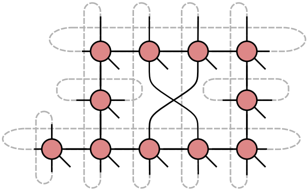
Tensor Networks, Fundamental Theorems, and Computional Complexity

Michael Walter (Uni Bochum)



ICMAT, March 2023

joint work with Arturo Acuaviva, Visu Makam, Harold Nieuwboer, David Pérez-García, Friedrich Sittner, Freek Witteveen (QIP 2013, arXiv:2209.14358)

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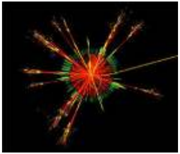
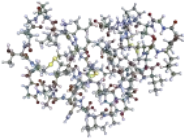
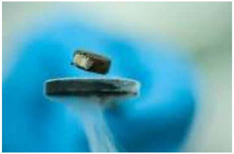
CASA
CYBER SECURITY IN THE AGE OF LARGE-SCALE ADVERSARIES

Complexity of many-body quantum physics


Many-body quantum states have exponentially large description:

$$|\Psi\rangle = \sum_{i_1,\ldots,i_n} \Psi_{i_1,\ldots,i_n} |i_1,\ldots,i_n\rangle$$

In practice, entanglement local $\rightsquigarrow$ compact description:

Start with local entangled pairs...

...and "glue" by applying local transformations:

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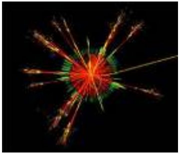
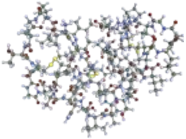
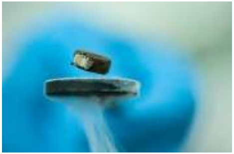


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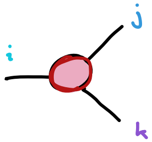
. . . and "glue" by applying local transformations:

What is a tensor network?

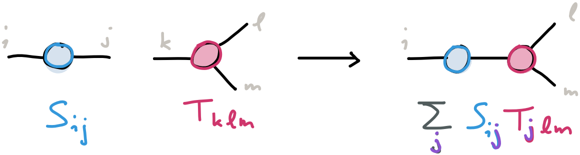
Given a tensor

$$T = \sum_{i,j,k} T_{ijk} \left|i\right\rangle \left|j\right\rangle \left|k\right\rangle$$

we represent it graphically as



Contraction of tensors is shown graphically as



The tensor network tool box

Tensor network: define many-body state by contracting "local" tensors

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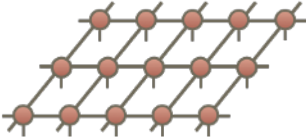
e.g.

MPS [White, Fannes-Nachtergaele-Werner, ...]



PEPS [Verstraete-Cirac]

Numerical tool on classical and quantum computers

Analytical tool that provides "dual descriptions" of complex phenomena: symmetries, topological phases, renormalization, ...

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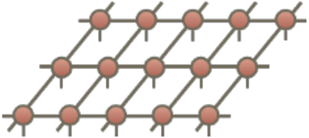

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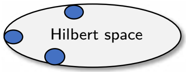

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Innocent or not? First examples

- Long-range entanglement: If  $= |000\rangle + |111\rangle$ then

 $= |00\cdots00\rangle + |11\cdots11\rangle$

- Quantum cellular automata:

Unitary, but *not* a quantum circuit!

- An example from TCS: $= \sum_{i,j,k} A_{ij} B_{jk} C_{ki} = \mathrm{tr}(ABC)$

and hence is the matrix multiplication tensor.

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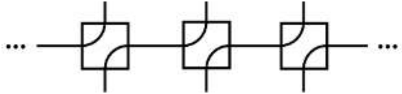

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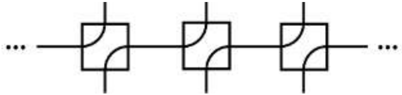

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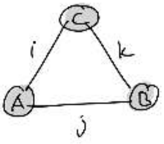
- An example from TCS: 

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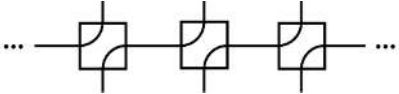

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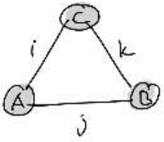
- An example from TCS: 

