Psi_0| &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t + \mathcal{O}(e^{-\frac{1}{2}\gamma^2 q}) \\ &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes H_M^{(\ell)}(\tau)\otimes \mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)^* e^{\mathrm{i}H_{L+R}t}e^{-\frac{t^2}{2q}}\,\mathrm{d}t \\ &\qquad + \mathcal{O}(e^{-\frac{1}{2}\gamma^2 q} + q^{3/2}e^{-a\ell}).\end{aligned}$$

We would be done if it were possible to write $e^{\mathrm{i}H_{L+R}t} \simeq O_L \otimes \mathrm{id}_{j+1:d}\,\mathrm{id}_{1:j}\otimes O_R$ for $O_L \in \mathcal{L}(\mathcal{H}_{1:j})$ and $O_R \in \mathcal{L}(\mathcal{H}_{j+1:d})$ that are independent of t. In order to do so, another transformation is applied to H_M and H_{L+R} to guarantee that such a step is justified.

Proof of Theorem 4.2.4

Lemma 4.2.7. *Let $q > 0$ and ρ_q be defined by*

$$\rho_q = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t. \tag{4.2.8}$$

Then we have

$$\|\rho_q - |\Psi_0\rangle\langle\Psi_0|\| \leq e^{-\frac{1}{2}\gamma^2 q}, \tag{4.2.9}$$

where γ is the spectral gap.

Proof. This follows from the spectral gap assumption 4.1.1 and the fact that the Fourier transform of $t \mapsto \frac{1}{\sqrt{2\pi q}}e^{-\frac{t^2}{2q}}$ is $\omega \mapsto e^{-\frac{1}{2}\omega^2}$. □

Lemma 4.2.8. *For $1 \leq j \leq d$ and $\ell > 0$, let*

$$H_M = \sum_{k=j-\frac{\ell}{3}}^{j+\frac{\ell}{3}} h_k, \quad H_L = \sum_{k<j-\frac{\ell}{3}} h_k, \quad H_R \sum_{k>j+\frac{\ell}{3}} h_k.$$

For $q > 0$, let

$$H_M(q) = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{-\mathrm{i}Ht}H_M e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle\Psi_0, H_M\Psi_0\rangle \tag{4.2.10}$$

$$H_L(q) = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{-\mathrm{i}Ht}H_L e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle\Psi_0, H_L\Psi_0\rangle \tag{4.2.11}$$

$$H_R(q) = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{-\mathrm{i}Ht}H_R e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle\Psi_0, H_R\Psi_0\rangle. \tag{4.2.12}$$

Then for all $q > 0$, we have

$$H = H_L(q) + H_M(q) + H_R(q), \tag{4.2.13}$$

and

$$\|H_M(q)\Psi_0\|, \|H_L(q)\Psi_0\|, \|H_R(q)\Psi_0\| \leq \gamma J e^{-\frac{1}{2}\gamma^2 q}. \tag{4.2.14}$$

Proof. Since $H = H_L + H_M + H_R$, eq. (4.2.13) is clear. For eq. (4.2.14), we have

$$\begin{aligned} H_M(q)\Psi_0 &= \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}Ht} H_M e^{\mathrm{i}Ht}\Psi_0 e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle \Psi_0, H_M\Psi_0\rangle \Psi_0 \\ &= \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{-\mathrm{i}Ht} P_0^{\perp} H_M \Psi_0 e^{-\frac{t^2}{2q}}\,\mathrm{d}t, \end{aligned}$$

where $P_0^{\perp} = \mathrm{id} - |\Psi_0\rangle\langle\Psi_0|$. We have

$$\|P_0^{\perp} H_M \Psi_0\| \leq \gamma \|H H_M \Psi_0\| \leq \gamma \|[H, H_M]\Psi_0\| \leq \gamma J.$$

Hence using again the spectral gap of H, we obtain

$$\|H_M(q)\Psi_0\| \leq \gamma J e^{-\frac{1}{2}\gamma^2 q}. \tag{4.2.15}$$

The same proof applies to H_L and H_R. □

The operators $H_L(q)$, $H_M(q)$ and $H_R(q)$ do not have the same support as H_L, H_M and H_R. In fact, their support is now the full Hilbert space $\mathcal{H}_{1:d}$. However, this can be solved by truncating the operators using Corollary 4.2.3.

Lemma 4.2.9. *There are self-adjoint operators $\widetilde{H}_L(q)$, $\widetilde{H}_M(q)$ and $\widetilde{H}_R(q)$ with respective support in $\mathcal{H}_{1:j}$, $\mathcal{H}_{j-2\ell/3:j+2\ell/3}$ and $\mathcal{H}_{j+1:d}$ such that*

$$\begin{aligned} \|H_M(q) - \widetilde{H}_M(q)\| &\lesssim \|h\| \ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}, \\ \|H_L(q) - \widetilde{H}_L(q)\| &\lesssim \|h\| \ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}, \\ \|H_R(q) - \widetilde{H}_R(q)\| &\lesssim \|h\| \ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}. \end{aligned}$$

Proof. We only give the proof for $\widetilde{H}_M(q)$ as it is identical for the other truncations. By Corollary 4.2.3, there is an operator $H_M^{(\ell)}(t)$ with support in $\mathcal{H}_{j-2\ell/3:j+2\ell/3}$ such that

$$\|e^{-\mathrm{i}Ht} H_M e^{\mathrm{i}Ht} - H_M^{(\ell)}(t)\| \leq \|h\| \ell^2 d \exp(-a(\ell/3 - v|t|)).$$

