Projected Entangled Pair States (PEPS)

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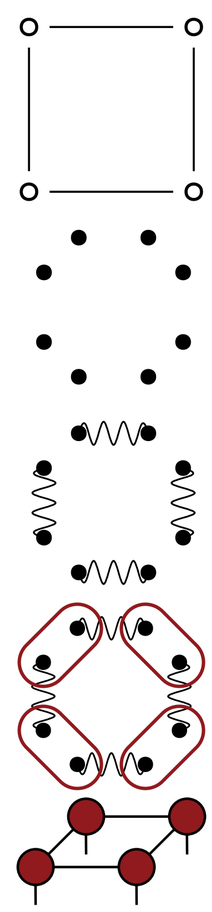
I. Definition

Projected Entangled Pair States (PEPS) are a class of tensor network states that efficiently parametrise quantum states with finite entanglement. They are a generalization of (1D) Matrix Product States (MPS) to arbitrary dimension.



- Given a physical sytem composed of local sites with site-Hilbertspaces $\mathcal{H}_i \equiv \mathbb{C}^{d_i}$ situated on a graph with edges $E = \{e_{i,j}\}$ and vertices $V = \{v_i\}$.
- For each vertex v_i, and for each edge $e_{i,j}$ connected to v_i (and v_j), associate an ancilla degree of freedom $a_{i,j} \in \mathcal{H}_{i,j} \equiv \mathbb{C}^{d_{i,j}}$.
- Maximally entangle ancillae $a_{i,j}$ and $a_{j,i}$ associated with each edge $e_{i,j}$:

$$|\Phi_{i,j}) = \sum_{l=1}^{d_{i,j}} |l\rangle \otimes |l\rangle \tag{1}$$

- Apply a linear map $\mathcal{P}_i : \bigotimes_{j_i} \mathcal{H}_{a_{i,j}} \to \mathcal{H}_i$ to the ancillae of site i, to obtain the projected entangled pair states (PEPS) $|\Psi\rangle = \bigotimes_{e\in E} \mathcal{P}_e \, |\Phi_e)$.
- The final PEPS is a tensor network state that has the same connectivity as the original graph and that lives in the total Hilbert space $\mathcal{H} = \bigotimes_i \mathcal{H}_i$.

[Cirac et. al. 2021]

II. Entanglement Area Law

Entanglement Area Law
The entanglement entropy of a region $\mathcal{A}$ of quantum state with finite (local) entanglement scales as $\partial\mathcal{A}$, the boundary of $\mathcal{A}$.

$$S_\mathcal{A} \sim \partial\mathcal{A} \tag{2}$$

This is in constrast with the volume law most states follow.
Given the Schmidt decomposition of a state $|\Psi\rangle$ across a bipartition of the system into the "In" system $\mathcal{A}$ and the "Out" system $\mathcal{B}$ (where $\sum_i \lambda_i^2 = 1$):

$$|\Psi\rangle = \sum_i \lambda_i \, |I_i\rangle \otimes |O_i\rangle \tag{3}$$

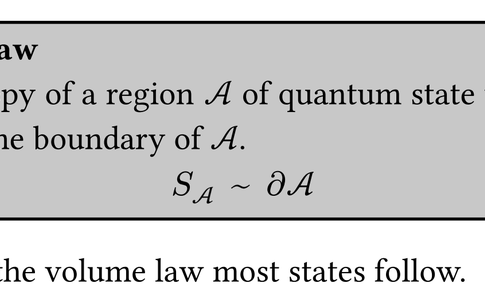
The entanglement entropy of the region $\mathcal{A}$ is given by:

$$S_\mathcal{A} = -\sum_i \lambda_i^2 \log(\lambda_i^2) \tag{4}$$

The maximal value this can take is when all the $\lambda_i = \frac{1}{N_S}$, with N_S the Schmidt rank. For finitely entangled systems, $S_\mathcal{A}$ is thus bounded by the finite Schmidt rank N_S.

$$S_\mathcal{A} \leq \log(N_S) \tag{5}$$

It turns out that PEPS satisfy an **area law** for their entanglement entropy **by construction**. This property makes PEPS an efficient representation of quantum states with finite (local) entanglement.



