DMRG: ground states, time evolution and spectral functions

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DMRG: a young adult

09.11.1992 S.R. White: *Density Matrix Formulation for Quantum Renormalization Groups* (PRL 69, 2863 (1992))

„This new formulation appears extremely powerful and versatile, and we believe it will become the leading numerical method for 1D systems; and eventually will become useful for higher dimensions as well.“

~2004 old insight „DMRG is linked to MPS (Matrix Product States)“ goes viral

Östlund, Rommer, PRL 75, 3537 (1995), Dukelsky, Martin-Delgado, Nishino, Sierra, EPL43, 457 (1998)

Vidal, PRL 93, 040502 (2004), Daley, Kollath, Schollwöck, Vidal, J. Stat. Mech. P04005 (2004), White, Feiguin, PRL 93, 076401 (2004), Verstraete, Porras, Cirac, PRL 93, 227205 (2004), Verstraete, Garcia-Ripoll, Cirac, PRL 93, 207204 (2004), Verstraete, Cirac, cond-mat/0407066 (2004)

reviews:

U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005) - „old“ statistical physics perspective, applications
U. Schollwöck, Ann. Phys. 326, 96 (2011) - „new“ MPS perspective, technical
F. Verstraete, V. Murg, J. I. Cirac, Adv. Phys. 57, 143 (2008) - as seen from quantum information

matrix product states: definitions

quantum system living on *L* lattice sites

d local states per site $\{\sigma_i\}$ $\quad i \in \{1, 2, \ldots, L\}$

example: spin 1/2: *d*=2 $\quad |\uparrow\rangle, |\downarrow\rangle$

Hilbert space:

$$\mathcal{H} = \otimes_{i=1}^{L} \mathcal{H}_i \qquad \mathcal{H}_i = \{|1_i\rangle, \ldots, |d_i\rangle\}$$

most general state (not necessarily 1D):

$$|\psi\rangle = \sum_{\sigma_1, \ldots, \sigma_L} c^{\sigma_1 \ldots \sigma_L} |\sigma_1 \ldots \sigma_L\rangle$$

abbreviations: $\{\sigma\} = \sigma_1 \ldots \sigma_L \qquad c^{\{\sigma\}}$

(matrix) product states

exponentially many coefficients!
standard approximation: mean-field approximation

$$c^{\sigma_1 \ldots \sigma_L} = c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L}$$

$d^L \to dL$ coefficients

often useful, but misses essential quantum feature: entanglement

consider 2 spin 1/2: $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ $\quad \mathcal{H}_i = \{|\uparrow_i\rangle, |\downarrow_i\rangle\}$

$$|\psi\rangle = c^{\uparrow\uparrow}|\uparrow\uparrow\rangle + c^{\uparrow\downarrow}|\uparrow\downarrow\rangle + c^{\downarrow\uparrow}|\downarrow\uparrow\rangle + c^{\downarrow\downarrow}|\downarrow\downarrow\rangle$$

singlet state: $|\psi\rangle = \frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle$ $\quad c^{\uparrow\downarrow} \neq c^{\uparrow}c^{\downarrow}$

generalize product state to matrix product state:

$$c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L} \to M^{\sigma_1} \cdot M^{\sigma_2} \cdot \ldots \cdot M^{\sigma_L}$$

matrix product states

useful generalization even for matrices of dimension 2:
AKLT (Affleck-Kennedy-Lieb-Tasaki) model

general matrix product state (MPS):

$$|\psi\rangle = \sum_{\sigma_1,\ldots,\sigma_L} M^{\sigma_1} M^{\sigma_2} \ldots M^{\sigma_L} |\sigma_1 \sigma_2 \ldots \sigma_L\rangle$$

matrix dimensions:

$$(1 \times D_1), (D_1 \times D_2), \ldots, (D_{L-2} \times D_{L-1}), (D_{L-1} \times 1)$$

non-unique: gauge degree of freedom

$$XX^{-1} = 1 \qquad M^{\sigma_i} \to M^{\sigma_i} X \qquad M^{\sigma_{i+1}} \to X^{-1} M^{\sigma_{i+1}}$$

matrix product states

Why are matrix product states interesting?

- any state can be represented as an MPS
  (even if numerically inefficiently)
- MPS are hierarchical: matrix size related to degree of entanglement
- MPS emerge naturally in renormalization groups
- MPS can be manipulated easily and efficiently
- MPS can be searched efficiently:
  which MPS has lowest energy for a given Hamiltonian?

singular value decomposition (SVD)

key workhorse of MPS manipulation and generally very useful!

general matrix *A* of dimension $(m \times n)$ $\qquad k = \min(m, n)$

then
$$A = USV^\dagger$$

with U dim. $(m \times k)$ $\quad U^\dagger U = I$ (ON col); if $m = k$: $UU^\dagger = I$

S dim. $(k \times k)$ diagonal: $s_1 \geq s_2 \geq s_3 \geq \ldots$ non-neg.: $s_i \geq 0$
singular values, non-vanishing = rank $r \leq k$

$V^\dagger$ dim. $(k \times n)$ $\quad V^\dagger V = I$ (ON row); if $k = n$: $VV^\dagger = I$

popular notation: (left) singular vectors $|u_i\rangle$

$$U = [|u_1\rangle|u_2\rangle \ldots]$$

SVD and EVD (eigenvalue decomp.)

singular value decomposition (always possible):

$$A = USV^\dagger \qquad s_1 \geq s_2 \geq s_3 \geq \ldots \qquad s_i \geq 0$$

eigenvalue decomposition (for special square matrices):

$$AU = U\Lambda \qquad \lambda_i \qquad U = [|u_1\rangle|u_2\rangle\ldots]$$ eigenvectors

connection by „squaring“ *A*: $A^\dagger A \qquad AA^\dagger$

$$AA^\dagger = USV^\dagger VSU^\dagger = US^2U^\dagger \Rightarrow (AA^\dagger)U = US^2$$

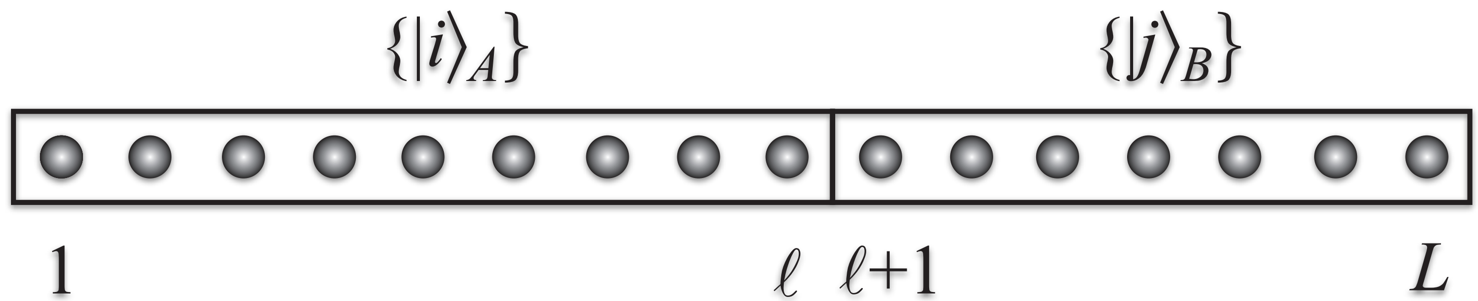
$$A^\dagger A = VSU^\dagger USV^\dagger = VS^2V^\dagger \Rightarrow (A^\dagger A)V = VS^2$$

eigenvalues = singular values squared
eigenvectors = left, right singular vectors

Schmidt decomposition

allows for direct readout of entanglement

bipartition of „universe“ AB into subsystems A and B:



$$|\psi\rangle = \sum_{i=1}^{\dim \mathcal{H}_A} \sum_{j=1}^{\dim \mathcal{H}_B} \psi_{ij} |i\rangle_A |j\rangle_B$$

read coefficients as matrix entries, carry out SVD:

$$|\psi\rangle = \sum_{\alpha=1}^{r} s_\alpha |\alpha\rangle_A |\alpha\rangle_B$$

Schmidt decomposition

$$|\alpha\rangle_A = \sum_{i=1}^{\dim \mathcal{H}_A} U_{i\alpha} |i\rangle_A \qquad |\alpha\rangle_B = \sum_{j=1}^{\dim \mathcal{H}_B} V^*_{j\alpha} |j\rangle_B$$

orthonormal sets!

