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Haldane's conjecture, and AKLT chain

References

- An introduction to lattice gauge theory and spin systems by John B. Kogut (1979)
- (Online Lecture) The Haldane Phase as a Symmetry-protected Topological Phase and Quantum Entanglement by Masaki Oshikawa
- Non-Invertible Duality Transformation Between SPT and SSB Phases by Linhao Li, Masaki Oshikawa, Yunqin Zheng (2024)

Heisenberg Model for Spin Chains and Haldane's conjecture

The Hamiltonian for a one-dimensional Heisenberg spin chain is given by:

$$H = -J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \tag{1}$$

where J is the exchange interaction between neighboring spins, and $\vec{S}_i$ represents the spin operator at site i. We will focus on the $J < 0$ case, which indicates anti-ferromagnetism.

Spin-$\frac{1}{2}$ Operators

For spin-$\frac{1}{2}$ particles, the spin operators are represented by Pauli matrices:

$$S^x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

Spin-1 Operators

For $S = 1$ spin chains, the spin operators expand to 3×3 matrices:

$$S^x = \frac{\sqrt{2}}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^y = \frac{\sqrt{2}}{2}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{3}$$

Haldane's Conjecture (1980)

Haldane's conjecture concerns the one-dimensional *antiferromagnetic* Heisenberg spin chain. It states that the low-energy behavior depends crucially on whether the spin S is integer or half-integer:

1. For *integer* spin S, the chain has a finite excitation gap above the ground state (the *Haldane gap*) and exhibits exponentially decaying spin correlations.
2. For *half-integer* spin S, the chain is gapless, with low-energy excitations extending down to zero energy and spin correlations that decay algebraically.

Thus, even though the Hamiltonian has the same form for different values of S, integer-spin and half-integer-spin antiferromagnetic chains belong to qualitatively different quantum phases.

AKLT model

In condensed matter physics, an **AKLT model**, also known as an **Affleck-Kennedy-Lieb-Tasaki model** is an extension of the one-dimensional quantum Heisenberg spin model. The proposal and exact solution of this model by Ian Affleck, Elliott H. Lieb, Tom Kennedy and Hal Tasaki provided crucial insight into the physics of the spin-1 Heisenberg chain. It has also served as a useful example for such concepts as valence bond solid order, *symmetry-protected topological order*, and matrix product state wavefunctions.

A major motivation for the AKLT model was the Majumdar–Ghosh chain. Because two out of every set of three neighboring spins in a Majumdar–Ghosh ground state are paired into a singlet, or valence bond, the three spins together can never be in a spin 3/2 state. In fact, the Majumdar–Ghosh Hamiltonian is nothing but the sum of all projectors of three neighboring spins onto a 3/2 state.

The main insight of the AKLT paper was that this construction could be generalized to obtain exactly solvable models for spin sizes other than 1/2. Just as one end of a valence bond is a spin-$\frac{1}{2}$, the ends of two valence bonds can be combined into a spin-1, three into a spin 3/2, etc.

Construction of the Spin-1 Chain

Affleck, Kennedy, Lieb, and Tasaki explored the formulation of a one-dimensional quantum state characterized by a valence bond between each pair of neighboring sites. This structure necessitates that the combined system exhibits spin-1 behavior at each site.

Hamiltonian Derivation

In the AKLT model, adjacent spin-1 particles cannot achieve a collective spin-2 state. This restriction is mathematically encoded using projection operators, leading to the AKLT Hamiltonian:

$$\hat{H} = \sum_i P_2(\boldsymbol{S}_i + \boldsymbol{S}_j) \sim \sum_j \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} + \frac{1}{3}(\boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1})^2 \tag{4}$$

up to a constant, where the $\boldsymbol{S}_j$ are spin-1 operators, and $P_2(\vec{S}_i + \vec{S}_{i+1})$ the local 2-point projector that favors the spin-2 state of an adjacent pair of spins. Let's provide the derivation here.

