ExQM Exploring Quantum Matter

Generic Construction of Tensor Product Operator Representations

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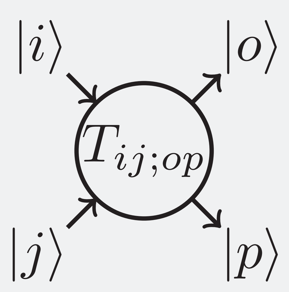
Tensor Networks

Tensor

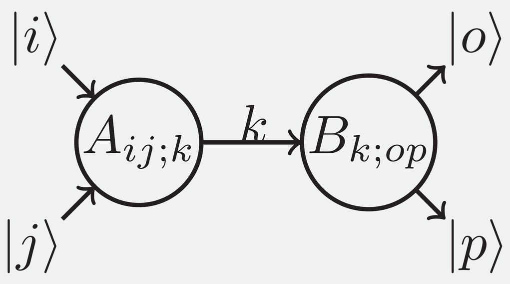
Maps from product space of input spaces to linear combinations of elements of product space of output spaces:

$$\bigotimes_{j=1}^{N_i} |i_j\rangle \to \sum_{o_1,\ldots,o_{N_o}} T_{i_1,\ldots,i_{N_i};o_1,\ldots,o_{N_o}} \bigotimes_{j=1}^{N_o} |o_j\rangle$$



Tensor Networks

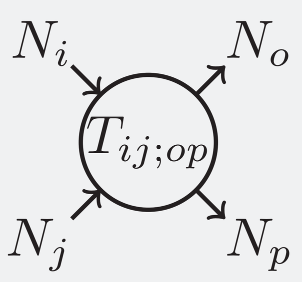
Decomposition of large tensor (e.g. Hamiltonian matrix) into smaller tensors with implied tensor contraction:



$$T_{ij;op} = \sum_k A_{ij;k} B_{k;op}$$

Abelian Symmetries

Tensors on spaces with good quantum numbers (e.g. particle number) should conserve them:[1]



$$N_i + N_j \neq N_o + N_p \quad \Rightarrow T_{ij;op} = 0$$

Nonabelian Symmetries

Tensors on spaces with non-abelian symmetries should preserve relations between different states (treat $S^z = \pm^1/_2$ of $S = {}^1/_2$ doublet the same).[2,3] Decompose $T_{ij;op}$ into reduced and symmetry-protected tensors:

$$T_{ij;op} \to T^R_{r_i r_j; r_o r_p} \bigotimes_{s=1}^{N_S} T^s_{s_i s_j; s_o s_p}$$

$\Rightarrow$ much smaller reduced tensor T^R and very sparse symmetry-protected tensors T^s

DMRG

- 1-D/MPS case: Write state (Hamiltonian) as Matrix Product State (Operator)
- Variationally optimise state sequentially and locally to find lowest eigenstate[4,5]
- **Requires MPO rep of Hamiltonian**
- DMRG3S[6] also generalises as Tensor Product State-DMRG to all loop-free tensor network topologies, using Tensor Product Operators

References

[1] I. P. McCulloch. JStatM 2007.10 (2007)

[2] I. P. McCulloch et al. PhilMag B 81 (2001)

[3] A. Weichselbaum. Ann. Phys. 327.12 (2012)

[4] S. R. White. PRL 69 (19 1992)

[5] U. Schollwöck. Ann. Phys. 326.1 (2011)

[6] C. Hubig et al. PRB 91 (15 2015)

[7] F. Fröwis et al. PRA 81 (6 2010)

[8] G. Ehlers et al. PRB 92 (23 2015)

Problem Setting

- DMRG requires Matrix Product Operator (MPO) rep

$$\hat{H} = \sum_{\boldsymbol{\sigma\tau}} W_1^{\sigma_1\tau_1} \cdot W_2^{\sigma_2\tau_2} \cdots W_L^{\sigma_L\tau_L} |\boldsymbol{\tau}\rangle\langle\boldsymbol{\sigma}| \quad (1)$$

- Generalised DMRG (e.g. on binary tree tensor networks) requires Tensor Product Operator (TPO) rep of $\hat{H}$
- Construction of these reps with smallest possible matrices $W_i^{\sigma_i\tau_i}$ by hand is hard
- Many algorithmic approaches cannot construct generic operators
- Many algorithmic approaches get extremely complicated quickly

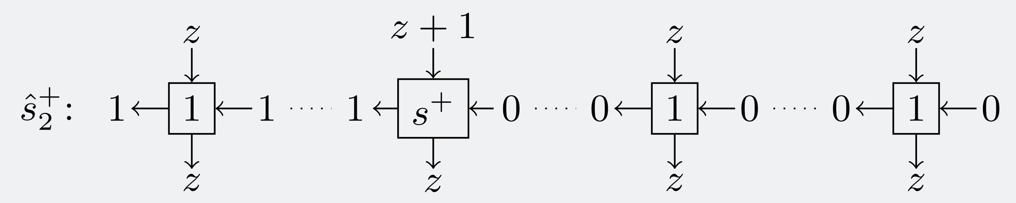
Generic Construction Method

Overview

- Define single-site TPOs by hand (easy)
- Implement addition, multiplication and scalar products of TPOs
- Use *compression* (similar to MPS compression with SVD) to achieve most efficient TPO rep
- With operator overloading in OOP, construction similar to usual formulaic expressions

