1 Lecture 1

When investigating *many-body quantum systems*, we generally want statistical properties, even as our models are too complicated to solve exactly.

Example (Spin chain)**.** A system of L spins has a Hilbert space $\{|\uparrow\rangle, |\downarrow\rangle\}^{\otimes L}$ with dimension 2^L making exact numerical calculations completely infeasible for $L \gtrsim 30$

Instead we must change our mindset from finding information about all of the states, and instead focus only on the relevant sectors. For most purposes the states we are interested are near the *ground state* or *thermal states*. Hence we want a method to calculate states in these sectors, which is where the matrix product state (MPS) method comes into play.

Remark (MPS (PEPS/TNS) methods)**.** Key things to think about are

- Sysems dimension is usually 1D (or 2D)
- Works for Bosons, fermions, spins
- Works best for 'low' entanglement states, which is quantified later.
- There is primarily a possibility of finding ground state and low excited states
- It is possible to find time evolution of both closed and open systems
- The method works with finite temperature states

1.1 Idea of DMRG/MPS (Variational method)

The matrix product state method is a variational method which relies heavily on Singular value decompositions(SVD) and the Schmidt decomposition.

Method (Singular Value decomposition)**.** Any rectangular matrix A of dimensions $(m \times n)$ can be decomposed as

$$A = USV^\dagger,$$

where the matrices $U, S, V^\dagger$ are matrices with the below properties

U **:** A $(m \times \min(m,n))$ matrix with $U^\dagger U = I$

S **:** A $(\min(m,n) \times \min(m,n))$ diagonal matrix with $S_{\alpha\alpha} = \sqrt{\lambda_\alpha} \geq 0$

$V^\dagger$**:** A $(\min(m,n) \times n)$ matrix with $V^\dagger V = I$

The rank of S will turn out to be especially important and so in general we will denote $r =$ rank of S.

Method (Schmidt decomposition)**.** Using SVD we can decompose a general element of a product space $\mathcal{H}_A \otimes \mathcal{H}_B$ from a double sum over tensor products of basis elements to a single sum over an orthonormal schmidt basis as follows

$$\begin{aligned}
|\psi\rangle &= \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B \\
&= \sum_{ij\alpha} U_{i\alpha} \sqrt{\lambda_\alpha} V^*_{j\alpha} |i\rangle_A |j\rangle_B \\
&= \sum_{\alpha=1}^{r} \sqrt{\lambda_\alpha} \left(\sum_i U_{i\alpha} |i\rangle_A \right) \left(\sum_j V^*_{j\alpha} |j\rangle_B \right) \\
&= \sum_{\alpha=1}^{r} \sqrt{\lambda_\alpha} |\alpha\rangle_A |\alpha\rangle_B \qquad (\star)
\end{aligned}$$

The Schmidt decomposition is exact and the coefficients λ_α tell us very useful information about what happens if we trace out one of the two subsystems. It also provides the minimal number r of coefficients by which we may describe $|\psi\rangle$ using a product basis.

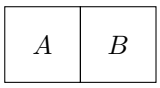
The point of matrix product states is now to find a way of implementing a variational technique for the states $|\tilde{\psi}\rangle$ which takes the form of ($\star$) with only $D \leq r$ terms. For given D we may vary the basis and coefficients to minimise $|| \, |\tilde{\psi}\rangle - |\psi\rangle \, ||$. Without loss of generality we may order the coefficients $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_r$, which allows us to calculate the minimal distance

$$\left\| |\tilde{\psi}\rangle - |\psi\rangle \right\|^2 = 1 - \sum_{\alpha=1}^{D} \lambda_\alpha.$$

It is therefore self-evident that this is good approximation if λ_α decay quickly.

1.2 Quantifying validity of approximation

By thinking of our total system as consisting of two subsystems, and tracing out one of them we can illuminate the meaning of the coefficients.



Suppose we are in a pure state of the total system so that $\rho = |\psi\rangle\langle\psi|$. The reduced density matrices for the subsystems may be found by tracing out the other part of the Hilbert space

$$\begin{aligned}
\rho_A &= \mathrm{Tr}_B \, \rho, \\
\rho_B &= \mathrm{Tr}_A \, \rho.
\end{aligned}$$

The coefficients λ_α are therefore the eigenvalues of the reduced density matrices. A measure of how mixed the state is the von-Neumann entropy

$$S = -\mathrm{Tr} \, \rho_A \ln \rho_A = -\sum_\alpha \lambda_\alpha \ln \lambda_\alpha,$$

which is small when λ_α decay fast, and maximal when they are all equal. Hence the approximation is good if S is small.

