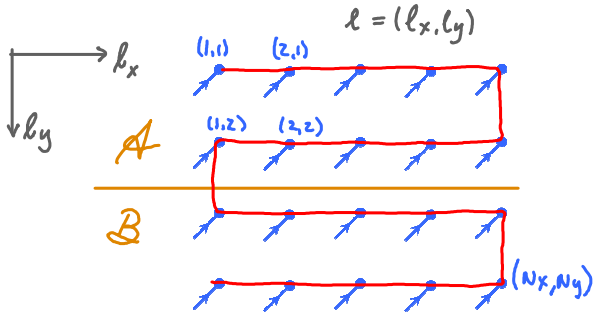
PEPS 1: Projected Entangled Pair States (Verstraete, Cirac, 2004)

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.

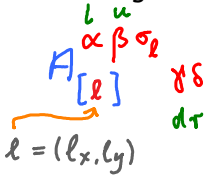
Main limitation: not enough entanglement: entanglement entropy $S_{AB}^{MPS} \sim \mathcal{O}(\ln_2 D)$

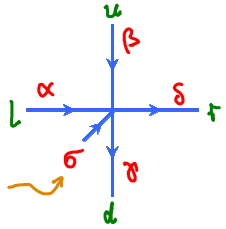
but according to area law, we need $S_{AB} \sim N_x \Rightarrow D \sim 2^{N_x}$

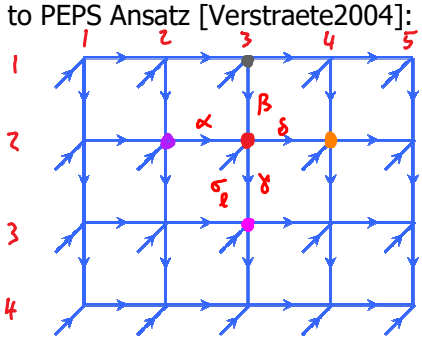
Reason for insufficiency: entanglement between $\mathcal{A}$ and $\mathcal{B}$ is encoded in a single bond.

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

Introduce 5-leg tensor for every site:







Sum over all virtual bonds linking neighboring sites:

$$|\psi\rangle = \sum_{\vec{\sigma}_\ell} |\vec{\sigma}_\ell\rangle \prod_\ell A^{\sigma_\ell}_{[\ell]} \quad (1)$$

PEPS

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

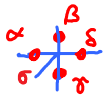
contraction pattern:

$$A_{[\ell_x-1,\ell_y]\,\alpha} \; A_{[\ell_x,\ell_y-1]\,\beta} \; A^{\sigma_{\ell\ell'}}_{[\ell_x,\ell_y]\,\alpha\beta\gamma\delta} \; A_{[\ell_x,\ell_y+1]\,\gamma} \; A_{[\ell_x+1,\ell_y]\,\delta} \quad (2)$$

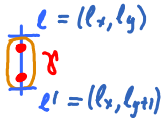
Variationally minimize $\langle\psi|\hat{H}|\psi\rangle$. # of variational parameters: $\mathcal{O}(d D^4 N_x N_y)$

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

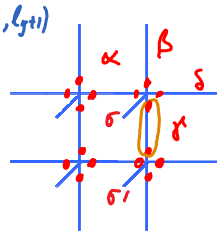
Associate 4 'auxiliary particles' with each site: $|\alpha\beta\gamma\delta\rangle_\ell = |\alpha\rangle^l_\ell |\beta\rangle^u_\ell |\gamma\rangle^d_\ell |\delta\rangle^r_\ell$ (3)



Construct entangled pairs along bonds: $|EP\rangle_{\ell,\ell'} = \sum_\gamma |\gamma\rangle^d_\ell |\gamma\rangle^u_{\ell'}$ e.g. (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 $|\psi\rangle = \bigotimes_\ell \hat{P}_\ell \bigotimes_{\langle\ell,\ell'\rangle} |EP\rangle_{\ell,\ell'}$