Using that for $p, q > 0$, $\int_0^{\infty} e^{pt} e^{-\frac{t^2}{2q}}\,\mathrm{d}t \lesssim q^{1/2} e^{p^2 q/2}$.We deduce that there is an operator $\widetilde{H}_M(q)$ such that

$$\|H_M(q) - \widetilde{H}_M(q)\| \lesssim \|h\| \ell^2 d e^{-a\ell/3} e^{qa^2v^2/2}.$$

□

Lemma 4.2.10. *Let $q > 0$ and $\widetilde{\rho}_q$ be given by*

$$\widetilde{\rho}_q = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} e^{-\frac{t^2}{2q}} \,\mathrm{d}t,$$

where $\widetilde{H}_L(q)$, $\widetilde{H}_M(q)$ and $\widetilde{H}_R(q)$ are defined in Lemma 4.2.9. Then we have

$$\left\| \widetilde{\rho}_q - |\Psi_0\rangle\langle\Psi_0| \right\| \lesssim \|h\| \ell^2 dq^{1/2} e^{-a\ell/3} e^{qa^2v^2/2} + e^{-\frac{1}{2}\gamma^2 q}. \tag{4.2.16}$$

Proof. The proof relies on a Duhamel formula:

$$\begin{aligned}
\|\widetilde{\rho}_q - |\Psi_0\rangle\langle\Psi_0|\| &\leq \|\widetilde{\rho}_q - \rho_q\| + \|\rho_q - |\Psi_0\rangle\langle\Psi_0|\|, \\
&\leq \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} \|e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} - e^{\mathrm{i}Ht}\| e^{-\frac{t^2}{2q}} \,\mathrm{d}t + e^{-\frac{1}{2}\gamma^2 q}, \\
&\lesssim \|h\| \ell^2 dq^{1/2} e^{-a\ell/3} e^{qa^2v^2/2} + e^{-\frac{1}{2}\gamma^2 q},
\end{aligned}$$

where we have used Lemma 4.2.9. □

Lemma 4.2.11. *Let $\widetilde{H}_L(q)$ and $\widetilde{H}_R(q)$ be the operators defined in Lemma 4.2.9. Let $\alpha > 0$ and $O_R(q)$ and $O_L(q)$ be the following spectral projections*

$$O_L(q) = \sum_{|\lambda| \leq \alpha} |\Phi_\lambda^{(L)}\rangle\langle\Phi_\lambda^{(L)}|, \quad O_R(q) = \sum_{|\lambda| \leq \alpha} |\Phi_\lambda^{(R)}\rangle\langle\Phi_\lambda^{(R)}|, \tag{4.2.17}$$

where $(\Phi_\lambda^{(L)})$ and $(\Phi_\lambda^{(R)})$ are the normalised eigenvectors of $\widetilde{H}_L(q)$ and $\widetilde{H}_R(q)$. Then we have

$$\|O_R O_L \Psi_0 - \Psi_0\| \leq \frac{1}{\alpha} \Big(\|\widetilde{H}_L(q) - H_L(q)\| + \|\widetilde{H}_R(q) - H_R(q)\| + \|H_L\Psi_0\| + \|H_R\Psi_0\| \Big), \tag{4.2.18}$$

and

$$\|(e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} - \mathrm{id}) O_L O_R\| \leq 2\alpha|t|. \tag{4.2.19}$$

Proof. We first prove the estimate (4.2.18). Since $O_L(q)$ and $O_R(q)$ commute and are bounded operators by 1, we have

$$\|O_L O_R \Psi_0 - \Psi_0\| \leq \|O_L\Psi_0 - \Psi_0\| + \|O_R\Psi_0 - \Psi_0\|. \tag{4.2.20}$$

We have

$$\begin{aligned}
\|O_L\Psi_0 - \Psi_0\| &\leq \Big\| \int_{|\lambda| \geq \alpha} \mathrm{d}P_\lambda^{\widetilde{H}_L(q)}(\Psi_0) \Big\| \\
&\leq \frac{1}{\alpha} \Big\| \int_{|\lambda| \geq \alpha} \lambda \mathrm{d}P_\lambda^{\widetilde{H}_L(q)}(\Psi_0) \Big\| \\
&\leq \frac{1}{\alpha} \|\widetilde{H}_L(q)\Psi_0\| \\
&\leq \frac{1}{\alpha} \big(\|\widetilde{H}_L(q) - H_L(q)\| + \|H_L\Psi_0\| \big).
\end{aligned}$$

Estimate (4.2.19) follows from the definition of O_L and O_R. □

A final lemma is needed before completing the proof of Theorem 4.2.4 about the splitting of the evolution $e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}$.

Lemma 4.2.12. *With the notation in Lemma 4.2.9, there is a family of operators $\widetilde{H}_M^{(\ell)}(t) \in \mathcal{L}(\mathcal{H}_{j-\ell:j+\ell})$ such that*

$$\left\| e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} - \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)^*\, e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}\right\| \leq t\|h\|\ell^2 d\exp(-a(\ell/3-v|t|)), \quad (4.2.21)$$

where for a family of operators $A(t)$, $\mathcal{T}\exp\big(\int_0^t A(\tau)\,\mathrm{d}\tau\big)$ is the time-ordered exponential.

