Mechanism of symmetry breaking in matrix product states

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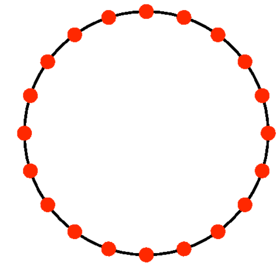
Outline

- **Optimization of periodic matrix product states**
- **Mechanism of symmetry breaking**
  - 1-d periodic transeverse-field Ising model
  - critical form of the magnetization curve (finite N, N=∞)
  - limitations of finite computer precision(?)
- **Use of discrete symmetries in MPSs (extension of MPS)**
  - Spin inversion, lattice reflection, translation
  - Tested on 1-d Heisenberg chain, including frustrated J_1-J_2 model

Matrix product states (MPSs)

Consider a periodic chain of S=1/2 spins



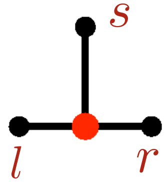
$$|\Psi\rangle = \sum_{\{s_i\}} W(s_1,s_2,\ldots,s_N)|s_1,s_2,\ldots,s_N\rangle, \qquad s_i = \uparrow,\downarrow$$

$$A(s) = \begin{pmatrix} a^s_{11} & \cdots & a^s_{1D} \\ a^s_{21} & \cdots & a^s_{2D} \\ \cdots & \cdots & \cdots \\ a^s_{D1} & \cdots & a^s_{DD} \end{pmatrix}$$

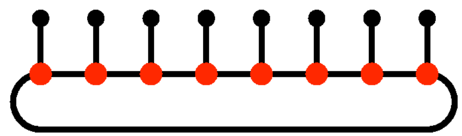
$$W(s_1,s_2,\ldots,s_N) = \mathrm{Tr}[A(s_1)A(s_2)\cdots A(s_N)]$$

- MPSs can be implicitly generated by DMRG (Ostlund & Romer, 1995)
- Can be used independently of DMRG as a class of variational states (1 dim)

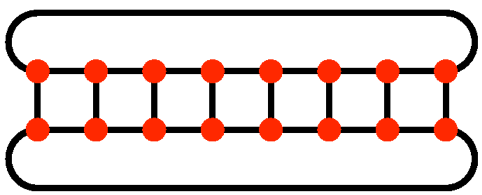
Graphical representation of a_{lr}^s and MPSs



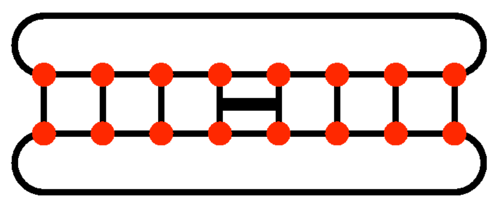
$$s = 1,2\ (\uparrow,\downarrow)$$
$$l,r = 1,\ldots,D$$



Normalization $\langle\Psi|\Psi\rangle$



Expectation value $\langle\Psi|S^a_i S^b_{i+1}\Psi\rangle$



These can be easily evaluated; scaling for periodic chain: standard way costs ND^5

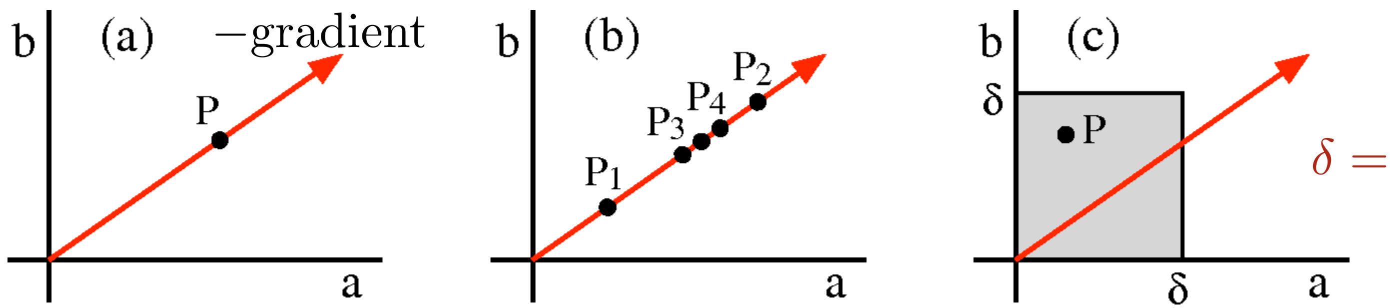
- Pippan, White, Evertz, ArXiv:0801.1947; good approximation (SVD) with ND^3 cost
- Monte Carlo sampling (Sandvik & Vidal, 2007); ND^3