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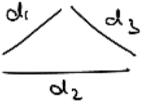
and hence 

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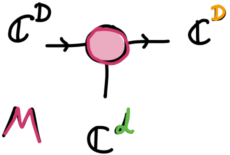
1D: Matrix product states (MPS)

Consider 3-leg tensor M with bond dimension D and physical dimension d:



This determines a quantum state on any n sites:

Its coefficients are $\langle i_1, \ldots, i_n | M_n \rangle = \mathrm{tr}(M^{(i_1)} M^{(i_2)} \cdots M^{(i_n)})$, hence the name.

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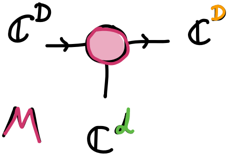

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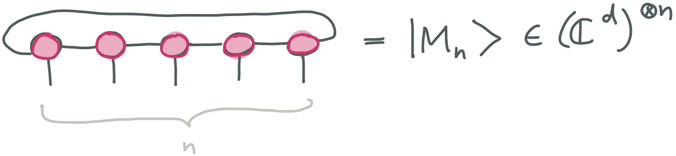

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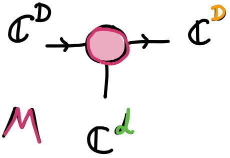

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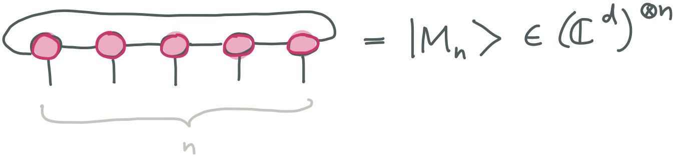

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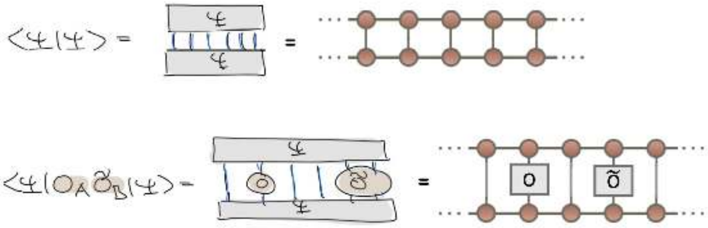
Computing with tensor networks

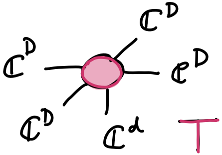
Essentially all computations amount to tensor contractions:



Computational complexity: Easy in 1D. In principle, hard in 2D and higher.

2D: Projected entangled pair states (PEPS)

Consider 5-leg tensor T with bond dimension D and physical dimension d:



This determines a quantum state on any $n \times m$ sites:

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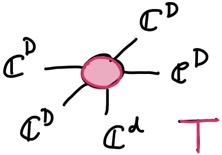

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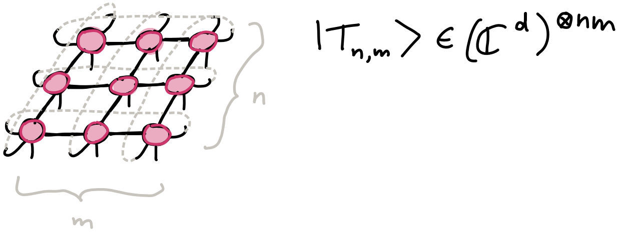
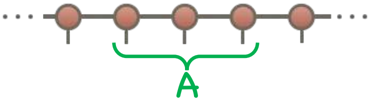
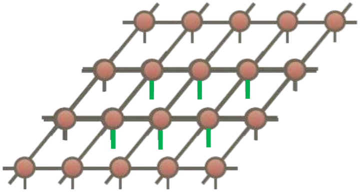


Geometry vs. entanglement

$S(A) = -\operatorname{tr} \rho_A \log \rho_A$





Area law: $S(A) \leqslant |\partial A| \log D.$

- Any tensor network satisfies an area law, determined by its geometry.
- In 1D, low-energy states of local gapped quantum systems satisfy *area law* and have accurate MPS representations [Hastings].
- These can be found in polynomial time [Landau-Vazirani-Vidick, Arad et al].
- In 2D and higher conjecture, many examples, proof only in special cases [Anshu-Arad-Gosset, ...]