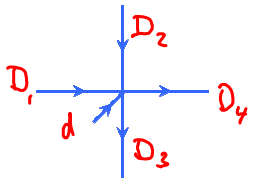
$$|\sigma\rangle_\ell |\sigma'\rangle_{\ell'} A^{\sigma}_{[\ell]\,\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}} A^{\sigma'}_{[\ell']\,\bar{\alpha}'\bar{\beta}'\bar{\gamma}'\bar{\delta}'} \langle\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}|\langle\bar{\alpha}'\bar{\beta}'\bar{\gamma}'\bar{\delta}'|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

$$|\sigma\rangle_\ell |\sigma'\rangle_{\ell'} A^{\sigma}_{[\ell]\alpha\beta\gamma\delta} A^{\sigma'}_{[\ell']\alpha'\beta'\gamma'\delta'} \langle\alpha\beta\gamma\delta|\langle\alpha'\beta'\gamma'\delta'| \sum |\gamma\rangle_\ell^d \gamma\rangle_{\ell'}^u$$

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:

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

number of bonds between A and B; maximal entanglement per bond

- Entanglement entropy between subsystems A, B is $S_{AB} \sim O(\underbrace{N_x}_{\text{number of bonds between A and B}} \underbrace{\ln_2 D}_{\text{maximal entanglement per bond}})$ $\Rightarrow$ 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 $\sim O(e^{N_x N_y})$

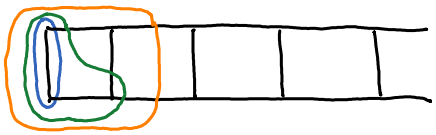
  #P-hard class of problems = count number of solutions of NP-complete problems

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

  'non-deterministic polynomial'

Why are exact contractions hard? Recall 1D situation:

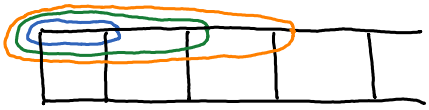
Cheap contraction pattern:



# of open indices remains constant (≤ 3)

cost: $O(D^2 \cdot d)$, $O(dD^2 \cdot D)$, $O(D^2 \cdot dD)$ $\sim O(dD^3)$

Expensive contraction pattern:

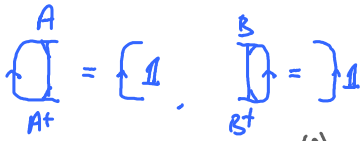


# of open indices grows linearly

cost: $O(d^2 D \cdot D)$, $O(d^3 D \cdot D)$, $O(d^4 D \cdot D)$ $O(d^L D^2)$

Moreover, if canonical form is used,

with

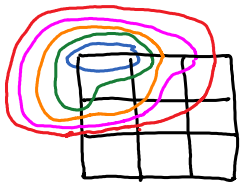


(7)

then contraction costs are very small:

(8)

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



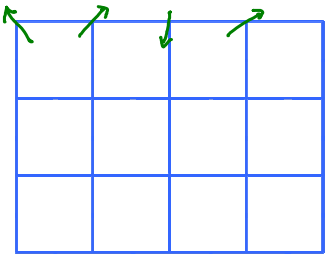
open indices: 3 4 4 5 5 just keeps growing...

- 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]

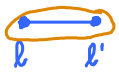
2. Example: RVB state



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':



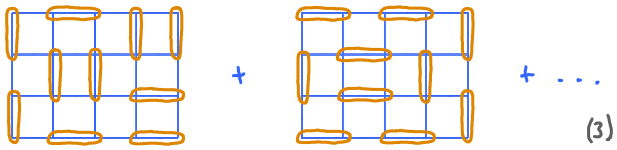
$$= \frac{1}{\sqrt{2}}\left(|\uparrow_\ell\downarrow_{\ell'}\rangle - |\downarrow_\ell\uparrow_{\ell'}\rangle\right)$$

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

[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.

