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- chain with Hamiltonian

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

and the operator triplet

Then the dot product term is:

The Hamiltonian can be expressed in the basis:

is a linear map acting on a direct product space:

where is the 2D representation space of site .

is a sum of single-site and two-site terms.

On-site terms:

Matrix representation in :

Nearest-neighbor interactions, acting on direct product space,

Matrix representation in :

We define the 3-leg tensors with index placements matching those of tensors for wave functions: incoming up, outgoing down, with (by convention) as middle index.

Diagonalize site 1

chain of length 1 site index

is diagonal, with matrix elements

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

Eigenvectors of operator are given by :

<u>Add site 2</u>

Diagonalize in enlarged Hilbert space,

chain of length 2

Matrix representation in corresponding to 'local' basis,

We seek matrix representation in corresponding to enlarged, 'site-1-diagonal'

basis, defined as

So, attach to in/out legs of site 1, and to in/out legs of site 2:

First term is diagonal. But others are not.

Now diagonalize in this enlarged basis:

is diagonal, with matrix elements

Eigenvectors of matrix are given by column vectors of the matrix

Eigenstates of the operator

Add site 3

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

For example, spin-spin interaction,

Local basis:

enlarged,

site-1,2 diagonal basis

Then diagonalize in this basis:

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:

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

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

Hilbert space: local index:

Operator action:

The operators

have matrix representations in

Shorthand: we write

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

Check anti-commutation relations:

For the number operator , matrix representation in reads:

where is a representation of

Useful relations:

Commuting produces a sign (check on your own).

Intuitive reason: both change eigenvalue by one,

hence change sign of .

Examples:

Now consider a chain of spinless fermions:

Complication: fermionic operators on different sites anti commute:

Hilbert space:

Define canonical ordering for fully filled state:

Now consider:

To keep track of such signs, matrix representations in need extra 'sign counters' tracking fermion numbers:

Here denotes a direct product operation; the order (space 1, space 2, …) matches that of the indices on the corresponding tensors:

Check whether

Algebraically:

Similarly:

More generally, each must produce sign change when moved past with . so, define the following matrix representations in

(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 spin index

Anti-commutation relations

Define canonical order for fully filled state:

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

Hilbert space: local index:

constructed via

To incorporate minus signs, introduce

We seek a matrix representation of in direct product space

(Matrices acting in this pace will carry tildes)

The factors account for signs. For example

Algebraic check:

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

Now consider a <u>chain</u> of spinful fermions (analogous to spinless case with)

Each must produce a sign change when moved past

so define the following matrix representations in

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

Example: hopping term

Bond indicates sum

Convention: annihilation - outgoing arrow, creation, incoming arrow

mnemonic: charge flows from annihilation to creation site

Similarly:

Translationally invariant MPS

1. Transfer matrix

Consider length-N chain with periodic boundary conditions

[Assume that all bonds have same dimension:]

Normalization:

regroup as:

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

Then

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

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

2. Eigenvalues of transfer matrix

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

Then we now the MPS is normalized to unity:

Therefore, the largest eigenvalue of the transfer matrix is

Hence all eigenvalues of transfer matrix must satisfy

The eigenvector, , having eigenvalue is

[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:

Define corresponding transfer matrix:

Correlator:

Let be eigenvectors, eigenvalues of transfer matrix

or explicitly with matrix indices:

Transform to eigenbasis of transfer matrix:

For , only contribution of largest eigenvalue, , survives:

Assume , and take their separation to be large.

If ‘long-range order’

If ‘exponential decay’,

with correlation length

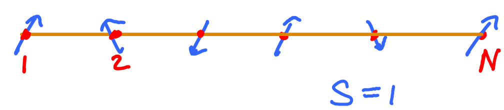
AKLT Model

[Affleck 1988, Schollwock2011, Sec 4.1.5, Tu2008]

