1. Original formulation of DMRG

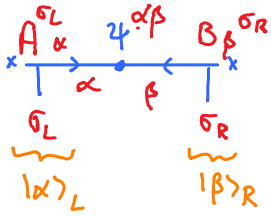
[White1992], [White1993], [Schollwöck2011, Sec 2.2]

Goal: finding ground state of infinite chain

Infinite-size DMRG (iDMRG)

Diagonalize small system (e.g. 2 sites), write ground state in the form

$$|\psi\rangle = \sum_{\alpha\beta} |\beta\rangle_R |\alpha\rangle_L \psi^{\alpha\beta}$$

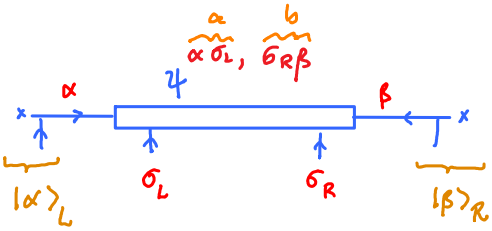


'Block L' describes left part of system, with basis $\{|\alpha\rangle_L\}$

'Block R' describes right part of system, with basis $\{|\beta\rangle_R\}$

Now add two sites between blocks L and R, and seek new ground state of the form

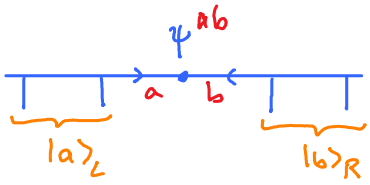
$$|\psi\rangle = |\beta\rangle_R |\sigma_R\rangle |\sigma_L\rangle |\alpha\rangle_L \psi^{\alpha\sigma_L,\sigma_R\beta}$$



by minimizing (Lanzcos) $\dfrac{\langle\psi|\hat{H}_{L\bullet R}|\psi\rangle}{\langle\psi|\psi\rangle}$

Split enlarged system in the middle, and call left side (new) block L, right side (new) block R.
Write ground state in the form

$$|\psi\rangle = |b\rangle_R |a\rangle_L \psi^{a,b}$$



with composite indices $a = (\alpha, \sigma_L), b = (\beta, \sigma_R)$

of dimension $D_a = D_\alpha d$. White's truncation prescription: compute reduced DM of $L\bullet$

$$\rho_{L\bullet} = \mathrm{Tr}_{\bullet R} |\psi\rangle\langle\psi| = |a'\rangle_L \underbrace{\psi^{a'b'} \overline{\psi}_{b'a}}_{(\rho_{L\bullet})^{a'}{}_a} {}_L\langle a| = \sum_c |\tilde{c}\rangle_L \rho_c {}_L\langle\tilde{c}|$$

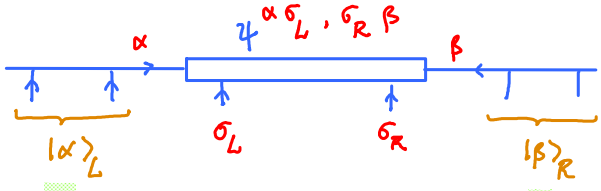
diagonalize

Construct truncated basis for block L , using the D eigenvectors $|\tilde{c}\rangle_L$ with the largest eigenvalues ρ_c . Rename: $|\alpha\rangle_L^{new} \equiv |\tilde{c}\rangle_L$.

here truncation happens

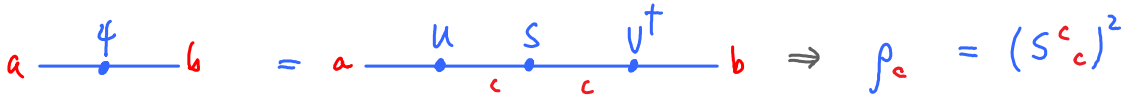
Ditto for block R.

Then iterate,: add two more sites, etc.



$|\alpha\rangle_L$ U_L U_R $|\beta\rangle_R$

Remark: we established early on (see MPS-I.4) that the eigenvalues ρ_c of reduced density matrix of L, are obtained by SVD of ψ^{ab}



So retaining the ρ_L-eigenstates with largest ρ_c is equivalent to just doing SVD-truncation on ψ^{ab}.