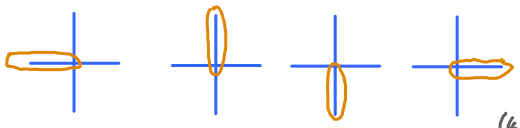


(3)

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

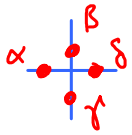
Defining properties of RVB state:

- 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, $|\alpha\beta\gamma\delta\rangle_\ell$



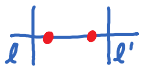
(5)

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

(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

$\ell = (\ell_x, \ell_y)$ is 2D index (6)

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

Projector on site ℓ :

$$\hat{P}_\ell = \sum_{\sigma_\ell=\uparrow,\downarrow} |\sigma_\ell\rangle\left(\ {}_\ell\langle\sigma eee| + {}_\ell\langle e\sigma ee| + {}_\ell\langle ee\sigma e| + {}_\ell\langle eee\sigma|\right)$$

physical spin

VB points left up down right (7)

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

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

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

all sites; all nearest neighbor pairs ℓ,ℓ'

Advantages of PEPS description of RBV state

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

  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

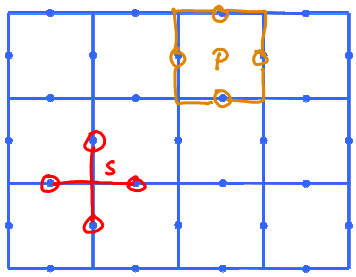
[Kitaev2003], [Kitaev2009] ← easy to read!

PEPS-I.3

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
- $\hat{H} = -J_e \sum_s \hat{A}_s - J_m \sum_p \hat{B}_p$ (1)

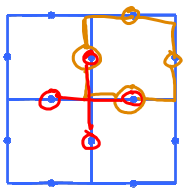
  s: sum over all stars; p: sum over all plaquettes



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

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

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



(3)

All terms in Hamiltonian commute

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

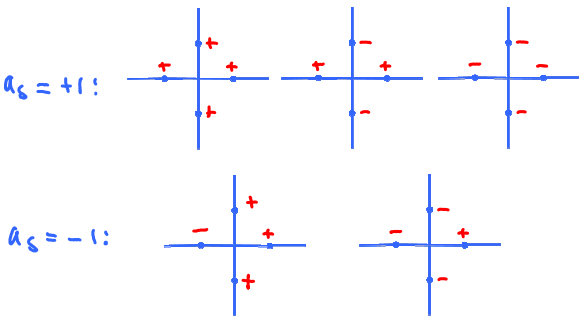
because all stars and plaquettes share an even number of edges (0 or 2);

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

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

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

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

Note: $a_s = 1$ $\Rightarrow$ all +, or all - , or two +, two -, on every star (11)

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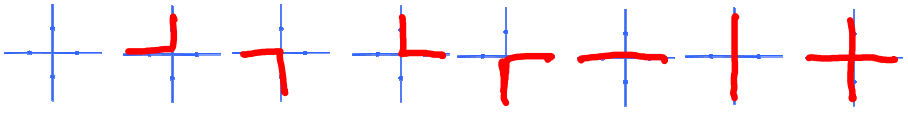
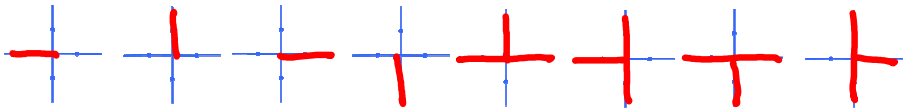
Graphical notation:  (12)

Allowed configurations: 

Forbidden configurations: 

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

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

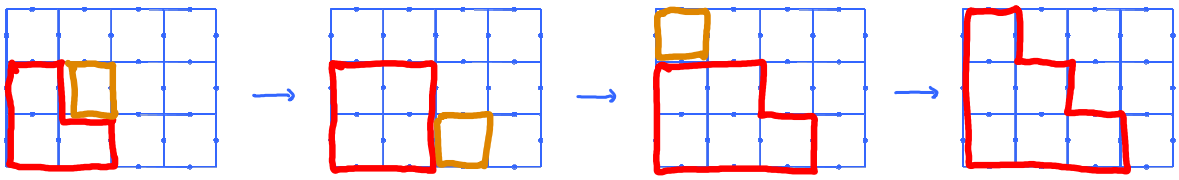
- $\hat{B}_p$ flips all spins on plaquette, hence maps 'allowed configuration' to 'allowed configuration'.

