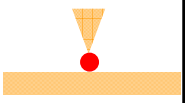
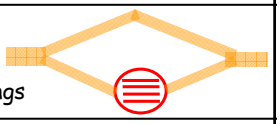
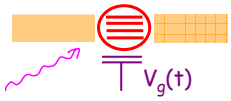
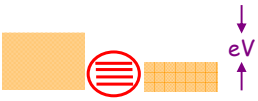
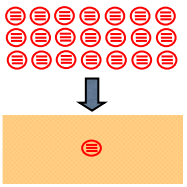
Numerical Renormalization group for Quantum Impurity Models

discrete quantum system + continuum 

Magnetic atom in metal (Kondo effect) 	STM-studies of adatoms on surfaces 
Transport through quantum dot(s) 	Phase-coherent transport Aharonov-Bohm rings 
Time-dependent driving 	Nonequilibrium steady-state transport 
Qubits (driving + dissipation)  $\Delta(t)\,\sigma_x + \varepsilon(t)\,\sigma_z$	Dynamical mean field theory (maps lattice model to self-consistent impurity model) 

Opening the NRG (and DMRG) black box

Numerical renormalization group (NRG) [Wilson, '75]

Quantum impurity models

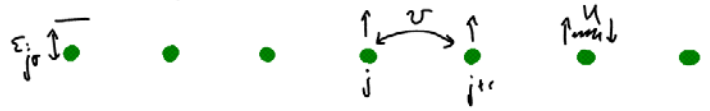
Density matrix renormalization group (DMRG) [White, '92]

Quantum chain models

- What is NRG good for?
- How does NRG work?
- How does DMRG work?
- Relation between NRG and DMRG
- Many-body dynamics meets quantum information theory

Many-Body Numerics: Matrix Product States 25.01.2011 MPS1

Consider 1-D quantum chain model, e.g. Hubbard model



$$H^{(N)} = \sum_{j=1}^{N}\sum_{\sigma} \varepsilon_{j\sigma} \underbrace{d^\dagger_{j\sigma} d_{j\sigma}}_{n_{j\sigma}} - \sum_{j=1}^{N}\sum_{\sigma} v_j \left(c^\dagger_{j\sigma} c_{j+1} + c^\dagger_{j+1} c_j \right) + \sum_{j=1}^{N} U_j \underbrace{d^\dagger_{j\uparrow} d_{j\uparrow}}_{n_{j\uparrow}} \underbrace{d^\dagger_{j\downarrow} d_{j\downarrow}}_{n_{j\downarrow}}$$

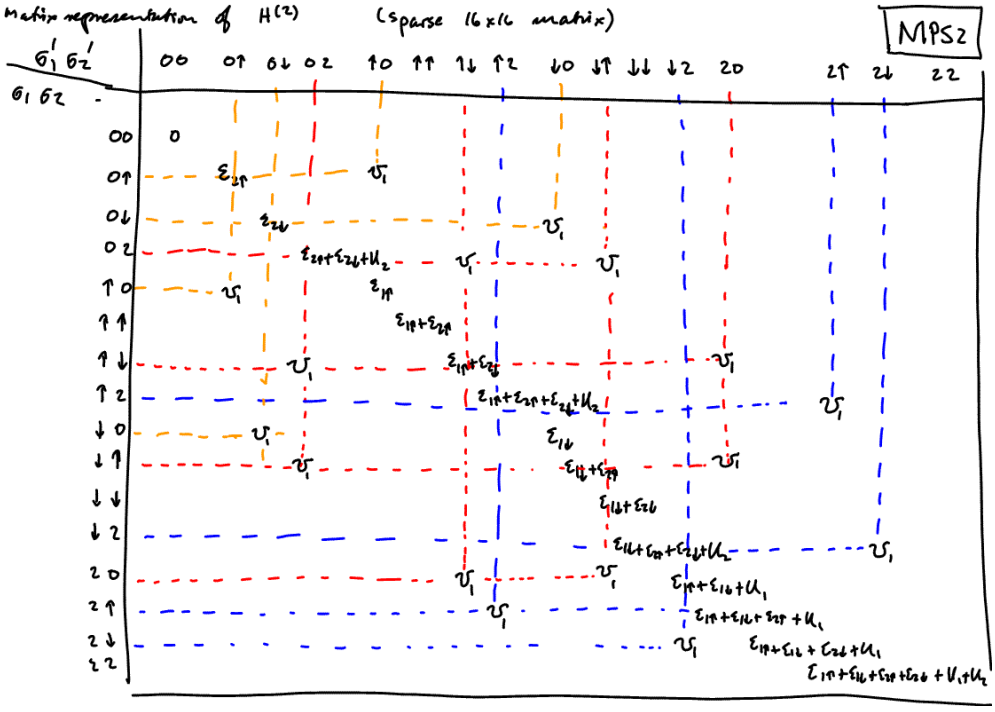
Local Hilbert space on site i: $|\sigma_i\rangle \in \{ |0\rangle, |\uparrow\rangle, |\downarrow\rangle, \underset{|\uparrow\downarrow\rangle}{|2\rangle} \} =: \mathcal{H}_1$

