ULRICH SCHOLLWOECK
(University of Munich)

DENSITY-MATRIX RENORMALIZATION GROUP, MATRIX PRODUCT STATES, TENSOR NETWORK STATES – AND ALL THAT:

EFFICIENT QUANTUM SIMULATIONS IN ONE AND, HOPEFULLY, TWO DIMENSIONS

1 WHY ARE QUANTUM SIMULATIONS DIFFICULT?

conventional argument:

quantum spin chain

spin-$\frac{1}{2}$ $\{|\uparrow\rangle, |\downarrow\rangle\}^{\otimes L}$

$\mathcal{H}|\psi_0\rangle = E_0|\psi_0\rangle$ ground state, energy

$\mathcal{H} = \sum_{i=1}^{L-1} \underline{S}_i \cdot \underline{S}_{i+1}$ is a $(2^L \times 2^L)$ dim. matrix

$\Rightarrow$ exponentially large in L $\rightarrow$ thermodynamic limit unreachable

techniques:

- exact diagonalization ($L \sim 40$)
- stochastic sampling of state space (QMC techniques ... negative sign problem: frustrated magnets, fermionic systems)
- <u>variational techniques</u>: <u>subspaces</u>

more modern argument:
intrinsic difference in complexity between classical and quantum world

⇒ WHAT IS SPECIAL ABOUT QUANTUM MECHANICS?

new notion of state: ray in Hilbert space

$|\psi\rangle \in H \equiv \{|\uparrow\rangle, |\downarrow\rangle\}$ for 1 spin-$\frac{1}{2}$

<u>superposition</u> principle: $|\psi\rangle = c_\uparrow |\uparrow\rangle + c_\downarrow |\downarrow\rangle$

$$\underbrace{H_{12}}_{\substack{\text{2 particles} \\ \text{with } S=1/2}} = \underbrace{H_1 \otimes H_2}_{\text{1 particle}}$$

multiparticle space: <u>tensor product</u> of state spaces

$$|\psi\rangle_{12} = c_{\uparrow\uparrow}|\uparrow\uparrow\rangle + c_{\uparrow\downarrow}|\uparrow\downarrow\rangle + c_{\downarrow\uparrow}|\downarrow\uparrow\rangle + c_{\downarrow\downarrow}|\downarrow\downarrow\rangle$$

immediate consequence:
(Einstein, Podolsky, Rosen; Schrödinger (1935))

there exist states that are <u>not</u> <u>separable</u>:

$$\underset{\in H_{12}}{|\psi\rangle_{12}} \neq \underset{\in H_1}{|\psi\rangle_1} \otimes \underset{\in H_2}{|\psi\rangle_2}$$

examples.
- separable state $|\psi\rangle_{12} = |\uparrow\rangle_1 \otimes |\downarrow\rangle_2$

- <u>entangled</u> state

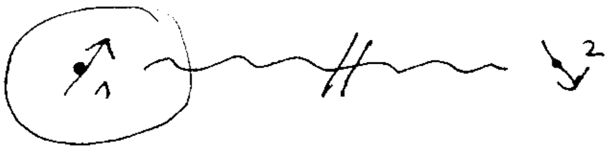
$$\boxed{|\psi\rangle_{12} = \frac{1}{\sqrt{2}}\left[|\uparrow\uparrow\rangle_{12} + |\downarrow\downarrow\rangle_{12}\right]}$$ (a <u>Bell</u> state)

(assume sep. $|\psi\rangle_{12} = |\psi\rangle_1 \otimes |\psi\rangle_2$. $|\psi_1\rangle = c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$;
$|\psi_2\rangle = d_\uparrow|\uparrow\rangle + d_\downarrow|\downarrow\rangle$.

$c_{\uparrow\uparrow} = c_\uparrow d_\uparrow$; $c_{\uparrow\downarrow} = c_\uparrow d_\downarrow$; $c_{\downarrow\uparrow} = c_\downarrow d_\uparrow$; $c_{\downarrow\downarrow} = c_\downarrow d_\downarrow$

$c_{\uparrow\downarrow} = 0 \Rightarrow c_\uparrow = 0 \vee d_\downarrow = 0 \Rightarrow c_{\uparrow\uparrow} = 0 \vee c_{\downarrow\downarrow} = 0$ ↯.)

<u>non-separability</u> of quantum mechanics :



bring 1, 2 far apart

knowledge on 1 encoded in reduced density operator:

$$\hat{\rho}_1 = \mathrm{tr}_2 |\psi\rangle_{12}\,{}_{12}\langle\psi| = \frac{1}{2}\left[|\uparrow\rangle_1\langle\uparrow| + |\downarrow\rangle_1\langle\downarrow|\right]$$

upon measurement: 50% $\uparrow$, 50% $\downarrow$: no knowledge

(Shannon information gain : $S = -\sum_i p_i \log_2 p_i = -2 \cdot \frac{1}{2}\log_2\frac{1}{2}$
$= 1$)

maximal!

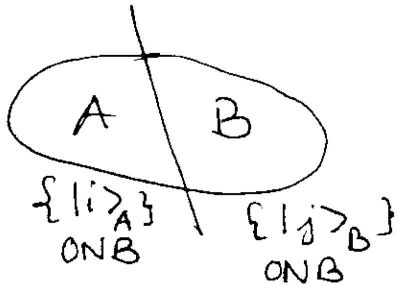
but: upon measurement of 1, 2 is fixed:
(in this case <u>all</u>) information is <u>non-local</u>.

<u>objective</u> lack of knowledge vs.
<u>subjective</u> lack of knowledge in classical physics
(statistical physics)

$\Rightarrow$ will need <u>information</u> measures, <u>entropy</u>.

object of study: encoding of <u>partial</u> quantum system:
<u>reduced density operator</u>

$$|\psi\rangle = \sum_{i,j} \psi_{ij} \, |i\rangle_A |j\rangle_B$$



$$\hat{\rho}_{AB} = |\psi\rangle\langle\psi|$$

$$(\hat{\rho}_{AB})_{ij,i'j'} = \cancel{\sum_{ii'jj'}} \psi_{ij} \psi^*_{i'j'} \, |i\rangle_A |j\rangle_B \, {}_B\langle j'| \, {}_A\langle i'|$$

$$\boxed{\hat{\rho}_A = \mathrm{tr}_B \, \hat{\rho}_{AB}}$$

$$(\hat{\rho}_A)_{i,i'} = \sum_j \psi_{ij} \psi^*_{i'j} \, |i\rangle_A \, {}_A\langle i'|$$

two important extreme cases:

$$\hat{\rho}_A = |\psi\rangle_A \, {}_A\langle\psi| \quad \Rightarrow \text{spectrum of } \hat{\rho}_A = \{1, 0, 0, 0, \dots\}$$

<u>full knowledge</u>

$$\hat{\rho}_A = \frac{1}{d^{|A|}} \sum_i |i\rangle_A \, {}_A\langle i|$$

$\{|i\rangle_A\}$ some ONB; $d^{|A|} = \dim(\mathcal{H}_A)$

size of lattice

local dimension
e.g. 2 for $S=\frac{1}{2}$

$$\Rightarrow \text{spectrum of } \hat{\rho}_A = \left\{ \frac{1}{d^{|A|}}, \frac{1}{d^{|A|}}, \dots \right\}$$

<u>full ignorance</u>

<u>minimally</u> entangled vs. <u>maximally</u> entangled
(full knowledge) (full ignorance)

Why are physicists interested?

- beginning: philosophical interest
- quantum cryptography, teleportation
  "few qubit quantum information"
- resource in quantum <u>computing</u>
- more recently:
  - characterization of quantum many body states
  - assessment of classical <u>simulatability</u> of quantum systems:
    <u>entanglement</u> as measure of <u>non-classicality</u>

2 MEASURES OF ENTANGLEMENT

would like to attribute a number S to a reduced density operator:

$$\underbrace{\begin{array}{c|c} \text{pure} & \text{separable} \\ \hat{\rho}_A & \hat{\rho}_{AB} \end{array}}_{S=0} \qquad \underbrace{\begin{array}{c|c} \text{mixed} & \text{entangled} \\ \hat{\rho}_A & \hat{\rho}_{AB} \end{array}}_{S>0}$$

reasonable demands on entanglement
(Horodecki et al 2000, Vidal 2000: entanglement monotones):

* $S=0 \Leftrightarrow$ state separable
* S continuous in state space
* invariant under subsystem basis changes (unitary trafos)
  (but not global: $\underbrace{\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)}_{\substack{S=1,\, S^z=0 \\ \text{entangled}}} \cdot \xleftrightarrow[\text{rot}]{} \underbrace{|\uparrow\uparrow\rangle}_{\substack{S=1,\, S^z=1 \\ \text{separable}}}$)
* under LOCC (local operations (generalised measurements) & classical communication):

$$\underset{\text{RDO}}{S(\hat{\rho})} \geq \sum p_i \, S(\hat{\rho}_i)$$

outcome i with probability p_i

on average, entanglement should decrease after measurement

* convexity:

$$S\left(\sum p_i \hat{\rho}_i\right) \leq \sum_i p_i \, S(\hat{\rho}_i)$$

classical mixing should reduce effect of non-classical correlations.

look for measures $S(\{w_\alpha\})$

$\{w_\alpha\}$ spectrum of reduced density operator

<u>non-unique and purpose-dependent!</u>

becomes unique upon following (reasonable) demands

* weak additivity

$$S\left((|\psi\rangle\langle\psi|)^n\right) = n \cdot S(|\psi\rangle\langle\psi|)$$

* continuity demand close to pure states

$\Rightarrow$ <u>von Neumann entropy</u> (for pure states only!)

$$\boxed{S_1(\hat{\rho}_A) = -\mathrm{tr}_A\, \hat{\rho}_A \log_2 \hat{\rho}_A = -\sum_{\alpha=1} w_\alpha \log_2 w_\alpha}$$

will mostly be dropped!

special cases: $\hat{\rho}_A = |\psi\rangle\langle\psi| \rightarrow S_1(\hat{\rho}_A) = 0$

$\hat{\rho}_A = \frac{1}{d^{|A|}} \sum_i |i\rangle_A\langle i| \Rightarrow S_1(\hat{\rho}_A) = |A| \log_2 d$

<u>extensive!</u>

von Neumann entropy is special case of

<u>Rényi entropy</u>

$$S_\alpha(\hat{\rho}_A) = \frac{1}{1-\alpha} \log_2 \mathrm{tr}\, \hat{\rho}_A^\alpha \qquad (0 \leq \alpha < \infty)$$

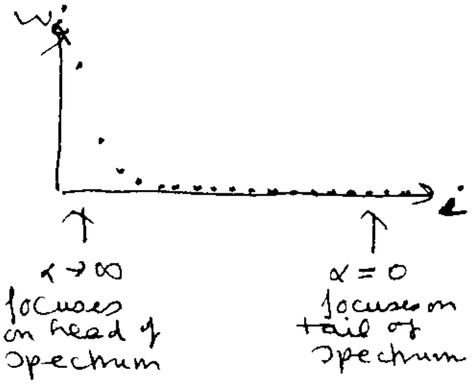
for $\alpha \searrow 1$.

limiting cases of entropy:

$\alpha = 0: \quad S_\alpha(\hat{\rho}_A) = \operatorname{rank}(\hat{\rho}_A)$

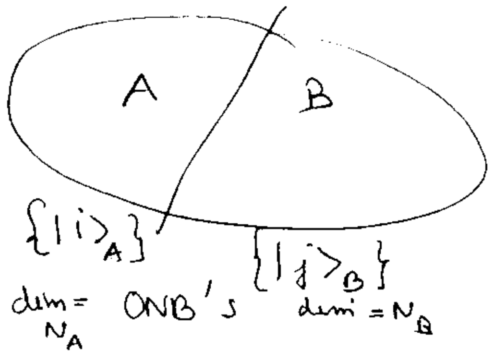
$\alpha \to \infty: \quad S_\alpha(\hat{\rho}_A) = -\log_2 w_1$

maximal eigenvalue of red. density op.



entanglement measures are "<u>executive summaries</u>" of the more complex entanglement information available through the spectrum.

(3) PURE STATE DECOMPOSITION AND REDUCED DENSITY OPERATORS



$$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$$

introduce matrix Ψ $(N_A \times N_B)$

$$(\Psi)_{ij} = \psi_{ij}$$

important tool from linear algebra:
<u>singular value decomposition</u> (SVD)

for <u>any</u> rectangular matrix A $(m \times n)$ [real, complex]

$$A = U \cdot D \cdot V^+$$

where:

* U : $(m \times \min(m,n))$: orthonormal <u>columns</u> $U^+U = I$
  (<u>unitary</u> if ~~A~~ U square) $(UU^+ = I)$
* D : $(\min(m,n) \times \min(m,n))$: non-negative diagonal:
  $D_{\alpha\alpha} \equiv \sqrt{w_\alpha} \geq 0$
* V^+ : $(\min(m,n) \times n)$: orthonormal <u>rows</u> $V^+V = I$
  (unitary if V^+ square) $(VV^+ = I)$

def: r = number of <u>non-zero</u> diagonal elements of D : <u>rank</u>

$$|\psi\rangle_{AB} = \sum_{ij\alpha} U_{i\alpha} \sqrt{w_\alpha}\, V^*_{j\alpha}\, |i\rangle_A |j\rangle_B$$

$$= \sum_{\alpha=1}^{r} \sqrt{w_\alpha} \left(\sum_i U_{i\alpha} |i\rangle_A\right) \left(\sum_j V^*_{j\alpha} |j\rangle_B\right)$$

$$= \sum_{\alpha=1}^{r} \sqrt{w_\alpha}\, |\alpha\rangle_A\, |\alpha\rangle_B$$

<u>Schmidt decomposition</u>; r <u>Schmidt rank</u>

* $r \leq \min(m,n)$
* $\{|\alpha\rangle_A\}$, $\{|\alpha\rangle_B\}$ form ON sets, that can be extended to bases of A and B (from ortho-properties of $\{|i\rangle_A\}$, $\{|j\rangle_B\}$, and U, V^+)

Why is this compact notation (much less coefficients!) useful?

$$\hat{\varrho}_A = tr_B|\psi\rangle\langle\psi| = \sum_{\alpha=1}^{r} w_\alpha |\alpha\rangle_A {}_A\langle\alpha|$$

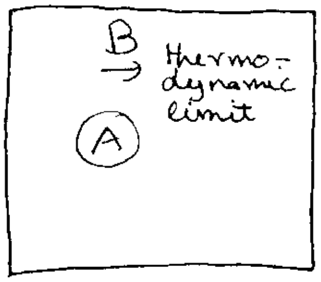
$$\hat{\varrho}_B = tr_A|\psi\rangle\langle\psi| = \sum_{\alpha=1}^{r} w_\alpha |\alpha\rangle_B {}_B\langle\alpha|$$

* direct link to reduced density operators

* reveals identity of non-vanishing parts of r.d.o. spectra

* $r=1 \Leftrightarrow$ separable; $r>1 \Leftrightarrow$ entangled.