Proof. We can write

$$e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} = e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}.$$

By differentiating we notice that $e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}$ is the solution to

$$\begin{cases} \mathrm{i}U'(t) = U(t)e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} \\ U(0) = \mathrm{id}\,. \end{cases}$$

Alternatively, the solution to the equation above can be written

$$e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} = \mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big)^*.$$

Using a Lieb-Robinson bound and Corollary 4.2.3, there is a family of operators $\widetilde{H}_M^{(\ell)}(t)$ such that for all $t\in\mathbb{R}$, $\widetilde{H}_M^{(\ell)}(t)\in\mathcal{L}(\mathcal{H}_{j-\ell:j+\ell})$ and

$$\left\| e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} - \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(t)\otimes\mathrm{id}_{j+\ell+1:d}\right\| \leq \|h\|\ell^2 d\exp(-a(\ell/3-v|t|)).$$

It remains to bound the difference between $\mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big)$ and $\mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)$. Recall that for a family of operators $A(t)$, the time-ordered exponential is defined by

$$\mathcal{T}\exp\Big(\int_0^t A(\tau)\,\mathrm{d}\tau\Big) = \lim_{N\to\infty} e^{A(t_N)\Delta t}e^{A(t_{N-1})\Delta t}\cdots e^{A(t_1)\Delta t}, \quad t_k = k\Delta t, \quad \Delta t = \frac{t}{N}.$$

By a Duhamel formula, the difference of the time-ordered exponentials can be bounded by

$$\Big\|\mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big) - \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)\Big\| \leq t\|h\|\ell^2 d\exp(-a(\ell/3-v|t|)).$$

This finishes the proof of the lemma. □

We have now all the ingredients to prove Hastings area law 4.2.4.

Proof of Theorem 4.2.4. Let O_L and O_R be the operators defined in Lemma 4.2.11. Then we have

$$|\Psi_0\rangle\langle\Psi_0| = |\Psi_0\rangle\langle\Psi_0|O_LO_R + \frac{1}{\alpha}\mathcal{O}(\|\widetilde{H}_L(q)-H_L(q)\|+\|\widetilde{H}_R(q)-H_R(q)\|+\|H_L\Psi_0\|+\|H_R\Psi_0\|).$$

Thus with Lemma 4.2.8 and Lemma 4.2.9, we obtain

$$|\Psi_0\rangle\langle\Psi_0| = |\Psi_0\rangle\langle\Psi_0|O_LO_R + \frac{1}{\alpha}\mathcal{O}\Big(\gamma J e^{-\frac{1}{2}\gamma^2 q} + \|h\|\ell^2 d q^{1/2}e^{-a\ell/3}e^{qa^2v^2}\Big).$$

Using that O_L and O_R are bounded operators by 1, in combination with Lemma 4.2.10, we get

$$\begin{aligned}|\Psi_0\rangle\langle\Psi_0| &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}e^{-\frac{t^2}{2q}}O_LO_R\,\mathrm{d}t + \mathcal{O}\Big(\frac{\|h\|\ell^2 d}{\alpha}q^{1/2}e^{-a\ell/3}e^{qa^2v^2} + \frac{\gamma J}{\alpha}e^{-\frac{1}{2}\gamma^2 q}\Big)\\ &= \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}}\mathcal{T}\exp\Big(\int_0^t e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}H_M e^{-\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))\tau}\,\mathrm{d}\tau\Big)^* e^{-\frac{t^2}{2q}}e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}O_LO_R\,\mathrm{d}t\\ &\quad + \mathcal{O}\Big(\frac{\|h\|\ell^2 d}{\alpha}q^{1/2}e^{-a\ell/3}e^{qa^2v^2} + \frac{\gamma J}{\alpha}e^{-\frac{1}{2}\gamma^2 q}\Big),\end{aligned}$$

where we have used Lemma 4.2.12. By Lemma 4.2.11, we thus have

$$\begin{aligned}|\Psi_0\rangle\langle\Psi_0| = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}}\mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)^* e^{-\frac{t^2}{2q}}O_LO_R\,\mathrm{d}t\\ + \mathcal{O}\Big(\alpha q^{1/2} + \frac{\|h\|\ell^2 d}{\alpha}q^{1/2}e^{-a\ell/3}e^{qa^2v^2} + \frac{\gamma J}{\alpha}e^{-\frac{1}{2}\gamma^2 q}\Big).\end{aligned}$$

All it remains to do is to set the parameters α and q to prove Theorem 4.2.4. Taking $q = \tilde{q}\ell$ such that $\big(\frac{\gamma^2}{2}+av^2\big)\tilde{q} < \frac{a}{3}$ and $\alpha < e^{-\frac{1}{2}\gamma^2\tilde{q}\ell}$ give (4.2.5). □

Chapter 5

DMRG for the electronic Schrödinger equation

Density matrix renormalisation group [Whi92] (DMRG) is an alternating scheme to solve linear problems or eigenvalue problems in the tensor train format. In the mathematical community, it is also referred to the *alternating linear scheme* (ALS) in its simplest version or to the *modified ALS (MALS)* [HRS12a], which is the equivalent to the two-site DMRG. In DMRG, given a hermitian matrix $H \in \mathbb{C}^{n_1 \cdots n_L \times n_1 \cdots n_L}$, we want to solve for $x \in \mathbb{C}^{n_1 \cdots n_L}$ the linear problem

$$Hx = b, \tag{5.0.1}$$

for a given $b \in \mathbb{C}^{n_1 \cdots n_L}$, or for $(\lambda, x) \in \mathbb{R} \times \mathbb{C}^{n_1 \cdots n_L}$ the lowest eigenvalue problem

$$Hx = \lambda x. \tag{5.0.2}$$

For both problems, a tensor train representation of the operator H is needed in order to efficiently implement the DMRG algorithm.

