New Development of Numerical Simulations in Low-Dimensional Quantum Systems:
From Density Matrix Renormalization Group to Tensor Network Formulations
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Matrix-Product states: Properties and Extensions

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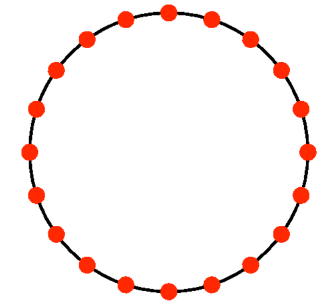
Outline

- **Variational optimization of periodic MPS**
- **Mechanism of symmetry breaking with MPS**
  - 1-d periodic transeverse-field Ising model
  - critical form of the magnetization curve (finite N, N=∞)
  - limitations of finite computer precision(?)
- **Criticality in 2D iPEPS (transverse-field Ising)**
- **MPS with variational Monte Carlo** (time permitting)

Matrix product states (MPS)

Consider a periodic chain of S=1/2 spins

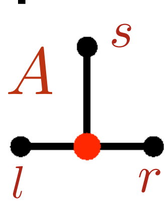


$$|\Psi\rangle = \sum_{\{s_i\}} W(s_1, s_2, \ldots, s_N)|s_1, s_2, \ldots, s_N\rangle, \qquad s_i = \uparrow, \downarrow$$

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

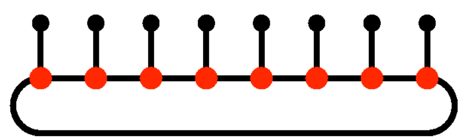
- MPSs can be implicitly generated by DMRG (Ostlund & Romer, 1995)
- Can be used independently of DMRG as a class of variational 1-d states

Graphical representation of a_{lr}^s and MPSs



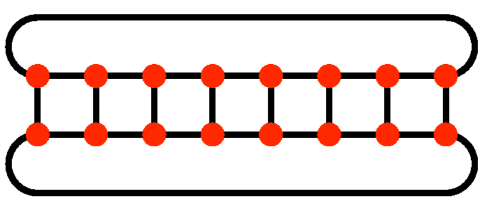
$s = 1, 2\ (\uparrow, \downarrow)$

$l, r = 1, \ldots, D$

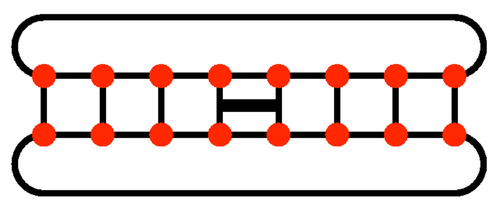


$$A(s) = \begin{pmatrix} a_{11}^s & \cdots & a_{1D}^s \\ a_{21}^s & \cdots & a_{2D}^s \\ \cdots & \cdots & \cdots \\ a_{D1}^s & \cdots & a_{DD}^s \end{pmatrix}$$

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



Expectation value $\langle \Psi | S_i^a S_{i+1}^b \Psi \rangle$



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

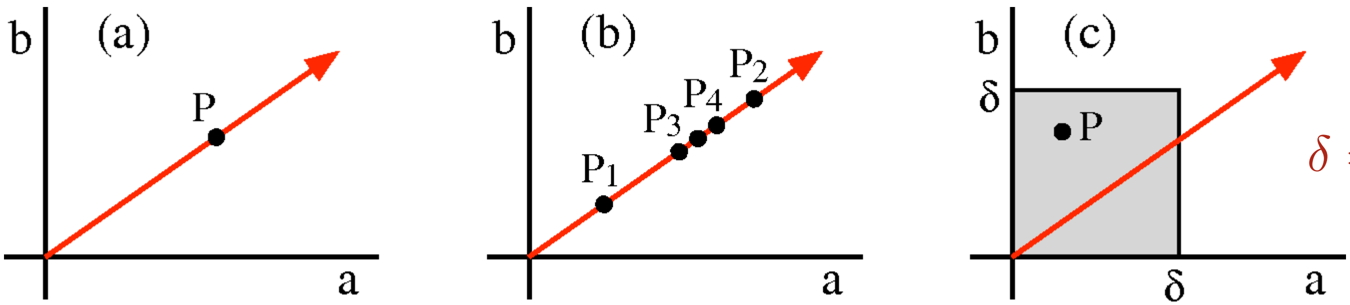
- Pippan, White, Evertz (PRB 2010); good approximation (SVD) with ND^3
- Monte Carlo sampling (Sandvik & Vidal, PRL 2007); ND^3

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 with maintained translational invariance?

