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DENSITY MATRIX RENORMALIZATION GROUP
(DMRG)

Uli Schollwöck

- most powerful numerical techniques for 1D quantum lattice systems

- invented in 1992 by Steve White — PRL 69, 2863 (1992)

- originally conceived as an RG method — US. RMP 77, 259 (2005)
  Flow in density matrices of subsystems

- close connection to <u>matrix product states</u> (MPS)
  realized 1995 onwards — U.S. Ann Phys. 326, 96 (2011)

- TODAY: DMRG <u>variational</u> method in space of <u>MPS</u>.

$$|\psi\rangle = \sum_{\sigma_1\ldots\sigma_L} \underbrace{c_{\sigma_1\sigma_2\ldots\sigma_L}}_{d^L \text{ coeffs for local state space of dim } d} |\sigma_1\ldots\sigma_L\rangle$$

unwieldy! first approx: <u>factorize</u>

$$|\psi\rangle = \sum_{\sigma_1\ldots\sigma_L} c_{\sigma_1}\cdot c_{\sigma_2}\cdot\ldots\cdot c_{\sigma_L} |\sigma_1\ldots\sigma_L\rangle$$

mean-field theory
product state
no entanglement

generalize this to non-local superpositions:

$$|\psi\rangle = \sum_{\sigma_1\cdot\sigma_L} \mathrm{tr}\,(\underbrace{M^{\sigma_1}\cdot M^{\sigma_2}\ldots M^{\sigma_L}}_{\text{at least } 2\times 2})|\sigma_1\ldots\sigma_L\rangle$$

(Kramer, Wannier; Baxter; Accardi; Affleck et al; Klümper/Schadschneider/Zittartz; Werner, Fannes, Nachtergaele)

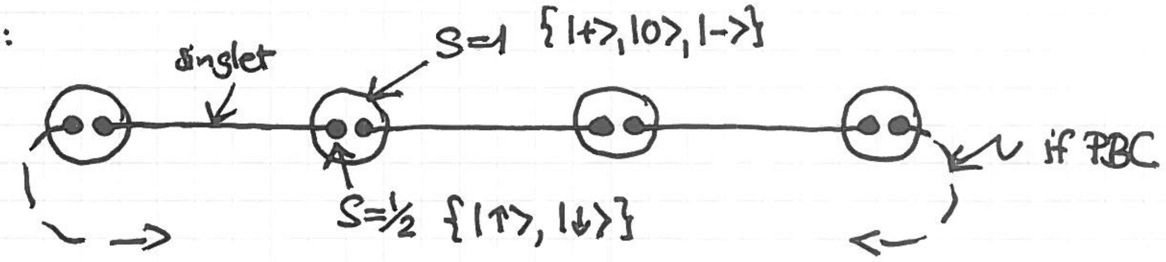
IS THIS ANY USEFUL?

Affleck-Kennedy-Lieb-Tasaki (AKLT) model

PRL **59**, 799 (87) Comm. Math. Phys. **115**, 477 (88)

parent Hamiltonian concept: interesting state → find $\hat{\mathcal{H}}$ where state is ground state

here:



- spin-1 states formed from totally symmetric (triplet) states of 2 $S=\frac{1}{2}$:

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

- spin-½ on neighboring sites linked by antisymmetric (singlet) state of 2 $S=\frac{1}{2}$

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

state reproduces almost all interesting features of $S=1$ <u>Haldane</u> chain: $\hat{H} = \sum \hat{\underline{S}}_i \cdot \hat{\underline{S}}_{i+1}$ $(S=1)$

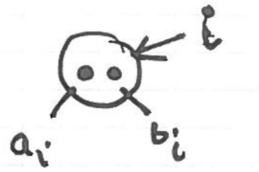
parent Hamiltonian: $\hat{H} = \sum_i \left\{ \hat{\underline{S}}_i \cdot \hat{\underline{S}}_{i+1} + \frac{1}{3}(\hat{\underline{S}}_i \cdot \hat{\underline{S}}_{i+1})^2 + \frac{2}{3} \right\}$

matrix product state of lowest non-trivial size $\boxed{D=2}$ is <u>exact</u> representation of ground state!

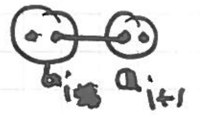
$S=1$ basis: $|\sigma_1 \ldots \sigma_L\rangle \equiv |\underline{\sigma}\rangle$

rep of GS in auxiliary $S=\frac{1}{2}$ basis:

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



Singlet bond between $i, i+1$:



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

$$\Sigma = \begin{bmatrix} 0 & +\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix} \quad (2\times 2) \text{ matrix}$$

Singlets everywhere:

$$|\psi_\Sigma\rangle = \sum_{\underline{a},\underline{b}} \Sigma_{b_1 a_2} \Sigma_{b_2 a_3} \ldots \Sigma_{b_{L-1} a_L} \overset{\text{PBC}}{\Sigma_{b_L a_1}} |\underline{a}\,\underline{b}\rangle$$

identification triplet $\Leftrightarrow$ $S=1$:

mapping $\{|\uparrow\rangle, |\downarrow\rangle\}^{\otimes 2} \rightarrow \{|+\rangle, |0\rangle, |-\rangle\}$

rep. by $M^\sigma_{ab} |\sigma\rangle\langle ab|$ $\quad M^\sigma$: (2×2) matrix $d=3$ of then

$$M^+ = \begin{array}{c|cc} & b\uparrow & \downarrow \\ \hline \uparrow & 1 & 0 \\ \downarrow\, a & 0 & 0 \end{array} \qquad M^0 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix} \qquad M^- = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$$

$|\psi_\Sigma\rangle$ mapped to

$$|\tilde{\psi}\rangle = \sum_{\underline{\sigma}} \sum_{\underline{a}\underline{b}} M^{\sigma_1}_{a_1 b_1} \Sigma_{b_1 a_2} M^{\sigma_2}_{a_2 b_2} \Sigma_{b_2 a_3} \cdots M^{\sigma_L}_{a_L b_L} \Sigma_{b_L a_1} |\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}} \mathrm{tr}\,(M^{\sigma_1}\Sigma M^{\sigma_2}\Sigma \ldots \overbrace{M^{\sigma_L}\Sigma}^{\tilde{A}^{\sigma_L}})|\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}} \mathrm{tr}\,(\tilde{A}^{\sigma_1} \ldots \tilde{A}^{\sigma_L})|\underline{\sigma}\rangle$$

$$\tilde{A}^+ = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix} \qquad \tilde{A}^0 = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & +\frac{1}{2} \end{bmatrix} \qquad \tilde{A}^- = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$ (2×2) (D×D) matric

normalized?

