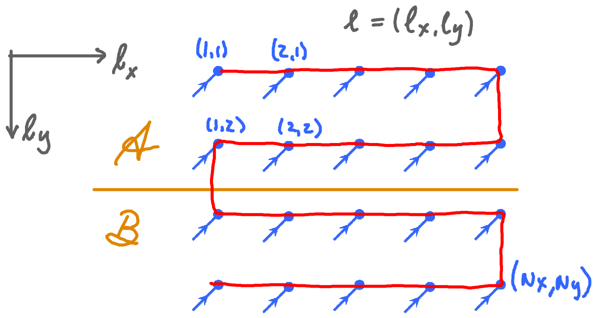
PEPS 1: Projected Entangled Pair States (Verstraete, Cirac, 2004)

PEPS-I.1

1. Motivation & Definition of PEPS



Goal: generalize MPS ideas to 2 dimension!

Most obvious idea: 2D-DMRG, using a 'snake-MPS':

[White1996] (2D Heisenberg, nn & nnn interactions)

[Stoudenmire2012] (brief review)

[He2016] (2D Kagome)

[Zheng2017] (recent high-end application: striped order in 2D Hubbard model)

2D-DMRG is one of the most powerful/accurate methods for studying 2D quantum lattice models.

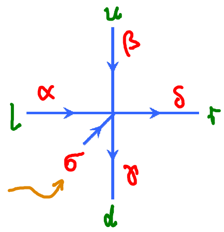
Main limitation: not enough entanglement: entanglement entropy $S^{MPS}_{\mathcal{AB}} \sim \mathcal{O}(\ln_2 D)$

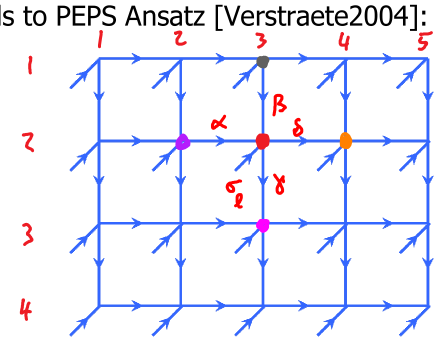
but according to area law, we need $S_{\mathcal{AB}} \sim L \quad \Rightarrow \quad D \sim 2^L$

Reason for insufficiency: entanglement between $\mathcal{A}$ and $\mathcal{B}$ is encoded in a single bond.

Natural generalization: add more bonds between rows! This leads to PEPS Ansatz [Verstraete2004]:

Introduce 5-leg tensor for every site: $A^{\alpha\beta\sigma_\ell}_{[\ell]\,\gamma\delta}$ with $\alpha \leftrightarrow l$, $\beta \leftrightarrow u$, $\gamma \leftrightarrow d$, $\delta \leftrightarrow r$, $\ell = (\ell_x, \ell_y)$





Sum over all virtual bonds linking neighboring sites:

$$\underset{\text{PEPS}}{|\psi\rangle} = \sum_{\vec{\sigma}_\ell} |\vec{\sigma}_\ell\rangle \prod_\ell A^{\cdot\cdot\,\sigma_\ell}_{[\ell]\,\cdot\cdot} \qquad (1)$$

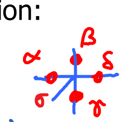
physical basis: $|\vec{\sigma}_\ell\rangle \equiv |\sigma_{N_xN_y}\rangle \otimes \dots |\sigma_{21}\rangle \otimes |\sigma_{11}\rangle$

contraction pattern: $A^{\cdots}_{[\ell_x-1,\ell_y]\cdot\alpha} \; A^{\cdots}_{[\ell_x,\ell_y-1]\beta\cdot} \; A^{\alpha\beta\sigma_{\ell\ell'}}_{[\ell_x,\ell_y]\,\gamma\delta} \; A^{\cdot\gamma\cdot}_{[\ell_x,\ell_y+1]} \; A^{\delta\cdot\cdot}_{[\ell_x+1,\ell_y]\cdot\cdot}$ (2)

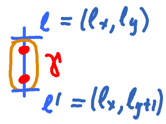
Variationally minimize $\langle\psi|\hat{H}|\psi\rangle$. # of variational parameters: $\mathcal{O}(d D^4 N_x N_y)$

Why the name 'PEPS'? Verstraete & Cirac envisioned generalization of AKLT construction:

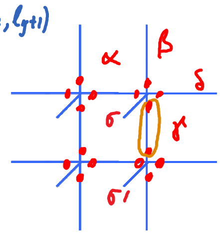
Associate 4 'auxiliary particles' with each site: $|\alpha\beta\gamma\delta\rangle_\ell = |\alpha\rangle^l_\ell |\beta\rangle^u_\ell |\gamma\rangle^d_\ell |\delta\rangle^r_\ell$ (3)



Construct entangled pairs along bonds: $|EP\rangle_{\ell\ell'} \overset{\text{e.g.}}{=} \sum_\gamma^D |\gamma\rangle^d_\ell |\gamma\rangle^u_{\ell'}$ (4)



Define projectors on each site: $\hat{P}_\ell = |\sigma\rangle_\ell A^{\sigma_\ell}_{[\ell]\bar\alpha\bar\beta\bar\gamma\bar\delta} \langle\bar\alpha\bar\beta\bar\gamma\bar\delta|$ (5)



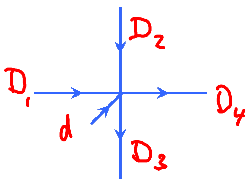
Then $|\psi\rangle = \prod_{\otimes\ell} \hat{P}_\ell \prod_{\otimes\langle\ell,\ell'\rangle} |EP\rangle_{\ell,\ell'}$

$$|\sigma\rangle_\ell |\sigma'\rangle_{\ell'} A^{\sigma}_{[\ell]\bar\alpha\bar\beta\underset{\gamma}{\bar\gamma}\bar\delta} A^{\sigma'}_{[\ell']\bar\alpha'\underset{u}{\bar\beta'}\bar\gamma'\bar\delta'} \langle\underset{l}{\bar\alpha}\underset{u}{\bar\beta}\underset{d}{\bar\gamma}\underset{r}{\bar\delta}| \langle\underset{l}{\bar\alpha'}\underset{u}{\bar\beta'}\underset{d}{\bar\gamma'}\underset{r}{\bar\delta'}| \sum_\gamma |\gamma\rangle^d_\ell |\gamma\rangle^u_{\ell'}$$

generates a γ-contraction between two A-tensors

General remarks: [Orus2014, Sec. 5.2]

- PEPS are dense: any 2D state can be written as a PEPS, though possibly with exponentially large D



If no truncations are performed:

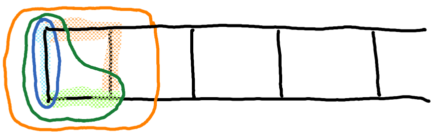
$$\Rightarrow \underbrace{d D_1 D_2}_{\text{in-dimension}} = \underbrace{D_3 D_4}_{\text{out-dimension}} \Rightarrow \underbrace{D_{\ell\ell'} \sim \sqrt{d}^{\,\ell_x+\ell_y}}_{\text{out-dimension grows exponentially}} \qquad (6)$$

- Entanglement entropy between subsystems A, B is $S_{AB} \sim \mathcal{O}(\underbrace{N_x}_{\text{number of bonds between A and B}} \underbrace{\ln_2 D}_{\text{maximal entanglement per bond}})$ $\Longrightarrow$ 2D area law is satisfied $S_{AB} \sim N_x$
- PEPS can handle polynomially-decaying correlations (in contrast to 1D MPS)
- Exact contraction is #P hard, $\Rightarrow$ contraction time $\sim \mathcal{O}(e^{N_x N_y})$

  #P-hard class of problems = count number of solutions of NP-complete problems
  NP-complete class = problems that cannot be solved in polynomial time
  'non-deterministic polynomial'

Why are exact contractions hard? Recall 1D situation:

Cheap contraction pattern:



# of open indices remains constant ($\lesssim 3$)

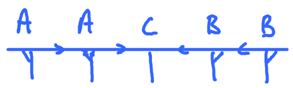
cost: $\left.\begin{array}{l} \mathcal{O}(d \cdot D^2) \\ \mathcal{O}(D \cdot D^2 d) \\ \mathcal{O}(Dd \cdot D^2 d) \end{array}\right\} \sim \mathcal{O}(d D^3)$

Expensive contraction pattern:

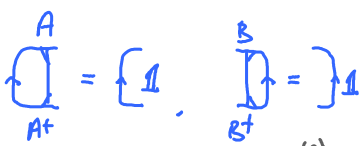
# of open indices grows linearly

cost: $\left.\begin{array}{l} \mathcal{O}(D \cdot d^2 D) \\ \mathcal{O}(D \cdot d^3 D) \\ \mathcal{O}(D \cdot d^4 D) \end{array}\right\} \mathcal{O}(d^L D^2)$

