10. Matrix product states

10.1 Introduction

* You know what a matrix product state is
* You know the AKLT state.
* You know the concept of fractionalization

We got acquainted with the fact that many-body Hilbert spaces are exponentially large. This quite generally prevents us from direct numerical searches of ground-states or from tracking the time evolution of large quantum systems.

We got used to the idea of approximate numerical solutions, may that be through variational mean-field calculations or the use of density functional theory. Here we want to learn about a powerful tool for gapped one-dimensional systems: matrix product state representations of quantum wave functions.

The principle idea is very simple. We know that any wave function can be written with respect to some basis as

$$|\psi\rangle = \sum_{\vec{\imath}} a_{\vec{\imath}} |i_1\rangle \otimes |i_2\rangle \otimes \cdots \otimes |i_N\rangle.$$

$$i_j = 1, \ldots, d$$

Here $\vec{\imath}$ is a multi-index $\vec{\imath} = \{i_1, i_2, \ldots, i_N\}$ where each i_α runs over all local quantum orders $|i_\alpha\rangle$. The full many-body wave-function is simply a *sum* of *tensorproducts* of such local configuration. For example a simple quantum ferro-magnet, where all spins are perfectly aligned has expansion coefficients

$$a_{\{\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \ldots \uparrow\}} = 1 \qquad a_{\vec{\imath}} = 0 \quad \forall \text{ other config.}$$

$$\Rightarrow \quad |\psi\rangle = \sum_{\vec{\imath}} a_{\vec{\imath}} |i_1\rangle \otimes \cdots |i_N\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \otimes \cdots \otimes |\uparrow\rangle.$$

A generic wave-function therefore need d^N numbers to be captured! The idea of matrix product states is to write the $a_{\vec{\imath}}$ in a way that gets away with significantly less effort and still does a good job in capturing a wide class of wave-functions. The idea is to simply write

$$|\psi\rangle = \sum_{\vec{\imath}} \text{Tr}\left[A_{i_1} \cdot A_{i_2} \cdot A_{i_3} \cdot \cdots A_{i_N}\right] |i_1\rangle \otimes \cdots \otimes |i_N\rangle,$$

where A_{i_α} are *matrices*. Let's try to understand this. For every state where α-th site is in state i_α, the contribution to the expansion coefficient is the same A_{i_α}. If we take all matrices to be 1×1, we only have

$N \cdot d$ different numbers to describe a state in a d^N sized Hilbert space. If, on the other hand, we take the matrices to be $\chi \times \chi$ and take $\chi \to \infty$, we don't loose degrees of freedom. The question is, what does χ signify and when is $\chi \ll \infty$ good enough.

To turn this approach into a useful numerical method, we need the following things:

1.) Understand which wave-functions are well-represented by a matrix product state (MPS).

2.) How do we find the matrices A_α^i of a ground-state of a given Hamiltonian H?

3.) How can we update the A_α^i's for time-evolution?

Before we address these points, we introduce the Affleck-Kennedy-Lieb-Tasaki (AKLT) state as a prime example of an MPS state. It can be seen as the Drosophila of 1D interacting phases of matter.

9.1.1 The Affleck-Kennedy-Lieb-Tasaki state

We present the AKLT-physics in the following way: First, we sketch the AKLT wave function and derive it's key properties. Second, we write it as an MPS to illustrate the concept of matrix product states. Finally

