Tensor trains for high-dimensional problems

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February 22, 2024

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Introduction

These notes are a short introduction to the tensor train decomposition, with a particular focus on solving linear equations within this format. 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. Approximation results for the tensor train format as well as the tensor train manifold are discussed.

The second part deals with the numerical resolution of linear systems or eigenvalue problems. The historical algorithm is an alternating scheme, known as the density matrix renormalisation group (DMRG) [Whi92, HRS12a], using the variational formulation of symmetric linear problems. Another way to solve linear problems is to adapt the classical iterative methods to the tensor train format [KU16]. Both approaches are presented and discussed in the present notes.

These notes are inspired by the following texts on the tensor train decomposition [Hac12, Hac14, Sch11, BSU16, UV20].

Chapter 1

Tensor trains

1.1 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.

1.1.1 The low-rank approximation for matrices

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

Theorem 1.1.1 (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:

$$s_k = \max_{\dim V_k = k} \min_{x \in V_k} \frac{\|Ax\|_2}{\|x\|_2}. \tag{1.1.1}$$

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 1.1.2 (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

$$\|A - A_r\|_F = \Big(\sum_{k\geq r+1} s_k^2\Big)^{1/2}. \tag{1.1.2}$$

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 $M, N \in \mathbb{R}^{p\times q}$

$$\forall\, 1 \leq i, j \leq \min(p, q), 0 \leq j \leq d - i, s_{i+j-1}(M + N) \leq s_i(M) + s_j(N), \tag{1.1.3}$$

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 (1.1.3) 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 1.1.3. *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

$$\mathrm{dist}(A, \mathcal{U}\otimes\mathcal{V}) = \|A - \Pi_{\mathcal{U}\otimes\mathcal{V}} A\| = \min_{\substack{\widetilde{\mathcal{U}}\subset\mathbb{C}^m, \dim\widetilde{\mathcal{U}}=r \\ \widetilde{\mathcal{V}}\subset\mathbb{C}^n, \dim\widetilde{\mathcal{V}}=r}} \|A - \Pi_{\widetilde{\mathcal{U}}\otimes\widetilde{\mathcal{V}}} A\|, \tag{1.1.4}$$

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 $(u_i \otimes v_j)_{1\leq i\leq m, 1\leq j\leq n}$:

$$A = \sum_{k=1}^{r_A} s_k u_k \otimes v_k. \tag{1.1.5}$$

Proposition 1.1.4. *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 (1.1.4) is given by*

$$\mathcal{U} = \mathrm{Span}(u_1,\dots,u_r), \quad \mathcal{V} = \mathrm{Span}(v_1,\dots,v_r). \tag{1.1.6}$$

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 (1.1.4) 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 (1.1.4) 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 $\widetilde{\mathcal{V}} = \mathrm{Span}(v_1,\dots,v_r)$. □

1.1.2 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 1.1. It is a powerful tool to avoid writing cumbersome operations between tensors, using the dictionary in Figure 1.2.

Definition 1.1.5 (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.

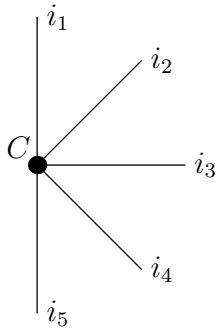
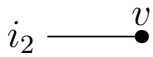
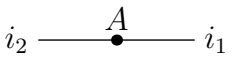


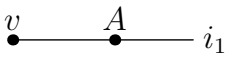
Figure 1.1: Graphical representation of C. The tensor C is represented by its vertex and its indices by the free edges.



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

1.1.3 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

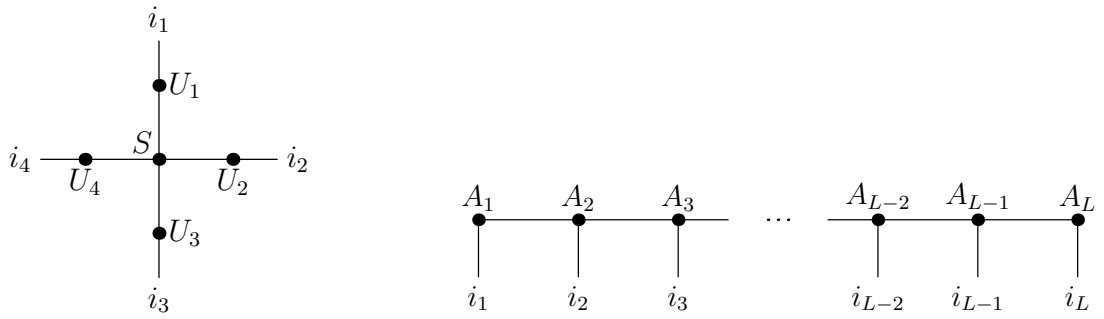
$$C - \left(\frac{1}{\varepsilon}(a + \varepsilon b) \otimes (a + \varepsilon b) \otimes (a + \varepsilon b) - \frac{1}{\varepsilon} a \otimes a \otimes a\right) = \mathcal{O}(\varepsilon). \tag{1.1.7}$$

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 1.3: Tucker and tensor train decompositions

1.2 Tensor train decomposition

1.2.1 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 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].

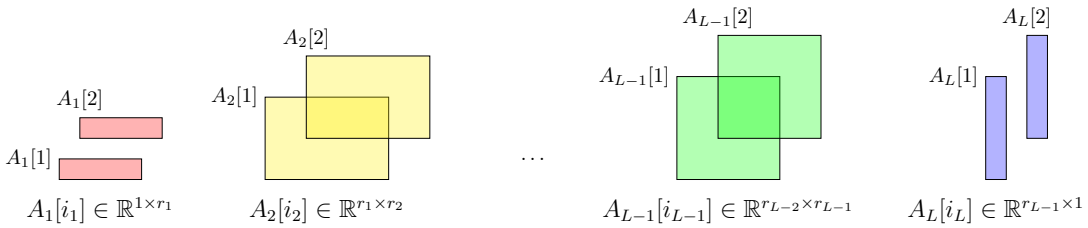


Figure 1.4: Schematic representation of the TT decomposition

Definition 1.2.1 ([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 $1 \le i_k \le n_k$*

$$C_{i_1\ldots i_L} = A_1[i_1]A_2[i_2]\cdots A_L[i_L] \tag{1.2.1}$$

$$= \sum_{\alpha_1=1}^{r_1}\sum_{\alpha_2=1}^{r_2}\cdots\sum_{\alpha_{L-1}=1}^{r_{L-1}} A_1[i_1]_{\alpha_1}A_2[i_2]_{\alpha_2}^{\alpha_1}\cdots A_L[i_L]^{\alpha_{L-1}}, \tag{1.2.2}$$

where for each $1 \le i_k \le n_k$, $A_k[i_k] \in \mathbb{C}^{r_{k-1}\times r_k}$ ($r_0 = r_L = 1$). 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 1.2.2.

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

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

  is a TT of rank 2: let $(B_k)_{1\le k\le 2L}$ 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 $\widetilde{B} \in \bigotimes_1^4\mathbb{C}^2$*

  $$\widetilde{B}_{i_1\ldots i_4} = \big(\delta_{1,i_1}\delta_{2,i_3} + \delta_{2,i_1}\delta_{1,i_3}\big)\big(\delta_{1,i_2}\delta_{2,i_4} + \delta_{2,i_3}\delta_{1,i_4}\big)$$

  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 1.2.3. *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 1.2.7.*

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 $(G_k)_{1 \le k \le L-1} \in \bigotimes_{k=1}^{L-1} \mathrm{GL}_{r_k}(\mathbb{C})$, 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 1.2.4 (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*

$$\begin{aligned} B_1[i_1] &= \begin{pmatrix} A_1[i_1] & \widetilde{A}_1[i_1] \end{pmatrix}, \quad B_L[i_L] = \begin{bmatrix} A_L[i_L] \\ \widetilde{A}_L[i_L] \end{bmatrix} \\ B_k[i_k] &= \begin{bmatrix} A_k[i_k] & 0 \\ 0 & \widetilde{A}_k[i_k] \end{bmatrix}, k = 2, \dots, L-1 \end{aligned} \tag{1.2.3}$$

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 (1.2.3) is in general not minimal and can be compressed as explained in Section 1.3.

Remark 1.2.5. *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.*

1.2.2 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 $C_{i_1 \dots i_{L-1}}^{i_L} \in \mathbb{C}^{n_1 \cdots n_{L-1} \times n_L}$, 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 $C_{i_1 \dots i_k}^{i_{k+1} \dots i_L} \in \mathbb{C}^{n_1 \cdots n_k \times n_{k+1} \cdots n_L}$ 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 1.3.

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.

1.2.3 Normalisation and gauge freedom

Definition 1.2.6. *We say that a TT decomposition $(A_1, \dots, A_L)$ is*

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

$$\sum_{i_k=1}^{n_k} A_k[i_k]^* A_k[i_k] = \mathrm{id}_{r_k}; \tag{1.2.4}$$

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

$$\sum_{i_k=1}^{n_k} A_k[i_k] A_k[i_k]^* = \mathrm{id}_{r_{k-1}}\,. \tag{1.2.5}$$

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 2).

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 $n+1 \leq k \leq L$

$$\sum_{i_k=1}^{n_k} A_k[i_k] A_k[i_k]^* = \mathrm{id}_{r_{k-1}}\,. \tag{1.2.6}$$

In that case, the norm of the tensor is carried by the TT core that is not normalised, using the following trick:

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

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

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

we repeat this process until we reach

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

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 1.2.7 (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 1.2.2 gives a TT decomposition of minimal TT rank;

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

$$r_k = \operatorname{Rank} C^{i_{k+1} \ldots i_L}_{i_1 \ldots i_k}. \tag{1.2.7}$$

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

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

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 $r_k = \operatorname{Rank} C^{i_{k+1} \ldots i_L}_{i_1 \ldots i_k}$. □

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

Proposition 1.2.8 (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 $(Q_k)_{1\leq k\leq L-1}$, $Q_k \in \mathbb{C}^{r_k \times r_k}$ such that for all $1 \leq i_k \leq n_k$ we have*

$$\begin{aligned} A_1[i_1]Q_1 = B_1[i_1], \quad Q_{L-1}^* A_L[i_L] = B_L[i_L] \\ Q_{k-1}^* A_k[i_k] Q_k = B_k[i_k], \ \text{for } k = 2, \dots, L-1. \end{aligned} \tag{1.2.8}$$

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

$$M_1 M_2 = N_1 N_2 \quad \text{and} \quad M_1^* M_1 = N_1^* N_1 = \mathrm{id}_r,$$

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

$$M_1 = N_1 Q \quad \text{and} \quad M_2 = Q^* N_2.$$

The proof of this lemma is straightforward:

$$N_2 = N_1^* M_1 M_2 = N_1^* M_1 M_1^* N_1 N_2,$$

which shows that $N_1^* M_1$ is a unitary matrix. Denote this matrix Q. Hence $N_2 = Q M_2$ and $M_1 N_1^* N_1 = M_1$ thus, $N_1 = M_1 Q^*$.

