MPS II: Diagonalization, fermonic signs; Translationally invariant MPS; AKLT model

[credit for course materials: Prof. Jan von Delft]

Iterative diagonalization and Fermionic signs

1. Iterative diagonalization

Consider spin-$\frac{1}{2}$ chain with Hamiltonian $H^N = \sum_{l=1}^{N} \hat{\vec{S}}_l \cdot \vec{h}_l + J \sum_{l=2}^{N} \hat{\vec{S}}_l \cdot \hat{\vec{S}}_{l-1}$

For later convenience, we write the spin-spin interaction in covariant notation. Define

$$\hat{S}_z \equiv \hat{S}^{+z} \; ; \quad \hat{S}_{\pm} \equiv \frac{1}{\sqrt{2}}\left(\hat{S}_x \pm i \hat{S}_y\right) \; ; \quad \hat{S}^{+\pm} \equiv \frac{1}{\sqrt{2}}\left(\hat{S}_x \mp i \hat{S}_y\right)$$

and the operator triplet $\hat{\vec{S}}_l \cdot \hat{\vec{S}}_{l-1} = \hat{S}^x_l \hat{S}^x_{l-1} + \hat{S}^y_l \hat{S}^y_{l-1} + \hat{S}^z_l \hat{S}^z_{l-1}$

$$= \hat{S}^{+}_{l} \hat{S}_{+\,l-1} + \hat{S}^{+-}_{l} \hat{S}_{-(l-1)} + \hat{S}^{+z}_{l} \hat{S}_{z\,l-1}$$

Then the dot product term is:

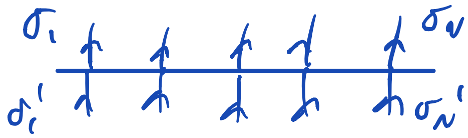
$$\hat{S}_a \equiv \{\hat{S}_+, \hat{S}_-, \hat{S}_z\} \qquad = \hat{S}^{+a}_l \hat{S}_{a,l-1}$$

$$\hat{S}^{+a} \equiv \{\hat{S}^{++}, \hat{S}^{+-}, \hat{S}^{+z}\}$$

The Hamiltonian can be expressed in the basis: $\{|\bar{\sigma}\rangle_N\} = \{|\sigma_N\rangle \ldots |\sigma_2\rangle|\sigma_1\rangle\}$

$$\hat{H}^N = |\bar{\sigma}'\rangle H^{\bar{\sigma}'}_{\bar{\sigma}} \langle \bar{\sigma}|$$

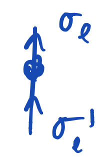
$H^{\bar{\sigma}'}_{\bar{\sigma}}$ is a linear map acting on a direct product space: $V^{\otimes N} = V_1 \otimes V_2 \ldots \otimes V_N$



where V_ℓ is the 2D representation space of site ℓ .

$\hat{H}^N$ is a sum of single-site and two-site terms.

one ~~On~~-site terms: $\hat{S}_{a\ell} = |\sigma_\ell'\rangle (S_a)^{\sigma_\ell'}{}_{\sigma_\ell} \langle\sigma_\ell|$

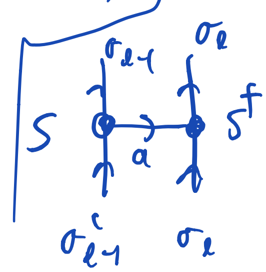


Matrix representation in V_ℓ : $(S_a)^{\sigma_\ell'}{}_{\sigma_\ell} = \langle\sigma_\ell'|\hat{S}_{a\ell}|\sigma_\ell\rangle = \begin{pmatrix} (S_a)^\uparrow{}_\uparrow & (S_a)^\uparrow{}_\downarrow \\ (S_a)^\downarrow{}_\uparrow & (S_a)^\downarrow{}_\downarrow \end{pmatrix}$

$$S_+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad S_- = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad S_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Nearest-neighbor interactions, acting on direct product space, $|\sigma_\ell\rangle \otimes |\sigma_{\ell-1}\rangle$

$$\hat{S}^{\dagger a}_\ell \otimes \hat{S}_{a\ell-1} = |\sigma_\ell'\rangle|\sigma_{\ell-1}'\rangle (S_a)^{\sigma_{\ell-1}'}{}_{\sigma_{\ell-1}} (S^{\dagger a})^{\sigma_\ell'}{}_{\sigma_\ell} \langle\sigma_{\ell-1}|\langle\sigma_\ell|$$



Matrix representation in $V_{\ell-1} \otimes V_\ell$:

(notation) $$S^{\sigma_{\ell-1}'}{}_{a\sigma_{\ell-1}} \; S^{\dagger\,\sigma_\ell' a}{}_{\sigma_\ell}$$

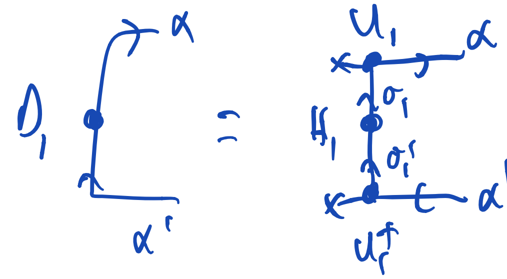
We define the 3-leg tensors $S, S^\dagger$ with index placements matching those of tensors for wave functions: incoming up, outgoing down, with a (by convention) as middle index. Arrow for a goes from annihilation to creation.

Diagonalize site 1

$H_1 =$ 

$$H_1 = \hat{S}^{\dagger}_{a1} \cdot h^{a}_{1} = U_1 D_1 U_1^{\dagger}$$

chain of length 1 site index $l=1$

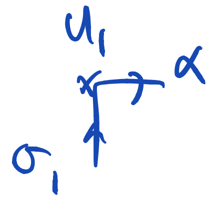


$D_1 = U_1^{\dagger} H_1 U_1$ is diagonal, with matrix elements

$$(D_1)^{\alpha'}_{\alpha} = (U_1^{\dagger})^{\alpha'}_{\sigma_1'} (H_1)^{\sigma_1'}_{\sigma_1} (U_1)^{\sigma_1}_{\alpha}$$

Eigenvectors of the matrix H_1 are given by column vectors of the matrix U_1 :

Eigenvectors of operator $\hat{H}_1$ are given by : $|\alpha\rangle = |\sigma_1\rangle (U_1)^{\sigma_1}_{\alpha}$



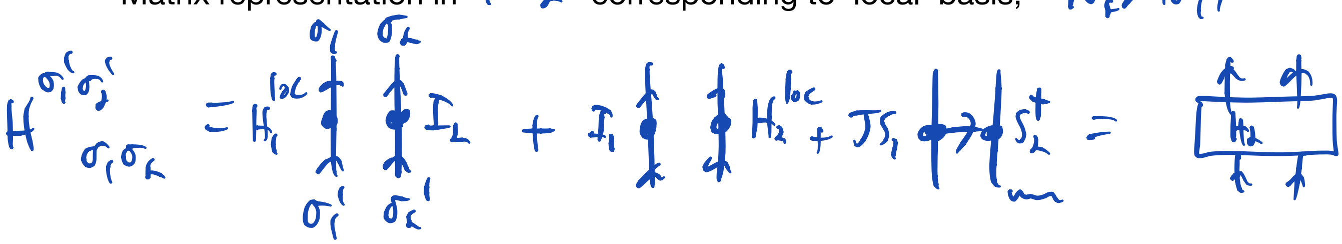
Add site 2

Diagonalize H_2 in enlarged Hilbert space, $\mathcal{H}_2 = \text{span}\{|\sigma_2\rangle|\sigma_1\rangle\}$

chain of length 2

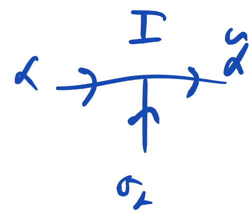
$$H_2 = I_2 \otimes \hat{S}_1 \cdot \bar{h}_1 + \hat{S}_2 \cdot \bar{h}_2 \otimes I_1 + J \hat{S}_{a1} \hat{S}_2^{\dagger a}$$

