Sparse and symmetry-preserving compression of matrix product operators

S. Badreddine[2] M. Beaupère[2] É. Cancès[3] M.-S. Dupuy[1] L. Grigori[2]

[1]LJLL, Sorbonne Université, Paris [2]INRIA, Paris [3]École des Ponts, INRIA, Paris

Workshop III: Large-Scale Certified Numerical Methods in Quantum Mechanics, May 2022

The many-body problem

Setting and occupation number representation

Want to solve the eigenvalue problem $\mathcal{H}^N \Psi = E\Psi$ with $\Psi \in \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$ and

$$\mathcal{H}^N = \sum_{i=1}^{N} -\frac{1}{2}\Delta_i + v(r_i) + \sum_{1 \le i < j \le N} \frac{1}{|r_i - r_j|}$$

Galerkin approximation $(\phi_i)_{1 \le i \le L}$ orthonormal family of $L^2(\mathbb{R}^3)$

- basis functions of $\bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$: Slater determinants $\phi_{i_1} \wedge \cdots \wedge \phi_{i_N} = \det(\phi_{i_k}(r_j))$

$$\Psi(r_1, \ldots, r_N) = \sum_{1 \le i_1 < \cdots < i_N \le L} C_{i_1 \ldots i_N} \phi_{i_1} \wedge \cdots \wedge \phi_{i_N}(r_1, \ldots, r_N).$$

- possibly $\binom{L}{N}$ nonzero coefficients $C_{i_1 \ldots i_N}$, hard to parametrize

Occupation number representation: reparametrize the Slater determinant wrt occupied states

$$\Psi = \sum_{(\mu_1, \ldots, \mu_L) \in \{0,1\}^L} \boldsymbol{\Psi}_{\mu_1 \ldots \mu_L} \Phi_{(\mu_1, \ldots, \mu_L)},$$

with $\Phi_{(\mu_1, \ldots, \mu_L)} = \phi_{i_1} \wedge \cdots \wedge \phi_{i_N}$ is the Slater determinant of occupied states (*i.e.* $\mu_j = 1$ iff $j = i_k$).

- example: $L = 5$, $\phi_1 \wedge \phi_3 \wedge \phi_4 = \Phi_{(10110)}$ and $\boldsymbol{\Psi}_{10110} = C_{134}$
- remark: since Ψ_0 is a function of N variables, $\boldsymbol{\Psi}_{\mu_1 \ldots \mu_L} = 0$ if $\sum \mu_k \neq N$

Setting and occupation number representation

Want to solve the eigenvalue problem $\mathcal{H}^N\Psi = E\Psi$ with $\Psi \in \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$ and

$$\mathcal{H}^N = \sum_{i=1}^{N} -\frac{1}{2}\Delta_i + v(r_i) + \sum_{1\leq i<j\leq N} \frac{1}{|r_i - r_j|}$$

Galerkin approximation $(\phi_i)_{1\leq i\leq L}$ orthonormal family of $L^2(\mathbb{R}^3)$

- basis functions of $\bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$: Slater determinants $\phi_{i_1} \wedge \cdots \wedge \phi_{i_N} = \det(\phi_{i_k}(r_j))$

$$\Psi(r_1,\dots,r_N) = \sum_{1\leq i_1<\cdots<i_N\leq L} C_{i_1\dots i_N}\phi_{i_1} \wedge \cdots \wedge \phi_{i_N}(r_1,\dots,r_N).$$

- possibly $\binom{L}{N}$ nonzero coefficients $C_{i_1\dots i_N}$, hard to parametrize

Occupation number representation: reparametrize the Slater determinant wrt occupied states

$$\Psi = \sum_{(\mu_1,\dots,\mu_L)\in\{0,1\}^L} \boldsymbol{\Psi}_{\mu_1\dots\mu_L}\Phi_{(\mu_1,\dots,\mu_L)},$$

with $\Phi_{(\mu_1,\dots,\mu_L)} = \phi_{i_1} \wedge \cdots \wedge \phi_{i_N}$ is the Slater determinant of occupied states (*i.e.* $\mu_j = 1$ iff $j = i_k$).

- example: $L = 5$, $\phi_1 \wedge \phi_3 \wedge \phi_4 = \Phi_{(10110)}$ and $\boldsymbol{\Psi}_{10110} = C_{134}$
- remark: since Ψ_0 is a function of N variables, $\boldsymbol{\Psi}_{\mu_1\dots\mu_L} = 0$ if $\sum \mu_k \neq N$

Setting and occupation number representation

Want to solve the eigenvalue problem $\mathcal{H}^N\Psi = E\Psi$ with $\Psi \in \bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$ and

$$\mathcal{H}^N = \sum_{i=1}^{N} -\frac{1}{2}\Delta_i + v(r_i) + \sum_{1\leq i<j\leq N} \frac{1}{|r_i - r_j|}$$

Galerkin approximation $(\phi_i)_{1\leq i\leq L}$ orthonormal family of $L^2(\mathbb{R}^3)$

- basis functions of $\bigwedge_{i=1}^{N} L^2(\mathbb{R}^3)$: Slater determinants $\phi_{i_1} \wedge \cdots \wedge \phi_{i_N} = \det(\phi_{i_k}(r_j))$

$$\Psi(r_1, \dots, r_N) = \sum_{1\leq i_1<\cdots<i_N\leq L} C_{i_1\dots i_N} \phi_{i_1} \wedge \cdots \wedge \phi_{i_N}(r_1, \dots, r_N).$$

- possibly $\binom{L}{N}$ nonzero coefficients $C_{i_1\dots i_N}$, hard to parametrize

Occupation number representation: reparametrize the Slater determinant wrt occupied states

$$\Psi = \sum_{(\mu_1,\dots,\mu_L)\in\{0,1\}^L} \boldsymbol{\Psi}_{\mu_1\dots\mu_L} \Phi_{(\mu_1,\dots,\mu_L)},$$

with $\Phi_{(\mu_1,\dots,\mu_L)} = \phi_{i_1} \wedge \cdots \wedge \phi_{i_N}$ is the Slater determinant of occupied states (*i.e.* $\mu_j = 1$ iff $j = i_k$).

- example: $L = 5$, $\phi_1 \wedge \phi_3 \wedge \phi_4 = \Phi_{(10110)}$ and $\boldsymbol{\Psi}_{10110} = C_{134}$
- remark: since Ψ_0 is a function of N variables, $\boldsymbol{\Psi}_{\mu_1\dots\mu_L} = 0$ if $\sum \mu_k \neq N$

Many-body Hamiltonian

Advantage

Easier to handle $\mathbf{\Psi} \in \mathbb{R}^{2^L}$ by tensor methods (here: matrix product states)

The many-body Hamiltonian in the occupation number representation: $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$

- $\mathbf{H}$ is symmetric

$$\forall(\mu_1, \nu_1, \ldots, \mu_L, \nu_L) \in \{0,1\}^{2L}, \; \mathbf{H}_{\mu_1 \ldots \mu_L}^{\nu_1 \ldots \nu_L} = \mathbf{H}_{\nu_1 \ldots \nu_L}^{\mu_1 \ldots \mu_L}$$

- $\mathbf{H}$ is particle-number preserving

$$\forall(\mu_1, \nu_1, \ldots, \mu_L, \nu_L) \in \{0,1\}^{2L}, \; \mathbf{H}_{\mu_1 \ldots \mu_L}^{\nu_1 \ldots \nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = \sum_{k=1}^{L} \nu_k$$

- $\mathbf{H}$ comes from a two-body Hamiltonian

$$(\mu_k)_{1 \leq k \leq L} \text{ and } (\nu_k)_{1 \leq k \leq L} \text{ differ by more than 2 pairs } \Rightarrow \mathbf{H}_{\mu_1 \ldots \mu_L}^{\nu_1 \ldots \nu_L} = 0.$$

Many-body Hamiltonian

Advantage

Easier to handle $\mathbf{\Psi} \in \mathbb{R}^{2^L}$ by tensor methods (here: matrix product states)

The many-body Hamiltonian in the occupation number representation: $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$

- $\mathbf{H}$ is symmetric

$$\forall (\mu_1, \nu_1, \dots, \mu_L, \nu_L) \in \{0,1\}^{2L}, \ \mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \mathbf{H}_{\nu_1 \dots \nu_L}^{\mu_1 \dots \mu_L}$$

- $\mathbf{H}$ is particle-number preserving

$$\forall (\mu_1, \nu_1, \dots, \mu_L, \nu_L) \in \{0,1\}^{2L}, \ \mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = \sum_{k=1}^{L} \nu_k$$

- $\mathbf{H}$ comes from a two-body Hamiltonian

$(\mu_k)_{1 \leq k \leq L}$ and $(\nu_k)_{1 \leq k \leq L}$ differ by more than 2 pairs $\Rightarrow \mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = 0.$

Many-body Hamiltonian

Advantage

Easier to handle $\mathbf{\Psi} \in \mathbb{R}^{2^L}$ by tensor methods (here: matrix product states)

The many-body Hamiltonian in the occupation number representation: $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$

- $\mathbf{H}$ is symmetric

$$\forall (\mu_1, \nu_1, \dots, \mu_L, \nu_L) \in \{0,1\}^{2L},\ \mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} = \mathbf{H}^{\mu_1 \dots \mu_L}_{\nu_1 \dots \nu_L}$$

- $\mathbf{H}$ is particle-number preserving

$$\forall (\mu_1, \nu_1, \dots, \mu_L, \nu_L) \in \{0,1\}^{2L},\ \mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = \sum_{k=1}^{L} \nu_k$$

- $\mathbf{H}$ comes from a two-body Hamiltonian

$$(\mu_k)_{1 \leq k \leq L} \text{ and } (\nu_k)_{1 \leq k \leq L} \text{ differ by more than 2 pairs } \Rightarrow \mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} = 0.$$