$$\langle\tilde\psi|\tilde\psi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}(\tilde A^{\sigma_1}\dots\tilde A^{\sigma_L})^* \,\mathrm{tr}(\tilde A^{\sigma_1}\dots\tilde A^{\sigma_L}) = \dots$$

$$\langle \text{use } \mathrm{tr}(ABC\dots)\,\mathrm{tr}(FGH\dots) = \mathrm{tr}\,(A\otimes F)(B\otimes G)(C\otimes H)\dots\rangle$$

$$\dots = \mathrm{tr}\Big[\underbrace{\Big(\sum_{\sigma_1}\tilde A^{\sigma_1 *}\otimes\tilde A^{\sigma_1}\Big)}_{=:\,\tilde E}\Big(\sum_{\sigma_2}\tilde A^{\sigma_2 *}\otimes\tilde A^{\sigma_2}\Big)\dots\Big]$$

$$= \mathrm{tr}\,\tilde E^L = \sum_{i=1}^{4=D^2}\tilde\lambda_i^L$$

a little calc shows: $\tilde E = \begin{bmatrix} 1/4 & 0 & 0 & 1/2 \\ 0 & -1/4 & 0 & 0 \\ 0 & 0 & -1/4 & 0 \\ 1/2 & 0 & 0 & 1/4 \end{bmatrix}$ $\quad \tilde\lambda_i = \{\frac{3}{4}, -\frac{1}{4}, -\frac{1}{4}, -\frac{1}{4}\}$

$$\Rightarrow \langle\tilde\psi|\tilde\psi\rangle = \left(\tfrac{3}{4}\right)^L + 3\left(-\tfrac{1}{4}\right)^L \longrightarrow 0 \text{ as } L\to\infty$$

rescale: $E = \frac{4}{3}\tilde E$, $\lambda_i = \frac{4}{3}\tilde\lambda_i$, $A^\sigma = \frac{2}{\sqrt3}\tilde A^\sigma$

$\boxed{|\psi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}(A^{\sigma_1}\dots A^{\sigma_L})|\underline{\sigma}\rangle}$ MPS $\qquad \lambda_i = \{1, -\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}\}$

$$\Rightarrow \boxed{\langle\psi|\psi\rangle = 1^L + 3\left(-\tfrac{1}{3}\right)^L \rightarrow 1 \text{ as } L\to\infty}$$

could we have had "correct"

$$A^+ = \begin{bmatrix} 0 & +\sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix} \quad A^0 = \begin{bmatrix} -\frac{1}{\sqrt3} & 0 \\ 0 & +\frac{1}{\sqrt3} \end{bmatrix} \quad A^- = \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$$

right away?

Want (left) eigenvector with eigenvalue 1 for E:

$$\sum_{ik} v_{ik} E_{(ik),(je)} = \sum_{ik} v_{ik}\sum_\sigma A^{\sigma *}_{ij} A^\sigma_{k,e} \overset{!}{=} v_{je}$$

$v_{ik} = \delta_{ik}$: eigenvector with eigenvalue 1 if

normalization condition

$$\sum_{\sigma i} A^{\sigma *}_{ij} A^\sigma_{ie} = \sum_\sigma (A^{\sigma\dagger}A^\sigma)_{je} = \delta_{je} \text{ or } \boxed{\sum_\sigma A^{\sigma\dagger}A^\sigma = 1}$$

(One has to show that then also all other eigenvalues < 1, which is more involved)

<u>observables, correlators?</u>

$\langle\psi|\hat{O}\hat{P}|\psi\rangle$ $\qquad$ $\hat{O}$ on site i, $\hat{P}$ on site j $\quad i<j$

$$= \sum_{\underline{\sigma}\underline{\sigma}'} \langle\psi|\underline{\sigma}\rangle\langle\underline{\sigma}|\hat{O}\hat{P}|\underline{\sigma}'\rangle\langle\underline{\sigma}'|\psi\rangle$$

$$= \sum_{\underline{\sigma},\sigma_i'\sigma_j'} \mathrm{tr}(A^{\sigma_1}\ldots A^{\sigma_i}\ldots A^{\sigma_j}\ldots A^{\sigma_L})^* \langle\sigma_i|\hat{O}|\sigma_i'\rangle\langle\sigma_j|\hat{P}|\sigma_j'\rangle \mathrm{tr}(A^{\sigma_1}\ldots A^{\sigma_i'}\ldots A^{\sigma_j'}\ldots A^{\sigma}$$

$$= \mathrm{tr}\Big(\sum_{\sigma_1} A^{\sigma_1 *}\otimes A^{\sigma_1}\Big)\ldots\Big(\sum_{\sigma_i\sigma_i'} A^{\sigma_i *}\otimes A^{\sigma_i'}\langle\sigma_i|\hat{O}|\sigma_i'\rangle\Big)\ldots$$
$$\Big(\sum_{\sigma_j\sigma_j'} A^{\sigma_j *}\otimes A^{\sigma_j'}\langle\sigma_j|\hat{P}|\sigma_j'\rangle\Big)\ldots\Big(\sum_{\sigma_L} A^{\sigma_L *}\otimes A^{\sigma_L}\Big)$$

$$E_O := \sum_{\sigma\sigma'} A^{\sigma *}\otimes A^{\sigma'}\langle\sigma|\hat{O}|\sigma'\rangle$$

$$\langle\psi|\hat{O}\hat{P}|\psi\rangle = \mathrm{tr}\, E^{i-1} E_O E^{j-i-1} E_P E^{L-j}$$
$$= \mathrm{tr}\, E_O E^{j-i-1} E_P E^{L-j+i-1} \qquad\qquad E|m\rangle = \lambda_m|m\rangle$$
$$= \sum_{m=1}^{4} \langle m|E_O E^{j-i-1} E_P \lambda_m^{L-j+i-1}|m\rangle$$

$\lambda_1 = 1$; $|\lambda_{m>1}| < 1$:

$$\langle\psi|\hat{O}\hat{P}|\psi\rangle \underset{L\to\infty}{=} \langle 1|E_O E^{j-i-1} E_P|1\rangle = \sum_{k=1}^{4}\langle 1|E_O|k\rangle \lambda_k^{j-i-1}\langle k|E_P|1\rangle$$

here: $|1\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 8 \\ 1/\sqrt{2} \end{bmatrix}$ $\quad |2\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}$ $\quad |3\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}$ $\quad |4\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}$

$\lambda_1 = 1$

2 standard examples:

$\langle\hat{S}_i^z\hat{S}_j^z\rangle$ $\qquad$ $E_{S^z} = A^{+*}\otimes A^{+} - A^{-*}\otimes A^{-} = \begin{bmatrix} 0 & 0 & 0 & 2/3 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -2/3 & 0 & 0 & 0 \end{bmatrix}$