Matrix representation in $V_1 \otimes V_2$ corresponding to 'local' basis, $|\sigma_2\rangle|\sigma_1\rangle$

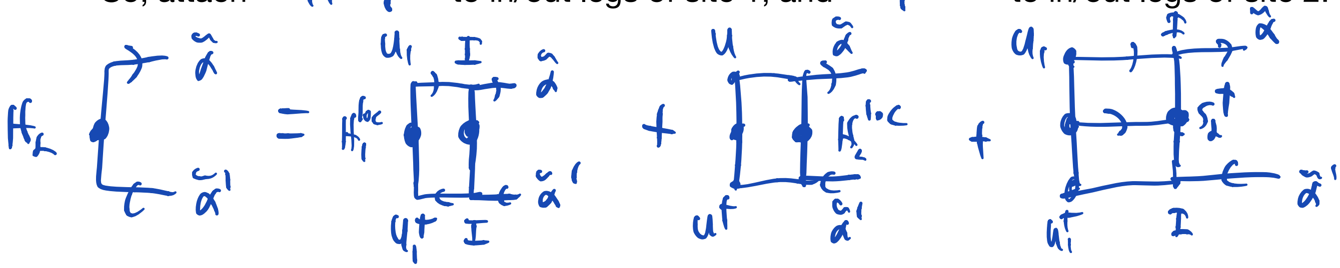


We seek matrix representation in $V_1 \otimes V_2$ corresponding to enlarged, 'site-1-diagonal' basis, defined as

$$|\tilde{\alpha}\rangle \equiv |\alpha \sigma_2\rangle \equiv |\sigma_2\rangle|\alpha\rangle$$



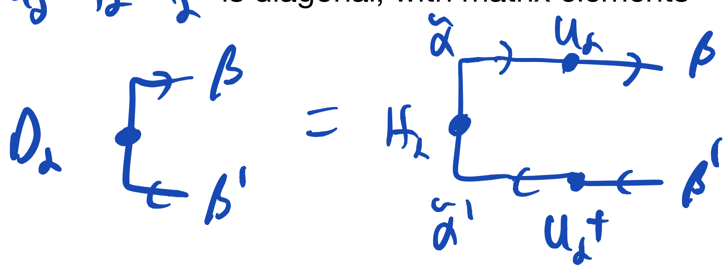
So, attach $U_1^\dagger, U_1$ to in/out legs of site 1, and I, I to in/out legs of site 2:



First term is diagonal. But others are not.

Now diagonalize H_2 in this enlarged basis: $H_2 = U_2 D_2 U_2^\dagger$

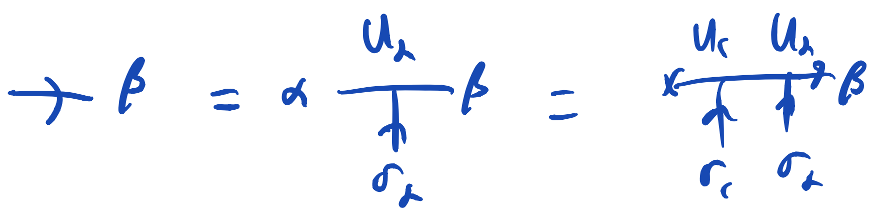
$D_2 = U_2^\dagger H_2 U_2$ is diagonal, with matrix elements



Eigenvectors of matrix H_2 are given by column vectors of the matrix $(U_2)^{\tilde\alpha}_{\beta} = (U_2)^{\alpha\sigma_2}_{\beta}$

Eigenstates of the operator $\hat{H}_2$

$$|\beta\rangle = |\tilde\alpha\rangle (U_2)^{\tilde\alpha}_{\beta} = |\sigma_2\rangle|\alpha\rangle (U_2)^{\alpha\sigma_2}_{\beta} = |\sigma_2\rangle|\sigma_1\rangle (U_1)^{\sigma_1}_{\alpha} (U_2)^{\alpha\sigma_2}_{\beta}$$

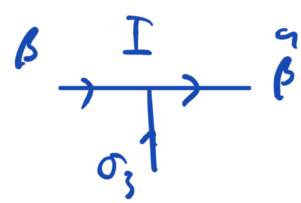


Add site 3

Transform each term involving new site into the 'enlarged, site 1,2 diagonal basis',

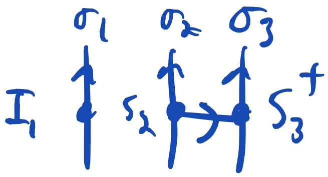
defined as:

$$|\tilde\beta\rangle \equiv |\beta\sigma_3\rangle \equiv |\sigma_3\rangle|\beta\rangle$$



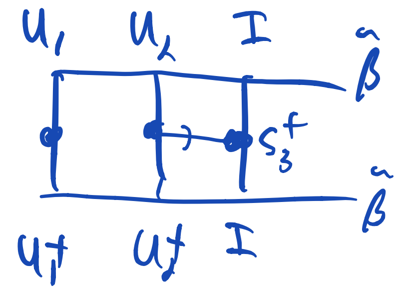
For example, spin-spin interaction, H^{int}_{32}

Local basis:



enlarged,

site-1,2 diagonal basis



Then diagonalize in this basis: $H_3 = U_3 D_3 U_3^\dagger$

Etc. At each iteration, Hilbert space grows by a factor of 2. Eventually, truncations needed.

2. Spinless fermions

Consider tight-binding chain of spinless fermions:

$$\hat{H} = \sum_{l=1}^{N} \varepsilon_l \hat{c}_l^\dagger \hat{c}_l + \sum_{l=2}^{N} t_l \left(\hat{c}_l^\dagger \hat{c}_{l-1} + \hat{c}_{l-1}^\dagger \hat{c}_l \right)$$

Goal: find matrix representation for this Hamiltonian, acting in direct product space while respecting fermionic minus signs:

$$\{ \hat{c}_l, \hat{c}_{l'} \} = 0 \qquad \{ \hat{c}_l^\dagger, \hat{c}_{l'}^\dagger \} = 0$$

$$\{ \ \} = \hat{c}_l \hat{c}_{l'} + \hat{c}_{l'} \hat{c}_l$$

$$\{ \hat{c}_l^\dagger, \hat{c}_{l'} \} = \underset{\sim}{\delta_{ll'}}$$

First consider a single site (dropping the site index ℓ):

Hilbert space: $\mathrm{span}(|0\rangle, |1\rangle)$ local index: $n = \sigma \in \{0,1\}$

Operator action: $\hat{c}^\dagger |0\rangle = |1\rangle$ $\hat{c}^\dagger |1\rangle = 0$

