Computation of ground states

A mathematical point of view

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Computation of ground states

Problem:

- Given: Hamiltonian

$$H = \sum_{k=1}^{M} \alpha_k Q_1^{(k)} \otimes \cdots \otimes Q_p^k.$$

- Problem: Computation of the ground state

$$\min_{x \neq 0} \frac{x^\dagger H x}{x^\dagger x}$$

- Trouble: exponential growth of the Hilbert space:

$$x = \sum_{k_1,\ldots,k_p=1}^{2} \beta_{k_1,\ldots,k_p} e_{k_1} \otimes \cdots \otimes e_{k_p}$$

- Goals:
    - Look for ”good” approximations/parametrisations,
    - Make use of the tensor structure.

Tensor-representation of the vector

- Idea: Choose a decomposition of the vector x:

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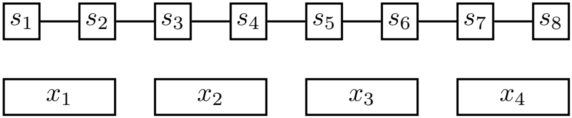

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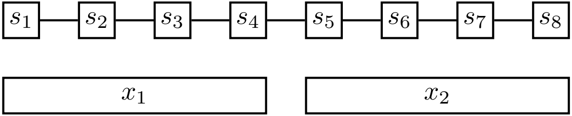

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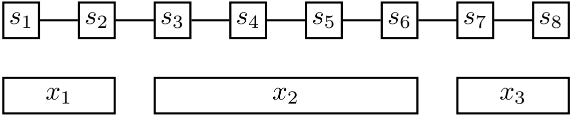

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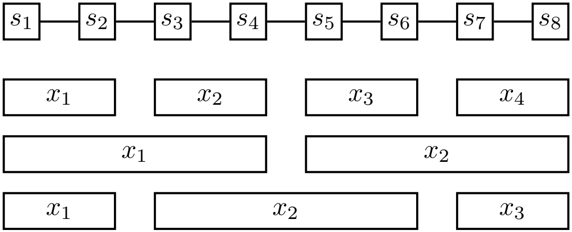

- The partitions x_i are small enough for numerical calculations.

Slice-wise optimisation

- Integration of this approximation into the variational ansatz

$$\min_{x_1,\ldots,x_q \neq 0} \frac{(x_1 \otimes \ldots \otimes x_q)^\dagger H (x_1 \otimes \ldots \otimes x_q)}{(x_1 \otimes \ldots \otimes x_q)^\dagger (x_1 \otimes \ldots \otimes x_q)}$$

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$$\min_{x_i \neq 0} \frac{(x_1 \otimes \dots \otimes x_i \otimes \dots \otimes x_q)^\dagger H (x_1 \otimes \dots \otimes x_i \otimes \dots \otimes x_q)}{(x_1 \otimes \dots \otimes x_i \otimes \dots \otimes x_q)^\dagger (x_1 \otimes \dots \otimes x_i \otimes \dots \otimes x_q)}$$

- This approach leads to the classical eigenvalue problem

$$\min_{x_i \neq 0} \frac{{x_i}^\dagger H_i x_i}{{x_i}^\dagger x_i}.$$

This eigenvalue problem is small enough to be solved with numerical methods (Krylov method, e.g. Lanczos).

Computation of ground states

This approach leads to the following algorithm:

1. Choose an appropriate decomposition $x = x_1 \otimes \cdots \otimes x_q$
2. Start with random guess
3. For all i compute

$$\min_{x_i \neq 0} \frac{(x_1 \otimes ... \otimes x_i \otimes ... \otimes x_q)^\dagger H (x_1 \otimes ... \otimes x_i \otimes ... \otimes x_q)}{(x_1 \otimes ... \otimes x_i \otimes ... \otimes x_q)^\dagger (x_1 \otimes ... \otimes x_i \otimes ... \otimes x_q)}$$

   by solving the respective eigenvalue problem.