$\langle 1 | E_{S^z} | 4 \rangle = -\frac{2}{3}$ $\langle 4 | E_{S^z} | 1 \rangle = +\frac{2}{3}$ all others zero

$$\langle \hat{S}^z_i \hat{S}^z_j \rangle = \left(-\frac{2}{3}\right)\left(+\frac{2}{3}\right)\underset{\lambda_4}{\left(-\frac{1}{3}\right)^{j-i-1}} = \frac{4}{3} \underbrace{(-1)^{j-i}}_{\text{AFM}} e^{-(j-i)/\xi}$$

$$\xi = -\frac{1}{\ln \lambda_4} = \frac{1}{\ln 3} \approx 0{,}91$$

exponential decay

$$\underbrace{\langle \hat{S}^z_i \left(\prod_{k=i+1}^{j-1} \overbrace{e^{i\pi \hat{S}^z_k}}^{\hat{P}_k} \right) \hat{S}^z_j \rangle}_{\text{hidden (string, topological) order}} \equiv \langle \hat{S}^z_i \prod_k \hat{P}_k \hat{S}^z_j \rangle$$

$$E_P = -A^{+*} \otimes A^+ + A^{0*} \otimes A^0 - A^{-*} \otimes A^- = \begin{bmatrix} 1/3 & 0 & 0 & -2/3 \\ 0 & -1/3 & 0 & 0 \\ 0 & 0 & -1/3 & 0 \\ -2/3 & 0 & 0 & 1/3 \end{bmatrix}$$

$$\underset{\tilde{\lambda}_1 = 1}{|\tilde{1}\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}} \quad \underset{-1/3}{|\tilde{2}\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}} \quad \underset{-1/3}{|\tilde{3}\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}} \quad \underset{-1/3}{|\tilde{4}\rangle = \begin{bmatrix} 1/\sqrt{2} \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix}}$$

$$\langle \hat{S}^z_i \prod_k \hat{P}_k S^z_j \rangle = \cancel{\sum_m} \langle 1 | E_{S^z} | 4 \rangle \langle 4 | E_P^{j-i-1} | 4 \rangle \langle 4 | E_{S^z} | 1 \rangle$$

$$= -\frac{4}{9} \langle 4 | E_P^{j-i-1} | 4 \rangle$$

$$= -\frac{4}{9} \sum_{\tilde{m}=1}^{4} \langle 4 | \tilde{m} \rangle \lambda_{\tilde{m}}^{j-i-1} \langle \tilde{m} | 4 \rangle \qquad \underset{\text{others } 0}{\langle \tilde{1} | 4 \rangle = 1}$$

$$= -\frac{4}{9} \cdot 1 \cdot 1^{j-i-1} \cdot 1 = -\frac{4}{9}$$

long-range order

both results are generic:

either superposition of exponentials or
LRO

not power law, not 1D Ornstein-Zernike $\frac{e^{-r/\xi}}{\sqrt{r}}$ mimic! it

our main workhorse: SVD

SVD ≡ $\underline{s}$ingular $\underline{v}$alue $\underline{d}$ecomposition

$$M = U \cdot S \cdot V^\dagger$$

M	U	S	$V^\dagger$
$(N_A \times N_B)$	$(N_A \times \min(N_A, N_B))$	$(\min(N_A,N_B) \times \min(N_A,N_B))$	$(\min(N_A,N_B) \times N_B)$
	orthonormal columns:	diagonal entries	orthonormal rows:
	$U^\dagger U = 1$	$S_{aa} \equiv s_a \geq 0$	$V^\dagger V = 1$
	$[\lvert u_a \rangle]$ column vectors	<u>singular values</u>	$[\langle v_a \rvert]$ row vectors
	$N_A \leq N_B$: $U^\dagger U = UU^\dagger = 1$ unitary	# of $s_a > 0$: <u>rank</u>	$N_A \geq N_B$: $V^\dagger V = VV^\dagger = 1$ unitary

$$M = \sum s_a |u_a\rangle\langle v_a|$$

$$M^\dagger M = \sum s_a^2 |v_a\rangle\langle v_a| \qquad MM^\dagger = \sum s_a^2 |u_a\rangle\langle u_a|$$

right singular vectors $|v_a\rangle$ eigenvectors of $M^\dagger M$

left singular vectors $|u_a\rangle$: eigenvectors of $MM^\dagger$

eigenvalues = (singular values)^2

<u>Schmidt decomposition:</u> composite (bipartite) sys AB

$$|\psi\rangle_{AB} = \sum_{ij} \underline{\Psi}_{ij} |i\rangle_A |j\rangle_B$$

ONB

read as matrix

$$= \sum_{ij} \sum_a^{r = \text{rank}} U_{ia} S_{aa} (V^*)_{ja} |i\rangle_A |j\rangle_B$$

$$= \sum_a^r \Big(\sum_i U_{ia} |i\rangle_A \Big) S_{aa} \Big(\sum_j (V^*)_{ja} |j\rangle_B \Big)$$

$$\boxed{= \sum_a s_a |a\rangle_A |a\rangle_B}$$

pairs of ONB!

Can any state be represented as an MPS?

Yes, but exact rep may be exponentially costly!

lattice L sites 1,…,d   not necessarily 1D, but think in 1D terms

$$|\psi\rangle = \sum_{\sigma} c_{\sigma_1\ldots\sigma_L} |\sigma_1\ldots\sigma_L\rangle$$

① reshape state vector with d^L components into

$$\Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} \equiv c_{\sigma_1\ldots\sigma_L} \qquad \text{dim}: d \times d^{L-1}$$

② SVD of Ψ

$$c_{\sigma_1\ldots\sigma_L} = \Psi_{\sigma_1,(\sigma_2\ldots\sigma_L)} = \sum_{a_1}^{r_1} U_{\sigma_1,a_1} \underbrace{S_{a_1,a_1}(V^\dagger)_{a_1,\sigma_2\ldots\sigma_L}}_{\text{reshape}}$$

$$\equiv \sum_{a_1}^{r_1} U_{\sigma_1 a_1} c_{a_1\sigma_2\ldots\sigma_L}$$

③ decompose U into d row vectors A^{σ_1}:

$$\underset{\text{dummy}}{A^{\sigma_1}_{1,a_1}} \equiv U_{\sigma_1 a_1}$$

④ reshape $c_{a_1\sigma_2\ldots\sigma_L}$ into

$$\Psi_{(a_1\sigma_2),(\sigma_3\ldots\sigma_L)} \equiv c_{a_1\sigma_2\ldots\sigma_L}$$

⑤ SVD of Ψ:

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{1,a_1} \underset{\downarrow}{U_{(a_1\sigma_2),a_2}} S_{a_2,a_2} \underset{\downarrow}{(V^\dagger)_{a_2,(\sigma_3\ldots\sigma_L)}}$$

$$= \sum_{a_1}^{r_1}\sum_{a_2}^{r_2} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} \Psi_{(a_2\sigma_3),(\sigma_4\ldots\sigma_L)}$$

$$U = \begin{array}{|c|}\hline A^1 \\ \hline A^2 \\ \hline A^3 \\ \hline A^d \\ \hline\end{array}$$

⟨decomposition⟩   …

finally:

$$c_{\sigma_1\ldots\sigma_L} = \sum_{a_1\ldots a_{L-1}} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} \cdots A^{\sigma_{L-1}}_{a_{L-2},a_{L-1}} A^{\sigma_L}_{a_{L-1},1}$$

$$= A^{\sigma_1}\ldots A^{\sigma_L} \quad \text{(matrix mult.)}$$

$$\boxed{|\psi\rangle = \sum_{\sigma_1\ldots\sigma_L} A^{\sigma_1}\ldots A^{\sigma_L}\,|\sigma_1\ldots\sigma_L\rangle}$$ <u>matrix product state</u>

- dimensions:

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

exp. large:
<u>can we truncate</u>?
at which price in accuracy?