link to entanglement

reduced density operators for A, B from Schmidt decomposition:

$$\hat{\rho}_A = \mathrm{tr}_B|\psi\rangle\langle\psi| = \sum_{\alpha=1}^{r} s_\alpha^2 |\alpha\rangle_A \; {}_A\langle\alpha| \qquad \hat{\rho}_B = \mathrm{tr}_A|\psi\rangle\langle\psi| = \sum_{\alpha=1}^{r} s_\alpha^2 |\alpha\rangle_B \; {}_B\langle\alpha|$$

entanglement between A, B: von Neumann entropy of reduced DOs:

$$S_{A|B}(|\psi\rangle) = -\mathrm{tr}_A \hat{\rho}_A \ln \hat{\rho}_A = -\mathrm{tr}_B \hat{\rho}_B \ln \hat{\rho}_B = -\sum_{\alpha=1}^{r} s_a^2 \ln s_a^2$$

product states: $|\psi\rangle = |\alpha\rangle_A |\alpha\rangle_B$ with $|\alpha\rangle_{A,B} = \sum_{\{\sigma_{A,B}\}} c^{\sigma_{A,B}} |\sigma_{A,B}\rangle$

spectrum: $(1, 0, 0, \ldots)$ entanglement 0 $\qquad 0 \ln 0 = \lim_{\epsilon \to 0^+} \epsilon \ln \epsilon = 0$

singlet state: $\hat{\rho}_A = \hat{\rho_B} = \mathrm{diag}(\frac{1}{2}, \frac{1}{2}) \qquad -2 \cdot \frac{1}{2} \ln \frac{1}{2} = \ln 2$

maximal entanglement: $-D \cdot D^{-1} \ln D^{-1} = \ln D$

states decomposed as MPS

reshape coefficient vector into matrix of dimension $(d \times d^{L-1})$ and SVD:

$$c^{\sigma_1\sigma_2\ldots\sigma_L} \to \Psi_{\sigma_1,\sigma_2\ldots\sigma_L} = \sum_{a_1} U_{\sigma_1,a_1} S_{a_1,a_1} V^\dagger_{a_1,\sigma_2\ldots\sigma_L}$$

slice *U* into *d* row vectors:

$$U_{\sigma_1,a_1} \to \{A^{\sigma_1}\} \quad \text{with} \quad A^{\sigma_1}_{1,a_1} = U_{\sigma_1,a_1}$$

rearrange SVD result:

$$c^{\sigma_1\sigma_2\ldots\sigma_L} = \sum_{a_1} A^{\sigma_1}_{1,a_1} c^{a_1\sigma_2\sigma_3\ldots\sigma_L} \qquad c^{a_1\sigma_2\sigma_3\ldots\sigma_L} = S_{a_1,a_1} V^\dagger_{a_1,\sigma_2\ldots\sigma_L}$$

reshape coefficient vector into matrix of dim. $(d^2 \times d^{L-2})$ and SVD:

$$c^{a_1\sigma_2\sigma_3\ldots\sigma_L} \to \Psi_{a_1\sigma_2,\sigma_3\ldots\sigma_L} = \sum_{a_2} U_{a_1\sigma_2,a_2} S_{a_2,a_2} V^\dagger_{a_2,\sigma_3\ldots\sigma_L}$$

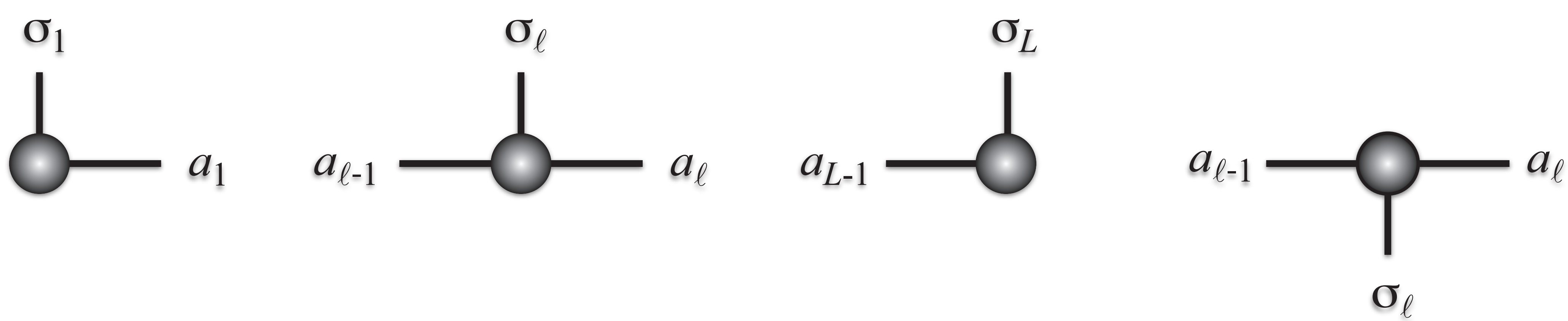
slice *U* into *d* matrices:

$$A^{\sigma_2}_{a_1,a_2} = U_{a_1\sigma_2,a_2}$$

rearrange SVD result: $c^{\sigma_1\sigma_2\ldots\sigma_L} = \sum_{a_1,a_2} A^{\sigma_1}_{1,a_1} A^{\sigma_2}_{a_1,a_2} c^{a_2\sigma_3\sigma_3\ldots\sigma_L}$ and so on!

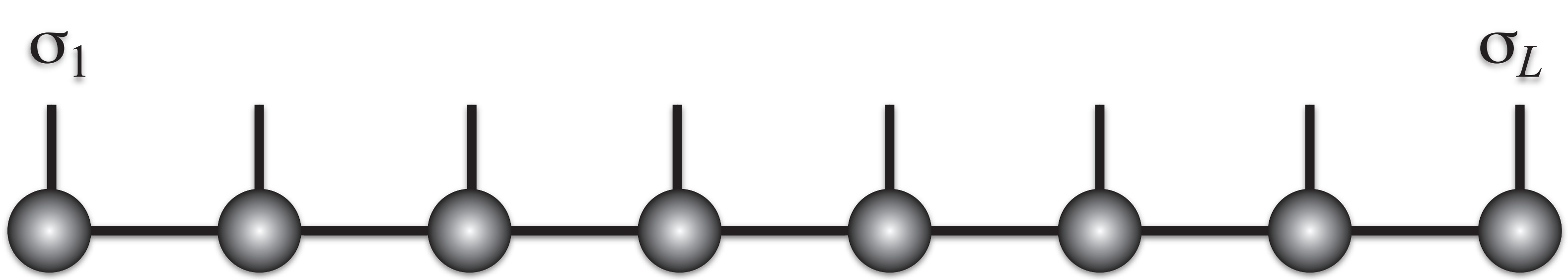
graphical representation

matrix: vertical lines = physical states, horizontal lines = matrix indices



left edge bulk right edge complex conjug.

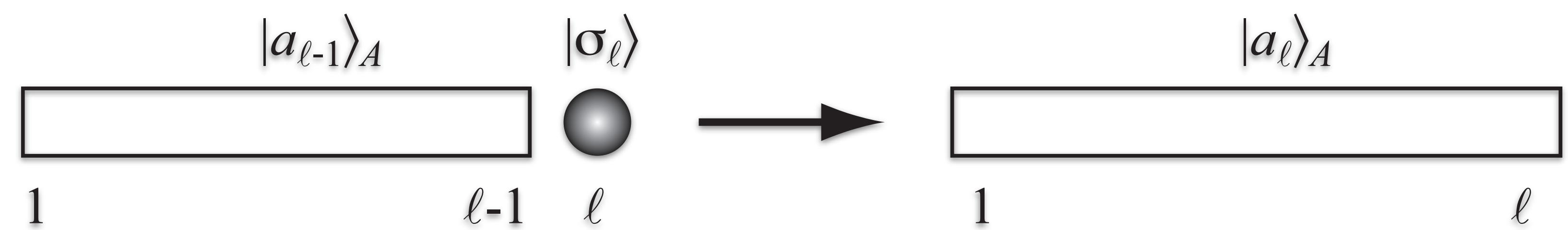
rule: connected lines are *contracted* (multiplied and summed)