we will construct a parent Hamiltonian to which the AKLT-state is the ground-state.
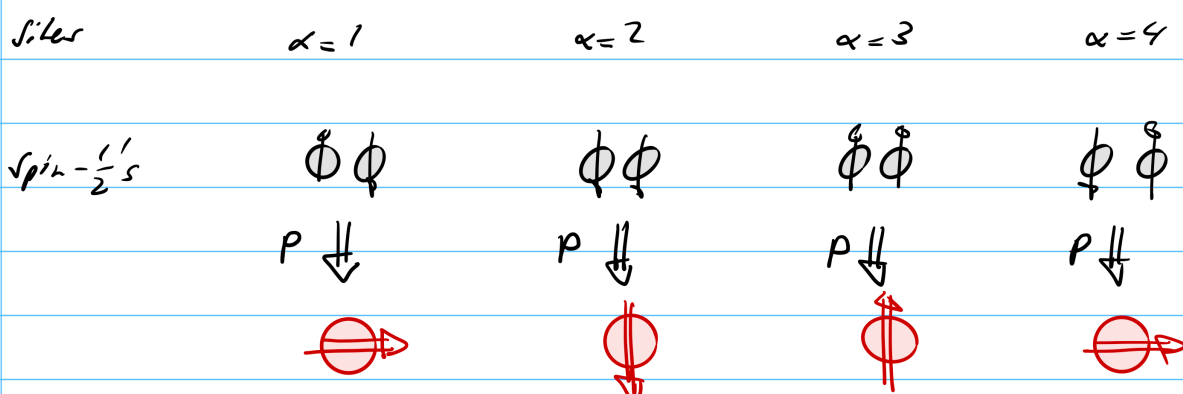
The AKLT state is a quantum state of spin-1 degrees of freedom on a one-dimensional chain. The key idea is to write each spin-1 site as one of two spin-$\frac{1}{2}$ degrees of freedom. We know that

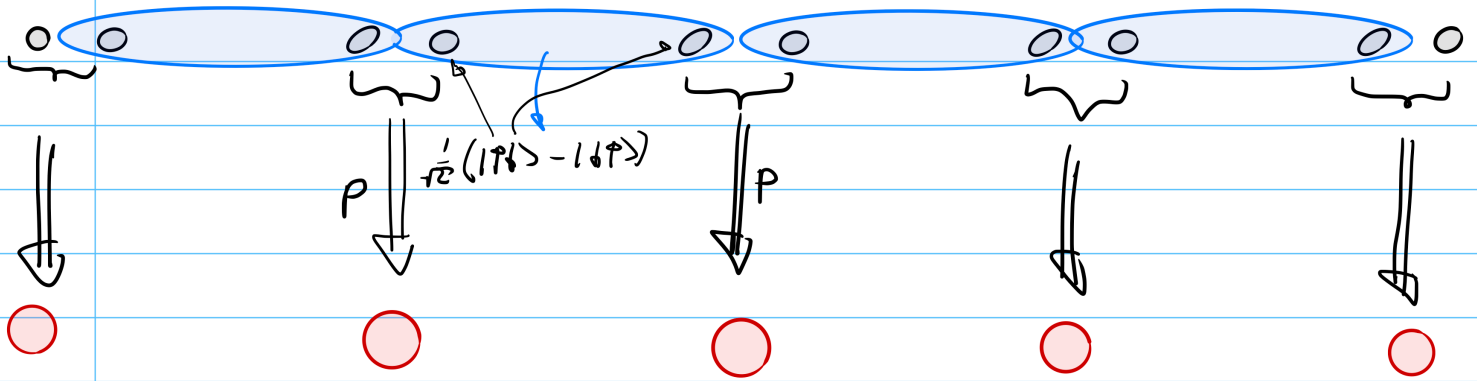$$\mathcal{H}_{\frac{1}{2}} \otimes \mathcal{H}_{\frac{1}{2}} = \mathcal{H}_1 \oplus \mathcal{H}_0$$

or

$$|\uparrow\downarrow\rangle \longrightarrow \frac{1}{\sqrt{2}}\left\{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right\} : \text{singlet} \quad \in \mathcal{H}_0$$

$$\begin{cases} |\uparrow\uparrow\rangle \\ |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle : \text{triplet} \quad \in \mathcal{H}_1 \\ |\downarrow\downarrow\rangle \end{cases}$$
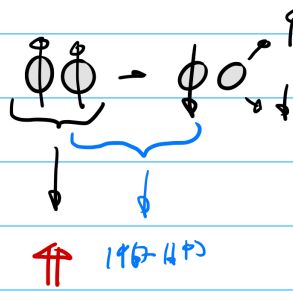
Therefore, we can write a arbitrary wave function of our auxiliary spin-$\frac{1}{2}$ degrees of freedom if we project at the end to the local triplet vector:

Sites $\alpha = 1$ $\alpha = 2$ $\alpha = 3$ $\alpha = 4$

spin-$\frac{1}{2}$'s

The key point is to form **singlets over bonds:**

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

What can we say about the structure of the spin-1 wave function? Let's say that site α projects to spin up. That means, both spin-$\frac{1}{2}$ were up! That means, the left spin-$\frac{1}{2}$ of site α is down! So what can the next projection on $\alpha+1$ yield? As the adjacent spin-$\frac{1}{2}$ over one bond are in a singlet, the moment we projected the left spin to $|\downarrow\rangle$, we know the right spin is $|\uparrow\rangle$. But that means $\alpha+1$ can only project to either ⇊ or ⇒!

What does that mean? In all S_z-configurations in our state we only have signatures such as

$$+ \ 0 \ - \ 0 \ 0 \ + \ - \ + \ 0 \ 0 \ - \ + \qquad\qquad \text{or}$$
$$- \ + \ 0 \ - \ + \ 0 \ - \ + \ 0 \ - \ + \ - \qquad\qquad \text{or}$$
$$0 \ 0 \ 0 \ 0 \ 0 \ + \ - \ + \ - \ + \ 0 \ - \ +$$

with other words, we know a "+" cannot be followed by a "−". But there might be arbitrary "0"'s in

between. This means there will be no long-range order detectable in

$$\lim_{n \to \infty} C(n) = \lim_{n \to \infty} \langle S_{i+n}^{\alpha} S_i^{\beta} \rangle$$

as knowing the spin at i doesn't allow us to infer the spin a $i+n$.

There is a trick however: Let us try to "strip away" the zeros. Remember that in an antiferromagnet we have long-range order in the staggered magnetization

$$\tilde{S}_i^z \to (-1)^i S_i^z \qquad \Rightarrow \qquad \tilde{C}^{zz}(n) = \langle \tilde{S}_{i+n}^z \tilde{S}_i^z \rangle.$$

Now, we need a way to flip, i.e. $(-1)^i$, the S_i^z operator, but "i" cannot be the site index, but an index that knows about the $S^z = 0$ sites... Let us try

$$O_{string}^z(n) = \langle S_{i+n}^z \, e^{i\pi \sum_{\ell=i+1}^{i+n-1} S_\ell^z} \, S_i^z \rangle.$$

This is called a string operator as we need to measure S^z on all sites between i and $i+n$! If we evaluate the above in an element of the z-basis, we see that if $S_\ell^z = 0$ we don't do anything, and for $S_\ell^z = \pm 1$ we we do times -1, essentially performing the transformation to a staggered magnetization but only for those sites that don't contribute a zero!
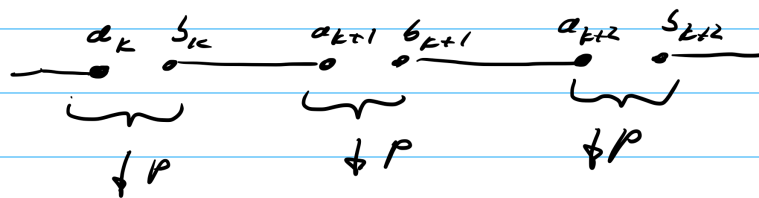
One can indeed calculate [Phys. Rev. B $\underline{40}$, 7, 1989] that

$$\sigma^2_{string}(n > 2) = \frac{4}{9}.$$

Let us now try to see how one can write this state as an MPS. We can write an arbitrary spin-$\frac{1}{2}$ state (i.e. before projection) as

$$|\psi\rangle = \sum_{\vec{a}, \vec{b}} C_{\vec{a}, \vec{b}} \; |\vec{a}\rangle \otimes |\vec{b}\rangle$$

where $\vec{a}$ and $\vec{b}$ are N-component vectors denoting the left and right auxiliary spin-$\frac{1}{2}$ on every site