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

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

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

$$C_{i_1,\ldots,i_L} = \Gamma_1[i_1]\Sigma_1\Gamma_2[i_2]\Sigma_2\cdots\Sigma_{L-1}\Gamma_L[i_L], \tag{1.2.9}$$

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

$$\sum_{i_1=1}^{n_1}\Gamma_1[i_1]^*\Gamma_1[i_1] = \mathrm{id}_{r_1}, \quad \sum_{i_L=1}^{n_L}\Gamma_L[i_L]\Gamma_L[i_L]^* = \mathrm{id}_{r_{L-1}} \tag{1.2.10}$$

$$\forall\, k = 2,\ldots,L-1,\ \sum_{i_k=1}^{n_k}\Gamma_k[i_k]^*\Sigma_{k-1}^2\Gamma_k[i_k] = \mathrm{id}_{r_k}, \quad \sum_{i_k=1}^{n_k}\Gamma_k[i_k]\Sigma_k^2\Gamma_k[i_k]^* = \mathrm{id}_{r_{k-1}}\,. \tag{1.2.11}$$

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

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

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 $C^{i_{k+1}\ldots i_d}_{i_1\ldots i_k}$. Then we have

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

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 1.1 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 1.2.10. *Let $(\Gamma_k)_{1\leq k\leq L}$, $(\Sigma_k)_{1\leq k\leq L-1}$ 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

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

□

1.3 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:

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

we repeat the process until we get

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

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 1.3.1 ([Gra10, Ose11, Hac12, Hac14]). *Let $C \in \mathbb{C}^{n_1\times\cdots\times n_L}$, $(\tilde r_1,\dots,\tilde r_{L-1}) \in \mathbb{N}^{L-1}$ and $\mathcal{M}_{\tilde{\mathbf{r}}}$ be the space of tensor trains of ranks bounded by $(\tilde r_1,\dots,\tilde r_{L-1})$. Then we have*

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

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

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:

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

hence by iteration

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

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 $(A_1, \dots, A_L)$ be a right-orthogonal TT representation of the tensor $C \in \mathbb{C}^{n_1 \times \cdots \times n_L}$. The first reshape is

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

and since the TT cores $(A_2, \dots, A_L)$ are right-orthogonal, the matrix $V_2 = \begin{bmatrix} A_2[1] \cdots A_L[1] & \dots & A_2[n_2] \cdots A_L[n_k] \end{bmatrix}$ 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 1.2.

Algorithm 1.2 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**
    $U_k, \Sigma_k, V_k^* = \mathtt{svd}\left(\begin{bmatrix} A_k[1] \\ \vdots \\ A_k[n_k] \end{bmatrix} \right)$
    $r_k = \arg\max_r \|\Sigma_k[1:r] - \Sigma_k\| \leq \varepsilon$
    $(A_k^\varepsilon)_{i_k \alpha_{k-1}}^{\alpha_k} = (U_k)_{i_k \alpha_{k-1}}^{\alpha_k}, \quad i_k = 1, \dots, n_k, \alpha_{k-1} = 1, \dots, r_{k-1}, \alpha_k = 1, \dots, r_k$
    $A_{k+1}[i_{k+1}] = \Sigma_k[1:r] V_k^*[1:r, :] A_{k+1}[i_{k+1}], \quad i_{k+1} = 1, \dots, n_{k+1}$
  end for
  $A_L^\varepsilon = A_L$
  return $(A_1^\varepsilon, \dots, A_L^\varepsilon)$
end function

1.4 Manifold of tensor trains

Even in finite-dimensions, the example exhibited in eq. (1.1.7) 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 1.4.1. *The set of tensor trains with TT rank less that r*

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

is a closed set.

Proof. The proof follows from the characterisation of the TT ranks given by Theorem 1.2.7: 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 $C_{i_1 \ldots i_k}^{i_{k+1} \ldots i_L}$. We conclude by recalling that the set of matrices with rank less than r is a closed set. □

Proposition 1.4.2. *The set of tensor trains with TT rank $\mathbf{r} = (r_1, \ldots, r_{L-1})$*

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

is of dimension

$$\dim \mathcal{M}_{\mathrm{TT}_{\mathbf{r}}} = \sum_{i=1}^{L} r_{i-1} n_i r_i - \sum_{i=1}^{L-1} r_i^2. \tag{1.4.1}$$

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

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

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 1.4.3 (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

$$\delta A = \sum_{k=1}^{L} \delta A^{(k)}, \tag{1.4.2}$$

with

$$\delta A^{(k)}_{i_1 \dots i_L} = A_1[i_1] \cdots A_{k-1}[i_{k-1}] W_k[i_k] A_{k+1}[i_{k+1}] \cdots A_L[i_L], \tag{1.4.3}$$

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

$$\sum_{i_k=1}^{n_k} A_k[i_k]^* W_k[i_k] = \mathbf{0}_{r_k \times r_k}. \tag{1.4.4}$$

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 $\Gamma(t) \in \mathcal{M}_{\mathrm{TT}_\mathbf{r}}$, we can choose a left-orthogonal TT representation of $\Gamma(t)$ such that

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

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

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

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

The tangent vectors are hence necessarily of the form given by eq. (1.4.2)-(1.4.4). Dimension counting and invoking Proposition 1.4.2 show the uniqueness of the representation. □

Chapter 2

DMRG algorithm

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 symmetric matrix $H \in \mathbb{R}^{n_1 \cdots n_L \times n_1 \cdots n_L}$, we want to solve for $x \in \mathbb{R}^{n_1 \cdots n_L}$ the linear problem

$$Hx = b, \tag{2.0.1}$$

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

$$Hx = \lambda x. \tag{2.0.2}$$

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

2.1 Tensor train operators

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

2.1.1 Definition and graphical representation

Definition 2.1.1 (Tensor train operator)**.** *Let $H \in \mathbb{R}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ be a matrix. A tensor train operator (TTO) representation of the matrix is any tuple of order 4 tensors $(H_1, \ldots, H_L)$, $H_k \in \mathbb{R}^{n_k \times n_k \times R_{k-1} \times R_k}$ ($R_0 = R_L = 1$) such that*

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

$(R_0, \ldots, R_L)$ are the TTO ranks of the TTO representation $(H_1, \ldots, H_L)$. $(H_1, \ldots, H_L)$ are the TTO cores of the TTO representation.

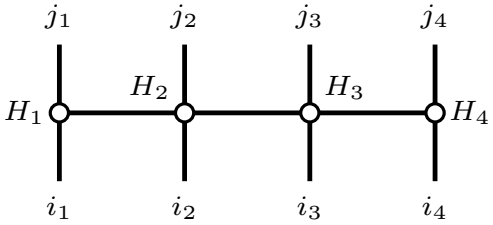


Figure 2.1: Diagrammatic representation of a TTO

In the context of tensor trains, this is the natural generalisation of the tensor product of operators. Indeed let $h_k \in \mathbb{R}^{n_k \times n_k}$ for $1 \leq k \leq L$, then the operator $H = h_1 \otimes \cdots \otimes h_L$ has a TTO representation of TTO rank 1 with TTO cores given by $H_k[i_k, j_k] = (h_k)_{i_k, j_k}$ for $1 \leq k \leq L$.

The diagrammatic representation of a TTO is similar to the diagrammatic of a TT as illustrated in Figure 2.1.

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

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

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

Proposition 2.1.2. *Let $H \in \mathbb{R}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ be a symmetric matrix. Then there is a TTO representation of H such that*

$$\forall\, 1 \leq i_k, j_k \leq n_k,\ H_k[i_k, j_k] = H_k[j_k, i_k], \quad k = 1, \ldots, L. \tag{2.1.1}$$

Proof. □

Example 2.1.3. *Let us consider the following matrix $H \in \mathbb{R}^{n^L \times n^L}$*

$$H = h \otimes \mathrm{id} \otimes \cdots \otimes \mathrm{id} + \cdots + \mathrm{id} \otimes \mathrm{id} \otimes \cdots \otimes h, \tag{2.1.2}$$

where $h \in \mathbb{R}^{n \times n}$ is a symmetric matrix and id *is the identity in $\mathbb{R}^{n \times n}$. The matrix $h \otimes \mathrm{id} \otimes \cdots \otimes \mathrm{id}$ is in fact a TTO of rank 1. A naïve application of Proposition 2.1.4 yields a TTO representation of H of rank L. However it is possible to achieve a rank 2 representation with the following construction*

$$\begin{aligned} H_1[i_1, j_1] &= \begin{pmatrix} h_{i_1 j_1} & \delta_{i_1 j_1} \end{pmatrix}, \quad H_L[i_L, j_L] = \begin{pmatrix} \delta_{i_L j_L} \\ h_{i_L j_L} \end{pmatrix} \\ H_k[i_k, j_k] &= \begin{pmatrix} \delta_{i_k j_k} & 0 \\ h_{i_k j_k} & \delta_{i_k j_k} \end{pmatrix}, \quad k = 2, \ldots, L-1. \end{aligned} \tag{2.1.3}$$

Note that this representation also satisfies the property stated in Proposition 2.1.2.

2.1.2 Algebraic properties

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

Proposition 2.1.4. *Let $G, H \in \mathbb{R}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ be matrices and $(G_1, \ldots, G_L)$, $G_k \in \mathbb{R}^{n_k \times n_k \times R^G_{k-1} \times R^G_k}$ and $(H_1, \ldots, H_L)$, $H_k \in \mathbb{R}^{n_k \times n_k \times R^H_{k-1} \times R^H_k}$ be respectively TTO representations of G and H. Let $A, B \in \mathbb{R}^{n_1 \cdots n_L}$ be vectors with respective TT representations $(A_1, \ldots, A_L)$, $A_k \in \mathbb{R}^{n_k \times r^A_{k-1} \times r^A_k}$, $(B_1, \ldots, B_L)$, $B_k \in \mathbb{R}^{n_k \times r^B_{k-1} \times r^B_k}$. Then*

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

$$\begin{aligned} S_1[i_1, j_1] &= \begin{pmatrix} G_1[i_1, j_1] & H_1[i_1, j_1] \end{pmatrix}, \quad S_L[i_L, j_L] = \begin{pmatrix} G_L[i_L, j_L] \\ H_L[i_L, j_L] \end{pmatrix} \\ S_k[i_k, j_k] &= \begin{pmatrix} G_k[i_k, j_k] & 0 \\ 0 & H_k[i_k, j_k] \end{pmatrix}, k = 2, \ldots, L-1 \end{aligned} \tag{2.1.4}$$

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

$$C_k[i_k] = \sum_{j_k=1}^{n_k} H_k[i_k, j_k] \otimes A_k[j_k], \quad k = 1, \ldots, L. \tag{2.1.5}$$

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

$$P_k[i_k, j_k] = \sum_{\ell_k=1}^{n_k} G_k[i_k, \ell_k] \otimes H_k[\ell_k, j_k], \quad k = 1, \ldots, L. \tag{2.1.6}$$

Proof. This is a direct computation. □

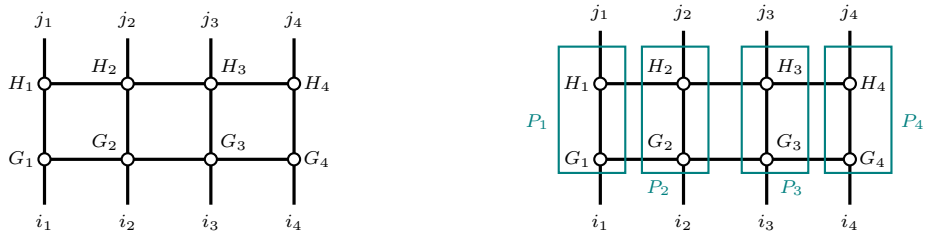
Remark 2.1.5. *The TTO representations of the sum and the product of the operators are not optimal. This is clear in the case of the sum $G + H$ when we consider $G = H$. A TT rounding step is required in order to reduce the TTO ranks of the representation. This is not innocuous as essential properties 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 2.2, avoiding cumbersome computations.

