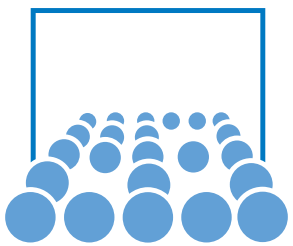
Numerical Linear and Multilinear Algebra in Quantum Tensor Networks

Konrad Waldherr

October 20, 2013

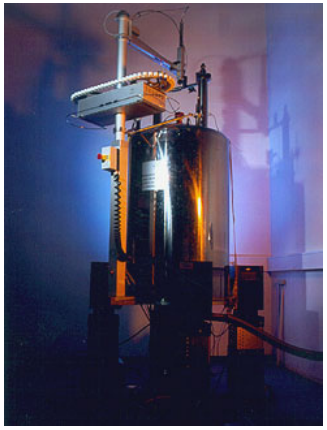


Joint work with Thomas Huckle

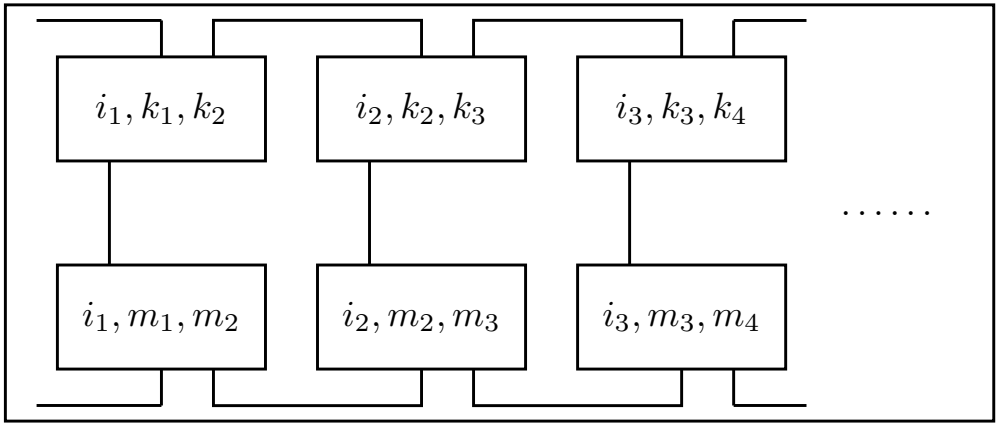
Outline

Numerical (Multi-) Linear Algebraic Approaches to...

- ...Quantum Control



- ...Quantum Tensor Networks



NMR Spectroscopy as Optimal Control Problem

- Goal: find optimal pulse amplitudes $\boldsymbol{u}(t)$ to steer nuclear spin states $\boldsymbol{x}(t)$ over the time interval $[0, T]$
- Optimality can be described by a scalar function f:

$$f(\boldsymbol{x}, \boldsymbol{u}) \;=\; \underbrace{f_T(\boldsymbol{x}(T))}_{\text{quality}}$$

- Application: Synthesization of a unitary target operator $\boldsymbol{U}_G$:

$$f(\boldsymbol{U}(T), \boldsymbol{u}) \;=\; \|\boldsymbol{U}(T) - \boldsymbol{U_G}\|_F^2$$

- The dynamics are governed by the equation of motion:

$$\dot{\boldsymbol{x}}(t) \;=\; -\mathrm{i} \underbrace{\left[\boldsymbol{H_0} + \sum_{m=1}^{M} \boldsymbol{u_m}(t) \boldsymbol{H_m}\right]}_{=\boldsymbol{H}(t)} \boldsymbol{x}(t)$$

Gradient Ascent Pulse Engineering Algorithm:

1: Set initial control amplitudes $u_m^{\{0\}}(t_k)$ for all times t_k and $\boldsymbol{U_0}$

2: **for** $\ell = 0, 1, 2, \ldots$ **until convergence**

a: Calculate **exponentials**

$$\boldsymbol{U_k} = e^{-\mathrm{i}\boldsymbol{H}(t_k)} \quad \text{for all} \quad k = 1, \ldots, K$$

b: Compute the **forward propagation**

$$\boldsymbol{U_{k:0}} = \boldsymbol{U_k U_{k-1}} \cdots \boldsymbol{U_1 U_0} \quad \text{for all} \quad k = 1, \ldots, K$$

c: Compute the **backward propagation**

$$\boldsymbol{W_{K+1:k+1}} = \boldsymbol{U_{K+1} U_K} \cdots \boldsymbol{U_{k+1} U_k} \quad \text{for all} \quad k = K, \ldots, 1$$

d: Calculate the **gradient**

$$\frac{\partial f}{\partial u_m(t_k)} = \mathrm{Re}\left[\mathrm{trace}\left(\boldsymbol{W}^{\mathbf{H}}_{\boldsymbol{K+1:k+1}}(-i\boldsymbol{H_m})\boldsymbol{U_{k:0}}\right)\right]$$

e: **Update** the controls $u_m(t_k)$

$$u_m^{\{\ell+1\}}(t_k) \;=\; u_m^{\{\ell\}}(t_k) + \epsilon \cdot \frac{\partial f}{\partial u_m(t_k)}$$

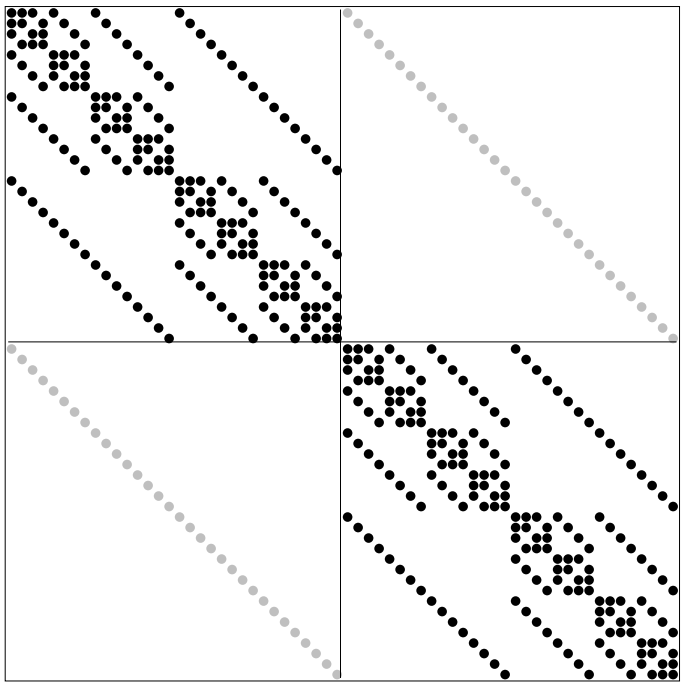
GRAPE: Computational Challenges

1. Computation of the matrix exponentials

$$\boldsymbol{U_k} = e^{-\mathrm{i}\left[\boldsymbol{H_0}+\sum_m u_m(t_k)\boldsymbol{H_m}\right]}$$

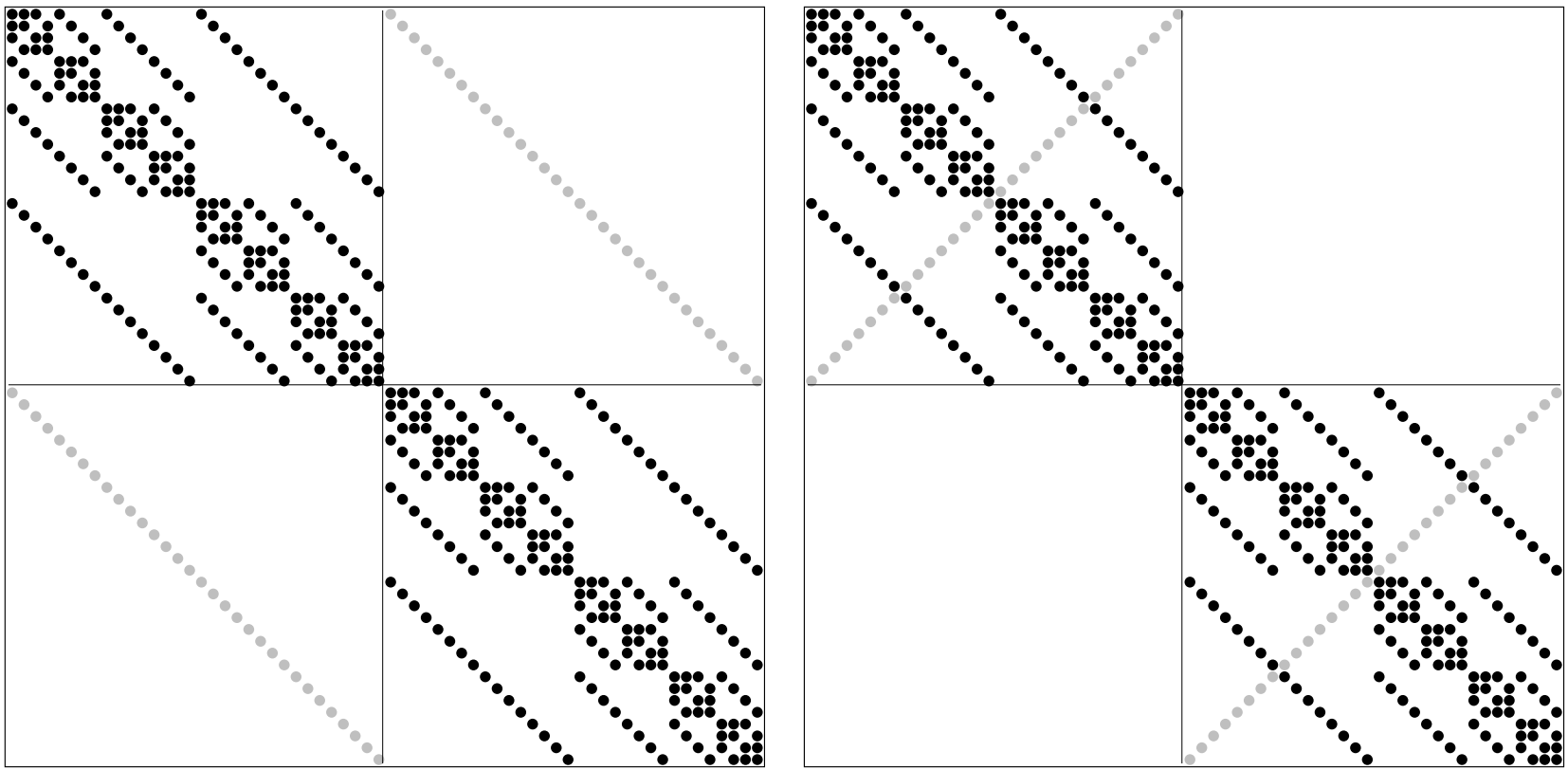
Challenges:

- Exponential of matrices are required in explicit form
- Operand matrices have certain properties (e.g., sparsity structure)



Matrix Exponentials

- **NMR setting:** Problem can be reduced to two problems of half size:
  cn^3 reduces to $2c\left(\frac{n}{2}\right)^3 = c\frac{n^3}{4}$
  $\Longrightarrow$ saves factor 4



Matrix Exponentials

- Old version: Eigendecomposition method
- New version: Chebyshev method

$$\boldsymbol{H} = \boldsymbol{V}\boldsymbol{\Lambda}\boldsymbol{V}^{\mathrm{H}} \quad \Longrightarrow$$

$$\mathrm{e}^{-\mathrm{i}\Delta t\boldsymbol{H}} = \boldsymbol{V}\mathrm{e}^{-\mathrm{i}\Delta t\boldsymbol{\Lambda}}\boldsymbol{V}^{\mathrm{H}} = \boldsymbol{V}\,\mathrm{diag}\left(\mathrm{e}^{-\mathrm{i}\Delta t\lambda_1}, \ldots, \mathrm{e}^{-\mathrm{i}\Delta t\lambda_n}\right)\boldsymbol{V}^{\mathrm{H}}.$$

Requires eigendecomposition of a typically sparse matrix.