Stochastic Optimization (using first derivatives)

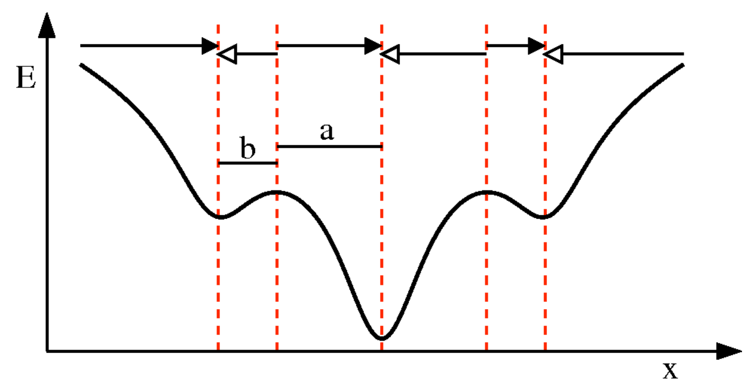


Steepest decent | Line minimization | Stochastic method

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

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

- “cooled” sufficiently slowly
- if all local minima on “funnel walls”: b<a



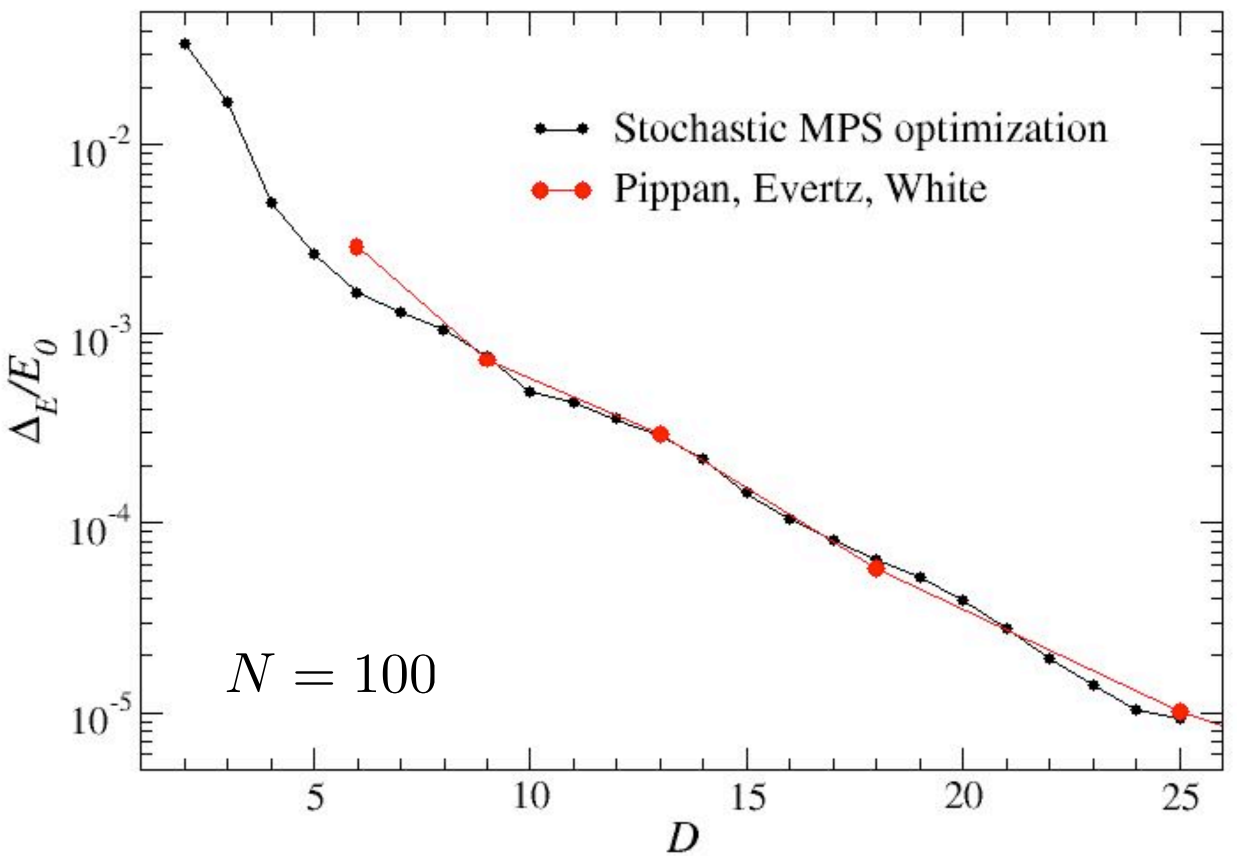
Seems to work well for MPS optimization

- Starting from random matrices or ones optimized for smaller D
- Steepest decent can be faster at final stages
- But much slower than conventional methods

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 (PRB 2010)