matrix product state in graphical representation

block growth, decimation and MPS

RG schemes: grow blocks while decimating basis



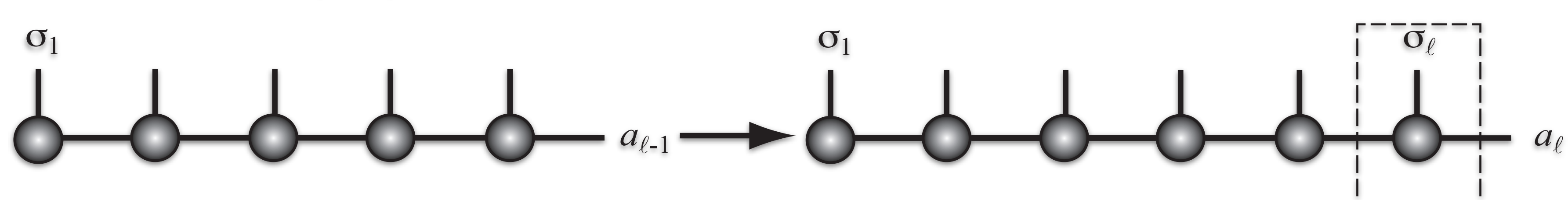
$$|a_\ell\rangle = \sum_{a_{\ell-1},\sigma_\ell} \langle a_{\ell-1},\sigma_\ell|a_\ell\rangle |a_{\ell-1}\rangle|\sigma_\ell\rangle \equiv \sum_{a_{\ell-1},\sigma_\ell} M^{\sigma_\ell}_{a_{\ell-1},a_\ell}|a_{\ell-1}\rangle|\sigma_\ell\rangle$$

simple rearrangement of expansion coefficients into matrices:

$$M^{\sigma_\ell}_{a_{\ell-1},a_\ell} = \langle a_{\ell-1},\sigma_\ell|a_\ell\rangle$$

recursion easily expressed as matrix multiplication:

$$|a_\ell\rangle = \sum_{\sigma_1,\ldots,\sigma_\ell} (M^{\sigma_1}M^{\sigma_2}\ldots M^{\sigma_\ell})_{1,a_\ell}|\sigma_1\sigma_2\ldots\sigma_\ell\rangle$$



(left and right) normalization

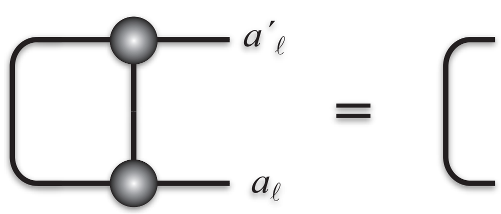
both state decomposition and block growth scheme give special gauge

$$\delta_{a'_\ell,a_\ell} = \langle a'_\ell | a_\ell \rangle = \sum_{a'_{\ell-1}\sigma'_\ell a_{\ell-1}\sigma_\ell} M^{\sigma'_\ell *}_{a'_{\ell-1},a'_\ell} M^{\sigma_\ell}_{a_{\ell-1},a'_\ell} \langle a'_{\ell-1}\sigma'_\ell | a_{\ell-1}\sigma_\ell \rangle$$

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

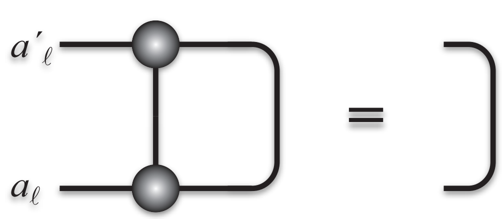
left normalization (called A); more compact representation:

$$I = \sum_{\sigma_\ell} M^{\sigma_\ell \dagger} M^{\sigma_\ell} \equiv \sum_{\sigma_\ell} A^{\sigma_\ell \dagger} A^{\sigma_\ell}$$



right normalization (called B):

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



mixed normalization:

$$AAAAAMBBBBBBBBB$$

matrix product operators (MPO)

general operator:

$$\hat{O} = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} c^{\sigma_1 \ldots \sigma_L, \sigma'_1 \ldots \sigma'_L} |\sigma_1 \ldots \sigma_L\rangle\langle\sigma'_1 \ldots \sigma'_L|$$

rearrange indices:

$$c^{\sigma_1 \ldots \sigma_L, \sigma'_1 \ldots \sigma'_L} \rightarrow c^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L}$$

„mean-field“ very useful: $c^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} \rightarrow c^{\sigma_1 \sigma'_1} \cdot c^{\sigma_2 \sigma'_2} \cdot \ldots \cdot c^{\sigma_L \sigma'_L}$

$$\hat{S}^z_i \rightarrow \hat{I}_1 \otimes \hat{I}_2 \otimes \ldots \otimes \hat{S}^z_i \otimes \ldots \otimes \hat{I}_L$$

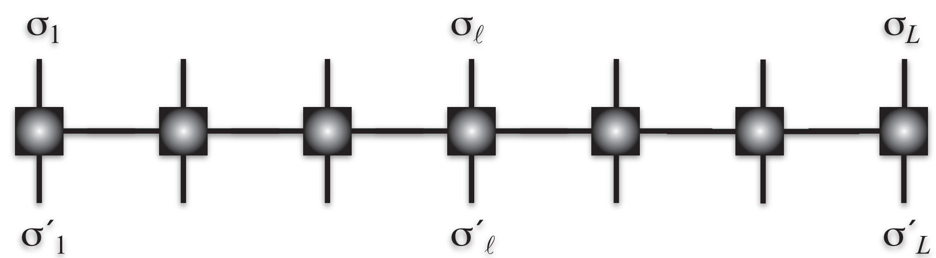
$$c^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L} = \delta_{\sigma_1, \sigma'_1} \cdot \delta_{\sigma_2, \sigma'_2} \cdot \ldots \cdot (\hat{S}^z)_{\sigma_i, \sigma'_i} \cdot \ldots \cdot \delta_{\sigma_L, \sigma'_L}$$

matrix product operator:

$$\hat{O} = \sum_{\{\sigma\}} \sum_{\{\sigma'\}} M^{\sigma_1 \sigma'_1} M^{\sigma_2 \sigma'_2} \ldots M^{\sigma_L \sigma'_L} |\sigma_1 \ldots \sigma_L\rangle\langle\sigma'_1 \ldots \sigma'_L|$$

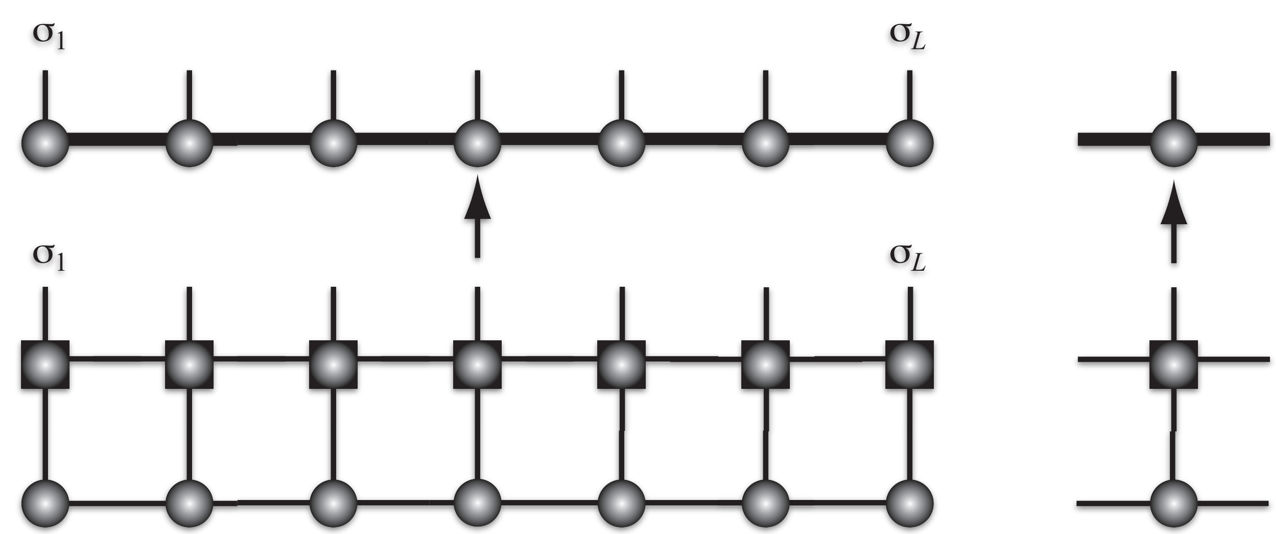
applying an MPO to an MPS

graphical representation with ingoing and outgoing physical states:



applying an MPO to an MPS: new MPS with matrix dims multiplied

$$\tilde{M}^{\sigma_i}_{(ab),(a'b')} = \sum_{\sigma_i'} N^{\sigma_i \sigma_i'}_{aa'} M^{\sigma_i'}_{bb'}$$



normalization and compression I

problem: matrix dimensions of MPS grow under MPO application

solution: compression of matrices with minimal state distance

assume state is given in mixed normalized form:

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1} A^{\sigma_2} \ldots A^{\sigma_\ell} M^{\sigma_{\ell+1}} B^{\sigma_{\ell+2}} \ldots B^{\sigma_L} |\sigma_1 \ldots \sigma_L\rangle$$

stack *M* matrices into one:

$$M_{a_\ell, \sigma_{\ell+1} a_{\ell+1}} = M^{\sigma_{\ell+1}}_{a_\ell, a_{\ell+1}}$$

carry out SVD, and use results: $M = USV^\dagger$

$$A^{\sigma_\ell} \leftarrow A^{\sigma_\ell} U$$ orthonormality of *U* !

$$B^{\sigma_{\ell+1}}_{a_\ell, a_{\ell+1}} = V^\dagger_{a_\ell, \sigma_{\ell+1} a_{\ell+1}}$$

normalization and compression II

now introduce orthonormal states:

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

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

read off Schmidt decomposition: $|\psi\rangle = \sum_{a_\ell} s_{a_\ell}|a_\ell\rangle_A|a_\ell\rangle_B$

compress matrices $A^{\sigma_\ell}, B^{\sigma_{\ell+1}}$ by keeping *D* largest singular values

$$A^{\sigma_\ell}S \rightarrow M^{\sigma_\ell}$$

$$|\psi\rangle = \sum_{\{\sigma\}} A^{\sigma_1}A^{\sigma_2}\ldots A^{\sigma_{\ell-1}}\boxed{M^{\sigma_\ell}}B^{\sigma_{\ell+1}}\ldots B^{\sigma_L}|\sigma_1\ldots\sigma_L\rangle$$

mixed rep shifted by 1 site: sweep through chain; also normalization

time-evolution

assume initial state in MPS representation; time evolution:

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\hat{H}t}|\psi(0)\rangle$$

how to express the evolution operator as an MPO?

one solution: Trotterization of evolution operator into small time steps

$$N \to \infty \qquad \tau \to 0 \qquad N\tau = T \qquad \tau \sim 0.01$$

Heisenberg model: $\hat{H} = \sum_{i=1}^{L-1} \hat{h}_i \qquad \hat{h}_i = \mathbf{S}_i \cdot \mathbf{S}_{i+1}$

$$\mathrm{e}^{-\mathrm{i}\hat{H}T} = \prod_{i=1}^{N} \mathrm{e}^{-\mathrm{i}\hat{H}\tau} = \prod_{k=1}^{N} \mathrm{e}^{-\mathrm{i}\sum_{i=1}^{L-1}\hat{h}_i\tau} \stackrel{!}{=} \prod_{k=1}^{N}\prod_{i=1}^{L-1} \mathrm{e}^{-\mathrm{i}\hat{h}_i\tau}$$

first-order Trotter decomposition

Trotter decomposition

calculation of $\mathrm{e}^{-\mathrm{i}\hat{h}_i\tau}$ as $(d^2 \times d^2)$ matrix:

$$H_i U = U\Lambda \quad H_i = U\Lambda U^\dagger \quad \Rightarrow \quad \mathrm{e}^{-\mathrm{i}H_i\tau} = U\mathrm{e}^{-\mathrm{i}\Lambda\tau}U^\dagger = U \cdot \mathrm{diag}(\mathrm{e}^{-\mathrm{i}\lambda_1\tau}, \mathrm{e}^{-\mathrm{i}\lambda_2\tau}, \ldots) \cdot U^\dagger$$

problem: exponential does not factorize if operators do not commute

$$\mathrm{e}^{\hat{A}+\hat{B}} = \mathrm{e}^{\hat{A}}\mathrm{e}^{\hat{B}}\mathrm{e}^{\frac{1}{2}[\hat{A},\hat{B}]}$$

but error is negligible as $\tau \to 0$

$$[\hat{h}_i\tau, \hat{h}_{i+1}\tau] \propto \tau^2$$

convenient rearrangement:

$$\hat{H} = \hat{H}_{\mathrm{odd}} + \hat{H}_{\mathrm{even}}; \qquad \hat{H}_{\mathrm{odd}} = \sum_i \hat{h}_{2i-1}, \quad \hat{H}_{\mathrm{even}} = \sum_i \hat{h}_{2i}$$

$$\mathrm{e}^{-\mathrm{i}\hat{H}T} = \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{even}}\tau}\mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau}; \qquad \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{even}}\tau} = \prod_i \mathrm{e}^{-\mathrm{i}\hat{h}_{2i}\tau}, \quad \mathrm{e}^{-\mathrm{i}\hat{H}_{\mathrm{odd}}\tau} = \prod_i \mathrm{e}^{-\mathrm{i}\hat{h}_{2i-1}\tau}$$

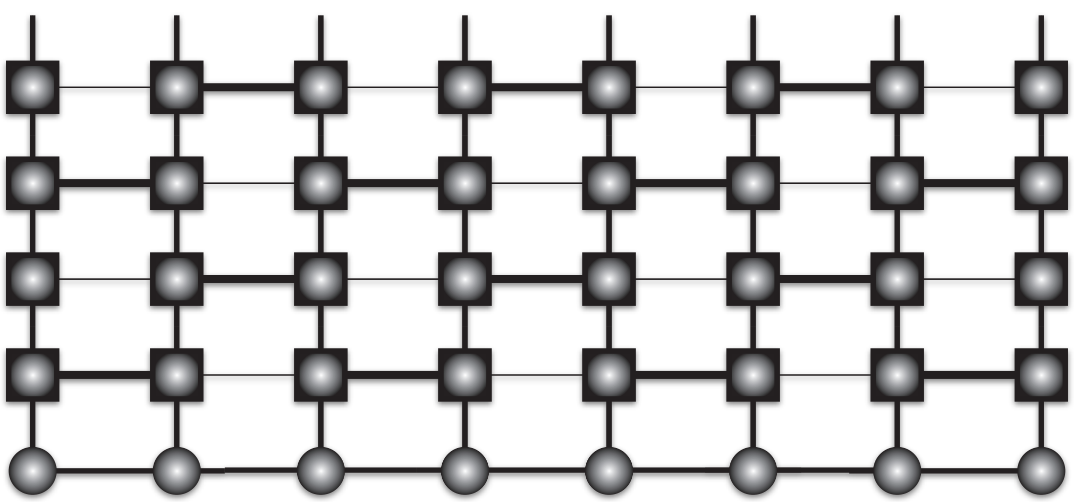
tDMRG, tMPS, TEBD

bring local evolution operator into MPO form:

$$U^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = \langle\sigma_1\sigma_2|\mathrm{e}^{-\mathrm{i}\hat{h}_1\tau}|\sigma_1'\sigma_2'\rangle$$

$$U^{\sigma_1\sigma_2,\sigma_1'\sigma_2'} = \overline{U}_{\sigma_1\sigma_1',\sigma_2\sigma_2'} \stackrel{SVD}{=} \sum_b W_{\sigma_1\sigma_1',b}S_{b,b}W_{b,\sigma_2\sigma_2'}$$

$$= \sum_b M_{1,b}^{\sigma_1\sigma_1'} M_{b,1}^{\sigma_2\sigma_2'}$$



one time step: dimension grows as d^2

- apply one infinitesimal time step in MPO form
- compress resulting MPS

some comments ...

real time evolution limited by entanglement growth:

$$S(t) \leq S(0) + \nu t \qquad S \sim \ln D$$

in the worst case, matrix dimensions grow exponentially!

ground states can be obtained by imaginary time evolution (SLOW!):