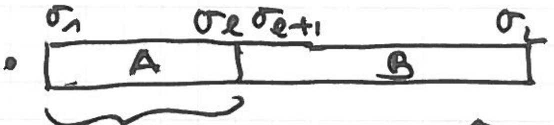
- SVD : $U^\dagger U = 1$:

$$\delta_{a_\ell a_\ell'} = \sum_{a_{\ell-1}\sigma_\ell} (U^\dagger)_{a_\ell,(a_{\ell-1}\sigma_\ell)} \cdot U_{(a_{\ell-1}\sigma_\ell),a_\ell'}$$

$$= \sum_{a_{\ell-1}\sigma_\ell} (A^{\sigma_\ell\dagger})_{a_\ell a_{\ell-1}} \cdot A^{\sigma_\ell}_{a_{\ell-1}a_\ell'}$$

$$= \sum_{\sigma_\ell} (A^{\sigma_\ell\dagger}A^{\sigma_\ell})_{a_\ell a_\ell'} \quad \text{or}$$

$$\boxed{\sum A^{\sigma_\ell\dagger}A^{\sigma_\ell} = I}$$ <u>left-normalized</u>;
state of A's: <u>left-canonical</u>

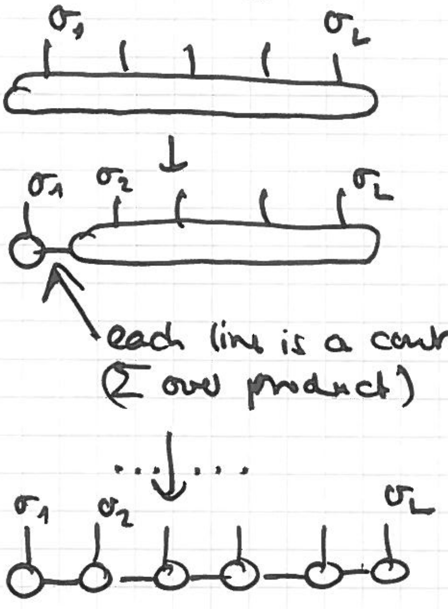
- 

$$|a_\ell\rangle_A := \sum_{\sigma_1\ldots\sigma_\ell} (A^{\sigma_1}\ldots A^{\sigma_\ell})_{1,a_\ell}\,|\sigma_1\ldots\sigma_\ell\rangle$$ <u>Orthonormal</u>

$$|a_\ell\rangle_B := \sum_{\sigma_{\ell+1}\ldots\sigma_L} (A^{\sigma_{\ell+1}}\ldots A^{\sigma_L})_{a_\ell,1}\,|\sigma_{\ell+1},\ldots\sigma_L\rangle$$ <u>not</u> orthonormal in general.

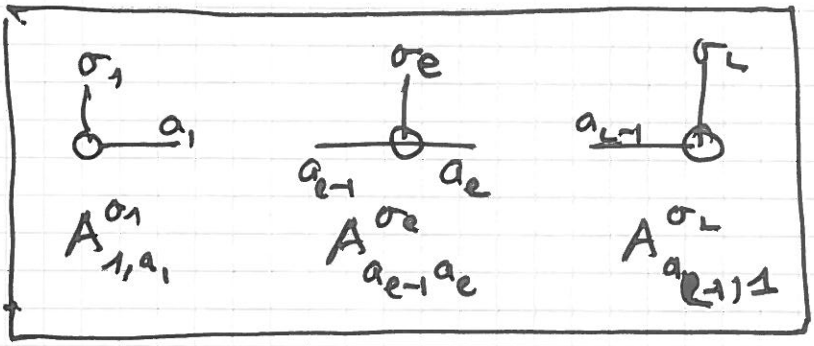
hence: $|\psi\rangle = \sum_{a_\ell} |a_\ell\rangle_A\,|a_\ell\rangle_B$ <u>no</u> Schmidt decomp!

too many indices! graphical representation



$\leftarrow c_{\sigma_1\ldots\sigma_L}$

$\leftarrow A^{\sigma_1}_{1,a_1}\; c_{a_1\sigma_2\ldots\sigma_L}$ ↙ each index is a leg sticking out



if we start decomposition from right, we obtain

$$|\psi\rangle = \sum_{\underline{\sigma}} B^{\sigma_1}\ldots B^{\sigma_L}|\sigma_1\ldots\sigma_L\rangle$$

with $\boxed{\sum_{\sigma} B^{\sigma}B^{\sigma\dagger} = 1}$ right-normalized / right-canonical (gauge freedom!)

leads to $|\psi\rangle = \sum_{a_\ell} \underset{\substack{\uparrow\\ \text{not orthon.}}}{|a_\ell\rangle_A}\, \underset{\substack{\uparrow\\ \text{orthonormal}}}{|a_\ell\rangle_B}$: reversed roles!

now mixed-canonical rep:

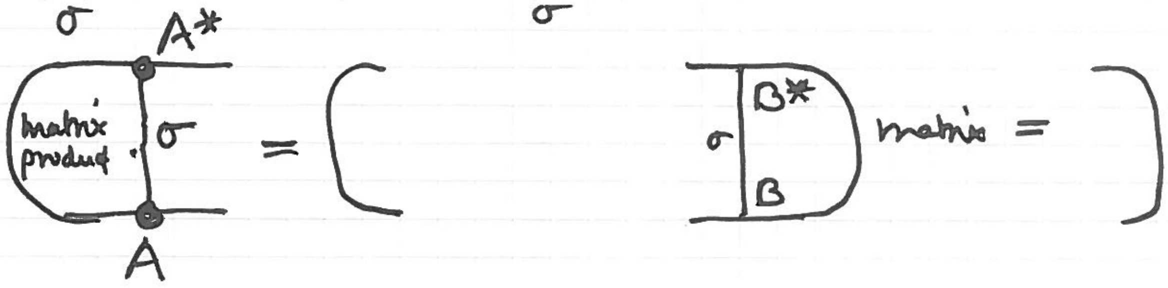
$$|\psi\rangle = \sum_{\sigma_1\ldots\sigma_L} \underbrace{A^{\sigma_1}\ldots A^{\sigma_\ell}}_{\substack{\text{generates}\\ \text{ONB}}}\, \underset{\substack{\uparrow\\ \text{singular values}}}{S}\, \underbrace{B^{\sigma_{\ell+1}}\ldots B^{\sigma_L}}_{\substack{\text{generates}\\ \text{ONB}}}|\sigma_1\ldots\sigma_L\rangle$$

$$|\psi\rangle = \sum_a s_a |a\rangle_A |a\rangle_B$$

Schmidt-decomp

some important graphics:

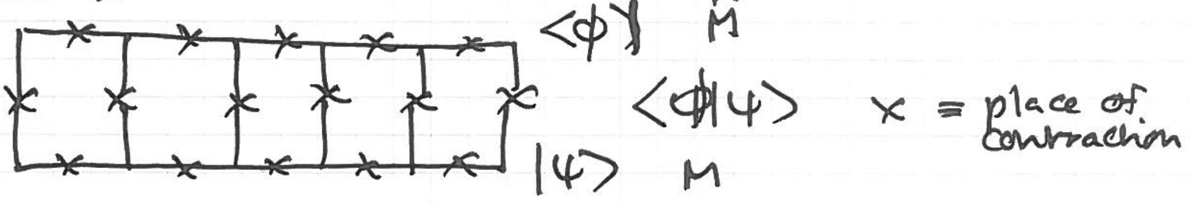
$$\sum_{\sigma} A^{+} A = 1 \qquad \sum_{\sigma} B B^{+} = 1$$



will show to lead to great simplifications!

Important operations with MPS

overlaps



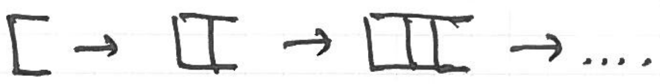
$$\langle\phi|\psi\rangle = \sum_{\sigma} \tilde{M}^{\sigma_1 *} \dots \tilde{M}^{\sigma_L *} M^{\sigma_1} \dots M^{\sigma_L}$$
$$= \sum_{\sigma} \tilde{M}^{\sigma_L +} \dots \tilde{M}^{\sigma_1 +} M^{\sigma_1} \dots M^{\sigma_L}$$

order of contraction crucial: like in formula: $O(d^L)$

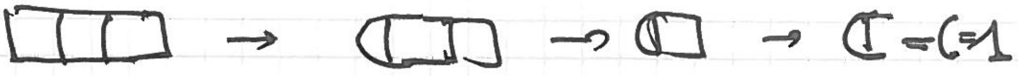
smart way:

$$\langle\phi|\psi\rangle = \sum_{\sigma_L} \tilde{M}^{\sigma_L +}\Big(\dots \underbrace{\Big(\sum_{\sigma_2} \tilde{M}^{\sigma_2 +} \underbrace{\Big(\sum_{\sigma_1} \tilde{M}^{\sigma_1 +} M^{\sigma_1}\Big)}_{O(dD^3)} M^{\sigma_2}\Big)\dots\Big)}_{2O(dD^3)} M^{\sigma_L}$$

altogether: $O((2L+1)dD^3) \rightarrow O(D^3)$ polynomial



if A Left-normalized:



expectation values, correlators:

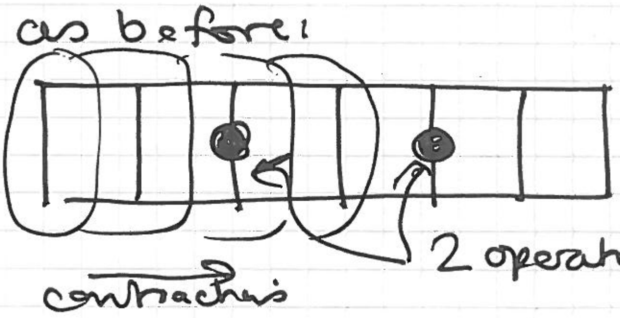
$$\hat{O}^{[\ell]} = \sum_{\sigma_\ell \sigma_\ell'} O^{\sigma_\ell \sigma_\ell'} |\sigma_\ell\rangle\langle\sigma_\ell'|$$

$$\langle\phi|\hat{O}^{[1]} \dots \hat{O}^{[L]}|\psi\rangle$$

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

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

as before:



2 operators ⇒ 2 point correlator.

general result for 2 points as a generalization of AKLT:

$$\boxed{\frac{\langle\psi|\hat{O}^{[i]}\hat{O}^{[j]}|\psi\rangle}{\langle\psi|\psi\rangle} = c_1 + \sum_{k=2}^{D^2} c_k e^{-r/\xi_k} \qquad \xi_k = -\frac{1}{\ln \lambda_k}}$$

λ_k eigenvalues of $E = \sum_{\sigma_\ell} M^{\sigma_\ell *} \otimes M^{\sigma_\ell}$

add 2 MPS: go to PBC (tr)

$$|\psi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}(M^{\sigma_1} \dots M^{\sigma_L}) |\underline{\sigma}\rangle \qquad |\phi\rangle = \sum_{\underline{\sigma}} \mathrm{tr}(\tilde{M}^{\sigma_1} \dots M^{\tilde{\sigma}_L}) |\underline{\sigma}\rangle$$

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

$$\begin{array}{|c|c|} \hline M & \\ \hline & \tilde{M} \\ \hline \end{array}$$

dimension grows! compression

Bring an MPS into <u>canonical form</u>, <u>compress it</u>

example: <u>left-canonical</u>

$$|\psi\rangle = \sum_{\underline{\sigma}} \sum_{a_1\ldots} M^{\sigma_1}_{1,a_1} M^{\sigma_2}_{a_1 a_2} M^{\sigma_3}_{a_2 a_3} \ldots |\underline{\sigma}\rangle$$

reshape (regroup) $M^{\sigma_1}_{1,a_1} \to M_{(1,\sigma_1),a_1}$ ⟨inverse of decomp⟩

SVD: $M = ASV^\dagger$

$$|\psi\rangle = \sum_{\underline{\sigma}} \sum_{a_1\ldots} \sum_{s_1} A_{(1\sigma_1),s_1} S_{s_1 s_1} V^\dagger_{s_1 a_1} M^{\sigma_2}_{a_1 a_2} \ldots |\underline{\sigma}\rangle$$

$$= \sum_{\underline{\sigma}} \sum_{a_2\ldots} \sum_{s_1} A^{\sigma_1}_{1,s_1} \underbrace{\left(\sum_{a_1} S_{s_1 s_1} V^\dagger_{s_1 a_1} M^{\sigma_2}_{a_1 a_2} \right)} M^{\sigma_3}_{a_2,a_3} \ldots |\underline{\sigma}\rangle$$

$$= \sum_{\sigma} \sum_{a_2\ldots} \sum_{s_1} \underbrace{A^{\sigma_1}_{1,s_1}}_{\text{left normalized due to SVD}} \underbrace{\tilde{M}^{\sigma_2}_{s_1,a_2}} M^{\sigma_3}_{a_2,a_3} \ldots |\sigma\rangle$$