(4) ENTANGLEMENT ENTROPY OF A PURE QUANTUM STATE – SCALING



$|A|, |B|$ # of lattice sites in A, B; $|B| \to \infty$

d # of local states ($d=2$ for $S=\frac{1}{2}$)

<u>handwaving argument</u>:

random numbers subject to normalization

<u>random</u> state $|\psi\rangle_{AB} = \sum c_{ij} |i\rangle_A |j\rangle_B$

$\Rightarrow \hat{\varrho}_A = \sum \varrho_{ii'} |i\rangle_A {}_A\langle i'|$ $\quad \varrho_{ii'} = \sum_j \varrho_{ij} \varrho^*_{i'j}$

also random (what distribution ??)

$\Rightarrow$ spectrum of $\hat{\rho}_A$, $\{w_\alpha\}$ random in $[0,1]$ $\quad \sum w_\alpha = 1$
(distribution?)

$$S(\hat{\varrho}_A) = -\sum_{\alpha=1}^{d^{|A|}} w_\alpha \log_2 w_\alpha \qquad w_\alpha \text{ are } O\left(\frac{1}{d^{|A|}}\right)$$

$$\approx -\log_2\left(\frac{1}{d^{|A|}}\right) = |A| \log_2 d$$

for a randomly picked state in $\mathcal{H}_{AB}$, entanglement entropy is

* extensive in $|A|$
* essentially maximal

All this can be done rigorously. Then:

$$\boxed{\mathbb{E}(S(\hat{\varrho}_A)) > |A| \log_2 d - \frac{d^{|A|-|B|}}{2 \log_2 2}}$$

Page 1993
Foong, Kanno 1994

expectation value taken over all states in $\mathcal{H}_{AB}$ with respect to the Haar measure

at the same time: $|A| \log_2 d \geq \mathbb{E}(S(\hat{\varrho}_A))$ [max.]

hence for $|B| \to \infty$:

$$\boxed{\mathbb{E}(S(\hat{\varrho}_A)) = |A| \log_2 d}$$

entanglement entropy is extensive and maximal except (possibly!) a subset of $\mathcal{H}_{AB}$ of (Haar) measure 0!

Fortunately, it turns out that many states of particular interest to us belong to this set of measure 0, where entanglement is not extensive and/or ~~a~~ maximal and states hence "more classical".

This might allow for an ~~more~~ efficient classical simulation!

This concerns in particular ground states (very little is known about excited states)

There are

- a few exact results (by exact solution or by conformal field theory)
- numerical results.

ONE DIMENSION

1) harmonic bosonic chain GS (Audenaert 2002)

$$S(\varrho_{\text{half-chain}}) \leq \frac{1}{2}\log_2\left(\frac{\|X\|^{1/2}}{\Delta E}\right)$$

operator norm of interaction matrix

gap

for $H = \frac{1}{2}\sum_{ij}\left(p_i P_{ij} p_j + x_i X_{ij} x_j\right)$

constant in size L (unless via gap!)

at criticality:

$$S(\varrho_{\text{half-chain}}) \leq \frac{1}{2}\log_2\left(\frac{2L}{m}\right)$$

logarithmic in size L!

for continuum limit (Klein-Gordon)

$$H = \frac{1}{2}\int_0^1 dx\ \left[\Pi^2(x) + \phi'(x) + m^2\phi^2\right]$$

This would indicate that in 1D:

subsystem size

(C) [
* gapped $\Rightarrow$ entanglement <u>constant</u> in ℓ
(in TD limit at least)
* critical $\Rightarrow$ entanglement <u>logarithmic</u> in ℓ

harmonic fermionic chain / XY model: at criticality

$$S(\hat{\rho}_A) = \xi \log_2 \ell + O(1)$$

subsystem size

But the world is not as simple... (Fannes 2003)

$\exists$ models with interaction strength $\leq \frac{\text{cst}}{r}$ that are <u>gapped</u> but have

$$S(\hat{\rho}_A) = \xi \log_2 \ell + O(1)$$

so the connection (C) is <u>not</u> true in general!

But (Hastings (2007)): compact support of interaction

H <u>local</u>, finite interaction strength ($\| h_{loc} \| < J$), gap ΔE to excitation:

$$\boxed{S(\hat{\rho}_A) \leq c_0 \xi \log_2(6\xi) \log_2 d \cdot 2^{6\xi \log_2 d}}$$

$$\begin{cases} \xi = \max\left(\frac{2v}{\Delta E}, \xi_c\right) \\ \xi_c \quad O(1) \\ v \quad \text{velocity of sound} \end{cases}$$

bounded by a <u>constant</u>.

conformal field theory (Cardy, Calabrese 2004-)

$S(\rho_A) = \frac{c}{3}\log_2 \ell + O(1)$ (ℓ subsystem size measured in lattice spacings)

$S_\alpha(\rho_A) = \frac{c}{6}\left(1+\frac{1}{\alpha}\right)\log_2 \ell + O(1)$

previously found numerically: Latorre, Rico, Vidal, Kitaev (2003,4)

So, at least for local Hamiltonians area laws with(out) logarithmic corrections are true for ground states at (not at) criticality!

TWO DIMENSIONS

More confused situation, but area laws do exist.
More later!

⑥ WHAT IS SIMULATABILITY?

Variational methods explore subsets of Hilbert space.
(like ansatzes $\psi(x) = e^{-(\alpha|x|+\beta|x|^2)}$ etc.)

Can we devise a variational method that works in the right "corner" of Hilbert space (which is so much smaller than the full one!)?

"Size of Hilbert space only an illusion"

If this is workable, I would call ground states "simulatable".

What do we need?

* identify "important" states in Hilbert space
* parametrize them efficiently
* "search" them efficiently

"efficiently" means with a numerical tool that is polynomial in system size (as opposed to exponential)

↳ will the power be small? other price to be paid?

Claim:

Matrix product states (MPS) good tool to do all this and highlight relationship to entanglement!

Literature:

US, RMP 77, 259 (2005)

US, Ann. Phys. 326, 96 (2011)

Verstraete, ~~~~ Murg, Cirac, Adv. Phys. 57, 143 (2008)

7 INTRODUCTION OF MATRIX PRODUCT STATES.

preliminary remarks.

(i) SVD can not only be used for decompositions, but also approximation of states:

$$|\psi\rangle = \sum_{\alpha=1}^{r} \sqrt{w_\alpha}\, |\alpha\rangle_A |\alpha\rangle_B$$

to be approx. in $\|\cdot\|_2$-norm by

$$|\tilde{\psi}\rangle = \sum_{\alpha=1}^{\tilde{r}} \sqrt{\tilde{w}_\alpha}\, |\alpha\rangle_A |\alpha\rangle_B \, ,$$

minimizing $\| |\psi\rangle - |\tilde{\psi}\rangle \|_2^2$.

On matrices, inner product $\langle M|N\rangle = \mathrm{tr}\, M^\dagger N$ induces Frobenius norm $\|M\|_F^2 = \sum_{ij} |M_{ij}|^2$.

Claim: optimal approx. of M (rank r) by $\tilde{M}$ (rank $\tilde{r}$) $\tilde{r} < r$ in Frobenius norm is given by

$$\tilde{M} = U \tilde{D} V^\dagger \qquad \tilde{D} = \mathrm{diag}\,(\underbrace{\sqrt{w_1}, \sqrt{w_2}, \sqrt{w_3}, \ldots \sqrt{w_{\tilde{r}}}}_{\text{largest } r' \text{ singular values.}}, 0, 0, 0)$$

But $\| |\psi\rangle \|_2^2 = \sum_{ij} |\psi_{ij}|^2 = \|\Psi\|_F^2$ if we define $(\Psi)_{ij} = \psi_{ij}$.

$$\hookrightarrow |\tilde{\psi}\rangle = \sum_{\alpha=1}^{\tilde{r}} \sqrt{w_\alpha}\, |\alpha\rangle_A |\alpha\rangle_B$$

└ leading singular values; for normalization rescaling!

(ii) SVD is a beautiful tool in mathematics, but costly in numerics.

we will often need $M = U D V^{+}$ only as

* $U^{+}U = I$
* (DV^{+})

$\Rightarrow$ better tool given by <u>QR-decomposition.</u>

$$M = Q \cdot R$$

M: $(N_A \times N_B)$, Q: $(N_A \times N_A)$, R: $(N_A \times N_B)$

* Q unitary: $Q^{+}Q = QQ^{+} = I$
* R upper triangular: $R_{ij} = 0$ if $i > j$

$N_A > N_B$:

all zero

$$M = Q \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = [Q_1 \, Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1$$

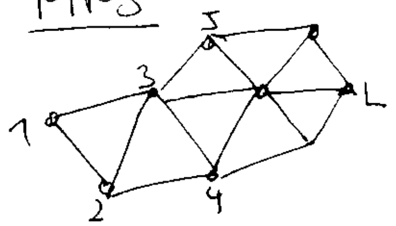
$(N_A \times N_B)$ only

will be used in the following

$Q_1^{+} Q_1 = I$, $Q_1 Q_1^{+} \neq I$ (in general)

$Q_{(1)}$ and U share properties, but are not the same!
(QR) (SVD)

Decomposition of arbitrary quantum states into MPS



d-dim state spaces $\{\sigma_i\}$; $i = 1, \dots, L$
(will focus on 1D ,
but at first arbitrary)

[MPS in higher than 1D theoretical, but not practical tool.]

$$|\psi\rangle = \sum_{\sigma_1, \dots, \sigma_L} \underbrace{c_{\sigma_1 \dots \sigma_L}}_{\text{exp. many!}} |\sigma_1, \sigma_2, \dots, \sigma_L\rangle$$

$\boxed{\text{LEFT-CANONICAL MPS}}$

reshape $\begin{pmatrix} \vdots \end{pmatrix}$ [d^L components] as matrix $d\Big\{\overbrace{\begin{pmatrix} \cdots \\ \cdots \end{pmatrix}}^{d^{L-1}}$ $(d \times d^{L-1})$

- $\Psi_{\sigma_1, (\sigma_2, \dots, \sigma_L)} := c_{\sigma_1, \sigma_2, \dots, \sigma_L}$.
- SVD of Ψ:

$$c_{\sigma_1 \dots \sigma_L} = \Psi_{\sigma_1, (\sigma_2 \dots \sigma_L)} = \sum_{a_1}^{r_1} U_{\sigma_1, a_1} \underbrace{S_{a_1 a_1} (V^\dagger)_{a_1, (\sigma_2 \dots \sigma_L)}}_{\text{back to vector}}$$
$$\equiv \sum_{a_1}^{r_1} U_{\sigma_1, a_1} c_{a_1 \sigma_2 \dots \sigma_L}$$

rank $r_1 \leq d$

- decompose U into collection of d row vectors A^{σ_1} with entries $A^{\sigma_1}_{a_1} = U_{\sigma_1, a_1}$.
- reshape $c_{a_1 \sigma_2 \dots \sigma_L} \to \Psi_{(a_1 \sigma_2), (\sigma_3 \dots \sigma_L)}$ $(r_1 d \times d^{L-2})$

$$c_{\sigma_1 \dots \sigma_L} = \sum_{a_1}^{r_1} A^{\sigma_1}_{a_1} \Psi_{(a_1 \sigma_2), (\sigma_3 \dots \sigma_L)}$$

- SVD of Ψ:

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} U_{(a_1\sigma_2),a_2} S_{a_2a_2} (V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)}$$
$$= \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{a_1} A^{\sigma_2}_{a_1a_2} \Psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}$$

- $U_{(a_1\sigma_2),a_2} \rightarrow A^{\sigma_2}_{a_1a_2}$ set of d matrices $(r_1 \times r_2)$

$r_2 \leq r_1 d \leq d^2$

- $(V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)} \rightarrow \Psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}$

and so on!

at the end: row vec's matrices col. vec's

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1\ldots a_{L-1}} A^{\sigma_1}_{a_1} \underbrace{A^{\sigma_2}_{a_1a_2} A^{\sigma_3}_{a_2a_3} \cdots A^{\sigma_{L-1}}_{a_{L-2}a_{L-1}}}_{\text{matrices}} A^{\sigma_L}_{a_{L-1}}$$

matrix multiplications

$$\boxed{c_{\sigma_1\ldots\sigma_L} = A^{\sigma_1}A^{\sigma_2}A^{\sigma_3}\ldots A^{\sigma_{L-1}}A^{\sigma_L}}$$

and we obtain a <u>matrix product state</u>:

$$\boxed{|\psi\rangle = \sum_{\sigma_1\ldots\sigma_L} A^{\sigma_1}A^{\sigma_2}A^{\sigma_3}\ldots A^{\sigma_{L-1}}A^{\sigma_L}\,|\sigma_1\sigma_2\ldots\sigma_{L-1}\sigma_L\rangle}$$

properties of A-matrices :

(i) maximal dimensions given by SVD's where # of non-zero singular values reaches theoretical maximum (smaller of two dimensions of matrix SVD'ed)

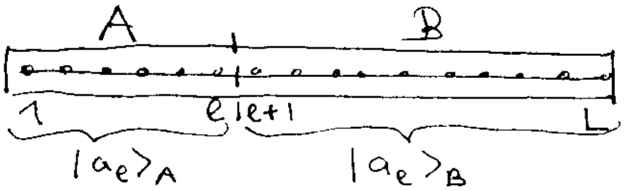
$(1\times d), (d\times d^2), (d^2\times d^3), \ldots, (d^{L/2-1}\times d^{L/2}), (d^{L/2}\times d^{L/2-1}), \ldots, (d^2\times d), (d\times 1)$

$\Rightarrow$ <u>exact</u> MPS decomposition impractical, will be exponentially large.