$$\vec{J}_i \equiv \vec{S}_i + \vec{S}_{i+1}$$

J_i	$P_2 J_i$
$j=0$	0
$j=1$	0
$j=2$	1

$$\Rightarrow P_2 \vec{J}_i = \frac{1}{24}\vec{J}_i^2(\vec{J}_i^2 - 2)$$

$$\begin{aligned}
\Rightarrow H &= \frac{1}{24}\sum(\vec{S}_i + \vec{S}_{i+1})^2\left((\vec{S}_i + \vec{S}_{i+1})^2 - 2\right) \\
&= \frac{1}{24}\sum(2\vec{S}_i \cdot \vec{S}_{i+1} + 4)(2\vec{S}_i \cdot \vec{S}_{i+1} + 2) \\
&= \frac{1}{2}\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{6}(\vec{S}_i \cdot \vec{S}_{i+1})^2 + \frac{1}{3} \\
\Rightarrow H_{\text{AKLT}} &= \sum\left[\vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2\right]
\end{aligned}$$

This Hamiltonian is similar to the spin-1, one-dimensional quantum Heisenberg spin model but has an additional "biquadratic" spin interaction term.

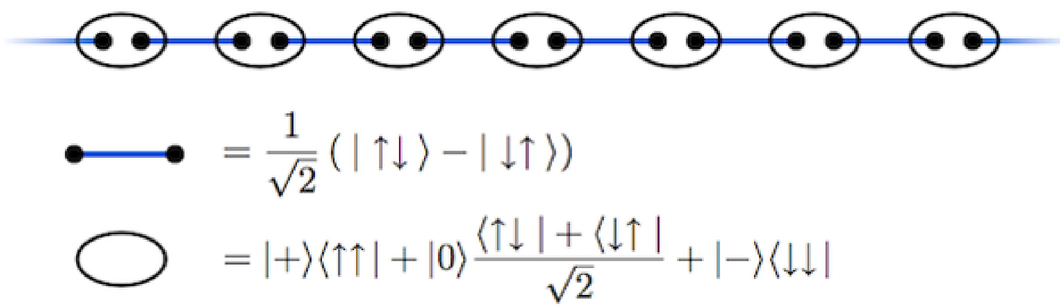


Figure 1: The ground state depiction of an AKLT chain: blue lines represent valence bonds forming spin singlets, and circles indicate the projection of two spin-$\frac{1}{2}$ particles into an effective spin-1 state.

Figure 2: Spin chain with residual spin-$\frac{1}{2}$ at each end and the effective coupling between them.

Consider a spin chain with boundary spins that are not fully paired, leading to residual spin-$\frac{1}{2}$ degrees of freedom at the ends of the chain. The Hamiltonian for such a system can be affected by the coupling between these residual spins across the chain. For a chain of length L, the effective coupling J can be expressed as a function of L and the correlation length ξ, as shown below:

- Two $s = \frac{1}{2}$ spins left at the end.
- The coupling of different spins $J \sim e^{-L/\xi}$.

This leads to $2 \times 2 = 4$ (nearly) degenerate ground states, due to the combinatorial possibilities of the boundary spins.

We analyze the spin chain using the S^z basis, where $+$ and $-$ alternate, ignoring the zero states.

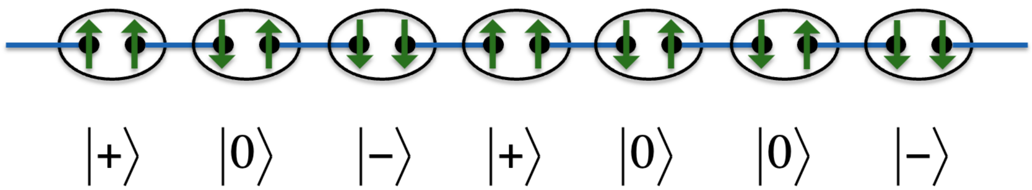


Figure 3: Spin chain representation in S^z basis.