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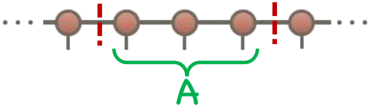

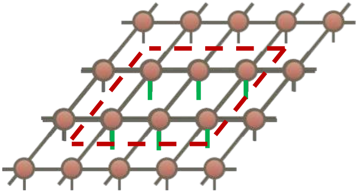

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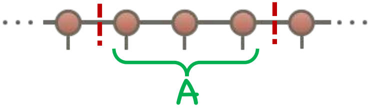

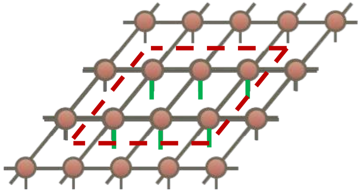

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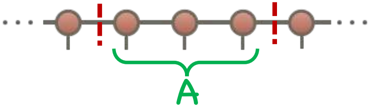

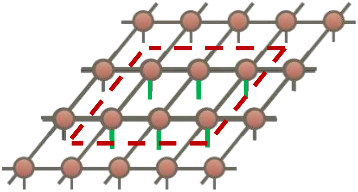

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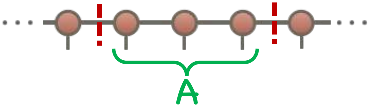

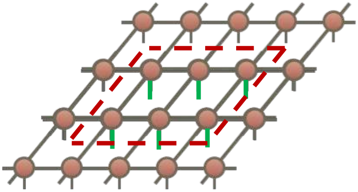

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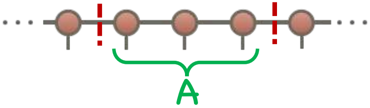

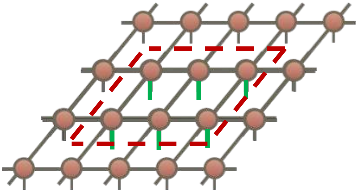

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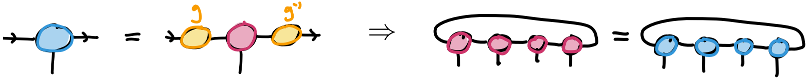
Fundamental theorems

A fundamental question

Given two tensors, when do they generate the *same* tensor network state?

Easy to find such situations! MPS:



PEPS:

$\Rightarrow$

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Moreover, can take limits of such symmetries...

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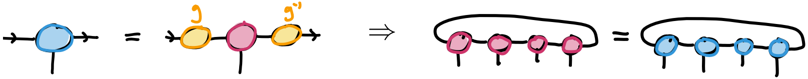

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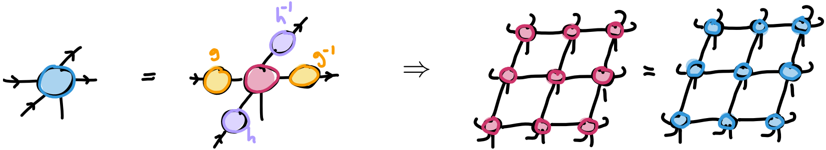

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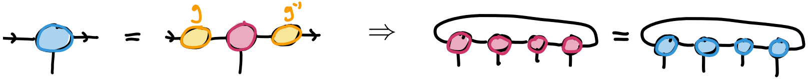

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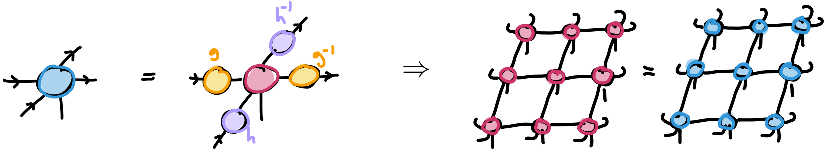

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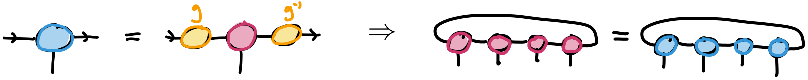

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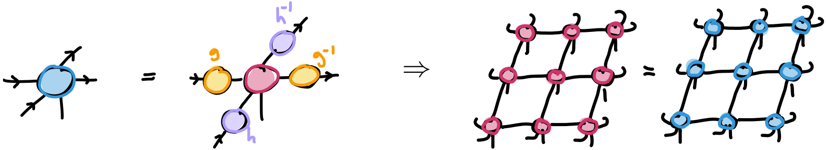

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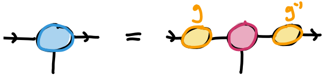
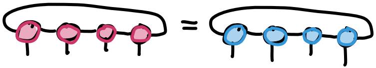
Fundamental theorem for MPS



vs.