(ii)
$$\begin{aligned}\delta_{a_\ell, a_\ell'} &= \sum_{a_{\ell-1}\sigma_\ell} (U^\dagger)_{a_\ell, a_{\ell-1}\sigma_\ell} U_{a_{\ell-1}\sigma_\ell, a_\ell'} \\ &= \sum_{a_{\ell-1}\sigma_\ell} (A^{\sigma_\ell \dagger})_{a_\ell a_{\ell-1}} A^{\sigma_\ell}_{a_{\ell-1}a_\ell} \\ &= \sum_{\sigma_\ell} (A^{\sigma_\ell\dagger}A^{\sigma_\ell})_{a_\ell a_\ell'}\end{aligned}$$

$$\Rightarrow \boxed{\sum_{\sigma_\ell} A^{\sigma_\ell\dagger}A^{\sigma_\ell} = I}$$ <u>left-normalized</u>

an MPS made from L-~~normalized~~ normalized A^σ we call left-canonical.



$$|a_\ell\rangle_A = \sum_{\sigma_1\ldots\sigma_\ell} (A^{\sigma_1}\cdots A^{\sigma_\ell})_{1,a_\ell} |\sigma_1,\ldots,\sigma_\ell\rangle$$

$$|a_\ell\rangle_B = \sum_{\sigma_{\ell+1}\ldots\sigma_L} (A^{\sigma_{\ell+1}}\cdots A^{\sigma_L})_{a_\ell,1} |\sigma_{\ell+1},\ldots,\sigma_L\rangle$$

$$|\psi\rangle = \sum_{a_\ell} |a_\ell\rangle_A |a_\ell\rangle_B$$

looks <u>almost</u> like Schmidt-decomposition, but:

$\{|a_\ell\rangle_A\}$ are ON-set

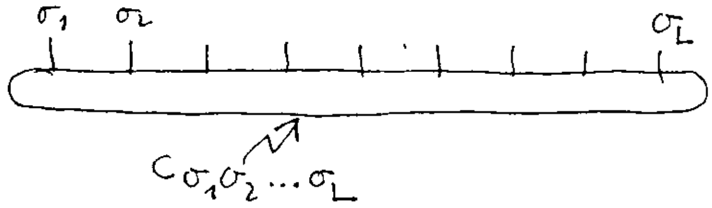
$\{|a_\ell\rangle_B\}$ are in general <u>not</u>.

$$
{}_A\langle a_\ell'|a_\ell\rangle_A = \sum_{\sigma_1\ldots\sigma_\ell} (A^{\sigma_1}\ldots A^{\sigma_\ell})^*_{1,a_\ell'} (A^{\sigma_1}\ldots A^{\sigma_\ell})_{1,a_\ell}
$$
$$
= \sum_{\sigma_1\ldots\sigma_\ell} (A^{\sigma_1}\ldots A^{\sigma_\ell})^\dagger_{a_\ell',1} (A^{\sigma_1}\ldots A^{\sigma_\ell})_{1,a_\ell}
$$
$$
= \sum_{\sigma_1\ldots\sigma_\ell} (A^{\sigma_\ell\dagger}\ldots \underbrace{\underbrace{A^{\sigma_1\dagger}A^{\sigma_1}}_{I \text{ after sum } \sigma_1}\ldots}_{I \text{ after sum } \sigma_2} A^{\sigma_\ell})_{a_\ell' a_\ell} = \delta_{a_\ell' a_\ell}. \quad \text{ON!}
$$

same calc ${}_B\langle a_\ell'|a_\ell\rangle_B$ leads to $\sum_{\sigma_\ell} A^{\sigma_\ell} A^{\sigma_\ell\dagger} \neq I$ in general.

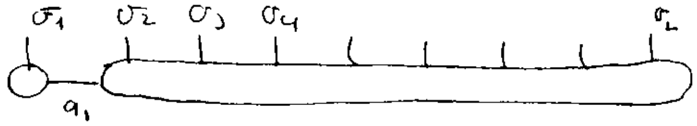
$\Rightarrow {}_B\langle a_\ell'|a_\ell\rangle_B \neq \delta_{a_\ell' a_\ell}$

<u>graphical</u> representation:



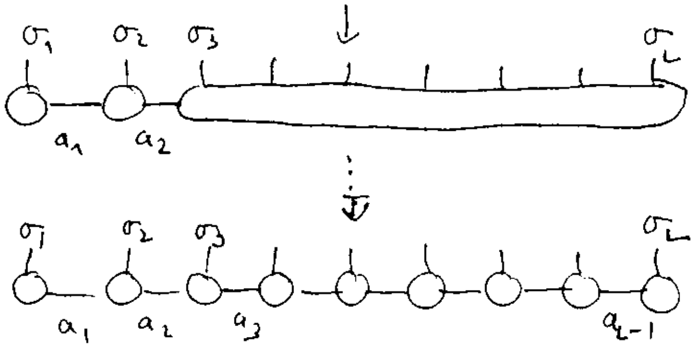
physical indices ≡ vertical legs

first decomposition:

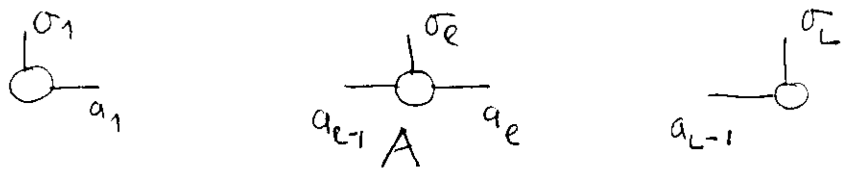


auxiliary indices ≡ horizontal legs

rule: <u>connected</u> lines are <u>summed</u> over (here $\sum_{a_1}$)



A-matrices are represented as:



<u>remark</u>: all this could also have been achieved by QR-decompositions (try for yourself!)

$\boxed{\text{RIGHT-CANONICAL MPS}}$

decomposition can also start from the right!

$$c_{\sigma_1 \dots \sigma_L} =$$

$$\Psi_{(\sigma_1 \dots \sigma_{L-1}),\sigma_L} = \sum_{a_{L-1}} U_{(\sigma_1 \dots \sigma_{L-1}),a_{L-1}} \underbrace{S_{a_{L-1}a_{L-1}} (V^\dagger)_{a_{L-1},\sigma_L}} =$$

$$\sum_{a_{L-1}} \Psi_{(\sigma_1 \dots \sigma_{L-2}),(\sigma_{L-1} a_{L-1})} B^{\sigma_L}_{a_{L-1}} =$$

$$\sum_{a_{L-2},a_{L-1}} U_{(\sigma_1 \dots \sigma_{L-2}),a_{L-2}} \underbrace{S_{a_{L-2}a_{L-2}} (V^\dagger)_{a_{L-2},(\sigma_{L-1} a_{L-1})}}_{B^{\sigma_{L-1}}_{a_{L-2},a_{L-1}}} B^{\sigma_L}_{a_{L-1}} = \dots$$

$$\sum_{a_1 \dots a_{L-1}} B^{\sigma_1}_{a_1} B^{\sigma_2}_{a_1,a_2} \dots B^{\sigma_{L-1}}_{a_{L-2}a_{L-1}} B^{\sigma_L}_{a_{L-1}}$$

$$\rightsquigarrow |\Psi\rangle = \sum_{\sigma_1 \dots \sigma_L} B^{\sigma_1} \dots B^{\sigma_L} |\sigma_1 \dots \sigma_L\rangle$$

with (decisive point!)

$$\sum_{\sigma_\ell} B^{\sigma_\ell} B^{\sigma_\ell \dagger} = I$$

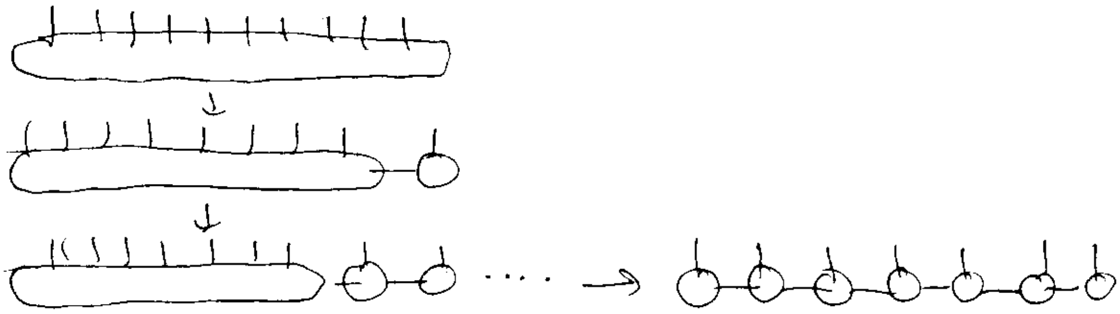
<u>right-normalized</u>, <u>right-canonical</u>

Again,

$$|a_\ell\rangle_A = \sum_{\sigma_1\dots\sigma_\ell} (B^{\sigma_1}\dots B^{\sigma_\ell})_{1,a_\ell}|\sigma_1\dots\sigma_\ell\rangle \quad \leftarrow \underline{\text{not}}\ \text{ON}$$

$$|a_\ell\rangle_B = \sum_{\sigma_{\ell+1}\dots\sigma_L} (B^{\sigma_{\ell+1}}\dots B^{\sigma_L})_{a_\ell,1}|\sigma_{\ell+1}\dots\sigma_L\rangle \quad \leftarrow \text{ON}$$

(following same argument!)



can also be achieved by QR-decomp, but instead of

$$\Psi = QR \;\rightarrow\; \Psi^\dagger = QR \;\text{ or }\; \Psi = R^\dagger \underbrace{Q^\dagger}_{B}.$$

$\boxed{\text{MIXED-CANONICAL MPS}}$

try to combine good properties from L-normalized and R-normalized states!

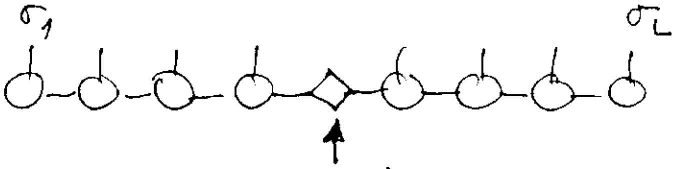
* start decomp from left up to site ℓ

$$c_{\sigma_1\dots\sigma_\ell} \rightarrow \sum (A^{\sigma_1}\dots A^{\sigma_\ell})_{a_\ell} \underbrace{S_{a_\ell a_\ell} V^\dagger_{a_\ell,(\sigma_{\ell+1}\dots\sigma_L)}}$$

* start decomp from right for $\Psi^\dagger$

$$c_{\sigma_1\dots\sigma_\ell} \rightarrow \underbrace{A^{\sigma_1}\dots A^{\sigma_\ell}}_{\text{L-normalized}}\, S\, \underbrace{B^{\sigma_{\ell+1}}\dots B^{\sigma_L}}_{\text{R-normalized}}$$

(by construction for $\ell+2\dots L$, by calculation for $\ell+1$: automatic!) (Exercise)



S singular values

direct link to Schmidt decomposition at bond $(\ell, \ell+1)$:

$$|a_\ell\rangle_A = \sum_{\sigma_1 \ldots \sigma_\ell} (A^{\sigma_1} \ldots A^{\sigma_\ell})_{1,a_\ell} |\sigma_1 \ldots \sigma_\ell\rangle \quad \text{ON}$$

$$|a_\ell\rangle_B = \sum_{\sigma_{\ell+1} \ldots \sigma_L} (B^{\sigma_{\ell+1}} \ldots B^{\sigma_L})_{a_\ell,1} |\sigma_{\ell+1} \ldots \sigma_L\rangle \quad \text{ON}$$

$$\Rightarrow |\psi\rangle = \sum_{a_\ell} S_{a_\ell} |a_\ell\rangle_A |a_\ell\rangle_B$$ Schmidt decomposition!

GAUGE DEGREES OF FREEDOM

same state represented in different MPS $\Rightarrow$ not unique!

consider general MPS : (A = L-norm, B = R-norm, M = anything

$$\ldots M^{\sigma_\ell} M^{\sigma_{\ell+1}} \ldots$$

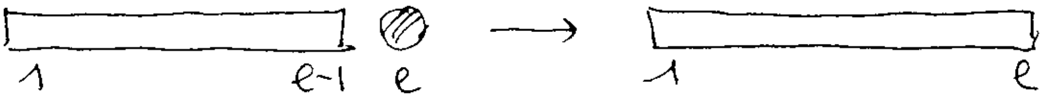
$$\equiv \ldots \underbrace{M^{\sigma_\ell} X}_{\tilde{M}^{\sigma_\ell}} \underbrace{X^{-1} M^{\sigma_{\ell+1}}}_{\tilde{M}^{\sigma_{\ell+1}}}$$

gauge degree of freedom

MPS and single-site decimation in one dimension

Can we link the MPS construction to something more typical of, say, statistical physics?

RG growth step:



$$|a_{\ell-1}\rangle_A \quad |\sigma_\ell\rangle \quad \rightarrow \quad |a_\ell\rangle_A$$
$$(\# = D) \qquad\qquad\qquad (\# = D)$$

state space grows $\times d$ $\Rightarrow$ <u>decimation</u> by (now) undefined procedure

$$|a_\ell\rangle_A = \sum_{\sigma_\ell a_{\ell-1}} {}_A\langle a_{\ell-1}\sigma_\ell | a_\ell\rangle_A \; |a_{\ell-1}\rangle_A |\sigma_\ell\rangle$$

now introduce d matrices $A^{[\ell]\sigma_\ell}$ at site ℓ of dim. $D\times D$:

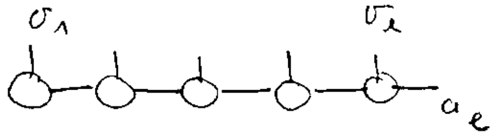
$$\boxed{\left(A^{[\ell]\sigma_\ell}\right)_{a_{\ell-1}a_\ell} := {}_A\langle a_{\ell-1}\sigma_\ell | a_\ell\rangle_A}$$

usually, notation overkill: drop $[\ell]$ marker.

why is this useful (beyond looking like MPS):

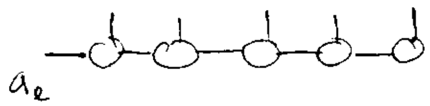
<u>recursion.</u>

$$|a_\ell\rangle_A = \sum_{a_{\ell-1}}\sum_{\sigma_\ell} A^{\sigma_\ell}_{a_{\ell-1}a_\ell} |a_{\ell-1}\rangle_A |\sigma_\ell\rangle$$
$$= \sum_{a_{\ell-2}a_{\ell-1}} \sum_{\sigma_{\ell-1}\sigma_\ell} A^{\sigma_{\ell-1}}_{a_{\ell-2}a_{\ell-1}} A^{\sigma_\ell}_{a_{\ell-1}a_\ell} |a_{\ell-2}\rangle_A |\sigma_{\ell-1}\rangle|\sigma_\ell\rangle = \dots$$
$$= \sum_{a_1\dots a_{\ell-1}} \sum_{\sigma_1\dots\sigma_\ell} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1a_2} \dots A^{\sigma_\ell}_{a_{\ell-1}a_\ell} |\sigma_1\rangle|\sigma_2\rangle\dots|\sigma_\ell\rangle$$
$$= \sum_{\sigma_i \in A} \left(A^{\sigma_1}\dots A^{\sigma_\ell}\right)_{1,a_\ell} |\sigma_1\dots\sigma_\ell\rangle .$$



$|a_\ell\rangle_A$

similarly, construction from the right:



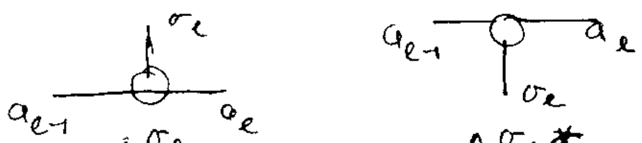
$|a_\ell\rangle_B$

$$|a_\ell\rangle_B = \sum_{\sigma_i \in B} (B^{\sigma_{\ell+1}} B^{\sigma_{\ell+2}} \cdots B^{\sigma_L})_{a_{\ell+1},1} |\sigma_{\ell+1}\sigma_{\ell+2}\cdots\sigma_L\rangle$$

if we demand that states $\{|a_\ell\rangle_A\}$ are ON, this implies L-normalization:

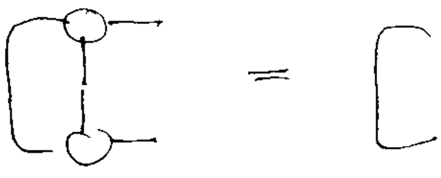
$$\boxed{\sum_\sigma A^{\sigma\dagger} A^\sigma = I}$$

graphical representation of normalization condition:



$A^{\sigma_\ell}_{a_{\ell-1}a_\ell}$ $\quad$ $A^{\sigma_\ell *}_{a_{\ell-1}a_\ell}$ $\quad$ complex conjugate

L-normalization:



$$\sum_{a_{\ell-1}} \sum_{\sigma_\ell} A^{\sigma_\ell *}_{a_{\ell-1}a_\ell'} A^{\sigma_\ell}_{a_{\ell-1}a_\ell} = \delta_{a_\ell a_\ell'}$$

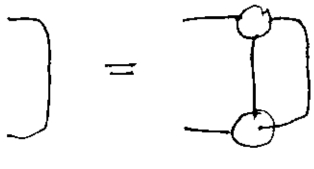
$$\parallel$$

$$\sum_{a_{\ell-1}} \sum_{\sigma_\ell} A^{\sigma_\ell \dagger}_{a_\ell' a_{\ell-1}} A^{\sigma_\ell}_{a_{\ell-1}a_\ell}$$

$$\parallel$$

$$\Big(\sum_{\sigma_\ell} A^{\sigma_\ell\dagger} A^{\sigma_\ell}\Big)_{a_\ell' a_\ell}$$

R-normalization:



9 AKLT model as a matrix product state

AKLT = Affleck, Kennedy, Lieb, Tasaki (1987)

$$H_{AKLT} = \sum_i \left\{ \underline{S}_i \cdot \underline{S}_{i+1} + \frac{1}{3}(\underline{S}_i \cdot \underline{S}_{i+1})^2 \right\}$$

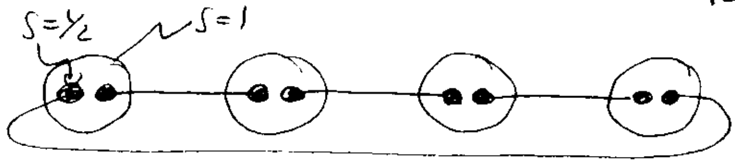
$S = 1$ (!)

claim: ground state given as follows:

build $S=1$ states from symmetric states of 2 $S=1/2$:

$$|\uparrow\uparrow\rangle \longrightarrow |+\rangle \qquad (S^z = 1)$$
$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \longrightarrow |0\rangle \qquad (S^z = 0)$$
$$|\downarrow\downarrow\rangle \longrightarrow |-\rangle \qquad (S^z = -1)$$

(discard antisymmetric state: $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$)



Connect 2 $S=1/2$ via singlet state $\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$.