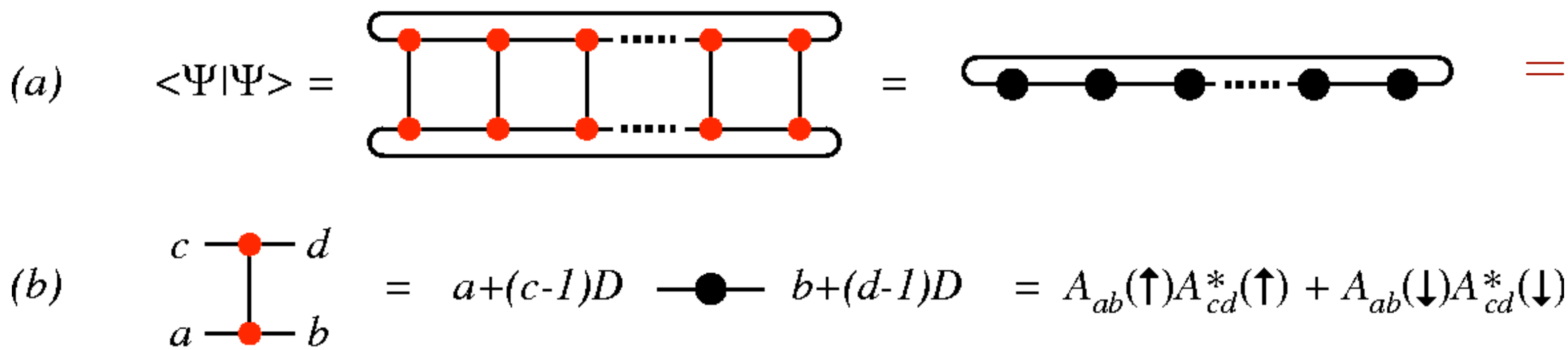


Good results, but the method is very slow

Infinite chain MPS

Exactly as in classical transfer-matrix method;

- keep only largest eigenvalue of P when N→∞
- Imaginary-time evolution (ground state projection) or DMRG-type optimization can be applied (Vidal, Cirac, McCulloch,...)



(a) $\langle\Psi|\Psi\rangle = \mathrm{Tr}\{P^N\}$

(b) $= A_{ab}(\uparrow)A^*_{cd}(\uparrow) + A_{ab}(\downarrow)A^*_{cd}(\downarrow) = P$

For some operator M (single-site, e.g., magnetization)

$$\langle M \rangle = \frac{\mathrm{Tr}\{MP^{N-1}\}}{\mathrm{Tr}\{P^N\}} \rightarrow \frac{1}{\lambda_1}\sum_{i,j} v^*_{1i} v_{1j} M_{ij}$$

Question: How is symmetry breaking manifested in MPS?

- for finite N and N→∞

Test: transverse-field Ising model

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

$$H = -\sum_{i=1}^{N} \sigma_i^z \sigma_{i+1}^z - \frac{h}{2} \sum_{i=1}^{N} (\sigma_i^+ + \sigma_i^-)$$

Stochastic optimization

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

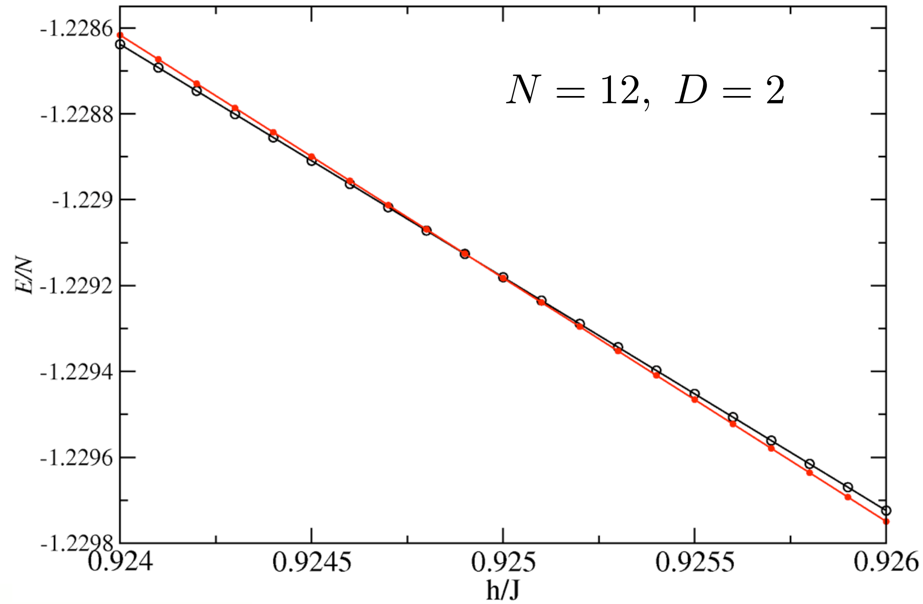
Optimize in a trivial (slow) way for N=∞