2.1.3 The electronic Hamiltonian as a TTO

The electronic Hamiltonian operator in second quantisation is given by

$$H = \sum_{i,j=1}^{L} h_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{i,j,k,\ell=1}^{L} V_{ijk\ell} c_i^\dagger c_j^\dagger c_\ell c_k, \tag{2.1.7}$$



(a) Diagrammatic representation of the product of two TTO

(b) Diagrammatic representation of the product of two TTO

Figure 2.2: 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.

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

$$c_i = Z \otimes \cdots \otimes Z \otimes C \otimes \mathrm{id}_2 \otimes \cdots \otimes \mathrm{id}_2 \in \mathbb{R}^{2^L \times 2^L}, \tag{2.1.8}$$

$$c_i^\dagger = Z \otimes \cdots \otimes Z \otimes C^* \otimes \mathrm{id}_2 \otimes \cdots \otimes \mathrm{id}_2 \in \mathbb{R}^{2^L \times 2^L}, \tag{2.1.9}$$

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 2.1.4, 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 conservation and the symmetry of the Hamiltonian, this procedure has to done with great care.

Remark 2.1.6. *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.*

2.2 The DMRG algorithm

The DMRG algorithm [Whi92] 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 *symmetric* and positive-definite matrices. In the following, we assume that H is a symmetric, positive-definite matrix.

Assumption 2.2.1. *The matrix $H \in \mathbb{R}^{n_1 \cdots n_L \times n_1 \cdots n_L}$ is symmetric and positive-definite.*

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

$$x_* = \underset{x \in \mathbb{R}^{n_1 \cdots n_L}}{\arg\min} \frac{1}{2}\langle x, Hx\rangle - \langle b, x\rangle. \tag{2.2.1}$$

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

$$x_* = \underset{x \in \mathbb{R}^{n_1 \cdots n_L}}{\arg\min} \frac{\langle x, Hx\rangle}{\langle x, x\rangle}. \tag{2.2.2}$$

2.2.1 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

$$\mathscr{M}_{\mathrm{TT}_{\leq r}} = \left\{C \mid \forall\, 1 \leq i_k \leq n_k, C_{i_1 \ldots i_L} = X_1[i_1] \cdots X_L[i_L], X_k[i_k] \in \mathbb{R}^{r_{k-1} \times r_k}, r_k \leq r\right\}. \tag{2.2.3}$$

The exact solution to $Hx_* = b$ (since H is symmetric positive-definite) is also the minimiser of the functional $J(x) = \frac{1}{2}\langle x, Hx\rangle - \langle b, x\rangle$. Let TT be the map

$$\mathrm{TT} \ : \begin{cases} \mathbb{R}^{n_1 \times r_0 \times r_1} \times \cdots \times \mathbb{R}^{n_L \times r_{L-1} \times r_L} \to \mathbb{R}^{n_1 \cdots n_L} \\ \qquad\qquad (X_1, \ldots, X_L) \mapsto (X_1[i_1] \cdots X_L[i_L]), \end{cases}$$

and j the map

$$j(X_1, \ldots, X_L) = J \circ \mathrm{TT}(X_1, \ldots, X_L). \tag{2.2.4}$$

Minimising J over the manifold $\mathscr{M}_{\mathrm{TT}_{\leq r}}$ is the same as minimising the functional j. In the one-site DMRG procedure, the minimisation of j is carried out sequentially by freezing all the TT cores but one and by solving the minimisation problem for the remaining core. The algorithm is described in Algorithm 2.1.

The optimisation steps (2.2.5) and (2.2.6) are called *microsteps*. An iteration over the loop n is called a sweep. Notice that at each microstep (2.2.5) or (2.2.6) the left TT cores are left-orthogonal and the right-TT cores are right-orthogonal.

Algorithm 2.1 One-site DMRG with sweeps

Input: $(X_1^{(0)}, \dots, X_L^{(0)})$ in right-orthogonal TT representation
Output: $(X_1^{(n)}, \dots, X_L^{(n)}) \in \mathscr{M}_{\mathrm{TT}_{\leq r}}$ approximation of the minimiser in $\mathscr{M}_{\mathrm{TT}_{\leq r}}$ of J

function ONE-SITE-DMRG($(X_1^{(0)}, \dots, X_L^{(0)})$)
  $n = 0$
  while `not converged` **do**
    for $k = 1, 2, \dots, L-1$ **do** ▷ Forward half-sweep

$$Y_k^{(n+\frac{1}{2})} = \underset{V_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}}{\arg\min} j(X_1^{(n+\frac{1}{2})}, \dots, X_{k-1}^{(n+\frac{1}{2})}, V_k, X_{k+1}^{(n)}, \dots, X_L^{(n)}) \tag{2.2.5}$$

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

$$Y_k^{(n+1)} = \underset{V_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}}{\arg\min} j(X_1^{(n+\frac{1}{2})}, \dots, X_{k-1}^{(n+\frac{1}{2})}, V_k, X_{k+1}^{(n+1)}, \dots, X_L^{(n+1)}) \tag{2.2.6}$$

$L, Q = \mathtt{lq}\Big(\big(Y_k^{(n+1)}\big)^{\beta_k i_k}_{\alpha_{k-1}}\Big)$ ▷ LQ decomposition
$\big(X_k^{(n+1)}[i_k]\big)^{\alpha_k}_{\alpha_{k-1}} = \big(Q\big)^{\alpha_k i_k}_{\alpha_{k-1}}$ ▷ Keep Q
$\big(X_{k-1}^{(n+\frac{1}{2})}[i_{k-1}]\big)^{\alpha_{k-1}}_{\alpha_{k-2}} \leftarrow \big(X_{k-1}^{(n+\frac{1}{2})}[i_{k-1}] L\big)^{\alpha_{k-1}}_{\alpha_{k-2}}$ ▷ Shift L to the left
    end for
    $n = n + 1$
  end while
  return $(X_1^{(n)}, \dots, X_L^{(n)})$
end function

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

$$(P_k V)_{i_1 \dots i_L} = X_1[i_1] \cdots X_{k-1}[i_{k-1}] V[i_k] X_{k+1}[i_{k+1}] \cdots X_L[i_L], \tag{2.2.7}$$

where $(X_1, \dots, X_L)$ are TT cores that are left-orthogonal for $j \leq k-1$ and right-orthogonal for $j \geq k+1$. The tensor $Y_k^{(n+\frac{1}{2})}$ of the microstep problem (2.2.5) is the solution to the linear system

$$P_k^* H P_k Y_k^{(n+\frac{1}{2})} = P_k^* b. \tag{2.2.8}$$

Proposition 2.2.2. *Assume that $(X_i^{(n+\frac{1}{2})})_{1 \leq i \leq k-1}$ are left-orthogonal and $(X_i^{(n)})_{k+1 \leq i \leq L}$ are right-orthogonal. Then the microstep (2.2.5) has a unique solution.*

Proof. It is equivalent to check that eq. (2.2.8) has a unique solution, *i.e.* that the matrix $P_k^* H P_k$ is invertible. As H is symmetric and positive-definite, it is sufficient to prove that P_k is an injective operator. Let $V \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ such that $\|P_k V\| = 0$. Then we have

$$\begin{aligned}
\|P_k V\|^2 &= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} \operatorname{Tr}\big(X_L[i_L]^* \cdots X_{k+1}[i_{k+1}]^* V[i_k]^* X_{k-1}[i_{k-1}]^* \cdots X_1[i_1]^* \\
&\qquad\qquad X_1[i_1] \cdots X_{k-1}[i_{k-1}] V[i_k] X_{k+1}[i_{k+1}] \cdots X_L[i_L] \big) \\
&= \sum_{i_1=1}^{n_1} \cdots \sum_{i_L=1}^{n_L} \operatorname{Tr}\big(V[i_k]^* X_{k-1}[i_{k-1}]^* \cdots X_1[i_1]^* X_1[i_1] \cdots X_{k-1}[i_{k-1}] V[i_k] \\
&\qquad\qquad X_{k+1}[i_{k+1}] \cdots X_L[i_L] X_L[i_L]^* \cdots X_{k+1}[i_{k+1}]^* \big) \\
&= \sum_{i_k=1}^{n_k} \operatorname{Tr}\big(V[i_k]^* V[i_k] \big),
\end{aligned}$$

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 $V = 0$. □

Remark 2.2.3. *With similar calculations, we could also have shown that $P_k^* P_k = \mathrm{id}$.*

The condition number of the microstep (2.2.8) is bounded by the condition number of the matrix H.

Proposition 2.2.4. *The condition number of the linear system (2.2.8) is bounded by the condition number of H,* i.e.

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

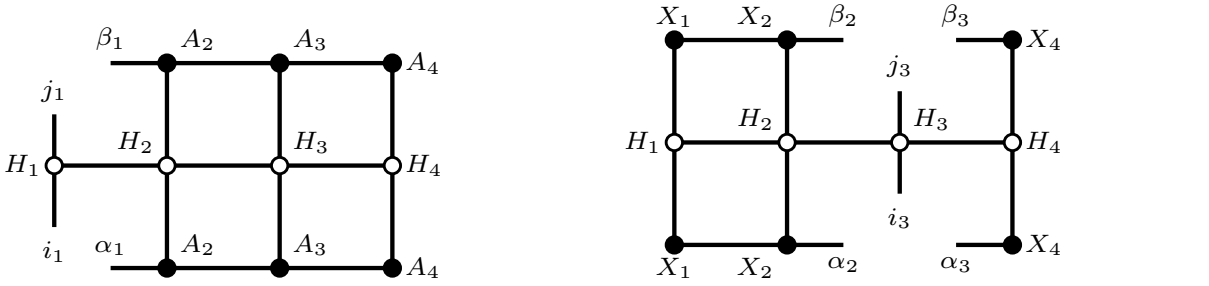
Proof. This follows from the inequalities $\lambda_{\min}(P_k^* H P_k) \geq \lambda_{\min}(H)$ and $\lambda_{\max}(P_k^* H P_k) \leq \lambda_{\max}(H)$. □

The QR steps that appear in the one-site DMRG algorithm 2.1 are not necessary when solving a linear system, however it is convenient to include them to solve eigenvalue problems.

2.2.2 Implementation details

In this part, we give some details about the implementation of the DMRG algorithm described in Algorithm 2.1, as well as the total computational cost of a sweep.

The matrix $P_k^* H P_k$ A critical step in DMRG, we want an efficient way to implement the effective matrix $P_k^* H P_k$ (see Figure 2.3).



