Mechanism of symmetry breaking in matrix product states

Anders W Sandvik
Boston University

Collaborators
Chen Liu (Boston University)
Ling Wang (Boston University → U of Vienna)
Ying-Jer Kao (National Taiwan University, Taipei)
Yu-Cheng Su (National Taiwan University, Taipei)
Outline

• Optimization of periodic matrix product states

• Mechanism of symmetry breaking
  ‣ 1-d periodic transverse-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 J₁-J₂ model
Matrix product states (MPSs)

Consider a periodic chain of $S=1/2$ spins

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

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

- 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

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)

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

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

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

Good results, but the method is very slow
Infinite chain MPS

\[ \langle \Psi | \Psi \rangle = \begin{array}{c}
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet
\end{array} = \begin{array}{c}
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet \\
\bullet \quad \bullet \quad \bullet \quad \bullet \quad \bullet
\end{array} = \text{Tr}\{P^N\} \]

Exactly as in classical transfer-matrix method;
• keep only largest eigenvalue of P when \( N \to \infty \)
• Imaginary-time evolution (ground state projection) can be applied (Vidal, Cirac et al.)

Test: transverse-field Ising model
• true exponent \( \beta = 1/8 \)
• 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 \( N \to \infty \)

Optimize in a trivial (stupid?) way
• Propose random changes in the matrix elements, accept if energy improves
• easy to do in quadruple precision

\[ \langle O_1 \rangle = \frac{\text{Tr}\{O_1 P^{N-1}\}}{\text{Tr}\{P^N\}} \]
\[ E/N \]

\[ m^z = \frac{1}{N} \sum_{i=1}^{N} S_i^z \]

\[ \delta = \text{max change in matrix elements} \]

\begin{align*}
-1.274624764007379568601740 & \quad 0.0107523120526 & 0.0000001652 \\
-1.274624764007380869060010 & \quad 0.0107537678231 & 0.0000001502 \\
-1.274624764007382167234777 & \quad 0.0107581552419 & 0.0000001366 \\
-1.274624764007383018499448 & \quad 0.0107499540804 & 0.0000001241 \\
-1.274624764007392878608852 & \quad 0.0107457713217 & 0.0000001128 \\
-1.27462476400740099225410 & \quad 0.0107333530705 & 0.0000001026 \\
-1.274624764007405559290561 & \quad 0.0107279581661 & 0.0000000933 \\
-1.274624764007410209949167 & \quad 0.0107265535218 & 0.0000000848 \\
-1.274624764007416468671250 & \quad 0.0107241180809 & 0.0000000771
\end{align*}

Relative change = \(3 \times 10^{-14}\)

Small change in \(E\) \\
Much larger (relative) change in \(m^z\)

- Can be serious close to \(h_c\)

### Messages:

- For \(N=\infty\) (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 $N \rightarrow \infty$
- level crossing between symmetric and symmetry-broken states ($E$ minima)

Behavior versus matrix size $D$
- for given $N$, $h_c(D) \rightarrow 0$
- no symmetry-breaking for $N < \infty$, $D = \infty$
Infinite chain MPS - optimization using derivatives

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

$$\frac{\partial E}{\partial a_{ij}^\sigma} = C_{ij}^\sigma + \sum_{l=1}^{N-2} D_{ij}^\sigma(l)$$

$$D(l) \sim \text{Tr}\{X B^l X B^{N-2-l}\}$$

$D(l)$ is a correlation function; $D(l) \to 0$ when $l \to \infty$

- impose cut-off $l_{\text{cut}}$ in optimization for $N=\infty$; investigate dependence on $l_{\text{cut}}$

\[ D = 2 \]
Limitations of computer (double) precision?

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

For large $l_{\text{cut}}$ 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 $E$
Dependence on matrix dimension D; D=2,3,4

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 precision (Vidal, McCulloch,...)