How to optimize the matrices in MPS calculations

- Local energy minimization, "sweep" through the lattice (Verstraete et al.)
- Imaginary-time evolution (projecting out the ground state) (Vidal)

Minimize the energy variationally with translational invariance?

Stochastic Optimization (using first derivatives)

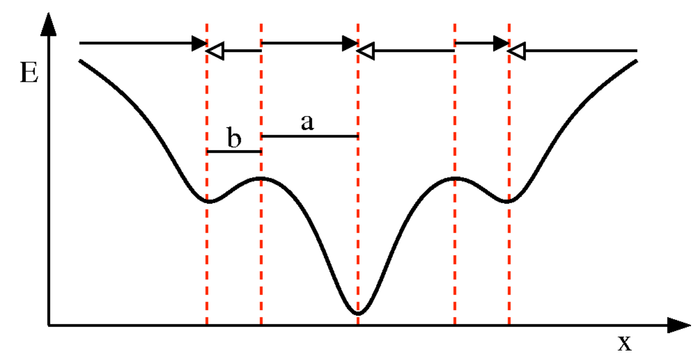


Steepest decent | Line minimization | Stochastic method

$$\delta = \frac{\delta_0}{k^\alpha}, \quad k = 1, 2, \ldots$$

The stochastic method is guaranteed to reach the global minimum if:

- "cooled" sufficiently slowly
- for all local minima on "funnel walls": b<a



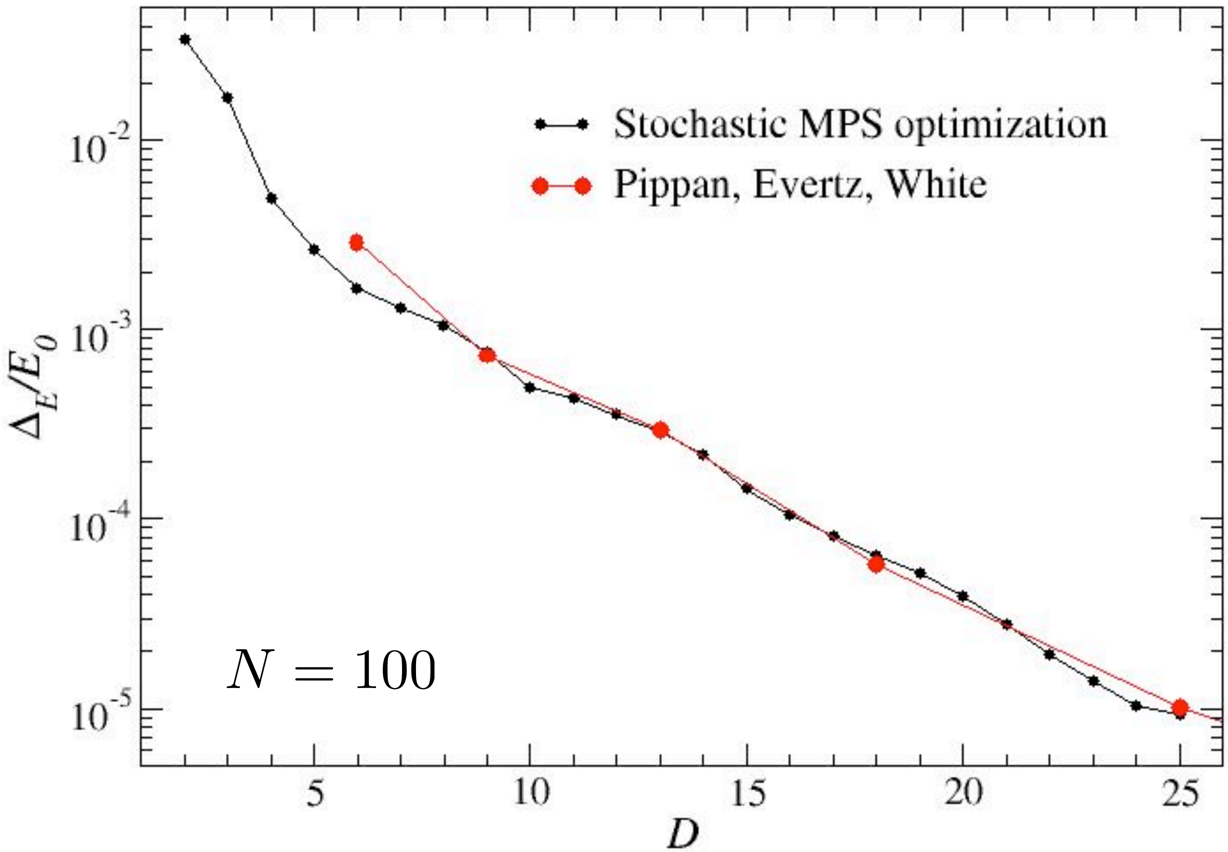
Seems to work well for MPS optimization

- Starting from random matrices or ones optimized for smaller D
- Steepest decent or line minimization can be faster at final stages

Test: Antiferromagnetic Heisenberg chain

$$H = \sum_{i=1}^{N} \mathbf{S}_i \cdot \mathbf{S}_{i+1} = \sum_{i=1}^{N} [S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)]$$

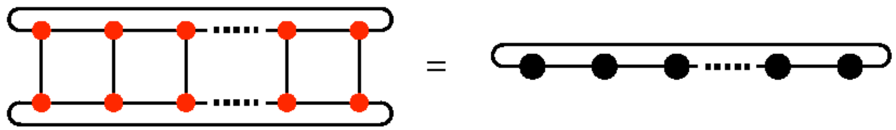
Comparison with N=100 results by: Pippan, White, Evertz, ArXiv: 0801.1947



Good results, but the method is very slow

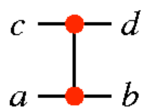
Infinite chain MPS

(a) $\langle\Psi|\Psi\rangle =$



$= \mathrm{Tr}\{P^N\}$

(b)



$= a+(c-1)D$ —●— $b+(d-1)D = A_{ab}(\uparrow)A^*_{cd}(\uparrow) + A_{ab}(\downarrow)A^*_{cd}(\downarrow) = P$

Exactly as in classical transfer-matrix method;

$$\langle O_1\rangle = \frac{\mathrm{Tr}\{O_1 P^{N-1}\}}{\mathrm{Tr}\{P^N\}}$$

- keep only largest eigenvalue of P when N→∞
- Imaginary-time evolution (ground state projection) can be applied (Vidal, Cirac et al.)