(a) Effective matrix $(P_1^* H P_1)^{\beta_1 j_1}_{\alpha_1 i_1} \in \mathbb{R}^{r_1 n_1 \times r_1 n_1}$ (b) Effective matrix $(P_3^* H P_3)^{\beta_2 j_3 \beta_3}_{\alpha_2 i_2 \alpha_3} \in \mathbb{R}^{r_2 n_3 r_3 \times r_2 n_3 r_3}$

Figure 2.3: 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 $P_k^* H P_k X_k$ where $X_k \in \mathbb{R}^{r_{k-1} n_k r_k}$. For this, a splitting of the effective Hamiltonian is used and it is written

$$\left(P_k^* H P_k\right)^{\beta_{k-1} j_k \beta_k}_{\alpha_{k-1} i_k \alpha_k} = \sum_{\nu_k=1}^{R_k} \left(\mathcal{L}_k\right)^{\beta_{k-1} j_k \nu_k}_{\alpha_{k-1} i_k} \left(\mathcal{R}_k\right)^{\beta_k}_{\alpha_k \nu_k}. \tag{2.2.9}$$

This splitting is illustrated in Figure 2.4.

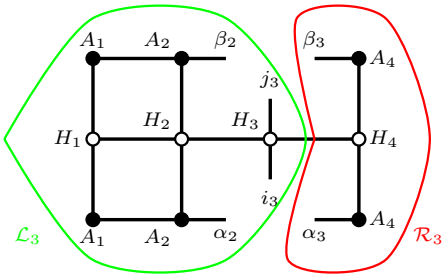


Figure 2.4: Splitting of the effective Hamiltonian

The computation of the matrix-vector multiplication goes as follows (see also Figure)

$$\left(P_k^* H P_k\right)^{\beta_{k-1} j_k \beta_k}_{\alpha_{k-1} i_k \alpha_k} \left(X_k\right)_{\beta_{k-1} j_k \beta_k} = \left(\left(\mathcal{L}_k\right)^{\beta_{k-1} j_k \nu_k}_{\alpha_{k-1} i_k} \left(X_k\right)_{\beta_{k-1} j_k \beta_k}\right) \left(\mathcal{R}_k\right)^{\beta_k}_{\alpha_k \nu_k}, \tag{2.2.10}$$

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

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

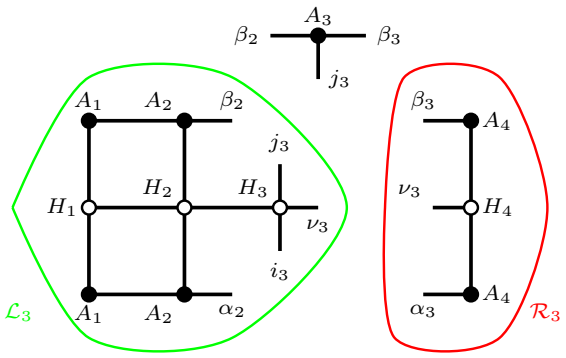
This scales as $\mathcal{O}(n^2 r^2 R)$.

(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

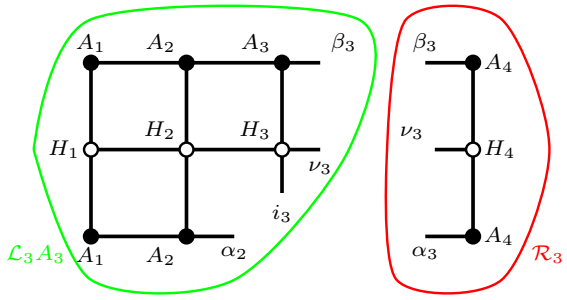
$$\sum_{\nu_k=1}^{R_k} \sum_{\beta_k=1}^{r_k} \left(\mathcal{L}_k X_k\right)_{\alpha_{k-1} i_k \beta_k}^{\nu_k} \left(\mathcal{R}_k\right)_{\alpha_k \nu_k}^{\beta_k}$$

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

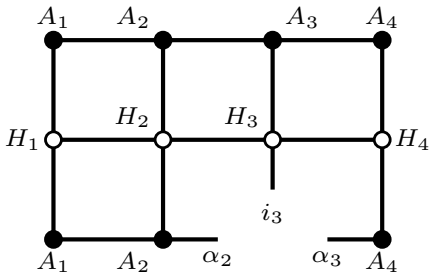
So overall the matrix-vector multiplication costs $\mathcal{O}(n^2 r^2 R + nRr^3)$.



(a) Tensors $\mathcal{L}_3$, X_3 and $\mathcal{R}_3$



(b) First step in the matrix-vector product

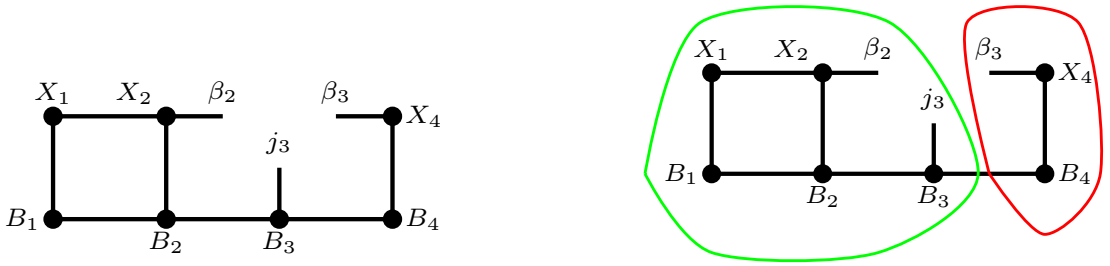


(c) Result of the matrix-vector product

Figure 2.5: Matrix-vector product (2.2.10)

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

The RHS $P_k^* b$ The assembly of the RHS is simpler than of the effective Hamiltonian. Similarly, it is possible to precompute the left and the right parts of the RHS as depicted in Figure 2.6b.



(a) $P_3^* b$ (b) Possible splitting of $P_3^* b$

Figure 2.6: Graphical representation of $P_3^* b$

2.3 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 2.3.1. *At the local minimiser X_*, the Hessian j'' is of full rank*

$$\operatorname{rank} j''(X_*) = \sum_{i=1}^{L} r_{i-1} n_i r_i - \sum_{i=1}^{L-1} r_i^2, \quad \textit{i.e.} \ \ker j''(X_*) = T_{X_*} \mathcal{M}_{\mathrm{TT}_{\leq r}}. \tag{2.3.1}$$

2.3.1 Local convergence of DMRG

Assumption 2.3.1 ensures that the Hessian is invertible at the solution to the DMRG equations.

Theorem 2.3.2 ([RU13, Theorem 2.7])**.** *There exists a neighbourhood W of X_* such that Algorithm 2.1 initiated with $X^{(0)} \in W$ converges to the minimiser X_*.*

2.3.2 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 2.7).

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

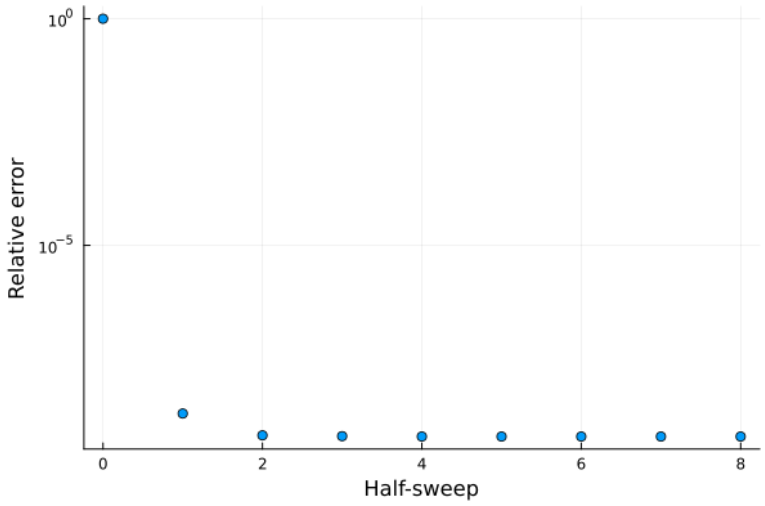


Figure 2.7: Convergence to the solution of $Hx = b$ with H the discrete Laplacian in $\mathbb{R}^{4^8 \times 4^8}$ b a random tensor of TT rank 2. The reference solution has TT rank 10.

Proposition 2.3.3 ([HRS12a, Lemma 4.2])**.** *Let $B \in \mathbb{R}^{n_1 \times \cdots \times n_L}$ with TT ranks $(r_0, \ldots, r_L)$. Let $(B_1, \ldots, B_L)$ be a left-orthogonal TT representation of B. Let $(X_1, \ldots, X_L)$ be a right-orthogonal TT with TT ranks $(r_0, \ldots, r_L)$. Suppose that $(X_1, \ldots, X_L)$ is such that for all $2 \leq k \leq L$, the matrix $G_k \in \mathbb{R}^{r_{k-1} \times r_{k-1}}$ defined by*

$$\big(G_k\big)_{\beta_{k-1}\alpha_{k-1}} = \sum_{i_k, \ldots, i_L} \sum_{\substack{\alpha_k \ldots \alpha_{L-1} \\ \beta_k \ldots \beta_{L-1}}} \big(X_k[i_k]\big)^{\alpha_k}_{\alpha_{k-1}} \cdots \big(X_L[i_L]\big)_{\alpha_{L-1}} \big(B_k[i_k]\big)^{\beta_k}_{\beta_{k-1}} \cdots \big(B_L[i_L]\big)_{\beta_{L-1}}.$$

is invertible. The DMRG algorithm applied with $H = \mathrm{id}$ converges in a half-sweep.

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

Proof. We are going to prove by recurrence that there are $Q_k \in \mathbb{R}^{r_k \times r_k}$ for $1 \leq k \leq L-1$ such that the solution of the DMRG microstep k can be written $X_k^{(\frac{1}{2})}[i_k] = Q_{k-1} B_k[i_k] Q_k^*$.