Second quantization

Matrix representation $\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} \in \mathbb{R}^{2^L\times 2^L}$ of the second quantized Hamiltonian

$$\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} = \begin{array}{c} \\ \text{0 electron sector} \\ \text{1 electron sector} \\ \vdots \\ \text{L electron sector} \end{array} \begin{array}{cccc} \text{0 electron sector} & \text{1 electron sector} & \cdots & \text{L electron sector} \\ \end{array}$$

$$\begin{pmatrix} H_0 & 0 & \cdots & 0 \\ 0 & H_1 & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & H_L \end{pmatrix}$$

Example: $L = 2$

$$\mathbf{H}^{\nu_1\nu_2}_{\mu_1\mu_2} = \begin{array}{c|cccc} {}_{\mu_1\mu_2}\backslash^{\nu_1\nu_2} & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & 0 \\ 01 & 0 & (H_1)^{01}_{01} & (H_1)^{10}_{01} & 0 \\ 10 & 0 & (H_1)^{01}_{10} & (H_1)^{10}_{10} & 0 \\ 11 & 0 & 0 & 0 & H_2 \end{array}$$

Second quantization

$$\mathbf{H} = \sum_{i,j=1}^{L} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{L} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

with $a_i^\dagger$ and a_j are creation and annihilation operators, $(h_{ij}) \in \mathbb{R}^{L\times L}$ are one-electron integrals, $V_{ijkl} \in \mathbb{R}^{L^4}$ two-electron integrals.

Second quantization

Matrix representation $\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} \in \mathbb{R}^{2^L\times 2^L}$ of the second quantized Hamiltonian

$$\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} = \begin{array}{r} \\ \text{0 electron sector} \\ \text{1 electron sector} \\ \vdots \\ \text{L electron sector} \end{array} \begin{array}{c} \begin{array}{cccc} \text{0 electron sector} & \text{1 electron sector} & \cdots & \text{L electron sector} \end{array} \\ \begin{pmatrix} H_0 & 0 & \cdots & 0 \\ 0 & H_1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & H_L \end{pmatrix} \end{array}$$

Example: $L = 2$

$$\mathbf{H}^{\nu_1\nu_2}_{\mu_1\mu_2} = \begin{array}{c|cccc} {}_{\mu_1\mu_2}\backslash^{\nu_1\nu_2} & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & 0 \\ 01 & 0 & (H_1)^{01}_{01} & (H_1)^{10}_{01} & 0 \\ 10 & 0 & (H_1)^{01}_{10} & (H_1)^{10}_{10} & 0 \\ 11 & 0 & 0 & 0 & H_2 \end{array}$$

Second quantization

$$\mathbf{H} = \sum_{i,j=1}^{L} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{L} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

with $a_i^\dagger$ and a_j are creation and annihilation operators, $(h_{ij}) \in \mathbb{R}^{L\times L}$ are one-electron integrals, $V_{ijkl} \in \mathbb{R}^{L^4}$ two-electron integrals.

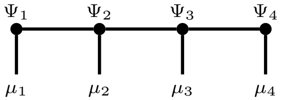
Matrix product operators

Matrix product state

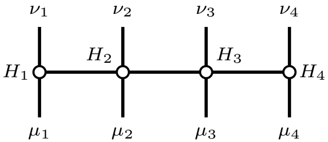
For $\mathbf{\Psi} \in \mathbb{R}^{2^L}$, $(\Psi_1, \ldots, \Psi_L)$ is an MPS representation of $\mathbf{\Psi}$ if

$$\forall (\mu_1, \ldots, \mu_L) \in \{0,1\}^L, \mathbf{\Psi}_{\mu_1 \ldots \mu_L} = \Psi_1[\mu_1]\Psi_2[\mu_2] \cdots \Psi_L[\mu_L], \quad \text{where } \Psi_k[\mu_k] \in \mathbb{R}^{r_{k-1} \times r_k}$$

$(r_k)_{k=0,\ldots,L}$ are called *MPS ranks* ($(r_0 = r_L = 1)$).



(a) Graphical representation of an MPS



(b) Graphical representation of an MPO

Matrix product operator

For $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$, $(H_1, \ldots, H_L)$ is an MPO representation of $\mathbf{H}$ if

$$\forall (\mu_1, \nu_1, \ldots, \mu_L, \nu_L) \in \{0,1\}^{2L}, \mathbf{H}^{\nu_1 \ldots \nu_L}_{\mu_1 \ldots \mu_L} = H_1[\mu_1, \nu_1] H_2[\mu_2, \nu_2] \cdots H_L[\mu_L, \nu_L],$$

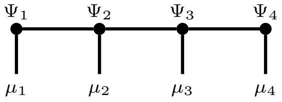
with $H_k[\mu_k, \nu_k] \in \mathbb{R}^{R_{k-1} \times R_k}$. $(R_k)_{k=0,\ldots,L}$ are called *MPO ranks* ($(R_0 = R_L = 1)$).

Matrix product state

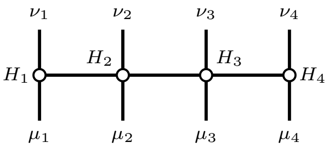
For $\mathbf{\Psi} \in \mathbb{R}^{2^L}$, $(\Psi_1, \dots, \Psi_L)$ is an MPS representation of $\mathbf{\Psi}$ if

$$\forall (\mu_1, \dots, \mu_L) \in \{0,1\}^L, \mathbf{\Psi}_{\mu_1 \dots \mu_L} = \Psi_1[\mu_1]\Psi_2[\mu_2] \cdots \Psi_L[\mu_L], \quad \text{where } \Psi_k[\mu_k] \in \mathbb{R}^{r_{k-1} \times r_k}$$

$(r_k)_{k=0,\dots,L}$ are called *MPS ranks* ($(r_0 = r_L = 1)$).



(a) Graphical representation of an MPS



(b) Graphical representation of an MPO

Matrix product operator

For $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$, $(H_1, \dots, H_L)$ is an MPO representation of $\mathbf{H}$ if

$$\forall (\mu_1, \nu_1, \dots, \mu_L, \nu_L) \in \{0,1\}^{2L}, \mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = H_1[\mu_1, \nu_1] H_2[\mu_2, \nu_2] \cdots H_L[\mu_L, \nu_L],$$

with $H_k[\mu_k, \nu_k] \in \mathbb{R}^{R_{k-1} \times R_k}$. $(R_k)_{k=0,\dots,L}$ are called *MPO ranks* ($(R_0 = R_L = 1)$).

Why the MPO?

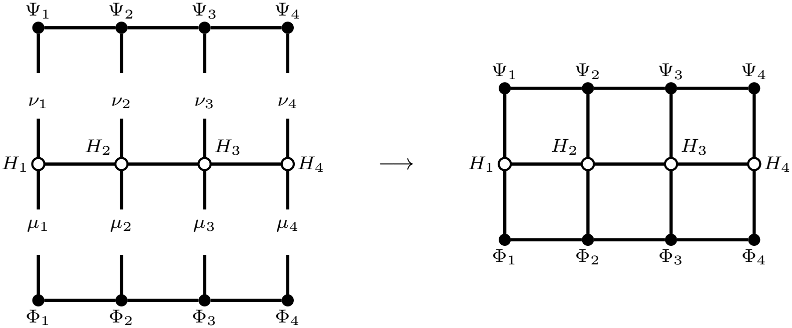
Computation of $\langle \Phi, H\Psi \rangle$

- MPO $\mathbf{H}$ of MPO rank R: $\mathbf{H}_{\mu_1\ldots\mu_L}^{\nu_1\ldots\nu_L} = H_1[\mu_1,\nu_1]H_2[\mu_2,\nu_2]\cdots H_L[\mu_L,\nu_L]$
- MPS $\mathbf{\Phi}, \mathbf{\Psi}$ of MPS rank r

$$\mathbf{\Psi}_{\nu_1\ldots\nu_L} = \Psi_1[\nu_1]\Psi_2[\nu_2]\cdots\Psi_L[\nu_L], \quad \mathbf{\Phi}_{\mu_1\ldots\mu_L} = \Phi_1[\mu_1]\Phi_2[\mu_2]\cdots\Phi_L[\mu_L]$$

Expectation value

$$\langle \Phi, H\Psi \rangle = \sum_{\mu_1\ldots\mu_L\in\{0,1\}^L} \sum_{\nu_1\ldots\nu_L\in\{0,1\}^L} \mathbf{\Phi}_{\mu_1\ldots\mu_L} \mathbf{H}_{\mu_1\ldots\mu_L}^{\nu_1\ldots\nu_L} \mathbf{\Psi}_{\nu_1\ldots\nu_L}$$



Computational cost: $\mathcal{O}(Rr^2)$

Algebraic properties of MPOs

Algebraic properties of MPO: consider $\mathbf{H}, \widetilde{\mathbf{H}} \in \mathbb{R}^{2^L \times 2^L}$ with respective MPO

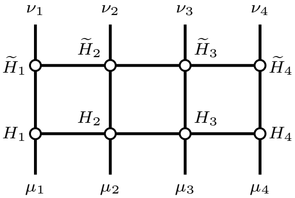
$$\mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = H_1[\mu_1, \nu_1] H_2[\mu_2, \nu_2] \cdots H_L[\mu_L, \nu_L], \quad \text{and} \quad \widetilde{\mathbf{H}}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \widetilde{H}_1[\mu_1, \nu_1] \widetilde{H}_2[\mu_2, \nu_2] \cdots \widetilde{H}_L[\mu_L, \nu_L].$$

- multiplication by a scalar: free
- addition of two MPOs: $\mathbf{F} = \mathbf{H} + \widetilde{\mathbf{H}}$

$$\mathbf{F}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \begin{pmatrix} H_1[\mu_1, \nu_1] & \widetilde{H_1}[\mu_1, \nu_1] \end{pmatrix} \begin{pmatrix} H_2[\mu_2, \nu_2] & 0 \\ 0 & \widetilde{H}_2[\mu_2, \nu_2] \end{pmatrix} \cdots \begin{pmatrix} H_{L-1}[\mu_{L-1}, \nu_{L-1}] & 0 \\ 0 & \widetilde{H}_{L-1}[\mu_{L-1}, \nu_{L-1}] \end{pmatrix} \begin{pmatrix} H_L[\mu_L, \nu_L] \\ \widetilde{H}_L[\mu_L, \nu_L] \end{pmatrix}$$

  - MPO rank of $\mathbf{F}$ = MPO rank of $\mathbf{H}$ + MPO rank of $\widetilde{\mathbf{H}}$.

