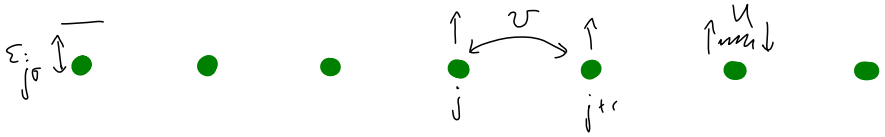
Many-Body Numerics: Matrix Product States

11.1.2010

MPS1

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



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

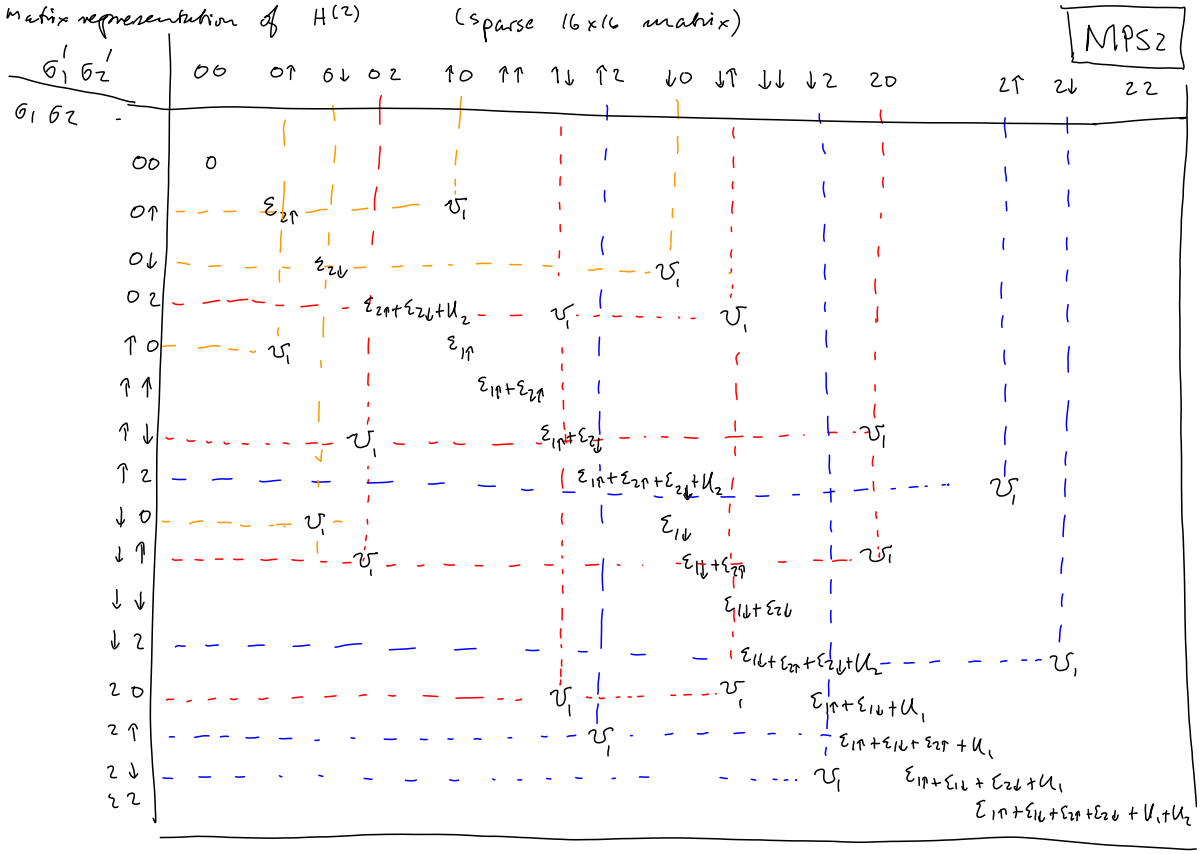
local Hilbert space on site i: $|\sigma_i\rangle \in \{ |0\rangle, |\uparrow\rangle, |\downarrow\rangle, \underset{|11\rangle}{|\uparrow\downarrow\rangle} \} =: \mathcal{H}_1$

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)



Full many-body Hilbert space:

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

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

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

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

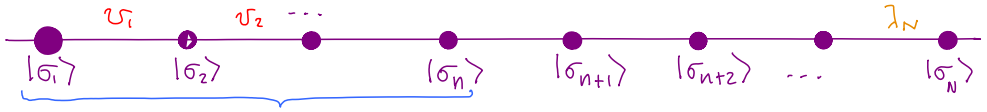
For small systems: "exact diagonalization", Lanczos algorithm

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

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

Iteration produces Matrix Product States

Verstraete, Weichselbaum, Schollwöck, Cirac, von Delft, cond-mat/0504305



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

$[A^{\sigma_{n+1}}]_{ss'}$: d matrices, $M \times (Md)$; old → new states

$\downarrow \lambda_{n+1} \neq 0$

$$|s'\rangle_{n+1} = \sum_{s\,\sigma_{n+1}} |s\rangle_n |\sigma_{n+1}\rangle \underbrace{\langle \sigma_{n+1}| \langle s|_n |s'\rangle_{n+1}}_{\mathbb{1}} \qquad (1)$$

$$|s'\rangle_{n+1} = \sum_{s\,\sigma_{n+1}} |s\rangle_n |\sigma_{n+1}\rangle [A^{\sigma_{n+1}}]_{ss'} \qquad (2)$$

$[N-1 \times N$ matrix$]$

truncation needed!

$\lambda_{n+2} \neq 0$

$\lambda_N \neq 0$

$$|s''\rangle_{\substack{n+2 \\ N}} = \sum |s\rangle_n |\sigma_{n+1}\rangle |\sigma_{n+2}\rangle \ldots |\sigma_N\rangle [A^{\sigma_{n+1}} A^{\sigma_{n+2}} \ldots A^{\sigma_N}]_{ss''} \qquad (3)$$

"matrix product state" (MPS)

Matrix product states:

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- Can give exact description of any $|\psi\rangle \in \mathcal{H}^{(N)}$ provided matrices are large enough: $A^{[\sigma_j]} = d^j \times d^{j+1}$

- Allow efficient approximations for ground state (low-lying excited states) of 1D chains with short-range interactions:

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

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

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

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

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

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

[Lagrange multiplyer.

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

quadratic in A's.

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

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

- fix all $A^{[\sigma]}$'s, except for site j: $A_j = \{A^{[\sigma_j]}, \sigma_j \in \{0,1,2,3\}\}$ (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)

Literature:

- 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,
  arXiv:0910.0753, Appendix A