Initialisation: since $(X_1, \ldots, X_L)$ is right-orthogonal, we have that $P_1^* P_1 = \mathrm{id}$. The solution to the first microstep is simply given by

$$Y_1[i_1]_{\alpha_1} = \sum_{\beta_1} B_1[i_1]_{\beta_1} (G_2)^{\beta_1}_{\alpha_1}.$$

Let Q_1^*, R_1 be the QR factorisation of G_2. Then

$$X_1^{(\frac{1}{2})}[i_1]_{\alpha_1} = \sum_{\beta_1} B_1[i_1]_{\beta_1} (Q_1)^{\alpha_1}_{\beta_1}.$$

Iteration: suppose that for all $1 \leq j \leq k-1$, we have

$$X_j^{(\frac{1}{2})}[i_j]_{\alpha_j}^{\alpha_{j-1}} = \sum_{\beta_{j-1},\beta_j} (Q_{j-1})_{\beta_{j-1}}^{\alpha_{j-1}} (B_j[i_j])_{\beta_j}^{\beta_{j-1}} (Q_j)_{\beta_j}^{\alpha_j}.$$

At microstep k, by left-orthogonality of $(X_j^{(\frac{1}{2})})_{1\leq j\leq k-1}$ and right-orthogonality of $(X_j)_{k+1\leq j\leq L}$, again the solution to the microstep k is given by

$$Y_k[i_k]_{\alpha_k}^{\alpha_{k-1}} = \sum_{\substack{\alpha_1\dots\alpha_{k-1}\\ \beta_1\dots\beta_k}} B_1[i_1]_{\beta_1}\cdots B_k[i_k]_{\beta_k}^{\beta_{k-1}} X_1^{(\frac{1}{2})}[i_1]_{\alpha_1}\cdots X_{k-1}^{(\frac{1}{2})}[i_{k-1}]_{\alpha_{k-1}}^{\alpha_{k-2}} (G_{k+1})_{\alpha_k}^{\beta_k}.$$

By the recurrence hypothesis and the orthogonality of the TT cores $(B_j)_{1\leq j\leq k-1}$, the above expression simplifies to

$$Y_k[i_k]_{\alpha_k}^{\alpha_{k-1}} = \sum_{\beta_{k-1},\beta_k} B_k[i_k]_{\beta_k}^{\beta_{k-1}} (Q_{k-1})_{\beta_{k-1}}^{\alpha_{k-1}} (G_{k+1})_{\alpha_k}^{\beta_k}.$$

Now let Q_k^*, R_k be the QR factorisation of G_{k+1}, then

$$X_k[i_k]_{\alpha_k}^{\alpha_{k-1}} = \sum_{\beta_{k-1},\beta_k} (Q_{k-1})_{\beta_{k-1}}^{\alpha_{k-1}} B_k[i_k]_{\beta_k}^{\beta_{k-1}} (Q_k)_{\beta_k}^{\alpha_k},$$

which is exactly $X_k[i_k] = Q_{k-1}B_k[i_k]Q_k^*$. This finishes the proof of the proposition. □

Remark 2.3.4. *A similar result holds for tensor rings, see [CLL20].*

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

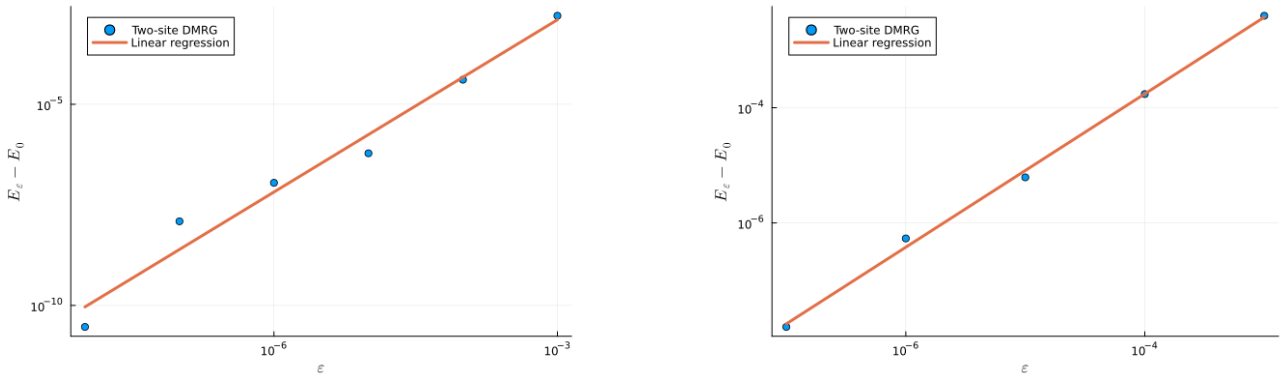
The main limitation of the one-site DMRG algorithm is the inability to dynamically adapt the TT ranks of the approximate solution during the course of the iterations. A small modification of the one-site DMRG makes it possible to have more flexibility in the TT ranks. The main idea is to solve the microstep in DMRG not only on one-site but on two neighbouring sites.

In that case, at each microstep k, the functional that is minimised is

$$j_2^{(k)} : \begin{cases} \mathbb{R}^{n_1\times r_0\times r_1}\times\cdots\times\mathbb{R}^{r_{k-1}\times n_k\times n_k\times r_{k+1}}\times\cdots\times\mathbb{R}^{n_L\times r_{L-1}\times r_L}\to\mathbb{R} \\ (X_1,\dots,X_{k-1},X,X_k,\dots,X_L)\mapsto J\circ\widetilde{\mathrm{TT}}_k(X_1,\dots,X_{k-1},X,X_k,\dots,X_L) \end{cases} \tag{2.4.1}$$

where

$$\widetilde{\mathrm{TT}}_k : \begin{cases} \mathbb{R}^{n_1\times r_0\times r_1}\times\cdots\times\mathbb{R}^{r_{k-1}\times n_k\times n_k\times r_{k+1}}\times\cdots\times\mathbb{R}^{n_L\times r_{L-1}\times r_L}\to\mathbb{R}^{n_1\cdots n_L} \\ (X_1,\dots,X_{k-1},X,X_{k+1},\dots,X_L)\mapsto (X_1[i_1]\cdots X_{k-1}[i_{k-1}]X[i_k,i_{k+1}]X_{k+1}[i_{k+1}]\cdots X_L[i_L]). \end{cases}$$



(a) Hubbard model with 10 sites

(b) Hubbard model with 20 sites

Figure 2.8: Extrapolation of the ground-state energy E_ε for the Hubbard model where E_ε is computed with the two-site DMRG algorithm with truncation ε

The TT rank adaptivity comes in the transformation of the microstep solution back to a suitable TT form by a truncated SVD

$$(X_{\alpha_{k-1} i_k}^{\alpha_{k+1} i_{k+1}}) = U_\varepsilon S_\varepsilon V_\varepsilon^* + \mathcal{O}(\varepsilon),$$

where $U_\varepsilon \in \mathbb{R}^{r_{k-1} n_k \times r}$, $S_\varepsilon \in \mathbb{R}^{r \times r}$ and $V_\varepsilon \in \mathbb{R}^{r_{k+1} n_{k+1} \times r}$ and r is chosen such that the truncated SVD has error ε. U_ε is (up to a reshape) the new TT core X_k and r is the corresponding TT rank. The full algorithm is given in Algorithm 2.2.

In practice, the truncation level ε is used to monitor the error in DMRG. It can also be used to extrapolate some quantities as the lowest eigenvalue as depicted in Figure 2.8 [WPAV14]. Theoretically, unlike the one-site algorithm, there is no convergence result on the two-site algorithm (except in the case where no truncation is made).

2.5 DMRG on eigenvalue problems

DMRG is primarily used to solve eigenvalue problems. In that case, the functional to minimise is $J(x) = \frac{\langle x, Hx \rangle}{\langle x, x \rangle}$. At each microstep, instead of solving a linear system, the following generalised eigenvalue problem has to be solved for the lowest eigenvalue

$$P_k^* H P_k V = \lambda P_k^* P_k V.$$

In that case, it is numerically beneficial to ensure the good orthogonality conditions for the approximate solution in the TT form, so that $P_k^* P_k = \mathrm{id}$.

Apart from this change, the algorithms 2.1 and 2.2 can be modified in a straightforward way to solve eigenvalue problems instead.

For multiple lowest eigenvalues, there are two main options

Algorithm 2.2 Two-site DMRG with sweeps

Input: $(X_1^{(0)}, \dots, X_L^{(0)})$ in right-orthogonal TT representation with initial TT ranks $(r_0^{(0)}, \dots, r_L^{(0)})$, $\varepsilon_{\mathrm{TT}}$

Output: $(X_1^{(n)}, \dots, X_L^{(n)}) \in \mathscr{M}_{\mathrm{TT}_{\leq r}}$ approximation of the minimiser of J

function TWO-SITE-DMRG($(X_1^{(0)}, \dots, X_L^{(0)}), \varepsilon_{\mathrm{TT}}$)
  $n = 0$
  while `not converged` **do**
    for $k = 1, 2, \dots, L-2$ **do** ▷ Forward half-sweep

$$Y_k^{(n+\frac{1}{2})} = \underset{V_k \in \mathbb{R}^{r_{k-1}^{(n+\frac{1}{2})} \times n_k \times n_k \times r_{k+1}^{(n)}}}{\arg\min} j_2^{(k)}(X_1^{(n+\frac{1}{2})}, \dots, X_{k-1}^{(n+\frac{1}{2})}, V_k, X_{k+2}^{(n)}, \dots, X_L^{(n)}) \tag{2.4.2}$$

$$U, S, V^* = \mathtt{svd}_{\varepsilon_{\mathrm{TT}}}\big(\big(Y_k^{(n+\frac{1}{2})}\big)_{\alpha_{k-1} i_k}^{\beta_{k+1} i_{k+1}}\big)$$ ▷ Truncated SVD of Y_k

$$r_k^{(n+\frac{1}{2})} = \text{rank of the SVD truncation to level } \varepsilon_{\mathrm{TT}}$$ ▷ Update TT rank

$$\big(X_k^{(n+\frac{1}{2})}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = U_{\alpha_{k-1} i_k}^{\alpha_k}$$ ▷ Update X_k

$$\big(X_{k+1}^{(n)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}} = \big(SV^*\big)_{\alpha_k}^{\alpha_{k+1} i_{k+1}}$$ ▷ Update X_{k+1}

    end for
    for $k = L-1, L-2, \dots, 2$ **do** ▷ Backward half-sweep

$$Y_k^{(n+1)} = \underset{V_k \in \mathbb{R}^{r_{k-2}^{(n+\frac{1}{2})} \times n_k \times n_k \times r_k^{(n+1)}}}{\arg\min} j_2^{(k)}(X_1^{(n+\frac{1}{2})}, \dots, X_{k-1}^{(n+\frac{1}{2})}, V_k, X_{k+2}^{(n+1)}, \dots, X_L^{(n+1)}) \tag{2.4.3}$$

$$U, S, V^* = \mathtt{svd}_{\varepsilon_{\mathrm{TT}}}\big(\big(Y_k^{(n+\frac{1}{2})}\big)_{\alpha_{k-1} i_k}^{\beta_{k+1} i_{k+1}}\big)$$ ▷ Truncated SVD of Y_k

$$r_k^{(n+1)} = \text{rank of the SVD truncation to level } \varepsilon_{\mathrm{TT}}$$ ▷ Update TT rank

$$\big(X_{k+1}^{(n+1)}[i_{k+1}]\big)_{\alpha_k}^{\alpha_{k+1}} = V_{\alpha_{k+1} i_{k+1}}^{\alpha_k}$$ ▷ Update X_{k+1}

$$\big(X_k^{(n)}[i_k]\big)_{\alpha_{k-1}}^{\alpha_k} = \big(US\big)_{\alpha_{k-1} i_k}^{\alpha_k}$$ ▷ Update X_k

    end for
    $n = n + 1$
  end while
  return $(X_1^{(n)}, \dots, X_L^{(n)})$
end function

(i). deflate the computed eigenvalues

(ii). use the following characterisation of the k smallest eigenvalues $(\lambda_1, \ldots, \lambda_k)$ of H

$$\sum_{i=1}^{k} \lambda_i = \min_{X \in \mathbb{R}^{n_1 \cdots n_L \times k}} \frac{\mathrm{Tr}(X^* H X)}{\mathrm{Tr}(X^* X)}.$$

This approach is described in [DKOS14]. Essentially, the TT representing $X \in \mathbb{R}^{n_1 \cdots n_L \times k}$ has an extra index accounting for the number of eigenvalues sought. At each microstep, this index is "moved" to the next microstep during the QR/SVD step.