Let us now write the singlet over one bond

$$|w_k\rangle = \sum_{b_k, a_{k+1} = 1}^{d} \mathcal{R}_{b_k, a_{k+1}} \; |b_k\rangle \otimes |a_{k+1}\rangle$$

with

$$\mathcal{R} = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}.$$

This might be an overkill to write

$$|w_k\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \right)$$

but it will turn out to be careful soon. If we write all of them find

$$|\psi_\omega\rangle = |\omega_1\rangle \otimes |\omega_2\rangle \otimes \cdots \otimes |\omega_N\rangle =$$

$$= \sum_{\vec{a},\vec{b}} \mathcal{R}_{b_1 a_2} \mathcal{R}_{b_2 a_3} \mathcal{R}_{b_3 a_4} \cdots \mathcal{R}_{b_N, a_1} |\vec{a}\rangle \otimes |\vec{b}\rangle$$

where we used periodic boundary conditions. Note that we don't multiply any matrices quite yet, as nothing binds a_2 to b_2, etc.. This is now done via the local projection P_k:

$$\hat{P}_k : \{|\uparrow\rangle, |\downarrow\rangle\} \otimes \{|\uparrow\rangle, |\downarrow\rangle\} \longrightarrow \{|+\rangle, |0\rangle, |-\rangle\}$$

$$|a_k\rangle \otimes |b_k\rangle \longmapsto |\sigma_k\rangle$$

where the spin-1 states σ_k are given by

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

It is now straight forward to write the projector

$$\hat{P}_k = \sum_{\sigma_k} \sum_{a_k, b_k} M^{\sigma_k}_{a_k b_k} |\sigma_k\rangle \langle a_k| \otimes \langle b_k| .$$

The M^{σ_k} are 2×2 matrices

$$M^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}; \quad M^0 = \begin{pmatrix} 0 & {}^1/\sqrt{2} \\ {}^1/\sqrt{2} & 0 \end{pmatrix}; \quad M^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Accordingly, generalizing this projection

$$\hat{P} = \hat{P_1} \otimes \hat{P_2} \otimes \hat{P_3} \otimes \cdots \otimes \hat{P_N} =$$

$$= \sum_{\vec{\sigma}, \vec{a}, \vec{b}} M^{\sigma_1}_{a_1 b_1} M^{\sigma_2}_{a_2 b_2} M^{\sigma_3}_{a_3 b_3} \cdot \cdots M^{\sigma_N}_{a_N b_N} |\vec{\sigma}\rangle \langle \vec{a}| \otimes \langle \vec{b}|$$

Now, we can apply this projection to $|\psi_\omega\rangle$:

$$\hat{P}|\psi_\omega\rangle = \sum_{\vec{\sigma}} \sum_{\vec{a}, \vec{b}} \sum_{\vec{a}', \vec{b}'} M^{\sigma_1}_{a_1 b_1} \Omega_{b_1' a_2'} M^{\sigma_2}_{a_2 b_2} \Omega_{b_2' a_3'} \cdots$$

$$\cdots M^{\sigma_N}_{a_N b_N} \Omega_{b_N', a_1'} |\vec{\sigma}\rangle \underbrace{\left(\langle \vec{b}| \otimes \langle \vec{a}|\right)\left(|\vec{a}'\rangle \otimes |\vec{b}'\rangle\right)}_{\delta_{\vec{a}\vec{a}'} \, \delta_{\vec{b}\vec{b}'}}$$

$$= \sum_{\vec{\sigma}} \sum_{\vec{a} \vec{b}} M^{\sigma_1}_{a_1 b_1} \Omega_{b_1 a_2} \cdots |\vec{\sigma}\rangle$$

$$= \sum_{\vec{\sigma}} \text{Tr}\left[M^{\sigma_1} \Omega \, M^{\sigma_2} \Omega \cdots M^{\sigma_N} \Omega \right] |\vec{\sigma}\rangle$$

$$= \sum_{\vec{\sigma}} \text{Tr}\left[\tilde{A}^{\sigma_1} \cdots \tilde{A}^{\sigma_N} \right] |\vec{\sigma}\rangle$$

