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

1. Motivation & Definition of PEPS

Goal: generalize MPS ideas to 2 dimension!

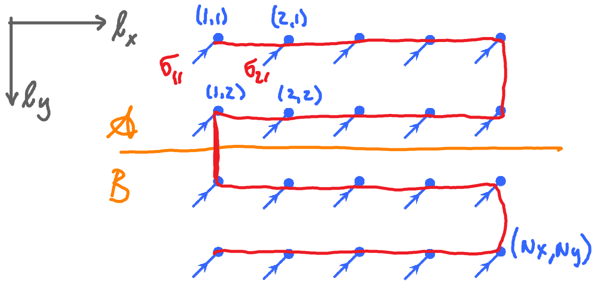
Most obvious idea: 2D-DMRG, using a 'snake-MPS':

[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 $S^{MPS}_{\mathcal{AB}} \sim \mathcal{O}(\ln_2 D)$

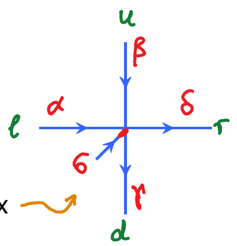
but according to area law, we need $S_{\mathcal{AB}} \sim N_x \Rightarrow D \sim 2^{N_x}$

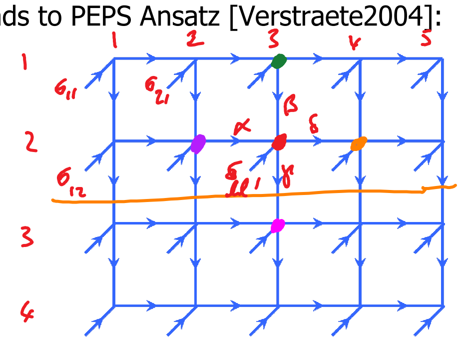
Reason for insufficiency: entanglement between $\mathcal{A}$ and $\mathcal{B}$ is encoded in a single bond.

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

Introduce 5-leg tensor for every site: $A^{\overset{\ell\ u}{\alpha\beta}\ \sigma_{\ell\ell'}}_{[\ell\ell']\ \underset{d\ r}{\gamma\delta}}$

physical index





Sum over all virtual bonds linking neighboring sites:

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

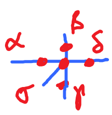
physical basis: $|\vec{\sigma}_{\ell\ell'}\rangle \equiv |\sigma_{N_x N_y}\rangle \otimes \dots |\sigma_{21}\rangle \otimes |\sigma_{11}\rangle$

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

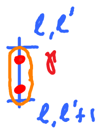
Variationally minimize $\langle\psi|\hat{H}|\psi\rangle$. # of variational parameters: $\mathcal{O}(d\,D^4 \cdot N_x N_y) \ll d^{N_x \cdot N_y}$

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

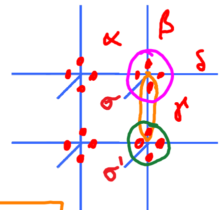
Associate 4 'auxiliary particles' with each site: $|\alpha\beta\gamma\delta\rangle_\ell = |\alpha\rangle^\ell \otimes |\beta\rangle^u \otimes |\gamma\rangle^d \otimes |\delta\rangle^r \qquad (3)$



Construct entangled pairs along bonds: e.g. $|EP\rangle_{\ell,\ell'} = \sum_{\gamma=1}^{D} |\gamma\rangle^d_{\ell,\ell'}\, |\gamma\rangle^u_{\ell,\ell'+1} \qquad (4)$



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



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

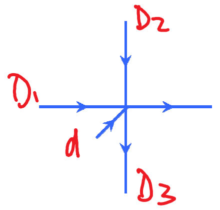
$$|\sigma\rangle_{\ell,\ell'}|\sigma'\rangle_{\ell,\ell'+1}\ \underline{A^{\sigma}_{[\ell,\ell']\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}}}\ \underline{A^{\sigma'}_{[\ell,\ell'+1]\bar{\alpha}'\bar{\beta}'\bar{\gamma}'\bar{\delta}'}}\ \langle\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}|\langle\bar{\alpha}'\bar{\beta}'\bar{\gamma}'\bar{\delta}'|\sum_{\gamma}|\gamma\rangle^d_{\ell,\ell'}|\gamma\rangle^u_{\ell,\ell'+1}$$

$$|\sigma\rangle_{\ell,\ell'} |\sigma'\rangle_{\ell,\ell'+1} \; A^{\sigma}_{[\ell,\ell']\bar\alpha\bar\beta\bar\gamma\underbrace{\bar\delta}_{=\gamma}} \; A^{\sigma'}_{[\ell,\ell'+1]\bar\alpha'\bar\beta'\underbrace{\bar\gamma'}_{=\gamma}\bar\delta'} \; \langle\bar\alpha\bar\beta\bar\gamma\bar\delta| \langle\bar\alpha'\bar\beta'\bar\gamma'\bar\delta'| \; \sum_{\gamma} |\gamma\rangle^{d}_{\ell,\ell'} |\gamma\rangle^{u}_{\ell,\ell'+1}$$

