1. Time-dependent DMRG (tDMRG)

[Daley2004], [White2004]

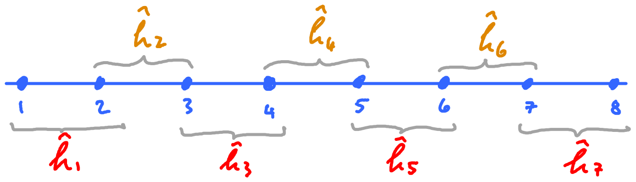
Invented 2004 by Daley, Kollath, Schollwöck, Vidal, and independently by White, Feiguin.

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

Time-evolution operator for nearest-neighbor interactions

(cf. iTEBD.1)

Even-odd decomposition of Hamiltonian:



$$\hat{H} = \sum_\ell \hat{h}_\ell = \hat{H}_o + \hat{H}_e \tag{2}$$

Trotterize: $t = \tau N_t$

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

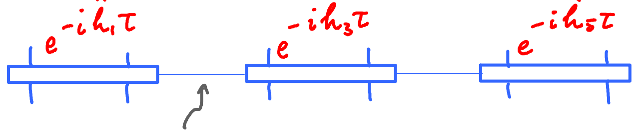
Time-evolution protocol

[Schollwöck2011, Sec. 7.1-7.3]

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

(i) MPO

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



bond dimension = 1, so consider factors separately

(6)

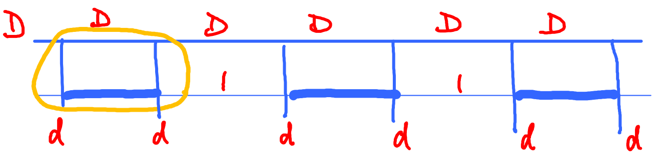
$$O^{\sigma_1'\sigma_2'}_{\sigma_1\sigma_2} = W^{\sigma_1'}_{\sigma_1\mu}\tilde{W}^{\mu\sigma_2'}_{\sigma_2}, \quad \mu = 1,\dots,d^2 \tag{7}$$

can be constructed explicitly

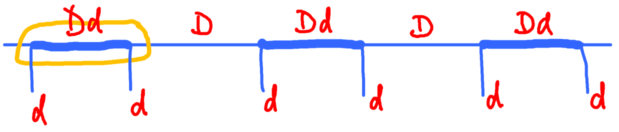
then SVD to yield

(ii) Evolve

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

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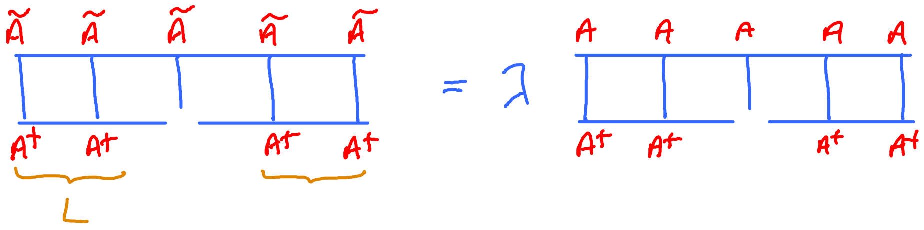
$$\| \underset{\text{target}}{|\psi(t+\tau)\rangle} - |\psi_{\text{compressed}}\rangle \|^2 \quad (10)$$

bond dimension $D \cdot d$ D

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

Explicitly:

$$\frac{\partial}{\partial A^{\dagger}_{[\ell]}}\Big[\langle \overset{A^\dagger A^\dagger A^\dagger}{\psi_{\text{compressed}}} | \overset{\tilde{A}\,\tilde{A}\,\tilde{A}}{\psi_{\text{target}}}\rangle - \lambda \langle \overset{A^\dagger A^\dagger A^\dagger}{\psi_{\text{compressed}}} | \overset{A\,A\,A}{\psi_{\text{compressed}}}\rangle\Big] = 0 \quad (11)$$



(12)

$$L \tilde{A} R = \lambda A$$

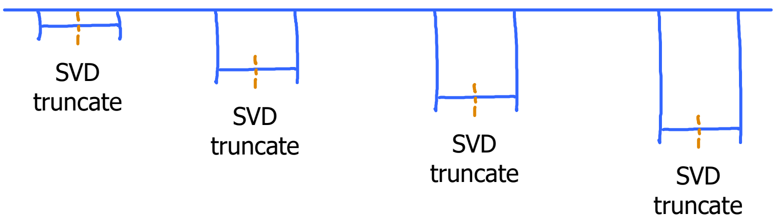
[λ is fixed by normalization condition: $A^{\dagger}_{\sigma} A^{\sigma} = \mathbb{1}$] (13)

Sweep back and forth, until overlap $\langle \psi_{\text{compressed}} | \psi_{\text{target}} \rangle$ no longer changes. Then apply $\hat{U}_e$.

