Density-Matrix Renormalisation Group/ Matrix Product States

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introduction

fundamental problem of solid state

- what do we need DMRG for? problem class:

  fundamental Hamiltonian (without lattice vibrations…!):

$$H = \sum_{j=1}^{e^-} \frac{\mathbf{p}_j^2}{2m_e} + \frac{1}{2}\frac{1}{4\pi\epsilon_0}\frac{q_e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_j^{e^-} V_{\text{eff}}(\mathbf{r}_j)$$

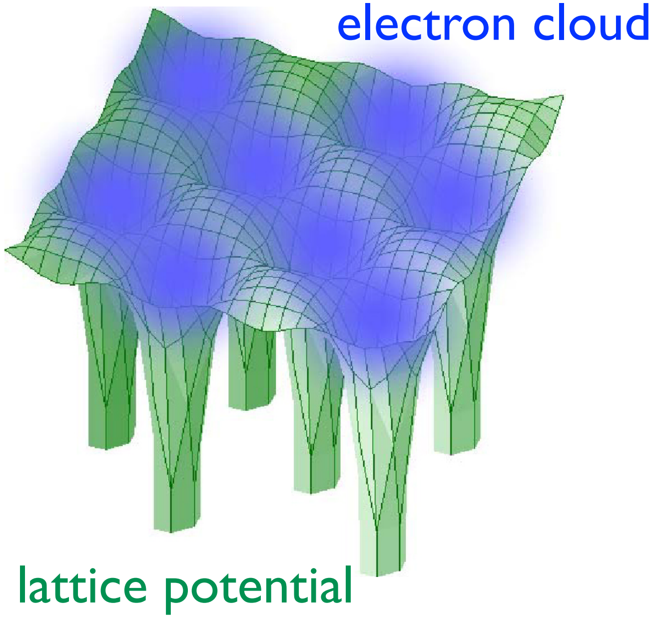
kinetic energy | electron-electron interaction | lattice potential

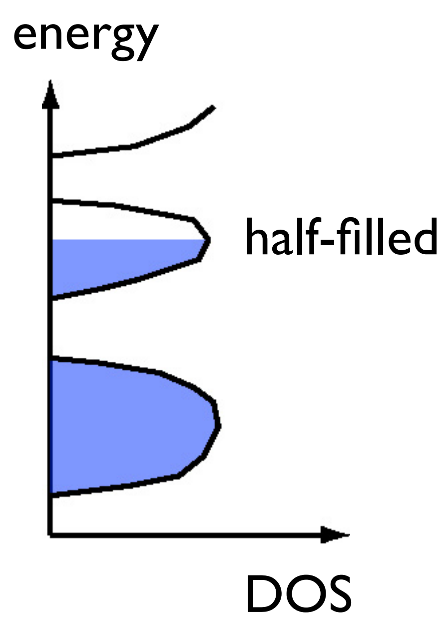
- we don't know how to solve the Schrödinger equation!

  problem: electron-electron interactions

electrons in solids

- **scenario I**
  valence electrons well delocalized
  interactions well screened





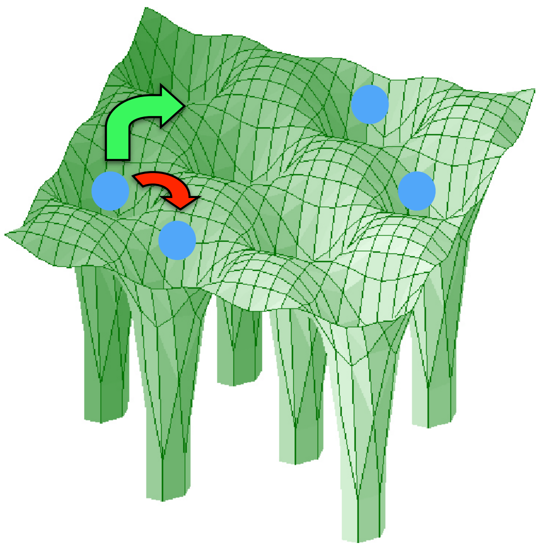
conductor

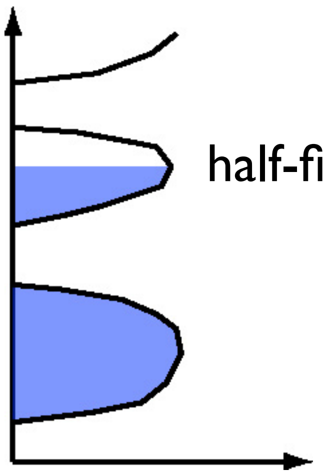
- many metals, semiconductors: single-electron picture OK