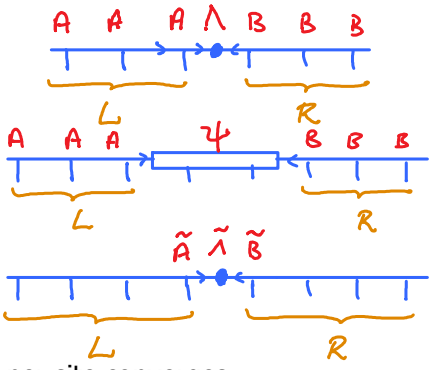
Modern formulation

Start with MPS in bond-canonical form:

Add two central sites and find ground state (Lanczos):

Do SVD to split chain into two larger blocks, and truncate:

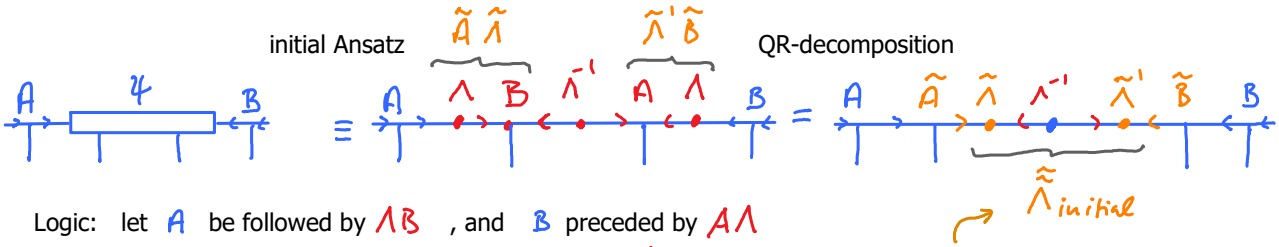
$\psi = U S V^\dagger = \tilde{A}\,\tilde{\Lambda}\,\tilde{B}$



Iterate: make chain longer and longer, until ground state energy per site converges.

'iDMRG state prediction' [McCulloch2008], [Schollwöck2011, Sec. 10.1]

To speed up Lanczos search for ground state, construct initial guess for ψ from previous data:



Logic: let A be followed by ΛB, and B preceded by $A\Lambda$

to reverse arrows between B and A, use Λ^{-1}

use this to initialize Lanczos

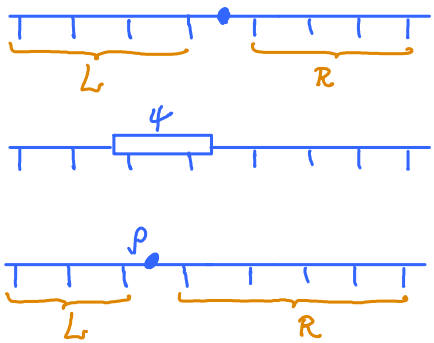
This leads to 'dramatic speedup' of iDMRG.

Finite-size DMRG

Grow chain to some length N using infinite-size DMRG algorithm.

Then reduce L, enlarge R, optimize ψ:

Diagonalize ρ_L, truncate.



Iterate: sweep back and forth until convergence.

This is conceptually identical to variational optimization with two-site update.

Single-site DMRG is also possible ⟷ variational single-site update.

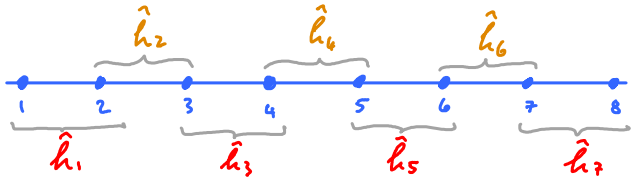
2. Time-dependent DMRG (tDMRG) [Daley2004], [White2004]

Invented 2004 by Daley, Kollath, Schollwöck, Vidal, and independently by White, Feiguin.