Chapter 3

Low-rank representation of solutions to elliptic PDEs

In this chapter, we state results on the low-rank approximability for two types of problems

- source problems $Hu = f$;
- eigenvalue problems $Hu = Eu$ for E the smallest eigenvalue of H,

where H is a symmetric operator acting on the tensor space $\bigotimes_{j=1}^{d} \mathcal{H}_j$ with $\dim \mathcal{H}_j = n_j$.

The main goal in this type of problems is to obtain an estimation of an approximate solution with TT ranks that do not depend exponentially with the dimension of the problem L, or on the quality of the approximation $u - u_{\text{approx}}$.

3.1 Source problems

For source problems, we have the following result.

Theorem 3.1.1 ([DDGS16],[Bac23, Theorem 4.6])**.** *Let H be a one-body operator,* i.e. *of the form*

$$H = \sum_{j=1}^{L} h_j, \tag{3.1.1}$$

where H is an operator acting on $\bigotimes_{j=1}^{d} \mathcal{H}$ with $\dim \mathcal{H} = n$ and h_j is a one-body operator of the form $\mathrm{id}_{1:j-1} \otimes h \otimes \mathrm{id}_{j+1:d}$. Suppose that for all $1 \leq j \leq L$, h is a symmetric positive-definite matrix with eigenvectors $(\phi_i)_{1 \leq i \leq n}$.

Let $f \in \bigotimes_{j=1}^{d} \mathcal{H}$ and $(f_I) \in \mathbb{R}^{Ln}$ be the coefficients of f in the canonical basis. Suppose that (f_I) has a TT representation with TT ranks bounded by r_f. Let $u \bigotimes_{j=1}^{d} \mathbb{R}^n$ be the solution to $Hu = f$.

Then for all $\varepsilon > 0$, there is $u_\varepsilon \in \bigotimes_{j=1}^d \mathcal{H}$ such that $\|u - u_\varepsilon\| \leq \varepsilon$ where u_ε has TT ranks bounded by $\frac{1}{\pi^2} \log\left(\frac{d\lambda\varepsilon\|f\|}{16}\right)^2 r_f$ in the canonical basis of $\bigotimes_{j=1}^d \mathcal{H}$.

Remark 3.1.2. *The L-dimensional discrete Laplacian is a one-body operator of the form (3.1.1), hence for low-rank RHS, the solution to the linear problem has a low-rank approximation in the TT format.*

The main idea of the proof is to use the spectral decomposition of H and an approximation of $1/x$ as a sum of exponentials:

$$\frac{1}{x} \approx \sum_{k=1}^K \omega_k e^{-\alpha_k x}, \text{ for some } \omega_k \in \mathbb{R} \text{ and } \alpha_k > 0. \tag{3.1.2}$$

Such an approximation can be obtained by noticing that for $x > 0$, we have

$$\frac{1}{x} = \int_0^\infty e^{-xt}\,\mathrm{d}t,$$

and using a quadrature rule for the integral.

Let $(\lambda_i, \phi_i) \in \mathbb{R} \times \mathbb{R}^n$ be the eigenpairs of h, then the eigenvalues Λ_I and the corresponding eigenvectors Φ_I of H are given by

$$\Lambda_I = \sum_{k=1}^d \lambda_{i_k}, \quad \Phi_I = \phi_{i_1} \otimes \cdots \otimes \phi_{i_d}.$$

Then the solution to the linear system $Hu = f$ is given by

$$u = \sum_I \frac{1}{\Lambda_I} \tilde{f}_I \Phi_I.$$

Since $\frac{1}{\Lambda_I}$ is not separable, the TT rank of u may be large. However it can be approximated by

$$u = \sum_I \frac{1}{\Lambda_I} \tilde{f}_I \Phi_I \approx \sum_{k=1}^K \sum_I \omega_k e^{-\alpha_k \Lambda_I} \tilde{f}_I \Phi_I.$$

Now since $\Lambda_I = \sum_{j=1}^d \lambda_{i_j}$, we have that $e^{-\alpha_k \Lambda_I} = \prod_{j=1}^d e^{-\alpha_k \lambda_{i_j}}$, which is now separable in each variable. Thus the TT rank of the approximation of u is simply bounded by Kr_f.

The factor K is related to the quality of the approximation of $1/x$ by a sum of the exponential (3.1.2). For this problem, we have the following bound.

Proposition 3.1.3 ([Hac19],[Bac23, Corollary 4.5])**.** *Let $a > 0$. Then for all $K \in \mathbb{N}$, there are $\omega_k, \alpha_k > 0$, $1 \leq k \leq K$ such that*

$$\sup_{t \in [a,\infty)} \left| \frac{1}{x} - \sum_{k=1}^K \omega_k e^{-\alpha_k t} \right| \leq \frac{16}{a} e^{-\pi\sqrt{K}}. \tag{3.1.3}$$

We can now give the proof of Theorem 3.1.1.

Proof of Theorem 3.1.1. Let $\widetilde{u}$ be defined as

$$\widetilde{u} = \sum_{k=1}^{K} \omega_k e^{-\alpha_k H} f,$$

where $(\omega_k), (\alpha_k)$ are chosen such that $\sup_{t\in[L\lambda,\infty)} \left|\frac{1}{x} - \sum_{k=1}^{K} \omega_k e^{-\alpha_k t}\right| \leq \varepsilon$ with λ the smallest eigenvalue of h. This means that $K \geq \frac{1}{\pi^2} \log\left(\frac{d\lambda\varepsilon\|f\|}{16}\right)^2$. Then we have

$$\|u - \widetilde{u}\| \leq \sup_{t\in[L\lambda,\infty)} \left|\frac{1}{x} - \sum_{k=1}^{K} \omega_k e^{-\alpha_k t}\right| \|f\|.$$

For $K \geq \frac{1}{\pi^2} \log\left(\frac{L\lambda\varepsilon\|f\|}{16}\right)^2$, we thus have $\|u - \widetilde{u}\| \leq \varepsilon$.

It remains to show that $\widetilde{u}$ has TT ranks at most $\frac{1}{\pi^2} \log\left(\frac{d\lambda\varepsilon\|f\|}{16}\right)^2 r_f$ in the basis of the eigenfunctions (Φ_I) of H. As $H = \sum_{j=1}^{d} h_j$ where h_j commute two-by-two, then $e^{-\alpha_k H} = \bigotimes_{j=1}^{d} e^{-\alpha_k h}$. Hence the TTO representation of $\bigotimes_{j=1}^{d} e^{-\alpha_k h}$ is of rank 1. Thus $e^{-\alpha_k H} f$ has the same TT rank as f. This finishes the proof. □

Remark 3.1.4. *The bound on the TT rank of the approximate solution does not depend on the dimension of the local space $\mathcal{H}$. We have thus the same bound at the continuous level, provided that we define rigorously a TT decomposition of functions.*

3.2 Eigenvalue problems

Eigenvalue problems have attracted more attention as DMRG and tensor trains in general have been applied in the context of quantum physics, where the properties of the system are derived from the eigenvector associated to the lowest eigenvalue of the many-body operator.

The first rigorous work on the approximability of eigenvectors by low-rank TT is due to Hastings [Has07]. Later, another strategy of proof has been proposed by Arad et al. [AKLV13].

We restrict ourselves to results for two-body Hamiltonians with nearest neighbour interactions of the form

$$H^{(d)} = \sum_{j=1}^{d-1} W_j \tag{3.2.1}$$

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

The main assumption needed to prove that the ground-state can be approximated well by a low-rank TT is the following.

Assumption 3.2.1. *Let $H^{(d)}$ be defined by (3.2.1). We assume that $H^{(d)}$ has a unique nondegenerate ground-state $\Psi_0^{(d)}$ and that $H^{(d)}$ has a spectral gap γ independent of L,* i.e. *$E_1^{(d)} - E_0^{(d)} \geq \gamma$ for all L where $E_0^{(d)}$ and $E_1^{(d)}$ are the lowest and second lowest eigenvalue of $H^{(d)}$.*

The approximation result on the ground-state can be written as follows.

Theorem 3.2.2 ([Has07, AKLV13])**.** *Let $H^{(d)}$ be given by (3.2.1) satisfying Assumption 3.2.1. Then for any $\varepsilon > 0$, there is a TT approximation $\mathrm{TT}_r\Psi_0^{(d)}$ with TT rank r independent of d of $\Psi_0^{(d)}$ such that*

$$\|\mathrm{TT}_r\Psi_0^{(d)} - \Psi_0^{(d)}\| \leq \varepsilon.$$

Remark 3.2.3. *Such approximation results are called* area laws *in physics. These approximation results in the physics litterature are usually written in terms of the ground-state projector $|\Psi_0^{(d)}\rangle\langle\Psi_0^{(d)}|$ which is an operator acting on $\bigotimes_{j=1}^d \mathcal{H}$. Looking at the partial trace of the ground-state projector on a block of neighbouring sites, it is possible to show that the approximation of the partial trace of the ground-state projector does not depend on the size of the block, but only on the "area", which in dimension one is a constant. In higher dimension, it is a folklore result that these types of result hold also for ground-state of nearest neighbour interactions Hamiltonians.*

3.2.1 Hastings area law

The full proof is given in Section 3.3 for the interested reader. We here give the essential ideas of the proof. First, we write an approximation of the projector onto the ground-state, using the energy gap assumption

$$|\Psi_0\rangle\langle\Psi_0| \approx \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}(H^{(d)} - E_0)t} e^{-\frac{t^2}{2q}} \,\mathrm{d}t, \tag{3.2.2}$$

with q sufficiently large.

The Hamiltonian $H^{(d)}$ is a sum of operators that are "almost" commuting, as only neighbouring operators do not commute. Hence if $H_A = \sum_{j\in A} W_j$, $H_{A^c} = H - H_A$ although we are not allowed to write $e^{iH^{(d)}t} = e^{iH_At}e^{iH_{A^c}t}$, we can quantify the difference in a rigorous way. The trick is to write

$$e^{\mathrm{i}H^{(d)}t} = e^{\mathrm{i}H_{L+R}t + \mathrm{i}H_Mt} e^{-\mathrm{i}H_{L+R}t} e^{\mathrm{i}H_{L+R}t},$$

with $H_M = \sum_{m-\ell\leq j\leq m+\ell} W_j$, $H_{L+R} = \sum_{j<m-\ell; m+\ell<j} W_j$ and realise that $e^{\mathrm{i}H_{L+R}t + \mathrm{i}H_Mt} e^{-\mathrm{i}H_{L+R}t}$ is the solution to

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

For small values of t by the Lieb-Robinson bound, proved for Hamiltonians with nearest neighbour interactions, $e^{\mathrm{i}H_{L+R}t} H_M e^{-\mathrm{i}H_{L+R}t}$ has support exponentially close to the support of H_M.

Denoting $\widetilde{U}_M(t) = e^{\mathrm{i}H_{L+R}t}H_M e^{-\mathrm{i}H_{L+R}t}$, we have then for small t

$$e^{\mathrm{i}H^{(d)}t} \approx \widetilde{U}_M(t)e^{\mathrm{i}H_{L+R}t},$$

with $\widetilde{U}_M(t)$ and $e^{\mathrm{i}H_{L+R}t}$ having exponentially small overlap.