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:

$\Rightarrow \quad d\, D_1 D_2 = D_3 D_4 \quad \Rightarrow \quad D_{\text{outgoing}} = D_{\text{incoming}} \sqrt{d}$ (6)

in-dimension out-dimension

$D_{\ell\ell'} \sim \sqrt{d}^{\,\ell+\ell'}$

- 2D area law is satisfied: $S_{AB} \sim \mathcal{O}(N_x \ln_2 D)$

- PEPS can handle polynomially-decaying correlations (in contrast to 1D MPS)

- Exact contraction is #P hard, $\Rightarrow$ contraction time $\sim \mathcal{O}(e^{N_x N_y})$

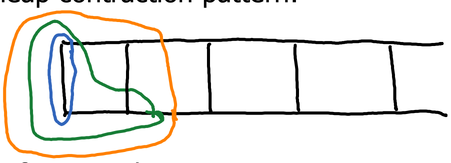
#P-hard class of problems = count number of solutions of NP-complete problems

NP-complete class = problems that cannot be solved in polynomial time

'non-deterministic polynomial'

Why are exact contractions hard? Recall 1D situation:

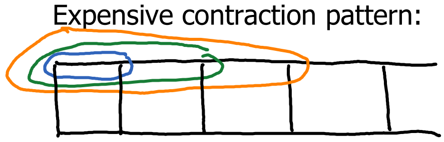
Cheap contraction pattern:



# of open indices

cost: $\mathcal{O}(D^2 \cdot d)$
$\mathcal{O}(d \cdot D^2 \cdot D)$
$\mathcal{O}(D^2 \cdot d D)$ $\Big\} \sim \mathcal{O}(d D^3 N)$

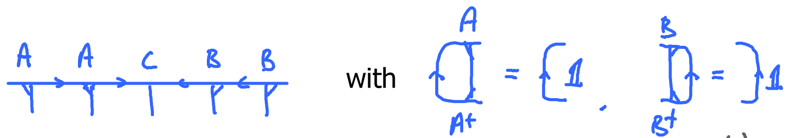
Expensive contraction pattern:



# of open indices

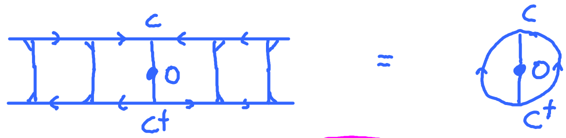
cost: $\mathcal{O}(d^2 D \cdot D)$
$\mathcal{O}(d^3 D \cdot D)$
$\mathcal{O}(d^4 D \cdot D)$ $\Big\} \; \mathcal{O}(d^N D^2)$

Moreover, if canonical form is used,



with (7)

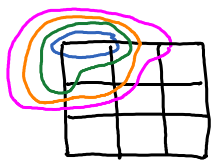
then contraction costs are very small:



(8)

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

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



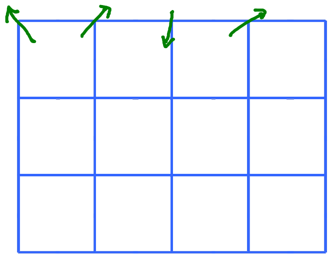
- Contraction costs would become manageable if a 'canonical form' were available!