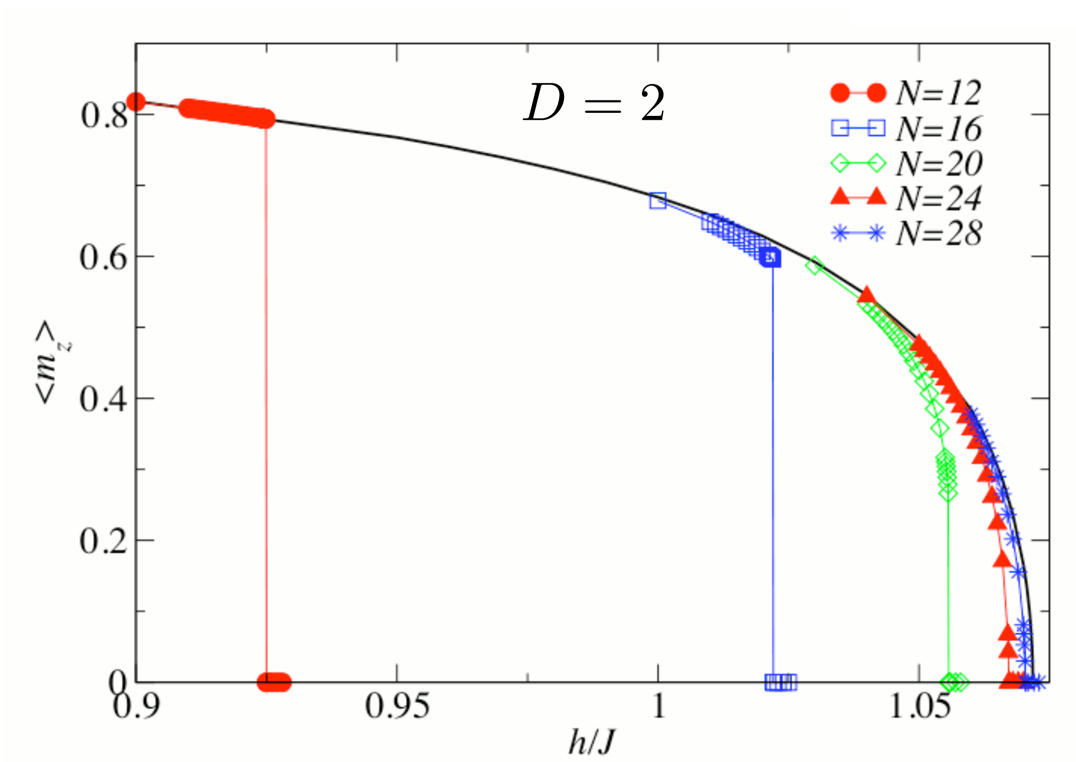
- Propose random changes in the matrix elements
  - accept if and only if the energy improves
- easy to do in **quadruple precision** (but very slow)

Symmetry breaking for finite N

First-order transition (D fixed)

- discontinuity decreases with increasing N
- continuous for N→∞
- two E minimums
  - symmetric and symmetry-broken states
- "level" crossing