density functional theory (DFT)

electrons in solids: strong correlations

- **scenario:**
  valence electrons tightly bound
  strong local interactions





insulator

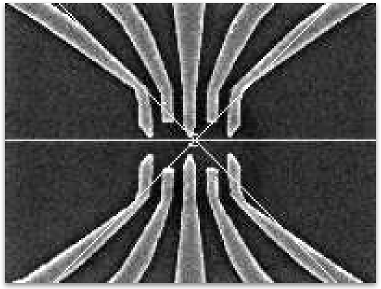
eg. high-Tc
parent compounds

- many particle picture: **strongly correlated materials**

model Hamiltonian methods - OUR TOPIC

why strong correlations?

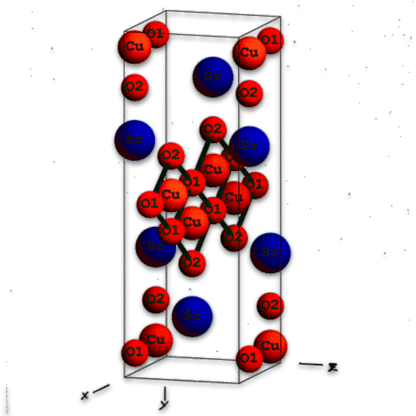
0 dimensions



magnetic
impurity physics

quantum dots

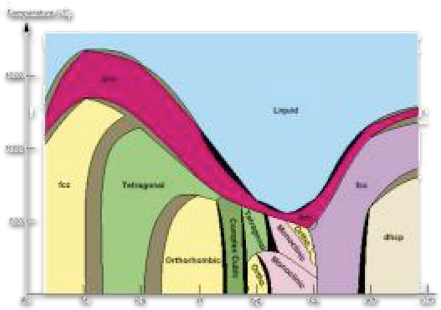
1 dimension



spin chains & ladders

Luttinger liquid

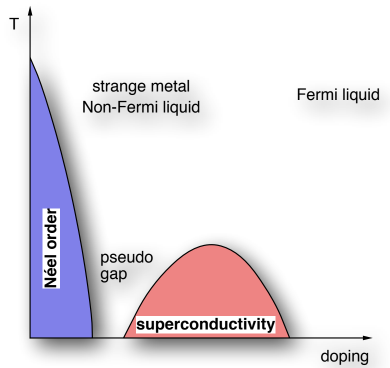
3 dimensions



realistic modelling:

transition metal,
rare earth compounds

2 dimensions



frustrated magnets

high-T_c superconductors

in equilibrium and out of/far from equilibrium!

which models?

- Hubbard model

$$H = -t \sum_{\langle i,j \rangle;\sigma} c^\dagger_{i\sigma} c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Wannier basis kinetic energy Coulomb energy

- Hilbert space: $\{|\emptyset\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle\}^{\otimes L}$ $d = 4$
- Heisenberg model (large-*U* Hubbard at half-filling)

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \tfrac{1}{2}(S_i^+ S_j^- + S_j^+ S_i^-) + S_i^z S_j^z$$

- Hilbert space: $\{|\uparrow\rangle, |\downarrow\rangle\}^{\otimes L}$ $d = 2$
- most simple cartoons of correlated problems
- computational methods needed …

compression of information

- compression of information necessary and desirable
  - diverging number of degrees of freedom
  - emergent macroscopic quantities: temperature, pressure, …

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \tfrac{1}{2}(S_i^+ S_j^- + S_j^+ S_i^-) + S_i^z S_j^z$$

- classical spins
  - thermodynamic limit: $N \to \infty$ $2N$ degrees of freedom (linear)
- quantum spins
  - superposition of states
  - thermodynamic limit: $N \to \infty$ 2^N degrees of freedom (exponential)

classical simulation of quantum systems

- compression of exponentially diverging Hilbert spaces
- what can we do with classical computers?
  - exact diagonalizations
    - limited to small lattice sizes: 40 (spins), 20 (electrons)
  - stochastic sampling of state space
    - quantum Monte Carlo techniques
    - negative sign problem for fermionic systems
  - physically driven selection of subspace: decimation
    - variational methods
    - renormalization group methods
    - **how do we find the good selection?** **DMRG/MPS!**