Moreover, if canonical form is used,

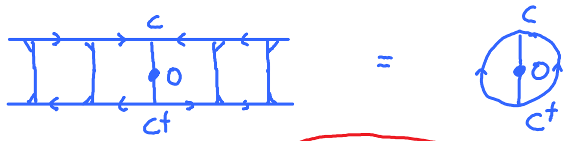


with



(7)

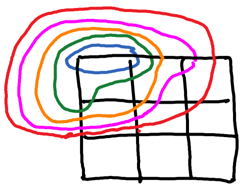
then contraction costs are very small:



(8)

In 2D, growth of # of open indices is unavoidable:

open indices: 3 4 4 5 5 just keeps growing...



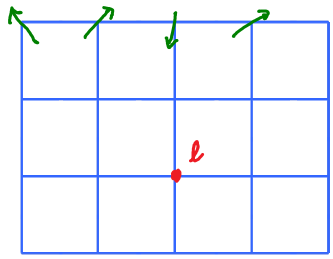
- Contraction costs would become manageable if a 'canonical form' were available!

  But this has not been explored systematically until recently.

- 'No exact canonical form exists' [Orus2014, Sec. 5.2] (but this claim might be outdated...)

- Restrictions to canonical forms are possible and probably useful. [Zaletel2019], [Hagshenas2019]

2. Example: RVB state

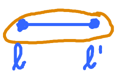


$\ell = (\ell_x, \ell_y)$ is 2D index

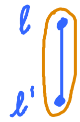
Resonating valence bond (RVB) states are of continued interest for constructing spin liquids.
[Anderson1987], [Rokhsar1988] (high-Tc context)

Canonical example: spin-1/2 Heisenberg model on square lattice

'Dimer' or 'valence bond':



$$= \frac{1}{\sqrt{2}}\left(|\uparrow_\ell \downarrow_{\ell'}\rangle - |\downarrow_\ell \uparrow_{\ell'}\rangle\right)$$

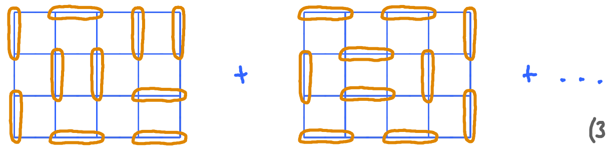


$$= \frac{1}{\sqrt{2}}\left(|\uparrow_\ell \downarrow_{\ell'}\rangle - |\downarrow_\ell \uparrow_{\ell'}\rangle\right) \qquad (1)$$

[sign conventions for bonds are needed and important]

RVB state: $|RVB\rangle =$ (equal-weight superposition of all possible dimer coverings of lattice) (2)

VB fluctuations lower energy due to Hamiltonian matrix elements connecting different configurations.

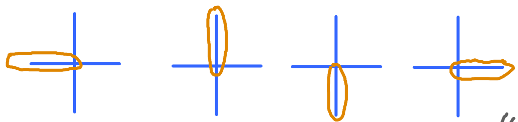


(3)

RVB state has a PEPS representation [Verstraete2004d], [Verstraete2006]

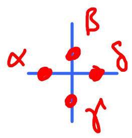
Defining properties of RVB state:

- each vertex has precisely one dimer attached to it, so it can be involved in one of four possible states:



(4)

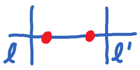
- introduce four auxiliary sites per physical site, $|\alpha\beta\gamma\delta\rangle_\ell$



  each in one of the states $|\alpha\rangle \in \{|e\rangle, |\uparrow\rangle, |\downarrow\rangle\}$ (5)
  empty up down (D= 3)

- for each bond, define 'entangled pairs' from the auxiliary states of the two sites connected by the bond:

$$|EP\rangle_{\langle \ell,\ell'\rangle} = \underbrace{\frac{1}{\sqrt{2}}\left(|\uparrow_\ell \downarrow_{\ell'}\rangle - |\downarrow_\ell \uparrow_{\ell'}\rangle\right)}_{\text{VB}} + \underbrace{|e_\ell e_{\ell'}\rangle}_{\text{no VB}} \qquad (6)$$



each bond is in an equal-weight superposition of VB or no-VB

- impose constraint: allow only one auxiliary spin-1/2 per physical site, and identify it with physical spin:

Projector on site ℓ :

$$\hat{P}_\ell = \sum_{\sigma_\ell = \uparrow,\downarrow} |\underbrace{\sigma_\ell}_{\text{physical spin}}\rangle \underbrace{\Big({}_\ell\langle \sigma e e e| + {}_\ell\langle e\sigma e e| + {}_\ell\langle e e \sigma e| + {}_\ell\langle e e e \sigma| \Big)}_{\text{VB points left, up, down, right}} \qquad (7)$$

(bra labels: $\ell\ u\ d\ r$)

projector assigns the spin on site ℓ to one of four possible VBs

$$:= \sum_{\sigma_\ell} \sum_{\alpha\beta\gamma\delta} A^{\sigma_\ell}_{\alpha\beta\gamma\delta} \, |\sigma_\ell\rangle\langle\alpha\beta\gamma\delta| \qquad \text{(no arrow convention here)} \qquad (8)$$

only nonzero elements of A tensor:

$= \sum_{\sigma_\ell} \sum_{\alpha\beta\gamma\delta} P^{\sigma}_{\alpha\beta\gamma\delta} \, |\sigma_\ell\rangle\langle\alpha\beta\gamma\delta|$ (no arrow convention here) (8)

only nonzero elements of A-tensor: $A^{\sigma}_{\sigma eee} = A^{\sigma}_{e\sigma ee} = A^{\sigma}_{ee\sigma e} = A^{\sigma}_{eee\sigma} = 1$ (9)

PEPS form for RVB state:

$$|RVB\rangle = \prod_{\otimes \ell} \hat{P}_\ell \prod_{\otimes\langle \ell, \ell'\rangle} |EP\rangle_{\ell\ell'} = \sum_{\vec{\sigma}_{\ell\ell'}} |\vec{\sigma}_{\ell\ell'}\rangle \prod_{\ell\ell'} A_{[\ell\ell']} \qquad (10)$$

all sites ($\otimes \ell$); all nearest neighbor pairs $\ell\ell'$ ($\otimes\langle \ell, \ell'\rangle$)

The action of (product of projectors on all sites) on (product of entangled pairs on all bonds) yields all coverings of the lattice for which each site is assigned to precisely one VB.

For example: for two neighboring sites ℓ, ℓ', action of $\hat{P}_\ell \hat{P}_{\ell'} |EP\rangle_{\ell\ell'}$ yields:

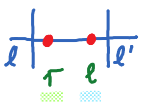
possible VBs for site ℓ possible VBs for site ℓ'

$$\sum_{\sigma_\ell = \uparrow\downarrow} |\sigma_\ell\rangle \Big({}_\ell\langle \sigma eee| + {}_\ell\langle e\sigma ee| + {}_\ell\langle ee\sigma e| + {}_\ell\langle eee\sigma| \Big) \sum_{\sigma'_\ell = \uparrow\downarrow} |\sigma'_{\ell'}\rangle \Big({}_{\ell'}\langle \sigma' eee| + {}_{\ell'}\langle e\sigma' ee| + {}_{\ell'}\langle ee\sigma' e| + {}_{\ell'}\langle eee\sigma'| \Big)$$

ℓ: $l\,u\,d\,r$ ℓ': $l\,u\,d\,r$

possible states for bond $\langle \ell, \ell'\rangle$

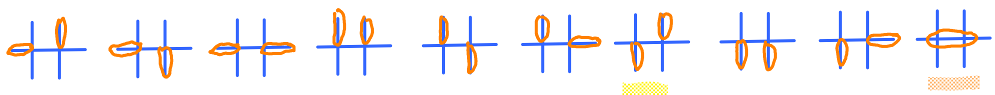
for this bond, we need auxiliary indices r for site ℓ and l for site ℓ'



$$\frac{1}{\sqrt{2}}\Big(|\uparrow_\ell \downarrow_{\ell'}\rangle - |\downarrow_\ell \uparrow_{\ell'}\rangle \Big) + |e_\ell \, e_{\ell'}\rangle$$

VB no VB

$=$



Advantages of PEPS description of RBV state

- Dimer basis is hard to work with, since individual components are not orthogonal:  $\neq 0$

  Therefore, explicit computations are easier in PEPS framework!