Local dimension: $d = 4$

Hilbert space for 2 sites: $|\sigma_1,\sigma_2\rangle \in \{ |00\rangle, |0\uparrow\rangle, |0\downarrow\rangle, |02\rangle, |\uparrow 0\rangle, |\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow 2\rangle, |\downarrow 0\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle, |\downarrow 2\rangle, |20\rangle, |2\uparrow\rangle, |2\downarrow\rangle, |22\rangle \}$

MPS2

Matrix representation of $H^{(2)}$ (sparse 16×16 matrix)



MPS 3

Full many-body Hilbert space:

$$\mathcal{H}^{(N)} = \bigotimes_{j=1}^{N} \mathcal{H}_j$$

Basis: $\{ |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \ldots \otimes |\sigma_N\rangle \}$, $\sigma_j \in 0, \uparrow, \downarrow, 2$ }

$\equiv |\sigma_1, \sigma_2, \ldots \sigma_N\rangle \equiv |\vec{\sigma}\rangle$

Dimension of $\mathcal{H}^{(N)} = d^N$ = exponentially large!

For small systems: "exact diagonalization", Lanczos algorithm

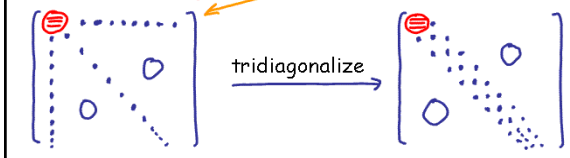
Basic problem: it is impossible to diagonalize $H^{(N)}$ numerically if N is large (say ≥ 10)

We need to truncate: throw away "useless" information!

How does NRG work?

$$H = H_0(d_j^\dagger, d_j) + \sum_k \varepsilon_k c_k^\dagger c_k + v\left(\sum_j d_j^\dagger \underbrace{\sum_k c_k}_{f_1} + \text{h.c.}\right)$$

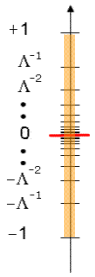
$d_j \to f_{0j}$



logarithmic discretization of cond. band:

$\omega_n = \Lambda^{-n}$

$\Lambda > 1$



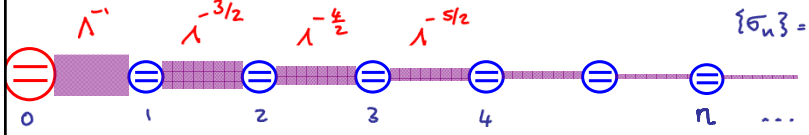
$$H = H_0(f_{0j}^\dagger, f_{0j}) + \sum_{n=1}^{\infty} \lambda_n \left(f_n^\dagger f_{n-1} + \text{h.c.}\right)$$

$\lambda_n \sim \Lambda^{-n/2}$

(Wilson chain)

local state space:

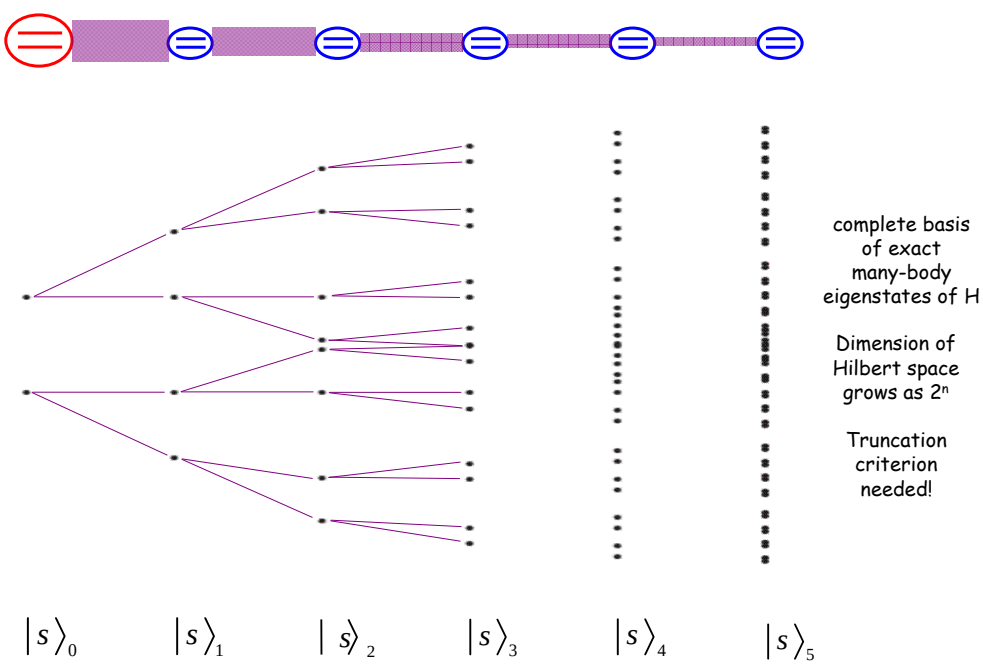
$\{\sigma_n\} = \{\underbrace{|0\rangle, |1\rangle}_{d=2}\}$



Diagonalize chain iteratively, discard high-energy states

Diagonalize Hamiltonian iteratively

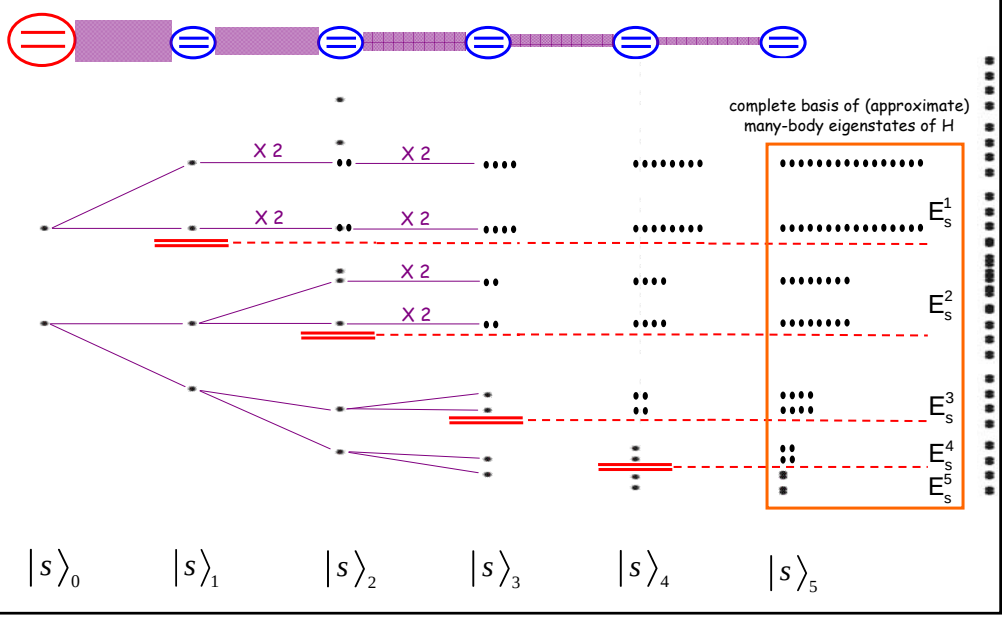
[Wilson, 1975]



Energy truncation, complete many-body basis

[Wilson, 1975] [Anders, Schiller, 2005]

build complete many-body basis from discarded states, keeping track of degeneracies



NRG yields Matrix Product States (MPS)

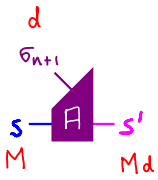
[Weichselbaum, Verstraete, Schollwoeck, Cirac, von Delft, 2005]