The entanglement entropy of the shaded area $\mathcal{A}$ is the sum of the entanglement entropy across the cut virtual bonds, which by construction all have a finite bond dimension (and Schmidt rank) χ.
The entanglement entropy of a single cut is bounded by $\log(\chi)$. The total entanglement entropy of the region $\mathcal{A}$ is thus proportional to the number of cut virtual bonds times $\log(\chi)$.

$$S_\mathcal{A} \sim \log(\chi) \cdot \partial\mathcal{A} \tag{6}$$

III. Parent Hamiltonians

Parent Hamiltonians for PEPS
Every injective PEPS is the unique ground state of a *local*, *frustration free* parent Hamiltonian.

Consider the same shaded region $\mathcal{A}$ as before. The support space $\mathcal{S}_\mathcal{A}$ of the reduced density matrix $\rho_\mathcal{A}$ grows as $\partial\mathcal{A}$ while the Hilbert space $\mathcal{H}_\mathcal{A}$ grows as $\mathcal{A}$.
Therefore we can always find a sufficiently large region such that $\rho_\mathcal{A}$ has a non-trivial kernel $\ker(\rho_\mathcal{A}) = \mathcal{H}_\mathcal{A} \setminus \mathcal{S}_\mathcal{A}$.
It is thus the groundstate of every Hamiltonian h with:

- $h \geq 0$
- $\ker(h) = \mathcal{S}_\mathcal{A}$

since by construction $\mathrm{tr}(\rho_\mathcal{A} h) = 0$.
The Hamiltonian can be extended to the entire lattice by assigning a region $\mathcal{R}_v$ to every vertex v of the lattice and defining

$$H = \sum_v h_v \otimes \mathbb{1} \tag{7}$$

The Hamiltonian is *local* since it is the sum of local terms h_v acting on bounded regions $\mathcal{R}_v$, and it is *frustration free* since every term h_v is minimized by the PEPS.

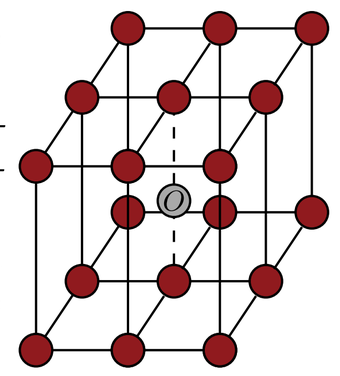
Examples
Many examples exist of the rather formal Parent Hamiltonian theorem. The groundstates of the following Hamiltonians can all be exactly expressed as PEPS.

1. The toric code
2. The 2d AKLT model

[Perez-Garcia et. al. 2007, Orus 2014]

IV. Computational complexity of PEPS contractions

Exact PEPS contraction is #P-Hard
The exact calculation of the scalar product between two PEPS is an exponentially hard problem.



For two arbitrary PEPS of N sites, it will always take a time $\mathcal{O}(\exp(N))$, no matter the contraction order.
Because in general *no canonical forms exist for PEPS*, calculating expecation values efficiently requires an approximate approach.
There exist many strategies for the approximate calculation of the contraction of PEPS which differ for finite and infinite systems.

Finite Systems
Boundary Matrix Product State (MPS) methods are an efficient technique for contracting finite Projected Entangled Pair States (PEPS), transforming the 2D contraction problem into a sequence of 1D contractions.

Infinite Systems
There exist several methods for the contraction of infinite PEPS. These include:

i. Boundary MPS methods
Boundary MPS methods transform the 2D contraction problem into a series of 1D contractions by representing the boundary of the PEPS as a Matrix Product State (MPS). The time complexity typically scales as $\mathcal{O}(\chi^{2N} + \chi^3 L)$, where L is the boundary length. These methods strike a balance between accuracy and computational feasibility, making them suitable for relatively large systems.

ii. Corner Transfer Matrix methods (CTM)
CTM methods approximate the environment tensors using corner and edge transfer matrices. These matrices are iteratively refined, with a typical time complexity of $\mathcal{O}(\chi^{10})$. CTM methods are particularly effective for large systems and are widely used to study critical phenomena.

iii. Tensor Renormalization Group methods (TRG)
Coarse-graining methods, such as Tensor Renormalization Group (TRG), reduce the tensor network size while preserving essential features. These methods involve iterative tensor decompositions and contractions, generally scaling as $\mathcal{O}(\chi^6)$. They are particularly useful for extracting long-range properties in large-scale systems.