5.1 Tensor train operators

Tensor train operators are also called *matrix product operators* in physics.

5.1.1 Definition and graphical representation

Definition 5.1.1 (Tensor train operator)**.** *Let $H \in \mathbb{C}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ be a matrix. A tensor train operator (TTO) representation of the matrix is any tuple of order 4 tensors $(H_1, \ldots, H_L)$, $H_k \in \mathbb{C}^{n_k \times n_k \times R_{k-1} \times R_k}$ ($R_0 = R_L = 1$) such that*

$$H^{j_1 \cdots j_L}_{i_1 \ldots i_L} = H_1[i_1, j_1] \cdots H_L[i_L, j_L], \forall\, i_k, j_k = 1, \ldots, n_k.$$

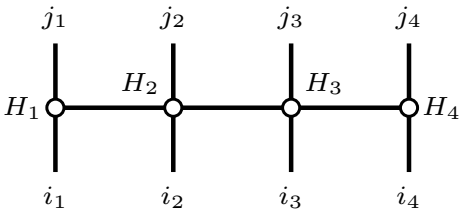


Figure 5.1: Diagrammatic representation of a TTO

The diagrammatic representation of a TTO is similar to the diagrammatic of a TT as illustrated in Figure 5.1.

A TTO representation of a matrix can be obtained by reordering the indices of the matrix H and performing a TT-SVD of the resulting tensor. More precisely, by defining the tensor $\widetilde{H} \in \mathbb{C}^{n_1^2 \times \cdots \times n_L^2}$

$$\widetilde{H}_{i_1 j_1 ; \ldots ; i_L j_L} = H_{i_1 \ldots i_L}^{j_1 \ldots j_L},$$

we realise that a TTO representation is simply a TT representation of $\widetilde{H}$.

Proposition 5.1.2. *Let $H \in \mathbb{C}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ be a hermitian matrix. Then there is a TTO representation of H such that*

$$\forall\, 1 \leq i_k, j_k \leq n_k, \;\; H_k[i_k, j_k] = H_k[j_k, i_k], \quad k = 1, \ldots, L. \tag{5.1.1}$$

Proof. □

Example 5.1.3. *Let us consider the following matrix $H \in \mathbb{C}^{n^L \times n^L}$*

$$H = h \otimes \mathrm{id} \otimes \cdots \otimes \mathrm{id} + \cdots + \mathrm{id} \otimes \mathrm{id} \otimes \cdots \otimes h, \tag{5.1.2}$$

where $h \in \mathbb{C}^{n \times n}$ is a hermitian matrix and id *is the identity in $\mathbb{C}^{n \times n}$. The matrix $h \otimes \mathrm{id} \otimes \cdots \otimes \mathrm{id}$ is in fact a TTO of rank 1. A naïve application of Proposition 5.1.4 yields a TTO representation of H of rank L. However it is possible to achieve a rank 2 representation with the following construction*

$$\begin{aligned} H_1[i_1, j_1] &= \begin{pmatrix} h_{i_1 j_1} & \delta_{i_1 j_1} \end{pmatrix}, \quad H_L[i_L, j_L] = \begin{pmatrix} \delta_{i_L j_L} \\ h_{i_L j_L} \end{pmatrix} \\ H_k[i_k, j_k] &= \begin{pmatrix} \delta_{i_k j_k} & 0 \\ h_{i_k j_k} & \delta_{i_k j_k} \end{pmatrix}, \quad k = 2, \ldots, L-1. \end{aligned} \tag{5.1.3}$$

Note that this representation also satisfies the property stated in Proposition 5.1.2.

5.1.2 Algebraic properties

Like the TT representation of vectors, the TTO format has some algebraic stability property.

Proposition 5.1.4. *Let $G, H \in \mathbb{C}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ be matrices and $(G_1, \ldots, G_L)$, $G_k \in \mathbb{C}^{n_k \times n_k \times R^G_{k-1} \times R^G_k}$ and $(H_1, \ldots, H_L)$, $H_k \in \mathbb{C}^{n_k \times n_k \times R^H_{k-1} \times R^H_k}$ be respectively TTO representations of G and H. Let $A, B \in \mathbb{C}^{n_1 \cdots n_L}$ be vectors with respcetive TT representations $(A_1, \ldots, A_L)$, $A_k \in \mathbb{C}^{n_k \times r^A_{k-1} \times r^A_k}$, $(B_1, \ldots, B_L)$, $B_k \in \mathbb{C}^{n_k \times r^B_{k-1} \times r^B_k}$. Then*

(i). the sum $G + H$ has a TTO representation $(S_1, \ldots, S_L)$ given by

$$\begin{gathered} S_1[i_1, j_1] = \begin{pmatrix} G_1[i_1, j_1] & H_1[i_1, j_1] \end{pmatrix}, \quad S_L[i_L, j_L] = \begin{pmatrix} G_L[i_L, j_L] \\ H_L[i_L, j_L] \end{pmatrix} \\ S_k[i_k, j_k] = \begin{pmatrix} G_k[i_k, j_k] & 0 \\ 0 & H_k[i_k, j_k] \end{pmatrix}, k = 2, \ldots, L-1 \end{gathered} \tag{5.1.4}$$

(ii). the matrix-vector product $C = HA$ has a TT representation $(C_1, \ldots, C_L)$ with $C_k[j_k] \in \mathbb{C}^{R^H_{k-1} r^A_{k-1} \times R^H_k r^A_k}$

$$C_k[i_k] = \sum_{j_k=1}^{n_k} H_k[i_k, j_k] \otimes A_k[j_k], \quad k = 1, \ldots, L. \tag{5.1.5}$$