This can be encoded easily as an MPS:

in auxiliary spin-1/2 language:

$$|\psi\rangle = \sum_{\underline{a}} \sum_{\underline{b}} c_{\underline{a}\underline{b}} |\underline{a}\underline{b}\rangle$$

$|\underline{a}\rangle = |a_1 \dots a_L\rangle$ 1st
$|\underline{b}\rangle = |b_1 \dots b_L\rangle$ 2nd
spin-1/2 on sites 1 ... L

singlet bond between sites i and $i+1$:

$$|\Sigma^{[i]}\rangle = \sum_{b_i a_{i+1}} \tilde{\Sigma}_{ba} |b_i\rangle |a_{i+1}\rangle$$

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

$$|\psi_\Sigma\rangle = \sum_{\underline{a}\,\underline{b}} \tilde{\Sigma}_{b_1 a_2} \tilde{\Sigma}_{b_2 a_3} \dots \tilde{\Sigma}_{b_{L-1} a_L} \Sigma_{b_L a_1} \, |\underline{a}\,\underline{b}\rangle$$

<u>mapping</u> from $|a_i\rangle|b_i\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}^{\otimes 2} \to |\sigma_i\rangle \in \{|-\rangle, |0\rangle, |+\rangle\}$

introduce $M^{\sigma}_{ab} |\sigma\rangle\langle ab|$ and write as 3 matrices $\underset{(2\times 2)}{}$ M^σ:

└ contains mapping

$$M^+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad M^0 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \qquad M^- = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

mapping reads:

$$\sum_{\underline{\sigma}} \sum_{\underline{a}\,\underline{b}} M^{\sigma_1}_{a_1 b_1} M^{\sigma_2}_{a_2 b_2} \dots M^{\sigma_L}_{a_L b_L} \, |\underline{\sigma}\rangle\langle \underline{a}\,\underline{b}|$$

$$|\psi_\Sigma\rangle \text{ maps to } \sum_{\underline{\sigma}} \sum_{\underline{a}\,\underline{b}} M^{\sigma_1}_{a_1 b_1} \tilde{\Sigma}_{b_1 a_2} M^{\sigma_2}_{a_2 b_2} \tilde{\Sigma}_{b_2 a_3} M^{\sigma_3}_{a_3 b_3} \dots |\underline{\sigma}\rangle$$

$$|\psi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}\,(\underbrace{M^{\sigma_1} \tilde{\Sigma}}_{\tilde{A}^{\sigma_1}} M^{\sigma_2} \tilde{\Sigma} \dots) \, |\underline{\sigma}\rangle$$

$$\tilde{A}^+ = \begin{bmatrix} 0 & 1/\sqrt{2} \\ 0 & 0 \end{bmatrix} \qquad \tilde{A}^0 = \begin{bmatrix} -1/2 & 0 \\ 0 & +1/2 \end{bmatrix} \qquad \tilde{A}^- = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}.$$

AKLT: $|\psi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}(\tilde{A}^{\sigma_1}\tilde{A}^{\sigma_2}\dots\tilde{A}^{\sigma_L})|\underline{\sigma}\rangle$

L-normalize $\tilde{A}$:

$$\sum_\sigma \tilde{A}^{\sigma\dagger}\tilde{A}^{\sigma} = \frac{3}{4} I \Rightarrow \text{rescale by } \frac{2}{\sqrt{3}}.$$

$$A^+ = \begin{bmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix} \quad A^0 = \begin{bmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \quad A^- = \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$$

normalizes state in TD limit:

$$\begin{aligned} \langle\psi|\psi\rangle &= \sum_{\underline{\sigma}} \mathrm{tr}(A^{\sigma_1}\dots A^{\sigma_L})^* \mathrm{tr}(A^{\sigma_1}\dots A^{\sigma_L}) \\ &= \mathrm{tr}\left(\sum_{\sigma_1} A^{\sigma_1 *}\otimes A^{\sigma_1}\right)\left(\sum_{\sigma_2} A^{\sigma_2 *}\otimes A^{\sigma_2}\right)\dots \\ &= \mathrm{tr}\, E^L = \sum_{i=1}^{4} \lambda_i^L \end{aligned}$$

λ_i eigenvalues of

$$E = \sum_\sigma A^{\sigma *}\otimes A^{\sigma} = \begin{bmatrix} \frac{1}{3} & 0 & 0 & \frac{2}{3} \\ 0 & -\frac{1}{3} & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 0 \\ \frac{2}{3} & 0 & 0 & \frac{1}{3} \end{bmatrix}$$

$$\Rightarrow \lambda_i = \left(1, -\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}\right)$$

$$\langle\psi|\psi\rangle = 1 + 3\left(-\tfrac{1}{3}\right)^L \to 1 \text{ for } L\to\infty.$$

Exercise:

show $\langle S_i^z S_j^z\rangle \propto (-1/3)^{i-j}$

$\langle S_i^z e^{i\pi\sum_{i<k<j} S_k^z} S_j^z\rangle = -\frac{4}{9}$ for $j-i>2$

("hidden order")

10 Calculating with MPS

overlaps: $|\phi\rangle \to \{\tilde{M}\}$; $|\psi\rangle \to \{M\}$

$$\langle\phi|\psi\rangle = \sum_{\underline{\sigma}} \underbrace{\tilde{M}^{\sigma_1 *}\dots\tilde{M}^{\sigma_L *}}_{\text{scalar}} M^{\sigma_1}\dots M^{\sigma_L}$$

$$= \sum_{\underline{\sigma}} \tilde{M}^{\sigma_L \dagger}\dots\tilde{M}^{\sigma_1 \dagger} M^{\sigma_1}\dots M^{\sigma_L}$$

right (optimal) order of contractions:

one might multiply matrices, and sum over $\underline{\sigma}$ in the end

$\Rightarrow$ exponentially complex in system size. NO!

instead:

$$\langle\phi|\psi\rangle = \sum_{\sigma_L} \tilde{M}^{\sigma_L \dagger}\Big(\dots\Big(\sum_{\sigma_2}\tilde{M}^{\sigma_2 \dagger}\underbrace{\Big(\sum_{\sigma_1}\tilde{M}^{\sigma_1 \dagger}M^{\sigma_1}\Big)}_{\text{multiply and sum}} M^{\sigma_2}\Big)\dots\Big) M^{\sigma_L}$$

multiply

multiply

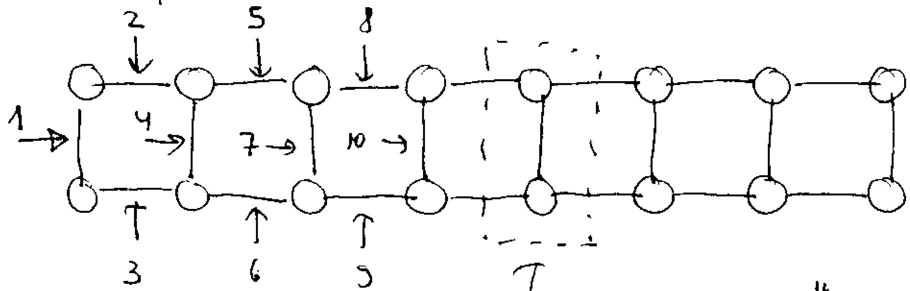
and sum

$$\sum (A \quad B) \; C$$

$(2L-1)d$ multiplications of $O(D^3)$ each

operation count $\boxed{O(LD^3d)}$

in a picture:

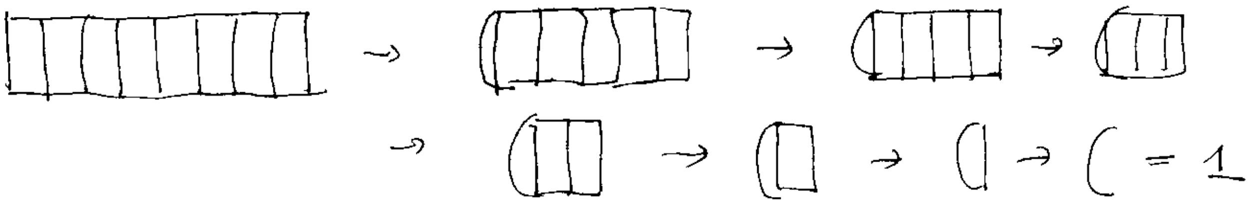


zipper.

$\tau_{E\text{-unit}} \approx D^4$ algorithm.

L-normalized A-matrices imply state normalized:

$$\langle\psi|\psi\rangle = \sum_{\sigma_L} A^{\sigma_L\dagger}(\cdot\cdot\underbrace{(\sum_{\sigma_2} A^{\sigma_2\dagger}\underbrace{(\sum_{\sigma_1} A^{\sigma_1\dagger}A^{\sigma_1})}_{I} A^{\sigma_2})}_{I}\dots) A^{\sigma_L} = 1.$$



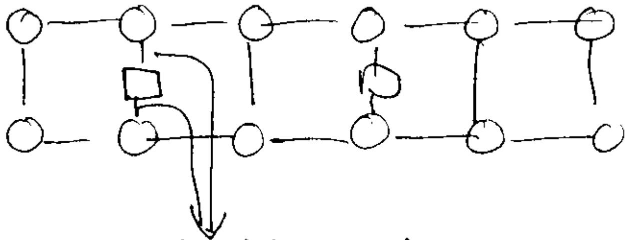
matrix elements:

$$\langle\phi|\hat{O}^{[i]}\hat{O}^{[j]}\dots|\psi\rangle \qquad \hat{O}^{[\ell]} = \sum_{\sigma_\ell\sigma_\ell'} O^{\sigma_\ell\sigma_\ell'}|\sigma_\ell\rangle\langle\sigma_\ell'|$$

$$= \sum_{\sigma\sigma'} \tilde{M}^{\sigma_1 *}\dots\tilde{M}^{\sigma_L *} O^{\sigma_1\sigma_1'}\dots O^{\sigma_L\sigma_L'} M^{\sigma_1'}\dots M^{\sigma_L'}$$

$$= \sum_{\sigma_L\sigma_L'} O^{\sigma_L\sigma_L'}\tilde{M}^{\sigma_L\dagger}(\dots(\sum_{\sigma_2\sigma_2'} O^{\sigma_2\sigma_2'}\tilde{M}^{\sigma_2\dagger}(\sum_{\sigma_1\sigma_1'} O^{\sigma_1\sigma_1'}\tilde{M}^{\sigma_1\dagger}M^{\sigma_1})M^{\sigma_2})\dots)M^{\sigma_L'}$$

as for simple overlap:



double sum here.

Comments.

(i) simplifies a lot for local op's if L- and R-normalized

AAAAAA ? BBBB

$\uparrow$ operator O sits here

Then $\sum A^\dagger A$, $\sum BB^\dagger$ collapse and:

$$\langle\psi|\hat{O}^{[\ell]}|\psi\rangle = \sum_{\sigma_\ell \sigma_\ell'} O^{\sigma_\ell \sigma_\ell'} \operatorname{tr}(M^{\sigma_\ell \dagger} M^{\sigma_\ell})$$

(ii) typically useful to have iterative procedure

$C^{[0]} = 1$

iterate overlap:

if necessary, insert $O^{\sigma_\ell\sigma_\ell'}$, $\sum_{\sigma_\ell'}$ here

$$C^{[\ell]} = \sum_{\sigma_\ell} \tilde{M}^{\sigma_\ell \dagger} C^{[\ell-1]} M^{\sigma_\ell}$$

contracts from the left (can also be set up from right)

attention: order of sums makes difference in efficiency!

(iii) structure of correlators

<u>map</u> from ops on block A (length $\ell-1$) to ops on block A (length ℓ)

$$\{|a_{\ell-1}\rangle\langle a_{\ell-1}'|\} \to \{|a_\ell\rangle\langle a_\ell'|\}$$

$$\hat{E}^{[\ell]} := \sum_{a_{\ell-1}a_{\ell-1}'} \sum_{a_\ell a_\ell'} \underbrace{\left(\sum_{\sigma_\ell} M^{\sigma_\ell *} \otimes M^{\sigma_\ell}\right)_{a_{\ell-1}a_{\ell-1}'; a_\ell a_\ell'}}_{\text{matrix elements of } E^{[\ell]} \ (\dim\ (D_{\ell-1}^2 \times D_\ell^2))} (|a_{\ell-1}\rangle\langle a_{\ell-1}'|)(|a_\ell\rangle\langle a_\ell'|)$$

$$E_O^{(\ell)} = \sum_{\sigma_\ell \sigma_\ell'} O^{\sigma_\ell \sigma_\ell'} M^{\sigma_\ell *} \otimes M^{\sigma_\ell'}$$

explicit notation:

$$E^{(\ell)}_{(a_{\ell-1} a_{\ell-1}'),(a_\ell a_\ell')} = \sum_{\sigma_\ell} M^{\sigma_\ell *}_{a_{\ell-1} a_\ell} \cdot M^{\sigma_\ell}_{a_{\ell-1}' a_\ell'}$$

$$E^{(\ell)}[O^{(\ell-1)}] = \sum_{\sigma_\ell} M^{\sigma_\ell \dagger} O^{(\ell-1)} M^{\sigma_\ell} \qquad \text{(action on matrix)}$$

or action on row vector (length $D_{\ell-1}^2$) $v_{aa'} = O^{[\ell-1]}_{aa'}$ from left:

$$\sum_{\sigma_\ell} \sum_{a_{\ell-1} a_{\ell-1}'} v_{a_{\ell-1} a_{\ell-1}'} M^{\sigma_\ell *}_{a_{\ell-1} a_\ell} M^{\sigma_\ell}_{a_{\ell-1}' a_\ell'}$$

Then $C^{[\ell]} = E^{[\ell]}(C^{[\ell-1]})$.

if $D_{\ell-1} = D_\ell$: eigenvalues, eigenvectors, ... ?