<u>continue here:</u> $\tilde{M}^{\sigma_2}_{s_1,a_2} \to \tilde{M}_{(s_1\sigma_2),a_2}$ and SVD

similarly, right-canonical

<u>compression</u>:

assume MPS in mixed canonical form:

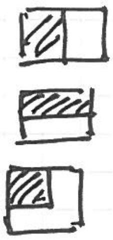
$$|\psi\rangle = \sum_{\underline{\sigma}} A^{\sigma_1} \ldots A^{\sigma_\ell} S B^{\sigma_{\ell+1}} \ldots B^{\sigma_L} |\underline{\sigma}\rangle$$

$\rightsquigarrow$ $|\psi\rangle = \sum s_{a_\ell} \underbrace{|a_\ell\rangle_A |a_\ell\rangle_B}_{\text{ONB}}$ $\Rightarrow$ $s^2_{a_\ell}$ EV of red. density operators for A, B:

$\rightsquigarrow$ compress A^{σ_ℓ} (col.)

$B^{\sigma_{\ell+1}}$ (row)

S (if ordered)



Keep <u>largest</u> contrib's!

<u>need</u> MPS in mixed can. form to do this everywhere!

⑭

$|\psi\rangle = MMMMMMMM$

$\xrightarrow{\text{rightcan}} = BBBBBBBBB$

now left-canonical (step by step):

$A\underbrace{SB}_{\text{truncate}}BBBB$

$A\,A\underbrace{SB}_{\text{truncate}}BBB \ldots \quad \rightarrow \quad AAAA\ldots$ (truncated)

one can also do a variational compression:

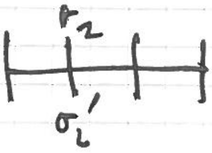
which (smaller dim.) MPS approx best $|\psi\rangle$ ~~$\exists$~~ in $\| . \|_2$ norm?

Matrix Product Operators

$\langle \underline{\sigma} | \psi \rangle = M^{\sigma_1} \ldots M^{\sigma_L}$

MPS

$\rightsquigarrow \langle \underline{\sigma} | \hat{O} | \underline{\sigma}' \rangle = M^{\sigma_1 \sigma_1'} \ldots M^{\sigma_L \sigma_L'}$



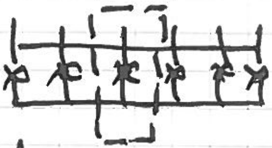
MPO

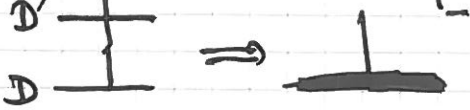
any operator can be rep as MPO:

$$\hat{O} = \sum_{\underline{\sigma}\underline{\sigma}'} M^{\sigma_1 \sigma_1'} \ldots M^{\sigma_L \sigma_L'} |\underline{\sigma}\rangle\langle\underline{\sigma}'|$$

proof: group indices $\hat{O}^{\sigma_1 \ldots \sigma_L, \sigma_1' \ldots \sigma_L'} \rightarrow \hat{O}^{(\sigma_1 \sigma_1')(\sigma_2 \sigma_2') \ldots}$ and use old proof for states

- even Hamiltonians find very simple rep (→ Miles)
- applying MPO to MPS:

$O|\psi\rangle$:

contract at ×



dim DD'

$\boxed{\text{MPO}|\text{MPS}\rangle = |\widetilde{\text{MPS}}\rangle}$ nice!

How useful are MPS? exponential size!

assume MPS in mixed rep:

$$\underbrace{AAAA}_{A}S\underbrace{BBBB}_{B} \qquad |\psi\rangle = \sum s_a |a\rangle_A |a\rangle_B \qquad \sum s_a^2 = 1$$

normalized

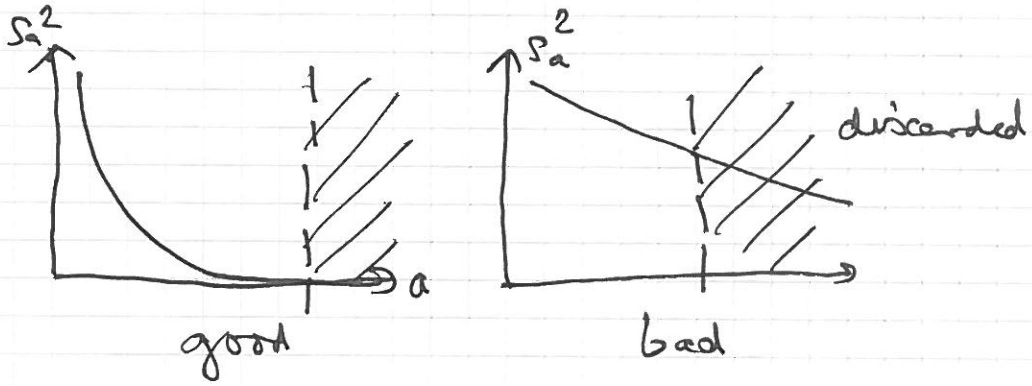
Can I reduce sum (matrix size)?

$$|\tilde{\psi}\rangle = \sum' s_a |a\rangle_A |a\rangle_B$$

$$\| |\psi\rangle - |\tilde{\psi}\rangle \|^2 = \sum_{\text{discarded}} s_a^2 \Rightarrow \text{kick out smallest } s_a$$

or:

$$\hat{\rho}_A = \sum s_a^2 |a\rangle_{A\,A}\langle a| \rightarrow \text{kick out smallest } s_a$$



Can be made more rigorous, but usually we do not know {s_a

Consider $S_1(|\psi\rangle_{AB}) = -\sum_a s_a^2 \ln s_a^2$

entanglement entropy of AB = subsystem entropy

special case of Renyi entropy : von Neumann entropy

"executive summary"

$\overbrace{\{1, 0, 0, \ldots\}}^{s_a^2}$: $S_1(|\psi\rangle) = 0$ product state

$\{\frac{1}{D}, \frac{1}{D}, \frac{1}{D}, \ldots\}$ $S_1(|\psi\rangle) = -D \cdot \frac{1}{D} \ln \frac{1}{D} = \ln D$ max. entangled

for D elements

$$\boxed{D \sim e^S}$$

D is just MPS dim:

⑯

$$|\psi\rangle = \sum S_a |a\rangle_A |a\rangle_B$$

$$\underbrace{AAAA}_{\dim(1,D)} \qquad \underbrace{BBBB}_{\dim(D,1)}$$

codeable entanglement less than $\underline{\ln D}$.

$$\boxed{D \gtrsim e^S}$$

What do we know about entanglement?