Hidden topological order can be characterized by the string order parameter, originally described by Den Nijs and Rommelse in 1989:

$$O^{\alpha}_{\text{str}} = \lim_{|j-k|\to\infty} \langle S^{\alpha}_j e^{-i\pi \sum_{l=j}^{k-1} S^{\alpha}_l} S^{\alpha}_k \rangle := \lim_{|j-k|\to\infty} \langle \sigma^{\alpha}_{ij} \rangle \tag{5}$$

This is analogous to the anti-ferromagnetic Néel order:

$$O^{\alpha}_{\text{Néel}} = \lim_{|j-k|\to\infty} (-1)^{j-k} \langle S^{\alpha}_j S^{\alpha}_k \rangle \tag{6}$$

Nonlocal Unitary Transform in Finite Spin Chains

- The transform leaves all 0's unchanged and affects $+$ or $-$ at site j.
- For a $+$ or $-$ at site j, count the number of $+$ and $-$ on the left, flipping the spin if the count is odd.
- Count the number of 0's at an odd site, and if the number is odd, multiply the state by -1.

$$\begin{aligned}
(0+0--0++-+0-0) &\to (0+0+-0-++0+0) \\
(0+-00+00-+0-0) &\to -(0++00+00++0+0) \\
(+-0+-00+0-0+-) &\to (++0++00+0+0++)
\end{aligned}$$

This unitary operator is defined as the Kennedy-Tasaki transformation:

$$U_{KT} = \prod_{j<k} \exp\big(i\pi S^z_j S^x_k\big). \tag{7}$$

For further details, refer to *Non-Invertible Duality Transformation Between SPT and SSB Phases* by Linhao Li, Masaki Oshikawa, and Yunqin Zheng.

Exercise to verify the rules above. Note that

$$\exp(i\pi S_x) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}. \tag{8}$$

This transformation converts the string order into spontaneous symmetry-breaking (SSB) order.

Hidden $\mathbb{Z}_2 \times \mathbb{Z}_2$ Symmetry

$$H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1} \tag{9}$$

$$H' = UHU^{-1} = \sum_j \left(-S_j^x S_{j+1}^x + S_j^y \exp\left[i\pi(S_j^z + S_{j+1}^x)\right] S_{j+1}^y + S_j^z \exp\left(i\pi S_j^z\right) S_{j+1}^z\right) \tag{10}$$

Another homework exercise.

- The transformed Hamiltonian H' remains invariant under π rotations about three coordinate axes.
- This defines a global discrete symmetry group $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$.

Spontaneous $\mathbb{Z}_2 \times \mathbb{Z}_2$ Symmetry Breaking

- Spontaneous symmetry breaking results in 4-fold degenerate ground states for H'.
- The presence of edge states indicates a nontrivial phase in H and ferromagnetic order $O^\alpha_{\text{ferro}} = \lim_{|j-k|\to\infty} \langle S_j^\alpha S_k^\alpha \rangle$ in H'.

4-fold degenerate ground states in H' $\Longleftrightarrow$ 4-fold degenerate ground states in H with open boundary condition

Ferromagnetic order in H' $\Longleftrightarrow$ String order in H

Nontrivial phase in H' $\Longleftrightarrow$ Nontrivial phase in H

The transformations between the operators under the unitary transformation are given by:

$$H' = UHU^{-1}$$

$$S_j^z S_k^z = U(S_j^z e^{-i\pi \sum_{l=j}^{k-1} S_l^z} S_k^z) U^{-1}$$

Hamiltonian H is described as local. Subjected to a specific nonlocal transformation, the resultant Hamiltonian H' retains its locality, implying the existence of a certain symmetry.

The existence of this symmetry indicates a protected topological phase within the Hamiltonian's structure. Therefore, there must exist global $D_2 = \mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in H. $S = 1$ Haldane phase is a topological phase protected by global D_2 symmetry.

Edge States in Spin Chains

The AKLT model is known for its edge states with spin-$\frac{1}{2}$, which raises the question of the existence of such states in more general models. When general perturbations are applied to the AKLT model, they can potentially lift the edge degeneracy.

Perturbation Analysis:

- Applying a general perturbation to the AKLT model may lift the edge degeneracy.
- If the perturbation respects time reversal symmetry, the Kramers degeneracy for spin-$\frac{1}{2}$ edge states is preserved.