$\hat{c}|0\rangle = 0$ $\hat{c}|1\rangle = |0\rangle$

The operators $\hat{c}^\dagger = |\sigma'\rangle C^{\dagger\sigma'}{}_{\sigma} \langle\sigma|$; same for $\hat{c}$

have matrix representations in V: $C^{\dagger\sigma'}{}_{\sigma} = \langle\sigma'|\hat{c}^\dagger|\sigma\rangle = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$C^{\sigma'}{}_{\sigma} = \langle\sigma'|\hat{c}|\sigma\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

Shorthand: we write

$\hat{c}^\dagger \longleftrightarrow C^\dagger$

lower case: operator in Fock space; upper case: matrix in 2-dim space V

Check anti-commutation relations:

$\{C^\dagger, C\} = C^\dagger C + C C^\dagger = I$

$C^\dagger C^\dagger = 0 = CC$

For the number operator $\hat{n} = \hat{c}^{\dagger}\hat{c}$, matrix representation in V reads:

$$n \equiv c^{\dagger}c = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \frac{1}{2}(I - Z)$$

where $Z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is a representation of $\hat{z} = 1 - 2\hat{n} = (-1)^{\hat{n}}$

Useful relations: $\hat{c}\hat{z} = -\hat{z}\hat{c}$; $\hat{c}^{\dagger}\hat{z} = -\hat{z}\hat{c}^{\dagger}$

Commuting $\hat{c}$ or $\hat{c}^{\dagger}$ past $\hat{z}$ produces a sign (check on your own).

Intuitive reason: $\hat{c}$ & $\hat{c}^{\dagger}$ both change $\hat{n}$ eigenvalue by one,

hence change sign of $(-1)^{\hat{n}}$.

Examples: $$\hat{c}^{\dagger}(-1)^{\hat{n}} = \hat{c}^{\dagger} = -\underbrace{(-1)^{\hat{n}}}_{(-1)^1 = -1}\hat{c}^{\dagger}$$

non-zero only on $|0\rangle$

Now consider a chain of spinless fermions:

Complication: fermionic operators on different sites anti commute:

$$c_\ell c_{\ell'}^\dagger = - c_{\ell'}^\dagger c_\ell \qquad (\text{for } \ell' \neq \ell)$$

Hilbert space:

$$\text{span}\left(|\vec{\sigma}\rangle_N = |n_1, n_2, \ldots, n_N\rangle \right)$$

Define canonical ordering for fully filled state:

$$|n_1 = 1, \ldots, n_N = 1\rangle = c_N^\dagger \ldots c_2^\dagger c_1^\dagger |\text{vacuum}\rangle$$

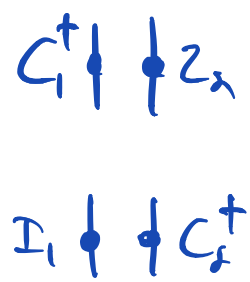
Now consider:

$$\hat{c}_1^\dagger |n_1 = 0, n_2 = 1\rangle = \hat{c}_1^\dagger \hat{c}_2^\dagger |\text{vac}\rangle = -\hat{c}_2^\dagger \hat{c}_1^\dagger |\text{vac}\rangle$$
$$= -|n_1 = 1, n_2 = 1\rangle$$

To keep track of such signs, matrix representations in $V_1 \otimes V_2$ need extra 'sign counters' tracking fermion numbers:

$$\hat{c}_1^\dagger = c_1^\dagger \otimes (-1)^{n_2} = c_1^\dagger \otimes Z_2$$

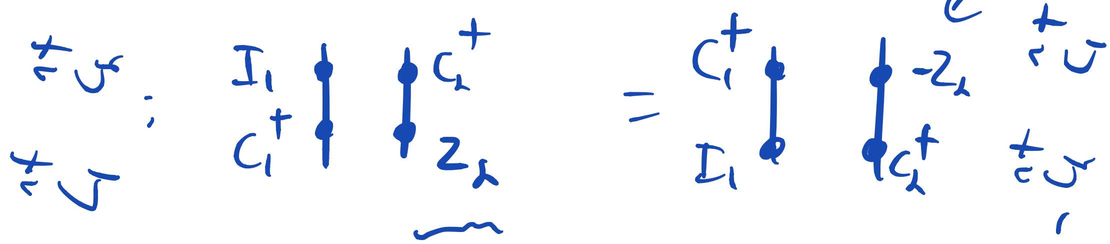
$$\hat{c}_2^\dagger = I_1 \otimes c_2^\dagger$$



Here $\otimes$ denotes a direct product operation; the order (space 1, space 2, …) matches that of the indices on the corresponding tensors: $A^{\sigma_1 \sigma_2 \ldots}$

Check whether $\hat{c}_1^\dagger \hat{c}_2^\dagger \stackrel{?}{=} -\hat{c}_2^\dagger \hat{c}_1^\dagger$

Moving Z past $c^\dagger$ gives $(-)$



Algebraically:

etc..

Similarly:

More generally, each $\hat{c}_\ell$ or $\hat{c}_\ell^\dagger$ must produce sign change when moved past with $\underbrace{\hat{c}_{\ell'}, \hat{c}_{\ell'}^\dagger}_{\ell' > \ell}$. so, define the following matrix representations in $V^{\otimes N} = V_1 \otimes \cdots \otimes V_N$

$$\hat{c}_\ell^\dagger = I_1 \otimes \cdots \otimes I_{\ell-1} \otimes c_\ell^\dagger \otimes Z_{\ell+1} \otimes \cdots Z_N$$
$$= c_\ell^\dagger Z_\ell^>$$

$$\hat{c}_\ell = I_1 \otimes \cdots \otimes I_{\ell-1} \otimes c_\ell \otimes Z_{\ell+1} \cdots Z_N$$
$$= c_\ell Z_\ell^> , \qquad Z_\ell^> \equiv \prod_{\otimes \ell' > \ell} Z_{\ell'} \to Z \text{ string}$$

(Jordan-Wigner transformation). **Exercise in HW to check.**

In bilinear combinations, all of Z's cancel. **Exercise in HW to check.**

Result: in spinless case, hopping terms are not changed by JW transform.

For spinful fermions, result will be different.

3. Spinful fermions

Consider a chain of spinful fermions.

Site index $\ell = 1 .. N$ spin index $s \in \{\uparrow, \downarrow\} \equiv \{+, -\}$

Anti-commutation relations $\{\hat{c}^\dagger_{\ell s}, \hat{c}_{\ell' s'}\} = \delta_{\ell\ell'}\delta_{ss'}$; $\{\hat{c}_{\ell s}, \hat{c}_{\ell' s'}\} = \{\hat{c}^\dagger_{\ell s}, \hat{c}^\dagger_{\ell' s'}\} = 0$

Define canonical order for fully filled state:

$$\hat{c}^\dagger_{N\downarrow}\hat{c}^\dagger_{N\uparrow} \dots \hat{c}^\dagger_{1\downarrow}\hat{c}^\dagger_{1\uparrow}|vac\rangle$$

To get a matrix rep, first consider a single site (drop index ℓ):

Hilbert space: $\text{span}\{|0\rangle, |\downarrow\rangle, |\uparrow\rangle, |\uparrow\downarrow\rangle\}$ local index: $\sigma = \{0, \downarrow, \uparrow, \uparrow\downarrow\}$

constructed via

$|0\rangle = |vac\rangle$ $\quad |\downarrow\rangle \equiv \hat{c}^\dagger_\downarrow |0\rangle$