In 1D, gauge symmetry and taking limits is the only redundancy. We can efficiently pick canonical form. It is unique up to *unitaries* & satisfies:

Fundamental Theorem of MPS (Cirac–PG–Schuch, de las Cuevas)

Two tensors M and N give rise to the same quantum states $|M_n\rangle = |N_n\rangle$ for all system sizes n if and only if they have same canonical forms.

Many applications!

- Classification of symmetries and topological phases
- Classification of quantum cellular automata
- Better-behaved numerics

No such result known in higher dimensions (before our work)!

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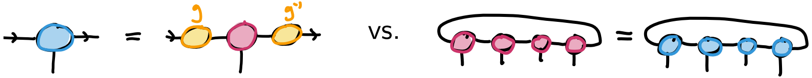

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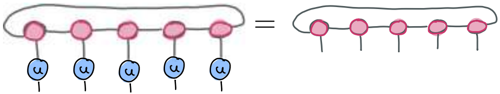
- Classification of quantum cellular automata
- Better-behaved numerics

No such result known in higher dimensions (before our work)!

Illustration: Classification of symmetries

Suppose M is tensor with global (on-site) symmetry for any system size n:

$$u^{\otimes n} |M_n\rangle = |M_n\rangle$$



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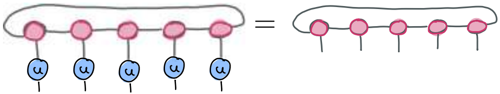

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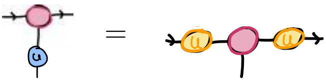

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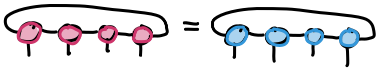
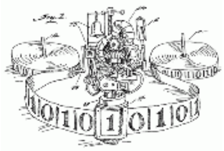
Computational complexity



In particular, "$|M_n\rangle = |N_n\rangle$ for all n?" can be decided in polynomial time.



Bad news: For PEPS, "$|T_{m,n}\rangle = |S_{m,n}\rangle$ for all m, n?" is undecidable!

Suggests in 2D and higher, *no* useful fundamental theorem should exist.
However, this is not so – need to change the perspective...

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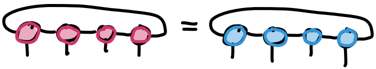

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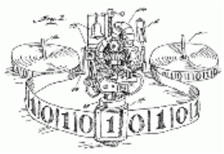

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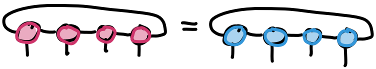

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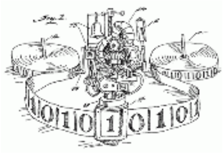

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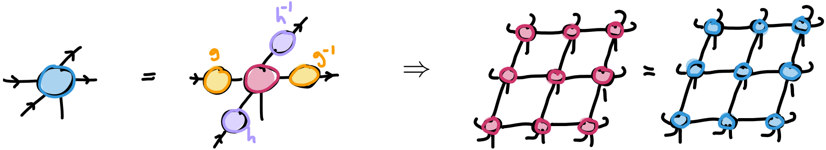
Gauge symmetry in higher dimension

When two PEPS tensors are related by gauge symmetry, they determine not only the same state on square grids. . .



Intuition: There are many inequivalent surfaces in 2D!