- multiplication of two MPOs: $\mathbf{G} = \mathbf{H} * \widetilde{\mathbf{H}}$



  - MPO rank of $\mathbf{G}$ = MPO rank of $\mathbf{H}$ × MPO rank of $\widetilde{\mathbf{H}}$

Algebraic properties of MPOs

Algebraic properties of MPO: consider $\mathbf{H}, \widetilde{\mathbf{H}} \in \mathbb{R}^{2^L \times 2^L}$ with respective MPO

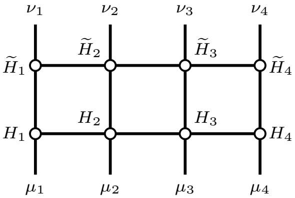
$$\mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} = H_1[\mu_1, \nu_1] H_2[\mu_2, \nu_2] \cdots H_L[\mu_L, \nu_L], \quad \text{and} \quad \widetilde{\mathbf{H}}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} = \widetilde{H}_1[\mu_1, \nu_1] \widetilde{H}_2[\mu_2, \nu_2] \cdots \widetilde{H}_L[\mu_L, \nu_L].$$

- multiplication by a scalar: free
- addition of two MPOs: $\mathbf{F} = \mathbf{H} + \widetilde{\mathbf{H}}$

$$\mathbf{F}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} = \begin{pmatrix} H_1[\mu_1, \nu_1] & \widetilde{H}_1[\mu_1, \nu_1] \end{pmatrix} \begin{pmatrix} H_2[\mu_2, \nu_2] & 0 \\ 0 & \widetilde{H}_2[\mu_2, \nu_2] \end{pmatrix} \cdots \begin{pmatrix} H_{L-1}[\mu_{L-1}, \nu_{L-1}] & 0 \\ 0 & \widetilde{H}_{L-1}[\mu_{L-1}, \nu_{L-1}] \end{pmatrix} \begin{pmatrix} H_L[\mu_L, \nu_L] \\ \widetilde{H}_L[\mu_L, \nu_L] \end{pmatrix}$$

  - MPO rank of $\mathbf{F}$ = MPO rank of $\mathbf{H}$ + MPO rank of $\widetilde{\mathbf{H}}$.

- multiplication of two MPOs: $\mathbf{G} = \mathbf{H} * \widetilde{\mathbf{H}}$



  - MPO rank of $\mathbf{G}$ = MPO rank of $\mathbf{H}$ × MPO rank of $\widetilde{\mathbf{H}}$

Algebraic properties of MPOs

Algebraic properties of MPO: consider $\mathbf{H}, \widetilde{\mathbf{H}} \in \mathbb{R}^{2^L \times 2^L}$ with respective MPO

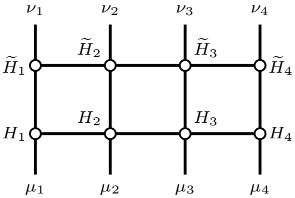
$$\mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = H_1[\mu_1, \nu_1] H_2[\mu_2, \nu_2] \cdots H_L[\mu_L, \nu_L], \quad \text{and} \quad \widetilde{\mathbf{H}}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \widetilde{H}_1[\mu_1, \nu_1] \widetilde{H}_2[\mu_2, \nu_2] \cdots \widetilde{H}_L[\mu_L, \nu_L].$$

- multiplication by a scalar: free
- addition of two MPOs: $\mathbf{F} = \mathbf{H} + \widetilde{\mathbf{H}}$

$$\mathbf{F}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \begin{pmatrix} H_1[\mu_1, \nu_1] & \widetilde{H_1}[\mu_1, \nu_1] \end{pmatrix} \begin{pmatrix} H_2[\mu_2, \nu_2] & 0 \\ 0 & \widetilde{H}_2[\mu_2, \nu_2] \end{pmatrix} \dots \begin{pmatrix} H_{L-1}[\mu_{L-1}, \nu_{L-1}] & 0 \\ 0 & \widetilde{H}_{L-1}[\mu_{L-1}, \nu_{L-1}] \end{pmatrix} \begin{pmatrix} H_L[\mu_L, \nu_L] \\ \widetilde{H}_L[\mu_L, \nu_L] \end{pmatrix}$$

  - MPO rank of $\mathbf{F}$ = MPO rank of $\mathbf{H}$ + MPO rank of $\widetilde{\mathbf{H}}$.

- multiplication of two MPOs: $\mathbf{G} = \mathbf{H} * \widetilde{\mathbf{H}}$



  - MPO rank of $\mathbf{G}$ = MPO rank of $\mathbf{H}$ × MPO rank of $\widetilde{\mathbf{H}}$

Algebraic properties of MPOs

Algebraic properties of MPO: consider $\mathbf{H}, \widetilde{\mathbf{H}} \in \mathbb{R}^{2^L \times 2^L}$ with respective MPO

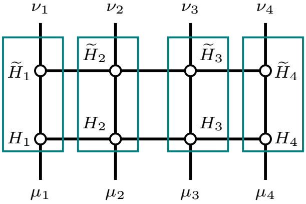
$$\mathbf{H}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = H_1[\mu_1, \nu_1] H_2[\mu_2, \nu_2] \cdots H_L[\mu_L, \nu_L], \quad \text{and} \quad \widetilde{\mathbf{H}}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \widetilde{H}_1[\mu_1, \nu_1] \widetilde{H}_2[\mu_2, \nu_2] \cdots \widetilde{H}_L[\mu_L, \nu_L].$$

- multiplication by a scalar: free
- addition of two MPOs: $\mathbf{F} = \mathbf{H} + \widetilde{\mathbf{H}}$

$$\mathbf{F}_{\mu_1 \dots \mu_L}^{\nu_1 \dots \nu_L} = \begin{pmatrix} H_1[\mu_1, \nu_1] & \widetilde{H_1}[\mu_1, \nu_1] \end{pmatrix} \begin{pmatrix} H_2[\mu_2, \nu_2] & 0 \\ 0 & \widetilde{H}_2[\mu_2, \nu_2] \end{pmatrix} \cdots \begin{pmatrix} H_{L-1}[\mu_{L-1}, \nu_{L-1}] & 0 \\ 0 & \widetilde{H}_{L-1}[\mu_{L-1}, \nu_{L-1}] \end{pmatrix} \begin{pmatrix} H_L[\mu_L, \nu_L] \\ \widetilde{H}_L[\mu_L, \nu_L] \end{pmatrix}$$

  - MPO rank of $\mathbf{F}$ = MPO rank of $\mathbf{H}$ + MPO rank of $\widetilde{\mathbf{H}}$.

- multiplication of two MPOs: $\mathbf{G} = \mathbf{H} * \widetilde{\mathbf{H}}$



  - MPO rank of $\mathbf{G}$ = MPO rank of $\mathbf{H}$ × MPO rank of $\widetilde{\mathbf{H}}$

Construction of the MPO of the Hamiltonian

Second quantized Hamiltonian

$$\mathbf{H} = \sum_{i,j=1}^{L} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{L} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

MPO of creation and annihilation operators

- a_i, $a_j^\dagger$ have MPO rank 1
- $a_i^\dagger a_j$ and $a_i^\dagger a_j^\dagger a_l a_k$ have MPO rank 1
- by summation $\mathbf{H}$ has MPO rank $\mathcal{O}(L^4)$

Theorem (Bachmayr, Götte, Pfeffer (2021)[1])

There is an explicit MPO representation of $\mathbf{H}$ *with MPO ranks bounded by* $\mathcal{O}(L^2)$.

Goal

Want to reduce the naive $\mathcal{O}(L^4)$ to $\mathcal{O}(L^2)$ (or even better)

[1] Chan, Garnet Kin-Lic, et al., JCP 145.1 (2016): 014102.

Construction of the MPO of the Hamiltonian

Second quantized Hamiltonian

$$\mathbf{H} = \sum_{i,j=1}^{L} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{L} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

MPO of creation and annihilation operators

- a_i, $a_j^\dagger$ have MPO rank 1
- $a_i^\dagger a_j$ and $a_i^\dagger a_j^\dagger a_l a_k$ have MPO rank 1
- by summation $\mathbf{H}$ has MPO rank $\mathcal{O}(L^4)$

Theorem (Bachmayr, Götte, Pfeffer (2021)[1])

There is an explicit MPO representation of $\mathbf{H}$ *with MPO ranks bounded by* $\mathcal{O}(L^2)$.

Goal

Want to reduce the naive $\mathcal{O}(L^4)$ to $\mathcal{O}(L^2)$ (or even better)

[1] Chan, Garnet Kin-Lic, et al., JCP 145.1 (2016): 014102.