$|\uparrow\rangle \equiv \hat{c}^\dagger_\uparrow |0\rangle$ $\quad |\uparrow\downarrow\rangle \equiv \hat{c}^\dagger_\downarrow \hat{c}^\dagger_\uparrow |0\rangle$

$$= \hat{c}^\dagger_\downarrow |\uparrow\rangle$$

$$= -\hat{c}^\dagger_\uparrow |\downarrow\rangle$$

To incorporate minus signs, introduce $\hat{z}_s = (-1)^{\hat{n}_s} = \frac{1}{2}\left(1 - \hat{n}_s\right)$

$$\left[s \in [\uparrow, \downarrow] \right]$$

We seek a matrix representation of $c_s^\dagger, c_s, z_s$ in direct product space $\tilde{V} \equiv V_\uparrow \otimes V_\downarrow$

(Matrices acting in this pace will carry tildes)

$$\hat{z}_\uparrow = z_\uparrow \otimes I_\downarrow = \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \equiv \tilde{z}_\uparrow$$

$$\hat{z}_\downarrow = I_\uparrow \otimes z_\downarrow = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} \equiv \tilde{z}_\downarrow$$

$$\hat{z}_\uparrow \hat{z}_\downarrow = z_\uparrow \otimes z_\downarrow = \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{pmatrix} \equiv \tilde{z}$$

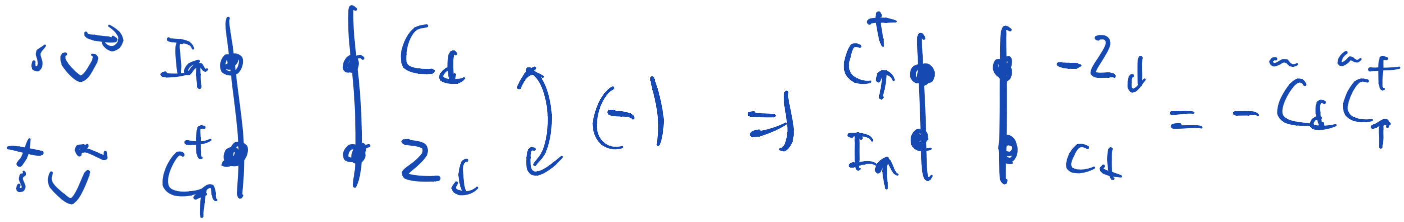
$$\hat{c}_\uparrow^\dagger \equiv c_\uparrow^\dagger \otimes z_\downarrow = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} 1 & \\ & -1 \end{pmatrix} = \left(\begin{array}{cc|cc} & & & \\ \hline 1 & & & \\ & -1 & & \end{array}\right) \equiv \tilde{c}_\uparrow^\dagger$$

$$\hat{c}_\uparrow \equiv c_\uparrow \otimes z_\downarrow \equiv \tilde{c}_\uparrow$$

$$\hat{c}_\downarrow^\dagger \equiv I_\uparrow \otimes c_\downarrow^\dagger = \begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \otimes \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \left(\begin{array}{cc|cc} 0 & 0 & & \\ 1 & 0 & & \\ \hline & & 0 & 0 \\ & & 1 & 0 \end{array}\right) \equiv \tilde{c}_\downarrow^\dagger$$

$$\hat{c}_\downarrow \equiv I_\uparrow \otimes c_\downarrow \equiv \tilde{c}_\downarrow$$

The factors Z_s account for signs. For example $\hat{c}^\dagger_\uparrow \hat{c}_d = -\hat{c}_d \hat{c}^\dagger_\uparrow$



Algebraic check:

$$\left(\qquad\right)\left(\qquad\right) = \ldots$$

Remark: for spinful fermions (in contrast to spinless fermions) we have

$$\hat{c}_s^\dagger \hat{Z} \neq \hat{c}_s^\dagger \quad , \quad \hat{Z}\hat{c}_s \neq \hat{c}_s$$

Now consider a chain of spinful fermions (analogous to spinless case with $\hat{V}_\ell$)

Each $\hat{c}_\ell, \hat{c}_\ell^\dagger$ must produce a sign change when moved past $\hat{c}_{\ell'}, \hat{c}_{\ell'}^\dagger$, $\ell' > \ell$.

so define the following matrix representations in $\hat{V}^{\otimes N} = \hat{V}_1 \otimes \cdots \otimes \hat{V}_N$

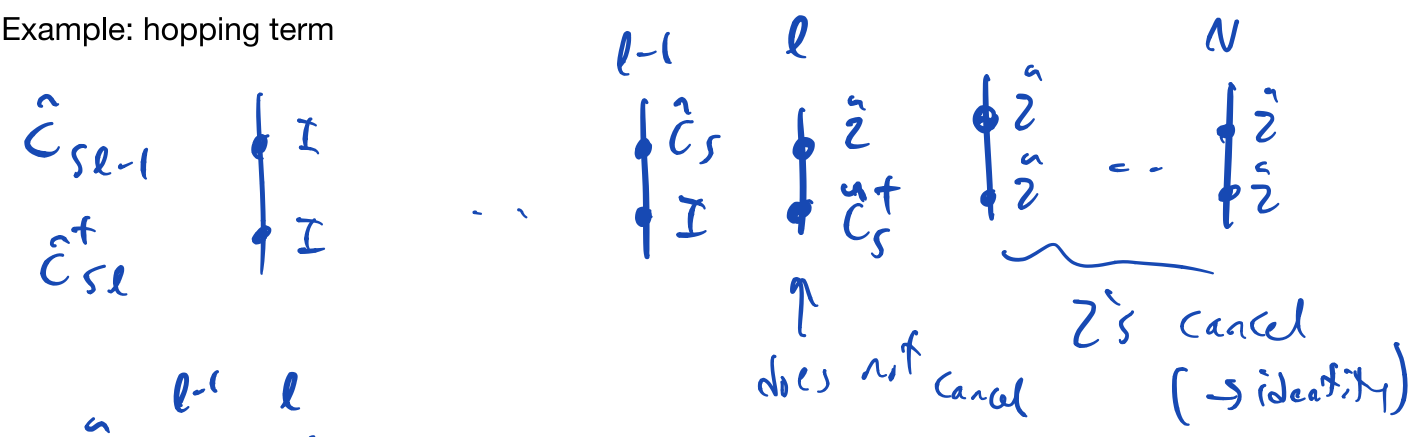
$$\hat{c}_\ell^\dagger \equiv \hat{I}_1 \otimes \cdots \otimes \hat{I}_{\ell-1} \otimes \hat{c}_\ell^\dagger \otimes \hat{z}_{\ell+1} \otimes \cdots \otimes \hat{z}_N$$

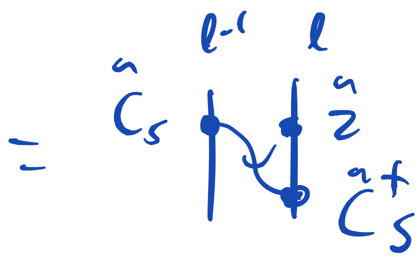
$$= \hat{c}_\ell^\dagger \hat{z}_\ell^>$$

$$\hat{c}_\ell = \hat{c}_\ell \hat{z}_\ell^>$$

In bilinear combinations, most (but not all!) of the z cancel.