IMPORTANT THEOREM:

If A are L-normalized, then E constructed from it has all eigenvalues $|\lambda_k| \leq 1$

<u>Proof.</u>

i) $v_{aa'} = \delta_{aa'}$ is left eigenvector to $\lambda_1 = 1$:

$$E(I) = \sum_\sigma A^{\sigma \dagger} \cdot I \cdot A^\sigma = \sum_\sigma A^{\sigma\dagger} A^\sigma = 1 \cdot I.$$

ii) but this is the <u>largest</u> eigenvalue:

consider $C' = E(C)$. If largest singular value $s_1' \leq s_1$, for E from L- or R-normalized matrices, all eigenvalues must be $|\lambda_i| \leq 1$: $C' = \lambda_i C \Rightarrow s_1' = |\lambda_i| s_1 \Rightarrow |\lambda_i| \leq 1$.

(but may be degenerate)

$C = U^+ S V$ (SVD)

C square $\Rightarrow U^+U = UU^+ = V^+V = VV^+ = I$

$$C' = \sum_\sigma A^{\sigma +} U^+ S V A^\sigma$$

$$= \left[(UA^1)^+ \dots (UA^d)^+\right] \begin{bmatrix} S & & & \\ & S & & \\ & & S & \\ & & & S \end{bmatrix} \begin{bmatrix} VA^1 \\ \vdots \\ VA^d \end{bmatrix}$$

$$= P^+ \begin{bmatrix} S & & \\ & S & \\ & & S \end{bmatrix} Q.$$

$P^+P = I$, $Q^+Q = I$ (but $PP^+ \neq I$, $QQ^+ \neq I$) for A L-norm:

$$P^+P = \sum_\sigma A^{\sigma +} U^+ U A^\sigma = \sum_\sigma A^{\sigma +} A^\sigma = I.$$

$\Rightarrow$ reduced basis trafos to ON subspaces

$\Rightarrow$ largest s.val. of C' must be less or equal to that of S.

now interesting insights in overlaps, matrix elements:

$$\langle\psi|\psi\rangle = E^{(1)} E^{(2)} \dots E^{(L)}$$

$$\langle\psi|\hat{O}^{[1]} \dots \hat{O}^{[L]}|\psi\rangle = E^{(1)}_{O_1} E^{(2)}_{O_2} \dots E^{(L)}_{O_L}$$

PBC, L-normalized A:

$$\langle\psi|\hat{O}^{[i]}\hat{O}^{[j]}|\psi\rangle = \mathrm{Tr}\left(E^{[1]} \dots E^{(i-1)} E^{(i)}_O E^{(i+1)} \dots E^{(j-1)} E^{(j)}_O E^{(j+1)} \dots E^{[L]}\right)$$

$$= \mathrm{tr}\left(E^{[i]}_O E^{j-i-1} E^{[j]}_O E^{L-j+i-1}\right)$$

$$= \sum_{l,k} \langle l|E^{[i]}_O|k\rangle \lambda_k^{j-i-1} \langle k|E^{[j]}_O|l\rangle \lambda_l^{L-j+i-1} =$$

$$= \sum_k \langle 1|E^{[i]}_O|k\rangle \lambda_k^{j-i-1} \langle k|E^{[j]}_O|1\rangle \quad (L \to \infty)$$

(assuming $\lambda_1 = 1$, $|\lambda_{i>1}| < 1$).

with $\xi_k = -\frac{1}{\ln \lambda_k}$:

$$\frac{\langle \psi | \hat{O}^{[i]} \hat{O}^{[j]} | \psi \rangle}{\langle \psi | \psi \rangle} = c_1 + \sum_{k=2}^{D^2} c_k e^{-r/\xi_k}$$

$c_k = \langle 1 | E_O^{[i]} | k \rangle \langle k | E_O^{[j]} | 1 \rangle \qquad i<j \, ; \; r = |j-i-1|$

correlators are <u>either</u> longranged (if $c_1 \neq 0$) or a <u>superposition</u> of <u>exponentials</u>

AKLT: $\xi = \frac{1}{\ln 3} = 0.9102$; for string correlator $c_1 \neq 0$.

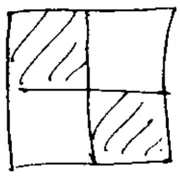
will approximate true behaviour (in 1D usually $\langle S(x) S(0) \rangle \sim x^{-\alpha}$ or $\frac{e^{-x/\xi}}{\sqrt{x}}$)

Adding 2 MPS

first for PBC: $\begin{matrix}|\psi\rangle \\ |\phi\rangle\end{matrix} = \sum_{\underline{\sigma}} \mathrm{tr} \begin{pmatrix} M^{\sigma_1} \dots M^{\sigma_L} \\ \tilde{M}^{\sigma_1} \dots \tilde{M}^{\sigma_L} \end{pmatrix} |\underline{\sigma}\rangle$

$|\psi + \phi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}(N^{\sigma_1} \dots N^{\sigma_L}) |\underline{\sigma}\rangle$

$N^{\sigma_i} = M^{\sigma_i} \oplus \tilde{M}^{\sigma_i}$



dimensions <u>add</u>.

$$\mathrm{tr}(NNNN) = \mathrm{tr} \begin{pmatrix} MMMM & 0 \\ 0 & \tilde{M}\tilde{M}\tilde{M}\tilde{M} \end{pmatrix} = \mathrm{tr}(MMMM) + \mathrm{tr}(\tilde{M}\tilde{M}\tilde{M}\tilde{M})$$

for OBC: difference on sites 1, L. (exercise.)

Bringing an MPS into canonical form

$$|\psi\rangle = \sum_{\underline{\sigma}} M^{\sigma_1}\dots M^{\sigma_L}|\underline{\sigma}\rangle \begin{array}{l} \nearrow |\psi\rangle = \sum_{\sigma} A^{\sigma_1}\dots A^{\sigma_L}|\underline{\sigma}\rangle \\ \searrow |\psi\rangle = \sum_{\sigma} B^{\sigma_1}\dots B^{\sigma_L}|\underline{\sigma}\rangle \end{array}$$

for OBC. (mixed constructions, AAAMBBB are easily generated from the stuff here.)

$\boxed{\text{LEFT CANONICAL}}$

$$\sum_{\sigma}\sum_{a_1,\dots} M_{(\sigma_1,1),a_1} M^{\sigma_2}_{a_1a_2} M^{\sigma_3}_{a_2a_3}\dots|\underline{\sigma}\rangle = \sum_{\sigma}\sum_{a_1\dots}\sum_{s_1} A_{(\sigma_1,1),s_1} S_{s_1,s_1} V^{\dagger}_{s_1,a_1} M^{\sigma_2}_{a_1a_2}\dots|\underline{\sigma}\rangle$$

restore explicit multiple.

$$= \sum_{\underline{\sigma}}\sum_{a_2,\dots}\sum_{s_1} A^{\sigma_1}_{1,s_1}\Big(\sum_{a_1} S_{s_1,s_1} V^{\dagger}_{s_1,a_1} M^{\sigma_2}_{a_1a_2}\Big) M^{\sigma_3}_{a_2a_3}\dots|\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}}\sum_{a_2\dots}\sum_{s_1} A^{\sigma_1}_{1,s_1}\tilde{M}^{\sigma_2}_{s_1,a_2} M^{\sigma_3}_{a_2a_3}\dots|\underline{\sigma}\rangle$$

$\sum_{\sigma} A^{\sigma\dagger}A^{\sigma} = 1$

reshape $\tilde{M}_{(\sigma_2 s_1),a_2}$; SVD; and so on

in the end, there will be a scalar factor left over. Keep it or set it to 1 for normalization.

$\boxed{\text{RIGHT CANONICAL}}$

exercise.

[start from right; reshape $M^{\sigma}_{ab} \to M_{a,(\sigma b)}$; SVD etc.]

reshape picture:

$$\left\{ \boxed{M^1}, \boxed{M^2}, \dots, \boxed{M^d} \right\} \to \begin{array}{|c|} \hline M^1 \\ \hline M^2 \\ \hline \dots \\ \hline M^d \\ \hline \end{array}$$

Approximate compression of an MPS

In many algorithms, we will be confronted by steps where the matrix dimensions of an MPS grow.
In order to keep the procedure numerically manageable, the MPS has to be <u>compressed</u> back to a manageable size:

$$(D'_{i-1} \times D'_i) \longrightarrow (D_{i-1} \times D_i) \qquad \begin{array}{l} D_{i-1} \leq D'_{i-1} \\ D_i \leq D'_i \end{array}$$

How can we do this optimally ~~of~~ and fast?

Two procedures exist currently:

- by SVD: quite fast, but not optimal approx (however almost optimal in many practical situations)
- by variational compression: slower, but optimal.

$\boxed{\text{COMPRESSION BY SVD}}$

assume MPS in <u>mixed-canonical</u> form:

$$|\psi\rangle = \sum_{\underline{\sigma}} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_\ell} \overset{D' \times D'}{\Lambda^{[\ell]}} B^{\sigma_{\ell+1}} \ldots B^{\sigma_L} |\underline{\sigma}\rangle$$

contains Schmidt coeffs as diagonal matrix

We know that <u>best</u> approximation is given by setting $\Lambda^{[\ell]} \to \tilde{\Lambda}^{[\ell]}$, keeping the D leading singular values $\Rightarrow$ A^{σ_ℓ} <u>column</u> dim $\downarrow D$; $B^{\sigma_{\ell+1}}$ <u>row</u> dim $\downarrow D$.

Works because of special form of state!

AAA Λ BBB

recepe : • start from BBBBBB
- 1 L-canon. step:
  $A\Lambda^{(1)}BBBB$
- truncate
- 1 L-canon. step:
  $AA\Lambda^{(2)}BBB$
- truncate
  ... and so on. → AAAA + compressed

or from AAAAAA and R-canon. steps. → BBBB + compressed

in details for starting from AAAAA configuration:

$$|\psi\rangle = \sum_\sigma A^{\sigma_1}A^{\sigma_2}\dots A^{\sigma_{L-1}}A^{\sigma_L}|\underline{\sigma}\rangle$$

$$|\psi^{(L-1)}\rangle = \sum_\sigma \underbrace{A^{\sigma_1}\dots \quad A^{\sigma_{L-1}}U}SB^{\sigma_L}|\underline{\sigma}\rangle \qquad \text{(reshape, SVD, reshape to B)}$$

as U is orthonormal, states on block

$\boxed{1 \qquad\qquad L-1}$ are orthonormal:

- those from $A^{\sigma_1}\dots A^{\sigma_{L-1}}$ are ON and
- we have an orthonormal transformation.
- can read state as correct Schmidt decomp with Schmidt coeffs in S.

$$|\tilde\psi^{(L-1)}\rangle = \sum_\sigma (A^{\sigma_1}\dots \underbrace{A^{\sigma_{L-1}}\tilde U \tilde S}) \tilde B^{\sigma_L}|\underline{\sigma}\rangle$$

$$= \sum_\sigma A^{\sigma_1}\dots A^{\sigma_{L-2}}M^{\sigma_{L-1}}\tilde B^{\sigma_L}|\underline{\sigma}\rangle$$

truncate U, S, B to D entries where they "meet" → $\tilde U, \tilde S, \tilde B$

SVD:

$$|\psi^{(L-2)}\rangle = \sum_{\underline{\sigma}} A^{\sigma_1} \ldots A^{\sigma_{L-2}} U S B^{\sigma_{L-1}} \tilde{B}^{\sigma_L} |\underline{\sigma}\rangle$$

with same argument as before $U, S, B^{\sigma_{L-1}} \to \tilde{U}, \tilde{S}, \tilde{B}^{\sigma_{L-1}}$ by truncation.

Why is this procedure not optimal?

- each M contains a truncated $\bar{U}$ from a previous step, hence the procedure is dependent on previous truncations
- truncations affect the ON system
- imbalance: if you go from right to left, right truncations influence left, but not vice versa
- if (e.g. in time dependent calculations) the effect of truncations is small, this dependence can be neglected without a lot of problems

ITERATIVE (VARIATIONAL) COMPRESSION

compress $|\psi\rangle$ (D') $\longrightarrow |\tilde{\psi}\rangle$ (D) minimizing

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|_2^2$$
$$= \langle\psi|\psi\rangle - \langle\tilde{\psi}|\psi\rangle - \langle\psi|\tilde{\psi}\rangle + \langle\tilde{\psi}|\tilde{\psi}\rangle$$

with respect to $|\tilde{\psi}\rangle$.

$$|\tilde{\psi}\rangle = \sum_{\underline{\sigma}} \tilde{M}^{\sigma_1} \tilde{M}^{\sigma_2} \ldots \tilde{M}^{\sigma_L} |\underline{\sigma}\rangle$$

highly nonlinear product of unknown variables $\Rightarrow$ no one knows how to do this!

standard trick (will ~~...~~ reoccur in MPS):
devolve this into sequence of linear optimization problems:

- start with a starting guess for $|\tilde{\psi}\rangle$
  (e.g. random, or from SVD compression)

  $|\tilde{\psi}\rangle = \sum_{\sigma} \tilde{M}^{\sigma_1} \ldots \tilde{M}^{\sigma_i} \ldots \tilde{M}^{\sigma_L} |\sigma\rangle$
- pick one $\tilde{M}^{\sigma_i}$, keep all others fixed
- optimize with respect to $\tilde{M}^{\sigma_i}$ (appears squared in $\langle\tilde{\psi}|\tilde{\psi}\rangle \Rightarrow$ extremum will be linear)
- sweep forth and back through all $\tilde{M}^{\sigma_i}$ until result stabilizes

~~$\tilde{M}^{\sigma_i}$ only shows up in~~

Take extremum with respect to $\tilde{M}^{\sigma_i *}_{a_{i-1} a_i}$

only in $-\langle\tilde{\psi}|\psi\rangle + \langle\tilde{\psi}|\tilde{\psi}\rangle$

$$\frac{\partial}{\partial \tilde{M}^{\sigma_i *}_{a_{i-1} a_i}} \left(\langle\tilde{\psi}|\tilde{\psi}\rangle - \langle\tilde{\psi}|\psi\rangle \right) = \sum_{\vec{\sigma}^*} (\tilde{M}^{\sigma_1 *} \ldots \tilde{M}^{\sigma_{i-1} *})_{1, a_{i-1}} (\tilde{M}^{\sigma_{i+1} *} \ldots \tilde{M}^{\sigma_L *})_{a_i, 1} \cdot \tilde{M}^{\sigma_1} \ldots \tilde{M}^{\sigma_i} \ldots \tilde{M}^{\sigma_L}$$