where we defined $\tilde{A}^{\sigma_k} := M^{\sigma_k} \Omega$. In order to simplify we define $A^{\sigma_k} = \frac{2}{\sqrt{3}} \tilde{A}^{\sigma_k}$, such that

$$\sum_{\sigma_k} A^{\sigma_k} \left(A^{\sigma_k}\right)^+ = \mathbb{1}.$$

We will see why this property is useful later. We now have

$$A^+ = \begin{pmatrix} 0 & \sqrt{2/3} \\ 0 & 0 \end{pmatrix}, \quad A^0 = \begin{pmatrix} -1/\sqrt{3} & 0 \\ 0 & 1/\sqrt{3} \end{pmatrix}, \quad A^- = \begin{pmatrix} 0 & 0 \\ -\sqrt{2/3} & 0 \end{pmatrix}.$$

And we write

$$|\psi_{AKLT}\rangle = \sum_{\vec{\sigma}} Tr\left[A^{\sigma_1} \cdots A^{\sigma_N}\right] |\vec{\sigma}\rangle$$

We have found an MPS with bond-dimension $\chi = 2$ for the AKLT state.

We finish by saying that the AKLT wave function is the ground state to

$$H = J \sum_{\dot{o}=1}^{N} \left[\vec{S}_i \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2\right],$$

which we can write as

$$H = J \sum_{\dot{o}=1}^{N} \left[2 P_2\left(\vec{S}_i + \vec{S}_{i+1}\right) - \frac{2}{3}\mathbb{1}\right],$$

where P_2 is the projector onto spin two over the pairs of spins over a bond. By our knowledge, that we never have

$$+ + \, o + - + - + \, o \, o + o -$$

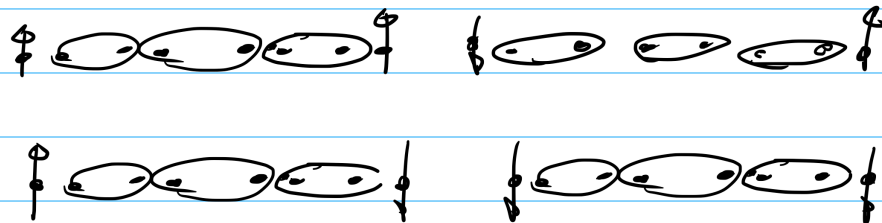never have this $\Rightarrow$ neighboring spins can only add up to 0 or 1, never 2!

This means that $|\psi_{AKLT}\rangle$ is in the kernel of

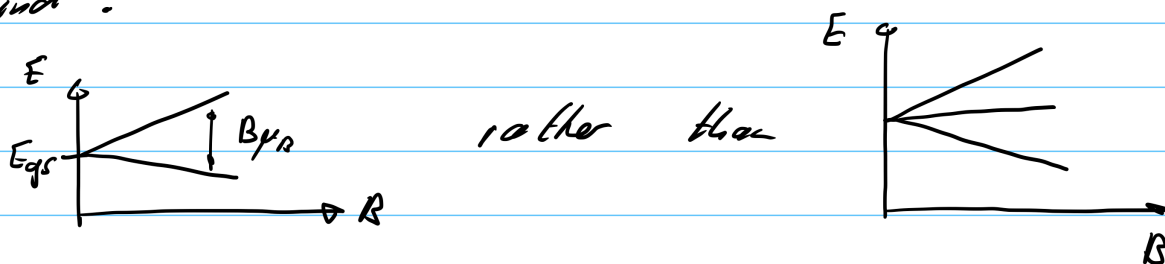P^2. As projectors are positive definite we found a ground state!

As a last thing, let us consider an *open chain*. The state looks like

We see that all bonds are in singlets and hence, also the open chain is a ground state! But, we have two *unpaired spin-$\frac{1}{2}$* at the ends. This means we have a *fourfold degenerat* ground state:

Moreover if we apply a magnetic field to the end of the chain and do spectroscopy we would find:

rather than

or one would expect for a spin-1! We have what we call *fractionalization*: A system made of spin-1 behaves locally like a spin-$\frac{1}{2}$.