- PEPS description can be extended to larger class of states, e.g. including longer-ranged bonds [Wang2013]

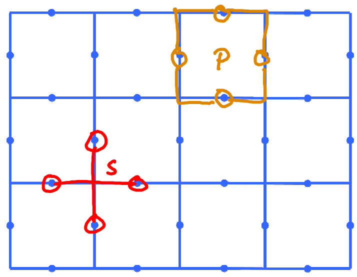
- 'Parent Hamiltonian' (for which RVB state is exact ground state) can be constructed systematically, but it is complicated: 19-site interaction [Schuch2012], 12-site interaction [Zhou2014]

3. Example: Kitaev's Toric Code

[Kitaev2003], [Kitaev2009] easy to read!

Simplest known model whose ground state displays topological order. Ground state on torus is four-fold degenerate, hence it can be used to define a 'topologically protected qubit'.

- Square lattice (on 2D plane, or on torus)
- Spin 1/2 on each edge

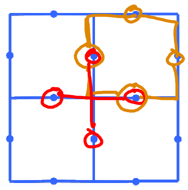


spins live on 'edges' of square lattice
index ℓ labels edges

- $$\hat{H} = -J_e \underbrace{\sum_s}_{\text{sum over all stars}} \hat{A}_s - J_m \underbrace{\sum_p}_{\text{sum over all plaquettes}} \hat{B}_p \qquad (1)$$

- $$\hat{A}_s \equiv \prod_{\ell \in \text{star}(s)} \hat{\sigma}^z_\ell \qquad \hat{B}_p \equiv \prod_{\ell \in \text{plaquette}(p)} \hat{\sigma}^x_\ell$$

[note: Kitaev uses $\hat{\sigma}^x$ for stars, $\hat{\sigma}^z$ for plaquettes]



All terms in Hamiltonian commute

Easy to check: $[\hat{A}_s, \hat{B}_p] = 0$ for all s, p (3)

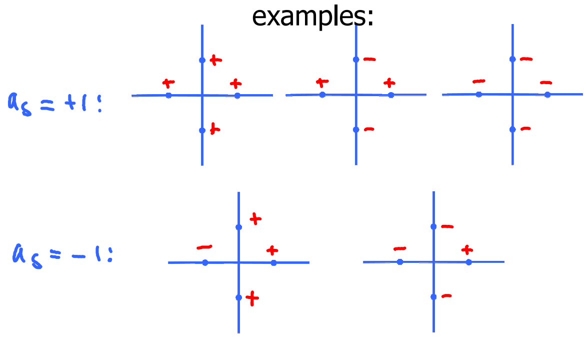
because all stars and plaquettes share an even number of edges (0 or 2);

hence minus signs from $\hat{\sigma}^z_\ell \hat{\sigma}^x_\ell = -\hat{\sigma}^x_\ell \hat{\sigma}^z_\ell$ cancel: $(-1)^0 = (-1)^2 = 1$ (4)

- All terms in $\hat{H}$ commute $\Rightarrow$ $\hat{H}$ should be solvable!
- Adopt eigenbasis of $\hat{\sigma}^z_\ell$: with eigenstates $|\sigma_\ell\rangle$, $\sigma_\ell = \pm 1$ (5)
- Star operator, $\hat{A}_s = \prod_{\ell \in \text{star}(s)} \hat{\sigma}^z_\ell$ (6)

  has eigenvalues $a_s = \pm 1$ 'star flux' (7)

  If $a_s = -1$, there is a 'vortex' on star. (8)



Ground state of toric code

- Due to (3), ground state must be an eigenstate of every $\hat{A}_s$, $\hat{B}_p$, (9)

$$\Rightarrow \quad \hat{A}_s|g\rangle = a_s|g\rangle, \qquad \hat{B}_p|g\rangle = b_p|g\rangle \quad \text{for all } s, p$$

- ground state must maximize energy of <u>all</u> $\hat{A}_s$, $\hat{B}_p$ terms, $\Rightarrow$ $a_s = b_p = +1$ (10)

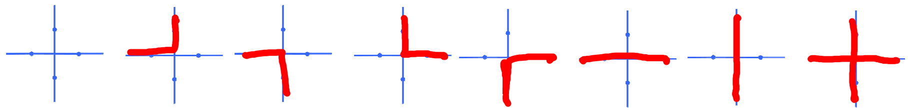
Note: $a_s = 1$ $\Rightarrow$ (all +), or (all -) , or (two +, two -), on every star

