Honeycomb-AKLT Model's Ground State as PEPS

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1 Introduction: Honeycomb AKLT

We want to calculate the PEPS representation of the ground state (GS) of the AKLT model for spin-3/2 on a Honeycomb bipartite lattice. According to [1] the GS is the projection on the spin-3/2 space of the collection of singlet-state on virtual spin-1/2 bonds between each real node of the lattice, so we will follow the procedure outlined in Tutorial #4.

According to [2] section 5.2.2 the singlet-bond state (SB, singlet on each bond on a Honeycomb lattice) is:

$$|\mathrm{SB}\rangle = \prod_{(i,j)\in\mathbb{B}} \frac{|\downarrow\rangle_i |\uparrow\rangle_j - |\uparrow\rangle_i |\downarrow\rangle_j}{\sqrt{2}}$$

While the projection operator is:

$$\begin{aligned} P_{\mathrm{sym}} &= \left|\frac{3}{2}\right\rangle \langle\uparrow\uparrow\uparrow| + \left|\frac{1}{2}\right\rangle \langle U| + \left|-\frac{1}{2}\right\rangle \langle D| + \left|-\frac{3}{2}\right\rangle \langle\downarrow\downarrow\downarrow| \\ |U\rangle &= \frac{1}{\sqrt{3}} \left(|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle\right) \\ |D\rangle &= \frac{1}{\sqrt{3}} \left(|\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\rangle\right) \end{aligned}$$

So the total ground state is:

$$|\psi\rangle = P_{\mathrm{sym}} |\mathrm{SB}\rangle$$

We will now convert this symbolic representation of the ground state into a proper PEPS.

2 Conversion to PEPS

In order to convert this state into a PEPS, we will follow a similar procedure to the one done on the MPS shown in class. First, we will define the singlet matrix:

$$\Sigma = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

Assuming a general PEPS network, in the ground state each bond $\mathcal{B} = (i,j) \in \mathbb{B}$ will have its corresponding $\Sigma_{\mathcal{B}}$. Next, we also define the projection operator:

$$\begin{aligned} \Theta^{3/2}_{abc} &= \delta_{a,\uparrow}\delta_{b,\uparrow}\delta_{c,\uparrow} \\ \Theta^{1/2}_{abc} &= \tfrac{1}{\sqrt{3}} \left(\delta_{a,\uparrow}\delta_{b,\uparrow}\delta_{c,\downarrow} + \delta_{a,\uparrow}\delta_{b,\downarrow}\delta_{c,\uparrow} + \delta_{a,\downarrow}\delta_{b,\uparrow}\delta_{c,\uparrow}\right) \\ \Theta^{-1/2}_{abc} &= \tfrac{1}{\sqrt{3}} \left(\delta_{a,\downarrow}\delta_{b,\downarrow}\delta_{c,\uparrow} + \delta_{a,\downarrow}\delta_{b,\uparrow}\delta_{c,\downarrow} + \delta_{a,\uparrow}\delta_{b,\downarrow}\delta_{c,\downarrow}\right) \\ \Theta^{-3/2}_{abc} &= \delta_{a,\downarrow}\delta_{b,\downarrow}\delta_{c,\downarrow} \end{aligned}$$

In the PEPS every site will correspond to an operator $\Theta^{\sigma}_{\mathcal{S}}$ like that, where $\mathcal{S} = (a,b,c) \in \mathbb{S}$ are the bond indices of each site. Note that the notation a,b,c and the notation i,j are different names for the same total set of indices in different permutations, and they contract with each other when multiplied.

So, the resulting final PEPS is:

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \left(\prod_{\mathcal{S}\in\mathbb{S}} \Theta^{\sigma}_{\mathcal{S}} \right) \left(\prod_{\mathcal{B}\in\mathbb{B}} \Sigma_{\mathcal{B}} \right) |\boldsymbol{\sigma}\rangle$$

Where the indices of $\mathbb{S}$ contract with indices of $\mathbb{B}$, as said before. But this is formally not a PEPS state yet – in order convert that into a PEPS, we need to assign each matrix $\Sigma_{\mathcal{B}}$ to an operator $\Theta^{\sigma}_{\mathcal{S}}$, and contract them together, converting the whole state into the following form:

$$|\psi\rangle = \sum_{\boldsymbol{\sigma}} \prod_{\mathcal{S}\in\mathbb{S}} A^{\sigma}_{\mathcal{S}} |\boldsymbol{\sigma}\rangle$$

This, theoretically, can be done in any order (as long as the contracted indices are compatible), and the resulting set of tensors $\{A^{\sigma}_{abc}\}$ is the final PEPS. In our case, we chose to just loop over the bonds of the lattice and assign randomly a Σ matrix for one of the vertices of the bonds.

3 Contraction

The contraction part of the code was the trickiest. First, we tried to use the `SVD` method we used for MPS, but this failed, since that method is base upon the assumption that it is possible to make all of the A tensors normalized to $\sum_{\sigma} (A^{\sigma})^{\dagger} A^{\sigma} = \mathbb{1}$ except for the orthogonality center, but this is impossible in any case where there are loops in the system.