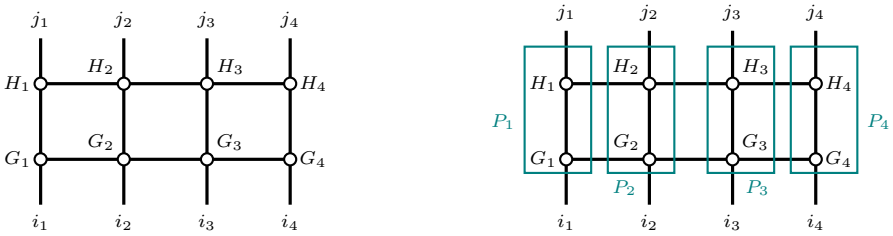
(iii). the product GH has a TTO representation $(P_1, \ldots, P_L)$ given by

$$P_k[i_k, j_k] = \sum_{\ell_k=1}^{n_k} G_k[i_k, \ell_k] \otimes H_k[\ell_k, j_k], \quad k = 1, \ldots, L. \tag{5.1.6}$$

Proof. This is a direct computation. □

Remark 5.1.5. *The TTO representations of the sum and the product of the operators are not optimal. This is clear in the case of the sum $G + H$ when we consider $G = H$. A TT rounding step is required in order to reduce the TTO ranks of the representation. This is not innocuous as essential properties of the matrix can be lost in the rounding procedure (symmetry for instance).*

A diagrammatic proof of the formula for the product of two TTO representations is given in Figure 5.2, avoiding cumbersome computations.



(a) Diagrammatic representation of the product of two TTO

(b) Diagrammatic representation of the product of two TTO

Figure 5.2: Diagrammatic proof of the product of two TTO. The left panel is the diagrammatic representation of the product of two TTO. On the right panel, the boxed tensors P_k are the TTO cores of a TTO representation of the product GH, provided that the double edges shared between neighbouring P_k are gathered into one edge.

5.1.3 The electronic Hamiltonian as a TTO

The electronic Hamiltonian operator in second quantisation is given by

$$H = \sum_{i,j=1}^{L} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,\ell=1}^{L} V_{ijk\ell} c_i^\dagger c_j^\dagger c_\ell c_k, \tag{5.1.7}$$

where h_{ij} (resp. $V_{ijk\ell}$) correspond to the one-electron integrals and two-electron integrals with Mulliken's convention [HJO14]. The tensor representation of the creation $c_i^\dagger$ and annihilation c_i operators can be written as a tensor product of 2×2 matrices

$$c_i = Z \otimes \cdots \otimes Z \otimes C \otimes \mathrm{id}_2 \otimes \cdots \otimes \mathrm{id}_2 \in \mathbb{R}^{2^L \times 2^L}, \tag{5.1.8}$$

$$c_i^\dagger = Z \otimes \cdots \otimes Z \otimes C^* \otimes \mathrm{id}_2 \otimes \cdots \otimes \mathrm{id}_2 \in \mathbb{R}^{2^L \times 2^L}, \tag{5.1.9}$$

where C (resp. C^*) appears in the i-th position and

$$C = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad \text{and} \quad Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Since the creation and annihilation operators are written as Kronecker products, their TTO rank is 1. Using the algebraic properties of TTOs in Proposition 5.1.4, a naïve implementation of the TTO of an electronic Hamiltonian has TTO rank scaling as L^4.

Noticing that the reshape of the two-body interaction at any cut is at most of rank L^2, we deduce that the TTO rank of the electronic Hamiltonian can be reduced to $\mathcal{O}(L^2)$ [CKN+16, BGP22]. The TT-SVD is useful to compress these ranks to the optimal ones. To preserve the particle and the Hermitian symmetries of the Hamiltonian, this procedure has to done with great care.

Remark 5.1.6. *In popular implementations of QC-DMRG, it is usual to work in the* space orbital picture*. Namely instead of having sites that can be either occupied or unoccupied, sites can be unoccupied, occupied with spin up or down, or doubly occupied. The expression of the electronic Hamiltonian is similar to the spin orbital case. The main reason of using this representation is that it is more suited for an implementation that preserves the $SU(2)$ symmetry.*

5.2 The DMRG algorithm

The DMRG algorithm is an algorithm to solve linear systems $Hx_* = b$ or the lowest eigenvalue problem $Hx_* = \lambda x_*$ using the variational characterisation of the solution to both problems. As such it is limited in the resolution of linear problems with *hermitian* matrices. In the following, we assume that H is a hermitian, positive-definite matrix.