Goal: to compute $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi\rangle$ (1)

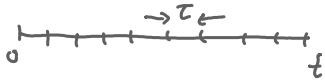
Time-evolution operator for nearest-neighbor interactions (cf. iTEBD.1)

Even-odd decomposition of Hamiltonian:



$$\hat{H} = \sum_\ell \hat{h}_\ell = \hat{H}_o + \hat{H}_e \quad (2)$$

Trotterize: $t = \tau N_t$

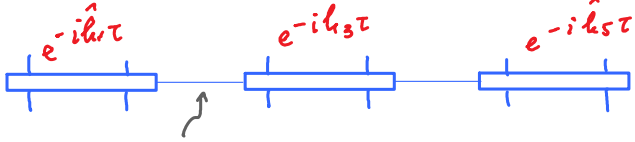


$$\hat{U}(t) = e^{-i\hat{H}t} = (e^{-i\tau(\hat{H}_o+\hat{H}_e)})^{N_t} \simeq (\underbrace{e^{-i\tau\hat{H}_e}}_{\hat{U}_e}\underbrace{e^{-i\tau\hat{H}_o}}_{\hat{U}_o} + \mathcal{O}(\tau^2))^{N_t} \quad (3)$$

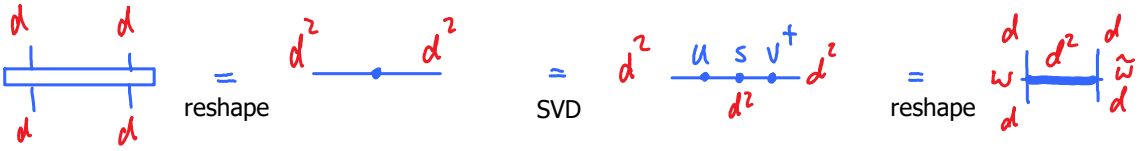
Time-evolution protocol [Schollwöck2011, Sec. 7.1-7.3]

Construct MPO representations for U_o and U_e, compute $|\psi(t+\tau)\rangle = \hat{U}_e\hat{U}_o|\psi(t)\rangle$ (4)

(i) MPO $\hat{U}_o =$ (5)



bond dimension = 1, so consider factors separately



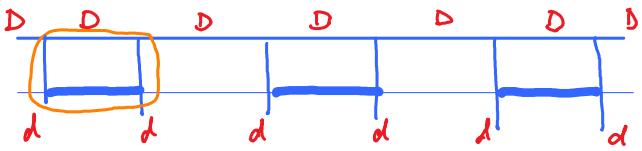
(6)

$$O^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2} = W^{\sigma_1'}_{\sigma_1\mu}\tilde{W}^{\mu\,\sigma_2'}_{\sigma_2}, \quad \mu = 1,\dots d^2 \quad (7)$$

can be constructed explicitly — then SVD to yield

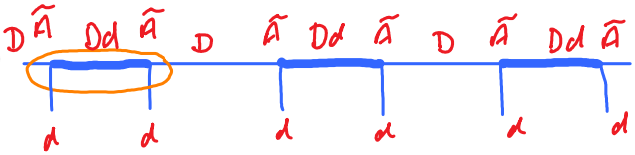
(ii) Evolve

$|\psi_o(t+\tau)\rangle = \hat{U}_o|\psi(t)\rangle =$



(8)

reshape, SVD =



(9)

(iii) Compress: either 'variationally' (global) or 'bond by bond' (local)

Variational compression: First apply full MPO for $\hat{U}_o$ to entire chain. Then variationally minimize

Variational compression: First apply full MPO for $\hat{U}_0$ to entire chain. Then variationally minimize

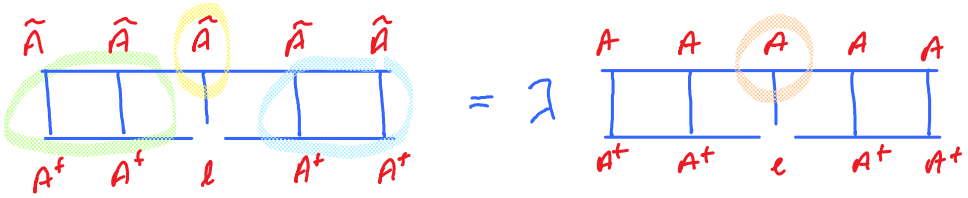
$$\| |\psi(t+\tau)\rangle - |\psi_{compressed}\rangle \|^2 \qquad (10)$$

bond dimension $D \cdot d$; D

. This yields optimal (in variational sense) way to compress $|\psi_{target}\rangle$ to $|\psi_{compressed}\rangle$ with given resources.