Question: How is symmetry breaking manifested in MPS (finite N and N→∞)**?**

Test: transverse-field Ising model

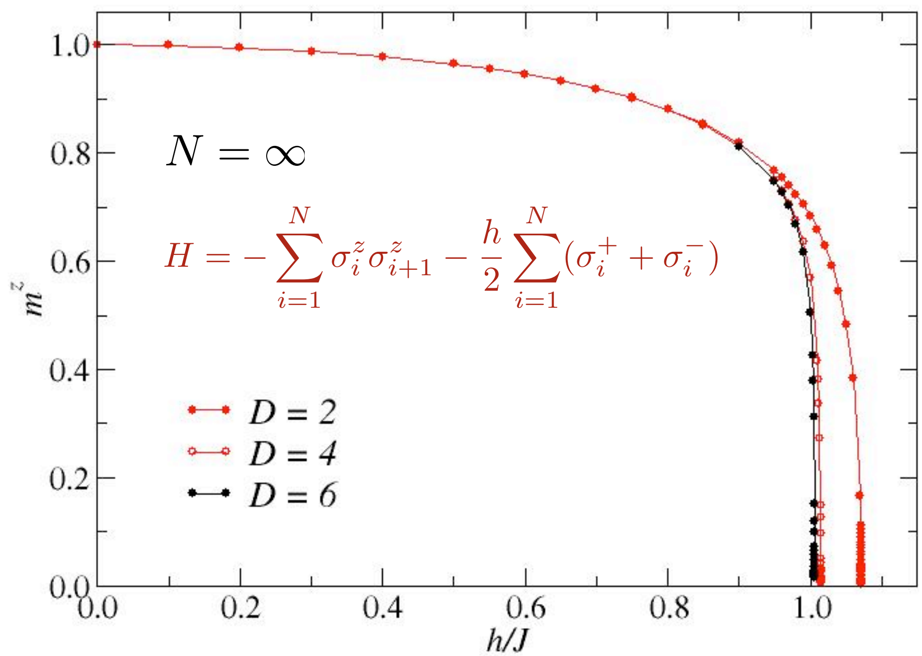
- true exponent β=1/8
- how does this exponent emerge?
- what is the $h\to h_c$ behavior for finite D?

Stochastic optimization?

Energy derivatives involve summing N contributions; time-consuming for N→∞

Optimize in a trivial (stupid?) way

- Propose random changes in the matrix elements, accept if energy improves
- easy to do in **quadruple precision**