Example: hopping term





Bond indicates sum $\sum_s$

Convention: annihilation - outgoing arrow, creation, incoming arrow

mnemonic: charge flows from annihilation to creation site

Similarly:

Translationally invariant MPS $\rightarrow A_{[l]} = A$ for all l

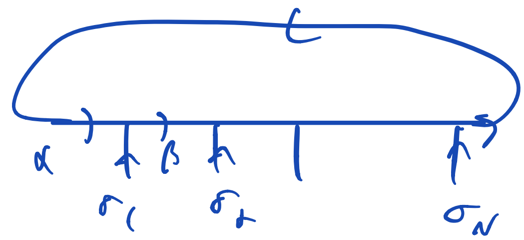
(infinite system, periodic BC)

1. Transfer matrix

Consider length-N chain with periodic boundary conditions

$$|\psi\rangle = |\vec{\sigma}_N\rangle A_{[1]}{}^{\alpha\sigma_1}{}_{\beta} A_{[2]}{}^{\beta\sigma_2}{}_{\gamma} \cdots A_{[N]}{}^{\lambda\sigma_N}{}_{\alpha}$$

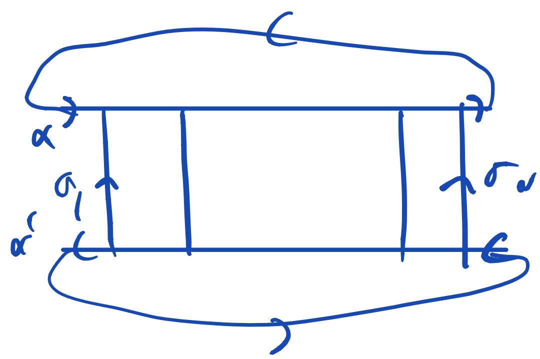
$$= |\vec{\sigma}_N\rangle \mathrm{Tr}\left[A_{[1]}^{\sigma_1} \cdots A_{[N]}^{\sigma_N}\right]$$



[Assume that all bonds have same dimension: $D_\alpha = D_\beta = \cdots = D$]

Normalization:

$$\langle\psi|\psi\rangle =$$



$$= A^{\dagger\alpha'}_{[N]\sigma_N\nu'} \cdots A^{\dagger\beta'}_{[1]\sigma_1\alpha'} A_{[1]}{}^{\alpha\sigma_1}{}_{\beta} \cdots A_{[N]}{}^{\nu\sigma_N}{}_{\alpha}$$

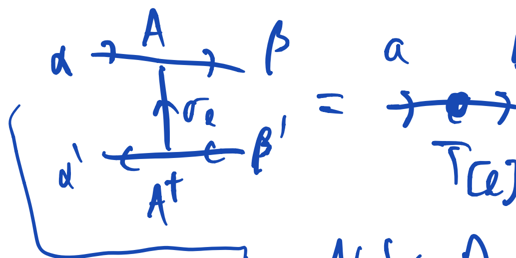
regroup as:

$$= \left(A^{\dagger\beta'}_{[1]\sigma_1\alpha'} A_{[1]}{}^{\alpha\sigma_1}{}_{\beta}\right) \cdots \left(A^{\dagger\alpha'}_{[N]\sigma_N\nu'} A_{[N]}{}^{\nu\sigma_N}{}_{\alpha}\right)$$

$$= T_{[1]\alpha'}{}^{\alpha\beta'}{}_{\beta} \cdots T_{[N]\nu'}{}^{\nu\alpha'}{}_{\alpha}$$

We define the 'transfer matrix' (collective indices chosen to reflect arrows on effective vertex).

$$T_{[\ell]}{}^{a}{}_{b} \equiv T_{[\ell]}{}^{\alpha\beta'}{}_{\underbrace{\alpha'}_{a}\,\underbrace{\beta}_{b}} \equiv A^{\dagger\beta'}_{[\ell]\,\sigma_\ell\alpha'}\, A^{\alpha\sigma_\ell}_{[\ell]\beta}$$



Note: $D_M = D^2$

Then

$$\langle\psi|\psi\rangle = T_{[1]}{}^{a}{}_{b}\, T_{[2]}{}^{b}{}_{c} \cdots T_{[N]}{}^{n}{}_{a}$$

$$= \mathrm{tr}\left(T_{[1]} \cdots T_{[N]}\right)$$

Assume all A tensors are identical, then the same is true for all T matrices.

Hence

$$\langle\psi|\psi\rangle = \mathrm{tr}\left(T^N\right) = \sum_j \left(t_j\right)^N \xrightarrow{N\to\infty} \left(t_1\right)^N$$

where t_j are the eigenvalues of the transfer matrix, and t_1 is the largest one of these.

2. Eigenvalues of transfer matrix

Assume now that A tensor is left-normalized (analogous discussion holds for RN)

Then we know the MPS is normalized to unity: $1 = \langle \psi | \psi \rangle$

Therefore, the largest eigenvalue of the transfer matrix is $(t_1)^N = 1 \Rightarrow t_1 = 1$

Hence all eigenvalues of transfer matrix must satisfy $|t_j| \le 1$

The eigenvector, $V^{j=1}$, having eigenvalue $t_{j=1} = 1$ is $(V^1)_a = I^{\alpha'}{}_a$

label $j=1$

component of eigenvector

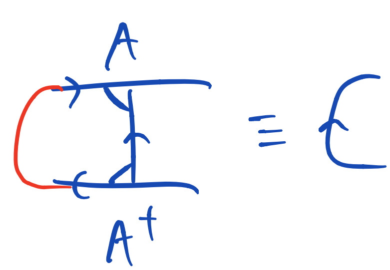
$$V_a T^a{}_b = A^{\dagger \beta'}{}_{\sigma \alpha'} I^{\alpha'}{}_{\alpha} A^{\alpha \sigma}{}_{\beta}$$

$$= A^{\dagger \beta}{}_{\sigma \alpha} A^{\alpha \sigma}{}_{\beta}$$

$$= I^{\beta'}{}_{\beta} = V_b$$

def of left norm

eigenvalue $= 1$



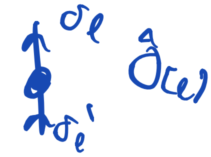
[A more rigorous proof exists but due to time constraints we will not do it in class.]

Overall result: all eigenvalues of transfer matrix built from left-normalized A-tensors have modulus less than or equation to unity.

3. Correlation functions

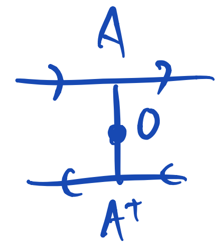
Consider local operator:

$$\hat{O}_{[l]} = |\sigma_l'\rangle O_{[l]\sigma_l}^{\sigma_l'} \langle\sigma_l|$$



Define corresponding transfer matrix:

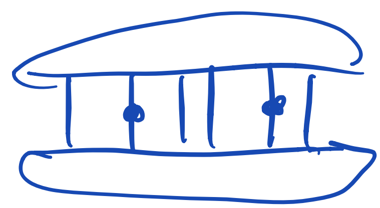
$$T_O^{[l]} = A^{\dagger}_{\sigma_l'} O_{[l]\sigma_l}^{\sigma_l'} A^{\sigma_l}$$