<u>Bond by bond compression</u>

Apply $\hat{U}_o$ to bond 1-2,

then reshape, SVD, truncate;
repeat for bond 3-4, then 5-6, etc.



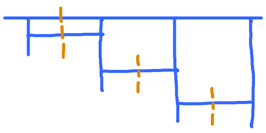
This protocal keeps bond dimensions low throughout, hence is cheaper. However, some interdependence of successive truncations may creep in, hence variational compression is, strictly speaking, cleaner.

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 truncations 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:

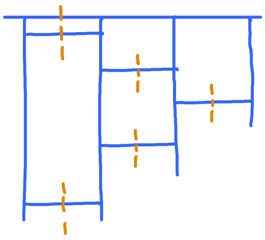
$$e^{-i\hat{H}\tau} = e^{-i\hat{h}_{N-1}\tau} \cdots e^{-i\hat{h}_2\tau} e^{-i\hat{h}_1\tau} + \mathcal{O}(\tau^2) \quad (15)$$



1st order Trotter

or

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



2nd order Trotter

Error analysis

for nth order Trotter scheme

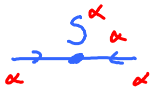
$$\varepsilon_{\text{Trotter}} = \text{(error per step) (\# of steps)} = \tau^{n+1} \frac{t}{\tau} = \tau^{n} t \qquad (17)$$

linear in time; controllable by reducing τ

Truncation error due to truncation of bond dimensions:

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

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



entanglement entropy is

$$S_E = -\sum_\alpha (S^\alpha_\alpha)^2 \ln (S^\alpha_\alpha)^2 \qquad (18)$$

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

$$S(t) \leq S(0) + ct \qquad (20)$$

[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]

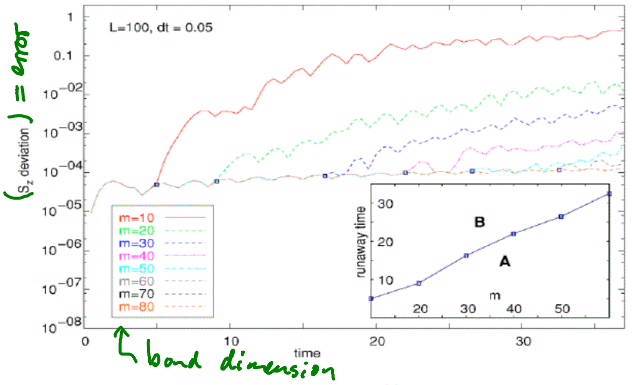


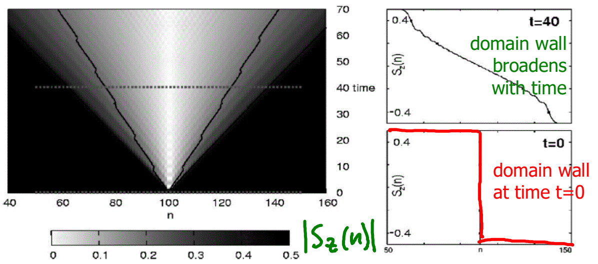
FIG. 6. Magnetization deviation $\Delta M(t)$ as a function of time for different numbers m of DMRG states. The Trotter time interval is fixed at dt=0.05. Again, two regimes can be distinguished: For early times, for which the Trotter error dominates, the error is slowly growing (essentially linearly) 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.

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

They performed quench, with initial state

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

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



2. Finite temperature: purification

[Verstraete2004b], [Schollwöck2011, Sec. 7.2.1]

$\boxed{\text{DMRG-III.2}}$

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

'p' denotes 'physical'

has three defining properties:

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

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

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

Expectation values: $\langle \hat{O} \rangle = \mathrm{Tr}(\hat{\rho}\,\hat{O})$ [or $\dfrac{\mathrm{Tr}(\hat{\rho}\,\hat{O})}{\mathrm{Tr}(\hat{\rho})}$ if one works with non-normalized $\hat{\rho}$] (5)

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

auxiliary physical

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

Norm yields trace: $\langle \Psi | \Psi \rangle = \sum_{\alpha'\alpha} \sqrt{\rho_{\alpha'}} \, {}_p\langle\alpha'| \underbrace{{}_a\langle\alpha'|\alpha\rangle_a}_{\mathbb{1}^{\alpha'}{}_{\alpha}} |\alpha\rangle_p \sqrt{\rho_\alpha} = \sum_\alpha \rho_\alpha = \mathrm{Tr}\,\hat{\rho}_p$ (7)