For $\underline{\text{ground states}}$: $\underline{\text{area law}}$ by Bekenstein (black holes)
(gapped systems)

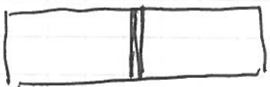
$\mathcal{D}$ dim.

$\sim L^0$ $\qquad \sim L$ $\qquad \sim L^2$ $\qquad \sim L^{\mathcal{D}-1}$

$\underline{\text{then}}$.

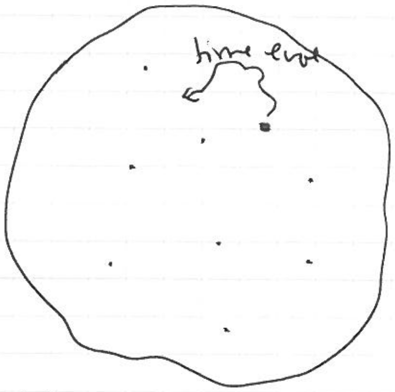
$D \sim \text{cst}$ $\qquad D \sim e^L$ $\qquad \cancel{D \sim e^{L^2}}$

very good!



long rectangles

in Fact: area law states are only subset of Hilbert space of measure zero (albeit an interesting one)



Hilbert space

if you time-evolve a GS with a (different) Hamiltonian, you will leave that cosy corner!

fundamental limitation of time-evolution with DMRG / MPS

Ground state search : DMRG

everything in place now: can do it graphically!

find MPS of (max) matrix dimension D minimizing

$$E_0 := \min \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

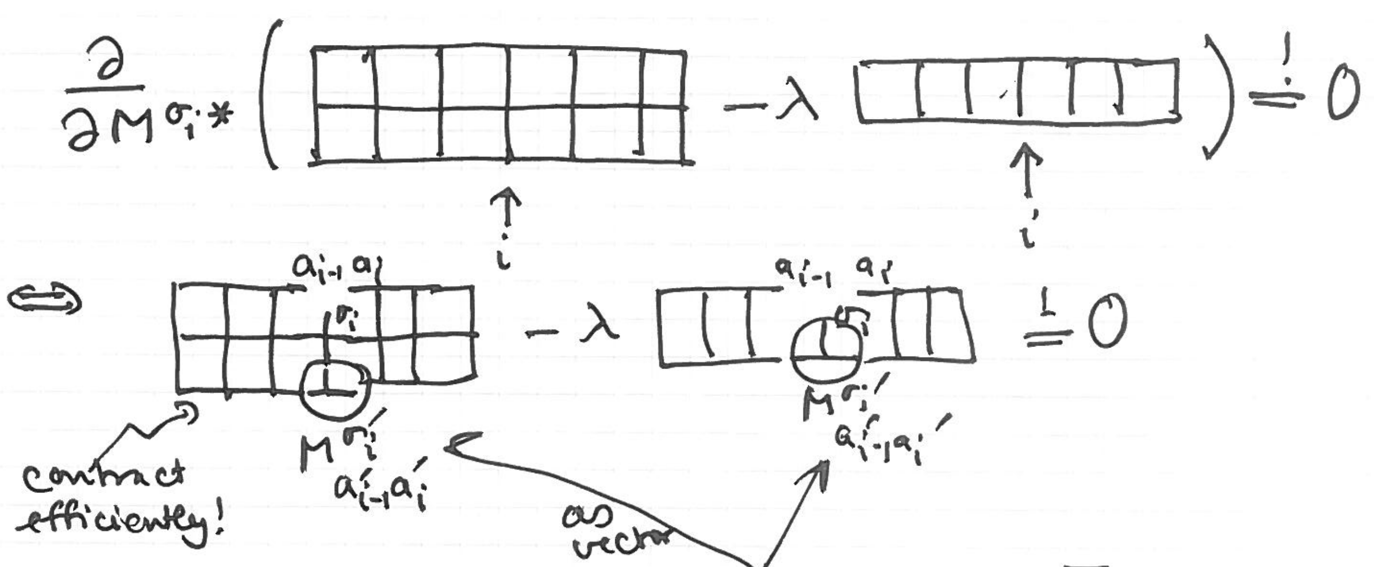
⇔ extremize

$$\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle \qquad \lambda \text{ will be } E_0 .$$

in MPS, this is a highly multilinear optimization problem

⇒ replace by <u>iterative</u> sequence of linear optimization problems: starting from guess $M^{\sigma_1} \dots M^{\sigma_L}$,

1) pick a site i
2) extremize wrt M^{σ_i} → <u>new</u> M^{σ_i}
3) continue going through all sites until energy converged

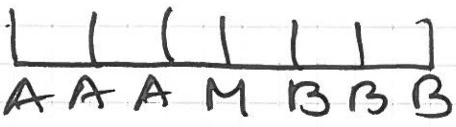


$$\sum_{\sigma_i' a_{i-1}' a_i'} H_{\sigma_i a_{i-1} a_i , \sigma_i' a_{i-1}' a_i'} \, v_{\sigma_i' a_{i-1}' a_i'} - \lambda \sum_{\sigma_i' a_{i-1}' a_i'} N_{\sigma_i a_{i-1} a_i , \sigma_i' a_{i-1}' a_i'} \, v_{\sigma_i' a_{i-1}' a_i'}$$

$Hv - \lambda N v = 0$ generalized eigenvalue problem

depending on N: very <u>badly</u> conditioned?

now assume:



then

due to normalization

$$\boxed{Hv - \lambda v = 0}$$

- <u>large</u> sp<u>arse</u> eigenvalue problem!
  $(dD^2 \times dD^2)$ most entries 0
  Davidson, Lanczos solvers

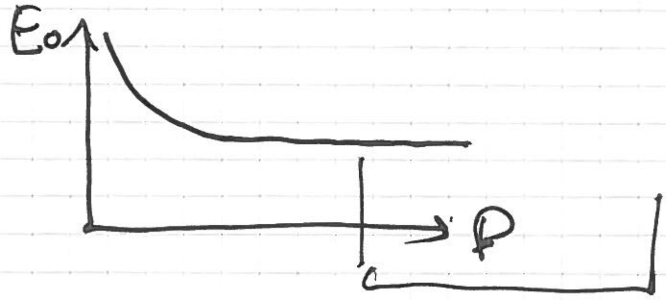
- while optimizing, keep proper mixed rep!
  ⟹ SWEEPING

$$\underset{\text{opt!}}{AMBBBBB} \rightarrow \underset{\text{opt}}{AAMBBBB} \rightarrow \ldots$$ and back (to beginning)

"sweeping"

- optimizing within ansatz class: DMRG is <u>variational</u> in MPS

- larger D (larger MPS matrices): strictly better energy



for spins: often O(100-300)
fermions: O(1000-3000)