Single-Site Operators

- MPO rep of e.g. $\hat{s}^z_i$ straightforward:
  - $k < i$: $W_k = \mathbf{1}_d$
  - $k = i$: $W_k = s^z$
  - $k > i$: $W_k = \mathbf{1}_d$
- If quantum numbers are used, left- and right identities may have to be different (labels are S^z quantum numbers):



Arithmetic Operations

- Addition of two TPOs increases bond dimension to the sum of the input bond dimensions
- Multiplication of two TPOs increases bond dimension to product of input bond dimensions
- Compression necessary to reduce bond dimension again and achieve optimal representation

Compression Methods

Deparallelisation (DPL)

- Attempts to find parallel rows/columns in W_i
- Often reproduces analytical form
- Works for simple MPOs, results in efficient reps for complicated MPOs

Rescaled SVD

- Like SVD for MPS, but rescales S (MPO not normalised to 1)
- Always results in optimal representation
- Sparse structure of many MPOs lost
- Discards exponentially small contributions (e.g. $\hat{1} + \hat{P}_{|\uparrow\ldots\uparrow\rangle} \approx \hat{1}$)
- Works well for most Hamiltonians

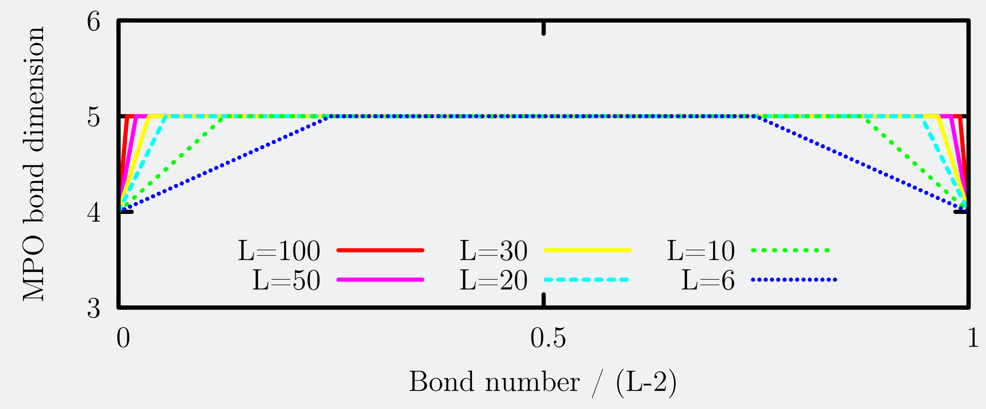
Delinearisation (DLN)

- More powerful variant of Deparallelisation
- Expresses rows and columns as sums of previously-kept rows and columns
- Usually results in optimal representation
- Keeps even exponentially small terms
- Keeps sparse structure of MPO

Example Constructions

Nearest-Neighbour Heisenberg Chain

- $S = {}^1/_2$-chain, $\hat{H} = \sum_{i=1}^{L-1} \hat{S}^i \cdot \hat{S}^{i+1}$
- Sum of scalar products of single-site operators
- Deparallelisation reproduces analytical result and optimal, constant bond dimension:

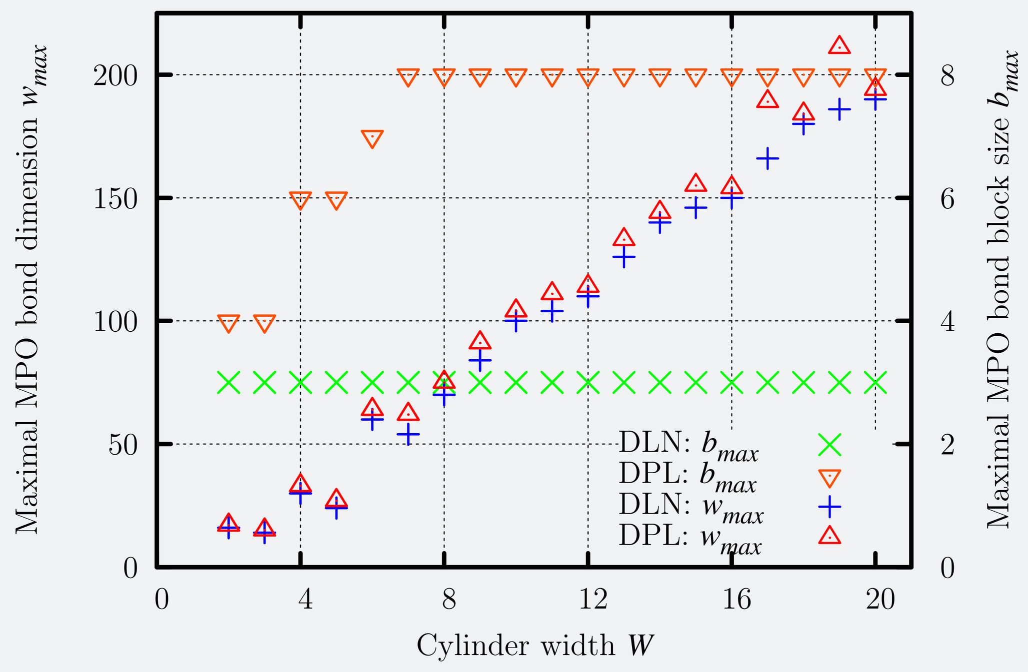


- Small powers of $\hat{H}$ can be constructed (bond dimensions and sparsity for DLN):

$\hat{H}^n$	1	2	3	4	5	6
SVD:	5	9	16	32	51	64
DLN:	5	9	16	32	51	81
DLN:	81%	84%	82%	89%	88%	88%
Fit:[7]	5	9	16	32	51	79

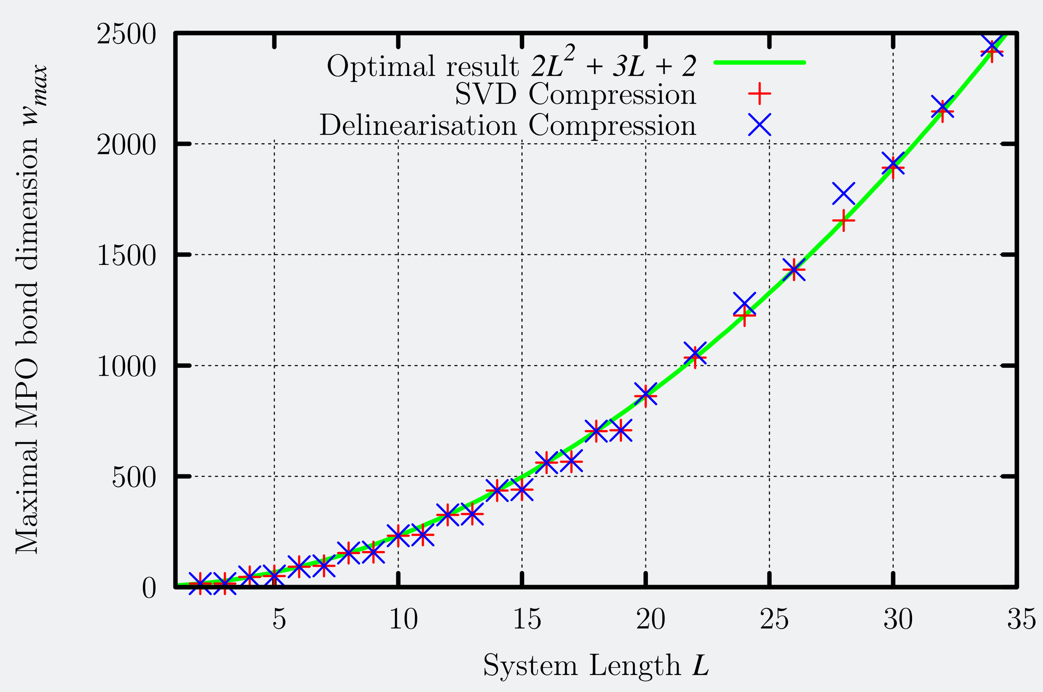
2-D Fermi-Hubbard in Hybrid Space

- Fourier Transformation from real to momentum space along rotational cylinder axis
- Very complicated interactions after mapping of 2-D cylindrical lattice to 1-D MPS chain
- Construction by hand impossible, using Finite State Machines[8] very complicated
- DLN, SVD give same result, DPL suboptimal



Proof of Principle: Full QC Hamiltonian

- $\hat{H} = V_{ijkl} \sum_{\sigma\tau=\uparrow\downarrow} \sum_{ijkl}^{L} \hat{c}^\dagger_{i\sigma} \hat{c}^\dagger_{k\tau} \hat{c}_{l\tau} \hat{c}_{j\sigma}$
- Construction very costly, $O(L^6)$ time at least, possible up to $L \approx 30$.
- SVD still optimal, DPL nearly optimal



Outlook

- Method allows construction of any operator, both as MPO and TPO
- Very flexible, new interactions or terms no challenge after initial implementation
- Underlying implementation can handle arbitrary-rank tensors & symmetries
- Extension to true 2-D tensor networks (PEPS, MERA etc.) possible
- Very useful for DMET and DMFT solvers, need algorithmic construction of TPOs
- Improvement of compression methods still possible: always-optimal and sparsity-preserving?