Construction of the MPO of the Hamiltonian

Second quantized Hamiltonian

$$\mathbf{H} = \sum_{i,j=1}^{L} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{L} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

MPO of creation and annihilation operators

- a_i, $a_j^\dagger$ have MPO rank 1
- $a_i^\dagger a_j$ and $a_i^\dagger a_j^\dagger a_l a_k$ have MPO rank 1
- by summation $\mathbf{H}$ has MPO rank $\mathcal{O}(L^4)$

Theorem (Bachmayr, Götte, Pfeffer (2021)[1])

There is an explicit MPO representation of $\mathbf{H}$ *with MPO ranks bounded by* $\mathcal{O}(L^2)$.

Goal

Want to reduce the naive $\mathcal{O}(L^4)$ to $\mathcal{O}(L^2)$ (or even better)

[1] Chan, Garnet Kin-Lic, et al., JCP 145.1 (2016): 014102.

Construction of the MPO of the Hamiltonian

Second quantized Hamiltonian

$$\mathbf{H} = \sum_{i,j=1}^{L} h_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{L} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k,$$

MPO of creation and annihilation operators

- a_i, $a_j^\dagger$ have MPO rank 1
- $a_i^\dagger a_j$ and $a_i^\dagger a_j^\dagger a_l a_k$ have MPO rank 1
- by summation $\mathbf{H}$ has MPO rank $\mathcal{O}(L^4)$

Theorem (Bachmayr, Götte, Pfeffer (2021)[1])

There is an explicit MPO representation of $\mathbf{H}$ *with MPO ranks bounded by* $\mathcal{O}(L^2)$.

Goal

Want to reduce the naive $\mathcal{O}(L^4)$ to $\mathcal{O}(L^2)$ (or even better)

[1] Chan, Garnet Kin-Lic, et al., JCP 145.1 (2016): 014102.

Compression of the MPO

Hierarchical SVD[1,2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$
\begin{aligned}
\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} &= \mathbf{H}^{\mu_1\nu_1}_{\mu_2\nu_2\cdots\mu_L\nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4\times 2^{2(L-1)}\text{)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha}_{\mu_2\nu_2\cdots\mu_L\nu_L} && \text{(SVD)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha\mu_2\nu_2}_{\mu_3\nu_3\cdots\mu_L\nu_L} && \text{(reshape of } V_1\text{)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta}_{\mu_3\nu_3\cdots\mu_L\nu_L} && \text{(SVD of } V_1\text{)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta\mu_3\nu_3}_{\mu_4\nu_4\cdots\mu_L\nu_L} && \text{(reshape of } V_2\text{)}
\end{aligned}
$$

And so on and so forth

$$
\begin{aligned}
\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} &= (U_1)^{\mu_1\nu_1}_{\alpha_1}(\Sigma_1)^{\alpha_1}_{\alpha_1}(U_2)^{\alpha_1\mu_2\nu_2}_{\alpha_2}(\Sigma_2)^{\alpha_2}_{\alpha_2}\cdots(U_{L-1})^{\alpha_{L-2}\mu_{L-1}\nu_{L-1}}_{\alpha_{L-1}}(\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}}(V_L)^{\alpha_{L-1}}_{\mu_L\nu_L}\\
&= H_1[\mu_1\nu_1] \quad H_2[\mu_2\nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1}\nu_{L-1}] \quad H_L[\mu_L\nu_L].
\end{aligned}
$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.

[2] Oseledets, SIAM J. Sci. Comput., 2011.

Hierarchical SVD[1,2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$\begin{aligned}
\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} &= \mathbf{H}^{\mu_1\nu_1}_{\mu_2\nu_2\dots\mu_L\nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4\times 2^{2(L-1)}) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha}_{\mu_2\nu_2\dots\mu_L\nu_L} && \text{(SVD)} \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha\mu_2\nu_2}_{\mu_3\nu_3\dots\mu_L\nu_L} && \text{(reshape of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta}_{\mu_3\nu_3\dots\mu_L\nu_L} && \text{(SVD of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta\mu_3\nu_3}_{\mu_4\nu_4\dots\mu_L\nu_L} && \text{(reshape of } V_2)
\end{aligned}$$

And so on and so forth

$$\begin{aligned}
\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} &= (U_1)^{\mu_1\nu_1}_{\alpha_1}(\Sigma_1)^{\alpha_1}_{\alpha_1}(U_2)^{\alpha_1\mu_2\nu_2}_{\alpha_2}(\Sigma_2)^{\alpha_2}_{\alpha_2}\cdots(U_{L-1})^{\alpha_{L-2}\mu_{L-1}\nu_{L-1}}_{\alpha_{L-1}}(\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}}(V_L)^{\alpha_{L-1}}_{\mu_L\nu_L} \\
&= \quad H_1[\mu_1\nu_1] \quad H_2[\mu_2\nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1}\nu_{L-1}] \quad H_L[\mu_L\nu_L].
\end{aligned}$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.

[2] Oseledets, SIAM J. Sci. Comput., 2011.

Hierarchical SVD[1,2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$
\begin{aligned}
\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} &= \mathbf{H}^{\mu_1\nu_1}_{\mu_2\nu_2\dots\mu_L\nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4 \times 2^{2(L-1)}) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha}_{\mu_2\nu_2\dots\mu_L\nu_L} && \text{(SVD)} \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha\mu_2\nu_2}_{\mu_3\nu_3\dots\mu_L\nu_L} && \text{(reshape of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta}_{\mu_3\nu_3\dots\mu_L\nu_L} && \text{(SVD of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta\mu_3\nu_3}_{\mu_4\nu_4\dots\mu_L\nu_L} && \text{(reshape of } V_2)
\end{aligned}
$$

And so on and so forth

$$
\begin{aligned}
\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} &= (U_1)^{\mu_1\nu_1}_{\alpha_1}(\Sigma_1)^{\alpha_1}_{\alpha_1}(U_2)^{\alpha_1\mu_2\nu_2}_{\alpha_2}(\Sigma_2)^{\alpha_2}_{\alpha_2}\cdots(U_{L-1})^{\alpha_{L-2}\mu_{L-1}\nu_{L-1}}_{\alpha_{L-1}}(\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}}(V_L)^{\alpha_{L-1}}_{\mu_L\nu_L} \\
&= \quad H_1[\mu_1\nu_1] \quad H_2[\mu_2\nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1}\nu_{L-1}] \quad H_L[\mu_L\nu_L].
\end{aligned}
$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.

[2] Oseledets, SIAM J. Sci. Comput., 2011.

Hierarchical SVD[1,2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$
\begin{aligned}
\mathbf{H}^{\nu_1\ldots\nu_L}_{\mu_1\ldots\mu_L} &= \mathbf{H}^{\mu_1\nu_1}_{\mu_2\nu_2\ldots\mu_L\nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4\times 2^{2(L-1)}\text{)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha}_{\mu_2\nu_2\ldots\mu_L\nu_L} && \text{(SVD)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha\mu_2\nu_2}_{\mu_3\nu_3\ldots\mu_L\nu_L} && \text{(reshape of } V_1\text{)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta}_{\mu_3\nu_3\ldots\mu_L\nu_L} && \text{(SVD of } V_1\text{)}\\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta\mu_3\nu_3}_{\mu_4\nu_4\ldots\mu_L\nu_L} && \text{(reshape of } V_2\text{)}
\end{aligned}
$$

And so on and so forth

$$
\begin{aligned}
\mathbf{H}^{\nu_1\ldots\nu_L}_{\mu_1\ldots\mu_L} &= (U_1)^{\mu_1\nu_1}_{\alpha_1}(\Sigma_1)^{\alpha_1}_{\alpha_1}(U_2)^{\alpha_1\mu_2\nu_2}_{\alpha_2}(\Sigma_2)^{\alpha_2}_{\alpha_2}\cdots(U_{L-1})^{\alpha_{L-2}\mu_{L-1}\nu_{L-1}}_{\alpha_{L-1}}(\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}}(V_L)^{\alpha_{L-1}}_{\mu_L\nu_L}\\
&= H_1[\mu_1\nu_1] \quad H_2[\mu_2\nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1}\nu_{L-1}] \quad H_L[\mu_L\nu_L].
\end{aligned}
$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.

[2] Oseledets, SIAM J. Sci. Comput., 2011.

Hierarchical SVD[1,2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$
\begin{aligned}
\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} &= \mathbf{H}^{\mu_1\nu_1}_{\mu_2\nu_2\ldots\mu_L\nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4\times 2^{2(L-1)}) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha}_{\mu_2\nu_2\ldots\mu_L\nu_L} && \text{(SVD)} \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha\mu_2\nu_2}_{\mu_3\nu_3\ldots\mu_L\nu_L} && \text{(reshape of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta}_{\mu_3\nu_3\ldots\mu_L\nu_L} && \text{(SVD of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta\mu_3\nu_3}_{\mu_4\nu_4\ldots\mu_L\nu_L} && \text{(reshape of } V_2)
\end{aligned}
$$

And so on and so forth

$$
\begin{aligned}
\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} &= (U_1)^{\mu_1\nu_1}_{\alpha_1}(\Sigma_1)^{\alpha_1}_{\alpha_1}(U_2)^{\alpha_1\mu_2\nu_2}_{\alpha_2}(\Sigma_2)^{\alpha_2}_{\alpha_2}\cdots(U_{L-1})^{\alpha_{L-2}\mu_{L-1}\nu_{L-1}}_{\alpha_{L-1}}(\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}}(V_L)^{\alpha_{L-1}}_{\mu_L\nu_L} \\
&= H_1[\mu_1\nu_1] \quad H_2[\mu_2\nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1}\nu_{L-1}] \quad H_L[\mu_L\nu_L].
\end{aligned}
$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.

[2] Oseledets, SIAM J. Sci. Comput., 2011.