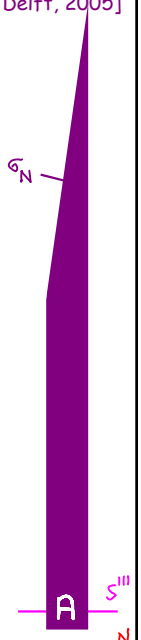
$H_n |s\rangle_n = E_s^n |s\rangle_n$ (M eigenstates)

$$|s'\rangle_{n+1} = \sum_{s\sigma_{n+1}} |s\rangle_n |\sigma_{n+1}\rangle [A^{\sigma_{n+1}}]_{ss'}$$

d matrices, M old states, Md new states

$${}_n\langle s|\langle\sigma_{n+1}|s'\rangle_{n+1}$$

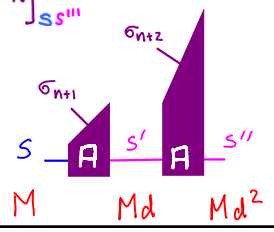




iterate:

$$|s'''\rangle_N = \sum |s\rangle_n |\sigma_{n+1}\rangle |\sigma_{n+2}\rangle \ldots |\sigma_N\rangle [A^{\sigma_{n+1}} A^{\sigma_{n+2}} \ldots A^{\sigma_N}]_{ss'''}$$

"matrix product state" (MPS)



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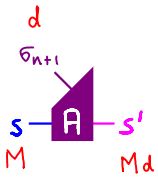

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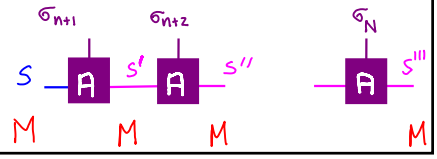
"matrix product state" (MPS)

Wilson truncation of high-energy states:



MPS 5

Matrix product states:

- Can give exact description of <u>any</u> $|\psi\rangle \in \mathcal{H}^{(N)}$ <u>provided</u> matrices are large enough: $A^{[\sigma_j]} = d^j \times d^{j+1}$
- Allow efficient <u>approximations</u> for ground state (low-lying excited states) of 1D chains with <u>short-range</u> interactions:

Take A^{σ_j} = $D \times D$ matrix for all j (D = "Matrix dimension")

Ansatz for ground state: $$|g\rangle = \sum_{\{\vec{\sigma}\}} |\sigma_1, \sigma_2, \ldots \sigma_N\rangle \, \mathrm{Tr}\left(A^{[\sigma_1]} A^{[\sigma_2]} \cdots A^{[\sigma_N]}\right)$$

MPS 6

Treat the elements of the matrices $A^{\sigma_j}_{\alpha\beta}[\,]$ as <u>variational</u> parameters, (there are $Nd\,D^2$ of them),

and <u>minimize</u> $\langle g | H^{(N)} | g \rangle$ with respect to $A^{[\sigma_j]}_{\alpha\beta}$ (1)

subject to the constraint that $\langle g | g \rangle = 1$. (2)

$$\Rightarrow \frac{\partial}{\partial A^{[\sigma_j]*}_{\alpha\beta}} \left[\langle g | \left(H^{(N)} - \lambda\right) | g \rangle \right] = 0 \qquad (\forall\, \sigma_j, \alpha, \beta) \quad (3)$$

(λ: Lagrange multiplyer.)

$$\frac{\partial}{\partial A^{[\sigma_j]*}_{\alpha\beta}} \mathrm{tr}\left(A^{[\sigma_N]\dagger} \cdots A^{[\sigma_1]\dagger}\right) \langle \vec{\sigma} | \left(H^{(N)} - \lambda\right) | \vec{\sigma}' \rangle \, \mathrm{tr}\left(A^{[\sigma'_1]} \cdots A^{[\sigma'_N]}\right) = 0 \quad (4)$$

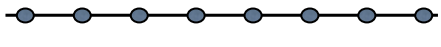
(quadratic in A's.)

Linear equation for $A^{\sigma_j}_{\alpha\beta}$, can be solved numerically

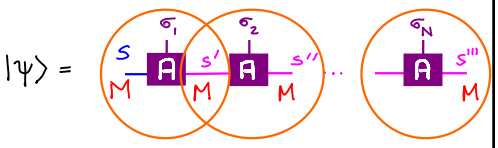
Strategy: (equivalent to DMRG "density matrix renormalization group") MPS-7

- fix all $A^{[\sigma_j]}$'s, except for site j: $A_j = \{A^{[\sigma_j]}, \sigma_j \in \{0,\uparrow,\downarrow,2\}\}$ (e.g. randomly)
- extremize $\langle\psi|(H-\lambda)|\psi\rangle$ w.r.t. A_j (i.e. also 6.4 for A_j), to obtain improved values for A_j
- move to neighboring site, and similarly improve A_{j+1}.
- "sweep" through chain back and forth a few times until ground state energy converges.
- (increase D, and repeat, until result no longer changes with D)