Summary of results: *If one allows for arbitrary graphs*, gauge symmetry and taking limits is the only redundancy. Can again find canonical form that satisfies all the same properties as before! *Let's see how this works. . .*

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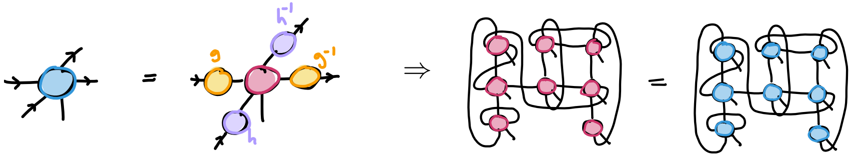

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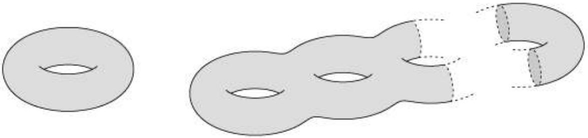

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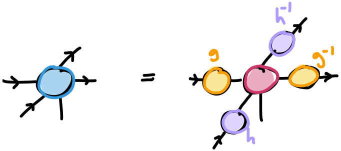

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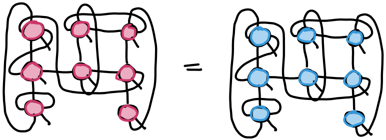

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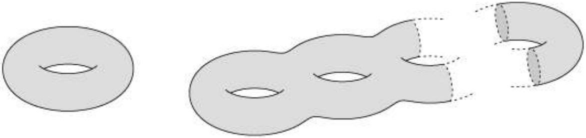

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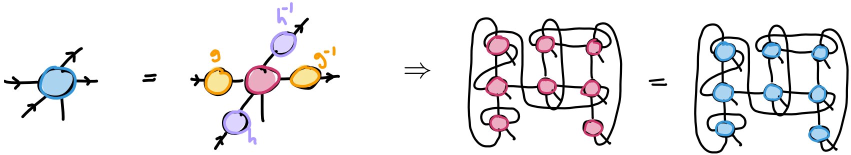

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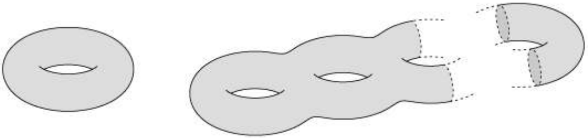

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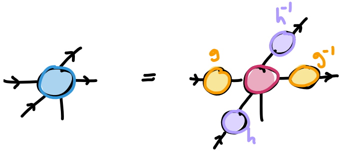
Our proposal: The minimal canonical form

Group action of $G = \mathrm{GL}(D) \times \mathrm{GL}(D)$:



$S = (g, h) \cdot T$

Define minimal canonical form of PEPS tensor T by minimizing ℓ^2-norm:

$$T_{\min} := \operatorname{argmin} \{\|S\|_2 : S \in \overline{G \cdot T}\}.$$

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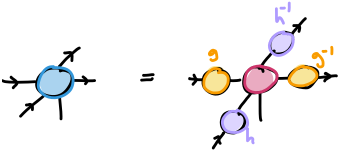

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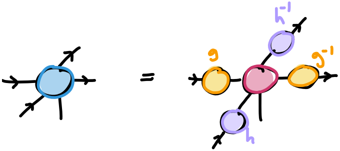

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We say T, T' are gauge equivalent if $\overline{G \cdot T}$ and $\overline{G \cdot T'}$ intersect. This implies that they give the same many-body states!

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1. The minimal canonical form exists and is unique up to $U(D) \times U(D)$.
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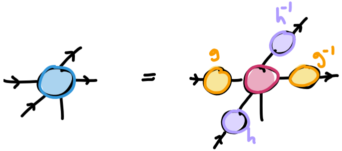

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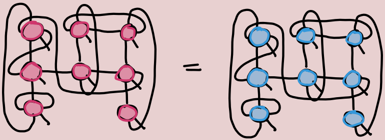
When are two tensors gauge equivalent?

Fundamental Theorem of PEPS

Two tensors T and T' give rise to the same tensor network state on any admissible graph Γ



if and only if they are gauge equivalent, so if and only if they have the same minimal canonical forms.

- In fact, $e^{O(D^2)}$ vertices suffice to distinguish two PEPS tensors, and $e^{\Omega(D)}$ vertices are necessary. For MPS, we note $\widetilde{O}(D)$ vertices suffice.