Behavior versus D

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

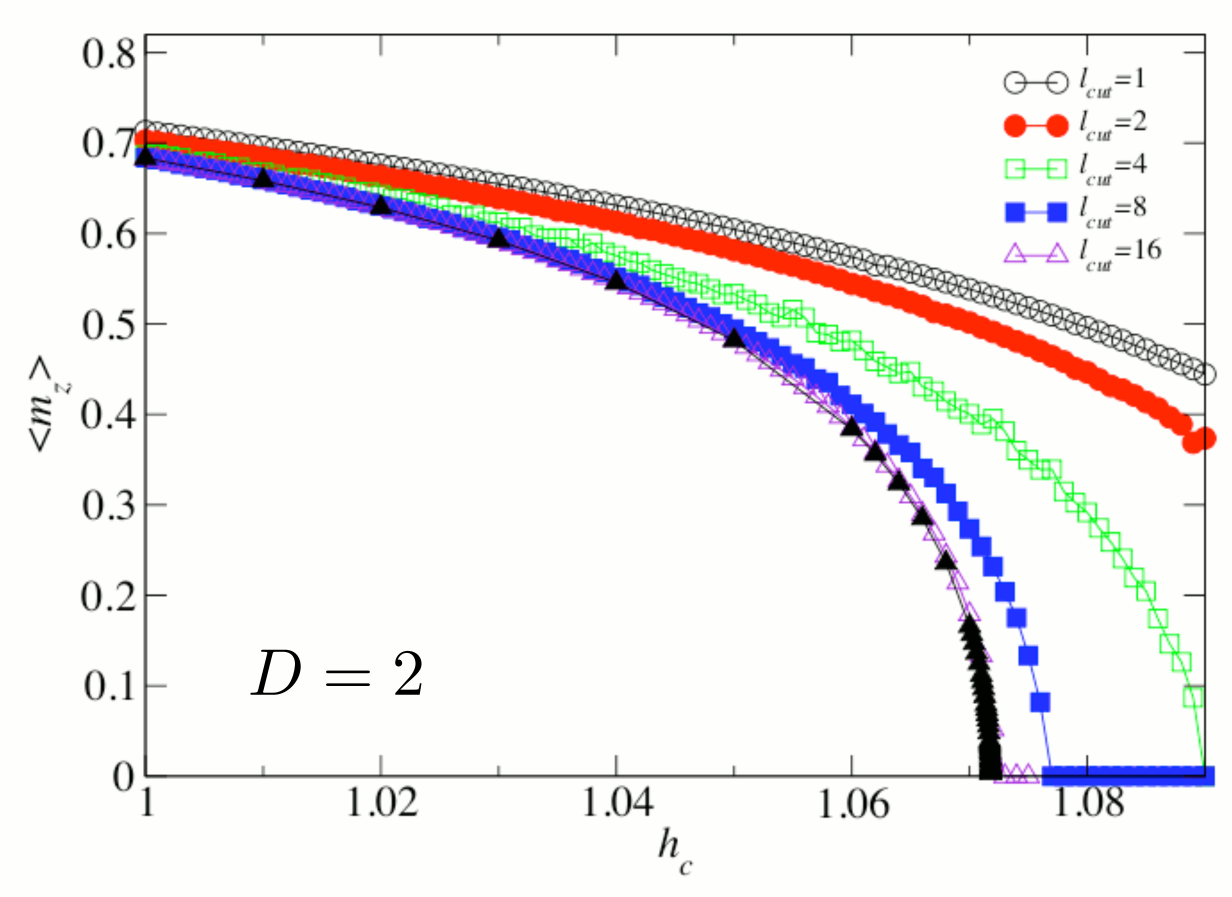
Infinite chain MPS - optimization using derivatives

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→∞

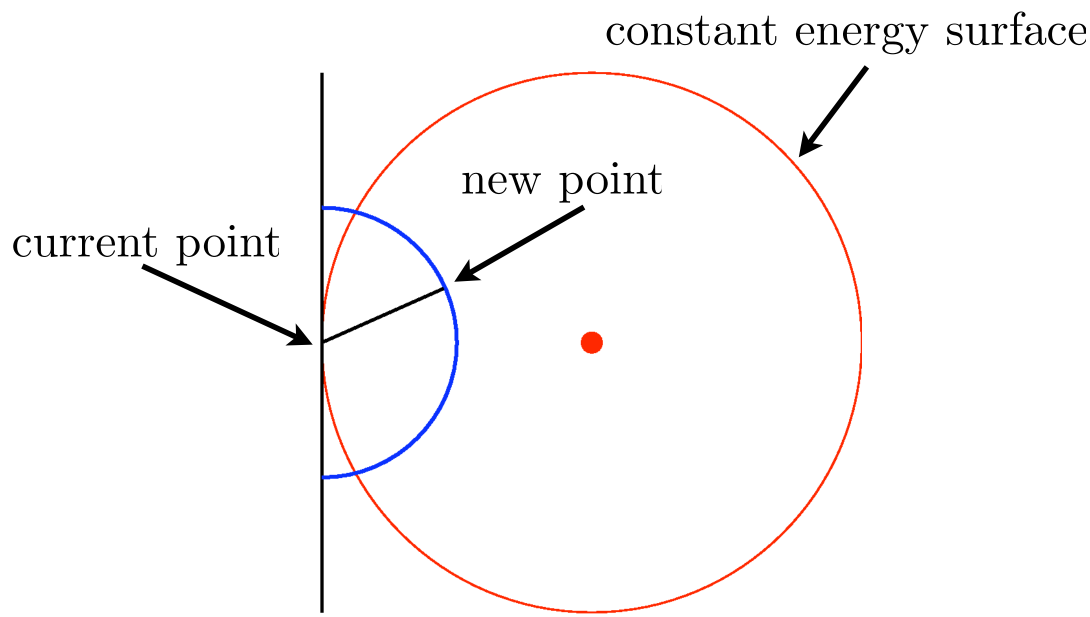
- impose cut-off l_{cut} in optimization for N=∞; dependence on l_{cut}



N=∞: Optimization using trivial random updates

Does not require derivatives

- propose random changes in all parameters; maximum change=δ
- accept only if the energy decreases
- for δ→0 the acceptance rate should be 50%
- adjust δ to give (e.g.) 10% acceptance rate