3.2.2 AGSP

A later strategy to obtain these results have been through the *approximate ground-state projector* (AGSP) construction, first proposed in [AKLV13]. As opposed to the proof by Hastings, where the central tool is the Lieb-Robinson bound, the AGSP is the result of an algorithm which terminates in finite time with polynomial complexity. This algorithm is called the *rigorous renormalisation group* (RRG) [RVM17]. It provides an alternative algorithm to DMRG for the computation of the ground-state energy. The scheme has been tested numerically in [RVM17, BMG+21], where RRG looked more stable than DMRG, but less efficient numerically. The other drawback of the RRG is that it is yet unclear how to adapt this algorithm to solve linear systems.

The idea of the proof uses a polynomial approximation of the ground-state projector. Indeed, because of the nearest neighbour interaction, the Hamiltonian $H^{(d)}$ has a TTO representation with ranks R independent of d. From algebraic properties of the TTO (see Chapter 2), the TTO representation of $P_n(H)$ of degree n will have a TTO representation with TT ranks bounded by R^{n+1}.

Suppose that $H^{(d)}$ is of the form (3.2.1) such that it has a nondegenerate ground-state. The ground-state projector can be written

$$|\Psi_0\rangle\langle\Psi_0| \approx T_m(H),$$

where T_m is the rescaled Chebyshev polynomial of degree m such that $T_m(E_0) = 1$ and it is the solution to

$$\|T_m\|_\infty = \min_{P_m\in\mathbb{R}^m[X]} \max_{E_1-E_0\leq x\leq E_{\max}-E_0} |P_m(x)|.$$

The error on the approximation is bounded by

$$\||\Psi_0\rangle\langle\Psi_0| - T_m(H)\| \leq 2\Big(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\Big)^m,$$

where $\kappa = \frac{E_{\max}-E_0}{E_1-E_0}$. For this problem, typically $E_{\max} - E_0$ would scale as the number of tensorised spaces L but the gap would remain bounded. Hence to have $\||\Psi_0\rangle\langle\Psi_0|-T_m(H)\| \leq \varepsilon$, n would have to be of the order $\sqrt{L}\log(\varepsilon)$, thus the TTO rank of the approximate projector would be of the order $R^{\sqrt{L}}$, where R is the TTO rank of H.

This strategy does not beat the curse of dimension, because the norm of the operator scales as L. An additional ingredient is required to prove an area law like Theorem 3.2.2, which is a truncation of the high-frequency component of parts of the Hamiltonian.

Let $\mathcal{J} \subset \{1, \dots, d\}$, $H_{\mathcal{J}} = \sum_{j\in\mathcal{J}} W_j$ and $E_0^{\mathcal{J}}$ its ground-state eigenvalue. For $\tau > 0$, let $\Pi_{E_0^{\mathcal{J}}+\tau}$ be the spectral projector associated to the eigenvalues of $H_{\mathcal{J}}$ below $E_0^{\mathcal{J}} + \tau$ and $\Pi^{\perp}_{E_0^{\mathcal{J}}+\tau} = \mathrm{id} - \Pi_{E_0^{\mathcal{J}}+\tau}$. The truncated Hamiltonian on J is then defined by

$$\widetilde{H}_{\mathcal{J}} = H_{\mathcal{J}}\Pi_{E_0^{\mathcal{J}}+\tau} + (\tau + E_0^{\mathcal{J}})\Pi^{\perp}_{E_0^{\mathcal{J}}+\tau}. \tag{3.2.3}$$

By definition, $\|\widetilde{H}_{\mathcal{J}} - E_0^{\mathcal{J}}\| \leq \tau$.

The core idea of the proof is to establish the following result on the overlap between the ground-state of the full Hamiltonian $H^{(d)}$ and the projector onto the high-frequency components of a part of $H^{(d)}$.

Lemma 3.2.4 ([AKL16, Theorem 2.3])**.** *For $\mathcal{J} \subset \{1, \dots, d-1\}$, let $E_0^{\mathcal{J}}$ and $E_0^{(d)}$ be respectively the lowest eigenvalue of $H_{\mathcal{J}} = \sum_{j\in\mathcal{J}} W_j$ and $H^{(d)}$. Let $\Pi_{[E,E']}$ be the spectral projector of $H_{\mathcal{J}}$ associated to the eigenvalues in $[E, E']$ $(E < E')$. Let $P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}$ be the spectral projector of $H^{(d)}$ associated to the eigenvalues in $[E_0^{(d)}, E_0^{(d)} + \varepsilon]$. Let $E_0^{\mathcal{J}}$ be the lowest eigenvalue of $H_{\mathcal{J}}$. Then there are constants C and α independent of $E, E', \varepsilon, \mathcal{J}$ such that we have*

$$\|\Pi_{[E_0^{\mathcal{J}}+E, E_0^{\mathcal{J}}+E']} P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}\| \leq C \exp\Big(-\alpha\big(E - \varepsilon + E_0^{(d)} - E_0^{\mathcal{J}}\big)\Big). \tag{3.2.4}$$

The proof of this lemma explicitly exploits the nearest neighbour interaction structure of the Hamiltonian $H^{(d)}$.

Sketch of the proof of Theorem 3.2.2 via AGSP

The proof of the area law requires a careful splitting of the Hamiltonian in two parts, such that the corresponding truncated Hamiltonian $\widetilde{H}_{\mathcal{J}}$ satisfies the following properties

(i). the ground-state of $\widetilde{H}_{\mathcal{J}}$ is exponentially close to $\Psi_0^{(d)}$;

(ii). for a given cut k, the polynomial $T_m(\widetilde{H}_{\mathcal{J}})$ has a controlled TTO rank at the cut k.

We want to show the following result.

Proposition 3.2.5. *There is a constant $\alpha > 0$ such that for each $1 \leq k \leq d$ and all $\varepsilon > 0$, there is an approximation of the ground-state projector $|\Psi_0\rangle\langle\Psi_0|$ such that*

$$\||\Psi_0\rangle\langle\Psi_0| - \widetilde{P}_0\| \leq \varepsilon, \tag{3.2.5}$$

where $(\widetilde{P}_0)^{j_1\dots j_d}_{i_1\dots i_d} \in \mathbb{R}^{n^d \times n^d}$ such that its reshape $(\widetilde{P}_0)^{i_{k+1}j_{k+1},\dots,i_dj_d}_{i_1j_1,\dots,i_kj_k} \in \mathbb{R}^{n^{2k}\times n^{2(d-k)}}$ has rank bounded by $CR^{\alpha(\log\varepsilon)^2}$ where R is the TTO rank of $H^{(d)}$ and C an irrelevant constant.

This means that the ground-state projector $|\Psi_0\rangle\langle\Psi_0|$ has a TTO approximation with error ε of TT rank $R^{\alpha(\log\varepsilon)^2}$. We then have the same bound on the TT approximation of the ground-state Ψ_0.

For $1 \leq k \leq d-1$, let $\widetilde{H}$ be the truncated Hamiltonian

$$\widetilde{H} = \widetilde{H}_{\mathcal{J}} + H_{\mathcal{J}^c}, \tag{3.2.6}$$

where $H_{\mathcal{J}^c} = \sum_{k-\ell\leq j\leq k+\ell} W_j$, $H_{\mathcal{J}} = H - H_{\mathcal{J}^c}$ and $\widetilde{H}_{\mathcal{J}} = H_{\mathcal{J}}\Pi_{E_0^{\mathcal{J}}+\tau} + (\tau + E_0^{\mathcal{J}})\Pi_\tau^\perp$, with $\Pi_{E_0^{\mathcal{J}}+\tau}$ being the spectral projector of $H_{\mathcal{J}}$ with eigenvalues below $E_0^{\mathcal{J}} + \tau$.

The proof has now two steps

(i). we show that $\||\Psi_0\rangle\langle\Psi_0| - |\widetilde{\Psi}_0\rangle\langle\widetilde{\Psi}_0|\| \leq C\exp(-\alpha(\tau - 2\ell))$

(ii). we prove that there is $\widetilde{P}_0$ such that $\||\widetilde{\Psi}_0\rangle\langle\widetilde{\Psi}_0| - \widetilde{P}_0\| \leq C\exp\Big(-\alpha\sqrt{\ell}\Big)$ for irrelevant constants α, C and where $\widetilde{P}_0$ has a reshape at the cut k with rank bounded by $R^{\ell+1}$.

Proof of step (i) The first step essentially follows from Lemma 3.2.4. Indeed we have

$$\|(\widetilde{H} - E_0)\Psi_0\| = \|(\widetilde{H} - H)\Psi_0\| = \|(H_{\mathcal{J}} - \tau - E_0^{\mathcal{J}})\Pi_{E_0^{\mathcal{J}}+\tau}\Psi_0\|.$$

Now we write

$$\begin{aligned}\|(H_{\mathcal{J}} - \tau - E_0^{\mathcal{J}})\Pi_{E_0^{\mathcal{J}}+\tau}\Psi_0\| &\leq \sum_{k\geq 0}\|(H_{\mathcal{J}} - \tau - E_0^{\mathcal{J}})\Pi_{[\tau_{k+1},\tau_k]}\Psi_0\| \\ &\leq C\exp\big(-\alpha(\tau - (E_0 - E_0^{\mathcal{J}}))\big)\sum_{k\geq 0}|\tau_k - \tau - E_0^{\mathcal{J}}|e^{-\alpha\tau_k},\end{aligned}$$

where we have used Lemma 3.2.4. Picking the right increasing sequence (τ_k), shows that

$$\|(\widetilde{H} - E_0)\Psi_0\| \leq C\exp\big(-\alpha(\tau - (E_0 - E_0^{\mathcal{J}}))\big). \tag{3.2.7}$$

Using the positivity of the interactions (W_j), we have that $E_0 - E_0^{\mathcal{J}} \leq 2\|W\|\ell$. From usual estimates on approximate eigenpairs [Saa11, Theorem 3.9], we then have that

$$\||\Psi_0\rangle\langle\Psi_0| - |\widetilde{\Psi}_0\rangle\langle\widetilde{\Psi}_0|\| \leq \frac{\|(\widetilde{H} - E_0)\Psi_0\|^2}{(\widetilde{E}_1 - E_0)^2} \leq C\exp(-\alpha(\tau - 2\ell)), \tag{3.2.8}$$

where $\widetilde{E}_1$ is the second lowest eigenvalue of $\widetilde{H}$ and where additionally one needs to prove that $\widetilde{E}_1 - E_0$ is bounded uniformly from below. This follows from Lemma 3.2.4 again and the spectral gap assumption 3.2.1. The proof is similar as to show that $\widetilde{E}_0 - E_0$ are close. This concludes the proof of the first step.

Proof of step (ii) Using the nearest neighbour nature of W_j, we have that for $m < \ell$, $T_m(\widetilde{H})$ has a TTO rank bounded by $R^{\ell+1}$.