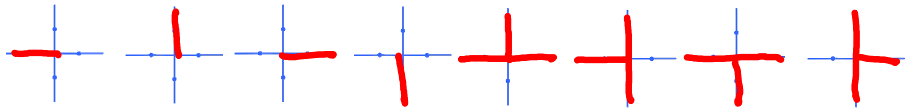
$\Rightarrow$ $\sum a_s = 0 \mod (4)$ 'even-parity condition' (11)

Note: $a_s = 1$ $\Rightarrow$ (all +), or (all -) , or (two +, two -), on every star

$\Rightarrow \sum_{s \in \text{star}} a_s = 0 \bmod (4)$ 'even-parity condition' (11)

Graphical notation:  (12)

Allowed configurations: 

Forbidden configurations: 

$\Rightarrow$ ground state is 'vortex free', i.e. it contains only closed loops of red edge lines

$$\Rightarrow \quad |g\rangle = \sum_{\text{all closed loops}} C^{\vec{\sigma}} |\vec{\sigma}\rangle \qquad \{\vec{\sigma}: \; a_s(\vec{\sigma}) = 1 \;\; \forall s\} \tag{13}$$

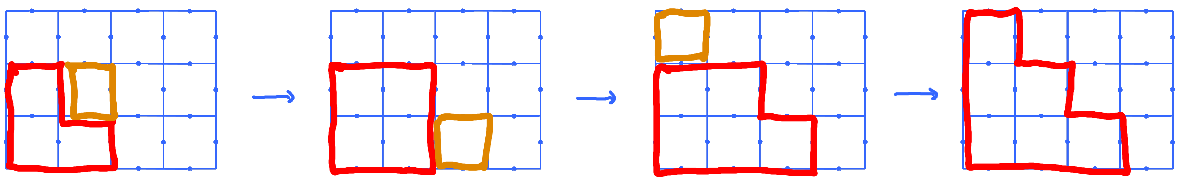
- $\hat{B}_p$ flips all spins on plaquette, hence maps 'allowed configuration' to 'allowed configuration'.

Since $|g\rangle$ sums over all allowed configurations, the condition $\hat{B}_p |g\rangle \overset{(9,10)}{=} |g\rangle$

can be satisfied provided that states connected by $\hat{B}_p$ have same amplitude:

$$\Rightarrow \quad \text{if} \quad \hat{B}_p |\vec{\sigma}\rangle = |\vec{\sigma}'\rangle, \quad \text{then} \quad C^{\vec{\sigma}} = C^{\vec{\sigma}'} \tag{14}$$

$\Rightarrow$ Along each 'orbit' of the action of plaquette operators, all coefficients must be equal:

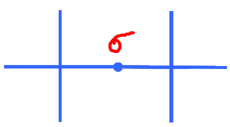
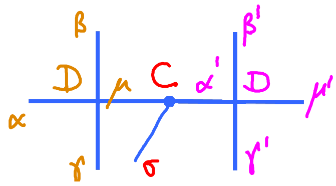
 (15)

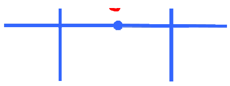
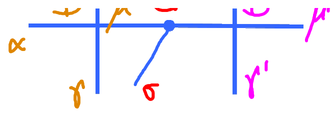
Toric code on plane

Spin flips of plaquette operator are 'ergodic', i.e. any closed loop $|\vec{\sigma}\rangle$ can be mapped to any other $|\vec{\sigma}'\rangle$ closed loop by a series of plaquette operators. Hence, all $C^{\vec{\sigma}}$ must be equal:

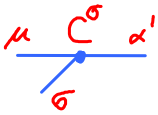
$$\boxed{|\bar{g}\rangle = \sum_{\text{all closed loops}} |\vec{\sigma}\rangle} \qquad \text{equal-weight superposition of all closed-loop configurations} \tag{16}$$

PEPS representation: [Verstraete2006]

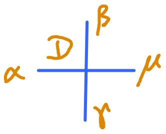
the local variable $\sigma = \pm 1$,  is represented by $\longrightarrow$ $\alpha, \beta, \gamma, \mu \in \{+, 1\}$  (17)

$\sigma = \pm 1$,  $\xrightarrow[\alpha,\beta,\gamma,\mu \in \{\pm 1\},\ D=2]{}$  (17)

with



$\equiv \delta_{\mu\sigma}\,\delta_{\alpha'\sigma}$ [on each edge: set both auxiliary indices equal to physical index σ] (18)