Remark. From this we may conclude that MPS methods approximates the true state well for low entropy states. An equivalent way of viewing these are as states with a low amount of entanglement *between the subsystems*[1]

Remark. Some general theorems about the growth of entropy as system size increases are known

- Ground state of 1D gapped system with short range interaction $S \to \text{const}$ as $L \to \infty$. Hence we only require our approximate state to have rank $D \sim 2^{\text{const}}$ indepedent of system size.[2]
- Ground state of 1D critical system $S \to R \ln L + \text{const}$ need $D \sim L^R$, which is polynomial in L, and therefore much more tractable than the exponential growth we see in the dimension of the full Hilbert space.

1.3 What are MPS?

So far we have no idea how we are going to implement our minimisation technique, or where the matrix product states come into play. Any $|\psi\rangle \in \mathcal{H}^{\otimes L}$ state can be decomposed into a so-called MPS by essentially unfolding the coefficients of into a product of matrices. Let

$$|\psi\rangle = \sum_{\sigma_1 \cdots \sigma_L} C_{\sigma_1,\ldots,\sigma_L} |\sigma_A\rangle \otimes \cdots \otimes |\sigma_L\rangle$$

be a representation of any given state. Now define a matrix ψ of dim $d \times d^{L-1}$ where $d = \dim\mathcal{H}$ by the relation

$$\psi_{\sigma_1,(\sigma_2,\ldots,\sigma_L)} = C_{\sigma_1\sigma_2\ldots\sigma_L}$$

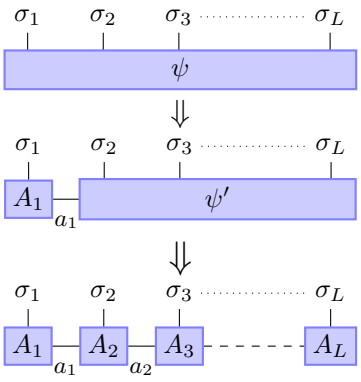
Clearly we can do SVDs iteratively on ψ

$$\begin{aligned}
\psi_{\sigma_1,(\sigma_2,\ldots\sigma_L)} &= \sum_{a_1=1}^{r_1} U_{\sigma_1,a_1} S_{a_1,a_1} (V^\dagger)_{a_1,(\sigma_2,\ldots,\sigma_L)} \\
&= \sum_{a_1=1}^{r_1} A^{\sigma_1}_{a_1} C_{a_1,\sigma_2,\ldots\sigma_L} \\
&= \sum_{a_1=1}^{r_1} \sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1,\sigma_2),a_2} S_{a_2a_2} (V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)} \\
&= \sum_{a_1,a_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1a_2} \psi_{(a_2,\sigma_3)(\sigma_4\cdots)} \\
&= \sum_{a_1\ldots a_{L-1}} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1 a2} \cdots A^{\sigma_{L-1}}_{a_{L-2}a_{L-1}} A^{\sigma_L}_{a_{L-1}}
\end{aligned}$$

Where we've decomposed the tensor coefficient into a product of matrices of dimension $(1 \times d)(d \times d^2)\ldots(d^{L/2-1} \times d^{L/2})(d^{L/2} \times d^{L/2-1})\ldots(d \times 1)$. It can be nice to think about what we are doing in diagrams, by representing a tensor as a square with lines corresponding to each index. Our matrix product state then is constructed by pulling apart each of the external indices as

[1] Ask lecturer to clarify that it is the entanglement between two subsystems which is small

[2] Shouldn't the ground state be a pure state? Ask follow up, if means ground state of combined system $A + B$.



2 Lecture 2

Now the MPS is an exact representation, but given that the matrices grow exponentially in size in the middle of the chain, it is necessary to approximate the matrices. This is where the Schmidt decomposition comes in.

Remark. We started from the left in our expansion; this is called *left-canonical* MPS or *left-normalised*. This means that

$$\sum_{\sigma_l} A^{\sigma_l\dagger} A^{\sigma_l} = I$$

This follows from

$$\begin{aligned}\sum_{\sigma_l} \left(A^{\sigma_l\dagger} A^{\sigma_l}\right)_{a_l a_l'} &= \sum_{\sigma_l, a_{l-1}} (U^\dagger)_{a_l, a_{l-1}\sigma_l} U_{a_{l-1}\sigma_l, a_l'} \\ &= \delta_{a_l, a_l'}\end{aligned}$$

Equivalently one can begin reshaping from right to get

$$|\psi\rangle = \sum_{\sigma_1 \dots \sigma_l} B^{\sigma_1} \cdots B^{\sigma_L} |\sigma_1 \dots \sigma_L\rangle$$