DMRG truncation strategy

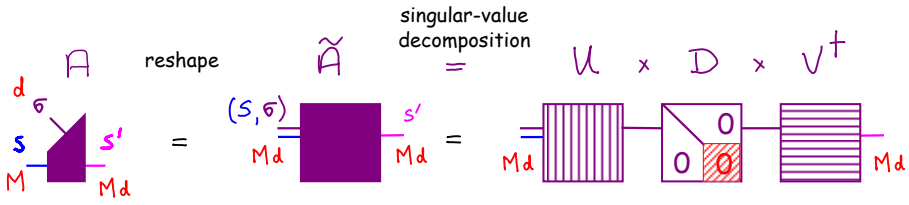


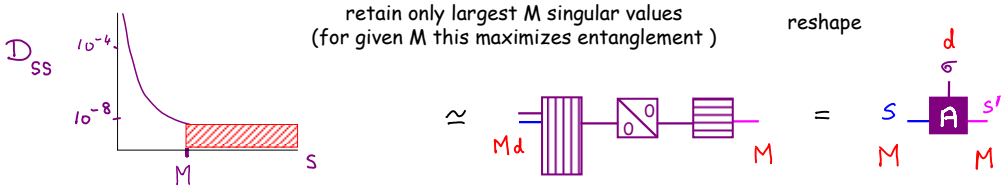
Fix size of matrices:



Variationally optimize ground state in space of matrix product states:

$$\frac{\partial}{\partial A^n}\ {}_{MPS}\langle\psi|H|\psi\rangle_{MPS} = 0$$





Advantages of MPS formulation

For quantum impurity problems:

- First truly "clean" algorithm for spectral functions at finite temperatures (full multi-shell DM) [Weichselbaum, von Delft, PRL 2007]

- Memory reduction by optimizing size of A-matrices

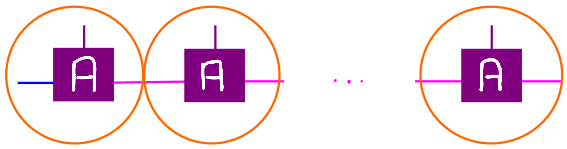
- Logarithmic discretization no longer needed [Weichselbaum et al, PRB 2009, Guo et al, 2009]

In general:

- Time-dependent problems !! (t-DMRG)
  [Daley, Kollath, Schollwöck, Vidal (2004)
  White, Feiguin, (2004)]

$$|\psi(t+\Delta t)\rangle = e^{-iH(t)\,\Delta t}\,|\psi(t)\rangle$$

$|\psi(t+\Delta t)\rangle$ =



Many-Body Numerics meets Quantum Information

Weichselbaum, Verstraete, Schollwöck, Cirac, von Delft (2005)
Weichselbaum, von Delft (2007)
Saberi, Weichselbaum, von Delft (2008)

MPS: matrix product states

Östlund, Rommer (1995)
Verstraete, Porras, Cirac (2004)

NRG: numerical renormalization group (Wilson, 1975)

⟷

DMRG: density matrix renormalization group (White, 1992)

quantum information theory

quantum impurity models
(discrete states + continuous bath)

magnetic moment + Fermi sea
atom/molecule + surface
quantum dot + leads
qubit + environment
dynamical mean-field theory

!!!

quantum chains

spin chains
1-d Hubbard model
quantum wires
polymers
1-d cold atoms

$$|\psi(t+\Delta t)\rangle = e^{-iH(t)\,\Delta t}\,|\psi(t)\rangle$$

nonequilibrium dynamics!!
(time-dependent driving, quantum quenches)

Daley, Kollath, Schollwöck, Vidal (2004)
White, Feiguin, (2004)

Literature:

-General Review of NRG (without MPS)
Bulla, R.; Costi, T. A. & Pruschke, T.
Numerical renormalization group method for quantum impurity systems
Reviews of Modern Physics, 80, 395 (2008)

- General Review on DMRG:
U. Schollwöck: The density-matrix renormalization group
Reviews of Modern Physics, 77, 259 (2005)

- Review of Matrix Product State approach to DMRG
W. Münder, A. Weichselbaum, A. Holzner, J. von Delft, C. Henley,
New J. Phys., 12, 075027 (2010), Appendix A

- DMRG in the age of Matrix Product States
U. Schollwöck
Annals of Physics, 326, 96 (2010)