$\equiv \begin{cases} 1 & \text{if } \alpha+\beta+\gamma+\mu = 0 \bmod (4) \\ 0 & \text{otherwise} \end{cases}$ [on each vertex: enforce even-parity condition] (19)

Summing over all $\alpha\beta\gamma\mu$ on each vertex generates all possible loop orderings!

$$|g\rangle = \sum_{\vec{\sigma}} |\vec{\sigma}\rangle \prod_{\ell} C^{\sigma_\ell}_{[\ell]} \prod_{s} D_{[s]}$$ [contraction of all auxiliary bonds implied] (20)

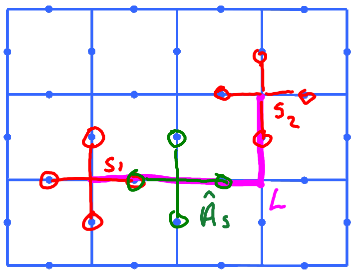
PEPS formulation is generalizable to all 'string-net' models', [Gu2009]
which realize all non-chiral topological order in 2+1 dimensions. [Buerschaper2009]

Excitations on plane

Excitations come in two varieties: (i) 'electric charges', (iii) 'magnetic vortices'.

(i) Define 'electric path operator', $\hat{E}_L = \prod_{\ell \in L} \hat{\sigma}^x_\ell$ (21)

with L = path from s_1 to s_2 .



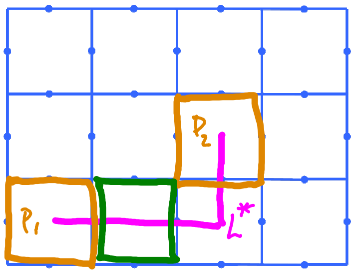
Then $[\hat{E}_L, \hat{B}_p] = 0$ (since both are built only from $\hat{\sigma}^x$) (22)

$$\hat{E}_L \hat{A}_s = \mp \hat{A}_s \hat{E}_L \quad \text{for } \begin{cases} s = s_1 \text{ or } s_2 & \text{[star flips only one spin on path]} \\ \text{otherwise} & \text{[star flips two or zero spins on path]} \end{cases}$$ (23)

So, electric path operator creates two 'charges', at s_1 and s_2 , each having energy $2J_e$. (24)

(i) Define 'magnetic path operator', $\hat{M}_{L^*} = \prod_{\ell \in L^*} \hat{\sigma}^z_\ell$ (25)

with L^* = path on 'dual lattice' from p_1 to p_2

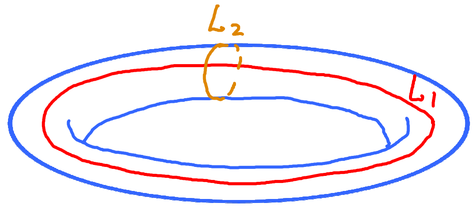


Then $[\hat{M}_{L^*}, \hat{A}_s] = 0$ (since both are built only from $\hat{\sigma}^z$) (26)

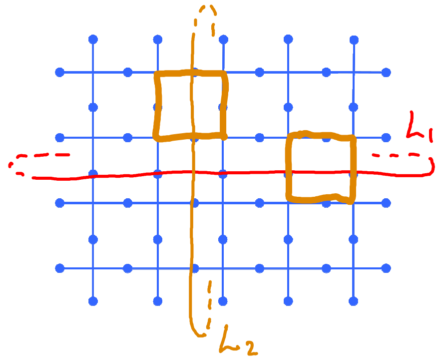
$$\hat{M}_{L^*} \hat{B}_p = \mp \hat{B}_p \hat{M}_{L^*} \quad \text{for } \begin{cases} p = p_1 \text{ or } p_2 & \text{[plaquette flips only one spin on path]} \\ \text{otherwise} & \text{[plaquette flips two or zero spins on path]} \end{cases}$$ (27)

So, magnetic path operator creates two 'vortices', at p_1 and p_2 , each having energy $2J_m$. (28)

Toric code on torus



Let L_1 and L_2 be 'global loops' wrapping around surface of torus, along the spin locations (i.e. between edges, on dual lattice)



For given L_1 and L_2, define the 'global loop operators'

$$\hat{A}_L = \prod_{\ell \in L} \hat{\sigma}^z_\ell \,, \qquad L = L_1 \text{ or } L_2$$

Possible eigenvalues: $a_{L_1} = \pm 1 \,, \quad a_{L_2} = \pm 1$

Any plaquette cuts L_1 and L_2 either 0 or 2 times,

i.e. B_p flips an even number of spins along a global loop, hence $[\hat{B}_p, \hat{A}_L] = 0$

Moreover, $[\hat{A}_s, \hat{A}_L] = 0$ (since both are built only from $\hat{\sigma}^z$)

Hence, $[\hat{H}, \hat{A}_L] = 0$.