4. Repeat step **3.** several times, until convergence against a stationary point is reached.

Generalization

- Consider a sum of such vector tensor representations:

$$x = x_1 \otimes ... \otimes x_q + \sum_{j=1}^{D} y_1^{(j)} \otimes ... \otimes y_{q(j)}^{(j)}.$$

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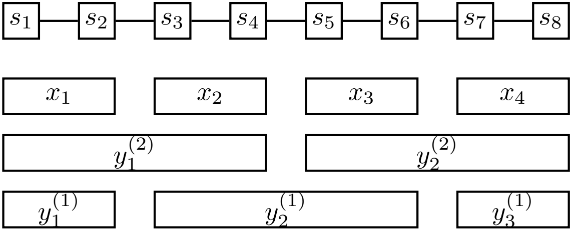

Generalization

- Integration in the variational approach leads to

$$\min_{x_1,\ldots,x_q \neq 0} \frac{\left(x_1 \otimes \ldots \otimes x_q + \sum_{j=1}^{D} y_1^{(j)} \otimes \ldots \otimes y_{q(j)}^{(j)}\right)^{\dagger} H \left(x_1 \otimes \ldots \otimes x_q + \sum_{j=1}^{D} y_1^{(j)} \otimes \ldots \otimes y_{q(j)}^{(j)}\right)}{\left(x_1 \otimes \ldots \otimes x_q + \sum_{j=1}^{D} y_1^{(j)} \otimes \ldots \otimes y_{q(j)}^{(j)}\right)^{\dagger} \left(x_1 \otimes \ldots \otimes x_q + \sum_{j=1}^{D} y_1^{(j)} \otimes \ldots \otimes y_{q(j)}^{(j)}\right)}$$

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$$\min_{x_1,\ldots,x_q\neq 0} \frac{\left(x_1\otimes\ldots\otimes x_q+\sum_{j=1}^{D} y_1^{(j)}\otimes\ldots\otimes y_{q(j)}^{(j)}\right)^\dagger H \left(x_1\otimes\ldots\otimes x_q+\sum_{j=1}^{D} y_1^{(j)}\otimes\ldots\otimes y_{q(j)}^{(j)}\right)}{\left(x_1\otimes\ldots\otimes x_q+\sum_{j=1}^{D} y_1^{(j)}\otimes\ldots\otimes y_{q(j)}^{(j)}\right)^\dagger \left(x_1\otimes\ldots\otimes x_q+\sum_{j=1}^{D} y_1^{(j)}\otimes\ldots\otimes y_{q(j)}^{(j)}\right)}$$

- Slice-wise optimisation of x_i leads to a generalized eigenproblem

$$\min_{x_i\neq 0} \frac{\begin{pmatrix} x_i & 1\end{pmatrix}^\dagger \begin{pmatrix} H_i & u \\ u^\dagger & \beta \end{pmatrix} \begin{pmatrix} x_i \\ 1 \end{pmatrix}}{\begin{pmatrix} x_i & 1\end{pmatrix}^\dagger \begin{pmatrix} I & v \\ v^\dagger & \rho \end{pmatrix} \begin{pmatrix} x_i \\ 1 \end{pmatrix}}$$

- Simple transformation to a classical eigenproblem possible.

Complexity of this method

- Let

M: length of the Hamiltonian representation,
D: length of the sum of vector tensors
m: length of the greatest subblock
p: number of sites
q: number of subblocks

- Computational-intensive parts:
  - calculation of the inner products:

$$\mathcal{O}(DMm^{3/2}) + \mathcal{O}(DMm^{3/2}) + \mathcal{O}(mp) + \mathcal{O}(Dm^{3/2}) = \mathcal{O}(DMm^{3/2}p$$

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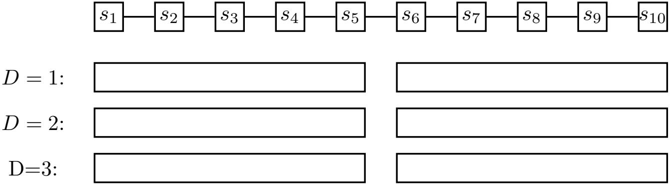
  - Solving the individual eigenproblems: $\mathcal{O}(Mqm)$
  - Total costs: $\mathcal{O}(MpD^2m^{3/2})$