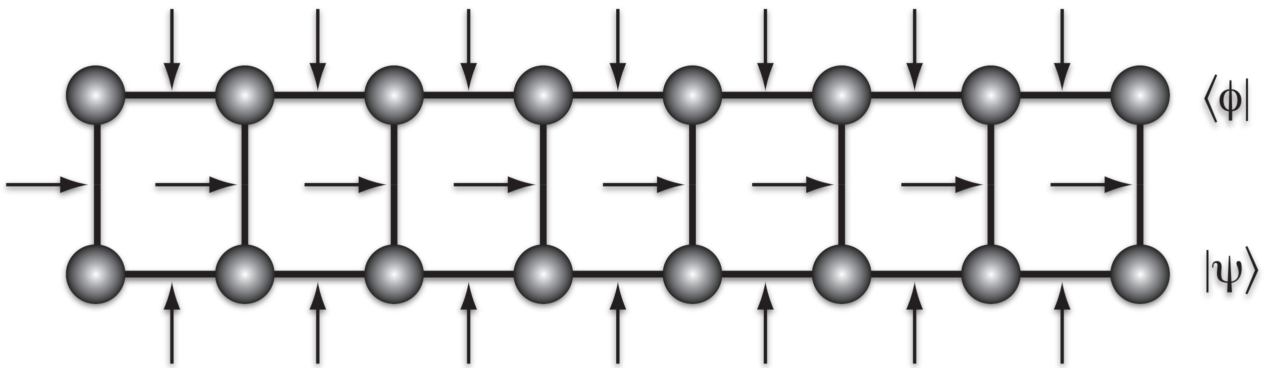
$$|\psi\rangle = \sum_n c_n |n\rangle \qquad \hat{H}|n\rangle = E_n|n\rangle \qquad E_0 \leq E_1 \leq E_2 \leq \ldots$$

$$\begin{aligned} \lim_{\beta\to\infty} \mathrm{e}^{-\beta\hat{H}}|\psi\rangle &= \lim_{\beta\to\infty} \sum_n \mathrm{e}^{-\beta E_n} c_n|n\rangle = \lim_{\beta\to\infty} \mathrm{e}^{-\beta E_0}\left(c_0|0\rangle + \sum_{n>0} \mathrm{e}^{-\beta(E_n - E_0)} c_n|n\rangle\right. \\ &= \lim_{\beta\to\infty} \mathrm{e}^{-\beta E_0} c_0|0\rangle \end{aligned}$$

overlaps

$$\langle\psi(t)|\psi(0)\rangle \qquad \langle S_i^z(t)\rangle = \langle\psi(t)|\hat{S}_i^z|\psi(t)\rangle$$

overlap contractions:



$$\langle\phi|\psi\rangle = \sum_{\{\sigma\}}\sum_{\{\sigma'\}}\langle\{\sigma'\}|\tilde{M}^{\sigma'_1 *}\ldots\tilde{M}^{\sigma'_L *}M^{\sigma_1}\ldots M^{\sigma_L}|\{\sigma\}\rangle = \sum_{\{\sigma\}}\tilde{M}^{\sigma_1 *}\ldots\tilde{M}^{\sigma_L *}M^{\sigma_1}\ldots M^{\sigma_L}$$

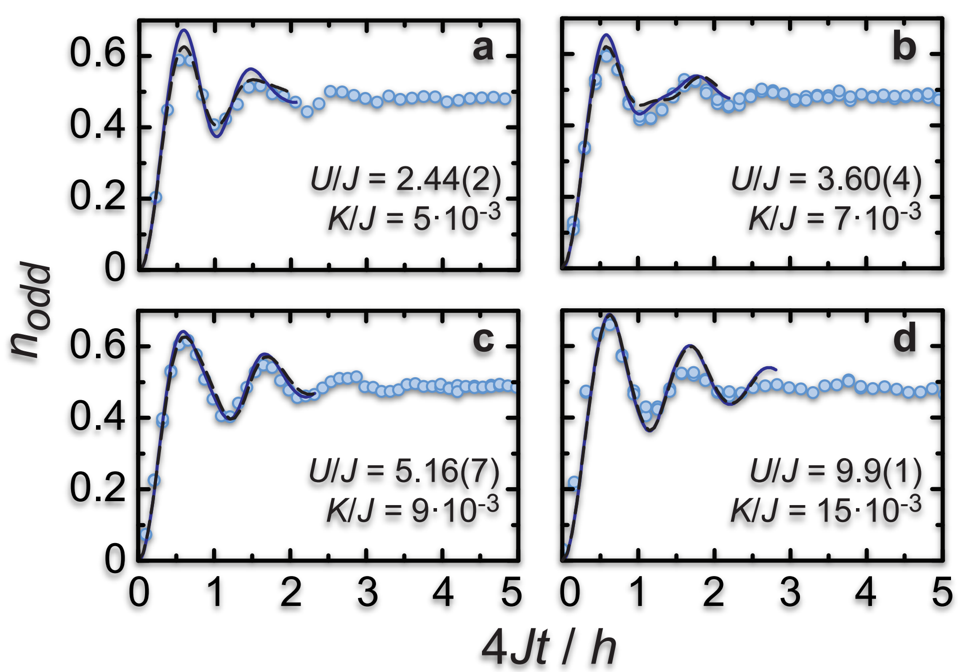
$$\begin{aligned}\langle\phi|\psi\rangle &= \sum_{\{\sigma\}}\tilde{M}^{\sigma_1 *}\ldots\tilde{M}^{\sigma_L *}M^{\sigma_1}\ldots M^{\sigma_L} \\ &= \sum_{\{\sigma\}}\tilde{M}^{\sigma_L \dagger}\ldots\tilde{M}^{\sigma_1 \dagger}M^{\sigma_1}\ldots M^{\sigma_L} \\ &= \sum_{\sigma_L}\tilde{M}^{\sigma_L \dagger}\left(\ldots\left(\sum_{\sigma_2}\tilde{M}^{\sigma_2 \dagger}\left(\sum_{\sigma_1}\tilde{M}^{\sigma_1 \dagger}M^{\sigma_1}\right)M^{\sigma_2}\right)\ldots\right)M^{\sigma_L}\end{aligned}$$

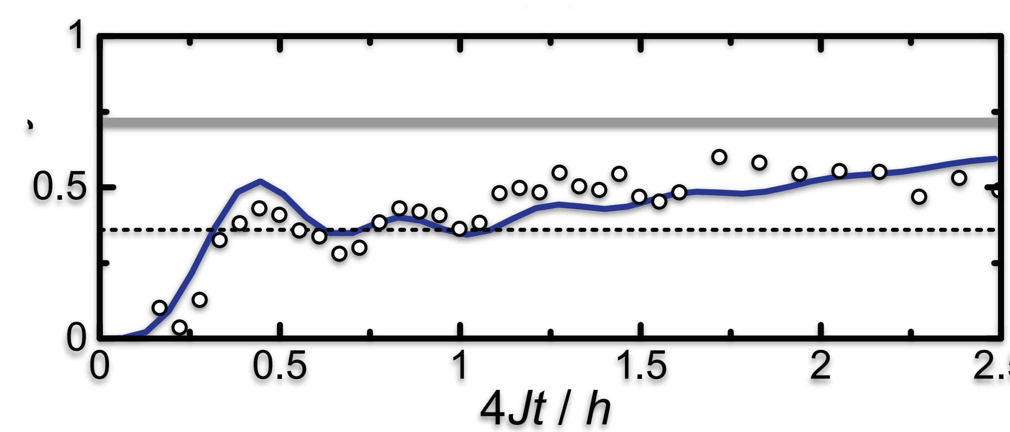
order of contractions: zip through the ladder; cost $O(dLD^3)$

expectation values and correlators

expectation value of local observable: simply replace sum

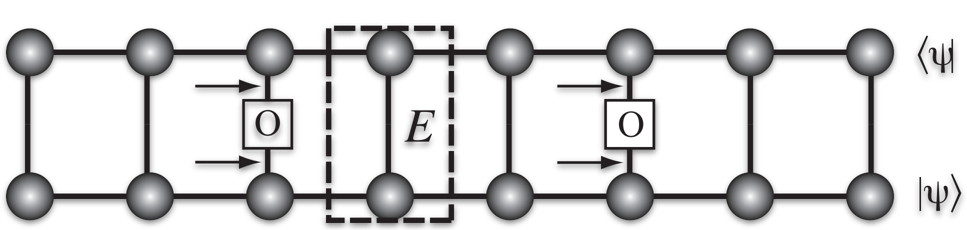
$$\sum_{\sigma_i} \quad \text{turns into} \quad \sum_{\sigma_i,\sigma_i'} O_{\sigma_i,\sigma_i'}$$





local densities and NN correlators in a bosonic ultracold atomic relaxation experiment: simulation vs. experiment

two-point correlators: long-range or superposition of exponentials



$$E^{(a_{\ell-1}a'_{\ell-1}),(a_\ell,a'_\ell)} := \sum_{\sigma_\ell} A^{\sigma_\ell *}_{a_{\ell-1},a_\ell} A^{\sigma_\ell}_{a'_{\ell-1},a'_\ell}$$

hence: power laws only „by approximation“

purification and finite-T evolution

purification: any mixed state can be expressed by a pure state on a larger system (P: physical, Q: auxiliary state space)

$$\hat{\rho}_P = \sum_n \rho_n |n\rangle_P \; {}_P\langle n| \qquad |\psi\rangle_{PQ} = \sum_n \sqrt{\rho_n} |n\rangle_P |n\rangle_Q$$