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]

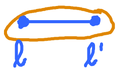
2. Example: RVB state



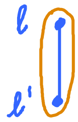
Resonating valence bond (RVB) states are of continued interest for constructing spin liquids.
[Anderson1987], [Rokhsar1988] (high-Tc context)

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

'Dimer' or 'valence bond':



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



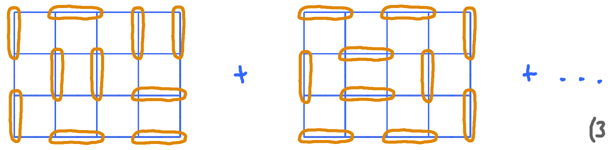
$$= \frac{1}{\sqrt{2}}\left(|\uparrow_\ell \downarrow_{\ell'}\rangle - |\downarrow_\ell \uparrow_{\ell'}\rangle\right) \quad (1)$$

[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.

$$\langle \#_1 | H | \#_2 \rangle \neq 0$$

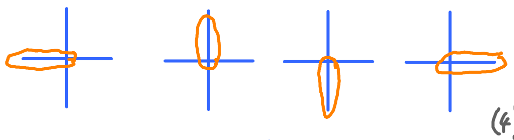


(3)

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

Defining properties of RVB state:

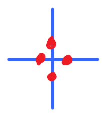
- each vertex has precisely one dimer attached to it, so it can be involved in one of four possible states:



(4)

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

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

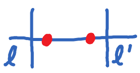


(5)

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

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

equal-weight superposition of VB or no-VB on bond



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

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

Projector on site ℓ:

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

$$\equiv \sum_{\sigma_\ell} \sum_{\alpha\beta\gamma\delta} A^{\sigma_\ell}_{\alpha\beta\gamma\delta} |\sigma_\ell\rangle\langle \alpha\beta\gamma\delta| \quad (8)$$

(no arrow convention here)

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

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

PEPS form for RVB state: $|RVB\rangle = \prod_{\otimes l} \hat{P}_l \prod_{\otimes \langle l,l' \rangle} |EP\rangle_{ll'} = \sum |\vec{\sigma}_{ll'}\rangle \prod_{ll'} A_{[ll']}$ (10)

all sites

all nearest neighbor pairs ll'

Advantages of PEPS description of RBV state

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

  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]

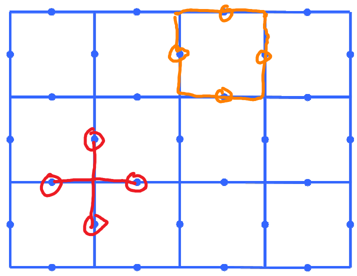
3. Example: Kitaev's Toric Code

[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 $\qquad J_s > 0, \quad J_e > 0$
- $\hat{H} = - J_s \sum_s \hat{A}_s \quad - J_e \sum_p \hat{B}_p$ (1)

  sum over all stars $\qquad$ sum over all plaquettes

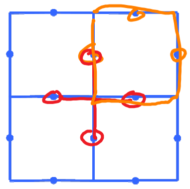


spins live on 'edges' of square lattice
index ℓ labels edges

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

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

All terms in Hamiltonian commute



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

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

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

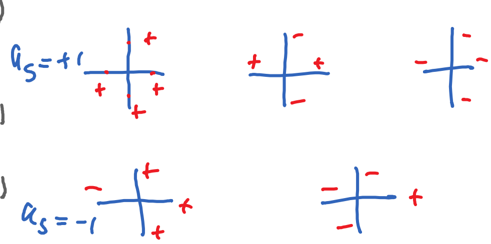
$A_s B_p \overset{?}{=} B_p A_s$

- All terms in $\hat{H}$ commute $\Rightarrow$ $\hat{H}$ should be solvable!
- Adopt eigenbasis of $\hat{\sigma}^z_\ell$: $\qquad$ with eigenstates $|\sigma_\ell\rangle, \quad \sigma_\ell = \pm 1$ (5)

- Star operator, $\quad \hat{A}_s = \prod_{\ell \in \text{star}(s)} \hat{\sigma}^z$ (6)

  has eigenvalues $\quad a_s = \pm 1 \quad$ '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)

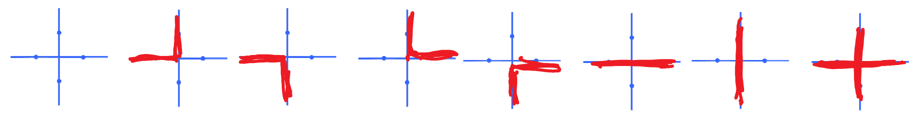
$\Rightarrow \quad \hat{A}_s |g\rangle = a_s |g\rangle, \qquad \hat{B}_p |g\rangle = b_p |g\rangle \quad$ for all s, p