$\vec{\sigma}^*$: all $\vec{\sigma}$ except on site i

$$- \sum_{\vec{\sigma}^*} (\tilde{M}^{\sigma_1 *} \ldots \tilde{M}^{\sigma_{i-1} *})_{1, a_{i-1}} (\tilde{M}^{\sigma_{i+1} *} \ldots \tilde{M}^{\sigma_L *})_{a_i, 1} \cdot M^{\sigma_1} \ldots M^{\sigma_i} \ldots M^{\sigma_L}.$$

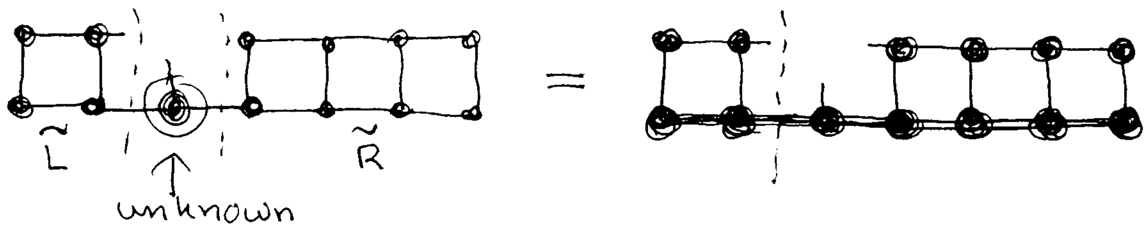
We may rewrite this seemingly complex system as

$$\sum_{a'_{i-1} a'_i} \underbrace{\tilde{O}_{a_{i-1} a_i, a'_{i-1} a'_i}}_{\text{matrix } P \; D^2 \times D^2} \underbrace{\tilde{M}^{\sigma_i}_{a'_{i-1} a'_i}}_{\text{vector length } D^2} = \underbrace{O^{\sigma_i}_{a_{i-1} a_i}}_{\text{vector length } D^2} .$$

For each σ_i:

$\Rightarrow P v = b$ linear equation system
(usually, matrices are big, hence sparse large ~~...~~ solver: conjugate gradient)

<u>graphical representation:</u>



—— : $\tilde{M}$ matrices

▬ : M matrices (higher dimension)

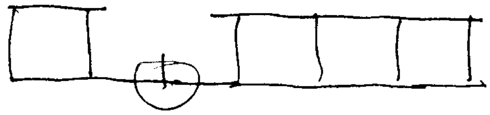
remarks:

(i) numerical cost drops if factorial structure of $\tilde{O}$ is realized:

$$\tilde{O}_{a_{i-1} a_i, a'_{i-1} a'_i} = \tilde{L}_{a_{i-1} a'_{i-1}} \cdot \tilde{R}_{a_i a'_i}$$

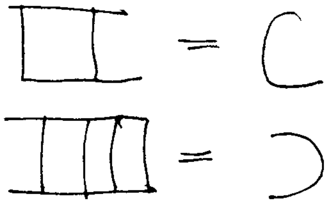
(can be evaluated as $O(D^3)$)

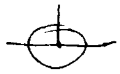
(ii) more importantly: the entire equation solving can be avoided <u>provided</u> the state $|\tilde{\psi}\rangle$ is in adequate L/R (mixed)-normalization.

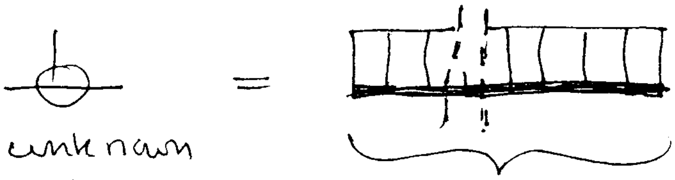


if state in form

$\tilde A \tilde A \tilde M \tilde B \tilde B \tilde B \tilde B \Rightarrow$



$\Rightarrow$  and system reads



unknown

x

fast calculation by

decomposition in 3 units as indicated

hence optimal compression algorithm:

- start with $|\tilde\psi\rangle$-guess in mixed canonical form,
  to improve matrix at boundary (as above: $x = b$)
  $\tilde A \tilde A \tilde A \tilde M \tilde B \tilde B \tilde B \tilde B$

- L- or R-canonize it, and shift by one site:

opt. $\Rightarrow \tilde A \tilde A \tilde A \tilde{\tilde M}^{*} \tilde B \tilde B \tilde B \tilde B$

$= \tilde A \tilde A \tilde A \tilde A \underbrace{\Lambda V^\dagger \tilde B}_{\tilde M} \tilde B \tilde B \tilde B$

$= \tilde A \tilde A \tilde A \tilde A \tilde M \tilde B \tilde B \tilde B$

- continue variational optimization on this one!

comments:

(i) can use QR, as singular values are not needed.

(ii) assess convergence by monitoring $\| |\psi\rangle - |\tilde{\psi}\rangle \|_2^2$ at each step. Easy in mixed normalization:

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = \overbrace{\langle\psi|\psi\rangle}^{1} + \langle\tilde{\psi}|\tilde{\psi}\rangle - \langle\tilde{\psi}|\psi\rangle - \langle\psi|\tilde{\psi}\rangle$$

$$= 1 - \sum_{\sigma_i} \mathrm{tr}\left(\tilde{M}^{\sigma_i \dagger} \tilde{M}^{\sigma_i}\right)$$

because:

$\underset{\tilde{M}^{\sigma_i}}{\perp}$ = 

$\uparrow$

$\langle\tilde{\psi}|\psi\rangle$ without $\tilde{M}^{\sigma_i *}$

$$\Rightarrow \langle\tilde{\psi}|\psi\rangle = \sum_{\sigma_i} \mathrm{tr}\left(\tilde{M}^{\sigma_i \dagger} M^{\sigma_i}\right)$$
$$\langle\tilde{\psi}|\tilde{\psi}\rangle = \sum_{\sigma_i} \mathrm{tr}\left(\tilde{M}^{\sigma_i \dagger} \tilde{M}^{\sigma_i}\right)$$

because of mixed normalization.

(iii) variational trapping in non-global minimum: there may be a danger of getting stuck!

may be helpful to reformulate as two-site-optimization:

$$|\tilde{\psi}\rangle = \sum_{\sigma} \tilde{A}^{\sigma_1} \dots \tilde{A}^{\sigma_{\ell-1}} \underbrace{\tilde{M}^{\sigma_\ell \sigma_{\ell+1}}}_{\text{two multiplied}} \tilde{B}^{\sigma_{\ell+2}} \dots \tilde{B}^{\sigma_L} |\underline{\sigma}\rangle$$

$\sim$ eq'n system for $\tilde{M}^{\sigma_\ell \sigma_{\ell+1}}$ (simplifies upon proper L-R-norm.)

major change: new $\tilde{M}^{\sigma_\ell \sigma_{\ell+1}} \xrightarrow[\text{reshape}]{\text{SVD}} \underbrace{\tilde{U}^{\sigma_\ell} S}_{\tilde{M}^{\sigma_\ell}} \underbrace{(V^\dagger)^{\sigma_{\ell+1}}}_{\tilde{B}^{\sigma_{\ell+1}}}$

if shift towards left is intended!

Matrix Product Operators

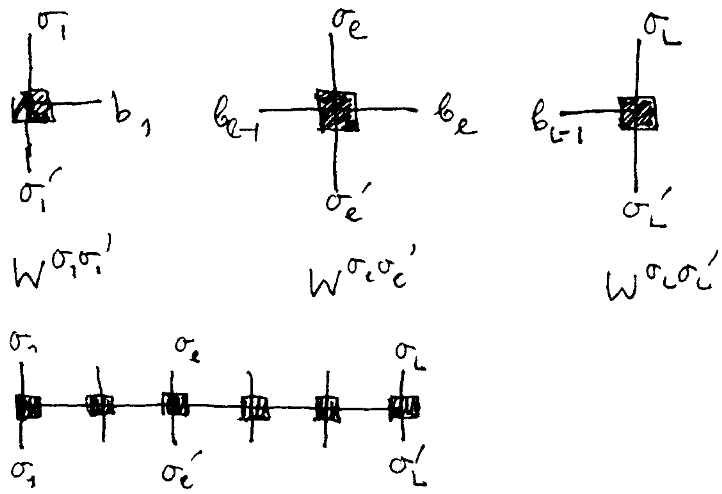
$$\langle \underline{\sigma} | \psi \rangle = M^{\sigma_1} M^{\sigma_2} \ldots M^{\sigma_{L-1}} M^{\sigma_L} \quad \longrightarrow$$

$$\langle \underline{\sigma} | \hat{O} | \underline{\sigma}' \rangle = \underbrace{W^{\sigma_1 \sigma_1'}}_{\text{matrices as in MPS}} W^{\sigma_2 \sigma_2'} \ldots W^{\sigma_{L-1} \sigma_{L-1}'} W^{\sigma_L \sigma_L'}$$

$$\boxed{\hat{O} = \sum_{\underline{\sigma}, \underline{\sigma}'} W^{\sigma_1 \sigma_1'} W^{\sigma_2 \sigma_2'} \ldots W^{\sigma_{L-1} \sigma_{L-1}'} W^{\sigma_L \sigma_L'} |\underline{\sigma}\rangle \langle \underline{\sigma}'|}$$

(MPO)

graphical representation:



any operator can be brought into MPO form:

$$\hat{O} = \sum_{\sigma_1 \ldots, \sigma_1' \ldots} c_{(\sigma_1 \ldots \sigma_L), (\sigma_1' \ldots \sigma_L')} |\sigma_1 \ldots \sigma_L \rangle \langle \sigma_1' \ldots \sigma_L'|$$

$$= \sum_{\sigma_1 \ldots, \sigma_1' \ldots} \underbrace{c_{(\sigma_1 \sigma_1') \ldots (\sigma_L \sigma_L')}}_{\text{decompose as for MPS; } (\sigma_\ell \sigma_\ell') \text{ instead of } (\sigma_\ell)\text{.}} |\sigma_1 \ldots \sigma_L \rangle \langle \sigma_1' \ldots \sigma_L'|$$

Applying an MPO to an MPS

$$\hat{O}|\psi\rangle = \sum_{\underline{\sigma}\underline{\sigma}'} (W^{\sigma_1\sigma_1'} W^{\sigma_2\sigma_2'} \ldots)(M^{\sigma_1'} M^{\sigma_2'} \ldots)|\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}\underline{\sigma}'} \sum_{\underline{a}\underline{b}} (W^{\sigma_1\sigma_1'}_{1,b_1} W^{\sigma_2\sigma_2'}_{b_1 b_2} \ldots)(M^{\sigma_1'}_{1,a_1} M^{\sigma_2'}_{a_1 a_2} \ldots)|\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}\underline{\sigma}'} \sum_{\underline{a}\underline{b}} (W^{\sigma_1\sigma_1'}_{1,b_1} M^{\sigma_1'}_{1,a_1})(W^{\sigma_2\sigma_2'}_{b_1 b_2} M^{\sigma_2'}_{a_1 a_2}) \ldots |\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}} \sum_{\underline{a}\underline{b}} N^{\sigma_1}_{(1,1),(b_1 a_1)} N^{\sigma_2}_{(b_1 a_1),(b_2 a_2)} \ldots |\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}} N^{\sigma_1} N^{\sigma_2} \ldots |\underline{\sigma}\rangle$$

MPO × MPS → MPS !!!

$|\phi\rangle = \hat{O}|\psi\rangle$ $\qquad$ $|\phi\rangle = \sum_{\underline{\sigma}} N^{\sigma_1} N^{\sigma_2} \ldots |\underline{\sigma}\rangle$

$$N^{\sigma_i}_{(b_{i-1} a_{i-1}),(b_i a_i)} = \sum_{\sigma_i'} W^{\sigma_i\sigma_i'}_{b_{i-1} b_i} M^{\sigma_i'}_{a_{i-1} a_i}$$

graphically:

dimensions multiply → calls for compression algorithm!

Ground state calculations with MPS

find $|\psi\rangle$ (MPS of dimension D) minimizing

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

MPO REPRESENTATION OF HAMILTONIANS

might seem hopeless in practice...!

$$\hat{H} = \sum_{i=1}^{L-1} \frac{J}{2}\hat{S}^+_i \hat{S}^-_{i+1} + \frac{J}{2}\hat{S}^-_i \hat{S}^+_{i+1} + J^z \hat{S}^z_i \hat{S}^z_{i+1} - h\sum_i \hat{S}^z_i$$

this is a shorthand for sums of tensor products of operators:

$$\hat{H} = \ldots + J^z \hat{S}^z_1 \otimes \hat{S}^z_2 \otimes \hat{I} \otimes \hat{I} \otimes \ldots +$$
$$+ \hat{I} \otimes J^z \hat{S}^z_2 \otimes \hat{S}^z_3 \otimes \hat{I} \otimes \hat{I} \ldots + \ldots$$

Convenient: $\hat{W}_{bb'} = \sum_{\sigma\sigma'} W^{\sigma\sigma'}_{bb'} |\sigma\rangle\langle\sigma'|$

(operator-valued matrix)

$$\hat{O} = \hat{W}^{[1]} \hat{W}^{[2]} \hat{W}^{[3]} \ldots \hat{W}^{[L]}$$

move through an arbitrary operator ~~st~~ string in $\hat{H}$:

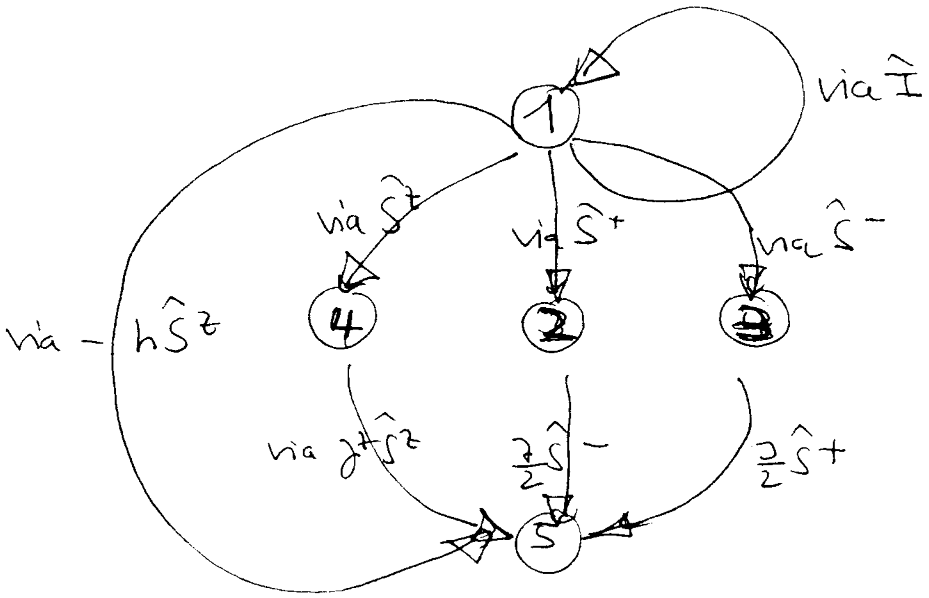
$$\hat{I} \otimes \hat{I} \otimes I \otimes I \otimes I \otimes S^z \otimes S^z \otimes I \otimes I$$

only I to the right (1)

S^z to the right (4)
S^+ " (2)
S^- " (3)

completed expression to the right
(e.g. S^+S^-, S^-S^+, S^zS^z) (5)
only identities to the left

this implies rules:



Can be encoded by following operator-valued matrix:

$$\hat{W}^{[i]} = \begin{bmatrix} \hat{I} & 0 & 0 & 0 & 0 \\ \hat{S}^+ & 0 & 0 & 0 & 0 \\ \hat{S}^- & 0 & 0 & 0 & 0 \\ \hat{S}^z & 0 & 0 & 0 & 0 \\ -h\hat{S}^z & \frac{J}{2}\hat{S}^- & \frac{J}{2}S^+ & J^z S^z & I \end{bmatrix}$$

$$\hat{W}^{[1]} = \begin{bmatrix} -h\hat{S}^z & \frac{J}{2}\hat{S}^- & \frac{J}{2}\hat{S}^+ & J^z\hat{S}^z & \hat{I} \end{bmatrix}$$

$$\hat{W}^{[L]} = \begin{bmatrix} \hat{I} \\ \hat{S}^+ \\ \hat{S}^- \\ \hat{S}^z \\ -h\hat{S}^z \end{bmatrix}$$

one can also construct longer-ranged Hamiltonians quite easily!