By definition of the truncated Hamiltonian $\widetilde{H}$, we have that $\|\widetilde{H} - E_0^{\mathcal{J}}\| \leq (2\ell\|W\| + \tau)$. By standard estimates of Chebyshev polynomials, we have that

$$\||\widetilde{\Psi}_0\rangle\langle\widetilde{\Psi}_0| - T_m(\widetilde{H})\| \leq 2\Big(\frac{\sqrt{\widetilde{\kappa}}-1}{\sqrt{\widetilde{\kappa}}+1}\Big)^m,$$

with $\widetilde{\kappa} = \frac{\widetilde{E}_{\max}-\widetilde{E}_0}{\widetilde{E}_1-\widetilde{E}_0}$ where $\widetilde{E}_{\max}$ is the largest eigenvalue of $\widetilde{H}$ and $\widetilde{E}_0$, $\widetilde{E}_1$ the lowest and second lowest eigenvalue of $\widetilde{H}$.

From Eq. (3.2.7) and the gap assumption on the Hamiltonian H, we have that $\widetilde{\kappa} \leq C(\ell+\tau)$ for some constant C independent from $\widetilde{H}$. Hence we get

$$\||\widetilde{\Psi}_0\rangle\langle\widetilde{\Psi}_0| - T_m(\widetilde{H})\| \leq C\Big(1 - \frac{C}{\sqrt{\ell+\tau}}\Big)^m.$$

Choosing $\tau = \mathcal{O}(\ell)$ and noting that $(1-\frac{a}{n})^n = \exp(-a) + o(1)$, we deduce that

$$\||\widetilde{\Psi}_0\rangle\langle\widetilde{\Psi}_0| - T_{\ell-1}(\widetilde{H})\| \leq C\exp\Big(-C\sqrt{\ell}\Big). \tag{3.2.9}$$

Picking $\tau = \ell + \sqrt{\ell}$ and combining Eq. (3.2.8) and Eq. (3.2.9), we obtain

$$\||\Psi_0\rangle\langle\Psi_0| - T_{\ell-1}(\widetilde{H})\| \leq C\exp\Big(-\alpha\sqrt{\ell}\Big), \tag{3.2.10}$$

where $T_{\ell-1}(\widetilde{H})$ has rank R^ℓ at cut k. This finishes the proof of Proposition 3.2.5.

3.3 Hastings area law

3.3.1 Hamiltonian with nearest neighbour interactions

The NNI Hamiltonian considered is of the form

$$H = \sum_{j=1}^{d-1} h_j, \tag{3.3.1}$$

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 3.3.1. *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.

3.3.2 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 3.3.2 (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 $A(t) = e^{\mathrm{i}Ht} A \otimes \mathrm{id}_{X^c} e^{-\mathrm{i}Ht}$ with H given by (3.3.1). Then there are constants $c, a, v > 0$ independent of A, B or d such that*

$$\|[A(t), \mathrm{id}_X \otimes B]\| \leq c|X||Y|\|A\|\|B\| \exp(-a(d(X,Y) - v|t|)), \tag{3.3.2}$$

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 3.3.3. *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*

$$\|[A, \mathrm{id} \otimes B]\| \leq \varepsilon \|B\|. \tag{3.3.3}$$

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

$$\|A - A_1 \otimes \mathrm{id}\| \leq \varepsilon. \tag{3.3.4}$$

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

Proof of Lemma 3.3.3. 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 3.3.4. *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 (3.3.1). Then for all $t \in \mathbb{R}$, there is an operator $A_\ell(t) \in \mathcal{L}(\mathcal{H}_{\widetilde{X}})$ such that*

$$\|A(t) - A_\ell(t) \otimes \mathrm{id}_{\widetilde{X}^c}\| \leq d|X|\|A\| \exp(-a(\ell - v|t|)). \tag{3.3.5}$$

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

Proof. Combining Lemma 3.3.3 with the Lieb-Robinson bonud (3.3.2), we directly get the result. □

3.3.3 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 3.3.5. *Let H be the Hamiltonian defined in (3.3.1) satisfying the assumptions 3.3.1. 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*

$$\left\|(\mathrm{id}_{1:j-\ell-1} \otimes O_M \otimes \mathrm{id}_{j+\ell+1:d})(O_L \otimes \mathrm{id}_{j+1:d})(\mathrm{id}_{1:j} \otimes O_R) - |\Psi_0\rangle\langle\Psi_0|\right\| \leq C \exp(-\beta\ell). \tag{3.3.6}$$

From eq. (3.3.6), the area law and the TT approximation of the ground-state follows.

Corollary 3.3.6. *Let Ψ_0 be the ground-state wave function of H given by (3.3.1). 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 3.3.7. *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 3.3.5 The proof of the theorem relies on the following approximation of the ground-state projection

$$\rho_q = \frac{1}{\sqrt{2\pi q}} \int_{\mathbb{R}} e^{\mathrm{i}Ht} e^{-\frac{t^2}{2q}} \,\mathrm{d}t, \tag{3.3.7}$$

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

$$\|\rho_q - |\Psi_0\rangle\langle\Psi_0|\| \leq e^{-\frac{1}{2}\gamma^2 q}, \tag{3.3.8}$$

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 3.3.4, 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 3.3.5

Lemma 3.3.8. *Let $q > 0$ and ρ_q be defined by*

$$\rho_q = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t. \tag{3.3.9}$$

Then we have

$$\|\rho_q - |\Psi_0\rangle\langle\Psi_0|\| \leq e^{-\frac{1}{2}\gamma^2 q}, \tag{3.3.10}$$

where γ is the spectral gap.

Proof. This follows from the spectral gap assumption 3.3.1 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 3.3.9. *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

$$H_M(q) = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{-\mathrm{i}Ht}H_M e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle\Psi_0, H_M\Psi_0\rangle \tag{3.3.11}$$

$$H_L(q) = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{-\mathrm{i}Ht}H_L e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle\Psi_0, H_L\Psi_0\rangle \tag{3.3.12}$$

$$H_R(q) = \frac{1}{\sqrt{2\pi q}}\int_{\mathbb{R}} e^{-\mathrm{i}Ht}H_R e^{\mathrm{i}Ht}e^{-\frac{t^2}{2q}}\,\mathrm{d}t - \langle\Psi_0, H_R\Psi_0\rangle. \tag{3.3.13}$$

Then for all $q > 0$, we have

$$H = H_L(q) + H_M(q) + H_R(q), \tag{3.3.14}$$

and

$$\|H_M(q)\Psi_0\|, \|H_L(q)\Psi_0\|, \|H_R(q)\Psi_0\| \leq \gamma J e^{-\frac{1}{2}\gamma^2 q}. \tag{3.3.15}$$

Proof. Since $H = H_L + H_M + H_R$, eq. (3.3.14) is clear. For eq. (3.3.15), 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

$$\|H_M(q)\Psi_0\| \leq \gamma J e^{-\frac{1}{2}\gamma^2 q}. \tag{3.3.16}$$

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 3.3.4.

Lemma 3.3.10. *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 3.3.4, 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 3.3.11. *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 3.3.10. Then we have

$$\left\|\widetilde{\rho}_q - |\Psi_0\rangle\langle\Psi_0|\right\| \lesssim \|h\|\ell^2 d q^{1/2} e^{-a\ell/3} e^{qa^2v^2/2} + e^{-\frac{1}{2}\gamma^2 q}. \tag{3.3.17}$$

Proof. The proof relies on a Duhamel formula:

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

where we have used Lemma 3.3.10. □

Lemma 3.3.12. *Let $\widetilde{H}_L(q)$ and $\widetilde{H}_R(q)$ be the operators defined in Lemma 3.3.10. Let $\alpha > 0$ and $O_R(q)$ and $O_L(q)$ be the following spectral projections*

$$O_L(q) = \sum_{|\lambda|\leq\alpha} |\Phi_\lambda^{(L)}\rangle\langle\Phi_\lambda^{(L)}|, \quad O_R(q) = \sum_{|\lambda|\leq\alpha} |\Phi_\lambda^{(R)}\rangle\langle\Phi_\lambda^{(R)}|, \tag{3.3.18}$$

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

$$\|O_R O_L \Psi_0 - \Psi_0\| \leq \frac{1}{\alpha}\Big(\|\widetilde{H}_L(q) - H_L(q)\| + \|\widetilde{H}_R(q) - H_R(q)\| + \|H_L\Psi_0\| + \|H_R\Psi_0\|\Big), \tag{3.3.19}$$

and

$$\|(e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t} - \mathrm{id})O_L O_R\| \leq 2\alpha|t|. \tag{3.3.20}$$

Proof. We first prove the estimate (3.3.19). Since $O_L(q)$ and $O_R(q)$ commute and are bounded operators by 1, we have

$$\|O_L O_R \Psi_0 - \Psi_0\| \leq \|O_L\Psi_0 - \Psi_0\| + \|O_R\Psi_0 - \Psi_0\|. \tag{3.3.21}$$

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

A final lemma is needed before completing the proof of Theorem 3.3.5 about the splitting of the evolution $e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t}$.

Lemma 3.3.13. *With the notation in Lemma 3.3.10, there is a family of operators $\widetilde{H}_M^{(\ell)}(t) \in \mathcal{L}(\mathcal{H}_{j-\ell:j+\ell})$ such that*

$$\left\| e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_M(q)+\widetilde{H}_R(q))t} - \mathcal{T}\exp\Big(\int_0^t \mathrm{id}_{1:j-\ell-1}\otimes\widetilde{H}_M^{(\ell)}(\tau)\otimes\mathrm{id}_{j+\ell+1:d}\,\mathrm{d}\tau\Big)^*\, e^{\mathrm{i}(\widetilde{H}_L(q)+\widetilde{H}_R(q))t}\right\| \leq t\|h\|\ell^2 d\exp(-a(\ell/3-v|t|)), \quad (3.3.22)$$

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 3.3.4, 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 3.3.5.

Proof of Theorem 3.3.5. Let O_L and O_R be the operators defined in Lemma 3.3.12. Then we have

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

Thus with Lemma 3.3.9 and Lemma 3.3.10, we obtain

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

Using that O_L and O_R are bounded operators by 1, in combination with Lemma 3.3.11, we get

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

where we have used Lemma 3.3.13. By Lemma 3.3.12, we thus have

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

All it remains to do is to set the parameters α and q to prove Theorem 3.3.5. 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 (3.3.6). □

3.4 Area laws via AGSP

The main goal of this section is to prove the following Lemma, which is central in the proof of the area law using AGSP.

Lemma 3.4.1 ([AKL16, Theorem 2.3]). *For $\mathcal{J} \subset \{1, \dots, d-1\}$, let $E_0^{\mathcal{J}}$ and $E_0^{(d)}$ be respectively the lowest eigenvalue of $H_{\mathcal{J}} = \sum_{j \in \mathcal{J}} W_j$ and $H^{(d)}$. Let $\Pi_{[E,E']}$ be the spectral projector of $H_{\mathcal{J}}$ associated to the eigenvalues in $[E, E']$ $(E < E')$. Let $P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}$ be the spectral projector of $H^{(d)}$ associated to the eigenvalues in $[E_0^{(d)}, E_0^{(d)} + \varepsilon]$. Let $E_0^{\mathcal{J}}$ be the lowest eigenvalue of $H_{\mathcal{J}}$. Then there are constants C and α independent of $E, E', \varepsilon, \mathcal{J}$ such that we have*

$$\|\Pi_{[E,E']} P_{[E_0^{(d)}, E_0^{(d)}+\varepsilon]}\| \leq C \exp\Big(-\alpha\big(E - (E_0^{(d)} + \varepsilon - E_0^{\mathcal{J}})\big)\Big). \tag{3.4.1}$$

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