Hierarchical SVD[1,2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$\begin{aligned}
\mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} &= \mathbf{H}^{\mu_1 \nu_1}_{\mu_2 \nu_2 \dots \mu_L \nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4 \times 2^{2(L-1)}) \\
&= (U_1)^{\mu_1 \nu_1}_{\alpha} (\Sigma_1)^{\alpha}_{\alpha} (V_1)^{\alpha}_{\mu_2 \nu_2 \dots \mu_L \nu_L} && \text{(SVD)} \\
&= (U_1)^{\mu_1 \nu_1}_{\alpha} (\Sigma_1)^{\alpha}_{\alpha} (V_1)^{\alpha \mu_2 \nu_2}_{\mu_3 \nu_3 \dots \mu_L \nu_L} && \text{(reshape of } V_1) \\
&= (U_1)^{\mu_1 \nu_1}_{\alpha} (\Sigma_1)^{\alpha}_{\alpha} (U_2)^{\alpha \mu_2 \nu_2}_{\beta} (\Sigma_2)^{\beta}_{\beta} (V_2)^{\beta}_{\mu_3 \nu_3 \dots \mu_L \nu_L} && \text{(SVD of } V_1) \\
&= (U_1)^{\mu_1 \nu_1}_{\alpha} (\Sigma_1)^{\alpha}_{\alpha} (U_2)^{\alpha \mu_2 \nu_2}_{\beta} (\Sigma_2)^{\beta}_{\beta} (V_2)^{\beta \mu_3 \nu_3}_{\mu_4 \nu_4 \dots \mu_L \nu_L} && \text{(reshape of } V_2)
\end{aligned}$$

And so on and so forth

$$\begin{aligned}
\mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} &= (U_1)^{\mu_1 \nu_1}_{\alpha_1} (\Sigma_1)^{\alpha_1}_{\alpha_1} (U_2)^{\alpha_1 \mu_2 \nu_2}_{\alpha_2} (\Sigma_2)^{\alpha_2}_{\alpha_2} \cdots (U_{L-1})^{\alpha_{L-2} \mu_{L-1} \nu_{L-1}}_{\alpha_{L-1}} (\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}} (V_L)^{\alpha_{L-1}}_{\mu_L \nu_L} \\
&= H_1[\mu_1 \nu_1] \quad H_2[\mu_2 \nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1} \nu_{L-1}] \quad H_L[\mu_L \nu_L].
\end{aligned}$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.

[2] Oseledets, SIAM J. Sci. Comput., 2011.

Hierarchical SVD[1][2]

Apply successive SVD to $\mathbf{H} \in \mathbb{R}^{2^L \times 2^L}$:

$$\begin{aligned}
\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} &= \mathbf{H}^{\mu_1\nu_1}_{\mu_2\nu_2\cdots\mu_L\nu_L} && \text{(reshape of } \mathbf{H} \text{ to } 4\times 2^{2(L-1)}) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha}_{\mu_2\nu_2\cdots\mu_L\nu_L} && \text{(SVD)} \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(V_1)^{\alpha\mu_2\nu_2}_{\mu_3\nu_3\cdots\mu_L\nu_L} && \text{(reshape of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta}_{\mu_3\nu_3\cdots\mu_L\nu_L} && \text{(SVD of } V_1) \\
&= (U_1)^{\mu_1\nu_1}_{\alpha}(\Sigma_1)^{\alpha}_{\alpha}(U_2)^{\alpha\mu_2\nu_2}_{\beta}(\Sigma_2)^{\beta}_{\beta}(V_2)^{\beta\mu_3\nu_3}_{\mu_4\nu_4\cdots\mu_L\nu_L} && \text{(reshape of } V_2)
\end{aligned}$$

And so on and so forth

$$\begin{aligned}
\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} &= (U_1)^{\mu_1\nu_1}_{\alpha_1}(\Sigma_1)^{\alpha_1}_{\alpha_1}(U_2)^{\alpha_1\mu_2\nu_2}_{\alpha_2}(\Sigma_2)^{\alpha_2}_{\alpha_2}\cdots(U_{L-1})^{\alpha_{L-2}\mu_{L-1}\nu_{L-1}}_{\alpha_{L-1}}(\Sigma_{L-1})^{\alpha_{L-1}}_{\alpha_{L-1}}(V_L)^{\alpha_{L-1}}_{\mu_L\nu_L} \\
&= H_1[\mu_1\nu_1] \quad H_2[\mu_2\nu_2] \quad \cdots \quad H_{L-1}[\mu_{L-1}\nu_{L-1}] \quad H_L[\mu_L\nu_L].
\end{aligned}$$

Compression of an MPO

Truncate the singular values Σ_k to a threshold ε

[1] Schollwoeck, Annals of physics, 2011.
[2] Oseledets, SIAM J. Sci. Comput., 2011.

Compression of an MPO

Basic properties to preserve

1. symmetry:

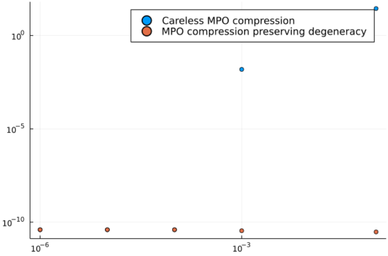
$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} = \mathbf{H}^{\mu_1\dots\mu_L}_{\nu_1\dots\nu_L}$$

2. particle number conservation:

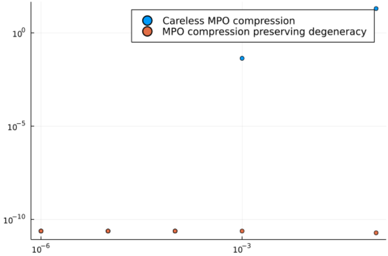
$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} \neq 0 \Rightarrow \sum_{k=1}^{L}\mu_k = \sum_{k=1}^{L}\nu_k$$

3. two-body interactions:

$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} \neq 0 \Rightarrow \sum_{k=1}^{L}|\mu_k-\nu_k| \leq 4$$



(a) Norm of $\mathbf{H} - \mathbf{H}^T$



(b) Norm of $\mathbf{H}\hat{N} - \hat{N}\mathbf{H}$

Keep degenerate singular values when truncating

Compression of an MPO

Basic properties to preserve

1. symmetry:

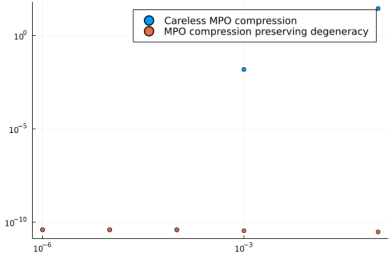
$$\forall(\mu_1, \nu_1, \ldots, \mu_L, \nu_L) \in \{0,1\}^{2L},\ \mathbf{H}_{\mu_1 \ldots \mu_L}^{\nu_1 \ldots \nu_L} = \mathbf{H}_{\nu_1 \ldots \nu_L}^{\mu_1 \ldots \mu_L}$$

2. particle number conservation:

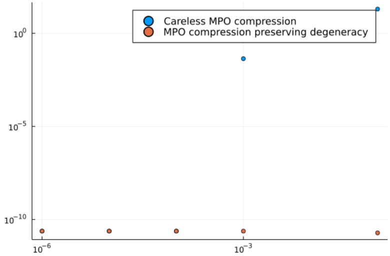
$$\forall(\mu_1, \nu_1, \ldots, \mu_L, \nu_L) \in \{0,1\}^{2L},\ \mathbf{H}_{\mu_1 \ldots \mu_L}^{\nu_1 \ldots \nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = \sum_{k=1}^{L} \nu_k$$

3. two-body interactions:

$$\forall(\mu_1, \nu_1, \ldots, \mu_L, \nu_L) \in \{0,1\}^{2L},\ \mathbf{H}_{\mu_1 \ldots \mu_L}^{\nu_1 \ldots \nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} |\mu_k - \nu_k| \leq 4$$



(a) Norm of $\mathbf{H} - \mathbf{H}^T$



(b) Norm of $\mathbf{H}\hat{N} - \hat{N}\mathbf{H}$

Keep degenerate singular values when truncating

Compression of an MPO

Basic properties to preserve

1. symmetry:

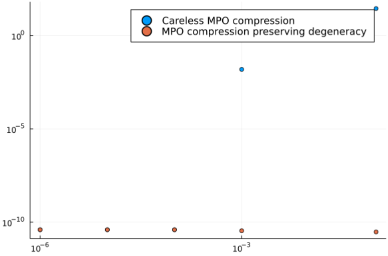
$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}=\mathbf{H}^{\mu_1\dots\mu_L}_{\nu_1\dots\nu_L}$$

2. particle number conservation:

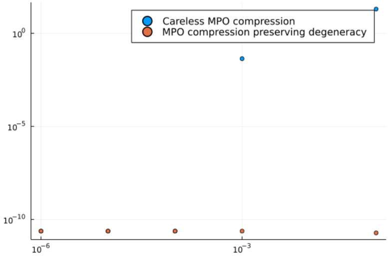
$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}\neq 0\Rightarrow\sum_{k=1}^{L}\mu_k=\sum_{k=1}^{L}\nu_k$$

3. two-body interactions:

$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}\neq 0\Rightarrow\sum_{k=1}^{L}|\mu_k-\nu_k|\leq 4$$



(a) Norm of $\mathbf{H}-\mathbf{H}^T$



(b) Norm of $\mathbf{H}\hat{N}-\hat{N}\mathbf{H}$

Keep degenerate singular values when truncating

Compression of an MPO

Basic properties to preserve

1. symmetry:

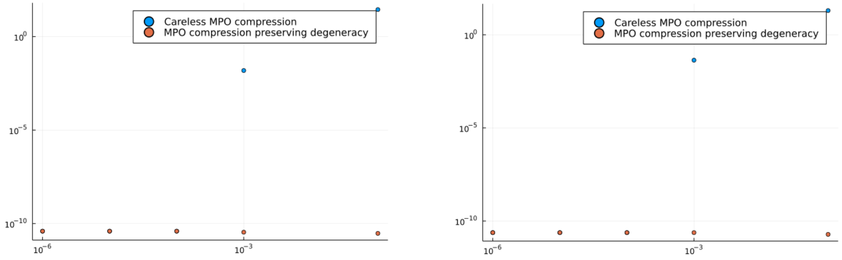
$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}=\mathbf{H}^{\mu_1\dots\mu_L}_{\nu_1\dots\nu_L}$$