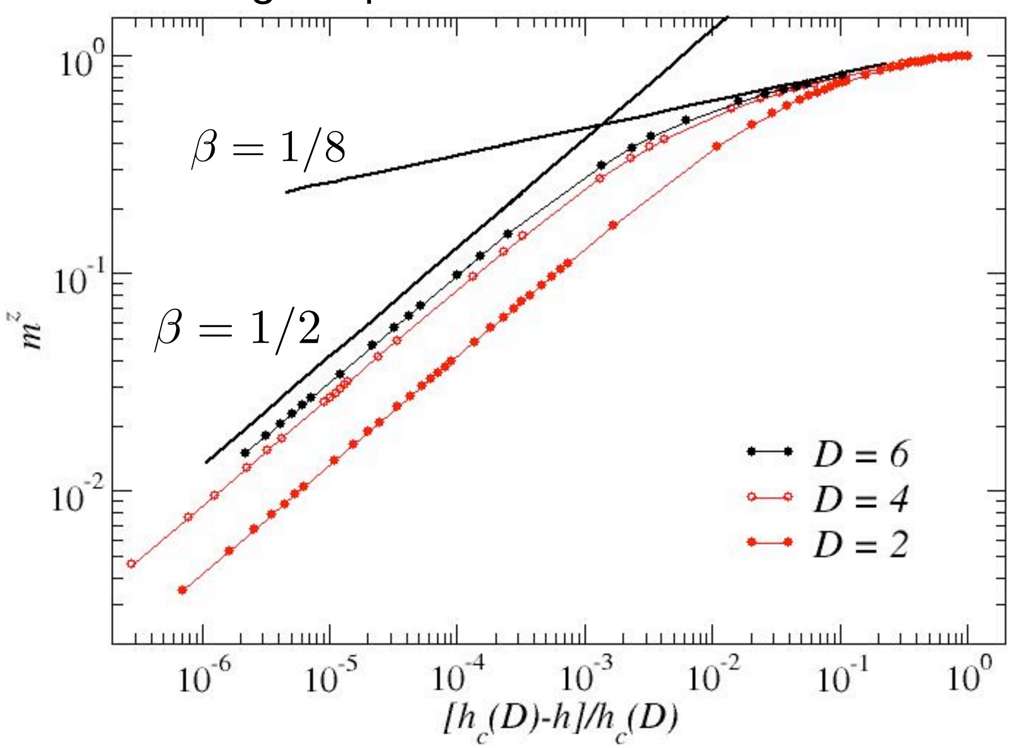


E/N	$m^z = \frac{1}{N}\sum_{i=1}^{N} S_i^z$	δ = max change in matrix elements
-1.274624764007379568601740	0.0107523120526	0.0000001652
-1.274624764007380869060010	0.0107537678231	0.0000001502
-1.274624764007382167234777	0.0107581552419	0.0000001366
-1.274624764007383018499448	0.0107499540804	0.0000001241
-1.274624764007392878608852	0.0107457713217	0.0000001128
-1.274624764007400992225410	0.0107333530705	0.0000001026
-1.274624764007405559290561	0.0107279581661	0.0000000933
-1.274624764007410209949167	0.0107265535218	0.0000000848
-1.274624764007416468671250	0.0107241180809	0.0000000771
relative change $= 3 \times 10^{-14}$	3×10^{-3}	

<u>Example</u>
Evolution of the energy and the magnetization

Small change in E→
much larger (relative) change in m^z
- can be serious close to h_c