Assumption 5.2.1. *The matrix $H \in \mathbb{C}^{n_1\cdots n_L \times n_1 \cdots n_L}$ is Hermitian and positive-definite.*

The solution to the linear system $Hx = b$ is also the minimiser of the functional

$$x_* = \underset{x\in\mathbb{C}^{n_1\cdots n_L}}{\arg\min} \frac{1}{2}\langle x, Hx\rangle - \langle b, x\rangle. \tag{5.2.1}$$

Using the Rayleigh-Ritz principle, the lowest eigenvalue of H is given by

$$x_* = \underset{x\in\mathbb{C}^{n_1\cdots n_L}}{\arg\min} \frac{\langle x, Hx\rangle}{\langle x, x\rangle}. \tag{5.2.2}$$

5.2.1 General algorithm

The DMRG algorithm, also known as *alternating linear scheme* (ALS) [HRS12a], is an alternating optimisation over the TT manifold. The general idea is to perform a descent step for each TT core separately. More precisely, the solution to the linear system $Hx_* = b$ is approximated on the TT manifold

$$\mathscr{M}_{\mathrm{TT}_{\leq r}} = \left\{C \mid \forall\, 1 \leq i_k \leq n_k, C_{i_1\ldots i_L} = A_1[i_1]\cdots A_L[i_L], A_k[i_k] \in \mathbb{C}^{r_{k-1}\times r_k}, r_k \leq r\right\}. \tag{5.2.3}$$

Denoting by j the map $J \circ \mathrm{TT}$ where

$$\mathrm{TT} \ : \begin{cases} \mathbb{C}^{n_1\times r_0\times r_1} \times \cdots \times \mathbb{C}^{n_L\times r_{L-1}\times r_L} \to \mathbb{C}^{n_1\cdots n_L} \\ \qquad\qquad (A_1, \ldots, A_L) \mapsto (A_1[i_1]\cdots A_L[i_L]), \end{cases}$$

and $J(x) = \frac{1}{2}\langle x, Hx\rangle - \langle b, x\rangle$.

Minimising J over the manifold $\mathscr{M}_{\mathrm{TT}_{\leq r}}$ is the same as minimising the functional j.

Algorithm 3 DMRG with sweeps

Input: $(A_1^{(0)}, \dots, A_L^{(0)})$ in right-orthogonal TT representation
Output: $(A_1^{(n)}, \dots, A_L^{(n)}) \in \mathscr{M}_{\mathrm{TT}_{\leq r}}$ approximation of the minimiser in of J

function DMRG($(A_1^{(0)}, \dots, A_L^{(0)})$)
  $n = 0$
  while `not converged` **do**
    for $k = 1, 2, \dots, L-1$ **do** ▷ Forward half-sweep

$$B_k^{(n+\frac{1}{2})} = \underset{V_k \in \mathbb{C}^{r_{k-1} \times n_k \times r_k}}{\arg\min} j(A_1^{(n+\frac{1}{2})}, \dots, A_{k-1}^{(n+\frac{1}{2})}, V_k, A_{k+1}^{(n)}, \dots, A_L^{(n)}) \tag{5.2.4}$$

$Q, R = \mathtt{qr}(\big(B_k^{(n+\frac{1}{2})}\big)_{\alpha_{k-1} i_k}^{\beta_k})$ ▷ QR decomposition
$\big(A_k^{(n+\frac{1}{2})}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = Q_{\alpha_{k-1} i_k}^{\alpha_k}$ ▷ Keep Q
$\big(A_{k+1}^{(n)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}} \leftarrow \big(R A_{k+1}^{(n)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}}$. ▷ Shift R to the right
    end for
    for $k = d, d-1, \dots, 2$ **do** ▷ Backward half-sweep

$$B_k^{(n+1)} = \underset{V_k \in \mathbb{C}^{r_{k-1} \times n_k \times r_k}}{\arg\min} j(A_1^{(n+\frac{1}{2})}, \dots, A_{k-1}^{(n+\frac{1}{2})}, V_k, A_{k+1}^{(n+1)}, \dots, A_L^{(n+1)}) \tag{5.2.5}$$

$L, Q = \mathtt{lq}\Big(\big(B_k^{(n+1)}\big)_{\alpha_{k-1}}^{\beta_k i_k}\Big)$ ▷ LQ decomposition
$\big(A_k^{(n+1)}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = \big(Q\big)_{\alpha_{k-1}}^{\alpha_k i_k}$ ▷ Keep Q
$\big(A_{k-1}^{(n+\frac{1}{2})}[i_{k-1}]\big)_{\alpha_{k-2}}^{\alpha_{k-1}} \leftarrow \big(A_{k-1}^{(n+\frac{1}{2})}[i_{k-1}] L\big)_{\alpha_{k-2}}^{\alpha_{k-1}}$ ▷ Shift L to the left
    end for
    $n = n + 1$
  end while
  return $(A_1^{(n)}, \dots, A_L^{(n)})$
end function

The optimisation steps (5.2.4) and (5.2.5) are called *microsteps*. An iteration over the loop n is called a sweep. Notice that at each microstep (5.2.4) or (5.2.5) the left TT cores are left-orthogonal and the right-TT cores are right-orthogonal.

The microsteps of the DMRG algorithm applied to the linear problem $Hx_* = b$ are linear problems involving an operator $P_k : \mathbb{C}^{r_{k-1}\times n_k\times r_k} \to \mathbb{C}^{n_1\times\cdots\times n_L}$ defined by

$$(P_k V)_{i_1\dots i_L} = A_1[i_1]\cdots A_{k-1}[i_{k-1}]V[i_k]A_{k+1}[i_{k+1}]\cdots A_L[i_L], \tag{5.2.6}$$

where $(A_1,\dots,A_L)$ are TT cores that are left-orthogonal for $j \le k-1$ and right-orthogonal for $j \ge k+1$. The tensor $B_k^{(n+\frac{1}{2})}$ of the microstep problem (5.2.4) is the solution to the linear system

$$P_k^* K P_k B_k^{(n+\frac{1}{2})} = P_k^* b. \tag{5.2.7}$$

Proposition 5.2.2. *Assume that $(A_i^{(n+\frac{1}{2})})_{1\le i\le k-1}$ are left-orthogonal and $(A_i^{(n)})_{k+1\le i\le L}$ are right-orthogonal. Then the microstep (5.2.4) has a unique solution.*