Explicitly:

$$\frac{\partial}{\partial A^\dagger_{[e]}} \left[\langle \psi_{compressed} | \psi_{target} \rangle - \lambda \langle \psi_{compressed} | \psi_{compressed} \rangle \right] \qquad (11)$$



(12)

$$L \tilde{A} R = \lambda A \qquad (13)$$

[λ is fixed by normalization condition:]

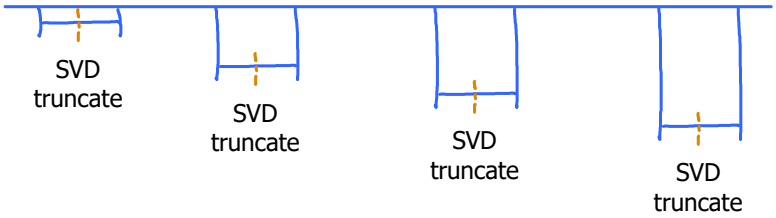
Sweep back and forth, until overlap $\langle \psi_{compressed} | \psi_{target} \rangle$ no longer changes.

Bond by bond compression

Apply U_0 to bond 1-2,

then reshape, SVD, truncate;

repeat for bond 3-4, then 5-6, etc.



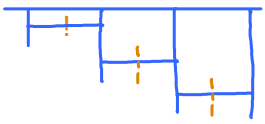
This protocal keeps bond dimensions low throughout, hence is cheaper. However, some interdependence of successive truncations may creep in, hence variational compression is, strictly speaking, cleaner.

The difference between variational and bond-by-bond compression strategies becomes negligible for sufficiently small τ , because then the state does not change much during a time step anyway, so trunctations are benign.

With bond-to-bond compression, there is no need to split $\hat{H} = \hat{H}_o + \hat{H}_e$, $\hat{U} = \hat{U}_e \cdot \hat{U}_o$ (14)

Instead, Trotterize as follows:

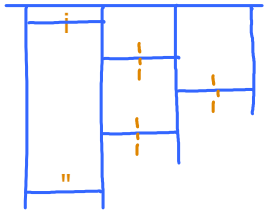
$$e^{-i\hat{H}\tau} = e^{-i\hat{h}_{N-1}\tau} \cdots e^{-i\hat{h}_2\tau} e^{-i\hat{h}_1\tau} + O(\tau^2) \qquad (15)$$



1st order Trotter

or

$$e^{-i\hat{H}\tau} = \left(e^{-i\hat{h}_1\tau/2} e^{-i\hat{h}_2\tau/2} \cdots e^{-i\hat{h}_{N-2}\tau/2}\right) e^{-i\hat{h}_{N-1}\tau} \left(e^{-i\hat{h}_{N-1}\tau/2} \cdots e^{-i\hat{h}_2\tau/2} e^{-i\hat{h}_1\tau/2}\right) + O(\tau^3) \qquad (16)$$



2nd order Trotter

Error analysis

$\varepsilon_{Trotter}$ = (error per step) (# of steps) = $\tau^{n+1} \frac{t}{\tau} = \tau^n t$ (17)

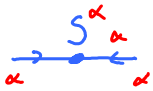
(for nth order Trotter scheme)

linear in time; controllable by reducing τ

Truncation error due to truncation of bond dimensions:

$\varepsilon_{trunc} \sim e^{\# t}$, grows exponentially! (until you 'hit the wall')

Reason: under time evolution, state becomes increasingly more entangled; on a bond



entanglement entropy is

$$S_E = -\sum_\alpha (S^\alpha{}_\alpha)^2 \ln (S^\alpha{}_\alpha)^2 \quad (18)$$

This is maximal if all singular values on bond are equal, $(S^\alpha{}_\alpha)^2 = \frac{1}{D}$, $\Rightarrow S_E \leq \ln_2 D$ (19)

If Hamiltonian $H(t)$ is changed abruptly (quench) such that global energy changes extensively, then

$$S(t) \leq S(0) + c\,t \quad (20)$$

[For less dramatic changes (e.g. local perturbation), entanglement growth is slower; but still significant.]