converged optimized data

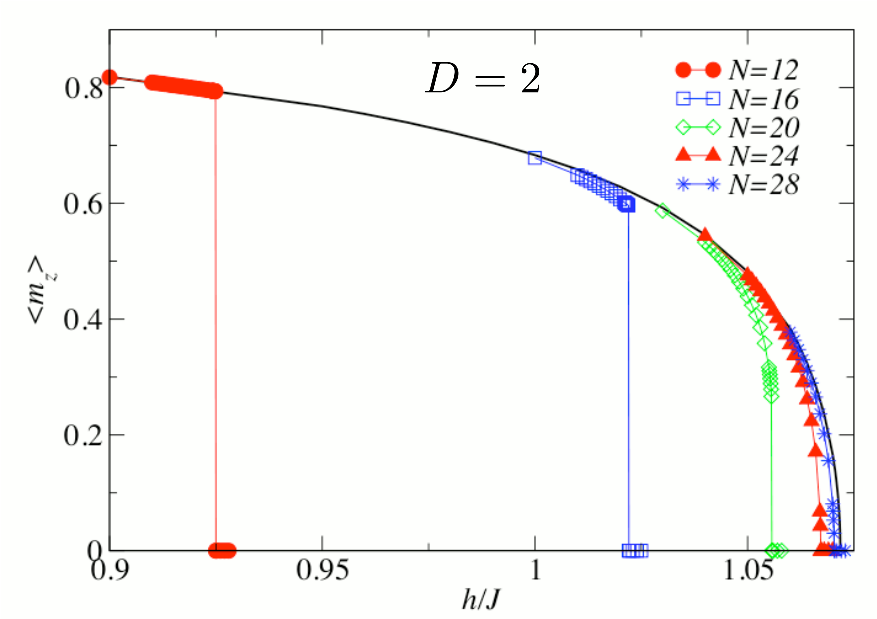


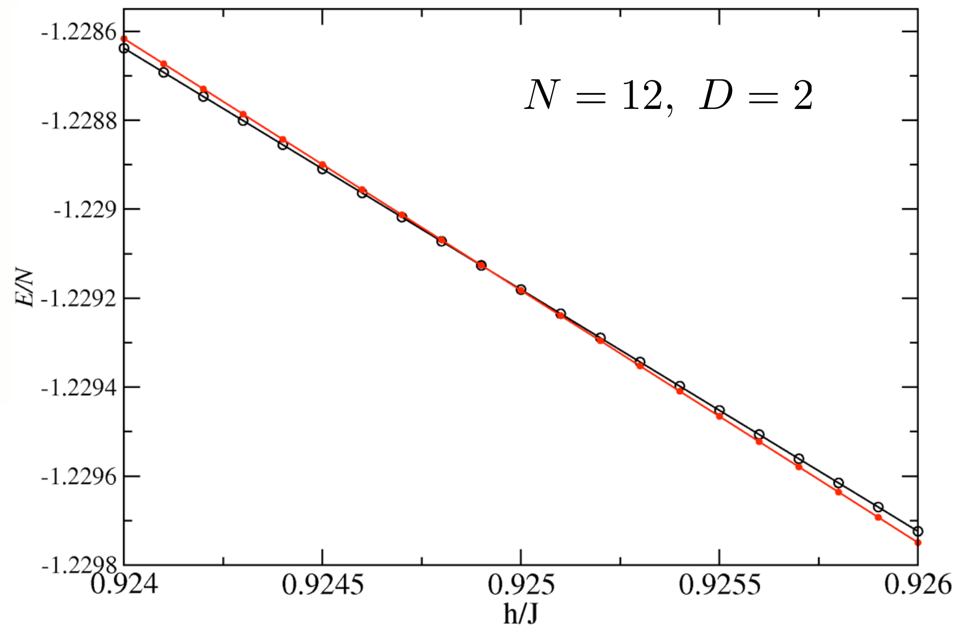
<u>Messages:</u>
- For N=∞ (or large N), numerical precision may limit access to critical behavior
- For finite D, asymptotic critical behavior is of mean-field type; cross-over to true exponent

Symmetry breaking for finite N

First-order transition (D fixed)

- discontinuity decreases with increasing N; continuous for N→∞
- level crossing between symmetric and symmetry-broken states (E minima)





Behavior versus matrix size D

- for given N, $h_c(D) \to 0$
- no symmetry-breaking for N<∞, D=∞

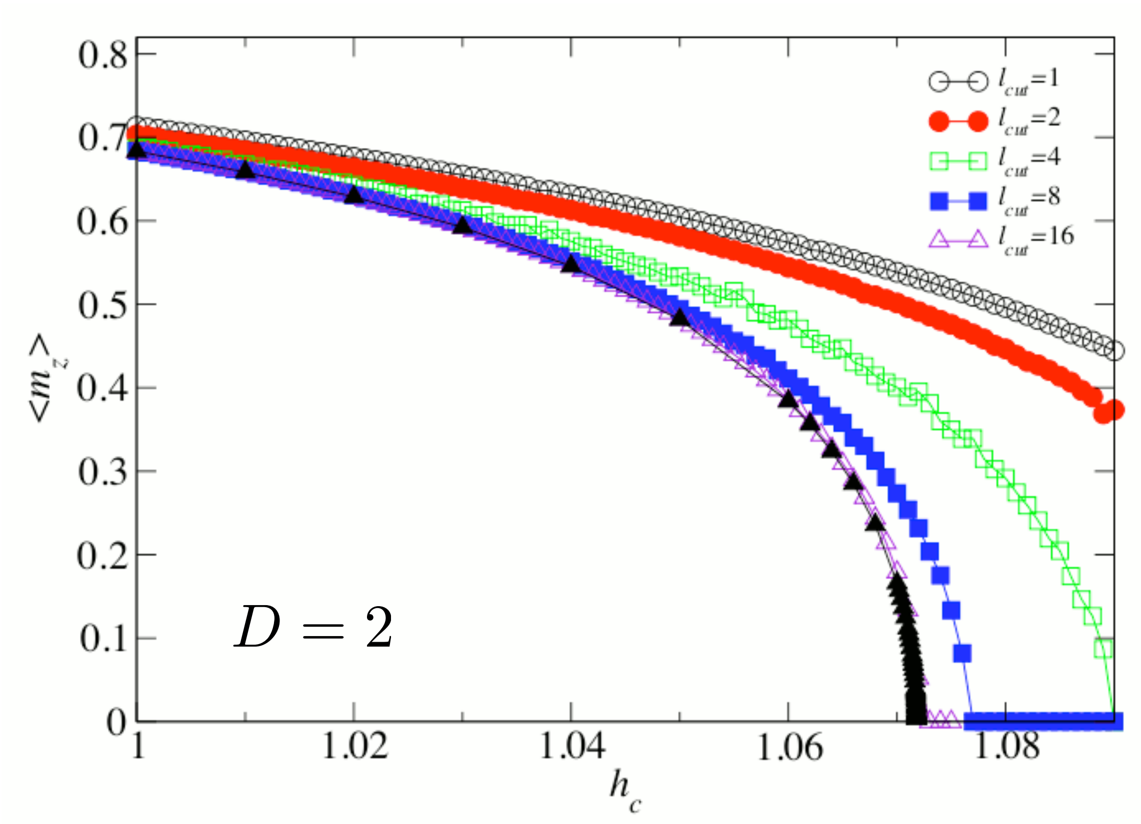
Infinite chain MPS - optimization using derivatives