$$\hat{\rho}_P = \mathrm{tr}_Q |\psi\rangle_{PQ} \; {}_{PQ}\langle\psi|$$

simplest way: Q copy of P

expectation values as before:

$$\langle \hat{O}_P \rangle_{\hat{\rho}_P} = \mathrm{tr}_P \hat{O}_P \hat{\rho}_P = \mathrm{tr}_P \hat{O}_P \mathrm{tr}_Q |\psi\rangle_{PQ} \; {}_{PQ}\langle\psi| = \mathrm{tr}_{PQ} \hat{O}_P |\psi\rangle_{PQ} \; {}_{PQ}\langle\psi| = \; {}_{PQ}\langle\psi|\hat{O}_P|\psi\rangle_{PQ}$$

time evolution as before:

$$\hat{\rho}_P(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t} \hat{\rho}_P \mathrm{e}^{+\mathrm{i}\hat{H}t} = \mathrm{e}^{-\mathrm{i}\hat{H}t} \mathrm{tr}_Q |\psi\rangle_{PQ} \; {}_{PQ}\langle\psi| \mathrm{e}^{+\mathrm{i}\hat{H}t} = \mathrm{tr}_Q |\psi(t)\rangle_{PQ} \; {}_{PQ}\langle\psi(t)|$$

$$|\psi(t)\rangle_{PQ} = \mathrm{e}^{-\mathrm{i}\hat{H}t} |\psi\rangle_{PQ}$$

time-evolution of thermal states

problem: usually we do not have mixed state in eigenrepresentation

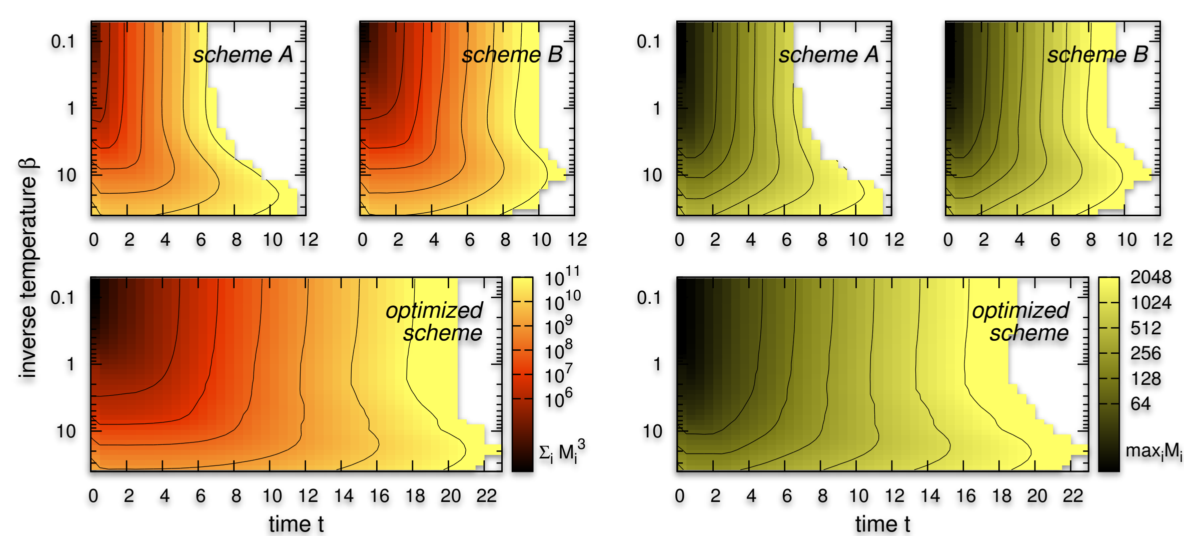
thermal states: easy way out by imaginary *t*-evolution

$$e^{-\beta\hat{H}} = e^{-\beta\hat{H}/2} \cdot \hat{I}_P \cdot e^{-\beta\hat{H}/2} = \mathrm{tr}_Q e^{-\beta\hat{H}/2} |\rho_0\rangle_{PQ} \;\; {}_{PQ}\langle\rho_0| e^{-\beta\hat{H}/2}$$

purification of infinite-T state: product of local totally mixed states

gauge degree of freedom: arbitrary unitary evolution on Q

lots of room for improvement: original, improved, and currently best scheme



build MPOs and compress them:

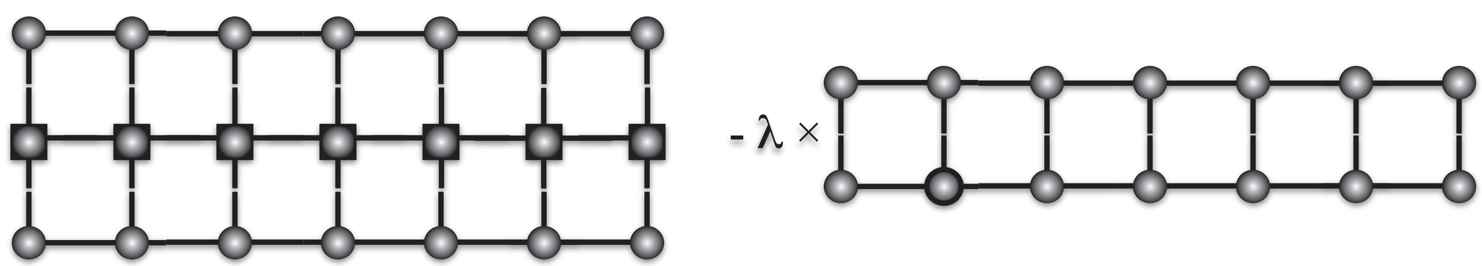
$$\langle\hat{B}(2t)\hat{A}\rangle_\beta = Z(\beta)^{-1}\mathrm{tr}\left(\left[e^{i\hat{H}t}e^{-\beta\hat{H}/2}\hat{B}e^{-i\hat{H}t}\right]\left[e^{-i\hat{H}t}\hat{A}e^{-\beta\hat{H}/2}e^{i\hat{H}t}\right]\right)$$

variational ground state search: DMRG

problem: find MPS (of a given dimension) that minimizes energy

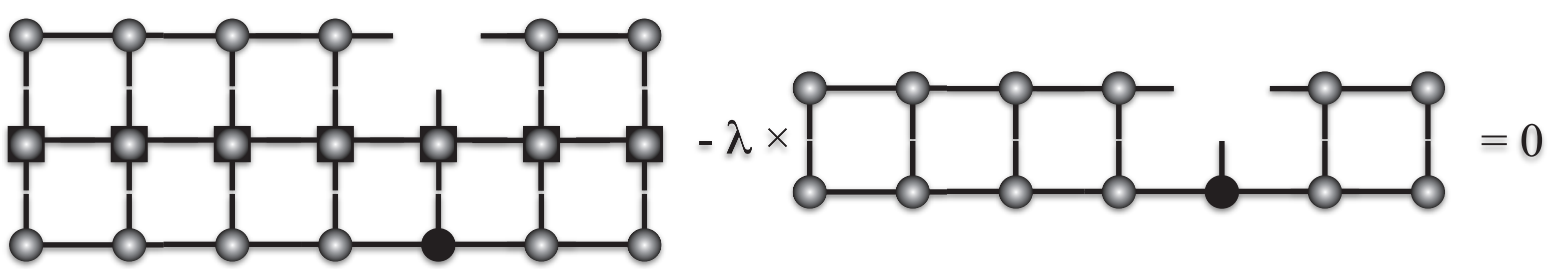
$$\min \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \quad \Leftrightarrow \quad \min\Big(\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle\Big)$$

graphical representation of expression to be minimized:

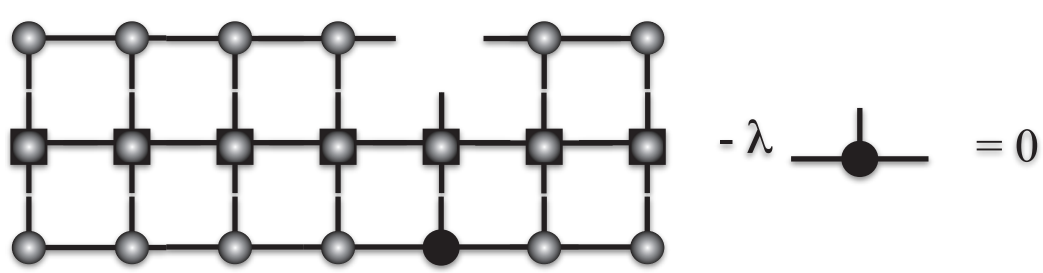


multilinear :-(

variational minimization with respect to one matrix:



unnormalized MPS:
generalized EV problem



mixed normalization MPS:
eigenvalue problem

ground state DMRG

analytical representation of variational problem:

$$\frac{\partial}{\partial M^{\sigma_i *}}\left(\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle\right) \stackrel{!}{=} 0$$

$$\sum_{\sigma_i' a_{i-1}' a_i'} H_{\sigma_i a_{i-1} a_i, \sigma_i' a_{i-1}' a_i'} M_{\sigma_i' a_{i-1}' a_i'} = \sum_{\sigma_i' a_{i-1}' a_i'} N_{a_{i-1} a_i, a_{i-1}' a_i'} \delta_{\sigma_i, \sigma_i'} M_{\sigma_i' a_{i-1}' a_i'} \equiv \sum_{\sigma_i' a_{i-1}' a_i'} N_{\sigma_i a_{i-1} a_i, \sigma_i' a_{i-1}' a_i'} M_{\sigma_i' a_{i-1}' a_i'}$$

$$H\mathbf{m} = \lambda N\mathbf{m}$$

DMRG algorithm:

- start with random or guess initial MPS
- maintaining mixed normalization, sweep „hot site“ forth and back
- at each step, optimize local matrices by solving eigenvalue problem

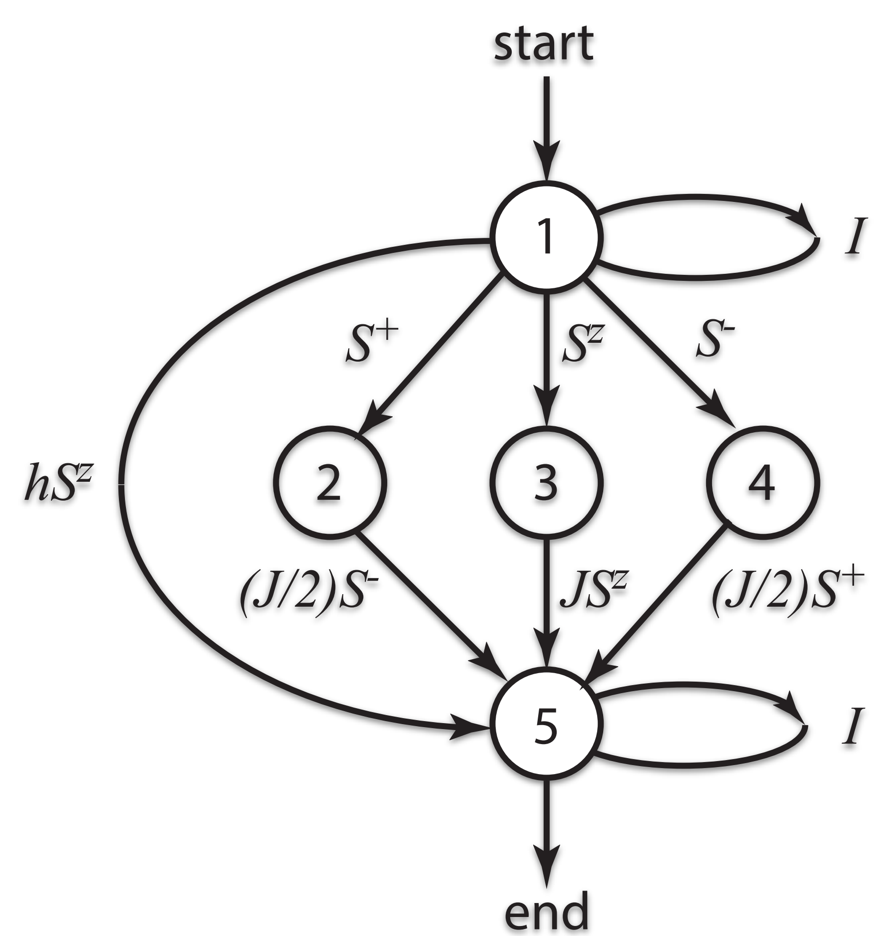
convergence: monitor $\langle\psi|\hat{H}^2|\psi\rangle - (\langle\psi|\hat{H}|\psi\rangle)^2$

Hamiltonians in MPO form

construct Hamiltonian as automaton that moves through chain (e.g. from right to left) building Hamiltonian

$$\hat{H} = \hat{M}^{[1]}\hat{M}^{[2]}\ldots\hat{M}^{[L]} \qquad \hat{M}^{[i]} = \sum_{\sigma_i,\sigma_i'} M^{\sigma_i,\sigma_i'}|\sigma_i\rangle\langle\sigma_i'|$$

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



Hamiltonians in MPO form II

short ranged Hamiltonians find very compact, exact representation!

$$\hat{M}^{[i]} = \begin{bmatrix} \hat{I} & 0 & 0 & 0 & 0 \\ \hat{S}^{+} & 0 & 0 & 0 & 0 \\ \hat{S}^{z} & 0 & 0 & 0 & 0 \\ \hat{S}^{-} & 0 & 0 & 0 & 0 \\ h\hat{S}^{z} & (J/2)\hat{S}^{-} & J^{z}\hat{S}^{z} & (J/2)\hat{S}^{+} & \hat{I} \end{bmatrix}$$

$$\hat{M}^{[1]} = \begin{bmatrix} h\hat{S}^{z} & (J/2)\hat{S}^{-} & J^{z}\hat{S}^{z} & (J/2)\hat{S}^{+} & \hat{I} \end{bmatrix} \qquad \hat{M}^{[L]} = \begin{bmatrix} \hat{I} \\ \hat{S}^{+} \\ \hat{S}^{z} \\ \hat{S}^{-} \\ h\hat{S}^{z} \end{bmatrix}$$

spectral functions I

time-dependent Green's function (Heisenberg picture)

$$\mathrm{i}G_O(t) = \langle 0|\hat{O}^\dagger(t)\hat{O}(0)|0\rangle \qquad (t > 0)$$

in frequency space (imaginary part: spectral function)

$$S_\eta(\omega) := \langle 0|\hat{O}^\dagger \frac{1}{E_0 + \omega + \mathrm{i}\eta - \hat{H}} \hat{O}|0\rangle$$

continuous fraction (Lanczos vector) approach (old, fast, imprecise):

$$|q_1\rangle = \hat{O}|0\rangle / \|\hat{O}|0\rangle\| \qquad \beta_m|q_{m+1}\rangle = \hat{H}|q_m\rangle - \alpha_m|q_m\rangle - \beta_{m-1}|q_{m-1}\rangle$$

$$\alpha_m = \langle q_m|\hat{H}|q_m\rangle \qquad \beta_m = \langle q_{m+1}|\hat{H}|q_m\rangle$$

$$S_\eta(\omega) = \cfrac{\langle 0|\hat{O}^\dagger\hat{O}|0\rangle}{E + \mathrm{i}\eta - \alpha_1 - \cfrac{\beta_1^2}{E + \mathrm{i}\eta - \alpha_2 - \cfrac{\beta_2^2}{E + \mathrm{i}\eta - \alpha_3 - \ldots}}}$$

spectral functions II

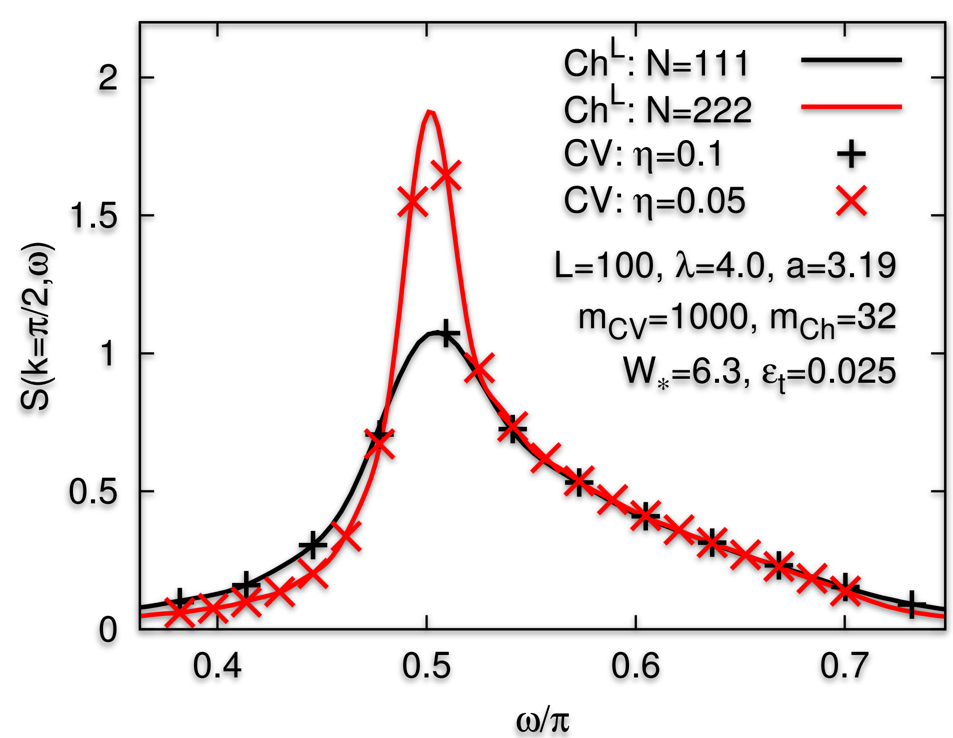
correction vector method (gold standard, slow, precise)

$$|c\rangle = \frac{1}{E_0 + \omega + \mathrm{i}\eta - \hat{H}} \hat{O}|0\rangle \qquad G_\eta(\omega) = \langle 0|\hat{O}^\dagger|c\rangle$$