Correlator:

$$C_{l'l} \equiv \langle\psi| \hat{O}_{[l']} \hat{O}_{[l]} |\psi\rangle$$

$$= \mathrm{Tr}\left(T^{l'-1} T_{O[l']} T^{l-l'-1} T_{O[l]} T^{N-l}\right)$$



$$= \mathrm{Tr}\left(T^{N-(l-l')-1} T_{O[l']} T^{l-l'-1} T_{O[l]}\right)$$

Let V^j, t_j be eigenvectors, eigenvalues of transfer matrix $\rightsquigarrow$ $V^j T = t_j V^j$

or explicitly with matrix indices: $(V^j)_a T^a_b = t_j (V^j)_b$

Transform to eigenbasis of transfer matrix:

$$C_{l'l} = \sum_{jj'} (t_{j'})^{N-(l-l')-1} \left(T_{O[l']}\right)^{j'}_{j} (t_j)^{l-l'-1} \left(T_{O[l]}\right)^{j}_{j'}$$

1. Def of trace
2. resolution of identity near $T_{O[l']}$

For $N \to \infty$, only contribution of largest eigenvalue, $t_{j'} = t_1$, survives:

$$C_{l'l} \xrightarrow{N\to\infty} t_1^N \sum_j \left(T_{O(l')}\right)^1{}_j \underbrace{\left(\frac{t_j}{t_1}\right)^{l-l'-1}}_{\text{requires } l-l' \gg 1} \left(T_{O(l)}\right)^j{}_1$$

Assume $\hat{O}_{(l)} = \hat{O}_{(l')} = \hat{O}$, and take their separation to be large. $l - l' \to \infty$

$$C_{l'l} \xrightarrow{l-l'\to\infty} t_1^N \left[\left|\left(T_0\right)^1{}_1\right|^2 + \left|\left(T_0\right)^1{}_2\right|^2 \left(\frac{t_2}{t_1}\right)^{l-l'-1} \dots \right]$$

If $\left(T_0\right)^1{}_1 \neq 0$ 'long-range order'

gapped?

Correlation remains as $l - l' \to \infty$

If $\left(T_0\right)^1{}_1 = 0$ 'exponential decay', $\sim e^{-|l-l'|/\xi}$

with correlation length

$$\xi = \left(\ln\left(t_1/t_2\right)\right)^{-1}$$

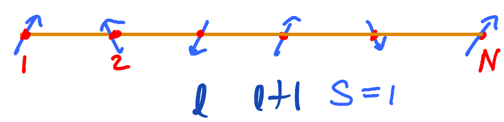
AKLT Model

[Affleck 1988, Schollwock2011, Sec 4.1.5, Tu2008]

1. General remarks:

- AKLT model was proposed by Affleck, Kennedy, Lieb, and Tasaki in 1988.
- Previously, Haldane had predicted that S=1 Heisenberg chain has finite excitation gap above a unique ground state, i.e. only 'massive' excitations [Haldane 1983a, b]
- AKLT then constructed the first solvable, isotropic, S=1 spin chain model that exhibits a 'Haldane gap'.
- Ground state of AKLT model is an MPS of lowest non-trivial bond dimension, D=2.
- Correlation functions decay exponentially - the correlation length can be computed analytically.

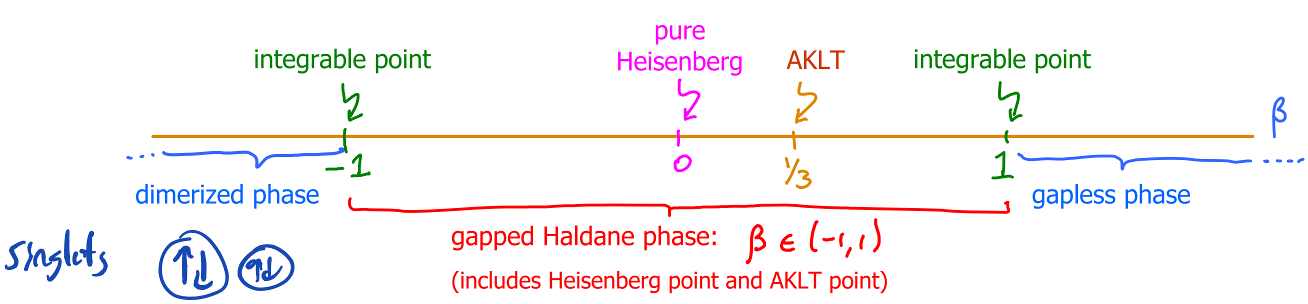
Haldane phase for S=1 spin chains



Consider a bilinear-quadratic (BB) Heisenberg model for 1D chain of spin S=1:

$$H_{BB} = \sum_{l=1}^{N-1} \bar{S}_l \cdot \bar{S}_{l+1} + \beta \left(\bar{S}_l \cdot \bar{S}_{l+1} \right)^2$$

Phase diagram:



Main idea of AKLT model: $H_{AKLT} = H_{BB}(\beta = 1/3)$

is built from projectors mapping spin on neighboring sites to total spin $S^{tot}_{l,l+1} = 2$.

Ground state satisfies $H_{AKLT}|g\rangle = 0$. To achieve this, ground state is constructed in such a manner that spins on neighboring sites can only be coupled to

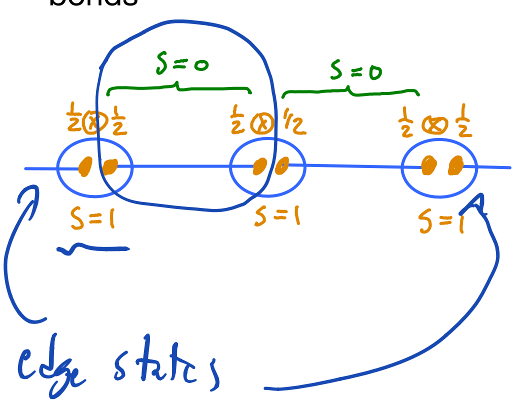
$$S^{tot}_{l,l+1} = 0 \quad \text{or} \quad 1,$$

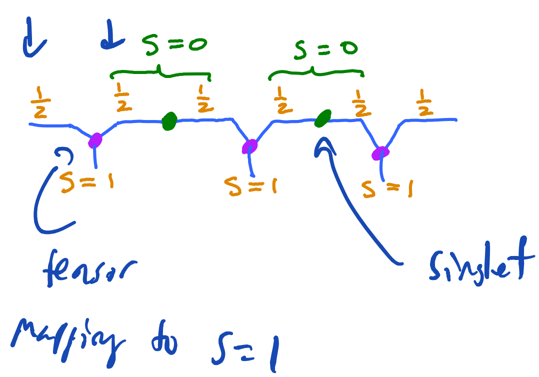
To this end, the spin-1 on each site is constructed from two auxiliary spin-1/2 degrees of freedom. One spin-1/2 each from neighboring sites is coupled to spin 0; this projects out the the S=2 sector in the direct-product space of neighboring sites, ensuring that H_{AKLT} annihilates ground state.

Traditional depiction:

MPS depiction: spin-1/2's live on bonds

bonds





2. Construction of AKLT Hamiltonian

Direct product of space spin 1 with spin 1 contains direct sum of spin 0,1,2:

$$\mathcal{H}_1 \otimes \mathcal{H}_1 = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2$$

Projector of $\mathcal{H}_1 \otimes \mathcal{H}_1$ onto $\mathcal{H}_s$ $(s = 0, 1, 2)$

eigenvalue of $\bar{S}^2$ for total spin s'.

$$\underbrace{P^{(s)}_{1,2}}_{\text{sites}} = P^{(s)}_{1,2}(\bar{S}_1, \bar{S}_2) = c \prod_{s' \neq s} \left[\underbrace{(\bar{S}_1 + \bar{S}_2)}_{\text{total spin}}{}^2 - s'(s'+1) \right]$$

normalization factor

yields zero if total spin $= s'$.