- find largest eigenvalue of P using

$$P^m v = \lambda_1^m v, \qquad m \to \infty$$

- efficient with m=1,2,4,8,.... → $P, P^2, P^4, P^8, \ldots$
- numerically stable
- easy to go to high precision (quadruple, 128 bit)

Example: D=4, h=1.01432

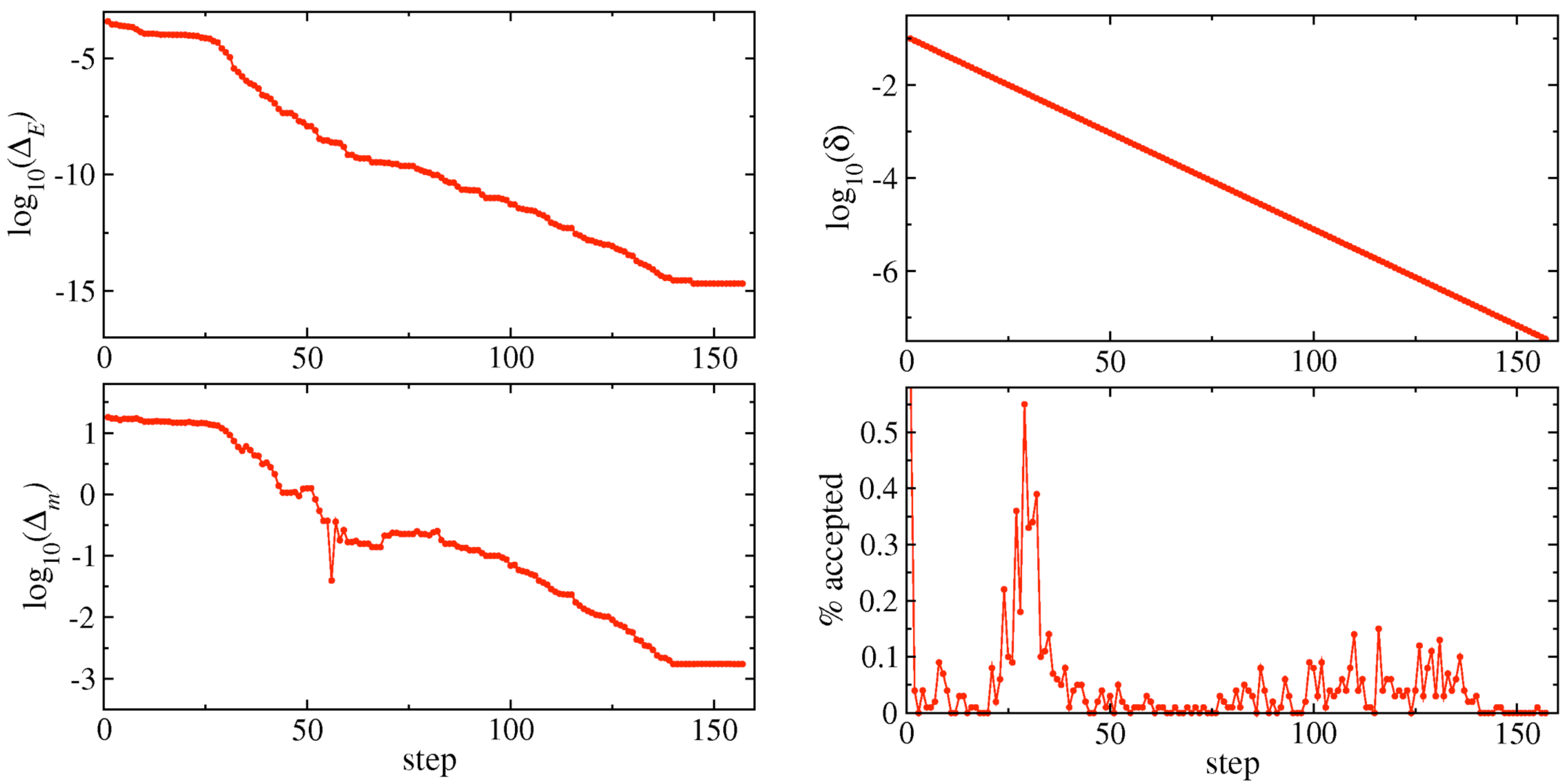
- 10^4 update attempts per “step”
- $\delta \rightarrow \delta/1.1$ after each step if <10% accepted updates
- **stage 1:** double precision, **stage 2:** quadruple precision
- E =-1.28244524657610764 2... , M_z=0.0318141670... (quad precision)