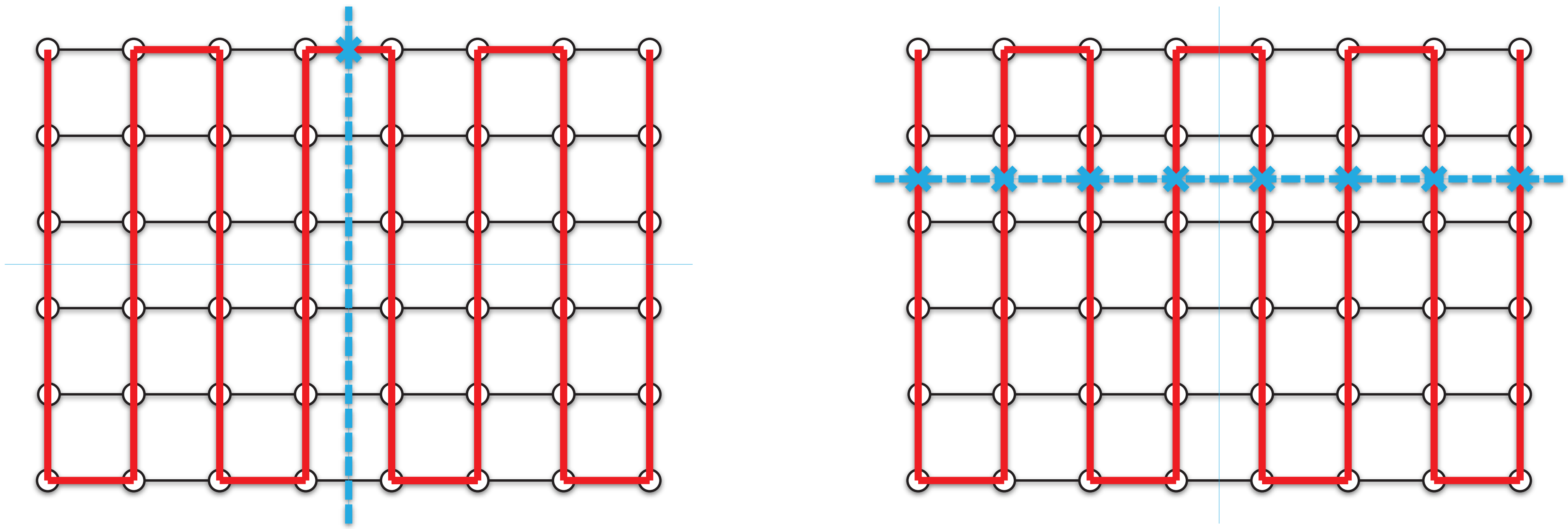
one has to solve large sparse equation system for correction vector:

$$(E_0 + \omega + \mathrm{i}\eta - \hat{H})|c\rangle = \hat{O}|0\rangle$$

recent alternative:
Chebyshev vector method
(fast, almost as precise)



DMRG in two dimensions



strategy: order 2D lattice as 1D snake with long-ranged interactions

problem: ground state entanglement grows as $S \sim L$ (linear dimension)

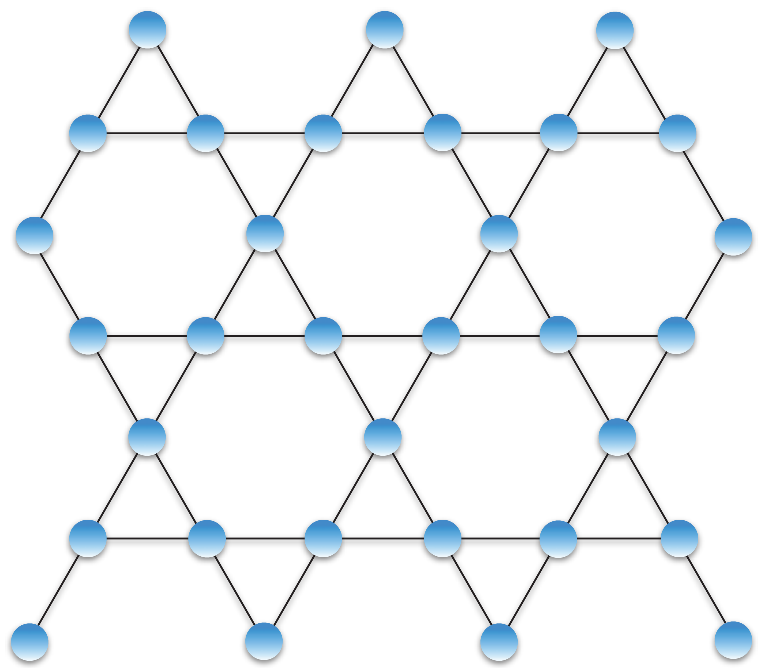
matrix dimension exponential in S !

vertical cut: 1 matrix carries all entanglement. Exponential!
horizontal cut: L matrices carry entanglement. Constant!

long horizontal stripes possible!

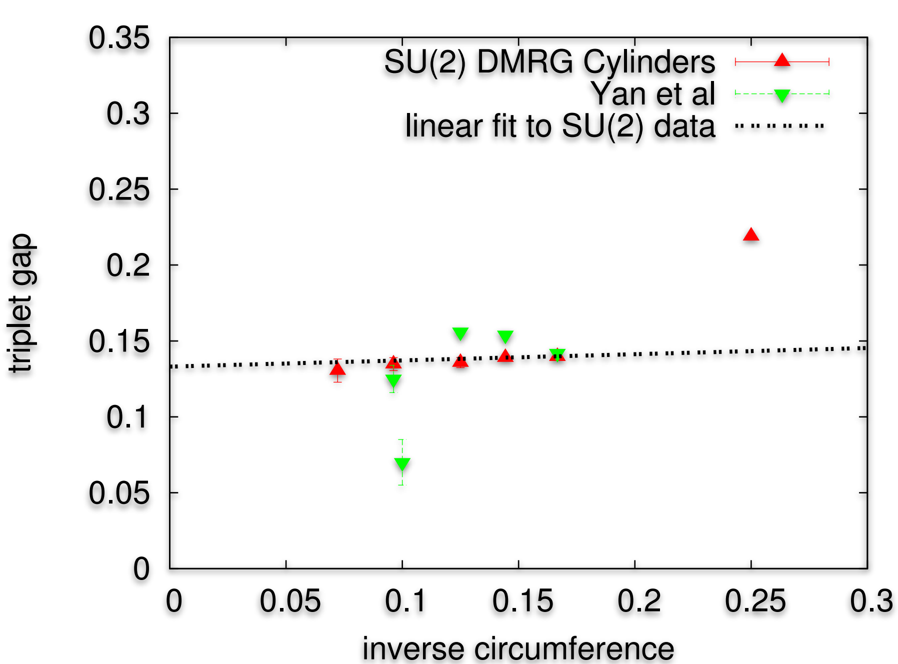
DMRG in 2D: kagomé lattice

Heisenberg spin-1/2 AFM on kagomé lattice: old, tough problem!



- no long-range order
- probably gap to first excitation
- various candidates for ground state:
  - valence bond solids (several types)
  - quantum spin liquids (several types)

DMRG on cylinders up to 17 lattice spacings:



- finite gap to first excitation
- no valence bond solid
- quantum spin liquid
- topological order: so-called Z_2 liquid

more to come!