Instead, in general 2D systems require full contraction of all of the tensors together. This is very hard to automate and is generally regarded as the main issue with PEPS models. So, we chose to use hard-coded orders for several lattice geometries:

- A Single Hexagon: This case is similar to the MPS case with 6 identical vertices, and the contraction just goes along the circle.
- A Triple Node: A central nofe connected to three other nodes. Since this is a very small configuration, we can just contract it in one sweep.
- An Arbitrary Length Line: Similar to the Hexagon, but with arbitrary length and OBC. The contraction here can be done by iterative manner along the line.

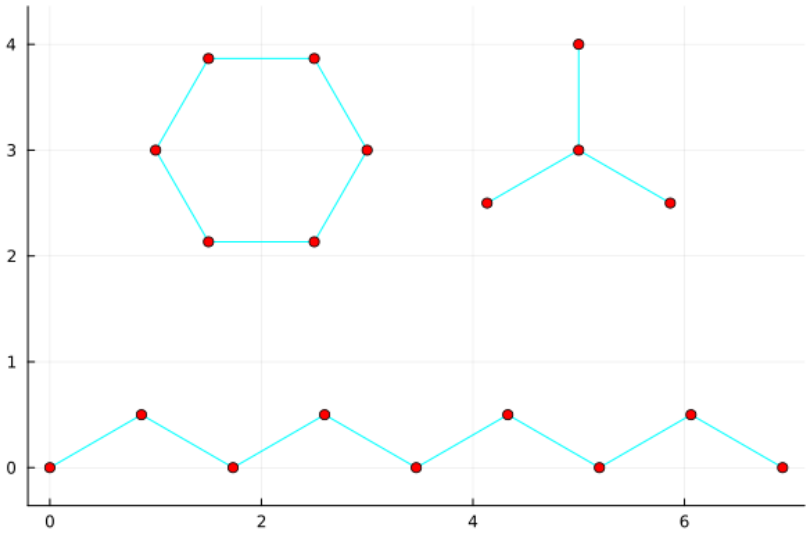

Figure 1: An example of the three lattices used in the script: a hexagon, triple junction and a line. Yes, it does look like a face.

4 Results

The results of the code **generally** followed what was expected from analytical theory: each vertex "split" into three virtual 1/2-spins, each pair corresponding to a single bond. The pairs were symmetric and their total spin is always 0, while the edge states where not canceled and their spin depended on the amount of free bonds: a single free bond corresponds to a spin 1/2 on the edge, while two correspond to spin 1.

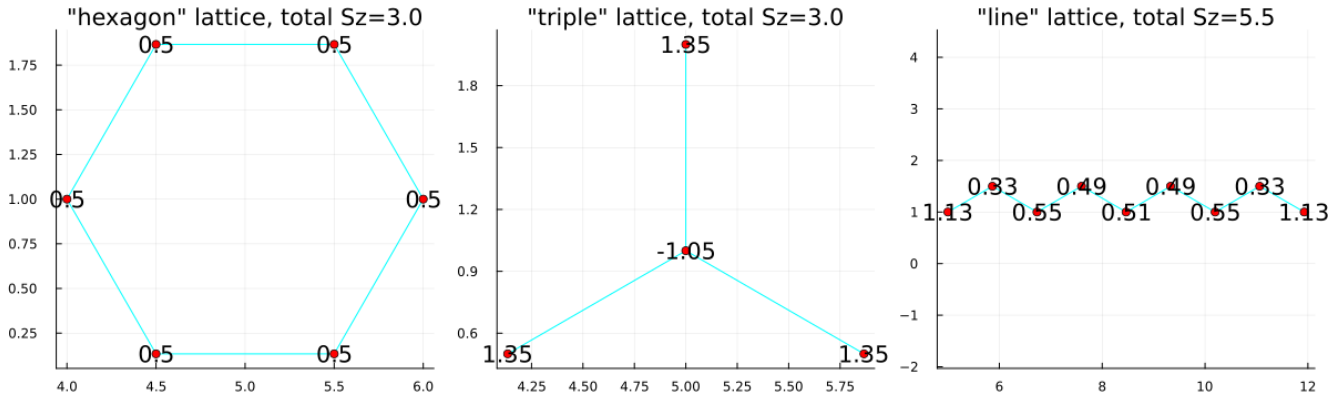

Figure 2: The results of the spin expectation value for each vertex in each PEPS geometry The expectation value for each vertex is written on it.

W say generally, since as can be seen in 2, this is not what is seen in reality. Boundary effects destroy the symmetry of the solution shown above, thus we resort to global measures of the correctness of our calculation. Specifically, we look at the total spin on each lattice, and observe that it indeed fits our expectations:

- Hexagon: $\frac{1}{2} \cdot 6 = 3$
- Triple: $0 + 1 \cdot 3 = 3$
- Line: $2 \cdot 1 + 7 \cdot \frac{1}{2} = 5.5$

So the boundaries only smeared the result, but not changed it in any massive manner.

References

[1] Ian Affleck, Tom Kennedy, Elliott H. Lieb, and Hal Tasaki. Rigorous results on valence-bond ground states in antiferromagnets. *Phys. Rev. Lett.*, 59(7):799–802, August 1987.

[2] Román Orús. A practical introduction to tensor networks: Matrix product states and projected entangled pair states. *Annals of Physics*, 349:117–158, October 2014.