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)

(some) 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

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: idea

proposal: let us do quantum mechanics entirely with
matrix product states (MPS):

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

- all basis states participate
- (variational) constraint is in expansion coefficients:
  - for each of the *d* local basis states, one matrix *M*
    dL matrices altogether
  - dimensions such that they can be multiplied to a scalar
  - matrix size has upper limit *D*
    up to dLD^2 coefficients instead of exponentially many
- look weird: do they make any sense at all? are they useful and practical?

product states and MPS

standard approximation: mean-field approximation / product state

$$c^{\sigma_1 \dots \sigma_L} = c^{\sigma_1} \cdot c^{\sigma_2} \cdot \ldots \cdot c^{\sigma_L} \qquad d^L \to dL \text{ coefficients}$$

often useful, but misses essential quantum feature: entanglement

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

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

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

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

$$M^{\uparrow_1} = [1 \;\; 0] \qquad M^{\uparrow_2} = \begin{bmatrix} 0 \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$$

$$M^{\downarrow_1} = [0 \;\; 1] \qquad M^{\downarrow 2} = \begin{bmatrix} +\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}$$

works!

AKLT model

MPS useful even for matrices of dimension 2!

Haldane chain (1982): $$H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} \quad (S=1)$$

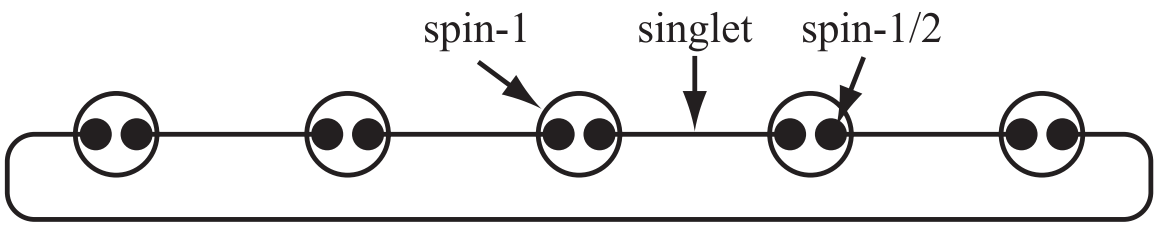
hidden order
topological
unexpected gap

AKLT (Affleck-Kennedy-Lieb-Tasaki) model (1987):

$$H = \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \frac{1}{3}(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2 \quad (S=1)$$

hidden order
topological
gapped

ground state:



MPS matrices: $$M^+ = \begin{bmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix} \quad M^0 = \begin{bmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \quad M^- = \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$$

matrix product states

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

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

non-uniqueness highly important/useful in practice!

MPS: beyond toy models

Why are matrix product states interesting beyond toy models?

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

technical tools

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

$$\boxed{A = USV^\dagger}$$

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*: $A^\dagger A \qquad AA^\dagger$

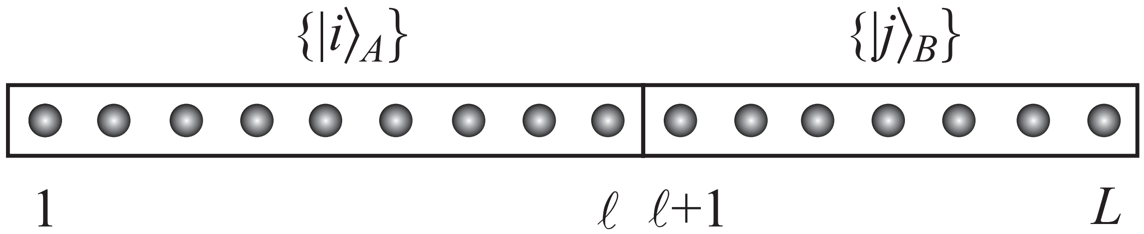
$$AA^\dagger = USV^\dagger VSU^\dagger = US^2U^\dagger \Rightarrow (AA^\dagger)U = US^2$$

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

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

SVD: Schmidt decomposition

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:

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

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!