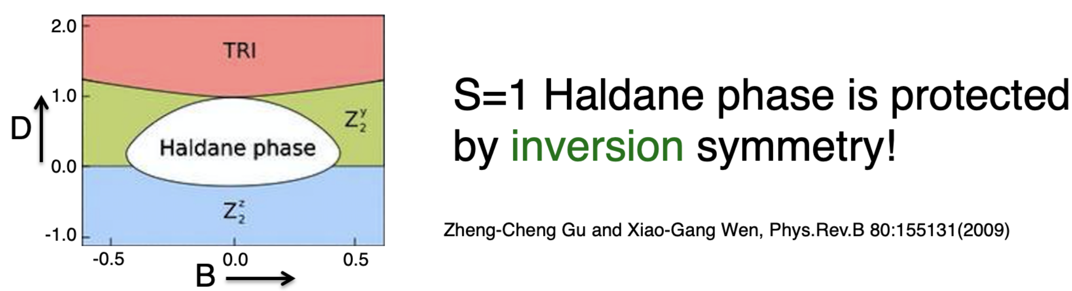
The Haldane phase for spin-1 systems is also noted for being protected by the time reversal symmetry, similar to edge states in $\mathbb{Z}_2$ topological insulators.

More symmetry

The Hamiltonian for a spin chain with anisotropy and external magnetic field can be expressed as:

$$H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + B_x \sum_j S_j^x + D \sum_j (S_j^z)^2 \tag{11}$$

where B_x the external magnetic field, and D the anisotropy parameter. This family of Hamiltonians has the following phase diagram:

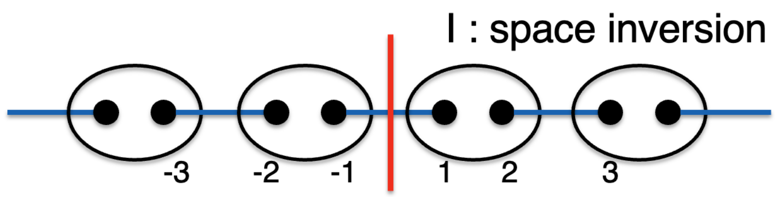


(12)

We examine the symmetries and their consequences:

- The D_2 symmetry, associated with π rotations around the x, y, and z axes, is generally not preserved in the presence of such perturbations.
- Time reversal symmetry is also broken.

There will still be an inversion symmetry:



Valence bond: $|a,b\rangle \equiv \frac{1}{\sqrt{2}}[|\uparrow\rangle_a |\downarrow\rangle_b - |\downarrow\rangle_a |\uparrow\rangle_b]$

$I|a,b\rangle = |-a,-b\rangle = -|-b,-a\rangle$

$\Rightarrow I|-1,1\rangle = -|-1,1\rangle$ → This bond make AKLT state parity odd

$I|2,3\rangle|-3,-2\rangle = +|2,3\rangle|-3,-2\rangle$

$$I|\Omega\rangle = -|\Omega\rangle \tag{13}$$

S=1 AKLT ground state has odd parity

↕ Can not be adiabatically connected
➔Phase transition

$|\Psi\rangle = \otimes_j |\psi\rangle_j$

The trivial ground state has even parity

The summary of the behavior of the Haldane chain under different symmetries is:

symmetry	string order	edge states	degeneracy
D_2 $(=Z_2 \times Z_2)$	yes	yes	yes
time reversal	no	yes	yes
inversion	no	no	yes

(14)

The 4-fold degeneracy always exists!

1 Symmetry protected topological order in 1D bosonic systems

1.1 Examples

Let's start by introducing some simple models with nontrivial SPT order in 1D. The AKLT model on a spin 1 chain discussed in Chap. 8 is a prototypical example. The Hamiltonian of the AKLT model is

$$H_{\text{AKLT}} = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2 \tag{15}$$

where S is the spin 1 spin operator. This Hamiltonian is obviously invariant under the $SO(3)$ spin rotation symmetry generated by S^x, S^y and S^z. The ground state wave function of this Hamiltonian can be explicitly constructed using a simple projected entangled pair picture.