Matrix Exponentials

- Old version: Eigendecomposition method
- New version: Chebyshev method

$$\mathrm{e}^{-\mathrm{i}\Delta t\boldsymbol{H}} = a_0\boldsymbol{I} + 2\sum_{k=1}^{m} a_k C_k\left(\frac{\boldsymbol{H}}{\|\boldsymbol{H}\|}\right),\ a_k = \mathrm{i}^k J_k\left(-\Delta t\|\boldsymbol{H}\|\right)\ .$$

Chebyshev recurrence translates into

for $k = m$ **downto** 0 **do**
$$a_k = \mathrm{i}^k J_k\left(-\Delta t\|\boldsymbol{H}\|\right)$$
$$\boldsymbol{D_k} = a_k\boldsymbol{I} + \tfrac{2}{\|\boldsymbol{H}\|}\boldsymbol{H}\boldsymbol{D_{k+1}} - \boldsymbol{D_{k+2}}$$
$$\mathrm{e}^{-\mathrm{i}\Delta t\boldsymbol{H}} = \boldsymbol{D_0} - \boldsymbol{D_2}$$

Computation relies solely on products of the form `sparse` $\times$ `dense`.
$\Longrightarrow$ No expensive operations such as inversion/eigendecomposition required

GRAPE: Computational Challenges

2. Computation of the intermediate matrix products

- Compute the **forward propagation**

$$\boldsymbol{U_{k:0}} = \boldsymbol{U_k U_{k-1}} \cdots \boldsymbol{U_1 U_0} \quad \text{for all} \quad k = 1, \ldots, K$$

- Compute the **backward propagation**

$$\boldsymbol{W_{K+1:k+1}} = \boldsymbol{U_{K+1} U_K} \cdots \boldsymbol{U_{k+1} U_k} \quad \text{for all} \quad k = K, \ldots, 1$$

Instances of the matrix-multiplication prefix problem:

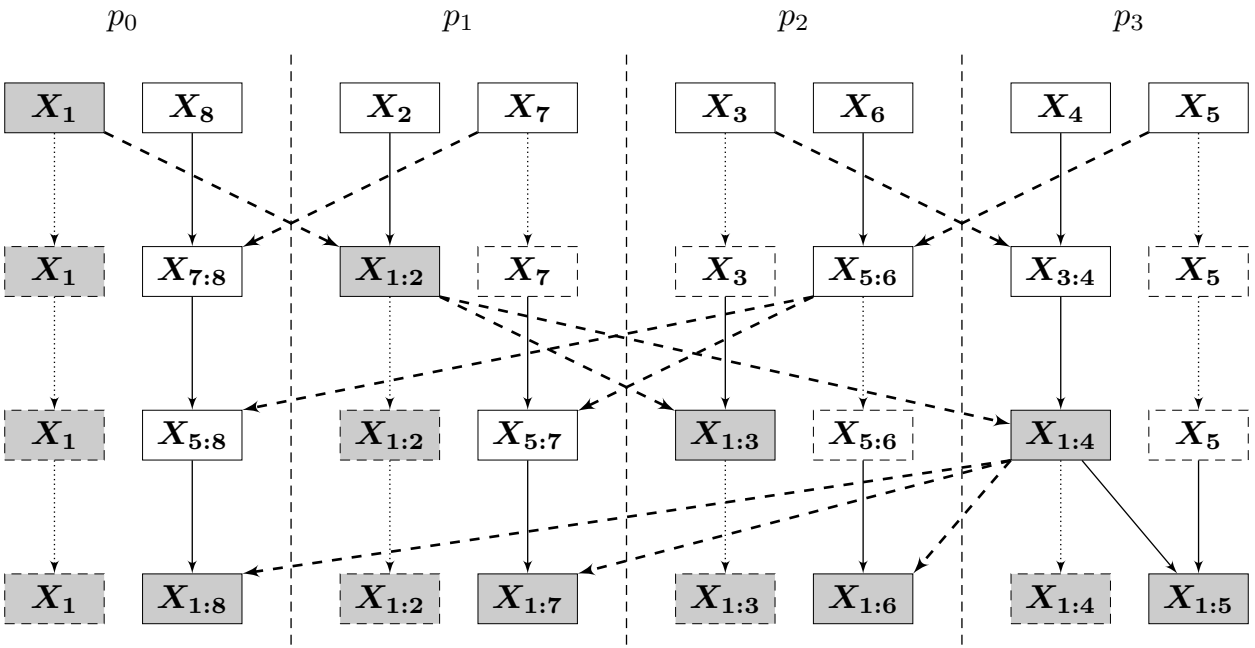
$$\forall k = 1 : K : \quad \left(\boldsymbol{X_1} \cdots \boldsymbol{X_{k-1}} \right) \boldsymbol{X_k}$$

Challenges:

- Parallelization
- Large number of matrices to be multiplied (e.g., $K = 1024$)
- Matrices comparably small (e.g., 1024×1024)

Computation of the Matrix Multiplications

- Old version: coarse-grain parallel prefix tree
- New version: fine-grain $3D$ parallelization:



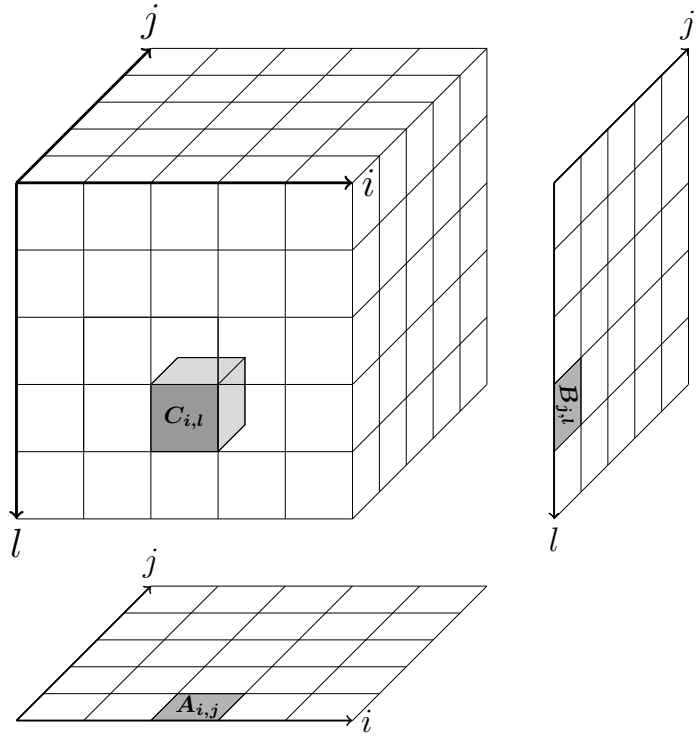
$\Longrightarrow$ individual matrix multiplications are computed **sequentially**

Computation of the Matrix Multiplications

- Old version: coarse-grain parallel prefix tree
- New version: fine-grain $3D$ parallelization:

$\Longrightarrow$ compute loop over k sequentially and
$\Longrightarrow$ **parallelize individual** matrix multiplications

- Total amount of work corresponds to a 3D cube.
- Each subblock corresponds to a block operation $C_{i,l} := C_{i,l} + A_{i,j}B_{j,l}$
- Find an appropriate "domain decomposition".
- 3D parallelization features lowest communication overhead



Numerical Results (10 spins)