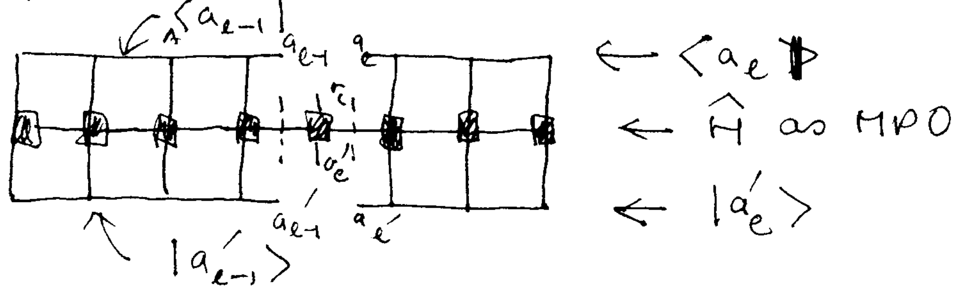
APPLYING A HAMILTONIAN MPO TO A MIXED CANONICAL STATE

$$|\psi\rangle = \sum_{\underline{\sigma}} A^{\sigma_1} \dots A^{\sigma_{\ell-1}} \psi^{\sigma_\ell} B^{\sigma_{\ell+1}} \dots B^{\sigma_L} |\underline{\sigma}\rangle$$

$$= \sum_{a_{\ell-1} a_\ell} |a_{\ell-1}\rangle_A \, \psi^{\sigma_\ell}_{a_{\ell-1} a_\ell} |a_\ell\rangle_B$$

want $\langle a_{\ell-1} \sigma_\ell a_\ell | \hat{H} | a'_{\ell-1} \sigma'_\ell a'_\ell \rangle$

pictorially:



The explicit formula looks nasty! And this shows why we want the pictorial representation:

$$\langle a_{\ell-1} \sigma_\ell a_\ell | \hat{H} | a'_{\ell-1} \sigma'_\ell a'_\ell \rangle$$

$$= \sum_{\underline{\sigma}\underline{\sigma}'} W^{\sigma_1\sigma'_1} \dots W^{\sigma_L\sigma'_L} \langle a_{\ell-1}\sigma_\ell a_\ell | \underline{\sigma}\rangle\langle\underline{\sigma}' | a'_{\ell-1}\sigma'_\ell a'_\ell\rangle$$

$$= \sum_{\underline{\sigma}^* \underline{\sigma}'^*} W^{\sigma_1\sigma'_1} \dots W^{\sigma_\ell\sigma'_\ell} \dots W^{\sigma_L\sigma'_L} \langle a_{\ell-1} | \sigma_1 \dots \sigma_{\ell-1}\rangle \langle a_\ell | \sigma_{\ell+1} \dots \sigma_L\rangle$$
$$\langle \sigma'_1 \dots \sigma'_{\ell-1} | a'_{\ell-1}\rangle \langle \sigma'_{\ell+1} \dots \sigma'_L | a'_\ell\rangle$$

$$= \sum_{\underline{\sigma}^* \underline{\sigma}'^*} W^{\sigma_1\sigma'_1} \dots W^{\sigma_\ell\sigma'_\ell} \dots W^{\sigma_L\sigma'_L} (A^{\sigma_1} \dots A^{\sigma_{\ell-1}})^*_{1, a_{\ell-1}} (B^{\sigma_{\ell+1}} \dots B^{\sigma_L})^*_{a_\ell, 1}$$
$$(A^{\sigma'_1} \dots A^{\sigma'_{\ell-1}})_{1, a'_{\ell-1}} (B^{\sigma'_{\ell+1}} \dots B^{\sigma'_L})_{a'_\ell, 1}$$

$$= \sum_{\{a_i, b_i, a'_i\}} \left(\sum_{\sigma_1\sigma'_1} A^{\sigma_1 *}_{1,a_1} W^{\sigma_1\sigma'_1}_{1,b_1} A^{\sigma'_1}_{1,a'_1} \right) \left(\sum_{\sigma_2\sigma'_2} A^{\sigma_2 *}_{a_1 a_2} W^{\sigma_2\sigma'_2}_{b_1 b_2} A^{\sigma'_2}_{a'_1 a'_2} \right) \dots \times W^{\sigma_\ell\sigma'_\ell}_{b_{\ell-1} b_\ell} \times$$
$$\left(\sum_{\sigma_{\ell+1}\sigma'_{\ell+1}} B^{\sigma_{\ell+1} *}_{a_\ell a_{\ell+1}} W^{\sigma_{\ell+1}\sigma'_{\ell+1}}_{b_\ell b_{\ell+1}} B^{\sigma'_{\ell+1}}_{a'_\ell a'_{\ell+1}} \right) \dots \left(\sum_{\sigma_L\sigma'_L} B^{\sigma_L *}_{a_{L-1},1} W^{\sigma_L\sigma'_L}_{b_{L-1},1} B^{\sigma'_L}_{a'_{L-1},1} \right).$$

But there is an obvious tripartite structure:

$$\langle a_{\ell-1}\sigma_\ell a_\ell|\hat{H}_\ell|a'_{\ell-1}\sigma'_\ell a'_\ell\rangle = \sum_{b_{\ell-1}b_\ell} L^{a_{\ell-1}a'_{\ell-1}}_{b_{\ell-1}} W^{\sigma_\ell\sigma'_\ell}_{b_{\ell-1}b_\ell} R^{a_\ell a'_\ell}_{b_\ell}$$

in the last equation.

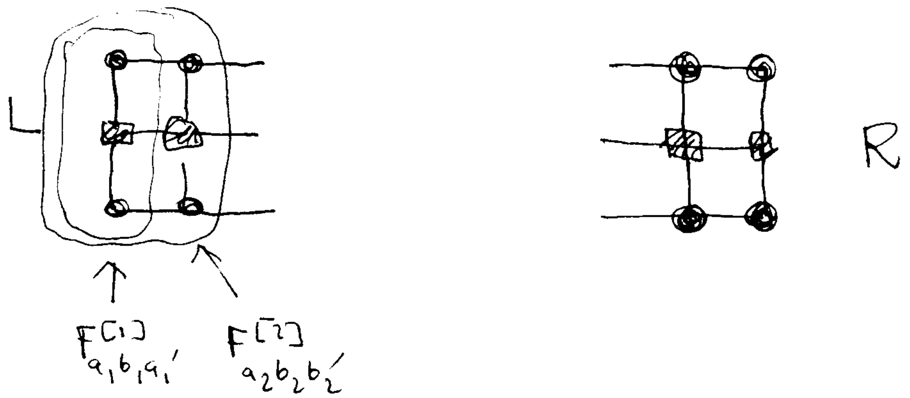
$$\hat{H}|\psi\rangle = \sum_{b_{\ell-1}b_\ell}\sum_{a'_{\ell-1}\sigma'_\ell a'_\ell} L^{a_{\ell-1}a'_{\ell-1}}_{b_{\ell-1}} W^{\sigma_\ell\sigma'_\ell}_{b_{\ell-1}b_\ell} R^{a_\ell a'_\ell}_{b_\ell} \Psi^{\sigma'_\ell}_{a'_{\ell-1}a'_\ell} |a_{\ell-1}\rangle_A |\sigma_\ell\rangle |a_\ell\rangle_B .$$

evaluating this expression is key in all ground state search algorithms $\Rightarrow$ must be made as fast as possible!

two lines of attack:

1. build L, R iteratively
2. arrange action of L, R, W on $|\psi\rangle$ efficiently

(1)



with dummy scalar $F^{[0]}_{a_0b_0a'_0} = 1$ (and $a_0, b_0, a'_0 = 1$ only):

$$F^{[i]}_{a_ib_ia'_i} = \sum_{\sigma_i\sigma'_i}\sum_{a_{i-1}b_{i-1}a'_{i-1}} W^{[i]\sigma_i\sigma'_i}_{b_{i-1}b_i} (A^{[i]\sigma_i})^\dagger_{a_ia_{i-1}} F^{[i-1]}_{a_{i-1}b_{i-1}a'_{i-1}} A^{[i]\sigma'_i}_{a'_{i-1}a'_i}$$

optimal bracketing of the sums is given as

$$F^{[i]}_{a_i b_i a_i'} = \sum_{\sigma_i a_{i-1}} (A^{[i]\sigma_i \dagger})_{a_i a_{i-1}} \left(\sum_{\sigma_i' b_{i-1}} W^{[i]\sigma_i \sigma_i'}_{b_{i-1} b_i} \left(\sum_{a_{i-1}'} F^{[i-1]}_{a_{i-1} b_{i-1} a_{i-1}'} A^{[i]\sigma_i'}_{a_{i-1}' a_i'} \right)\right)$$

This construction is a simple extension of the representation update for operators (which are usually MPOs with one non-trivial site).

(2) efficient bracketing of $\hat{H}|\psi\rangle$:

$$\hat{H}|\psi\rangle = \sum_{b_{\ell-1} a_{\ell-1}'} L^{a_{\ell-1} a_{\ell-1}'}_{b_{\ell-1}} \left(\sum_{b_\ell \sigma_\ell'} W^{\sigma_\ell \sigma_\ell'}_{b_{\ell-1} b_\ell} \left(\sum_{a_\ell'} R^{a_\ell a_\ell'}_{b_\ell} \Psi^{\sigma_\ell'}_{a_{\ell-1}' a_\ell'} \right)\right) |a_{\ell-1}\rangle_A |\sigma_\ell\rangle |a_\ell\rangle_B$$

Iterative ground state search:

Find $|\psi\rangle$ that minimizes

$$E = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

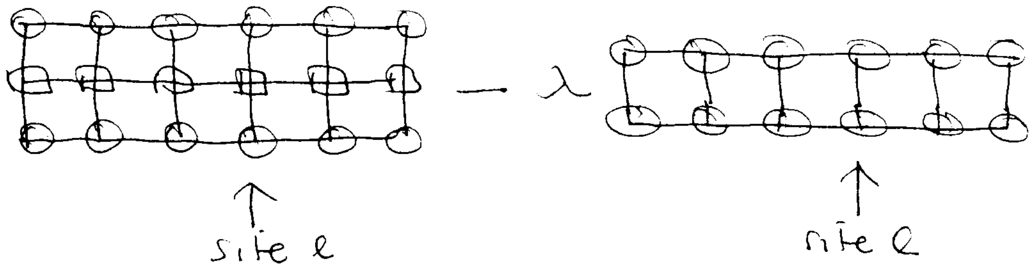
$\rightsquigarrow$ extremize $\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle$; $\lambda \to E$

problem: $M^{\sigma}_{aa'}$ appear as products in expression, making problem highly non-linear

$\rightsquigarrow$ transformation into iterative problem (DMRG)

KEEP ALL MATRICES CONSTANT EXCEPT ON ONE SITE (CALLED ℓ) AND CONSIDER ONLY MATRIX ELEMENTS ON SITE AS VARIABLES!

Extremizing will lower the energy an produce a variationally better state; continuing to shift the position of the "free site" where entries are variable will continue to lower the energy $\rightarrow$ proceed until convergence is reached.



$$\langle\psi|\psi\rangle = \sum_{\sigma_\ell} \sum_{a_{\ell-1}a_\ell} \sum_{a'_{\ell-1}a'_\ell} \psi^A_{a_{\ell-1}a'_{\ell-1}} M^{\sigma_\ell *}_{a_{\ell-1}a_\ell} M^{\sigma_\ell}_{a'_{\ell-1}a'_\ell} \psi^B_{a_\ell a'_\ell}$$

$$\psi^A_{a_{\ell-1}a'_{\ell-1}} = \sum_{\sigma_1\ldots\sigma_{\ell-1}} (M^{\sigma_{\ell-1}\dagger}\ldots M^{\sigma_1\dagger} M^{\sigma_1}\ldots M^{\sigma_{\ell-1}})_{a_{\ell-1}a'_{\ell-1}} \boxed{= \delta_{a_{\ell-1}a'_{\ell-1}}}$$

if L-norm!!

$$\psi^B_{a_\ell a'_\ell} = \sum_{\sigma_{\ell+1}\ldots\sigma_L} (M^{\sigma_{\ell+1}}\ldots M^{\sigma_L} M^{\sigma_L\dagger}\ldots M^{\sigma_{\ell+1}\dagger})_{a'_\ell a_\ell} \boxed{= \delta_{a_\ell a'_\ell}}$$

if R-norm!!

$$\langle\psi|H|\psi\rangle = \sum_{\sigma_\ell\sigma'_\ell} \sum_{a_{\ell-1}a_\ell} \sum_{a'_{\ell-1}a'_\ell} \sum_{b_{\ell-1}b_\ell} L^{a_{\ell-1}a'_{\ell-1}}_{b_{\ell-1}} W^{\sigma_\ell\sigma'_\ell}_{b_{\ell-1}b_\ell} R^{a_\ell a'_\ell}_{b_\ell} M^{\sigma_\ell *}_{a_{\ell-1}a_\ell} M^{\sigma'_\ell}_{a'_{\ell-1}a'_\ell}$$

now take extremum of $\langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle$ with respect to $M^{\sigma_\ell *}_{a_{\ell-1}a_\ell}$:

$$\sum_{\sigma'_\ell a'_{\ell-1} a'_\ell} \sum_{b_{\ell-1} b_\ell} \sum L^{a_{\ell-1} a'_{\ell-1}}_{b_{\ell-1}} W^{\sigma_\ell \sigma'_\ell}_{b_{\ell-1} b_\ell} R^{a_\ell a'_\ell}_{b_\ell} M^{\sigma'_\ell}_{a'_{\ell-1} a'_\ell} - \lambda \sum_{a'_{\ell-1} a'_\ell} \Psi^A_{a_{\ell-1} a'_{\ell-1}} \Psi^B_{a_\ell a'_\ell} M^{\sigma_\ell}_{a'_{\ell-1} a'_\ell} = 0.$$

simple eigenvalue equation:

H: $$H_{(\sigma_\ell a_{\ell-1} a_\ell),(\sigma'_\ell a'_{\ell-1} a'_\ell)} := \sum_{b_{\ell-1} b_\ell} L^{a_{\ell-1} a'_{\ell-1}}_{b_{\ell-1}} W^{\sigma_\ell \sigma'_\ell}_{b_{\ell-1} b_\ell} R^{a_\ell a'_\ell}_{b_\ell}$$

N: $$N_{(\sigma_\ell a_{\ell-1} a_\ell),(\sigma'_\ell a'_{\ell-1} a'_\ell)} := \Psi^A_{a_{\ell-1} a'_{\ell-1}} \Psi^B_{a_\ell a'_\ell} \delta_{\sigma_\ell \sigma'_\ell}$$

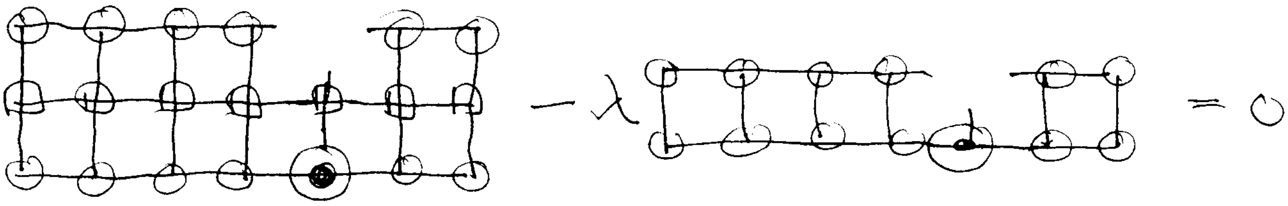
v: $$v_{(\sigma_\ell a_{\ell-1} a_\ell)} = M^{\sigma_\ell}_{a_{\ell-1} a_\ell}$$

$$\boxed{Hv - \lambda N v = 0} \qquad (dD^2 \times dD^2 \text{ matrices})$$

gives new v to reshape into new M

~~remarks~~ generalized eigenproblem

graphical representation:



remarks:

i) problem is Hermitian

ii) $dD^2 \times dD^2$ usually too large for exact diagonalization, but large sparse eigensolvers (Lanczos, Jacobi-Davidson) will do, as only the extreme eigenvalue is wanted. (initial guess vector important!)

iii) exploiting L- and R-normalization turns problem into standard eigenproblem, $N = \mathbb{1}$!

Algorithm.

- start with initial guess for $|\psi\rangle$, (e.g.) R-normalized (B only)
- calculate R-expressions iteratively from site $L-1, \dots, 1$.
- RIGHT SWEEP: starting from site 1 through $L-1$, move through the lattice to the right
  - solve standard eigenproblem for M^{σ_ℓ} (with current value as starting point)
  - left-normalize $M^{\sigma_\ell} \to A^{\sigma_\ell}$, via SVD/QR multiply remainder to the right into $M^{\sigma_{\ell+1}}$ (this will be starting guess for next site)
  - iteratively build up L-expression by one more site
  - move on: $\ell \to \ell+1$
- LEFT SWEEP: starting from site ~~L-1~~ L through 2, move through the lattice to the left:
  - solve eigenproblem
  - right-normalize $M^{\sigma_\ell} \to B^{\sigma_\ell}$, via SVD/QR, multiply remainder to the left into $M^{\sigma_{\ell-1}}$
  - iteratively build up R-expression by one more site
  - move on $\ell \to \ell-1$.

Time evolution with MPS

$\hat{H} = \sum_i \hat{h}_i$ nearest-neighbor (sites $i, i+1$)

$t = N\tau$, $\tau \to 0$, $N \to \infty$

first-order Trotter:

$$e^{-i\hat{H}t} = e^{-i\hat{h}_1\tau} e^{-i\hat{h}_2\tau} e^{-i\hat{h}_3\tau} \cdots e^{-i\hat{h}_{L-1}\tau} + O(\tau^2)$$

error because of $[\hat{h}_i, \hat{h}_{i+1}] \neq 0$

odd, even bonds commute among each other!

$$e^{-i\hat{H}\tau} \cong \underbrace{e^{-i\hat{H}_{odd}\tau}} \underbrace{e^{-i\hat{H}_{even}\tau}}$$

need MPO for this – must exist. (dim will be $\leq d^2$)

MPO $\times$ MPS: $D \to d^2 D$: compression needed!

Time evolution algorithm:

$$|\psi(t)\rangle \to \underbrace{e^{-i\hat{H}_{odd}\tau}}_{MPO} |\psi(t)\rangle$$

$$e^{-i\hat{H}_{odd}\tau} \to e^{-i\hat{H}_{even}\tau} e^{-i\hat{H}_{odd}\tau} |\psi(t)\rangle \equiv |\tilde{\psi}(t+\tau)\rangle$$

compress from $d^2 D \to D$: $|\tilde{\psi}(t+\tau)\rangle \to |\psi(t+\tau)\rangle$

and restart:

monitor error, extrapolate in $D \to \infty$, $\varepsilon \to 0$.

expectation values

$$\langle \hat{O}(t) \rangle = \langle \psi(t) | \hat{O} | \psi(t) \rangle$$

$$\langle \hat{O}(t) \hat{P} \rangle = \langle \psi | e^{+i\hat{H}t} \hat{O} e^{-i\hat{H}t} \hat{P} | \psi \rangle = \langle \psi(t) | \hat{O} | \varphi(t) \rangle$$

$$|\varphi(t)\rangle = e^{-i\hat{H}t} \hat{P} |\psi\rangle$$

$$\rightsquigarrow \langle S^z_i(t) S^z_j(0) \rangle \rightsquigarrow S^{zz}(k,\omega) \sim \int dt \sum_n \langle S^z_i(t) S^z_{i+n} \rangle e^{ikn} e^{-i\omega t}$$

simple improvements: higher-order Trotter decompositions.

2nd order:

$$e^{-i\hat{H}t} = e^{-i\hat{H}_{odd}\tau/2} e^{-i\hat{H}_{even}\tau} e^{-i\hat{H}_{odd}\tau/2} + O(\tau^3)$$

if evaluations not after every time step: cost as in first order (except evaluation times)

4th order:

$$e^{-i\hat{H}\tau} = \hat{U}(\tau_1)\hat{U}(\tau_2)\hat{U}(\tau_3)\hat{U}(\tau_2)\hat{U}(\tau_1)$$

$$U(\tau_i) = e^{-i\hat{H}_{odd}\tau_i/2} e^{-i\hat{H}_{even}\tau_i} e^{-i\hat{H}_{odd}\tau_i/2}$$

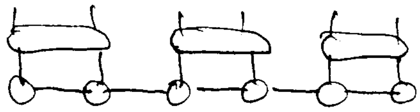
$$\tau_1 = \tau_2 = \frac{1}{4-4^{1/3}}\tau \qquad \tau_3 = \tau - 2\tau_1 - 2\tau_2 .$$

MPO for pure state evolution:

① pure states.

$$\underbrace{e^{-i\hat{h}_1\tau}} \otimes e^{-i\hat{h}_1\tau} \otimes \dots$$

$$\sum_{\sigma_1\sigma_2\sigma_1'\sigma_2'} O^{\sigma_1\sigma_2;\sigma_1'\sigma_2'} |\sigma_1\sigma_2\rangle\langle\sigma_1'\sigma_2'|$$



destroys MPS form.

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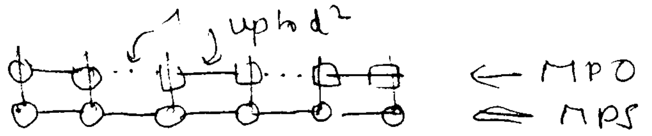
$$\hat{O}^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = P_{(\sigma_1\sigma_1'),(\sigma_2\sigma_2')}$$

$$= \sum_k U_{\sigma_1\sigma_1',k} S_{kk} (V^+)_{k,(\sigma_2\sigma_2')}$$

$$= \sum_k U_k^{\sigma_1\sigma_1'} \bar{U}_k^{\sigma_2\sigma_2'} \qquad 1 \le k \le d^2$$

$$= \sum_k U_{1,k}^{\sigma_1\sigma_1'} \bar{U}_{k,1}^{\sigma_2\sigma_2'}$$

$$U_k^{\sigma_1\sigma_1'} = U_{(\sigma_1\sigma_1'),k}\sqrt{S_{kk}} \qquad \bar{U}_k^{\sigma_2\sigma_2'} = \sqrt{S_{kk}}(V^+)_{k,(\sigma_2\sigma_2')}$$



and similarly even bonds!

② <u>mixed states</u>

purification: P is physical state space

dummy state in aux space.

$$\hat{\rho}_P = \sum_{a=1}^{r} s_a^2 |a\rangle_P \langle a|_P \rightarrow |\psi\rangle = \sum_{a=1}^{r} s_a |a\rangle_P |a\rangle_Q$$

$$\hat{\rho}_P = \mathrm{tr}_Q |\psi\rangle\langle\psi|$$

aux state space Q can be taken as copy of original.

chain → ladder.

but we don't know the s_a^2 ...! ~~but~~

generation is possible for thermal density operators:

$$\hat{\rho}_\beta = \frac{1}{Z(\beta)} e^{-\beta\hat{H}} \qquad Z(\beta) = \mathrm{tr}_P\, e^{-\beta\hat{H}}$$

$$\hat{\rho}_\beta = \frac{1}{Z(\beta)} e^{-\beta \hat{H}} = \frac{1}{Z(\beta)} e^{-\beta \hat{H}/2} \cdot \hat{I} \cdot e^{-\beta \hat{H}/2}$$

$\hat{I} = Z(0)\, \hat{\rho}_0$ (infinite-T density operator).

assume we know purification of $\hat{\rho}_0$ as MPS $|\psi_{\beta=0}\rangle$

Then

$$\hat{\rho}_\beta = \frac{Z(0)}{Z(\beta)} e^{-\beta \hat{H}/2} \, \mathrm{tr}_Q |\psi_0\rangle\langle\psi_0| e^{-\beta \hat{H}/2} = \frac{Z(0)}{Z(\beta)} \mathrm{tr}_Q\, e^{-\beta \hat{H}/2} |\psi_0\rangle\langle\psi_0| e^{-\beta \hat{H}/2}$$

trace acts on Q
$\hat{H}$ acts on P $\Rightarrow$ can be pulled in front!

$\Rightarrow$ carry out imaginary time evolution $|\psi_\beta\rangle = e^{-\beta \hat{H}/2} |\psi_0\rangle$.

expectation values:

$$\langle \hat{O} \rangle_\beta = \mathrm{tr}_P\, \hat{O} \hat{\rho}_\beta = \frac{Z(0)}{Z(\beta)} \mathrm{tr}_P\, \hat{O}\, \mathrm{tr}_Q |\psi_\beta\rangle\langle\psi_\beta| = \underbrace{\frac{Z(0)}{Z(\beta)}}_{d^L/Z(\beta)} \langle \psi_\beta | \hat{O} | \psi_\beta \rangle$$

$$1 \stackrel{!}{=} \langle \hat{I} \rangle_\beta = \mathrm{tr}_P\, \hat{\rho}_\beta = \frac{Z(0)}{Z(\beta)} \mathrm{tr}_P \mathrm{tr}_Q |\psi_\beta\rangle\langle\psi_\beta| = \frac{Z(0)}{Z(\beta)} \underbrace{\langle \psi_\beta | \psi_\beta \rangle}_{\Rightarrow Z(\beta)/Z(0)}$$

$$\Rightarrow \quad \langle \hat{O} \rangle_\beta = \frac{\langle \psi_\beta | \hat{O} | \psi_\beta \rangle}{\langle \psi_\beta | \psi_\beta \rangle}$$

as for pure states — no algorithmic changes!

thermodynamics:

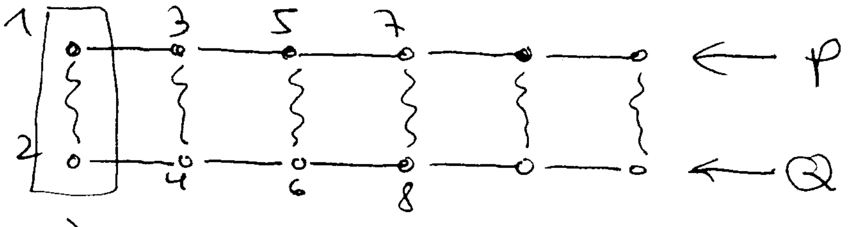
$Z(\beta)/Z(0) = \langle \psi_\beta | \psi_\beta \rangle$; $Z(0) = d^L \Rightarrow Z(\beta)$.

$\Rightarrow F(\beta) = -\beta^{-1} \ln Z(\beta)$

$U(\beta) = \langle \hat{H} \rangle_\beta = \langle \psi_\beta | \hat{H} | \psi_\beta \rangle / \langle \psi_\beta | \psi_\beta \rangle$.

$\Rightarrow S(\beta) = \beta (U(\beta) - F(\beta))$ $\Longrightarrow$ further TD quantities!

<u>last step:</u> purification $\hat{\rho}_{\beta=0} \to |\psi_{\beta=0}\rangle$



one big site

$$\hat{\rho}_0 = \frac{1}{d^L}\hat{I} = \left(\frac{1}{d}\hat{I}\right)^{\otimes L}$$ on each physical site

factorizes ⇒

$$|\psi_0\rangle = |\psi_{1,0}\rangle |\psi_{2,0}\rangle |\psi_{3,0}\rangle$$

rung number i

rung i: $|\sigma\rangle_P$, $|\sigma\rangle_Q$ on phys site $2i-1$ and aux site $2i$:

$$\frac{1}{d}\hat{I} = \sum_\sigma \frac{1}{d}\, {}_P|\sigma\rangle\langle\sigma|_P = \mathrm{tr}_Q\left[\left(\sum_\sigma \frac{1}{\sqrt{d}}|\sigma\rangle_P|\sigma\rangle_Q\right)\left(\sum_\sigma \frac{1}{\sqrt{d}}\,{}_P\langle\sigma|\,{}_Q\langle\sigma|\right)\right]$$

purification given by <u>maximally entangled</u> state

$$|\psi_{i0}\rangle = \sum_\sigma \frac{1}{\sqrt{d}}|\sigma\rangle_P|\sigma\rangle_Q \qquad (\text{entropy } \log_2 d)$$

unitary transformations on P and Q can be used to make optimal use of good quantum numbers, e.g. spin chain ($U(1)$ $[S^z]$, $SU(2)$ $[\vec{S}]$):

$$|\psi_{i0}\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\rangle_P|\downarrow\rangle_Q - |\downarrow\rangle_P|\uparrow\rangle_Q\right].$$

then:

$A^{\uparrow\uparrow} = 0$ $\quad A^{\uparrow\downarrow} = \frac{1}{\sqrt{2}}$ $\quad A^{\downarrow\uparrow} = -\frac{1}{\sqrt{2}}$ $\quad A^{\downarrow\downarrow} = 0$ $\quad \boxed{D=1}$

product state!