Each lattice site (big oval) contains two spin 1/2s (small circle), which form singlet pairs (connected bonds) $|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle$ with another spin 1/2 on a neighboring site. By projecting the two spin 1/2s on each lattice site to a spin 1, we obtain the ground state wave function H_{AKLT}.

On a ring with periodic boundary condition, the ground state preserves spin rotation symmetry and is unique and gapped. On a chain with boundary, on the other hand, there are isolated spin 1/2s at each end of the chain which are not coupled with anything and give rise to a two fold degenerate edge state. The full ground state on an open chain is hence four fold degenerate. The degenerate edge state is stable as long as spin rotation symmetry is preserved. In particular, spin 1/2s transform under spin rotation in a very special way with a 2π rotation around any axis giving rise to a -1 phase factor. Because of this, the edge state cannot be smoothly connected to a trivial spin 0, which gets a phase factor of 1 under 2π rotation, without closing the bulk gap. With a gapped symmetric bulk and degenerate edge states protected by spin rotation symmetry, the AKLT model is hence in a nontrivial SPT phase.

SPT order of the AKLT model The 1D AKLT model has a nontrivial symmetry-protected topological order protected by $SO(3)$ spin rotation symmetry, as indicated by its degenerate spin 1/2 edge state.

The 1D cluster state on a spin 1/2 chain provides another example of a nontrivial SPT order. The Hamiltonian of the 1D cluster state is

$$H_{\text{clu}} = -\sum_j Z_j X_{j+1} Z_{j+2} \tag{16}$$

For a 1D ring without boundary, the ground state of H_{clu} is the unique graph state stabilized by $\{Z_j X_{j+1} Z_{j+2}\}$. For a chain with boundary, where the summation index j runs from 2 to $N-1$, the ground state is then 4-fold degenerate.

This 4-fold degeneracy is a result of two edge states, each being 2-fold degenerate protected by a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry. The $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is generated by

$$\tilde{X}_1 = \prod_k X_{2k-1}, \quad \tilde{X}_2 = \prod_k X_{2k}, \tag{17}$$

Any local perturbation to the system cannot lift the degeneracy as long as this $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry is preserved. To see this, first we notice that the effective Pauli $\tilde{X}$ and $\tilde{Z}$ operators on the 2-fold degenerate edge states (at the left end of the chain for example) can be chosen as $\tilde{X} = X_1 Z_2$ and $\tilde{Z} = Z_1$, which commute with all the bulk Hamiltonian terms and anti-commute with each other. Next, we find that the effective action of $\tilde{X}_1$ and $\tilde{X}_2$ on the edge state is the same as $\tilde{X}$ and $\tilde{Z}$ because

$$\tilde{X}_1 \prod_{k=2}^{\infty}(Z_{2k-2}X_{2k-1}Z_{2k}) = X_1 Z_2 = \tilde{X}, \quad \tilde{X}_2 \prod_{k=1}^{\infty}(Z_{2k-1}X_{2k}Z_{2k+1}) = Z_1 = \tilde{Z} \tag{18}$$

From this, we can see that the $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry acts on the edge state in a very special way: the two $\mathbb{Z}_2$'s anti-commute with each other! Because of this, the edge state must be at least two-fold degenerate, and the degeneracy cannot be removed without breaking the symmetry or going through a bulk phase transition. This demonstrates the nontrivialness of the SPT order in the cluster state.

SPT order of the cluster state model The 1D cluster state model has nontrivial symmetry protected topological order protected by a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry, as indicated by its two-fold degenerate edge state.

Through the AKLT model and the cluster state model, we see some common features of SPT order in 1D: the bulk wave function is gapped and symmetric. In contrast, the edge state must be degenerate because it transforms in a nontrivial way under the symmetry. This picture can be generalized to all kinds of symmetries, and we want to understand what 1D SPT phases exist in general with any given symmetry. The matrix product formalism again provides a powerful tool for addressing this question.