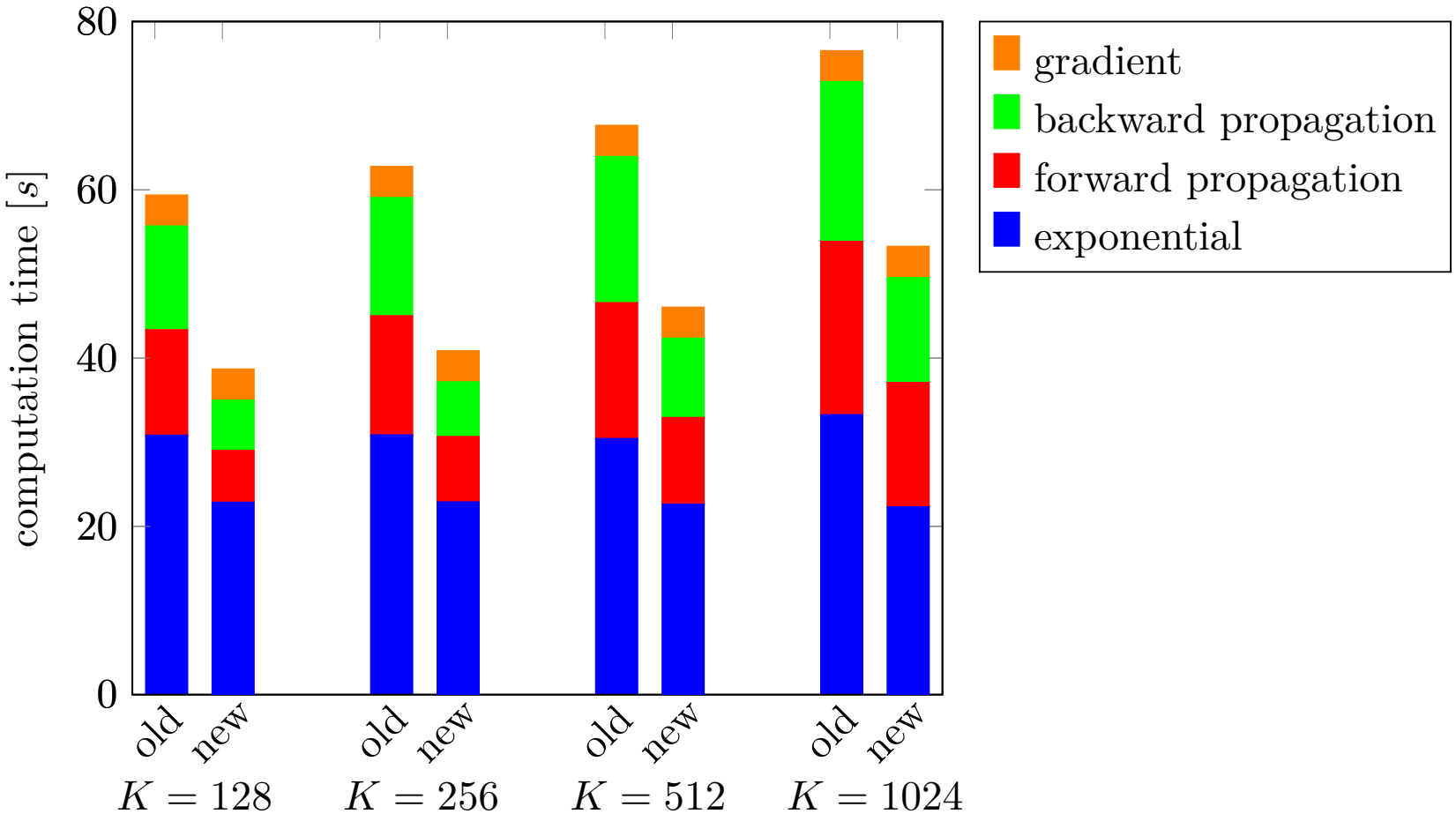


Figure : Runtime of one GRAPE iteration on the HLRB2 using $\frac{K}{2}$ processors.

Numerical Results (11 spins)

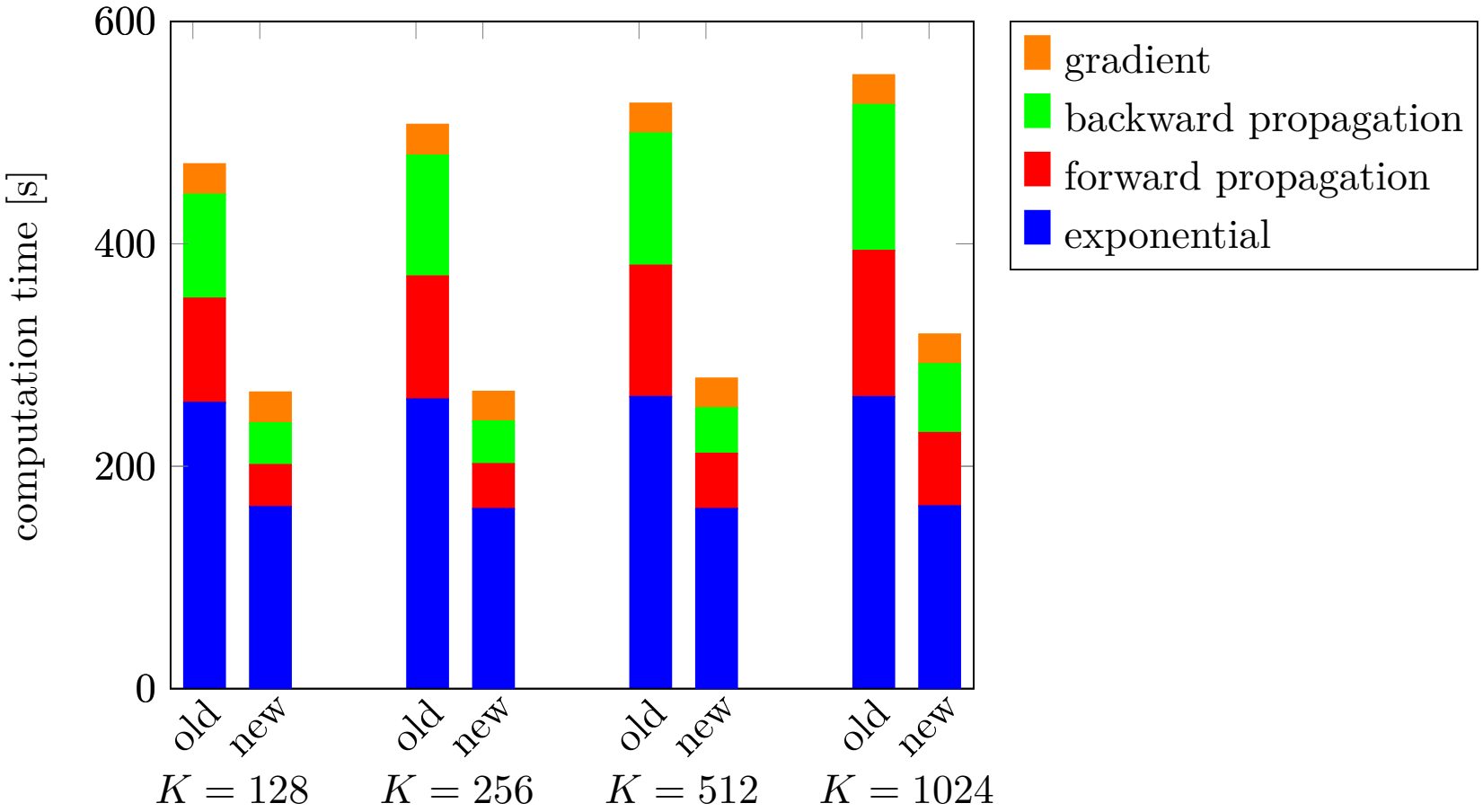


Figure : Runtime of one GRAPE iteration on the HLRB2 using $\frac{K}{2}$ processors.

Ground State of Quantum Systems

- Ground state: Compute lowest eigenvalue of the Hamiltonian

$$\boldsymbol{H} = \sum_{k=1}^{M} \alpha_k \boldsymbol{Q}_{\boldsymbol{1}}^{(\boldsymbol{k})} \otimes \cdots \otimes \boldsymbol{Q}_{\boldsymbol{N}}^{(\boldsymbol{k})} \in \mathbb{C}^{2^N \times 2^N}$$

- Challenges:
  - the vector space $\mathcal{V} = \mathbb{C}^{2^N}$ grows **exponentially** in N
  - for large N (e.g., $N = 100$) traditional matrix methods fail
- **Solution: data-sparse representation format** that allows
  - to overcome the curse of dimensionality,
  - to describe the right “corner” of the Hilbert space,
  - for efficient computations and algorithms.

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- **Solution: data-sparse representation format** that allows
  - to overcome the curse of dimensionality,
  - to describe the right “corner” of the Hilbert space,
  - for efficient computations and algorithms.
- Two approaches:
  - subspace method in the MPS format,
  - symmetry-adapted variational ground-state search.

Matrix Product States

- In physical simulations, **Matrix Product States** (MPS) are in use:

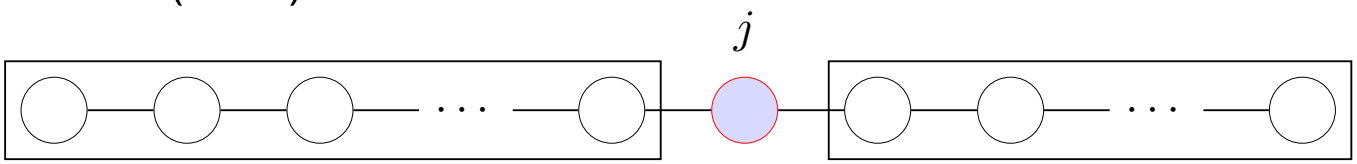
$$x = \sum_{i_1,\ldots,i_N} \operatorname{tr}\left(\boldsymbol{A}_{\mathbf{1}}^{(i_1)} \cdot \boldsymbol{A}_{\mathbf{2}}^{(i_2)} \cdots \boldsymbol{A}_{\boldsymbol{N}}^{(i_N)}\right) \boldsymbol{e}_{i_1 i_2 \ldots i_N} \cdot$$

  with $D_j \times D_{j+1}$ matrices $\boldsymbol{A}_{\boldsymbol{j}}^{(i_j)}$.

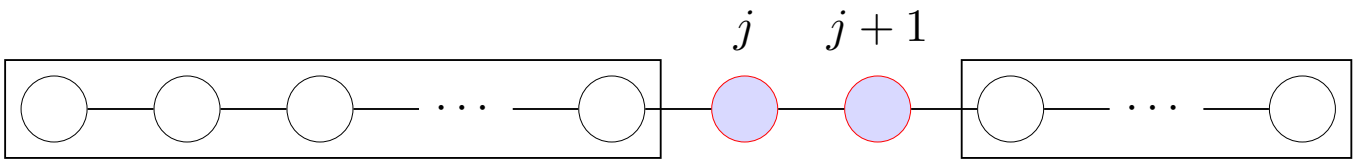
- MPS representation requires $2ND^2$ instead of 2^N entries.