Using $(\bar{S}_1 + \bar{S}_2)^2 = \underbrace{\bar{S}_1^2}_{1\cdot(1+1)} + 2\bar{S}_1 \cdot \bar{S}_2 + \underbrace{\bar{S}_2^2}_{1\cdot(1+1)} = 2\bar{S}_1 \cdot \bar{S}_2 + 4$

we find for spin-2 projector:

$$P^{(2)}_{1,2} = c\left[2\bar{S}_1 \cdot \bar{S}_2 + 4 - 0(0+1)\right]\left[2\bar{S}_1 \cdot \bar{S}_2 + 4 - 1(1+1)\right]$$

$$= c\left[4(\bar{S}_1 \cdot \bar{S}_2)^2 + 12(\bar{S}_1 \cdot \bar{S}_2) + 8\right]$$

Normalization is fixed by demanding that $P^{(2)}_{1,2}$ must yield 1 when acting on spin-2 subspace:

$$1 = P^{(2)}_{1,2}\Big|_{(\bar{S}_1 + \bar{S}_2)^2 = 2(2+1)} = c\left[2(2+1) - 0\right]\left[2(2+1) - 1(1+1)\right]$$

$$= c \cdot 6 \cdot 4 \Rightarrow c = \frac{1}{24}$$

Final projector on spin-2 subspace:

$$P^{(2)}_{1,2} = \frac{1}{6}\left(\bar{S}_1 \cdot \bar{S}_2\right)^2 + \frac{1}{2}\,\bar{S}_1 \cdot \bar{S}_2 + \frac{1}{3}$$

$$= P^{(2)}_{1,2}\left(\bar{S}_1, \bar{S}_2\right)$$

AKLT Hamiltonian is sum over spin-2 projectors for all neighboring pairs of spins:

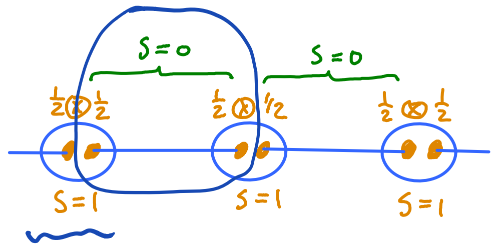
$$H_{AKLT} \equiv \sum_{\ell} P^{(2)}_{\ell,\ell+1}\left(\bar{S}_\ell, \bar{S}_{\ell+1}\right)$$

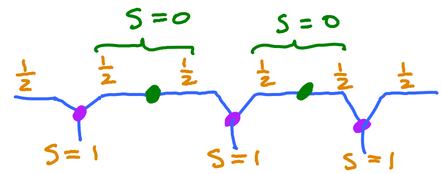
For a finite chain of N sites, use periodic boundary conditions, i.e. $\bar{S}_{\ell+N} = \bar{S}_\ell$

Each term is a projector, hence has only non-negative eigenvalues. Hence same is true for H_{AKLT}.

A state satisfying $H_{AKLT}|\psi\rangle = 0$ must be a ground state!

3. AKLT ground state





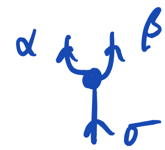
On every site, represent spin 1 as symmetric combination of two auxiliary spin-1/2s:

$$|S=1,\sigma\rangle \equiv |\sigma\rangle = \begin{cases} |+1\rangle = |\uparrow\rangle|\uparrow\rangle \\ |0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle|\downarrow\rangle + |\downarrow\rangle|\uparrow\rangle\right) \\ |-1\rangle = |\downarrow\rangle|\downarrow\rangle \end{cases}$$

On-site projector that maps $\mathcal{H}_{\frac{1}{2}} \otimes \mathcal{H}_{1/2}$ to $\mathcal{H}_1$

$$\hat{C} = |+1\rangle\langle\uparrow|\langle\uparrow| + |0\rangle\frac{1}{\sqrt{2}}\left(\langle\uparrow|\langle\downarrow| + \langle\downarrow|\langle\uparrow|\right) + |-1\rangle\langle\downarrow|\langle\downarrow|$$

Use such a projector on every site ℓ :



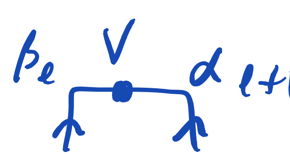
$$\hat{C}_{[\ell]} = |\sigma\rangle_\ell \, C^{\sigma}_{\alpha\beta} \, {}_\ell\langle\alpha| \, {}_\ell\langle\beta|$$

index $\rightarrow$ $C^{+1} = \begin{array}{c c} & \begin{array}{cc} \uparrow & \downarrow \end{array} \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \end{array}$; $C^{0} = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$; $C^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

Now construct nearest-neighbor valence bonds from auxiliary spin-1/2 states:

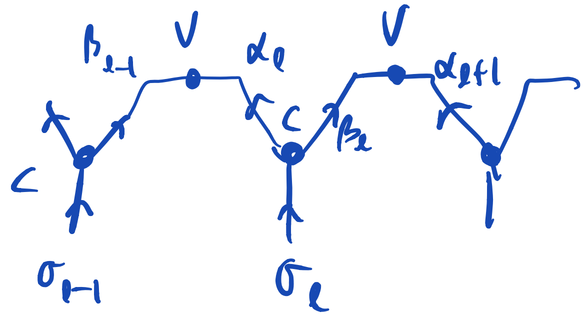
$$|V\rangle_\ell = |\beta_\ell\rangle_\ell \, |\alpha_{\ell+1}\rangle_{\ell+1} \, V^{\beta_\ell \alpha_{\ell+1}} = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_\ell|\downarrow\rangle_{\ell+1} - |\downarrow\rangle_\ell|\uparrow\rangle_{\ell+1}\right)$$

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



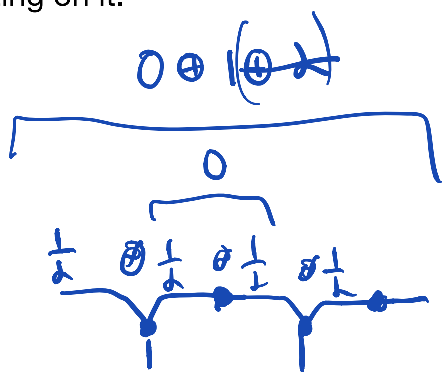
AKLT ground state = (direct product of spin-1 projectors) acting on (direct product of valence bonds)

$$|g\rangle \equiv \prod_{\otimes \ell} \hat{C}_{[\ell]} \prod_{\otimes \ell} |V\rangle_\ell$$



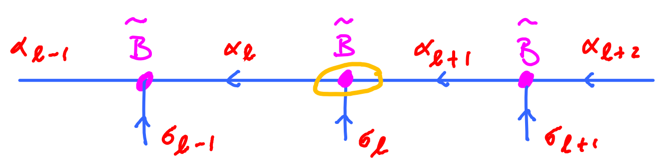
Why is this a ground state?

Coupling two auxiliary spin-1/2 to total spin 0 (valence bond) eliminates the spin-2 sector in direct product space of two spin-1. Hence spin-2 projector in H_{AKLT} yields zero when acting on it.