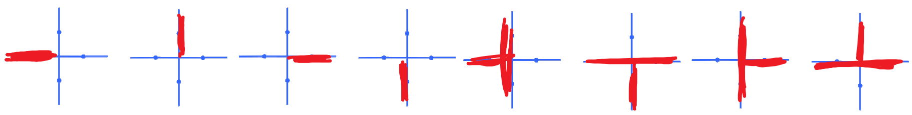
- ground state must maximize energy of <u>all</u> $\hat{A}_s, \hat{B}_p$ terms, $\Rightarrow a_s = b_p = +1$ (10)

Note: $\quad a_s = 1 \quad \Rightarrow \quad$ all ~~up~~ +, or all ~~down~~ −, or two ~~up~~ +, two ~~down~~ −, on every star (11) ground state must maximize energy of all A_s, B_p terms, $\Rightarrow$ $a_s = b_p = +1$ (10)

Note: $a_s = 1$ $\Rightarrow$ all up, or all down, or two up, two down, on every star (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

$$\Rightarrow \quad |g\rangle = \sum_{\text{all closed loops}} C^{\vec\sigma}\, |\vec\sigma\rangle \qquad (13)$$

all closed loops $\leftarrow$ $\{\vec\sigma : a_s(\vec\sigma) = 1 \;\; \forall s\}$

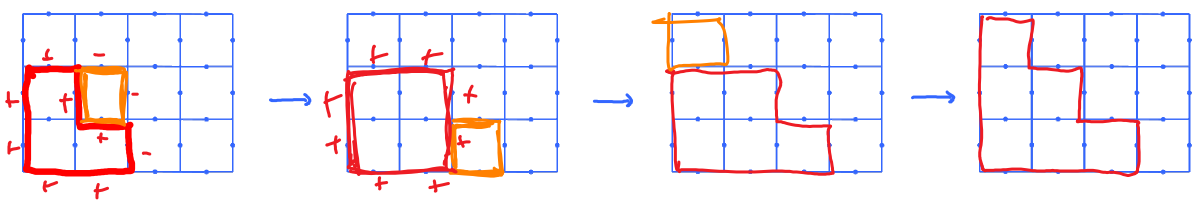
- $\hat B_p$ flips all spins on plaquette, hence maps 'allowed configuration' to 'allowed configuration'.

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:

if $\hat B_p |\vec\sigma\rangle = |\vec\sigma'\rangle$, then $C^{\vec\sigma} = C^{\vec\sigma'}$ (14)

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

 (15)

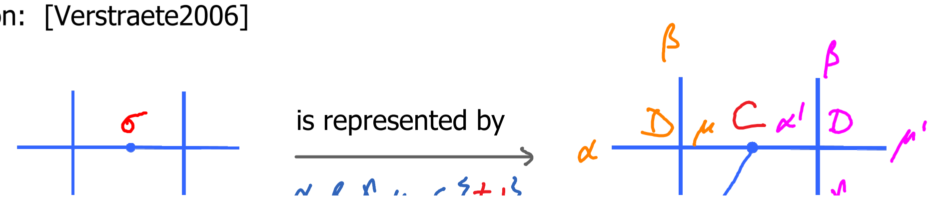
Toric code on plane

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:

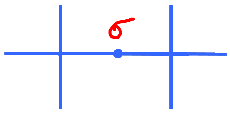
$$\boxed{|g\rangle = \sum_{\text{all closed loops}} |\vec\sigma\rangle}$$

equal-weight superposition of all closed-loop configurations (16)

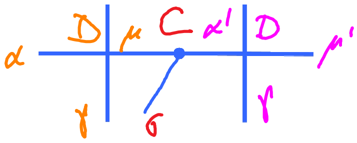
PEPS representation: [Verstraete2006]

the local variable $\sigma = \pm 1$,  is represented by (17) the local variable

$\sigma = \pm 1$,

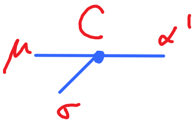


is represented by $\xrightarrow[\alpha,\beta,\gamma,\mu \in \{\pm 1\}]{}$ $D = 2$

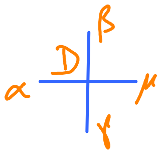


(17)

with



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



$$\equiv \begin{cases} 1 & \text{if } \alpha+\beta+\gamma+\mu = 0 \bmod (4) \\ 0 & \text{otherwise} \end{cases}$$

[on each vertex: enforce closed-loop 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)

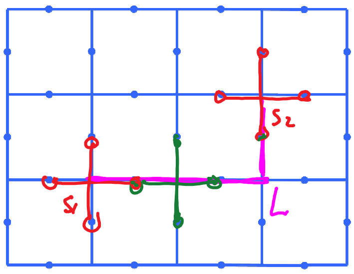
PEPS formulation is generalizable to all 'string-net' models', [Gu2009]
which realize all non-chiral topological order in 2+1 dimensions. [Buerschaper2009]