Errors relative to converged results (for given D)

$$\Delta_E = (E - E_{\rm conv})/E_{\rm conv}$$

$$\Delta_m = (m - m_{\rm conv})/m_{\rm conv}$$

evolution of δ and acceptance rate



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 $= 3 \times 10^{-14}$ $\quad 3 \times 10^{-3}$

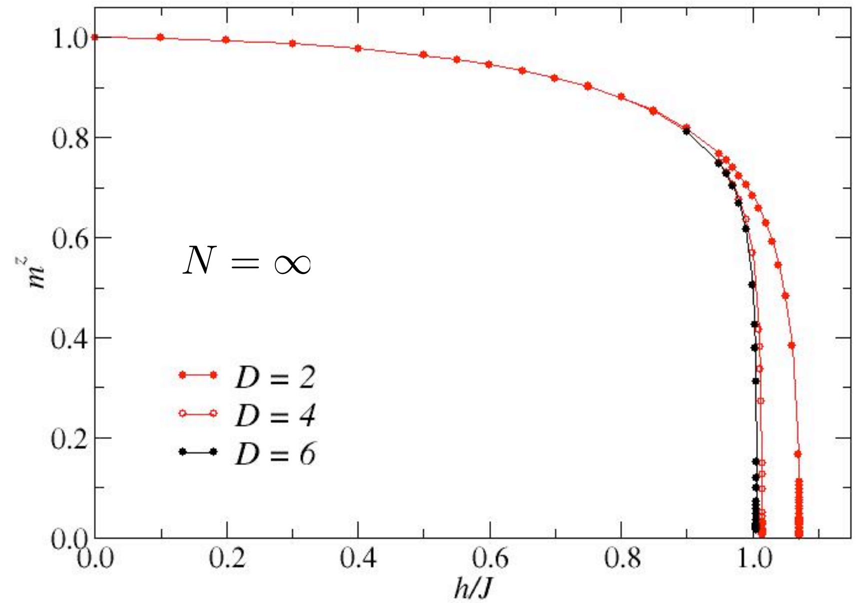
<u>Example</u>

Evolution of the energy and the magnetization

Close to the critical point:

Small change in E→
large (relative) change in m^z

- can be a serious issue when analyzing the critical behavior



Comparison with imaginary-time projection (TEBD); D=4, h=1.014334

E=-1.282454538906097 m=0.004589923026775 (I. McCulloch, standard)

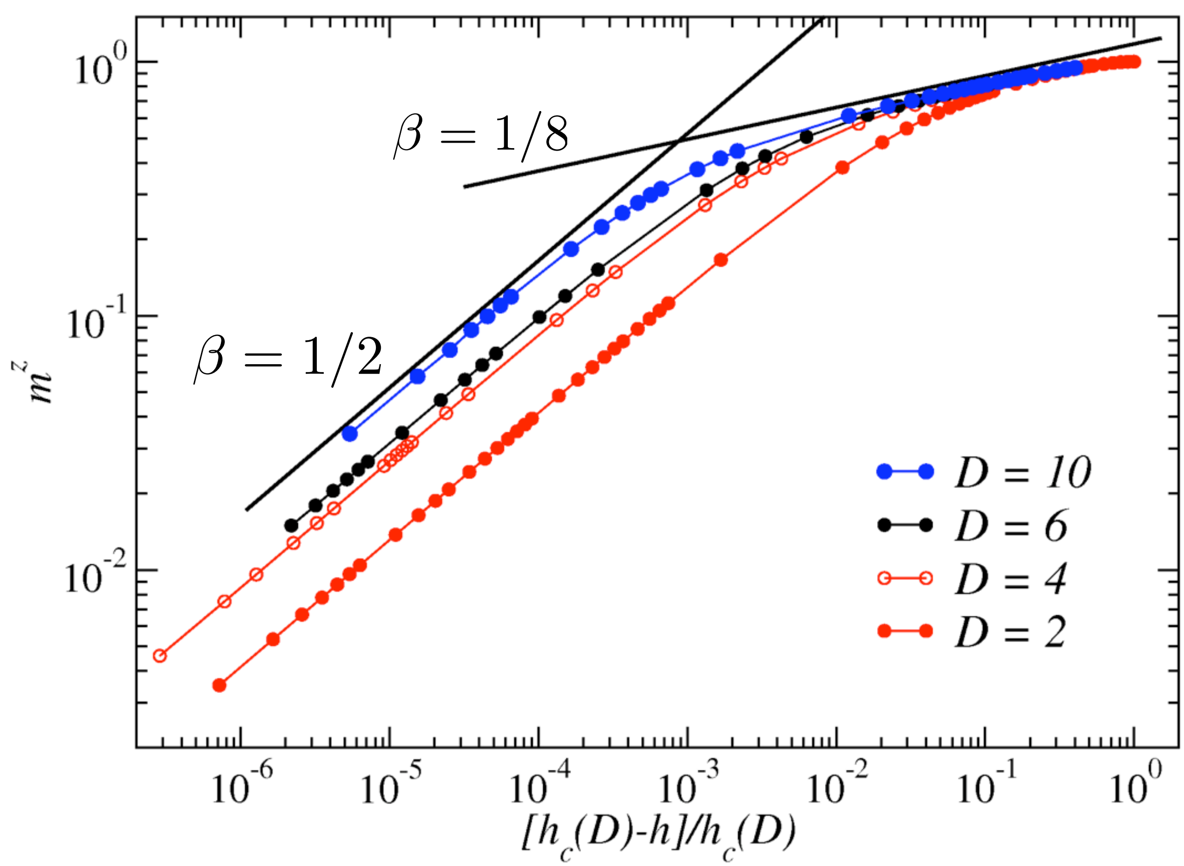
E=-1.28245453890609554713490 m=0.004589765790234 (Random optimization)