So, ground state(s) are also characterized by their a_L-eigenvalues:

$$\hat{A}_{L_1} |g, a_{L_1}, a_{L_2}\rangle = a_{L_1} |g, a_{L_1}, a_{L_2}\rangle \,, \qquad \hat{A}_{L_2} |g, a_{L_1}, a_{L_2}\rangle = a_{L_2} |g, a_{L_1}, a_{L_2}\rangle$$

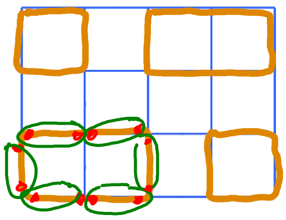
$\Rightarrow$ there are 4 degenerate ground states $\Rightarrow$ topological property!

4. Example: Resonating AKLT loop state (RAL)

Consider square lattice, spin 1 on every site:

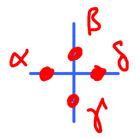
$|RAL\rangle$ = (equal-weight superposition of all fully packed AKLT loop coverings) [Yao2010]

- Loops don't touch (each site is visited by exactly one loop)
- Each loop is a periodic AKLT-type state



PEPS representation: [Li2014]

- introduce four auxiliary sites per physical site, $|\alpha\beta\gamma\delta\rangle_\ell$

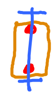


each in one of the states $|\alpha\rangle \in \{\,|e\rangle,\ |\uparrow\rangle,\ |\downarrow\rangle\,\}$
empty, up, down

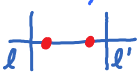
$\underbrace{\text{up} \quad \text{down}}_{\text{form auxiliary spin-1/2}}$

(D= 3)

- define 'entangled pairs' using adjacent auxiliary sites from nearest neighbors of given site:



$$|EP\rangle_{\langle \ell\ell'\rangle} = \underbrace{\frac{1}{\sqrt2}\left(|\uparrow_\ell\downarrow_{\ell'}\rangle - |\downarrow_\ell\uparrow_{\ell'}\rangle\right)}_{\text{VB}} + \underbrace{|e_\ell\, e_{\ell'}\rangle}_{\text{no VB}}$$



equal-weight superposition of VB or no-VB on bond (same as for RVB)

- impose constraint: allow only two auxiliary spin-1/2 per physical site, combined to form physical spin-1:

Projector on site ℓ :

$$\hat P_\ell = |1_\ell\rangle\left({}_\ell\langle ee\uparrow\uparrow| + {}_\ell\langle e\uparrow e\uparrow| + {}_\ell\langle \uparrow e e\uparrow| + \dots\right)$$

$$+ \frac{1}{\sqrt2}|0_\ell\rangle\left({}_\ell\langle ee\uparrow\downarrow| + {}_\ell\langle e\uparrow e\downarrow| + {}_\ell\langle \uparrow e e\downarrow| + \dots\right)$$

Clebsch-Gordan

$$|{-1}_\ell\rangle\left({}_\ell\langle ee\downarrow\downarrow| + {}_\ell\langle e\downarrow e\downarrow| + {}_\ell\langle \downarrow e e\downarrow| + \dots\right)$$

[two edges are bound into a spin-1, other two are 'empty']

$$\equiv \sum_{\sigma_\ell} \sum_{\alpha\beta\gamma\delta} A^{\sigma_\ell}_{\alpha\beta\gamma\delta}\, |\sigma_\ell\rangle\langle\alpha\beta\gamma\delta|$$

PEPS form for RAL state:

$$|RAL\rangle = \prod_{\otimes \ell} \hat P_\ell \prod_{\otimes \langle \ell,\ell'\rangle} |EP\rangle_{\ell\ell'} = \sum_{\vec\sigma_{\ell\ell'}} |\vec\sigma_{\ell\ell'}\rangle \prod_{\ell\ell'} A_{[\ell\ell']}$$

all sites

all nearest neighbor pairs $\ell\ell'$