Decidability

In particular, "$|T_\Gamma\rangle = |T'_\Gamma\rangle$ for all graphs Γ?" is decidable. ☺

Intuition: Undecidability for $|T_{n,m}\rangle$ reduces to periodic tiling problem.
Its undecidability in turn relies on existence of aperiodic tile sets such as:

There exist $T \neq 0$ such that all $|T_{n,m}\rangle = 0$, but no algorithm can recognize them! [Scarpa et al]

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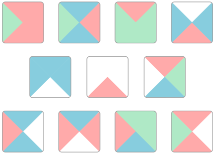

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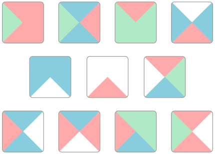

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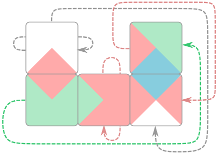
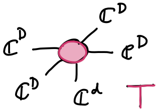
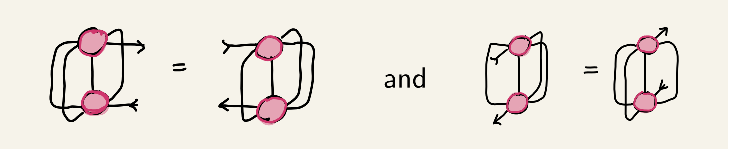


How to characterize the canonical form?

We show that a tensor T



is in minimal canonical form if and only if



This means the state $\rho = |T\rangle\langle T|$ satisfies $\rho_{\text{right}} = \overline{\rho_{\text{left}}}$ & $\rho_{\text{bottom}} = \overline{\rho_{\text{top}}}$.
Physical interpretation?

Why does it work? Geometric invariant theory (GIT)

A field of mathematics that studies equivalence for "nice" actions of group G on vector space V. In our case:

$$G = \mathrm{GL}(D) \quad \text{and} \quad V = \text{MPS tensors of fixed format,}$$
$$G = \mathrm{GL}(D) \times \mathrm{GL}(D) \quad \text{and} \quad V = \text{PEPS tensors of fixed format.}$$

Notion of equivalence: $\overline{G \cdot v}$ and $\overline{G \cdot v'}$ intersect. ☺ GIT tells us:

- Minimum norm vectors unique up to unitaries. [Kempf-Ness]
- Equivalent iff $P(v) = P(v')$ for all G-invariant polynomials P. [Mumford]

What are the invariant polynomials in our case? Quantum states!

$P(M) = \langle i_1, \ldots, i_n | M_n \rangle$ for $n = \widetilde{O}(D)$.
New perspective gives stronger results!

[Procesi-Razmyslov-Formanek, Derksen-Makam]

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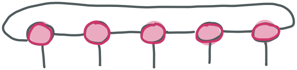

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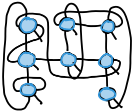

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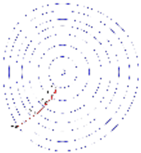
Algorithms for the minimal canonical form

Given a tensor T, how to compute $T_{\min}$? Nontrivial, even for MPS!



Result (Algorithms)

For fixed bond dimension D, can approximate $T_{\min}$ in polynomial time.

Combines computer science ideas from the solution of *Paulsen's problem* with recent results on optimization on groups *(operator, tensor scaling)*.

Key idea: $g \mapsto \|g \cdot v\|$ is convex along geodesics of curved space arising from noncommutative group. Accordingly, local algorithms can find canonical form. Versatile framework, many applications. [Bürgisser-...-W-Wigderson]

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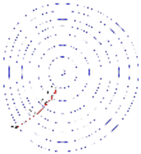

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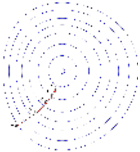 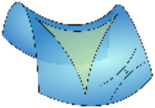

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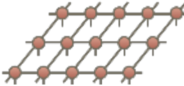
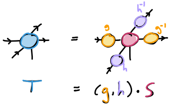
Summary and outlook

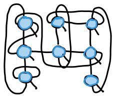
Tensor networks describe high-dimensional data succinctly.
Applications from physics to numerics to computer science.



Fundamental theorems and canonical forms are key tools.
We propose first rigorous general such tools beyond 1D.



To achieve this, we connect tensor networks to powerful tools from geometric invariant theory and recent progress on optimization algorithms in theoretical computer science.



Many exciting open questions: Faster algorithms for large bond dimension? Flexible framework – how about other tensor networks? Connection to topological order? Impact on numerics? **Thank you for your attention!**