Minimization in terms of MPS

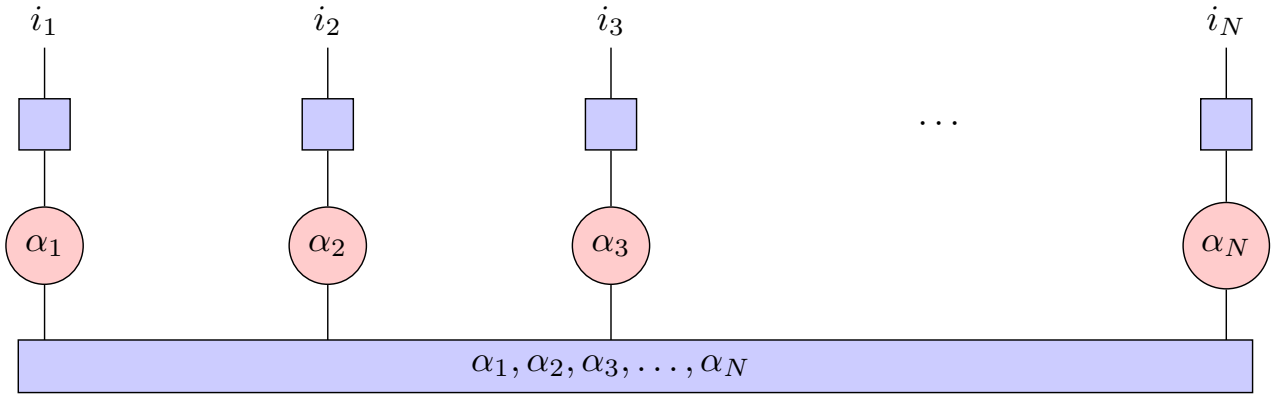
- vMPS (ALS):



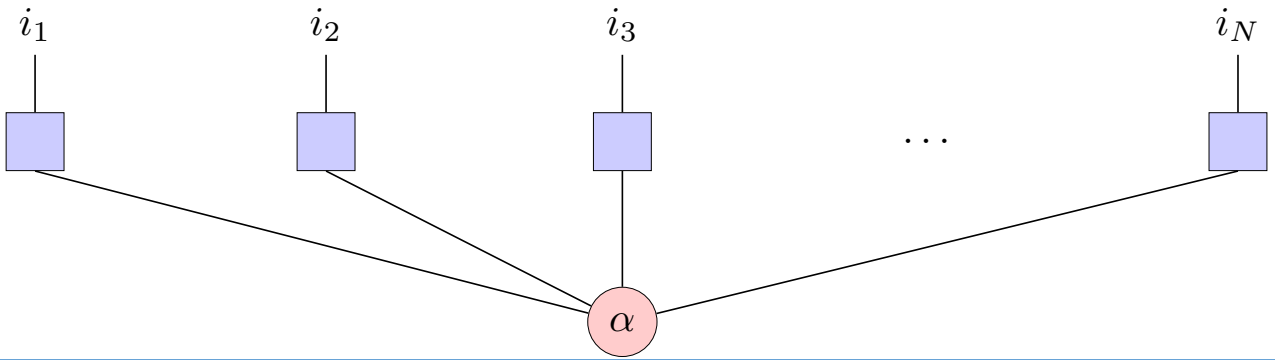
- DMRG (MALS):



Tucker:


i_1
i_2
i_3
i_N
$\cdots$
α_1
α_2
α_3
α_N
$\alpha_1, \alpha_2, \alpha_3, \ldots, \alpha_N$

CP:


i_1
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α

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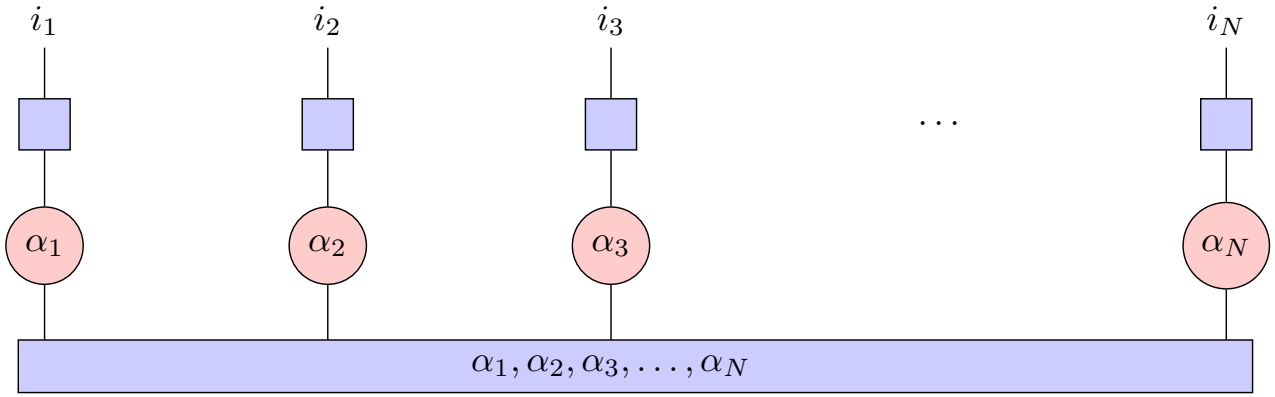
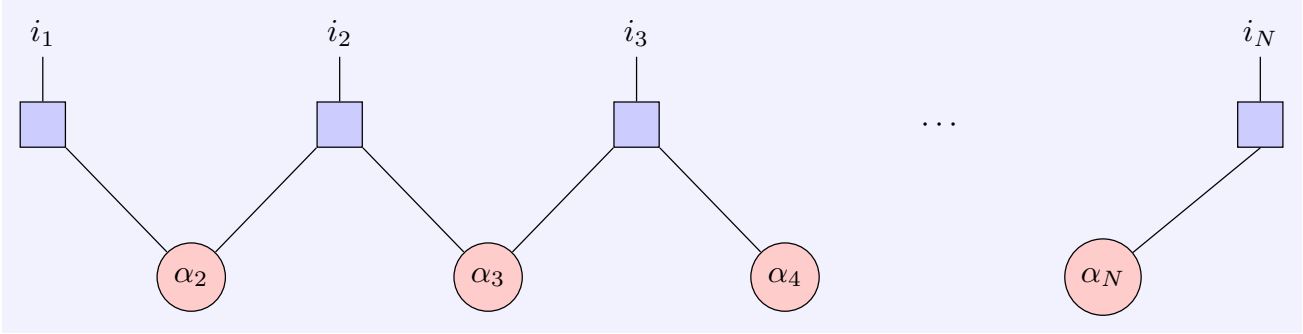


TT/MPS:



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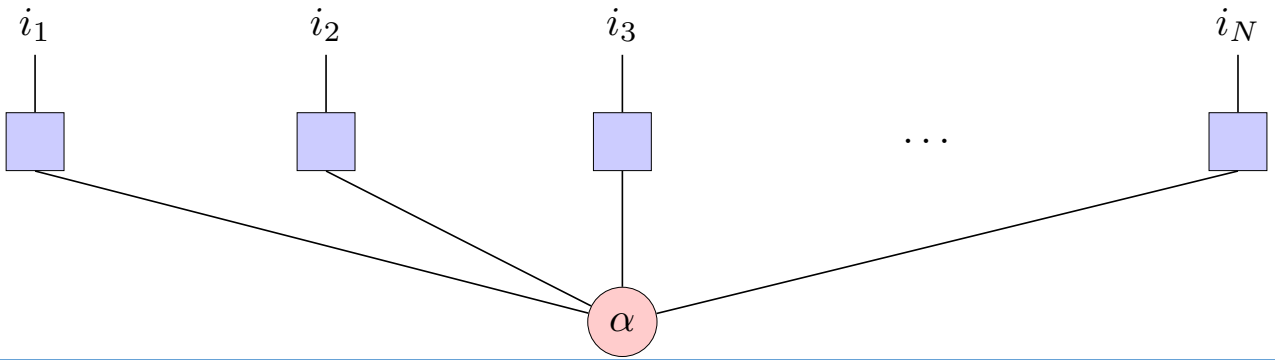

The Lanczos Algorithm

Algorithm: Lanczos iteration for Hermitian matrix $\boldsymbol{H}$

Choose initial guess $\boldsymbol{r_0} \neq \boldsymbol{0}$
Define $\beta_0 = \|\boldsymbol{r_0}\|$ and $\boldsymbol{q_0} = \boldsymbol{0}$
for $j = 1, 2, \ldots, m$ **do**

$$\boldsymbol{q_j} = \boldsymbol{r_{j-1}} / \beta_{j-1}$$
$$\boldsymbol{u_j} = \boldsymbol{H q_j}$$
$$\alpha_j = \boldsymbol{q_j^H u_j}$$
$$\boldsymbol{r_j} = \boldsymbol{u_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1} \boldsymbol{q_{j-1}}$$
$$\beta_j = \|\boldsymbol{r_j}\|$$

$$\boldsymbol{T_m} = \mathrm{tridiag}(\boldsymbol{\beta}, \boldsymbol{\alpha}, \boldsymbol{\beta})$$
$$(\lambda, \boldsymbol{y}) = \mathrm{eig}(\boldsymbol{T_m})$$
$$\boldsymbol{v} = \boldsymbol{Q y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m}) \boldsymbol{y}$$

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Computational tasks:

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Computational tasks:

1. Application of the matrix to a vector

The Lanczos Algorithm

Algorithm: Lanczos iteration for Hermitian matrix H

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Define $\beta_0 = \|r_0\|$ and $q_0 = 0$
for $j = 1, 2, \ldots, m$ **do**

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$$u_j = H q_j$$
$$\alpha_j = q_j^H u_j$$
$$r_j = u_j - \alpha_j q_j - \beta_{j-1} q_{j-1}$$
$$\beta_j = \|r_j\|$$

$$T_m = \text{tridiag}(\beta, \alpha, \beta)$$
$$(\lambda, y) = \text{eig}(T_m)$$
$$v = Qy = (q_1, \ldots, q_m)y$$

Computational tasks:

1. Application of the matrix to a vector
2. Computation of inner products

The Lanczos Algorithm

Algorithm: Lanczos iteration for Hermitian matrix H

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Define $\beta_0 = \|r_0\|$ and $q_0 = 0$
for $j = 1, 2, \ldots, m$ **do**

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$$u_j = H q_j$$
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$$\beta_j = \|r_j\|$$

$$T_m = \text{tridiag}(\beta, \alpha, \beta)$$
$$(\lambda_{\min}, y) = \text{eig}(T_m)$$
$$v = Qy = (q_1, \ldots, q_m)y$$

Computational tasks:

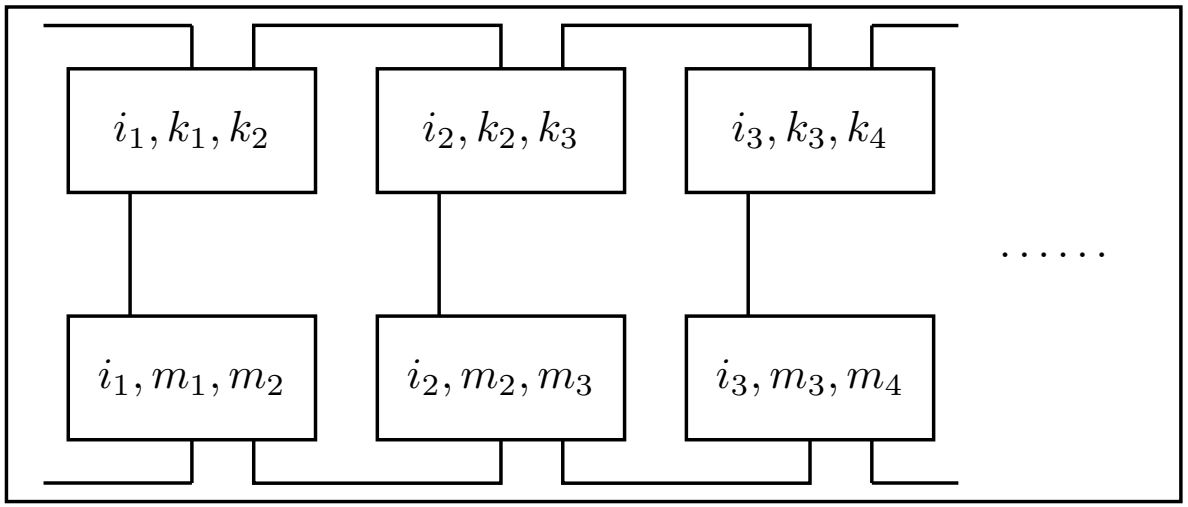
1. Application of the matrix to a vector
2. Computation of inner products
3. Sums and linear combinations of vectors

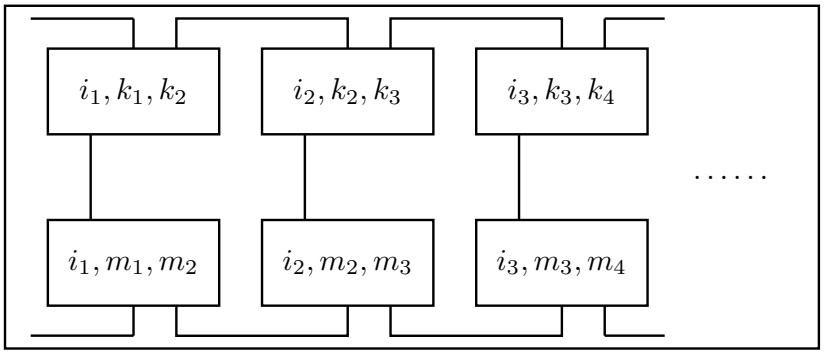
Computation of Inner Products

$$\boldsymbol{x}^{\mathrm{H}}\boldsymbol{y} = \sum_{i_1,\ldots,i_N} \left(\operatorname{tr}\left(\bar{\boldsymbol{A}}_{\boldsymbol{1}}^{(\boldsymbol{i_1})} \cdots \bar{\boldsymbol{A}}_{\boldsymbol{N}}^{(\boldsymbol{i_N})}\right)\right) \cdot \left(\operatorname{tr}\left(\boldsymbol{B}_{\boldsymbol{1}}^{(\boldsymbol{i_1})} \cdots \boldsymbol{B}_{\boldsymbol{N}}^{(\boldsymbol{i_N})}\right)\right)$$

$$= \sum_{i_j} \sum_{k_j} \overline{a_{1;k_1,k_2}^{(i_1)}} \cdots \overline{a_{N;k_N,k_1}^{(i_N)}} \sum_{m_j} b_{1;m_1,m_2}^{(i_1)} \cdots b_{N;m_N,m_1}^{(i_N)}$$

$\Longrightarrow$ Find an efficient ordering of the summations m_j, k_j, i_j.
Consider the tensor network

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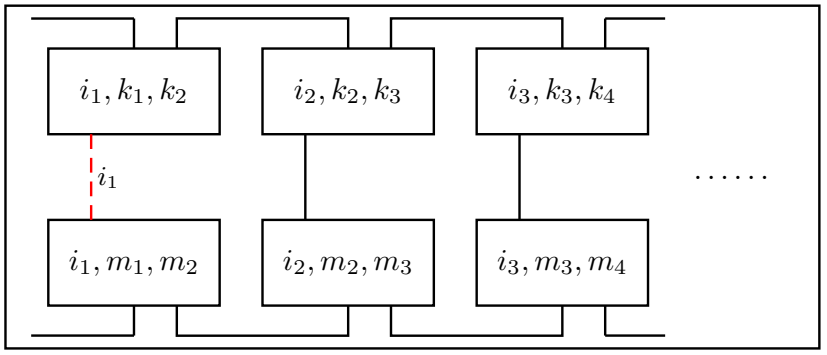
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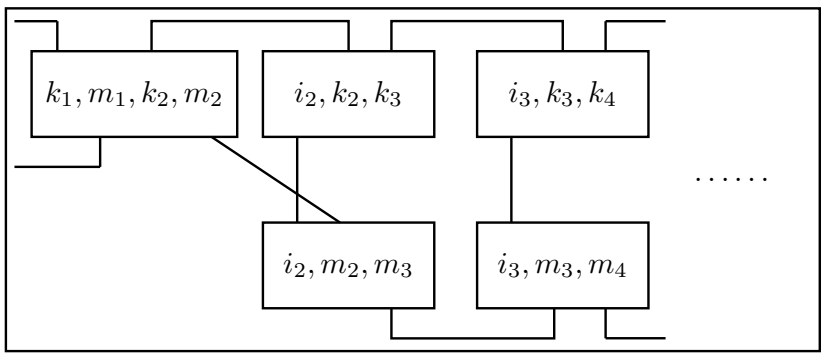
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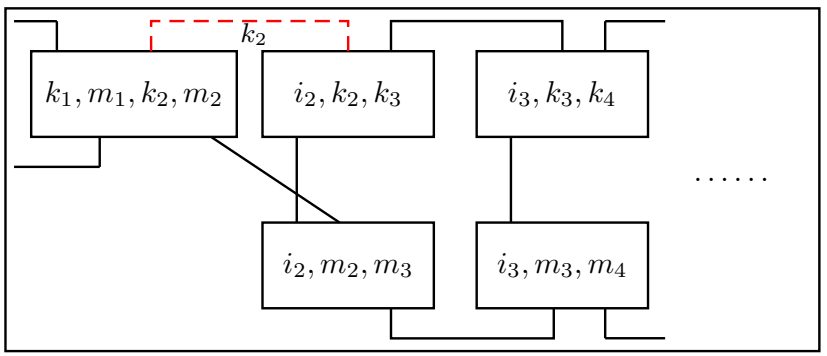
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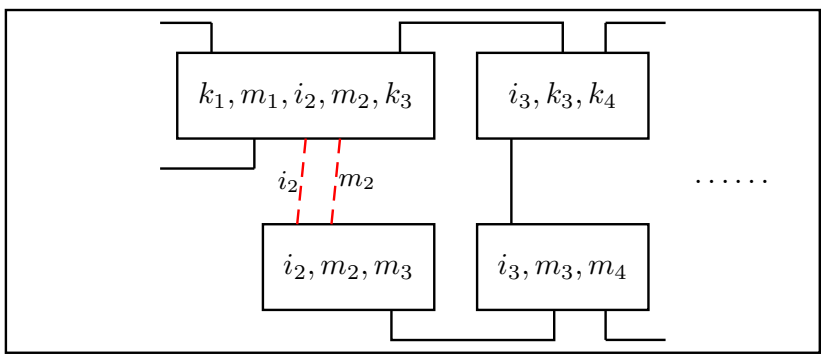
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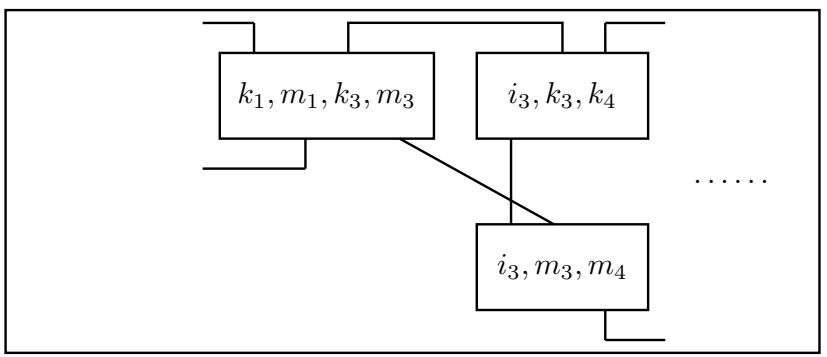
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i_3, k_3, k_4
i_3, m_3, m_4

Computation of the Sum of Two MPS

- Sum of two MPS vectors

$$\boldsymbol{x} = \sum_{i_1,\ldots,i_N} \operatorname{tr}\left(\boldsymbol{A}_1^{(i_1)} \boldsymbol{A}_2^{(i_2)} \ldots \boldsymbol{A}_N^{(i_N)}\right) \boldsymbol{e}_{i_1 \ldots i_N}$$

$$\boldsymbol{y} = \sum_{i_1,\ldots,i_N} \operatorname{tr}\left(\boldsymbol{B}_1^{(i_1)} \boldsymbol{B}_2^{(i_2)} \ldots \boldsymbol{B}_N^{(i_N)}\right) \boldsymbol{e}_{i_1 \ldots i_N}$$

$$(\boldsymbol{x}+\boldsymbol{y})_{i_1,\ldots,i_N} =$$

$$\operatorname{tr}\left[\begin{pmatrix} \boldsymbol{A}_1^{(i_1)} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}_1^{(i_1)} \end{pmatrix} \begin{pmatrix} \boldsymbol{A}_2^{(i_2)} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}_2^{(i_2)} \end{pmatrix} \cdots \begin{pmatrix} \boldsymbol{A}_N^{(i_N)} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}_N^{(i_N)} \end{pmatrix}\right]$$

- Adding MPS leads to an **increase** of the bond dimensions:

$$\boldsymbol{x}_{\mathrm{MPS}_D} + \boldsymbol{y}_{\mathrm{MPS}_D} = \boldsymbol{z}_{\mathrm{MPS}_{2D}}$$

Matrix Product Operators (MPO)

The MPS concept

$$x_{i_1,i_2,\ldots,i_N} = \mathrm{tr}\left(\boldsymbol{A}_{\boldsymbol{1}}^{(\boldsymbol{i_1})}\boldsymbol{A}_{\boldsymbol{2}}^{(\boldsymbol{i_2})}\cdots\boldsymbol{A}_{\boldsymbol{N}}^{(\boldsymbol{i_N})}\right)$$

can be generalized to operators:

$$O_{\substack{i_1,\ldots,i_N\\ j_1,\ldots,j_N}} = \mathrm{tr}\left(\boldsymbol{W}_{\boldsymbol{1}}^{(\boldsymbol{i_1},\boldsymbol{j_1})}\boldsymbol{W}_{\boldsymbol{2}}^{(\boldsymbol{i_2},\boldsymbol{j_2})}\cdots\boldsymbol{W}_{\boldsymbol{N}}^{(\boldsymbol{i_N},\boldsymbol{j_N})}\right)$$

Application of such an MPO to an MPS leads to

$$\mathrm{tr}\left[\left(\sum_{j_1}\boldsymbol{W}_{\boldsymbol{1}}^{(\boldsymbol{i_1},\boldsymbol{j_1})}\otimes\boldsymbol{A}_{\boldsymbol{1}}^{(\boldsymbol{j_1})}\right)\cdots\left(\sum_{j_N}\boldsymbol{W}_{\boldsymbol{N}}^{(\boldsymbol{i_N},\boldsymbol{j_N})}\otimes\boldsymbol{A}_{\boldsymbol{N}}^{(\boldsymbol{j_N})}\right)\right],$$

i.e., an MPS of larger size $D_{\mathrm{MPS}}D_{\mathrm{MPO}}$.