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

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

MPS details

any state can be 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:

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

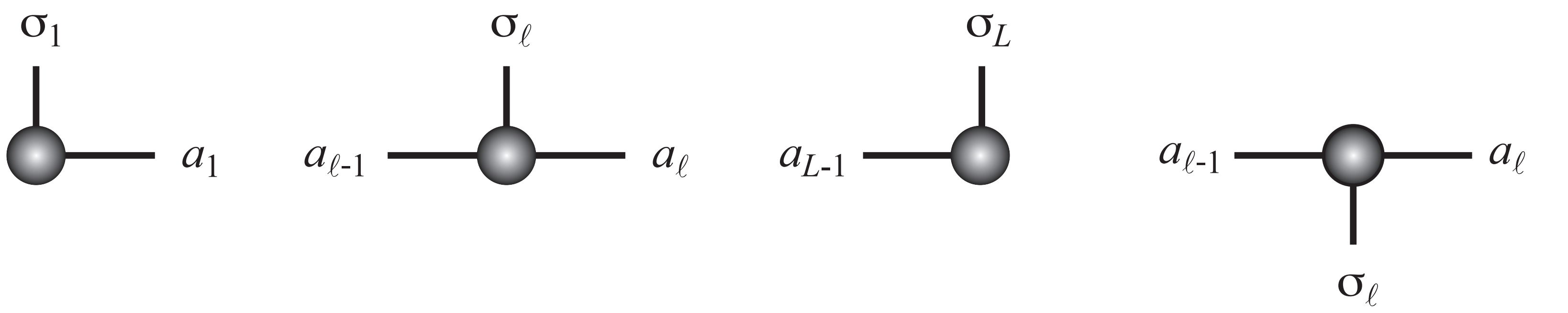
slice *U* into *d* matrices:

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

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!

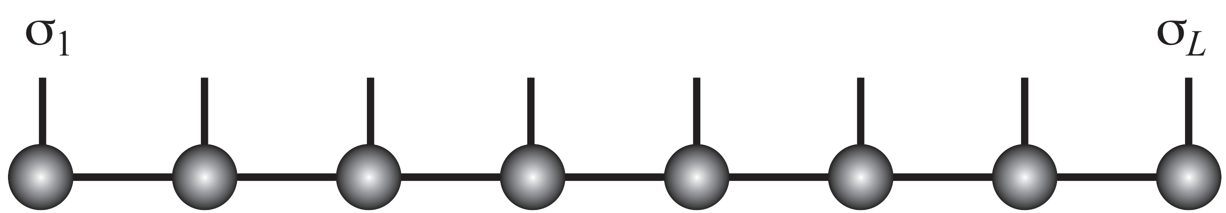
work with MPS: diagrammatics

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



left edge bulk right edge complex conjug.

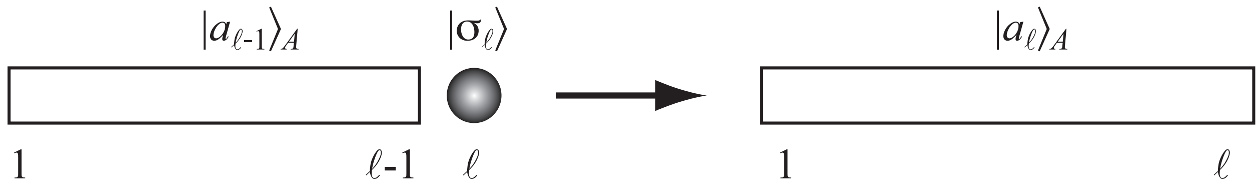
rule: connected lines are *contracted* (multiplied and summed)



matrix product state in graphical representation

block growth, decimation and MPS

RG schemes: grow blocks while decimating basis



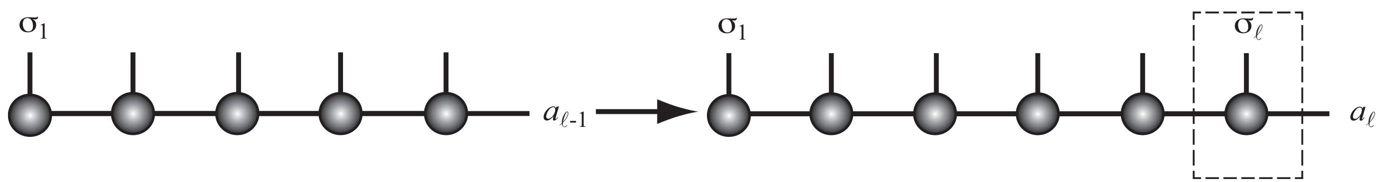
$$|a_\ell\rangle = \sum_{a_{\ell-1},\sigma_\ell} \langle a_{\ell-1},\sigma_\ell|a_\ell\rangle |a_{\ell-1}\rangle|\sigma_\ell\rangle \equiv \sum_{a_{\ell-1},\sigma_\ell} M^{\sigma_\ell}_{a_{\ell-1},a_\ell}|a_{\ell-1}\rangle|\sigma_\ell\rangle$$

