Tensor Networks, Fundamental Theorems, and Computational Complexity

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joint work with Arturo Acuaviva, Visu Makam, Harold Nieuwboer, David Pérez-García, Friedrich Sittner, Freek Witteveen (QIP 2023, arXiv:2209.14358)
Complexity of many-body quantum physics

Many-body quantum states have \textit{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 \textit{local} \xrightarrow{\sim} \textit{compact} description:

Start with local \textit{entangled} pairs...

...and "glue" by applying local transformations:
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In practice, entanglement \textit{local} \( \sim \) compact description:

Start with local \textit{entangled} pairs...

\[ \cdots \]

\[ \cdots \text{and "glue" by applying local transformations:} \cdots \]
What is a tensor network?

Given a tensor

\[ T = \sum_{i,j,k} T_{ijk} |i\rangle |j\rangle |k\rangle \]

we represent it graphically as

Contraction of tensors is shown graphically as

\[ \sum_{j} S_{ij} T_{jklm} \]
The tensor network tool box

**Tensor network:** define many-body state by contracting “local” tensors

\[
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\]

e.g.

\[\cdots \cdots \cdots \]

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

\[\cdots \cdots \cdots \]

**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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Innocent or not? First examples

- **Long-range entanglement:** If \( |000\rangle + |111\rangle \) then

\[
\ldots \quad \ldots = |00 \cdots 00\rangle + |11 \cdots 11\rangle
\]

- **Quantum cellular automata:**

Unitary, but *not* a quantum circuit!

- **An example from TCS:**

\[
\sum_{i,j,k} A_{ij} B_{jk} C_{ki} = \text{tr}(ABC)
\]

and hence is the matrix multiplication tensor.
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\[
\begin{tikzpicture}
\end{tikzpicture}
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and hence \( \alpha_1 \otimes \alpha_2 \) is the matrix multiplication tensor.
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 $\langle i_1, \ldots, i_n | M_n \rangle = \text{tr}(M^{(i_1)} M^{(i_2)} \cdots M^{(i_n)})$, hence the name.
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$$C^D \rightarrow C^D$$

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Computing with tensor networks

Essentially all computations amount to tensor contractions:

\[
\langle \psi | \psi \rangle = \begin{array}{c}
\text{vector}
\end{array} = \begin{array}{c}
\text{matrix}
\end{array}
\]

\[
\langle \psi | 0 \delta | \psi \rangle = \begin{array}{c}
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\]

**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:
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:

$$|T_{n,m} \rangle \in (\mathbb{C}^d)^{\otimes nm}$$
Geometry vs. entanglement

\[ S(A) = - \text{tr} \rho_A \log \rho_A \]

Area law: \[ S(A) \leq |\partial A| \log D. \]

- 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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Fundamental theorems
A fundamental question

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

Easy to find such situations! MPS:

![Diagram of MPS tensors](image)

PEPS:

![Diagram of PEPS tensors](image)

These gauge symmetries preserve the quantum state for any system size! Moreover, can take limits of such symmetries...
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\text{\begin{tikzpicture}
\node[cloud,fill=blue!30] (a) at (0,0) {};
\node[cloud,fill=orange!30] (b) at (1,0) {};
\node[cloud,fill=lightgray!30] (c) at (2,0) {};
\end{tikzpicture}}
\quad =
\quad \begin{tikzpicture}
\node[cloud,fill=blue!30] (a) at (0,0) {};
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These gauge symmetries preserve the quantum state for any system size! Moreover, can take limits of such symmetries...
Fundamental theorem for MPS

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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Illustration: Classification of symmetries

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

$$u^\otimes n \ket{M_n} = \ket{M_n}$$

Fundamental theorem implies that there is unitary $U$ such that

In this way, classification of SPT phases $\rightsquigarrow$ classification of projective representations. [Chen-Gu-Wen, Schuch-Perez-Garcia-Cirac, Pollman et al].
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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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Gauge symmetry in higher dimension

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

\[ \Rightarrow \]

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...
Gauge symmetry in higher dimension

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

\[ \implies \]

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Our proposal: The minimal canonical form

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

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

Define minimal canonical form of PEPS tensor $T$ by minimizing $\ell^2$-norm:

$$T_{\text{min}} := \arg\min \left\{ \|S\|_2 : S \in G \cdot T \right\}.$$

- Closure is needed so that minimum is attained, but also natural since taking limits is allowed.
- First rigorous canonical form in 2D (+ similarly works in higher dim)!
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Define **minimal canonical form** of PEPS tensor $T$ by minimizing $\ell^2$-norm:

$$T_{\text{min}} := \arg\min \{ \|S\|_2 : S \in \overline{G \cdot T} \}.$$
What does it characterize?

Recall the group action of $G = \text{GL}(D) \times \text{GL}(D)$:

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

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!

Result (Canonical form)

1. The minimal canonical form exists and is unique up to $U(D) \times U(D)$.
2. Two tensors have the same minimal canonical forms if and only if they are gauge equivalent.
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Result (Canonical form)

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2. Two tensors have the same minimal canonical forms if and only if they are gauge equivalent.
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 $\Gamma$ 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 $\tilde{O}(D)$ vertices suffice.
Decidability

In particular, “$|\Gamma\rangle = |\Gamma'\rangle$ for all graphs $\Gamma$?” 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]

However, if allow arbitrary graphs (topologies) this distinction collapses!
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![Tile Set Example]

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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

$$\rho = |T\rangle\langle T|$$

satisfies $\rho_{\text{right}} = \overline{\rho_{\text{left}}}$ and $\rho_{\text{bottom}} = \overline{\rho_{\text{top}}}$. 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:

\[
G = \text{GL}(D) \quad \text{and} \quad V = \text{MPS tensors of fixed format},
\]
\[
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Notion of equivalence: $G \cdot v$ and $G \cdot v'$ 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!

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

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P(T) = \langle i_1, \ldots, i_n | T_\Gamma \rangle \text{ for arbitrary graphs } \Gamma.
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[Procesi-Razmyslov-Formanek, Derksen-Makam]
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[Pčesi-Razmyslov-Formanek, Derksen-Makam]  

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New perspective gives **stronger results**!

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$$P(T) = \langle i_1, \ldots, i_n | T_\Gamma \rangle \text{ for arbitrary graphs } \Gamma$$
Algorithms for the minimal canonical form

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

Result (Algorithms)

For fixed bond dimension $D$, can approximate $T_{\text{min}}$ 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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For fixed bond dimension $D$, can approximate $T_{\text{min}}$ 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]
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!**