1. General remarks:

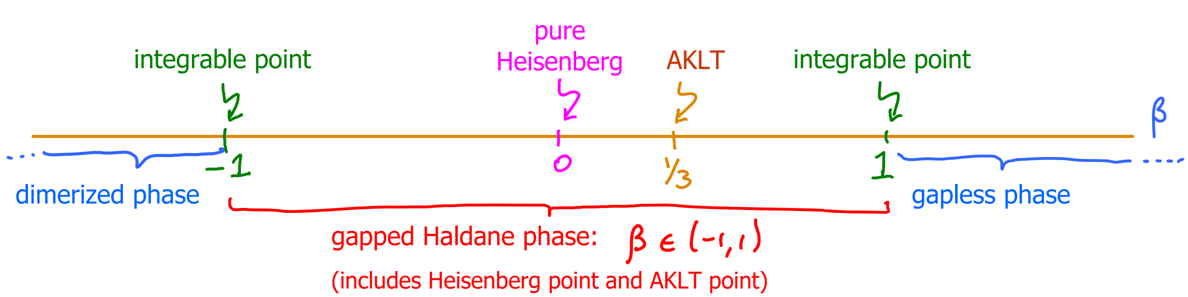
- AKLT model was proposed by Affleck, Kennedy, Lieb, and Tasaki in 1988.
- Previously, Haldane had predicted that S=1 Heisenberg chain has finite excitation gap above a unique ground state, i.e. only 'massive' excitations [Haldane 1983a, b]
- AKLT then constructed the first solvable, isotropic, S=1 spin 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) Heisenber model for 1D chain of spin S=1:

Phase diagram:



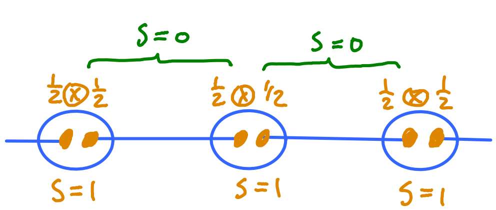
Main idea of AKLT model:

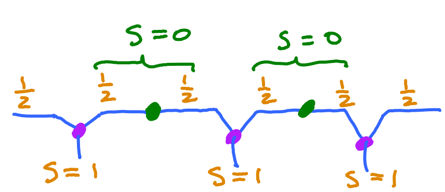
is built from projectors mapping spin on neighboring sites to total spin

Ground state satisfies . To achieve this, ground state is constructed in such a manner that spins on neighboring sites can only be coupled to

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 annihilates ground state.

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





2. Construction of AKLT Hamiltonian

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

Projector of onto

Using

we find for spin-2 projector:

Normalization is fixed by demanding that must yield when acting on spin-2 subspace:

Final projector on spin-2 subspace:

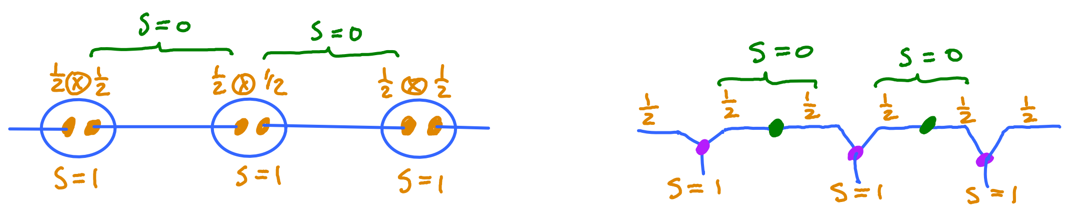
AKLT Hamiltonian is sum over spin-2 projectors for all neighboring pairs of spins:

For a finite chain of sites, use periodic boundary conditions, i.e.

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

A state satisfying must be a ground state!

3. AKLT ground state



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

On-site projector that maps

Use such a projector on every site :

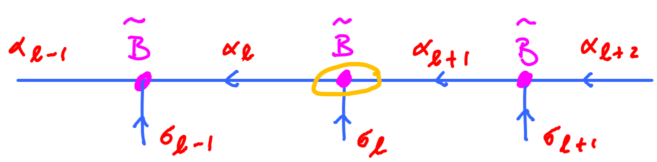
Now construct nearest-neighbor valence bonds from auxiliary spin-1/2 states:

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

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 yields zero when acting on it.

-> AKLT ground state is an MPS!



with

Explicitly:

Not normalized:

Define right-normalized tensors, satisfying

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

This approach leads to left-normalized tensors, with

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

Hint: use spin-1 representation for

Boundary conditions:

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

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

4. Transfer operator

To compute spin-spin correlator,

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:

with Pauli matrices

Now, note that

Thus, all ‘allowed configurations’ (having non-zero coefficients) in AKLT ground state

have the property that every is followed by a string of , then .

Allowed:

Not allowed:

String order parameter:

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