- Usually exact representation with small ranks
- Not dependent on N

Augmentation of ranks

- Increase of the bond dimension during the Lanczos algorithm

Lanczos algorithm	Bond dimension
for $j = 1, 2, \ldots, m$	
$\boldsymbol{q_j} = \boldsymbol{r_{j-1}} / \beta_{j-1}$	$D^{(j)}$
$\boldsymbol{u_j} = \boldsymbol{H}\boldsymbol{q_j}$	$D_O D^{(j)}$
$\alpha_j = \boldsymbol{q_j^{\mathrm{H}}} \boldsymbol{u_j}$	
$\boldsymbol{r_j} = \boldsymbol{H}\boldsymbol{q_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1}\boldsymbol{q_{j-1}}$	$D_O D^{(j)} + D^{(j)} + D^{(j-1)} =$
$\beta_j = \lVert \boldsymbol{r_j} \rVert$	$= D^{(j+1)}$
$\boldsymbol{v} = \boldsymbol{Q}\boldsymbol{y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m})\boldsymbol{y}$	$D^{(1)} + D^{(2)} + \cdots + D^{(m)}$

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$\boldsymbol{r_j} = \boldsymbol{H}\boldsymbol{q_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1}\boldsymbol{q_{j-1}}$	$D_O D^{(j)} + D^{(j)} + D^{(j-1)} =$
$\beta_j = \lVert \boldsymbol{r_j} \rVert$	$= D^{(j+1)}$
$\boldsymbol{v} = \boldsymbol{Q}\boldsymbol{y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m})\boldsymbol{y}$	$D^{(1)} + D^{(2)} + \cdots + D^{(m)}$

- Solution: keep the ranks $D^{(j)}$ bounded
  $\Longrightarrow$ Projection required

Compression/Projection of MPS

$$\mathcal{P}_D : \boldsymbol{y}_{MPS_{D'}} \mapsto \underset{\boldsymbol{x}_{MPS_D}}{\arg\min} \left\| \boldsymbol{y}_{MPS_{D'}} - \boldsymbol{x}_{MPS_D} \right\|_2^2 =$$

$$\underset{\boldsymbol{A}}{\arg\min} \left\| \left[\operatorname{tr}\left(\boldsymbol{B}_{\boldsymbol{1}}^{(i_1)} \cdots \boldsymbol{B}_{\boldsymbol{N}}^{(i_N)} \right) - \operatorname{tr}\left(\boldsymbol{A}_{\boldsymbol{1}}^{(i_1)} \cdots \boldsymbol{A}_{\boldsymbol{N}}^{(i_N)} \right) \right]_{i_1,\ldots,i_N} \right\|_2^2$$

SVD-based truncation:

- Suppose $\boldsymbol{A_1}, \ldots, \boldsymbol{A_{r-1}}$ are already constructed. $\boldsymbol{B_r}$ is $D \times D'$

$$\begin{pmatrix} \boldsymbol{B}_{\boldsymbol{r}}^{(0)} \\ \boldsymbol{B}_{\boldsymbol{r}}^{(1)} \end{pmatrix} = \begin{pmatrix} \boldsymbol{U}_{\boldsymbol{r}}^{(0)} \\ \boldsymbol{U}_{\boldsymbol{r}}^{(1)} \end{pmatrix} \boldsymbol{\Sigma_r} \boldsymbol{V_r^H} \overset{trunc}{\approx} \begin{pmatrix} \tilde{\boldsymbol{U}}_{\boldsymbol{r}}^{(0)} \\ \tilde{\boldsymbol{U}}_{\boldsymbol{r}}^{(1)} \end{pmatrix} \tilde{\boldsymbol{\Sigma}}_{\boldsymbol{r}} \tilde{\boldsymbol{V}}_{\boldsymbol{r}}^{\mathbf{H}}$$

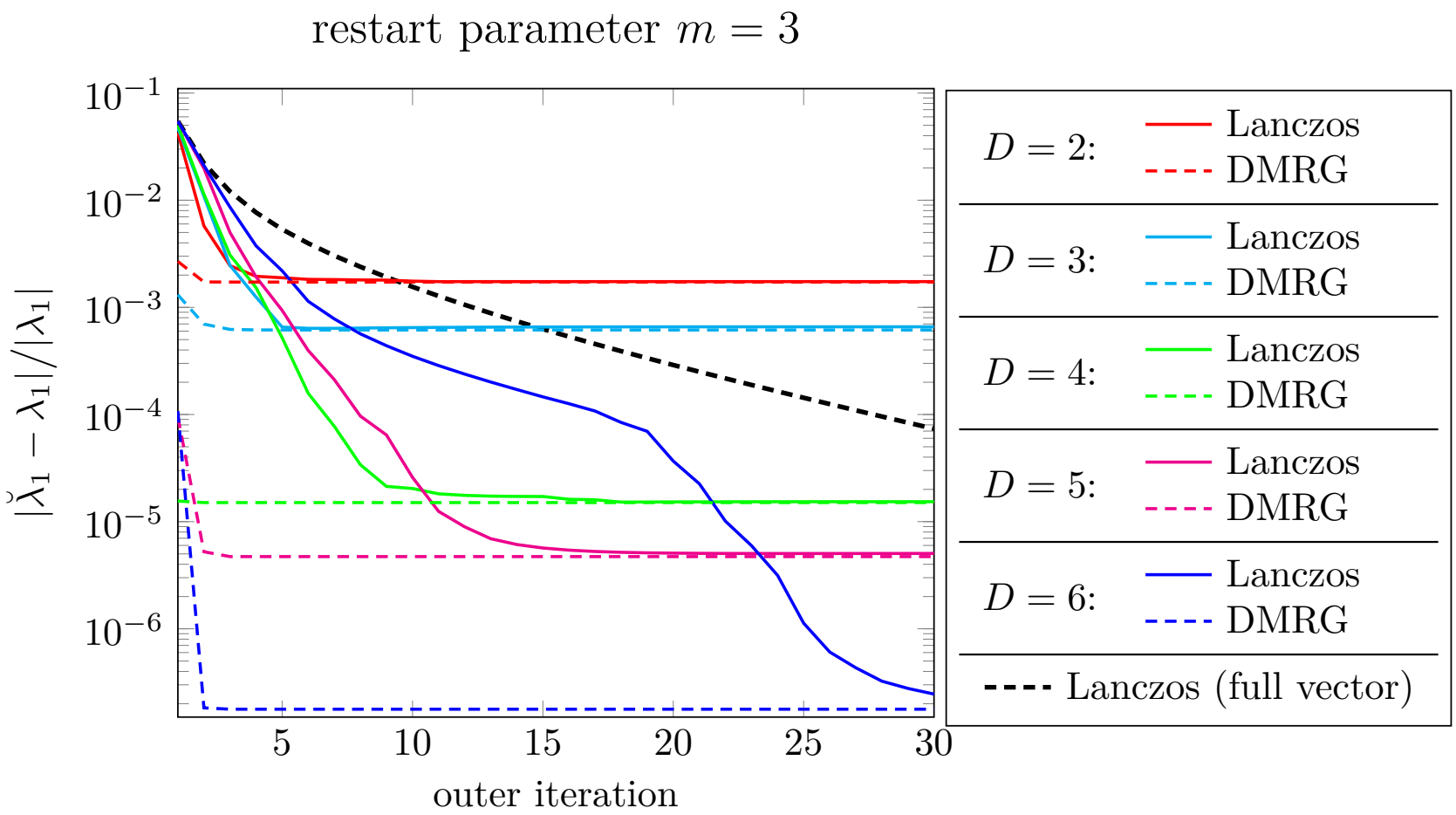
- Define $\boldsymbol{A}_{\boldsymbol{r}}^{(i_r)} = \tilde{\boldsymbol{U}}_{\boldsymbol{r}}^{(i_r)}$, a $D \times D$ matrix
- proceed with the $D \times D'$ matrix $\tilde{\boldsymbol{\Sigma}}_{\boldsymbol{r}} \tilde{\boldsymbol{V}}_{\boldsymbol{r}}^{\mathbf{H}} \boldsymbol{B}_{\boldsymbol{r+1}}^{(i_{r+1})}$

Restarted Lanczos

Algorithm: Restarted Lanczos iteration

Choose initial guess $\boldsymbol{r_0} \neq \boldsymbol{0}$;
for $iter = 1, 2, \ldots$ **do**
  Define $\beta_0 = \|\boldsymbol{r_0}\|$ and $\boldsymbol{q_0} = \boldsymbol{0}$;
  for $j = 1, 2, \ldots, m$ **do**
    $\boldsymbol{q_j} = \boldsymbol{r_{j-1}} / \beta_{j-1}$;
    $\boldsymbol{u_j} = \boldsymbol{H q_j}$;
    $\alpha_j = \boldsymbol{q_j}^{\mathrm{H}} \boldsymbol{u_j}$;
    $\boldsymbol{r_j} = \boldsymbol{u_j} - \alpha_j \boldsymbol{q_j} - \beta_{j-1} \boldsymbol{q_{j-1}}$;
    $\beta_j = \|\boldsymbol{r_j}\|$;
  $\boldsymbol{T_m} = \mathrm{tridiag}(\boldsymbol{\beta}, \boldsymbol{\alpha}, \boldsymbol{\beta})$;
  $(\lambda_{\min}, \boldsymbol{y}) = \mathrm{eig}(\boldsymbol{T_m})$;
  $\boldsymbol{v} = \boldsymbol{Q y} = (\boldsymbol{q_1}, \ldots, \boldsymbol{q_m}) \boldsymbol{y}$;
  $\boldsymbol{r_0} = \mathcal{P}_D(\boldsymbol{v})$