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

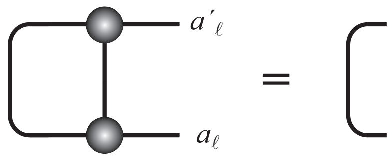
both state decomposition and block growth scheme give special gauge

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

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

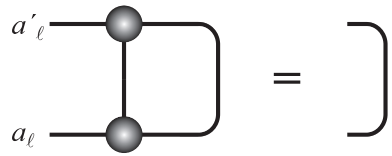
left normalization (called A); more compact representation:

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



right normalization (called B):

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



mixed normalization:

$$AAAAAMBBBBBBBBB$$

$$|\psi\rangle = \sum_{\alpha\beta\sigma} M^{\sigma}_{\alpha\beta} |\alpha\rangle |\sigma\rangle |\beta\rangle$$ block ONBs!

matrix product operators

matrix product operators (MPO)

general operator:

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

matrix product operator:

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

always possible, cf. MPS: $c^{\sigma_1 \ldots \sigma_L, \sigma'_1 \ldots \sigma'_L} \to c^{\sigma_1 \sigma'_1 \sigma_2 \sigma'_2 \ldots \sigma_L \sigma'_L}$

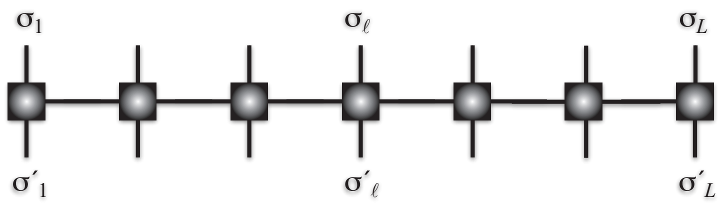
simple operators MPO of dimension *D*=1:

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

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

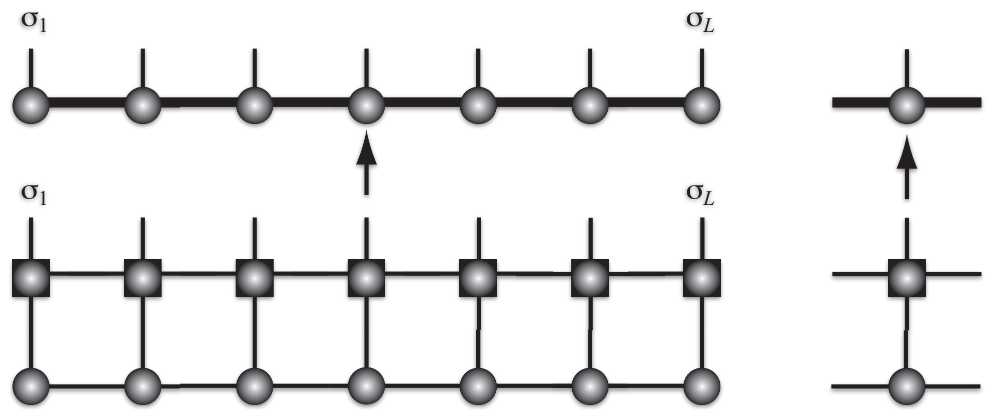
applying an MPO to an MPS

graphical representation with ingoing and outgoing physical states:



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

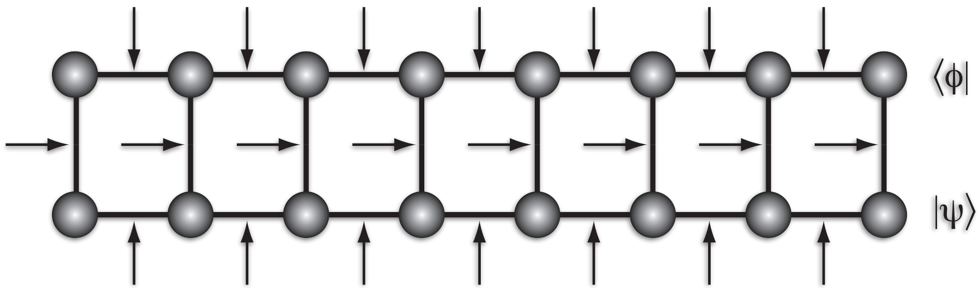
$$\tilde{M}^{\sigma_i}_{(ab),(a'b')} = \sum_{\sigma'_i} N^{\sigma_i \sigma'_i}_{aa'} M^{\sigma'_i}_{bb'}$$



overlaps

$$\langle \phi | \psi \rangle$$

overlap contractions:



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

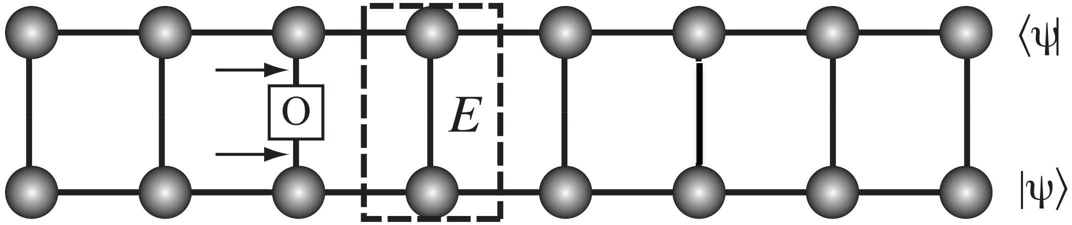
$$\begin{aligned} \langle \phi | \psi \rangle &= \sum_{\{\sigma\}} \tilde{M}^{\sigma_1 *} \dots \tilde{M}^{\sigma_L *} M^{\sigma_1} \dots M^{\sigma_L} \\ &= \sum_{\{\sigma\}} \tilde{M}^{\sigma_L \dagger} \dots \tilde{M}^{\sigma_1 \dagger} M^{\sigma_1} \dots M^{\sigma_L} \\ &= \sum_{\sigma_L} \tilde{M}^{\sigma_L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

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

expectation values

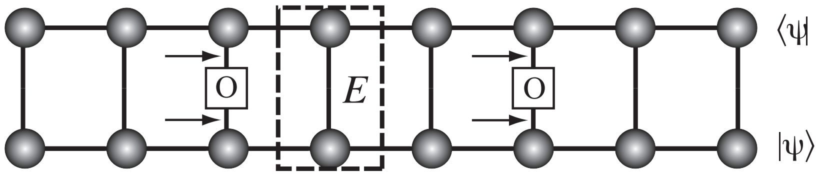
$$\langle\psi|\hat{O}|\psi\rangle$$

overlap contractions:



contractions again cost *O(dLD³)*

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



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

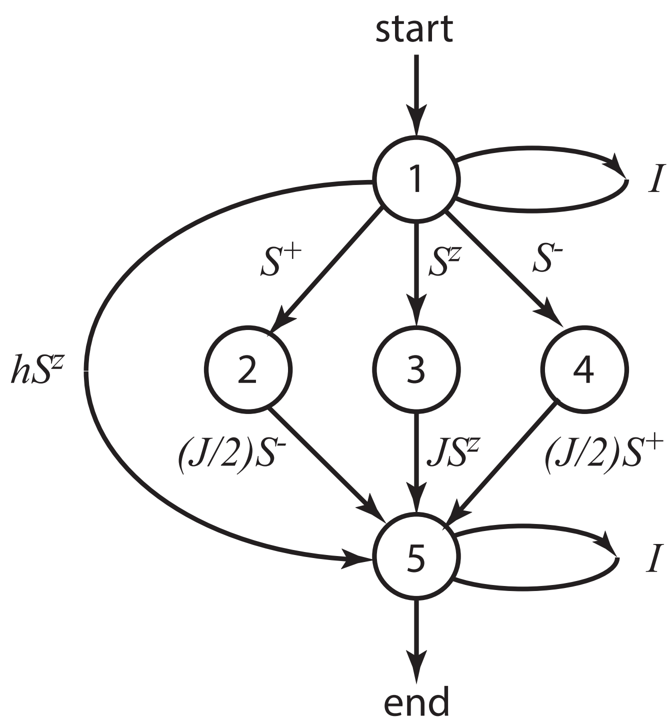
hence: power laws only „by approximation“

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!