Analysis of the critical behavior

Power-law fit for small m^z always gives $\beta \approx 0.50$

- indicates asymptotic mean-field behavior

converged optimized data



- For finite D, asymptotic critical behavior is of mean-field type
  - cross-over to the true critical exponent
- numerical precision may limit access to critical behavior

The asymptotic mean-field behavior for MPS is not surprising

- finite D → maps to classical 1D transfer matrix
- criticality in 1D classical system requires long-range interactions

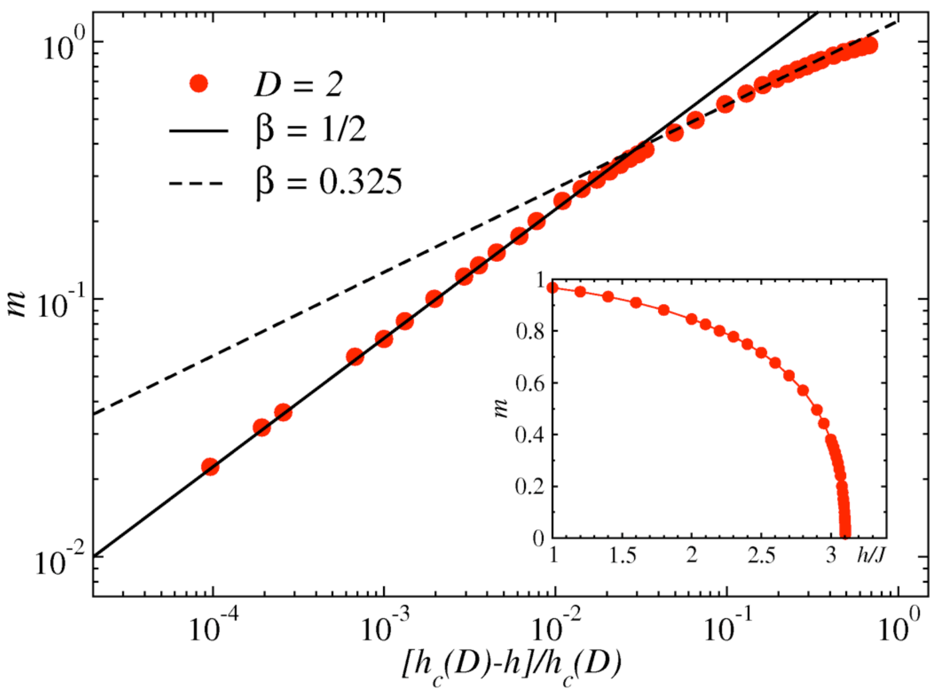
How about 2D PEPS?

Finite D → classical 2D partition function; critical points exist

- non-trivial exponents have been seen (?) for D=2,3 iPEPS

Infinite-size PEPS (iPEPS) [Orus & Vidal (2009)]

- Generalization of the N=∞ MPS (but more complicated, approximations)
- We use new stable optimization/contraction [Wang & Verstraete]



← 2D transverse-field Ising

- mean-field cross-over
- to extract the true exponent requires careful check of convergence with D
- the true exponent emerges in a window away from h_c
- similar cross-overs in classical systems (Baxter, Nishino et al.,...)

Conclusions

Symmetry-breaking in MPS

- **first-order for finite N, finite D**
- **continuous mean-field transition for N=∞, finite D**
  - mean-field window shrinks as D→∞
  - true exponents emerge through cross-over behavior

Numerical precision issues (variational optimization)

- **N=∞ optimization difficult close to phase transition**
  - relative error of order parameter large even if E converged
  - difficult to extract the critical point precisely

N=∞ PEPS (IPEPS)

- **mean-field criticality for finite D**
  - existence of non-trivial critical points for finite D does not mean that one automatically obtains correct critical behavior for a given H