The derivative of the energy with respect to a matrix element is of the form

$$\frac{\partial E}{\partial a_{ij}^{\sigma}} = C_{ij}^{\sigma} + \sum_{l=1}^{N-2} D_{ij}^{\sigma}(l) \qquad D(l) \sim \mathrm{Tr}\{XB^{l}XB^{N-2-l}\}$$

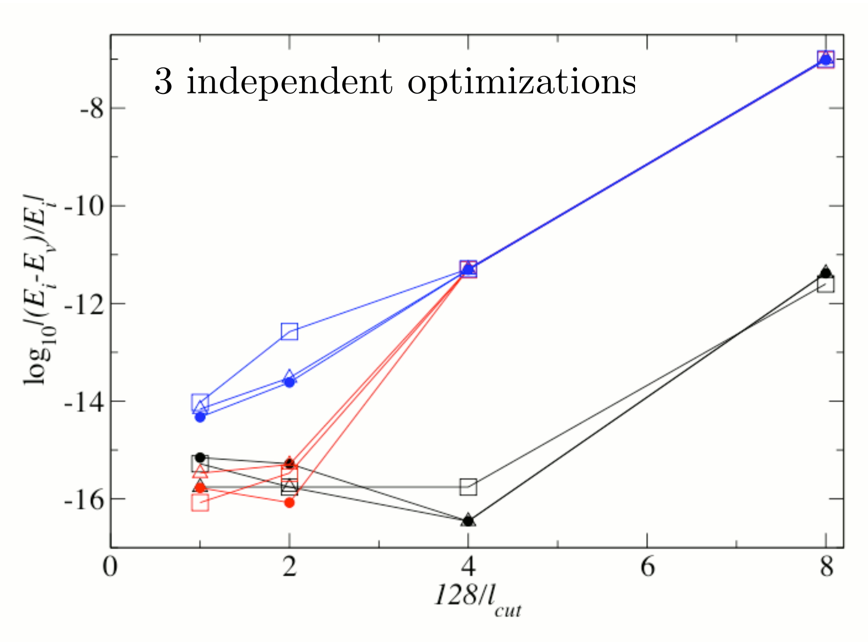
D(l) is a correlation function; D(l)→0 when l→∞

- impose cut-off l_{cut} in optimization for N=∞; investigate dependence on l_{cut}



Limitations of computer (double) precision?

