PEPS I: Projected entangled-pair state

1. Motivation

Goal: generalize MPS ideas to 2D.

Most obvious idea: 2D-DMRG

[White 1996]
[Stanley-Drummond 2012]
[He 2015] (2D Kagome)
[Zheng 2017] (2D-Hubbard)

Main limitation: not enough entanglement

Entangled pair entropy \( S_{AB} \sim O(\ln^{2} D) \quad D \sim 2^{d} \)

but even here, map \( S_{AB} \sim 1 \)

To build MPS-like generalized theory for 2D:

- reformulate 1D-MPS into 2D projected entangled pairs
- generalize to 2D.

\( \psi_{\text{MPS}} \), with dim \( D \):

\[
|\psi\rangle = \sum_{\sigma} (10^{D}) \delta_{\sigma}^{\chi_{1}} \delta_{\sigma}^{2} \delta_{\sigma}^{3} \delta_{\sigma}^{4}
\]

Reinterpretation:

- introduce auxiliary particles
- combine them into entangled pair
- map auxiliary state onto physical state
\( |\Phi\rangle = \sum_{\alpha, \beta} \frac{1}{\sqrt{2}} \left( |\alpha\rangle |\beta\rangle + |\beta\rangle |\alpha\rangle \right) \)  

\( |\psi\rangle = \prod_i |\psi_i\rangle \)  

\( \hat{\rho}_i = \sum_{\alpha_i, \beta_i} \lambda_{\alpha_i}^* \lambda_{\beta_i} \left( |\alpha_i\rangle \langle\beta_i| \right) \)  

\( (\text{with} \quad \lambda_i = \begin{cases} 1 & \text{if } i = 1 \\ \text{if } i = 2 \\ \end{cases} \)  

\( |\psi\rangle = \sum_{\alpha, \beta} (\alpha_1 \alpha_2 \beta_3 \beta_4) A_{\alpha_1 \beta_1} A_{\alpha_2 \beta_2} A_{\alpha_3 \beta_3} A_{\alpha_4 \beta_4} = \rho_{\psi} \)  

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2D generalization (square lattice)  

\( i = (x, y) \)  

Introduce auxiliary sites:

\( N \) per lattice site, \( W = K \times n \)  

Apply linear map to physical state space:

\( \hat{\rho}_i = \sum_{\alpha, \beta} \frac{1}{\lambda_i} \lambda_i^* \lambda_i \left( |\alpha\rangle \langle\beta| \right) \)  

\( |\psi\rangle = \prod_i |\psi_i\rangle \)  

\( (\text{phys})_{\alpha_i, \beta_i} = \sum_{\mu_i} |\mu_i\rangle \langle\mu_i| \)  

\( \lambda_i = \begin{cases} 1 & \text{if} \; i = 1 \\ \text{if} \; i = 2 \\ \end{cases} \)  

\( |\psi\rangle = \prod_i |\psi_i\rangle \)  

\( \text{parameters:} \quad C(N, D^4) \)
Various graphical representations

[Ours 2014]

\[ |w_D \rangle = \sum_{i=1}^{D} |i\rangle |i\rangle \]

(b) (a) D\_MEG

2D - D\_MEG

PEPS

Tensor Network Notation:

\[
\begin{align*}
\rho_{ij}^{\alpha\beta} &= \sum_{\gamma} \rho_{ij}^{\alpha\beta} \\
\rho_{ij}^{\alpha\beta} &= \sum_{\gamma} \rho_{ij}^{\alpha\beta} 
\end{align*}
\]

[Schuch 2017] Computational complexity of PEPS

- **expectation values** in PEPS (e.g. correlation functions):

  \[ \langle \psi | \hat{O} \hat{O}^{\dagger} | \psi \rangle \]

- resembles 1D situation, but ...

  \[ \begin{array}{c}
  \text{transfer operator}
  \end{array} \]

  \[ \begin{array}{c}
  \text{exact contraction is a hard problem}
  \end{array} \]
  (more precisely, #P-hard)

- **approximation methods** necessary – e.g. by again using MPS
2. Examples of PEPS states: RVB state

Resonating valence bond (RVB) states in square lattice:
[Anderson 1987] [Horsch 1988] (holographic inspired)
RVB: combined interest for spin liquids!
“diagonal”, “valence bond”

\[
\rho (i; j) = \frac{1}{2} (| \uparrow \downarrow \rangle - | \downarrow \uparrow \rangle)
\]

\[
\delta_i = \frac{1}{2} (| \uparrow \rangle \langle \uparrow | - | \downarrow \rangle \langle \downarrow |)
\]

[sign conventions matter!]

|RVB\rangle = (equal superposition of all possible dimer ensembles)

RVB fluctuation lower energy due to
matrix elements connecting different configurations.

 RVB state has a PEPS representation!  [ Verstraete 2004 d]  

Defining properties of RVB state:

1. 1 dimer per vertex

2. 4 possible states for a vertex:

3. Assistance of ancillary sites for physical spin:

Each site in one of the states \( \{ \uparrow \downarrow, \uparrow \uparrow, \downarrow \uparrow \} \)

\(D = 3\) empty

4. Define entangled pairs: \( | E \rangle_{ij} = \frac{1}{2} (| \uparrow \downarrow \rangle - | \downarrow \uparrow \rangle) \) for nearest neighbors

Equal weight superposition.
- Improve constraint: only the antiholing spins in per physical site; identify it with physical spin.

\[
\hat{p}_i = (\mathbb{C} \hat{e}_1 + \mathbb{C} \hat{e}_2 + \mathbb{C} \hat{e}_3 + \mathbb{C} \hat{e}_4) + (\mathbb{C} \hat{e}_1 + \mathbb{C} \hat{e}_2 + \mathbb{C} \hat{e}_3 + \mathbb{C} \hat{e}_4)
\]

\[
|RVB\rangle = \prod_j \hat{p}_j \prod_j |E_j\rangle
\]

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**Advantages of PEPS description of RVB state**

(a) dimer basis is not orthogonal: \( \langle \hat{E}|0\rangle \to 0 \)

PEPS formulation is easier to work with

(b) PEPS description can be generalized to include larger-range dimer bonds.

(c) "parent Hamiltonian" can be constructed systematically:

Preprocessing: 19x19 interactions: \([\text{Scherer 2012}]\)

[2x2m 2019]
3. **Example of 1RS state: Kitaev’s Toric Code**

[Kitaev 2003], [Kitaev 2009]

Simplist known model whose ground state displays topological order.

- Square lattice (a 2D plane, or torus)
- Spin $\sigma$ in each edge

$$H = - \sum_s A_s - \sum_p B_p$$

- $A_s = \prod_{i \in \text{stars}} \sigma_i^z$
- $B_p = \prod_{j \in \text{plaq}} \sigma_j^x$

[note: Kitaev 2009: $\sigma_x^x = \sigma^z$].

All terms in Hamiltonian commute easy to check: $[A_s, B_p]$ for all $s, p$.

Because all stars and plaquettes share an even # of edges ($0, 2$).

Minor sign from $6x \cdot 5z = -6z \cdot 6x \Rightarrow (-1)^0 = (-1)^2 = 1$

$\Rightarrow$ All terms in $H$ commute $\Rightarrow H$ should be exactly solvable.

Adapt