Bond dimension needed to encode entanglement entropy S_E is given by $D(t) \gtrsim 2^{S(t)}$ (21)

If, however, bond dimension D is held fixed during time evolution, errors will grow exponentially.

A quantitative error analysis has been performed by [Gobert2005] on the exactly solvable XX model:

[Gobert2005]

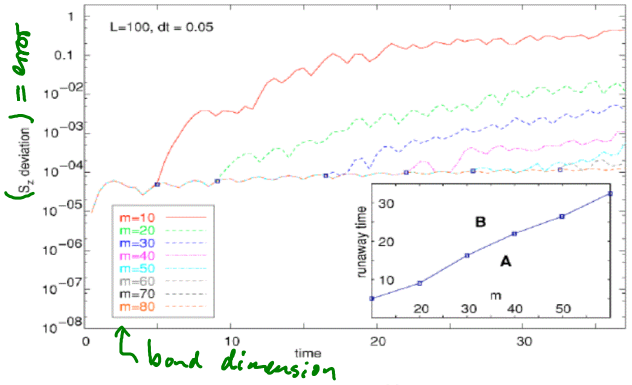


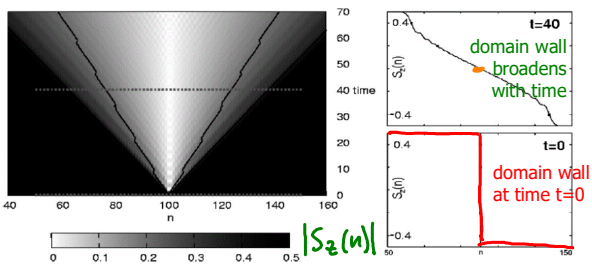
FIG. 6. Magnetization deviation $\Delta M(t)$ as a function of time for different numbers m of DMRG states. The Trotter time interval is fixed at dt=0.05. Again, two regimes can be distinguished: For early times, for which the Trotter error dominates, the error is slowly growing (essentially linearly) and independent of m (regime A); for later times, the error is entirely given by the truncation error, which is m-dependent and growing fast (almost exponential up to some saturation; regime B). The transition between the two regimes occurs at a well-defined "runaway time" t_R (small squares). The inset shows a monotonic, roughly linear dependence of t_R on m.

$$H_{XX} = J \sum_\ell S^x_{[\ell]} S^x_{[\ell+1]} + S^y_{[\ell]} S^y_{[\ell+1]} \quad (22)$$

They performed quench, with initial state

$|\psi\rangle_{J=0} = \uparrow\uparrow\uparrow\uparrow\,!\,\downarrow\downarrow\downarrow\downarrow$

For $t>0$: $J \neq 0$, domain wall widens…



3. Finite temperature: purification [Verstraete2004b], [Schollwöck2011, Sec. 7.2.1]

General quantum-mechanical density matrix for a mixed state, $\hat{\rho} = \sum_{\mu\nu} |\mu\rangle_p \rho^{\mu}{}_{\nu} {}_p\langle\nu|$ (1)

'p' denotes 'physical'

has three defining properties:

(i) Hermiticity: $\hat{\rho}^\dagger = \hat{\rho}$ (2)

(ii) Positivity: Eigenvalues are non-~~zero~~ negative: $\hat{\rho}_{\text{diagonalized}} = \sum_\alpha |\alpha\rangle_p \rho_\alpha {}_p\langle\alpha|$ (3), $\rho_\alpha \geq 0$

(iii) Normalized: $\mathrm{Tr}\,\hat{\rho} = 1 \Rightarrow \sum_\alpha \rho_\alpha = 1$ (4)

Expectation values: $\langle\hat{O}\rangle = \mathrm{Tr}(\hat{\rho}\hat{O})$ (5)

[or $\frac{\mathrm{Tr}(\hat{\rho}\hat{O})}{\mathrm{Tr}(\hat{\rho})}$ if one works with non-normalized $\hat{\rho}$]

'Purification'

Can we represent $\hat{\rho}$ in terms of a pure state?