Which now satisfy $\sum_{\sigma_l} B^{\sigma_l} B^{\sigma_l\dagger}$. Finally we may do both from left and right, and meet at l, so get *mixed-canonical*, where

$$C_{\sigma_1 \cdots \sigma_L} = A^{\sigma_1} \cdots A^{\sigma_l} S B^{\sigma_{l+1}} \cdots B^{\sigma_L}$$

which essentially gives us a Schmidt decomposition

$$|\psi\rangle = \sum_{a_l} S_{a_l, a_l} |a_l\rangle_A |a_l\rangle_B$$

$$|a_l\rangle_A = \sum_{\sigma_1 \dots \sigma_l} (A^{\sigma_1} \cdots A^{\sigma_l})_{1, a_l} |\sigma_1 \dots \sigma_l\rangle$$

$$|a_l\rangle_B = \sum_{\sigma_{l+1} \dots \sigma_L} B^{\sigma_{l+1}} \cdots B^{\sigma_L})a_l, 1 |\sigma_{l+1} \dots \sigma_L\rangle$$

Now what we do is cut down the rank of S to a managable number. This approximation is called *compression*. A: is left normalised B: is right normalised M: is

Method (Compression by SVD)**.** Matrix dimension initially D'. Want to decrease this to dimension $D < D'$.

$$\sum_{\sigma_1 \dots \sigma_L} A^{\sigma_1} \cdots A^{\sigma_{l-1}} M^{\sigma_l} B^{\sigma_{l+1}} \cdots B^{\sigma_L} |\sigma_1 \dots \sigma_L\rangle$$

Now use SVD on $M^{\sigma_l} = USV^\dagger$ where S is of dim $D' \times D'$. Keep only D largest eigenvalues of S, to replace M with $\tilde{U}\tilde{S}\tilde{V}^\dagger$. Now reshape to A^{σ_l}, and move through σ_l iteratively.

Matrix product operators (MPO)

$$\begin{aligned} O &= \sum_{\sigma,\sigma'} W^{\sigma_1 \sigma_1'} \dots W^{\sigma_L \sigma_L'} |\sigma\rangle\langle\sigma'| \\ &= \sum C_{(\sigma_1 \dots \sigma_L)(\sigma_1' \dots \sigma_L')} |\sigma\rangle\langle\sigma'| \end{aligned}$$

where we have performed SVD to reshape (σ_l, σ_l') extract the sigma indices s1 s2 — — O = [ ]-[ ]-.. — — sp1 sp2

Can apply to operator

$$O|\psi\rangle = \sum_{\sigma\sigma'} W^{\sigma_1 \sigma_1'} M^{\sigma_1'} \dots |\sigma'\rangle$$

Graphical form

— — — [ ]-[ ]-[ ]- — — — — — — — =¿ o=o=o= * - * - * -

Example (Heisenberg Hamiltonia)**.**

$$H = \sum_i^{L-1} \frac{J}{2} \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+ + \right) + J^z \sum_{i=1}^{L-1} S_i^z S_{i+1}^z - h \sum_{i=1}^{L} S_i^z$$

This is a XXZ model

Now convert to MPO

$W_{b_{l-1} b_l}^{\sigma_l \sigma_l'} \to \left(W_{b,b'}^{[l]} \right)_{\sigma_l \sigma_l'}$ a $d \times d$ matrix

$$W^{[i]} =$$

Will not describe how to find W, but is not hard for standard hamiltonians.

2.1 Time evolution with MPS

Why is it interesting? Recent experimental setups have allowed us to control time evolution. Literature: TEBD algorithm G.Vidal PRL 91,147902(2003) t-DMRG: A Daley et all JStatMech: Theo Exp P04005(2004) : SR white and A Feighah PRL93.076401

Here focus on Trotter-Suzuki decomposition.

Assume XXZ model from before $H = \sum_i h_i$ where h_i only depends on site i and $i+1$. Want to follow time evolution of state $|\psi_0\rangle$. Use Schrödinger equation

$$i\partial_t |\psi\rangle = H |\psi\rangle \longrightarrow U(t, t+\Delta t |\psi(t)\rangle = e^{-i\Delta t H} |\psi(t)\rangle$$

Want to reach time t, discretize to time steps Δt, so that $t = N\Delta t$, where Δt compared to the energy scale.

Remark. In practice need $\Delta t \lesssim \frac{1}{100 E_{\text{char}}}$

Perform Trotter Suzuki decomposition of time evolution operator

$$e^{-i\Delta t H} \simeq \prod_{j\in\text{odd}} e^{-ih_j\Delta t} \prod_{j\in\text{even}} e^{-ih_j\Delta t} + \mathcal{O}(\Delta t^2)$$

error from non-commutitativty of h_i and h_{i+1}.

Remark. Typically one uses second order

$$e^{-i\Delta t H} \simeq \prod_{j\in\text{odd}} e^{-ih_j\Delta t/2} \prod_{j\in\text{even}} e^{-ih_j\Delta t} \prod_{j\in\text{odd}} e^{-ih_j\Delta t/2} + \mathcal{O}(\Delta t^3)$$

N times gives order of $N\Delta t^3 = t\delta t^2$ error

Remark. MPS vs Polynomial with monte carlo for ground state. MPS deals better with fermion sign problem and frustrated systems.