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 $[\hat E_L, \hat B_p] = 0$ (22) (since both are built only from $\hat\sigma^x$)

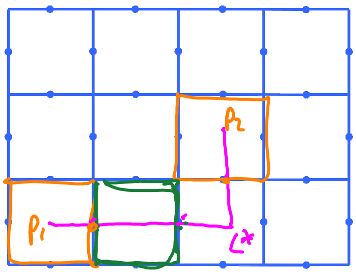
$$\hat E_L \hat A_s = \mp \hat A_s \hat E_L \quad \text{for} \begin{cases} s = s_1 \text{ or } s_2 & \text{[star flips only one spin on path]} \\ \text{otherwise} & \text{[star flips two or zero spins on path]} \end{cases}$$ (23)

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

$\hat E_L |g\rangle$ has eigenenergy $2J_e$

(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 $[\hat M_{L^*}, \hat A_s] = 0$ (26) (since both are built only from $\hat\sigma^z$)

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

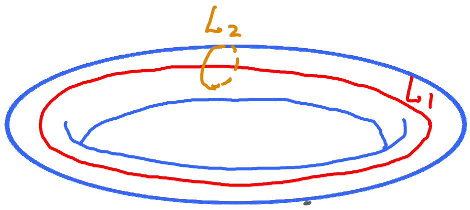
So, plaquette operator creates two 'vortices', at p_1 and p_2, each having energy $2J_p$ (28)

otherwise [plaquette flips two or zero spins on path]

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

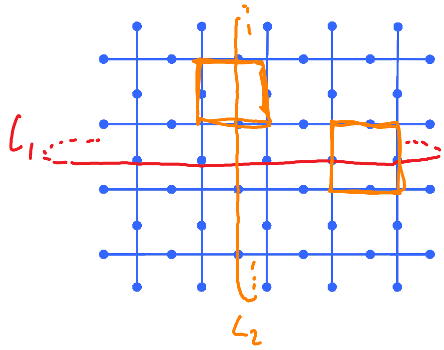
Toric code on torus

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



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

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



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

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

i.e. flips an even number of spins, hence $[\hat{B}_p, \hat{A}_L] = 0$; $[\hat{A}_s, \hat{A}_L] = 0$

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

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

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

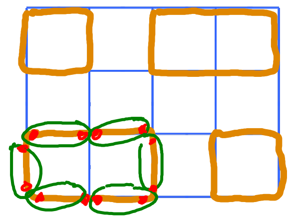
$\Rightarrow$ there are 4 degenerate ground states $\Rightarrow$ topological property!

4. Example: Resonating AKLT loop state (RAL)

Consider square lattice, spin 1 on every site:

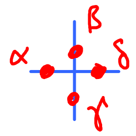
$|RAL\rangle$ = (equal-weight superposition of all fully packed AKLT loop coverings) [Yao2010]

- 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, $|\alpha\beta\gamma\delta\rangle_\ell = |\alpha\rangle^{l}_{\ell}|\beta\rangle^{u}_{\ell}|\gamma\rangle^{d}_{\ell}|\delta\rangle^{r}_{\ell}$



each in one of the states $|\alpha\rangle \in \{\underset{\text{empty}}{|e\rangle},\ \underbrace{\underset{\text{up}}{|\uparrow\rangle},\ \underset{\text{down}}{|\downarrow\rangle}}_{\text{form auxiliary spin-1/2}}\}$ (D= 3)

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

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

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 : $$\hat{P}_\ell = |1_\ell\rangle\left({}_\ell\langle ee\uparrow\uparrow| + {}_\ell\langle e\uparrow e\uparrow| + {}_\ell\langle\uparrow ee\uparrow| + \dots\right)$$
$$+ \frac{1}{\sqrt{2}}|0_\ell\rangle\left({}_\ell\langle ee\uparrow\downarrow| + {}_\ell\langle e\uparrow e\downarrow| + {}_\ell\langle\uparrow ee\downarrow| + \dots\right)$$
$$|-1_\ell\rangle\left({}_\ell\langle ee\downarrow\downarrow| + {}_\ell\langle e\downarrow e\downarrow| + {}_\ell\langle\downarrow ee\downarrow| + \dots\right)$$

Clebsch-Gordan

[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 $\ell\ell'$