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):

$$\mathrm{Tr}_a |\Psi\rangle\langle\Psi| = \sum_\beta \sum_{\alpha'\alpha} \underbrace{{}_a\langle\beta|\alpha'\rangle_a}_{\mathbb{1}^{\beta}{}_{\alpha'}} |\alpha'\rangle_p \sqrt{\rho_{\alpha'}}\sqrt{\rho_\alpha} \, {}_p\langle\alpha| \underbrace{{}_a\langle\alpha|\beta\rangle_a}_{\mathbb{1}^{\alpha}{}_{\beta}} \qquad (8)$$

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

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

$$\langle \Psi | \mathbb{1}_a \otimes \hat{O}_p | \Psi \rangle = \sum_{\alpha'\alpha} \sqrt{\rho_{\alpha'}} \, {}_p\langle\alpha'| \underbrace{{}_a\langle\alpha'| \mathbb{1}_a \otimes \hat{O}_p |\alpha\rangle_a}_{\delta^{\alpha'}{}_{\alpha}} |\alpha\rangle_p \sqrt{\rho_\alpha} \qquad (10)$$

$$= \sum_\alpha {}_p\langle\alpha| \hat{O} |\alpha\rangle_p \, \rho_\alpha = \mathrm{Tr}_p \, \hat{\rho}_p \hat{O}_p = \langle \hat{O}_p \rangle \qquad (11)$$

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

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: $\mathrm{Tr}_p\, \hat\rho_\beta = \sum_\alpha e^{-\beta E_\alpha} = Z(\beta) =$ partition function $\neq 1$ (14)

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

acts only on physical space!

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

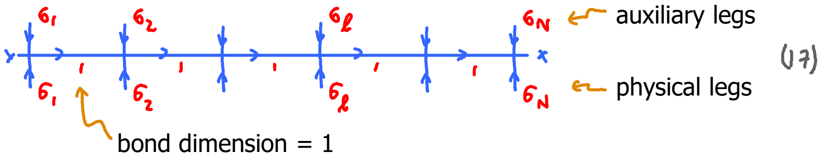
$=$ product state, with each factor describing maximal aux-phys entanglement at site ℓ

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

Check: $$\langle\Psi_\beta|\hat O_p|\Psi_\beta\rangle = \sum_{\vec\sigma\vec\sigma'} \underbrace{{}_a\langle\vec\sigma|\, {}_p\langle\vec\sigma| e^{-\beta\hat H_p/2}\, \hat O_p\, e^{-\beta \hat H_p/2}|\vec\sigma'\rangle_p |\vec\sigma'\rangle_a}_{\delta_{\vec\sigma\vec\sigma'}}$$
$$= \sum_{\vec\sigma} {}_p\langle\vec\sigma| e^{-\beta\hat H_p/2}\, \hat O_p\, e^{-\beta\hat H_p/2}|\vec\sigma\rangle_p$$
$$= \mathrm{Tr}\{e^{-\beta\hat H_p/2}\, \hat O_p\, e^{-\beta\hat H_p/2}] = \mathrm{Tr}[\hat\rho_p\hat O_p] \quad ✓$$

Protocol for finite-T DMRG calculations

Start from pure product state in doubled Hilbert space: $|\Psi_0\rangle =$



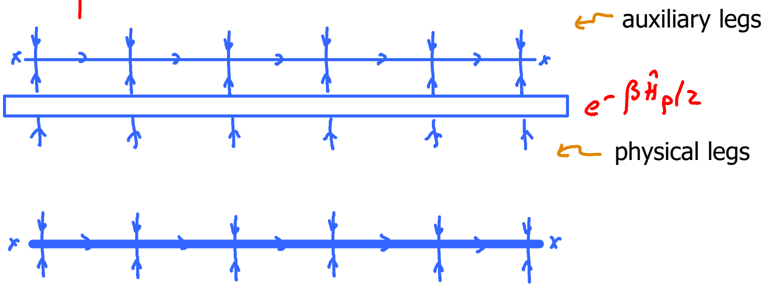
(17)

Perform imaginary-time evolution over a 'time' $\beta/2$, 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:

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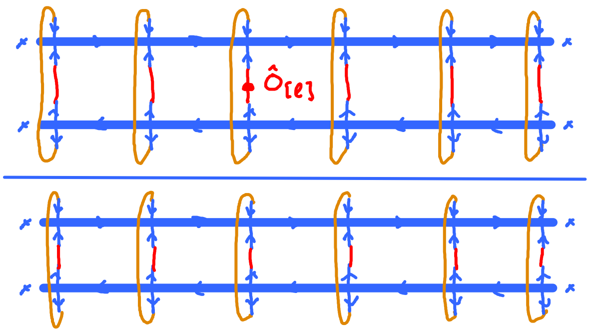
$$\langle \hat{O}_{[\ell]P} \rangle = \frac{\langle \Psi_\beta | \mathbb{1}_a \otimes \hat{O}_P | \Psi_\beta \rangle}{\langle \Psi_\beta | \Psi_\beta \rangle} =$$