Numerical Results (Ising Hamiltonian $N = 25$)



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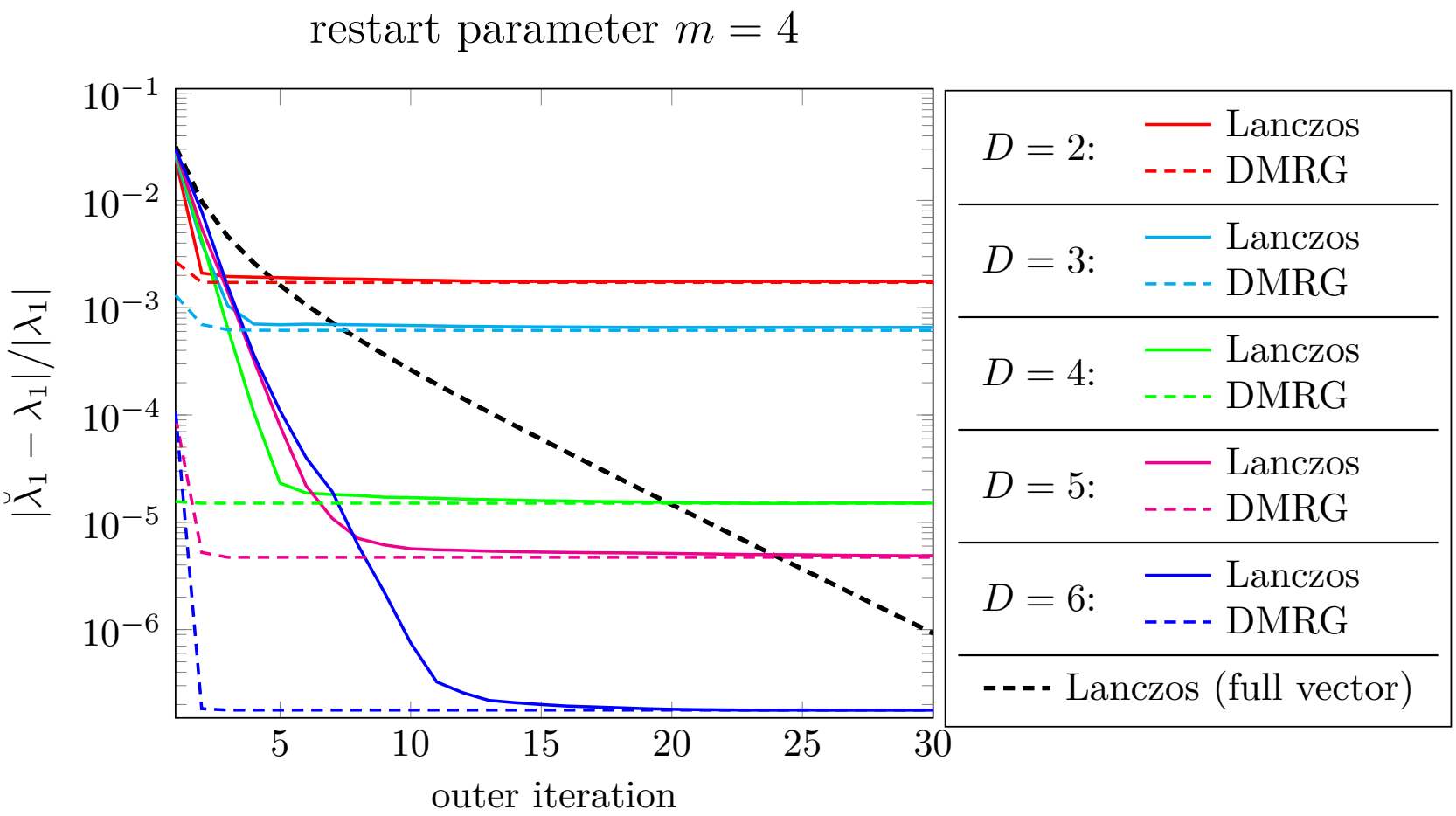

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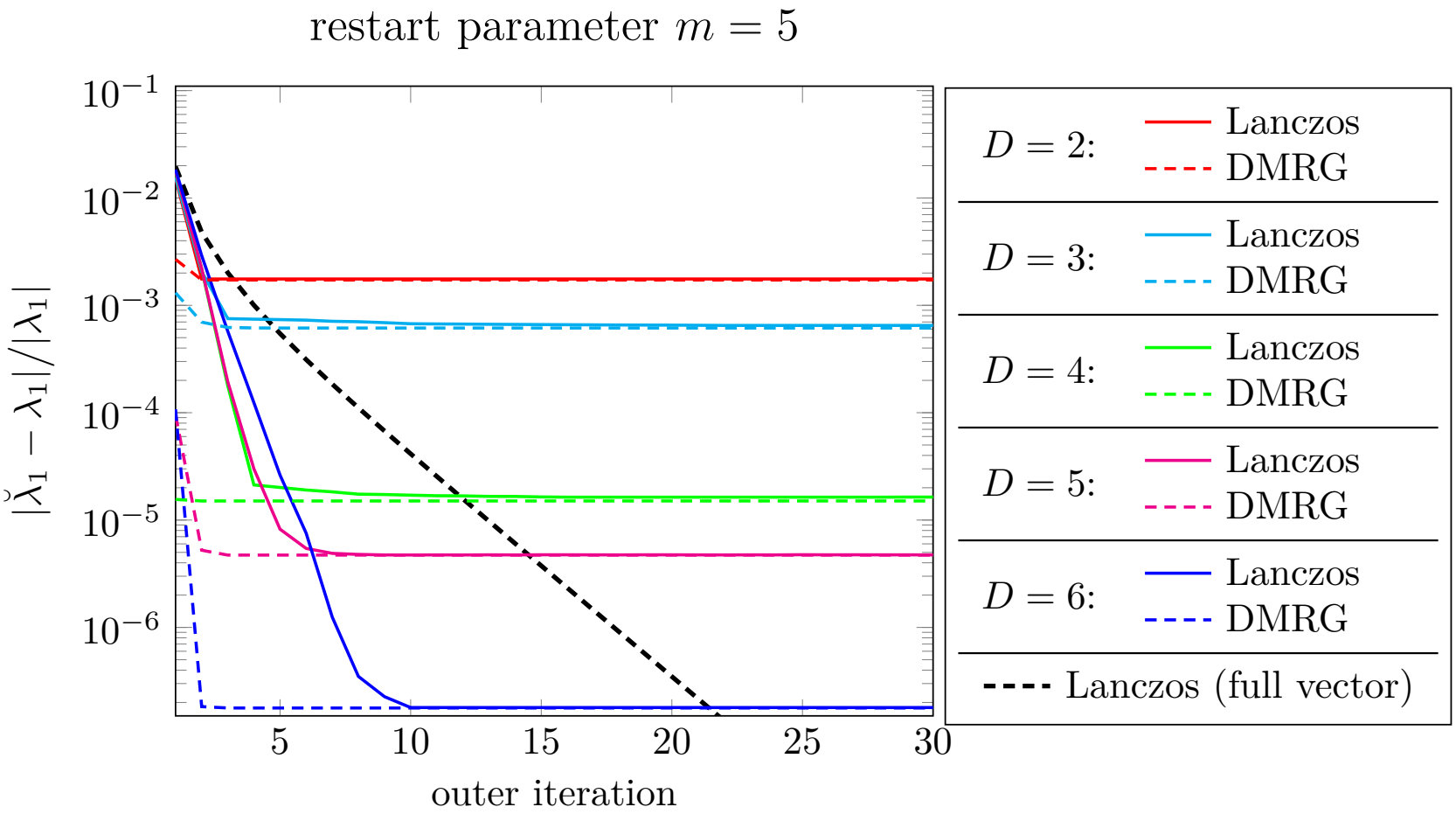

Matrix and Vector Symmetries

- $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric, if $a_{i,j} = a_{j,i}$
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$$\boldsymbol{A} = \begin{pmatrix} a & b & c & d \\ b & e & f & g \\ c & f & h & i \\ d & g & i & j \end{pmatrix}$$

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$$\boldsymbol{A} = \begin{pmatrix} 0 & b & c & d \\ -b & 0 & f & g \\ -c & -f & 0 & i \\ -d & -g & -i & 0 \end{pmatrix}$$

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$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ v_n \end{pmatrix} = \begin{pmatrix} v_n \\ v_{n-1} \\ \vdots \\ v_2 \\ v_1 \end{pmatrix} = \underbrace{\begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & \iddots & & \\ & 1 & & & \\ 1 & & & & \end{pmatrix}}_{=:J} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_{n-1} \\ v_n \end{pmatrix}$$

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Symmetries of Spin-$\frac{1}{2}$ Hamiltonians

$$\boldsymbol{H} = \sum_{k=1}^{M} \alpha_k \boldsymbol{Q_1^{(k)}} \otimes \cdots \otimes \boldsymbol{Q_N^{(k)}} \ , \quad \boldsymbol{Q_i^{(k)}} \in \{\boldsymbol{I}, \boldsymbol{\sigma_x}, \boldsymbol{\sigma_y}, \boldsymbol{\sigma_z}\} \subset \mathbb{C}^{2\times 2}$$

$$\boldsymbol{\sigma_x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \boldsymbol{\sigma_y} = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \ \boldsymbol{\sigma_z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ \boldsymbol{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} .$$

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- $\boldsymbol{\sigma_x}$, $\boldsymbol{\sigma_y}/\mathrm{i}$ and $\boldsymbol{I}$ are persymmetric, $\boldsymbol{\sigma_z}$ is skew-persymmetric,
- Kronecker product of two skew-symmetric matrices is symmetric,
- Kronecker product of two skew-persymmetric matrices is persymmetric.

Symmetries of Spin-$\frac{1}{2}$ Hamiltonians

$$\boldsymbol{H} = \sum_{k=1}^{M} \alpha_k \boldsymbol{Q}_1^{(k)} \otimes \cdots \otimes \boldsymbol{Q}_N^{(k)} \ , \quad \boldsymbol{Q}_i^{(k)} \in \{\boldsymbol{I}, \boldsymbol{\sigma_x}, \boldsymbol{\sigma_y}, \boldsymbol{\sigma_z}\} \subset \mathbb{C}^{2\times 2}$$

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- Kronecker product of two skew-symmetric matrices is symmetric,
- Kronecker product of two skew-persymmetric matrices is persymmetric.