Numerical results

- example: Hamiltonian of the Ising-type

$$H = \sum_{i=1}^{9} \sigma_z^{(i)} \sigma_z^{(i+1)} + \sum_{i=1}^{10} \sigma_x^{(i)}$$

- Unique decomposition $x = x_1 \otimes x_2 \in \mathbb{C}^{2^5} \otimes \mathbb{C}^{2^5}$:

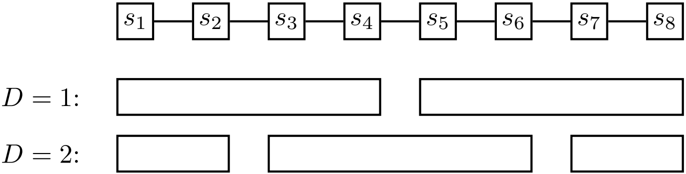


- Comparison MPS-DMRG vs. tensor product:

"D"	error dmrg-mps	error tensor-approach
2	0.0094	0.0089
3	0.0022	0.0054

Advantages of this approach

- Matrix-free formulation (enables great subblocks)
- offers possibilities for generalization and improvement:
  - Introduction of overlaps



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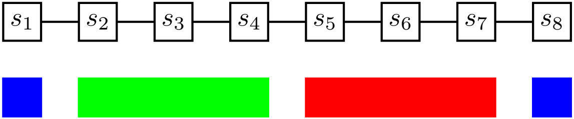

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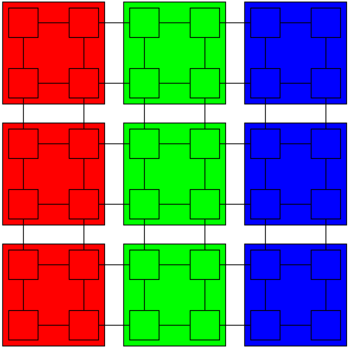

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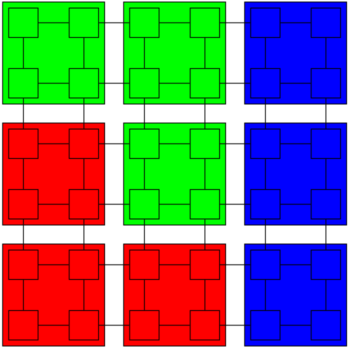

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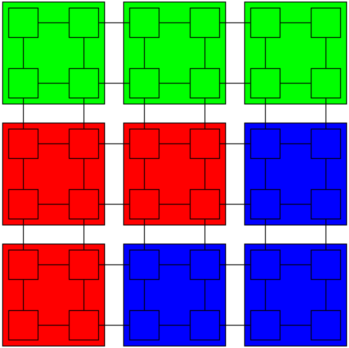

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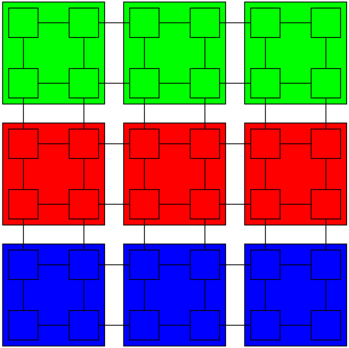

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Thanks go to

- Thomas Huckle
- Thomas Schulte-Herbrüggen

Thank you very much for your attention!

Discussion

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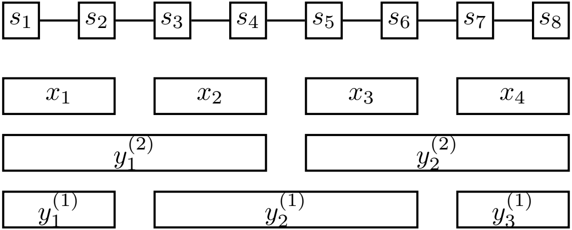

- Relation to physically motivated approaches (MPS, PEPS,...)?