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:

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

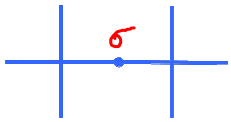
Spin flips of plaquette operator are 'ergodic', i.e. any closed loop $|\vec{\sigma}\rangle$ can be mapped to any other $|\vec{\sigma}'\rangle$ closed loop by a series of plaquette operators. Hence, all $c^{\vec{\sigma}}$ must be equal:

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

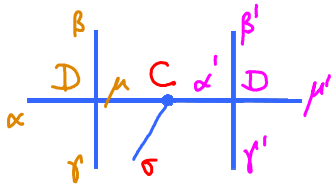
equal-weight superposition of all closed-loop configurations (16)

PEPS representation: [Verstraete2006]

the local variable $\sigma = \pm 1$,



is represented by

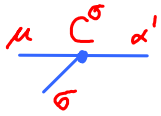


(17)

$\alpha, \beta, \gamma, \mu \in \{\pm 1\}$

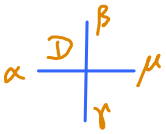
$D = 2$

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)

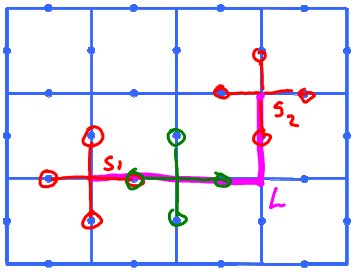
PEPS formulation is generalizable to all 'string-net' models', [Gu2009]
which realize all non-chiral topological order in 2+1 dimensions. [Buerschaper2009]

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 .



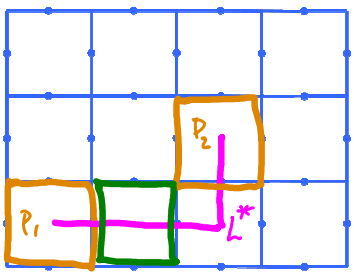
Then $[\hat{E}_L, \hat{B}_p] = 0$ (since both are built only from $\hat{\sigma}^x$) (22)

$\hat{E}_L \hat{A}_s = \mp \hat{A}_s \hat{E}_L$ 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



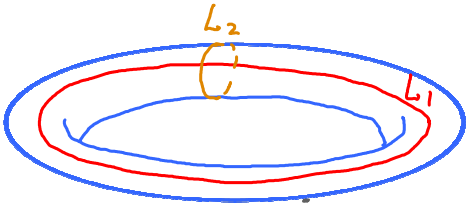
Then $[\hat{M}_{L^*}, \hat{A}_s] = 0$ (since both are built only from σ^z) (26)

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

$\hat{M}_{L^*} \hat{B}_p = \mp \hat{B}_p \hat{M}_{L^*}$ 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 $2 J_M$. (28)

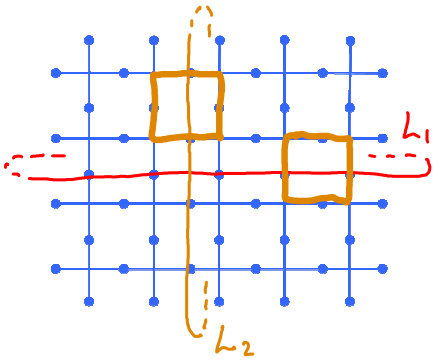
Toric code on torus



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'

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



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

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

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

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:

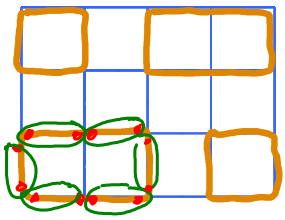
$$\hat{A}_{L_1} |g, a_{L_1}, a_{L_2}\rangle = a_{L_1} |g, a_{L_1}, a_{L_2}\rangle \,, \quad \hat{A}_{L_2} |g, a_{L_1}, a_{L_2}\rangle = a_{L_2} |g, a_{L_1}, a_{L_2}\rangle$$

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

4. Example: Resonating AKLT loop state (RAL)

Consider square lattice, spin 1 on every site:

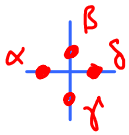
$|RAL\rangle$ = (equal-weight superposition of all fully packed AKLT loop coverings) [Yao2010]



- 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 $|\alpha\rangle \in \{|e\rangle, |\uparrow\rangle, |\downarrow\rangle\}$

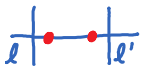
empty up down

(D= 3)

form auxiliary spin-1/2

- 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 :

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

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 ℓ,ℓ'