Symmetry of Spin Hamiltonians

Hamiltonians of typical physical models (Ising-ZZ, various Heisenberg models) are real-valued and symmetric persymmetric.

Matrix Symmetries and Eigenvectors

Eigenvectors of Symmetric Persymmetric Matrices ([CB76])

A symmetric persymmetric matrix $\boldsymbol{A}$ can be orthogonally transformed to a block diagonal matrix:

$$\boldsymbol{A} = \begin{pmatrix} \boldsymbol{B} & \boldsymbol{C} \\ \boldsymbol{C}^{\mathrm{T}} & \boldsymbol{JBJ} \end{pmatrix} = \frac{1}{2} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{I} \\ \boldsymbol{J} & -\boldsymbol{J} \end{pmatrix} \begin{pmatrix} \boldsymbol{B}+\boldsymbol{JC} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}-\boldsymbol{JC} \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{J} \\ \boldsymbol{I} & -\boldsymbol{J} \end{pmatrix} .$$

Hence, the eigenvectors of $\boldsymbol{A}$ are of the form

$$\begin{pmatrix} \boldsymbol{v_i} \\ \boldsymbol{Jv_i} \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \boldsymbol{v_i} \\ -\boldsymbol{Jv_i} \end{pmatrix} .$$

Matrix Symmetries and Eigenvectors

Eigenvectors of Symmetric Persymmetric Matrices ([CB76])

A symmetric persymmetric matrix A can be orthogonally transformed to a block diagonal matrix:

$$A = \begin{pmatrix} B & C \\ C^{\mathrm{T}} & JBJ \end{pmatrix} = \frac{1}{2} \begin{pmatrix} I & I \\ J & -J \end{pmatrix} \begin{pmatrix} B + JC & 0 \\ 0 & B - JC \end{pmatrix} \begin{pmatrix} I & J \\ I & -J \end{pmatrix} .$$

Hence, the eigenvectors of A are of the form

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Ground States of Spin Hamiltonians

Ground states of typical physical models (Ising-ZZ, various Heisenberg models) are either symmetric or skew-symmetric.

MPS Representation of Symmetric Vectors

$$x_{i_1,i_2,i_3,\ldots,i_{N-1},i_N} = x_{\bar{i}_1,\bar{i}_2,\bar{i}_3,\ldots,\bar{i}_{N-1},\bar{i}_N} \iff \boldsymbol{J}\boldsymbol{x} = \boldsymbol{x} \qquad \text{(BF)}$$

Flip-operator $\bar{i} := 1 - i$.

Example (N=3): $\boldsymbol{x} = \begin{pmatrix} a & b & c & d & d & c & b & a \end{pmatrix}^{\mathrm{T}}$

Theorem: MPS Representation of the Vector Symmetry ([Huckle13])

1. If all MPS matrix pairs $(\boldsymbol{A}_j^{(0)}, \boldsymbol{A}_j^{(1)})$ are connected via

$$\boldsymbol{A}_j^{(i_j)} = \boldsymbol{U}_j \boldsymbol{A}_j^{(\bar{i}_j)} \boldsymbol{U}_{j+1} \ , \ j = 1, \ldots, N \ , \qquad (1)$$

   with involutions $\boldsymbol{U}_j$ ($\boldsymbol{U}_j^2 = \boldsymbol{I}$), the represented vector is symmetric (BF).
2. Any symmetric vector (BF) can be represented by an MPS fulfilling relations (1).

- Reduction factor: ≈ 2

MPS Representation of Symmetric Vectors

Theorem: Uniqueness Result for Symmetric Vectors ([Huckle13])

Assume that the MPS matrices (over $\mathbb{K}$) are related by

$$\boldsymbol{A_j^{(1)}} = \boldsymbol{U_{j-1}} \boldsymbol{A_j^{(0)}} \boldsymbol{V_j} \ ,$$

with square matrices $\boldsymbol{V_j}$ and $\boldsymbol{U_j}$ of appropriate size ($j = 1, \ldots, N$). If any choice of matrices $\boldsymbol{A_j^{(0)}}$ results in the symmetry of the represented vector $\boldsymbol{x}$, i.e.,

$$\boldsymbol{Jx} \ = \ \boldsymbol{x} \ ,$$

then $\boldsymbol{U_j}$ and $\boldsymbol{V_j}$ are—up to a scalar factor—involutions for all j: $\boldsymbol{U_j^2} = u_j \boldsymbol{I}$, $\boldsymbol{V_j^2} = v_j \boldsymbol{I}$. Furthermore, $\boldsymbol{U_j} = c_j \cdot \boldsymbol{V_j}$, $j = 1, ..., N$ with constants c_j.

- This theorem gives an argument to use involutions as heuristic.
- An involution has as eigenvalues $\pm 1 \Longrightarrow$ choose $\boldsymbol{U_j} = \boldsymbol{J}$.

Exploiting Symmetries in Computations

- Impose symmetry conditions into variational ground-state search
- Suppose that the desired ground-state vector x is symmetric, i.e., $Jx = x$

$$0 \leq x^{\mathrm{H}} (I - J) x = x^{\mathrm{H}} \underbrace{(x - Jx)}_{=0} = 0 .$$

- Therefore,

$$\lambda_{\min} \leq \frac{y^{\mathrm{H}} H y}{y^{\mathrm{H}} y} \leq \frac{y^{\mathrm{H}} H y}{y^{\mathrm{H}} y} + \rho \frac{y^{\mathrm{H}} (I - J) y}{y^{\mathrm{H}} y} = \frac{y^{\mathrm{H}} (H + \rho(I - J)) y}{y^{\mathrm{H}} y} .$$

- Apply ground-state algorithm (e.g., DMRG) to modified Hamiltonian

$$H(\rho) := H + \rho(I - J) \quad \text{for some} \quad \rho > 0 .$$

Numerical Results: Number of Iterations

Table : Heisenberg-XXX model of $N = 100$ spins: Number of DMRG sweeps until convergence.

	D								
ρ	2	3	4	5	6	7	8	9	10
0	66	71	28	13	16	35	13	11	22
0.1	48	24	22	8	12	43	9	8	27
0.5	13	10	14	6	9	31	9	8	17
1	8	10	15	5	8	20	9	8	15
2	6	14	16	5	8	20	9	8	14
10	4	6	46	5	10	9	9	8	9
100	5	5	29	10	9	9	9	9	10

Numerical Studies: Convergence

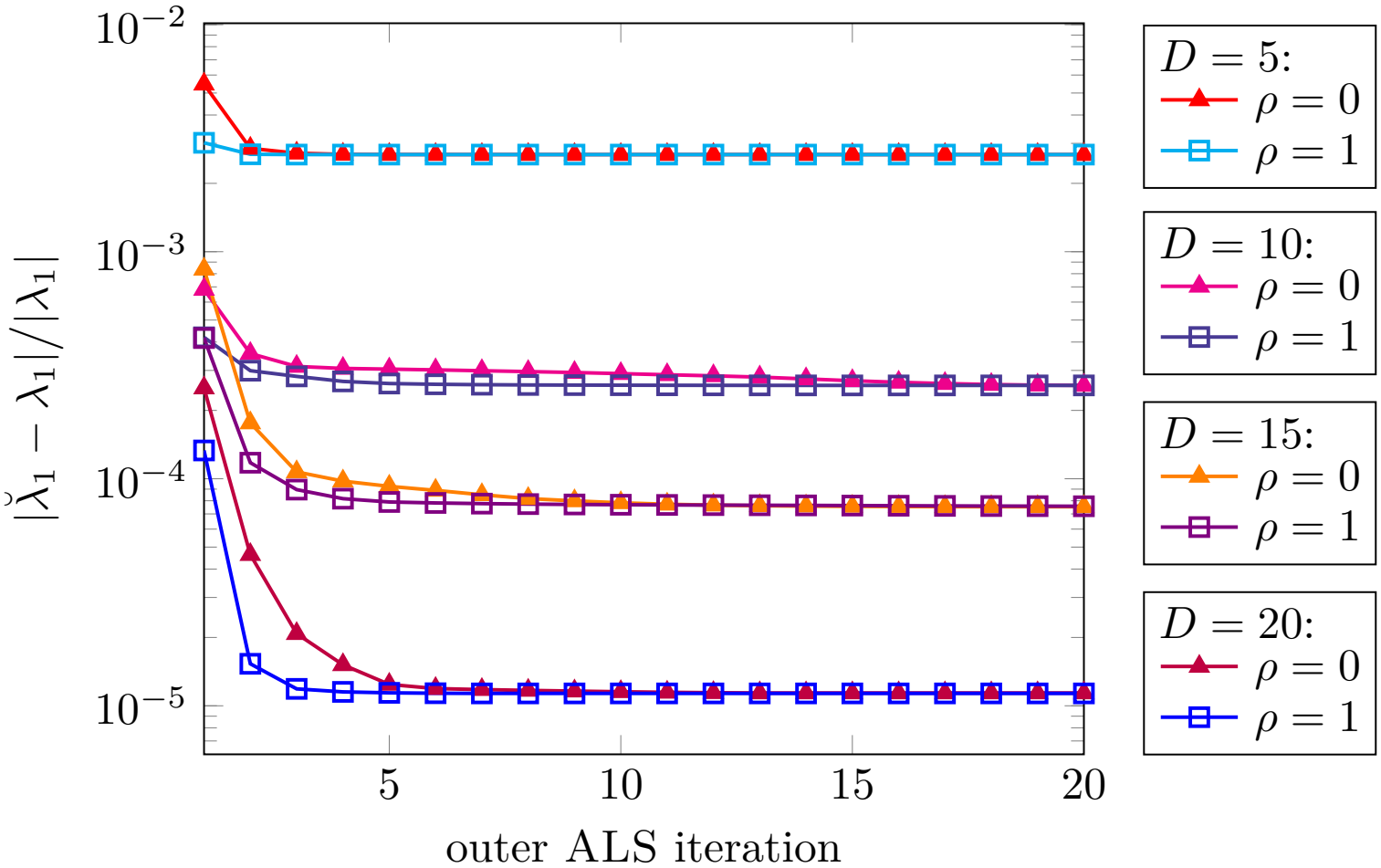

Figure : Heisenberg-XXX model of $N = 100$ spins: Approximation error.

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Thank you for your attention.


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