Yes: double Hilbert space by introducing an 'auxiliary' state for each physical state, and define

'purified state': $|\Psi\rangle = \sum_\alpha |\alpha\rangle_a |\alpha\rangle_p \sqrt{\rho_\alpha} \in \mathcal{H}_a \otimes \mathcal{H}_p$ (6)

auxiliary, physical

This can be viewed as Schmidt decomposition of a pure state in doubled Hilbert space.

Norm yields trace: $\langle\Psi|\Psi\rangle = \sum_{\alpha\alpha'} \sqrt{\rho_{\alpha'}} {}_p\langle\alpha'| {}_a\langle\alpha'|\alpha\rangle_a |\alpha\rangle_p \sqrt{\rho_\alpha} = \sum_\alpha \rho_\alpha = \mathrm{Tr}\,\hat{\rho}_p$ (7), $\langle\alpha'|\alpha\rangle_a = \delta^{\alpha'}_{\alpha}$

Tracing out auxiliary state space from $|\Psi\rangle\langle\Psi|$ (a pure DM in doubled Hilbert space) (7)

yields physical density matrix $\hat{\rho}_p$ (a mixed DM in physical Hilbert space):

$$\mathrm{Tr}_a |\Psi\rangle\langle\Psi| = \sum_\beta \sum_{\alpha'\alpha} {}_a\langle\beta|\alpha'\rangle_a |\alpha'\rangle_p \sqrt{\rho_{\alpha'}} \sqrt{\rho_\alpha} {}_p\langle\alpha| {}_a\langle\alpha|\beta\rangle_a \quad (8)$$

$\langle\beta|\alpha'\rangle_a = \delta^{\beta}_{\alpha'}$, $\langle\alpha|\beta\rangle_a = \delta^{\alpha}_{\beta}$

$$= \sum_\alpha |\alpha\rangle_p \rho_\alpha {}_p\langle\alpha| = \hat{\rho}_p \quad (9)$$

Purified-state expectation values in doubled Hilbert space yield thermal averages in physical space:

$$\langle\Psi| \mathbb{1}_a \otimes \hat{O}_p |\Psi\rangle = \sum_{\alpha'\alpha} \sqrt{\rho_{\alpha'}} {}_a\langle\alpha'| {}_p\langle\alpha'| \mathbb{1}_a \otimes \hat{O}_p |\alpha\rangle_p |\alpha\rangle_a \sqrt{\rho_\alpha} \quad (10)$$

$\langle\alpha'|\alpha\rangle_a = \delta^{\alpha'}_{\alpha}$

$$= \sum_\alpha \langle\alpha|\hat{O}|\alpha\rangle \rho_\alpha = \mathrm{Tr}_p\left(\hat{\rho}_p \hat{O}_p\right) = \langle\hat{O}_p\rangle \quad (11)$$

If $\hat{\rho}$ is not normalized, use $\langle\Psi| \mathbb{1}_a \otimes \hat{O}_p |\Psi\rangle$ $\mathrm{Tr}\,\hat{\rho}\,\hat{O}_p$

If $\hat{\rho}$ is not normalized, use $$\frac{\langle \Psi | \mathbb{1}_a \otimes \hat{O}_p | \Psi \rangle}{\langle \Psi | \Psi \rangle} = \frac{\mathrm{Tr}\, \hat{\rho}_p \hat{O}_p}{\mathrm{Tr}\, \hat{\rho}_p} = \langle \hat{O}_p \rangle \qquad (12)$$

Thermal density matrix

Thermal equilibrium is described by $$\hat{\rho}_\beta = e^{-\beta \hat{H}_p} = \sum_\alpha |\alpha\rangle_p\, e^{-\beta E_\alpha}\, {}_p\langle \alpha| \qquad (13)$$

Not normalized: $$\mathrm{Tr}_p\, \hat{\rho}_\beta = \sum_\alpha e^{-\beta E_\alpha} = Z(\beta) = \text{partition function} \neq 1 \qquad (14)$$