3. Exponential thermal renormalization group (XTRG)

[Chen2018a]

Goal: computation of the thermal density matrix, $\hat\rho(\beta) = e^{-\beta\hat H}$, $\beta = 1/T$ (1)

for arbitrary temperature T , in particular large to intermediate T , (i.e. small to intermediate β)

Once $\hat\rho$ is known, thermal expectation values follow from $\langle\hat O\rangle_\beta = \mathrm{Tr}\,[\hat\rho(\beta)\,\hat O]$ (2)

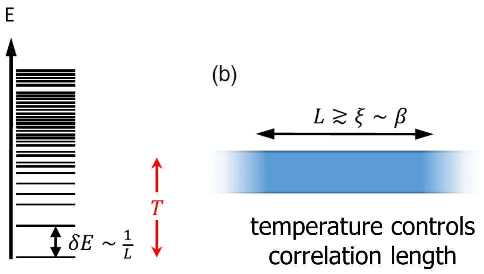
Further application: to obtain ground state projector, take $\beta \to \infty$.

One option: imaginary time evolution with Trotter decomposition, $\hat\rho(\beta) = \left[e^{-\tau\hat H}\right]^N$, $\tau = \beta/N$

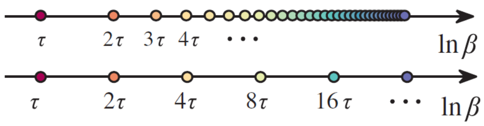
However, then number of time steps increases linearly with β , so reaching low T is numerically costly.

Key observation 1: If $\hat\rho(\beta)$ is represented as an MPO, the MPO entanglement entropy grows only logarithmically with decreasing temperature: [Barthel2017], [Dubail2017]

$S_E(\beta) \sim \ln(\beta)$ (for 1D systems) (4)



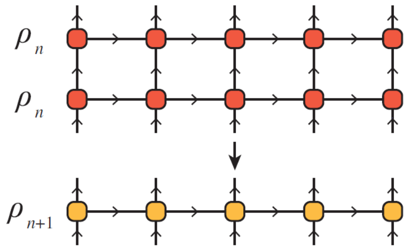
Thus, seek algorithm which lowers temperature in exponential steps!



Key observation 2: multiplying the density matrix by itself lowers the temperature by a factor of 2 :

$$e^{-2\beta\hat H} = e^{-\beta\hat H}\cdot e^{-\beta\hat H} \qquad (3)$$

$$\Rightarrow \quad \boxed{\hat\rho(2\beta) = \hat\rho(\beta)\,\hat\rho(\beta)} \qquad (4)$$



XTRG algorithm exploits this:

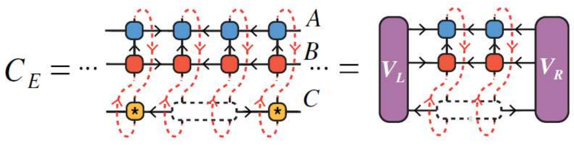
(i) Initialize density matrix at very high temperature, as an MPO (with small bond dimension):

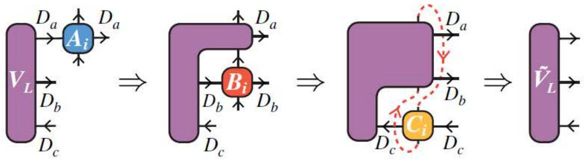
$$\hat\rho(\beta_0) \simeq 1 - \beta_0\hat H \; , \quad \beta_0 \simeq 10^{-6} \qquad (5)$$

(ii) Compute $\hat\rho^\dagger(\beta)\,\hat\rho(\beta)$ via MPO multiplication.

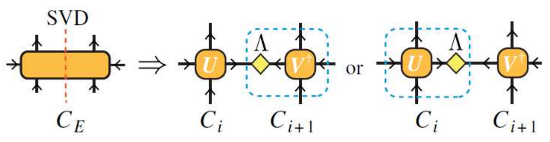
(iii) Reduce bond dimension by global variational optimization:

$$\frac{\partial}{\partial C^\dagger_{[\ell+1]}}\frac{\partial}{\partial C^\dagger_{[\ell]}} \Big\| \underbrace{\underset{\hat\rho^\dagger(\beta)}{A}\cdot\underset{\hat\rho(\beta)}{B}}_{\text{(fat) input MPO, large bond dim}} - \underset{\substack{\hat\rho(2\beta)\\ \text{compressed MPO,}\\ \text{smaller bond dim.}}}{C} \Big\|^2_{\underset{\text{Frobenius norm}}{F}} = 0 \qquad (7)$$





Compute environment of bond to be updated iteratively, use SVD to bring updated MPO bond into canonical form.



Iterate (ii,iii) until desired temperature is reached.