Time evolution (real and imaginary) with MPS

Trotter decomp:

$$e^{-iHt} = \left(e^{-iH\tau}\right)^N \qquad \tau N = t \qquad \begin{matrix} N \to \infty \\ \tau \to 0 \end{matrix}$$

$$\hat{H} = \sum_i \hat{h}_i \quad \text{nearest-neighbors}$$

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

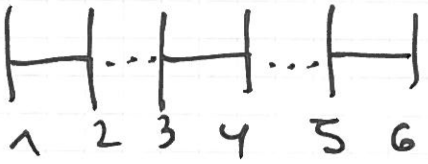
$$[\hat{h}_i, \hat{h}_{i+1}] \neq 0$$

$$e^{A+B} = e^A e^B \underbrace{e^{\frac{1}{2}[A,B]}}_{O(\tau^2)}$$

$$e^{-i\tilde{H}_{odd}\tau} \, e^{-i\hat{H}_{even}\tau}$$

<u>must</u> be MPO representable!

product of operators factorizes into MPO:



but we have  at the moment

$e^{-i\hat{h}_1\tau}$: is an operator $O^{\sigma_1\sigma_2, \sigma_1'\sigma_2'} =$

regroup:

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

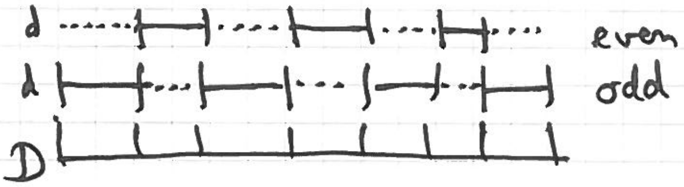
$$= \sum_k^{d^2} U_{(\sigma_1\sigma_1'),k} S_{kk} (V^\dagger)_{k,(\sigma_2\sigma_2')}$$

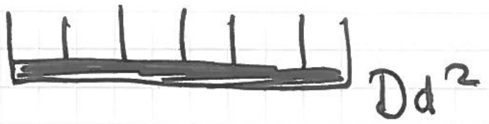
$$= \sum_k U^{\sigma_1\sigma_1'}_{\underset{\text{dummy}}{1},k} \overline{U}^{\sigma_2\sigma_2'}_{k,\underset{\text{dummy}}{1}}$$

$$U^{\sigma_1\sigma_1'}_{1,k} = U_{(\sigma_1\sigma_1'),k} \sqrt{S_{kk}} \qquad \overline{U}^{\sigma_2\sigma_2'}_{k,1} = (V^\dagger)_{k,(\sigma_2\sigma_2')} \sqrt{S_{kk}} \, .$$

algorithm:  $(|\psi(0)\rangle)$

① apply odd/even MPO:



→ 

② Compress back to D → 

③ next τ-step.

- higher-order Trotter decompositions reduce error

- FT in space / time gives rise to $S(k,\omega)$

$$\langle \hat{O}(t)\hat{P}\rangle = \langle\psi|e^{+iHt}\hat{O}e^{-iHt}\underbrace{\hat{P}|\psi\rangle}_{|\phi\rangle}$$

$$\|$$

$$\langle\psi(t)|\hat{O}|\phi(t)\rangle$$ reduced to single-time expectation value

- go to imaginary times to calculate

$$\underset{\text{random}}{e^{-\beta\hat{H}}|\psi\rangle} \longrightarrow \underset{\text{ground state}}{|\psi_0\rangle} \text{ for } \beta\to\infty$$

easy, but not as efficient as direct search!

- Trotter error can be taken to zero. Problem is: can we compress? depends on entanglement in $|\psi(t)\rangle$

worst case: global quench $\hat{H}\to\hat{H}'$ then $S(t)\le S(0)+\text{cst}\cdot t$

$\Rightarrow \underline{D(t)\le D(0)\cdot e^{\text{cst}\cdot t}}$ exp. growth of resource

For $e^{-iHt}\hat{O}|\psi\rangle$ only polynomial growth in t

no growth for adiabatic evolution: stay in GS set

Mixed states: finite temperatures

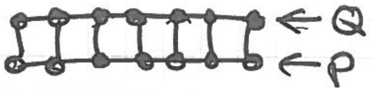
purification $|\psi\rangle_{AB} = \sum s_a |a\rangle_A |a\rangle_B \rightarrow \hat\rho_A = \sum s_a^2 |a\rangle_A \langle a|_A$

now inverse:

$$\hat\rho_P = \sum s_a^2 |a\rangle_P \langle a|_P \longrightarrow |\psi\rangle_{PQ} = \sum s_a |a\rangle_P |a\rangle_Q \Big| \rho_P = \mathrm{tr}|\psi\rangle\langle\psi|_{PQ}$$

phys system

aux system: easiest choice: copy of P

chain:  turns into ladder 

Can recycle code for states.

BUT: how do we know $\hat\rho_\beta$ to purify it?

thermal states: $\hat\rho_\beta = \frac{1}{Z(\beta)} e^{-\beta\hat H}$ $\quad Z(\beta) = \mathrm{tr}\, e^{-\beta\hat H}$

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

$$\hat I_{id} = Z(0)\hat\rho_0 \quad (\text{density op at } T=\infty)$$

assume purification of $\hat\rho_0$ $\Leftarrow$ is $|\psi_0\rangle$:

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

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

$|\psi_\beta\rangle = e^{-\beta\hat H/2}|\psi_0\rangle$ by tDMRG for imag. time!

$$\langle\hat O\rangle_\beta = \mathrm{tr}_P \hat O\hat\rho_\beta = \frac{Z(0)}{Z(\beta)} \mathrm{tr}_P\, \hat O\, \mathrm{tr}_Q |\psi_\beta\rangle\langle\psi_\beta|$$

$$= \frac{Z(0)}{Z(\beta)} \langle\psi_\beta|\hat O|\psi_\beta\rangle$$

$$1 \overset{!}{=} \langle\hat I\rangle_\beta = \frac{Z(0)}{Z(\beta)}\langle\psi_\beta|\psi_\beta\rangle$$

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

as always.... !

Last ingredient: purification of $\hat{\rho}_0 = Z^{-1}(0)\hat{I}$:

$Z(0) = d^L$.

$$\hat{\rho}_0 = \frac{1}{d^L}\hat{I} = \left(\frac{1}{d}I\right)^{\otimes L}$$ (factorizes)

purify <u>local</u> mixed state.

Example: spin-$\frac{1}{2}$:

$$\hat{\rho}_0 = \frac{1}{\sqrt{Q}}\left(|\uparrow_p\rangle\langle\uparrow_p| + |\downarrow_p\rangle\langle\downarrow_p|\right)$$

$$\Rightarrow |\Psi_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow_P\uparrow_Q\rangle + |\downarrow_P\downarrow_Q\rangle\right)$$ (check!)

<u>maximally entangled state</u>

gauge freedom: any max. entangled state will do:

$$|\tilde{\Psi}_0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right),$$

$$\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$ (best for conserved quantum numbers)