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

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

complicated for long-ranged, generic Hamiltonians
efficient automated construction: Hubig, McCulloch, US(2017)

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:

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

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: $\qquad M = USV^\dagger$

$$A^{\sigma_\ell} \leftarrow A^{\sigma_\ell} U$$

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

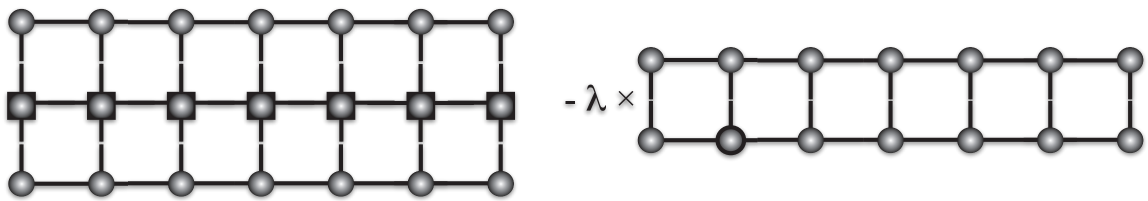
ground states with MPS: DMRG

variational ground state search: DMRG

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

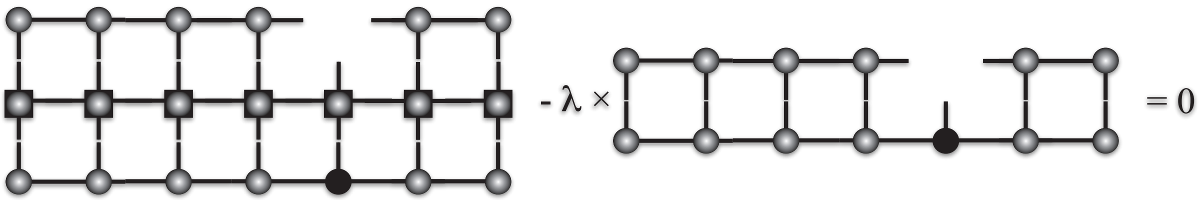
$$\min \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \quad \Leftrightarrow \quad \min \Big(\langle\psi|\hat{H}|\psi\rangle - \lambda\langle\psi|\psi\rangle\Big)$$

graphical representation of expression to be minimized:

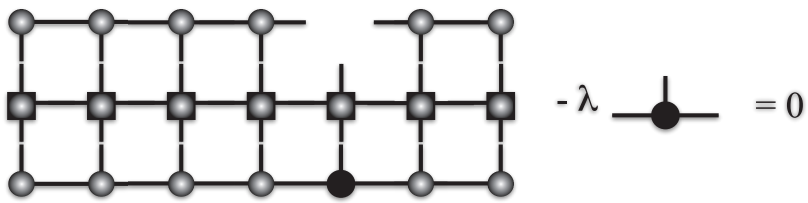


multilinear :-(

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:

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

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

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

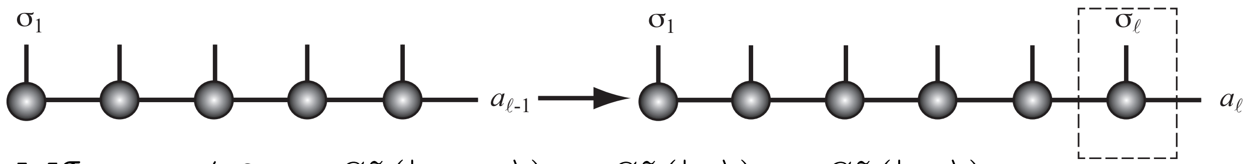
DMRG algorithm:

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

bells and whistles

- solving the eigenproblem is a large sparse matrix problem:
  - Lanczos, Davidson methods for „extreme“ eigenvalues/vectors of large sparse matrices *A* (dimension may be millions).
  - calculate powers $A|\psi\rangle, A^2|\psi\rangle = A(A|\psi\rangle), \ldots$
  - efficient implementation crucial!
- symmetries make MPS smaller and operations more efficient
  - Abelian symmetries (particle number, magnetisation) easy to implement



$M^{\sigma}_{a_{\ell-1}a_\ell} \neq 0 \Rightarrow S^z(|a_{\ell-1}\rangle) + S^z(|\sigma\rangle) = S^z(|a_\ell\rangle)$

block structures

saves O(10-100)

  - non-Abelian symmetries (e.g. SU(2)) much harder (McCulloch 2002, later Vidal, Weichselbaum)

further huge savings

- ensuring convergence: how do we get into a global minimum? (White 2005, e.g. Hubig et al 2015)