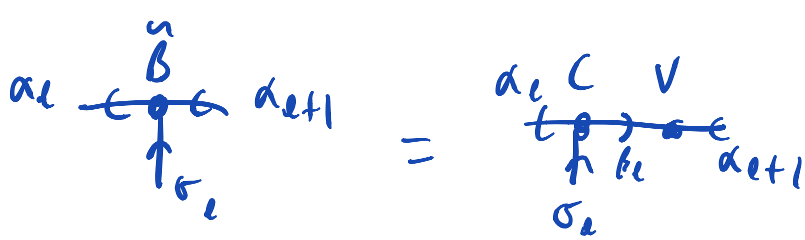
-> AKLT ground state is an MPS!

$$|g\rangle = \prod_{\otimes \ell} |\sigma_\ell\rangle \tilde{B}_{\alpha_\ell}^{\sigma_\ell \alpha_{\ell+1}}$$



with

$$\tilde{B}_{\alpha_\ell}^{\sigma_\ell \alpha_{\ell+1}} = C^{\sigma_\ell}_{\alpha_\ell \beta_\ell} V^{\beta_\ell \alpha_\ell}$$



Explicitly:

$\sigma_\ell = +1:$ $\quad \tilde{B}^{+1} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \cdot \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

$\sigma_\ell = 0:$ $\quad \tilde{B}^{0} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$

$\sigma_\ell = -1:$ $\quad \tilde{B}^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$

Not normalized: $\quad \tilde{B}^{\sigma} \tilde{B}^{+}_{\sigma} = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} + \ldots$

$$= \frac{3}{4} \cdot I$$

Define right-normalized tensors, satisfying

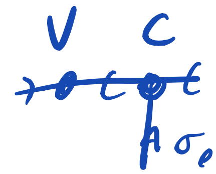
$$B^{\sigma} B^{+}_{\sigma} = I \quad , \quad B^{\sigma} \equiv \sqrt{\frac{4}{3}}\, \tilde{B}^{\sigma}$$

$$B^{+1} = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad B^{0} = \frac{1}{\sqrt{3}} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$B^{-1} = \sqrt{\frac{2}{3}} \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}$$

Note: we could have also grouped B and C in opposite order, defining

$$\tilde{A}^{\beta_{\ell-1}\sigma_\ell}{}_{\beta_\ell} = V^{\beta_{\ell-1}\alpha_\ell}\, C^{\sigma_\ell}{}_{\alpha_\ell\beta_\ell} =$$



This approach leads to left-normalized tensors, with

$$A^{\pm 1} = B^{\mp 1}$$

$$A^{0} = B^{0}$$

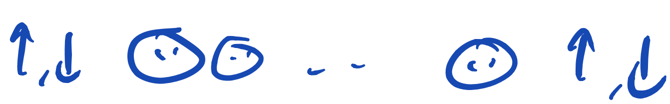
Exercise: verify that spin-2 projector yields zero when acting on sites l, l+1.

Hint: use spin-1 matrix representation for $\left(\bar{S}_\ell \cdot \bar{S}_{\ell+1}\right)^{\sigma\bar{\sigma}}{}_{\sigma'\bar{\sigma}'}$

<u>Boundary conditions:</u>

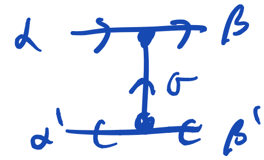
For periodic boundary conditions, Hamiltonian includes projector connecting sites 1 and N. Then the ground state is unique.

For <u>open</u> boundary conditions, there are 'left-over spin-1/2' degrees of freedom at both ends of chain. Ground state is <u>four-fold degenerate</u>.



4. Transfer operator (for Haldane gap)

$$T^{a}{}_{b} = T_{\alpha'}{}^{\alpha\beta'}{}_{\beta} = B^{+\beta'}{}_{\sigma\alpha'}\, B^{\alpha\sigma}{}_{\beta} = \overline{\left(B^{\alpha'\sigma}{}_{\beta'}\right)}\, B^{\alpha\sigma}{}_{\beta}$$



$$T = \overline{B^{\sigma}} \otimes B^{\sigma}$$

$$= \sqrt{\tfrac{2}{3}}\left(\begin{array}{c|c} 0 & \sqrt{\tfrac{2}{3}}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \\ \hline 0 & 0 \end{array}\right) + \frac{1}{\sqrt{3}}\left(\begin{array}{c|c} -\frac{1}{\sqrt{3}}\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} & 0 \\ \hline 0 & +1\cdot\left(\quad\right) \end{array}\right)$$

$$+ \sqrt{\tfrac{2}{3}}\left(\begin{array}{c|c} 0 & 0 \\ \hline -\sqrt{\tfrac{2}{3}}\begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} & 0 \end{array}\right)$$

To compute spin-spin correlator,
$$C^{zz}_{\ell\ell'} = \frac{\langle g|\, S^{z}_{(\ell)} S^{z}_{(\ell')}\, |g\rangle}{\langle g|g\rangle}$$

$\rightarrow$ Need
$$T_{S^z} = B^{+}_{\sigma'} \left(S^{z}\right)^{\sigma'}{}_{\sigma}\, B^{\sigma}$$

$$\boxed{S_z = \begin{pmatrix} 1 & & \\ & 0 & \\ & & -1 \end{pmatrix}}$$

$$= +1\left(\quad\right) + 0\cdot\left(\quad\right) + (-1)\cdot\left(\quad\right)$$

$$= \frac{2}{3}\left(\begin{array}{c|c} 0 & \begin{matrix} 0 & 1 \\ 0 & 0 \end{matrix} \\ \hline \begin{matrix} 0 & 0 \\ -1 & 0 \end{matrix} & 0 \end{array}\right)$$

Exercise: Compute eigenvalues and eigenvectors of T. Show that correlator decays exponentially and hence that model is gapped.

5. String order parameter

AKLT ground state: $|g\rangle = |\sigma_N\rangle \, \mathrm{Tr}\left(B^{\sigma_1} \ldots B^{\sigma_N}\right) \; ; \sigma_\ell \in \{-1, 0, 1\}$

$$B^{+1} = \frac{1}{\sqrt{3}} \tau^+ , \quad B^0 = -\frac{1}{\sqrt{3}} \tau^z , \quad B^{-1} = -\frac{1}{\sqrt{3}} \tau^-$$

with Pauli matrices $\rightarrow \tau^+, \tau^z, \tau^- \quad \left(\tau^+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \right)$

Now, note that $B^{\pm 1} B^0 \ldots B^0 B^{\pm 1} = 0$

Thus, all 'allowed configurations' (having non-zero coefficients) in AKLT ground state have the property that every ± 1 is followed by a string of 0, then ∓ 1.

Allowed: $|\sigma_N\rangle = \ldots 1 \, 0 0 0 -1 \, 0 \, 1 \, 0 \ldots$

Not allowed: $|\sigma_N\rangle = \underline{\underline{1}} \, 0 0 0 \, \underline{\underline{1}} \ldots$

String order parameter: $\hat{O}^{\text{string}}_{\ell\ell'} = S^z_{[\ell]} \prod_{\bar{\ell}=\ell+1}^{\ell'-1} e^{i\pi S^z_{[\bar{\ell}]}} S^z_{[\ell']}$

Exercise: show that ground state expectation value of string order parameter is non-zero.

$$\lim_{\ell-\ell' \to \infty} \lim_{N \to \infty} \langle g | \hat{O}^{\text{string}}_{\ell\ell'} | g \rangle = -\frac{4}{9}$$

Hint: find $T_{e^{i\pi s_2}}$