2. particle number conservation:

$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}\neq 0\Rightarrow\sum_{k=1}^{L}\mu_k=\sum_{k=1}^{L}\nu_k$$

3. two-body interactions:

$$\forall(\mu_1,\nu_1,\dots,\mu_L,\nu_L)\in\{0,1\}^{2L},\ \mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}\neq 0\Rightarrow\sum_{k=1}^{L}|\mu_k-\nu_k|\leq 4$$



(a) Norm of $\mathbf{H}-\mathbf{H}^T$

(b) Norm of $\mathbf{H}\hat{N}-\hat{N}\mathbf{H}$

Keep degenerate singular values when truncating

Compression of an MPO

Basic properties to preserve

1. symmetry:

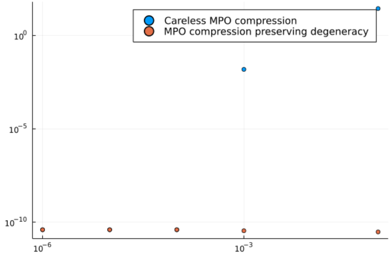
$$\forall(\mu_1,\nu_1,\ldots,\mu_L,\nu_L) \in \{0,1\}^{2L},\ \mathbf{H}_{\mu_1\ldots\mu_L}^{\nu_1\ldots\nu_L} = \mathbf{H}_{\nu_1\ldots\nu_L}^{\mu_1\ldots\mu_L}$$

2. particle number conservation:

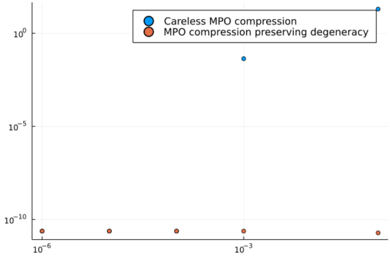
$$\forall(\mu_1,\nu_1,\ldots,\mu_L,\nu_L) \in \{0,1\}^{2L},\ \mathbf{H}_{\mu_1\ldots\mu_L}^{\nu_1\ldots\nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L}\mu_k = \sum_{k=1}^{L}\nu_k$$

3. two-body interactions:

$$\forall(\mu_1,\nu_1,\ldots,\mu_L,\nu_L) \in \{0,1\}^{2L},\ \mathbf{H}_{\mu_1\ldots\mu_L}^{\nu_1\ldots\nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L}|\mu_k-\nu_k| \leq 4$$



(a) Norm of $\mathbf{H} - \mathbf{H}^T$



(b) Norm of $\mathbf{H}\hat{N} - \hat{N}\mathbf{H}$

Keep degenerate singular values when truncating

Conservation of Hermitian symmetry

Singular values Σ_k related to the reshape $\mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} \in \mathbb{R}^{4^k\times 4^{L-k}}$:

- symmetry

$$\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} = \mathbf{H}^{\mu_1\cdots\mu_L}_{\nu_1\cdots\nu_L} \Rightarrow \mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} = \mathbf{H}^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k}$$

  stability by permuting all the pairs of indices

- SVD of $\mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k}$

$$\mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} = \sum_j \sigma_j \left(U_j V_j^T\right)^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} \qquad \sigma_j \text{ distinct}, U_j \in \mathbb{R}^{4^k\times r_j}, V_j^T \in \mathbb{R}^{4^{L-k}\times r_j}$$

$$\mathbf{H}^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k} = \sum_j \sigma_j \left(U_j V_j^T\right)^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k}$$

  by uniqueness of the SVD: for all j

$$\left(U_j V_j^T\right)^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} = \left(U_j V_j^T\right)^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k}.$$

Theorem

Not breaking the degeneracy of the singular values ⇒ preserve the symmetry

Conservation of Hermitian symmetry

Singular values Σ_k related to the reshape $\mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} \in \mathbb{R}^{4^k\times 4^{L-k}}$:

- symmetry

$$\mathbf{H}^{\nu_1\cdots\nu_L}_{\mu_1\cdots\mu_L} = \mathbf{H}^{\mu_1\cdots\mu_L}_{\nu_1\cdots\nu_L} \Rightarrow \mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} = \mathbf{H}^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k}$$

  stability by permuting all the pairs of indices

- SVD of $\mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k}$

$$\mathbf{H}^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} = \sum_j \sigma_j \left(U_j V_j^T\right)^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} \qquad \sigma_j \text{ distinct}, U_j \in \mathbb{R}^{4^k\times r_j}, V_j^T \in \mathbb{R}^{4^{L-k}\times r_j}$$

$$\mathbf{H}^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k} = \sum_j \sigma_j \left(U_j V_j^T\right)^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k}$$

  by uniqueness of the SVD: for all j

$$\left(U_j V_j^T\right)^{\mu_{k+1}\nu_{k+1}\cdots\mu_L\nu_L}_{\mu_1\nu_1\cdots\mu_k\nu_k} = \left(U_j V_j^T\right)^{\nu_{k+1}\mu_{k+1}\cdots\nu_L\mu_L}_{\nu_1\mu_1\cdots\nu_k\mu_k}.$$

Theorem

Not breaking the degeneracy of the singular values $\Rightarrow$ preserve the symmetry

Preservation of the particle number: a basic example

Example

$$\mathbf{H}_{\mu_1\mu_2}^{\nu_1\nu_2} = \begin{array}{c|cccc} \mu_1\mu_2 \backslash \nu_1\nu_2 & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & 0 \\ 01 & 0 & (H_1)_{01}^{01} & (H_1)_{01}^{10} & 0 \\ 10 & 0 & (H_1)_{10}^{01} & (H_1)_{10}^{10} & 0 \\ 11 & 0 & 0 & 0 & H_2 \end{array}$$

- reshape

$$\mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \begin{array}{c|cccc} \mu_1\nu_1 \backslash \mu_2\nu_2 & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & (H_1)_{01}^{01} \\ 01 & 0 & 0 & (H_1)_{10}^{01} & 0 \\ 10 & 0 & (H_1)_{01}^{10} & 0 & 0 \\ 11 & (H_1)_{10}^{10} & 0 & 0 & H_2 \end{array}$$

- $$\text{SVD of } \mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \text{SVD of } \begin{pmatrix} H_0 & (H_1)_{01}^{01} \\ (H_1)_{10}^{10} & H_2 \end{pmatrix} \bigotimes \begin{pmatrix} 0 & (H_1)_{10}^{01} \\ (H_1)_{01}^{10} & 0 \end{pmatrix}$$
- by symmetry of H_1: $(H_1)_{01}^{10} = (H_1)_{10}^{01}$

$\Rightarrow$ degenerate singular values

$\Rightarrow$ preserve the 0 by keeping degeneracy

Theorem

Not breaking the degeneracy of the singular values $\Rightarrow$ preserve the particle number conservation

Preservation of the particle number: a basic example

Example

$$\mathbf{H}_{\mu_1\mu_2}^{\nu_1\nu_2} = \begin{array}{c|cccc} {}_{\mu_1\mu_2}\backslash^{\nu_1\nu_2} & 00 & 01 & 10 & 11 \\ 00 & H_0 & 0 & 0 & 0 \\ 01 & 0 & (H_1)_{01}^{01} & (H_1)_{01}^{10} & 0 \\ 10 & 0 & (H_1)_{10}^{01} & (H_1)_{10}^{10} & 0 \\ 11 & 0 & 0 & 0 & H_2 \end{array}$$

- reshape

$$\mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \begin{array}{c|cccc} {}_{\mu_1\nu_1}\backslash^{\mu_2\nu_2} & 00 & 01 & 10 & 11 \\ 00 & H_0 & 0 & 0 & (H_1)_{01}^{01} \\ 01 & 0 & 0 & (H_1)_{10}^{01} & 0 \\ 10 & 0 & (H_1)_{01}^{10} & 0 & 0 \\ 11 & (H_1)_{10}^{10} & 0 & 0 & H_2 \end{array}$$

- $$\text{SVD of } \mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \text{SVD of } \begin{pmatrix} H_0 & (H_1)_{01}^{01} \\ (H_1)_{10}^{10} & H_2 \end{pmatrix} \bigotimes \begin{pmatrix} 0 & (H_1)_{10}^{01} \\ (H_1)_{01}^{10} & 0 \end{pmatrix}$$
- by symmetry of H_1: $(H_1)_{01}^{10} = (H_1)_{10}^{01}$

$\Rightarrow$ degenerate singular values

$\Rightarrow$ preserve the 0 by keeping degeneracy

Theorem

Not breaking the degeneracy of the singular values $\Rightarrow$ preserve the particle number conservation

Preservation of the particle number: a basic example

Example

$$\mathbf{H}_{\mu_1\mu_2}^{\nu_1\nu_2} = \begin{array}{c|cccc} \mu_1\mu_2 \backslash \nu_1\nu_2 & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & 0 \\ 01 & 0 & (H_1)_{01}^{01} & (H_1)_{01}^{10} & 0 \\ 10 & 0 & (H_1)_{10}^{01} & (H_1)_{10}^{10} & 0 \\ 11 & 0 & 0 & 0 & H_2 \end{array}$$

- reshape

$$\mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \begin{array}{c|cccc} \mu_1\nu_1 \backslash \mu_2\nu_2 & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & (H_1)_{01}^{01} \\ 01 & 0 & 0 & (H_1)_{10}^{01} & 0 \\ 10 & 0 & (H_1)_{01}^{10} & 0 & 0 \\ 11 & (H_1)_{10}^{10} & 0 & 0 & H_2 \end{array}$$