Proof. It is equivalent to check that eq. (5.2.7) has a unique solution, *i.e.* that the matrix $P_k^* H P_k$ is invertible. As H is hermitian and positive-definite, it is sufficient to prove that P_k is an injective operator. Let $V \in \mathbb{C}^{r_{k-1}\times n_k\times r_k}$ such that $\|P_k V\| = 0$. Then we have

$$\begin{aligned}
\|P_k V\|^2 &= \sum_{i_1=1}^{n_1}\cdots\sum_{i_L=1}^{n_L} \operatorname{Tr}\big(A_L[i_L]^*\cdots A_{k+1}[i_{k+1}]^* V[i_k]^* A_{k-1}[i_{k-1}]^*\cdots A_1[i_1]^* \\
&\qquad\qquad A_1[i_1]\cdots A_{k-1}[i_{k-1}]V[i_k]A_{k+1}[i_{k+1}]\cdots A_L[i_L]\big) \\
&= \sum_{i_1=1}^{n_1}\cdots\sum_{i_L=1}^{n_L} \operatorname{Tr}\big(V[i_k]^* A_{k-1}[i_{k-1}]^*\cdots A_1[i_1]^* A_1[i_1]\cdots A_{k-1}[i_{k-1}]V[i_k] \\
&\qquad\qquad A_{k+1}[i_{k+1}]\cdots A_L[i_L]A_L[i_L]^*\cdots A_{k+1}[i_{k+1}]^*\big) \\
&= \sum_{i_k=1}^{n_k} \operatorname{Tr}\big(V[i_k]^* V[i_k]\big),
\end{aligned}$$

where we have used the cyclicity of the trace and the orthogonality of the TT cores. Hence $P_k V = 0$ if and only if $V = 0$. □

The condition number of the microstep (5.2.7) is bounded by the condition number of the matrix H.

Proposition 5.2.3. *The condition number of the linear system (5.2.7) is bounded by the condition number of H,* i.e.

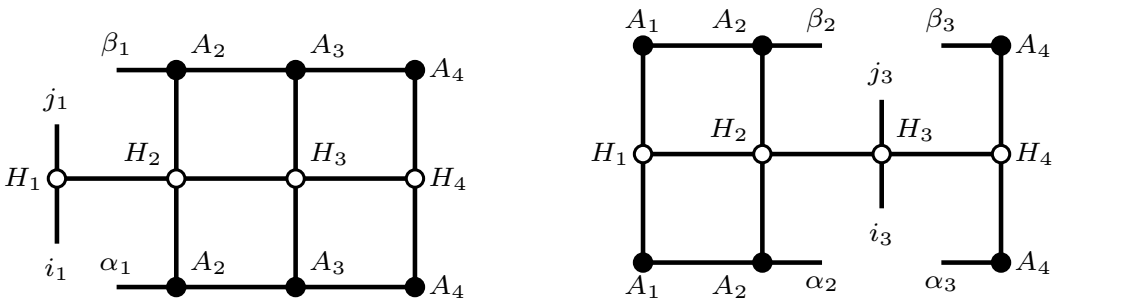
$$\operatorname{cond}_2 P_k^* H P_k \le \operatorname{cond}_2 A.$$

Proof. This follows from the inequalities $\lambda_{\min}(P_k^* A P_k) \ge \lambda_{\min}(A)$ and $\lambda_{\max}(P_k^* A P_k) \le \lambda_{\max}(A)$. □

5.2.2 Implementation details

In this part, we give some details about the implementation of the DMRG algorithm described in Algorithm 3, as well as the total computational cost of a sweep.

The matrix $P_k^* A P_k$ A critical step in DMRG, we want an efficient way to implement the effective matrix $P_k^* A P_k$ (see Figure 5.3).



(a) Effective matrix $(P_1^* H P_1)_{\alpha_1 i_1}^{\beta_1 j_1} \in \mathbb{R}^{r_1 n_1 \times r_1 n_1}$

(b) Effective matrix $(P_3^* H P_3)_{\alpha_2 i_2 \alpha_3}^{\beta_2 j_3 \beta_3} \in \mathbb{R}^{r_2 n_3 r_3 \times r_2 n_3 r_3}$

Figure 5.3: Examples of $P_k^* H P_k$

As the TT ranks can be large (of the order of $10^3 - 10^4$), it is inefficient and useless to build the effective matrix $P_k^* H P_k$. Instead, what is needed is the matrix-vector product $P_k^* H P_k A_k$ where $A_k \in \mathbb{R}^{r_{k-1} n_k r_k}$. For this, a splitting of the effective Hamiltonian is used and it is written

$$\left(P_k^* H P_k\right)_{\alpha_{k-1} i_k \alpha_k}^{\beta_{k-1} j_k \beta_k} = \sum_{\nu_k=1}^{R_k} \left(\mathcal{L}_k\right)_{\alpha_{k-1} i_k}^{\beta_{k-1} j_k \nu_k} \left(\mathcal{R}_k\right)_{\alpha_k \nu_k}^{\beta_k}. \tag{5.2.8}$$

This splitting is illustrated in Figure 5.4.