Purified version: $$|\Psi_\beta\rangle = \sum_\alpha |\alpha\rangle_a |\alpha\rangle_p\, e^{-\beta E_\alpha/2} = e^{-\beta \hat{H}_p/2} \underbrace{\sum_\alpha |\alpha\rangle_a |\alpha\rangle_p}_{\equiv |\Psi_0\rangle} \qquad (15)$$

($e^{-\beta \hat{H}_p/2}$ acts only on physical space!)

$$|\Psi_0\rangle = \sum_{\vec{\sigma}} |\vec{\sigma}\rangle_a |\vec{\sigma}\rangle_p = \sum_{\vec{\sigma}} |\sigma_N\rangle_a |\sigma_N\rangle_p \ldots |\sigma_1\rangle_a |\sigma_1\rangle_p = \prod_{\ell=1}^{N} \underbrace{\left(\sum_{\sigma_\ell} |\sigma_\ell\rangle_a |\sigma_\ell\rangle_p \right)}_{\text{maximal a-p entanglement}} \qquad (16)$$

= product state, with each factor describing maximal a-p entanglement at site ℓ

Note: at $T = \infty$, i.e. $\beta = 0$, we have $|\Psi_\infty\rangle = |\Psi_0\rangle$ (all states $|\vec{\sigma}\rangle$ are equally likely).

Check: ($\sum_{\vec{\sigma}\vec{\sigma}'} \delta_{\vec{\sigma}\vec{\sigma}'}$)

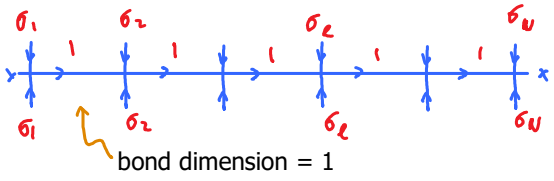
$$\langle \Psi_\beta | \hat{O}_p | \Psi_\beta \rangle = \sum_{\vec{\sigma}\vec{\sigma}'} {}_a\langle \vec{\sigma}| {}_p\langle \vec{\sigma}|\, e^{-\beta \hat{H}_p/2}\, \hat{O}_p\, e^{-\beta \hat{H}_p/2}\, |\vec{\sigma}'\rangle_p |\vec{\sigma}'\rangle_a$$

$$= \sum_{\vec{\sigma}} {}_p\langle \vec{\sigma}|\, e^{-\beta \hat{H}_p/2}\, \hat{O}_p\, e^{-\beta \hat{H}_p/2}\, |\vec{\sigma}\rangle_p$$

$$= \mathrm{Tr}\left[e^{-\beta \hat{H}/2}\, \hat{O}\, e^{-\beta \hat{H}/2} \right] = \mathrm{Tr}\, \hat{\rho}_p \hat{O}_p \quad \checkmark$$

Protocol for finite-T DMRG calculations

Start from pure product state in doubled Hilbert space:



(17)

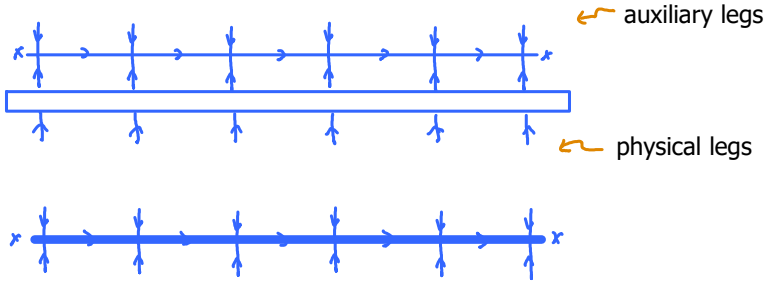
Perform imaginary-time evolution over a 'time' , acting only on physical space:

$$|\Psi_\beta\rangle = e^{-\beta \hat{H}_p/2} |\Psi_0\rangle =$$

(Trotterize…)

compress

$\simeq$



For thermal averages, trace out auxiliary space:

$$\langle \hat{O}_{[\ell]_p} \rangle = \frac{\langle \Psi_\beta | \mathbb{1}_a \otimes \hat{O}_p | \Psi_\beta \rangle}{\langle \Psi_\beta | \Psi_\beta \rangle} =$$