- $$\text{SVD of } \mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \text{SVD of } \begin{pmatrix} H_0 & (H_1)_{01}^{01} \\ (H_1)_{10}^{10} & H_2 \end{pmatrix} \bigotimes \begin{pmatrix} 0 & (H_1)_{10}^{01} \\ (H_1)_{01}^{10} & 0 \end{pmatrix}$$
- by symmetry of H_1: $(H_1)_{01}^{10} = (H_1)_{10}^{01}$

$\Rightarrow$ degenerate singular values

$\Rightarrow$ preserve the 0 by keeping degeneracy

Theorem

Not breaking the degeneracy of the singular values $\Rightarrow$ preserve the particle number conservation

Preservation of the particle number: a basic example

Example

$$\mathbf{H}_{\mu_1\mu_2}^{\nu_1\nu_2} = \begin{array}{c|cccc} \mu_1\mu_2 \backslash \nu_1\nu_2 & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & 0 \\ 01 & 0 & (H_1)_{01}^{01} & (H_1)_{01}^{10} & 0 \\ 10 & 0 & (H_1)_{10}^{01} & (H_1)_{10}^{10} & 0 \\ 11 & 0 & 0 & 0 & H_2 \end{array}$$

- reshape

$$\mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \begin{array}{c|cccc} \mu_1\nu_1 \backslash \mu_2\nu_2 & 00 & 01 & 10 & 11 \\ \hline 00 & H_0 & 0 & 0 & (H_1)_{01}^{01} \\ 01 & 0 & 0 & (H_1)_{10}^{01} & 0 \\ 10 & 0 & (H_1)_{01}^{10} & 0 & 0 \\ 11 & (H_1)_{10}^{10} & 0 & 0 & H_2 \end{array}$$

- $$\text{SVD of } \mathbf{H}_{\mu_1\nu_1}^{\mu_2\nu_2} = \text{SVD of } \begin{pmatrix} H_0 & (H_1)_{01}^{01} \\ (H_1)_{10}^{10} & H_2 \end{pmatrix} \bigotimes \begin{pmatrix} 0 & (H_1)_{10}^{01} \\ (H_1)_{01}^{10} & 0 \end{pmatrix}$$
- by symmetry of H_1: $(H_1)_{01}^{10} = (H_1)_{10}^{01}$

$\Rightarrow$ degenerate singular values

$\Rightarrow$ preserve the 0 by keeping degeneracy

Theorem

Not breaking the degeneracy of the singular values $\Rightarrow$ preserve the particle number conservation

Sparse representation of the MPO

MPS of an N-particle state[1]

Consider $\boldsymbol{\Psi}_{\mu_1\dots\mu_L} \in \mathbb{R}^{2^L}$ an N-particle state: $\boldsymbol{\Psi}_{\mu_1\dots\mu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = N$
Construct an MPS representation by successive SVDs

- first SVD

$$\boldsymbol{\Psi}_{\mu_1}^{\mu_2\cdots\mu_L} = \begin{pmatrix} U_{1,0} & 0 \\ 0 & U_{1,1} \end{pmatrix} \begin{pmatrix} \Sigma_{1,0} & 0 \\ 0 & \Sigma_{1,1} \end{pmatrix} \begin{pmatrix} V_{1,0}^T \\ V_{1,1}^T \end{pmatrix}.$$

  - first MPS core: $\Psi_1[0] = \begin{pmatrix} U_{1,0} & 0 \end{pmatrix}$ and $\Psi_1[1] = \begin{pmatrix} 0 & U_{1,1} \end{pmatrix}$.

- second SVD: reshape $(V_1)_{\alpha}^{\mu_2\cdots\mu_L} = \begin{pmatrix} V_{1,0}^T \\ V_{1,1}^T \end{pmatrix} \in \mathbb{R}^{r_1 \times 2^{L-1}}$ to $(V_1)_{\alpha\mu_2}^{\mu_3\cdots\mu_L} \in \mathbb{R}^{2r_1 \times 2^{L-2}}$

$$(V_1)_{\alpha\mu_2}^{\mu_3\cdots\mu_L} = \begin{matrix} \alpha\mu_2 \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix} \begin{pmatrix} U_{2,0} & 0 & 0 \\ 0 & U_{2,01} & 0 \\ 0 & U_{2,10} & 0 \\ 0 & 0 & U_{2,2} \end{pmatrix} \begin{pmatrix} \Sigma_{2,0} & & \\ & \Sigma_{2,1} & \\ & & \Sigma_{2,2} \end{pmatrix} \begin{pmatrix} V_{2,0}^T \\ V_{2,1}^T \\ V_{2,2}^T \end{pmatrix}.$$

  - second MPS core

$$\Psi_2[0] = \begin{pmatrix} U_{2,0} & 0 & 0 \\ 0 & U_{2,10} & 0 \end{pmatrix} \quad \Psi_2[1] = \begin{pmatrix} 0 & U_{2,01} & 0 \\ 0 & 0 & U_{2,2} \end{pmatrix}$$

[1] Bachmayr, Markus, Michael Götte, and Max Pfeffer. "Particle Number Conservation and Block Structures in Matrix Product States." arXiv (2021).

MPS of an N-particle state[1]

Consider $\mathbf{\Psi}_{\mu_1\dots\mu_L} \in \mathbb{R}^{2^L}$ an N-particle state: $\mathbf{\Psi}_{\mu_1\dots\mu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = N$
Construct an MPS representation by successive SVDs

- first SVD

$$\mathbf{\Psi}_{\mu_1}^{\mu_2\cdots\mu_L} = \begin{pmatrix} U_{1,0} & 0 \\ 0 & U_{1,1} \end{pmatrix} \begin{pmatrix} \Sigma_{1,0} & 0 \\ 0 & \Sigma_{1,1} \end{pmatrix} \begin{pmatrix} V_{1,0}^T \\ V_{1,1}^T \end{pmatrix}.$$

  - first MPS core: $\Psi_1[0] = \begin{pmatrix} U_{1,0} & 0 \end{pmatrix}$ and $\Psi_1[1] = \begin{pmatrix} 0 & U_{1,1} \end{pmatrix}$.

- second SVD: reshape $(V_1)_{\alpha}^{\mu_2\cdots\mu_L} = \begin{pmatrix} V_{1,0}^T \\ V_{1,1}^T \end{pmatrix} \in \mathbb{R}^{r_1 \times 2^{L-1}}$ to $(V_1)_{\alpha\mu_2}^{\mu_3\cdots\mu_L} \in \mathbb{R}^{2r_1 \times 2^{L-2}}$

$$(V_1)_{\alpha\mu_2}^{\mu_3\cdots\mu_L} = \begin{matrix} \alpha\mu_2 \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix} \begin{pmatrix} U_{2,0} & 0 & 0 \\ 0 & U_{2,01} & 0 \\ 0 & U_{2,10} & 0 \\ 0 & 0 & U_{2,2} \end{pmatrix} \begin{pmatrix} \Sigma_{2,0} & & \\ & \Sigma_{2,1} & \\ & & \Sigma_{2,2} \end{pmatrix} \begin{pmatrix} V_{2,0}^T \\ V_{2,1}^T \\ V_{2,2}^T \end{pmatrix}.$$

  - second MPS core

$$\Psi_2[0] = \begin{pmatrix} U_{2,0} & 0 & 0 \\ 0 & U_{2,10} & 0 \end{pmatrix} \quad \Psi_2[1] = \begin{pmatrix} 0 & U_{2,01} & 0 \\ 0 & 0 & U_{2,2} \end{pmatrix}$$

[1] Bachmayr, Markus, Michael Götte, and Max Pfeffer. "Particle Number Conservation and Block Structures in Matrix Product States." arXiv (2021).

MPS of an N-particle state[1]

Consider $\mathbf{\Psi}_{\mu_1 \dots \mu_L} \in \mathbb{R}^{2^L}$ an N-particle state: $\mathbf{\Psi}_{\mu_1 \dots \mu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} \mu_k = N$
Construct an MPS representation by successive SVDs

- first SVD

$$\mathbf{\Psi}_{\mu_1}^{\mu_2 \cdots \mu_L} = \begin{pmatrix} U_{1,0} & 0 \\ 0 & U_{1,1} \end{pmatrix} \begin{pmatrix} \Sigma_{1,0} & 0 \\ 0 & \Sigma_{1,1} \end{pmatrix} \begin{pmatrix} V_{1,0}^T \\ V_{1,1}^T \end{pmatrix}.$$

  - first MPS core: $\Psi_1[0] = \begin{pmatrix} U_{1,0} & 0 \end{pmatrix}$ and $\Psi_1[1] = \begin{pmatrix} 0 & U_{1,1} \end{pmatrix}$.

- second SVD: reshape $(V_1)_{\alpha}^{\mu_2 \cdots \mu_L} = \begin{pmatrix} V_{1,0}^T \\ V_{1,1}^T \end{pmatrix} \in \mathbb{R}^{r_1 \times 2^{L-1}}$ to $(V_1)_{\alpha\mu_2}^{\mu_3 \cdots \mu_L} \in \mathbb{R}^{2r_1 \times 2^{L-2}}$

$$(V_1)_{\alpha\mu_2}^{\mu_3 \cdots \mu_L} = \begin{matrix} \alpha\mu_2 \\ 00 \\ 01 \\ 10 \\ 11 \end{matrix} \begin{pmatrix} U_{2,0} & 0 & 0 \\ 0 & U_{2,01} & 0 \\ 0 & U_{2,10} & 0 \\ 0 & 0 & U_{2,2} \end{pmatrix} \begin{pmatrix} \Sigma_{2,0} & & \\ & \Sigma_{2,1} & \\ & & \Sigma_{2,2} \end{pmatrix} \begin{pmatrix} V_{2,0}^T \\ V_{2,1}^T \\ V_{2,2}^T \end{pmatrix}.$$

  - second MPS core

$$\Psi_2[0] = \begin{pmatrix} U_{2,0} & 0 & 0 \\ 0 & U_{2,10} & 0 \end{pmatrix} \quad \Psi_2[1] = \begin{pmatrix} 0 & U_{2,01} & 0 \\ 0 & 0 & U_{2,2} \end{pmatrix}$$

[1] Bachmayr, Markus, Michael Götte, and Max Pfeffer. "Particle Number Conservation and Block Structures in Matrix Product States." arXiv (2021).