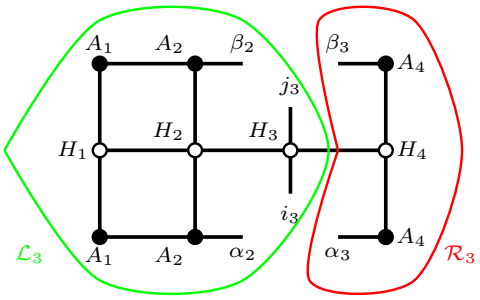


Figure 5.4: Splitting of the effective Hamiltonian

The computation of the matrix-vector multiplication goes as follows

$$\left(P_k^* H P_k\right)_{\alpha_{k-1} i_k \alpha_k}^{\beta_{k-1} j_k \beta_k} \left(A_k\right)_{\beta_{k-1} j_k \beta_k} = \left(\left(\mathcal{L}_k\right)_{\alpha_{k-1} i_k}^{\beta_{k-1} j_k \nu_k} \left(A_k\right)_{\beta_{k-1} j_k \beta_k}\right) \left(\mathcal{R}_k\right)_{\alpha_k \nu_k}^{\beta_k},$$

i.e.

(i). first, we compute for $1 \leq i_k \leq n_k, 1 \leq \nu_k \leq R_k, 1 \leq \alpha_{k-1}, 1 \leq \beta_k \leq r_k$ the sum

$$\sum_{\beta_{k-1}=1}^{r_{k-1}} \sum_{j_k=1}^{n_k} \left(\mathcal{L}_k\right)_{\alpha_{k-1} i_k}^{\beta_{k-1} j_k \nu_k} \left(A_k\right)_{\beta_{k-1} j_k \beta_k}.$$

This scales as $\mathcal{O}(n^2 r^2 R)$.

(ii). in the second step, the previous tensor is contracted with $\mathcal{R}_k$: for $1 \leq \alpha_{k-1} \leq r_{k-1}, 1 \leq \alpha_k \leq r_k, 1 \leq i_k \leq n_k$, we sum

$$\sum_{\nu_k=1}^{R_k} \sum_{\beta_k=1}^{r_k} \left(\mathcal{L}_k A_k\right)_{\alpha_{k-1} i_k \beta_k}^{\nu_k} \left(\mathcal{R}_k\right)_{\alpha_k \nu_k}^{\beta_k}$$

This scales as $\mathcal{O}(nRr^3)$.

So overall the matrix-vector multiplication costs $\mathcal{O}(n^2 r^2 R + nRr^3)$.

The assembly of the left $\mathcal{L}_k$ and right $\mathcal{R}_k$ splitting of the effective Hamiltonian has a similar cost.

The RHS $P_k^* b$

5.3 Convergence of DMRG

The global convergence of DMRG is a difficult problem, as the TT manifold is not a convex set. The convergence results on DMRG are local and assume that the Hessian of the functional j is of full-rank.

Assumption 5.3.1. *At the local minimiser A_*, the Hessian j'' is of full rank*

$$\operatorname{rank} j''(A_*) = \sum_{i=1}^{L} r_{i-1} n_i r_i - \sum_{i=1}^{L-1} r_i^2, \quad \textit{i.e. } \ker j''(A_*) = T_{A_*} \mathcal{M}_{\mathrm{TT}_{\leq r}}. \tag{5.3.1}$$

5.3.1 Local convergence of DMRG

Assumption 5.3.1 ensures that the Hessian is invertible at the solution to the DMRG equations.

Theorem 5.3.2 ([RU13, Theorem 2.7]). *There exists a neighbourhood W of A_* such that Algorithm 3 initiated with $A^{(0)} \in W$ converges to the minimiser A_*.*

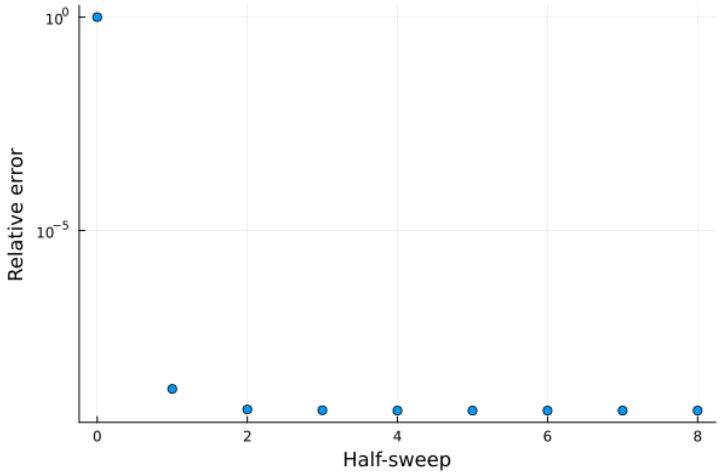


Figure 5.5: Convergence to the solution of $Hx = b$ with H the discrete Laplacian in $\mathbb{R}^{4^8 \times 4^8}$ b a random tensor of TT rank 2. The reference solution has TT rank 10.

5.3.2 Half-sweep convergence

A more surprising result states that if the TT ranks in the DMRG algorithm are exactly the TT ranks of the sought solution, then DMRG returns the *exact* solution in a half-sweep (see Figure 5.5).

This result is shown in the case of $H = \mathrm{id}$ in [HRS12a].

Proposition 5.3.3 ([HRS12a, Lemma 4.2])**.** *The DMRG algorithm applied with $H = \mathrm{id}$ converges in a half-sweep for almost all initial guess with the same TT rank as the right hand side.*

The condition on the initial guess is related to a nondeficiency of the initialisation of the DMRG algorithm.

Remark 5.3.4. *A similar result holds for tensor rings, see [CLL20].*

5.4 Two-site DMRG: how to dynamically adapt the TT ranks

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