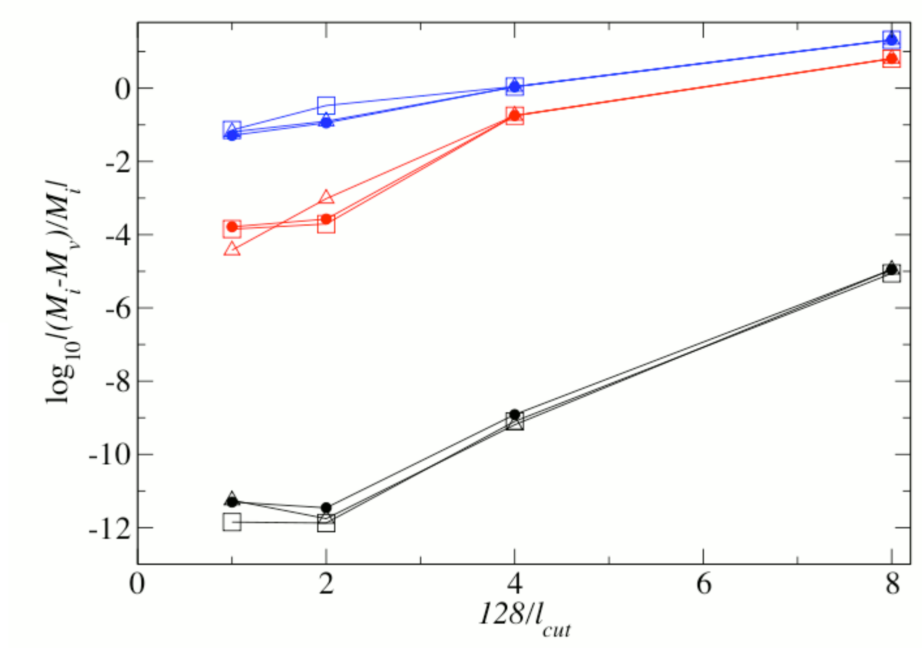
- optimizations using increasing l_{cut}
- compare with quadruple-precision derivative-free stochastic optimization



For large l_{cut} the limitation on E is the truncation error of double precision

The magnetization close to $h_c(D)$ is limited by the precision achievable for E

- $h = 1.071796$
- $h = 1.07179$
- $h = 1$

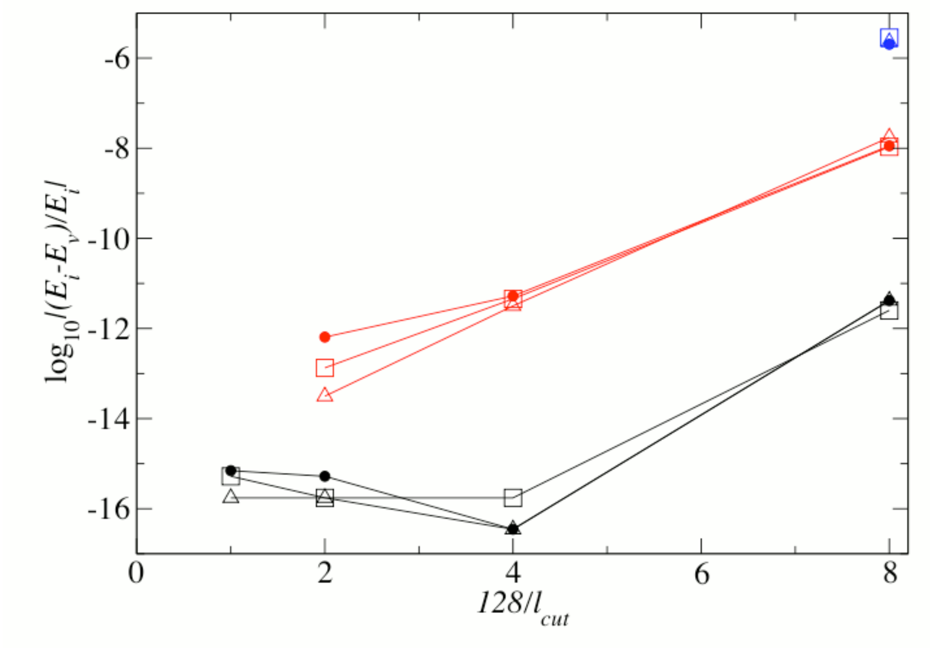


Dependence on matrix dimension D; D=2,3,4

$D = 4$

$D = 3$

$D = 2$



Message: Computer precision may be a limitation when studying critical properties

- seems to affect also imaginary-time proj
- but... critical long-distance correlation functions have been reproduced to high presision (Vidal, McCulloch,...)