Block structure of MPO

Block structure MPS: $\mathbf{\Psi}_{\mu_1\dots\mu_L}$ an N particle state, $(\Psi_1, \dots, \Psi_L)$ MPS cores

$$\Psi_k[0] = \begin{pmatrix} \Psi_k[0]_0 & & & \\ & \Psi_k[0]_1 & & \\ & & \ddots & \\ & & & \Psi_k[0]_N \end{pmatrix} \quad \Psi_k[1] = \begin{pmatrix} 0 & \Psi_k[1]_0 & & & \\ & 0 & \Psi_k[1]_1 & & \\ & & \ddots & \ddots & \\ & & & 0 & \Psi_k[1]_{N-1} \\ & & & & 0 \end{pmatrix}$$

Block structure MPO: $\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L} \in \mathbb{R}^{2^L\times 2^L}$ particle-number preserving and two-body operator

- MPO of $\mathbf{H}^{\nu_1\dots\nu_L}_{\mu_1\dots\mu_L}$ = MPS of $\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\dots;\mu_L\nu_L}$
- $\mathbf{H}$ particle-number preserving:

$$\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\dots;\mu_L\nu_L} \neq 0 \Rightarrow \sum_k^L \mu_k - \nu_k = 0.$$

the difference $\mu_k - \nu_k$ only takes values -1,0 and 1.

Block structure of MPO

Block structure MPS: $\boldsymbol{\Psi}_{\mu_1\dots\mu_L}$ an N particle state, $(\Psi_1,\dots,\Psi_L)$ MPS cores

$$\Psi_k[0] = \begin{pmatrix} \Psi_k[0]_0 & & & \\ & \Psi_k[0]_1 & & \\ & & \ddots & \\ & & & \Psi_k[0]_N \end{pmatrix} \quad \Psi_k[1] = \begin{pmatrix} 0 & \Psi_k[1]_0 & & & \\ & 0 & \Psi_k[1]_1 & & \\ & & \ddots & \ddots & \\ & & & 0 & \Psi_k[1]_{N-1} \\ & & & & 0 \end{pmatrix}$$

Block structure MPO: $\mathbf{H}_{\mu_1\dots\mu_L}^{\nu_1\dots\nu_L} \in \mathbb{R}^{2^L\times 2^L}$ particle-number preserving and two-body operator

- MPO of $\mathbf{H}_{\mu_1\dots\mu_L}^{\nu_1\dots\nu_L}$ = MPS of $\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\dots;\mu_L\nu_L}$
- **H** particle-number preserving:

$$\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\dots;\mu_L\nu_L} \neq 0 \Rightarrow \sum_k^L \mu_k - \nu_k = 0.$$

the difference $\mu_k - \nu_k$ only takes values -1,0 and 1.

Block structure MPO

MPO of particle-number preserving operator: $\mathbf{H}^{\nu_1\ldots\nu_L}_{\mu_1\ldots\mu_L} \in \mathbb{R}^{2^L \times 2^L}$

$$
\begin{aligned}
H_k[00] &= \mathrm{Diagonal}(H_k[00]_{-L}, H_k[00]_{-L+1}, \ldots, H_k[00]_{L})\\
H_k[11] &= \mathrm{Diagonal}(H_k[11]_{-L}, H_k[11]_{-L+1}, \ldots, H_k[11]_{L-2})\\
H_k[01] &= \mathrm{UpperDiagonal}(H_k[01]_{-L}, H_k[01]_{-L+1}, \ldots, H_k[01]_{L-1})\\
H_k[10] &= \mathrm{LowerDiagonal}(H_k[10]_{-L+1}, H_k[10]_{-L+2}, \ldots, H_k[10]_{L})
\end{aligned}
$$

MPO of two-body Hamiltonian: $\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\ldots;\mu_L\nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} |\mu_k - \nu_k| \leq 4$

$$
\begin{aligned}
H_k[00] &= \mathrm{Diagonal}(H_k[00]_{-2}, H_k[00]_{-1}, \ldots, H_k[00]_{2})\\
H_k[11] &= \mathrm{Diagonal}(H_k[11]_{-2}, H_k[11]_{-1}, \ldots, H_k[11]_{0})\\
H_k[01] &= \mathrm{UpperDiagonal}(H_k[01]_{-2}, H_k[01]_{-1}, \ldots, H_k[01]_{1})\\
H_k[10] &= \mathrm{LowerDiagonal}(H_k[10]_{-1}, H_k[10]_{0}, \ldots, H_k[10]_{2})
\end{aligned}
$$

Theorem

$H_k[i_k, j_k]$ is a block matrix with at most 5 nonzero blocks.

Block structure MPO

MPO of particle-number preserving operator: $\mathbf{H}_{\mu_1 \cdots \mu_L}^{\nu_1 \cdots \nu_L} \in \mathbb{R}^{2^L \times 2^L}$

$$H_k[00] = \mathrm{Diagonal}(H_k[00]_{-L}, H_k[00]_{-L+1}, \dots, H_k[00]_{L})$$
$$H_k[11] = \mathrm{Diagonal}(H_k[11]_{-L}, H_k[11]_{-L+1}, \dots, H_k[11]_{L-2})$$
$$H_k[01] = \mathrm{UpperDiagonal}(H_k[01]_{-L}, H_k[01]_{-L+1}, \dots, H_k[01]_{L-1})$$
$$H_k[10] = \mathrm{LowerDiagonal}(H_k[10]_{-L+1}, H_k[10]_{-L+2}, \dots, H_k[10]_{L})$$

MPO of two-body Hamiltonian: $\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\dots;\mu_L\nu_L} \neq 0 \Rightarrow \sum_{k=1}^{L} |\mu_k - \nu_k| \leq 4$

$$H_k[00] = \mathrm{Diagonal}(H_k[00]_{-2}, H_k[00]_{-1}, \dots, H_k[00]_{2})$$
$$H_k[11] = \mathrm{Diagonal}(H_k[11]_{-2}, H_k[11]_{-1}, \dots, H_k[11]_{0})$$
$$H_k[01] = \mathrm{UpperDiagonal}(H_k[01]_{-2}, H_k[01]_{-1}, \dots, H_k[01]_{1})$$
$$H_k[10] = \mathrm{LowerDiagonal}(H_k[10]_{-1}, H_k[10]_{0}, \dots, H_k[10]_{2})$$

Theorem

$H_k[i_k, j_k]$ is a block matrix with at most 5 nonzero blocks.

Block structure MPO

MPO of particle-number preserving operator: $\mathbf{H}^{\nu_1 \dots \nu_L}_{\mu_1 \dots \mu_L} \in \mathbb{R}^{2^L \times 2^L}$

$$H_k[00] = \mathrm{Diagonal}(H_k[00]_{-L}, H_k[00]_{-L+1}, \dots, H_k[00]_L)$$
$$H_k[11] = \mathrm{Diagonal}(H_k[11]_{-L}, H_k[11]_{-L+1}, \dots, H_k[11]_{L-2})$$
$$H_k[01] = \mathrm{UpperDiagonal}(H_k[01]_{-L}, H_k[01]_{-L+1}, \dots, H_k[01]_{L-1})$$
$$H_k[10] = \mathrm{LowerDiagonal}(H_k[10]_{-L+1}, H_k[10]_{-L+2}, \dots, H_k[10]_L)$$

MPO of two-body Hamiltonian: $\mathbf{H}_{\mu_1\nu_1;\mu_2\nu_2;\dots;\mu_L\nu_L} \neq 0 \Rightarrow \sum_{k=1}^L |\mu_k - \nu_k| \leq 4$

$$H_k[00] = \mathrm{Diagonal}(H_k[00]_{-2}, H_k[00]_{-1}, \dots, H_k[00]_2)$$
$$H_k[11] = \mathrm{Diagonal}(H_k[11]_{-2}, H_k[11]_{-1}, \dots, H_k[11]_0)$$
$$H_k[01] = \mathrm{UpperDiagonal}(H_k[01]_{-2}, H_k[01]_{-1}, \dots, H_k[01]_1)$$
$$H_k[10] = \mathrm{LowerDiagonal}(H_k[10]_{-1}, H_k[10]_0, \dots, H_k[10]_2)$$

Theorem

$H_k[i_k, j_k]$ is a block matrix with at most 5 nonzero blocks.

Conclusion

Conclusion

- Hermitian preserving and particle number preserving MPO compression by not breaking the degeneracy in the truncation
- sparse MPO representation of two-body Hamiltonians

Perspectives

- implementation to exploit the sparse structure of the MPO and of the MPS

Reference

- Badreddine, Beaupère, Cancès, MD, Grigori, *Sparse and symmetry-preserving compression of matrix product operators*, soon.

Conclusion

- Hermitian preserving and particle number preserving MPO compression by not breaking the degeneracy in the truncation
- sparse MPO representation of two-body Hamiltonians

Perspectives

- implementation to exploit the sparse structure of the MPO and of the MPS

Reference

- Badreddine, Beaupère, Cancès, MD, Grigori, *Sparse and symmetry-preserving compression of matrix product operators*, soon.