Matrix Product States and the Thermodynamic Limit

Order parameters and scaling relations

Ian McCulloch

University of Queensland

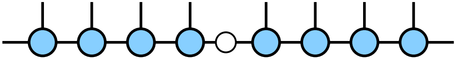
19/12/2009

Outline

MPS representations

Matrix Product State: approximate an exponential number of coefficients with a product of $D \times D$ matrices

$$|\Psi\rangle = \mathrm{Tr} \sum_{s_1, s_2, \ldots} A^{s_1} A^{s_2} A^{s_3} A^{s_4} \cdots |s_1\rangle |s_2\rangle |s_3\rangle |s_4\rangle \cdots$$



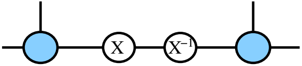
$$A^{\sigma_1} \; A^{\sigma_2} A^{\sigma_3} \; A^{\sigma_4} \Lambda \; A^{\sigma_5} A^{\sigma_6} A^{\sigma_7} A^{\sigma_8}$$

Λ is the wavefunction in the bipartite basis
$|\Psi\rangle = \sum_{ij} \Lambda_{ij} |i\rangle_L |j\rangle_R$

This is the variational form underlying the Density Matrix Renormalization Group Algorithm (White, 1992)

Orthonormality conditions

- Without any attention to conditioning the matrices, an MPS calculation is ill-conditioned

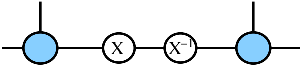


We make use of this gauge freedom to condition the matrices

- This is necessary to construct an orthonormal basis

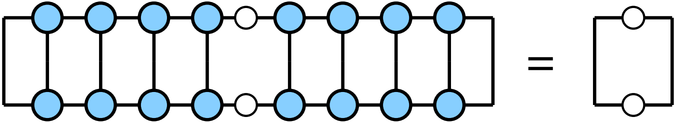
Orthonormality conditions

- Without any attention to conditioning the matrices, an MPS calculation is ill-conditioned



We make use of this gauge freedom to condition the matrices

- This is necessary to construct an orthonormal basis

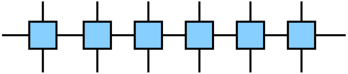


$$= \sum \Lambda_{ij}^2 = 1$$

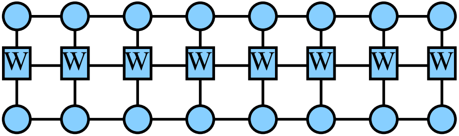
Matrix representation of the Hamiltonian

I P McCulloch, J. Stat. Mech. P10014 (2007)

Convenient representation: the Hamiltonian operator as a 4-index *MPO*



DMRG cast as variational optimization of a tensor network for the energy



Some examples:

Sum of local terms $H = \sum_i X_i$

$W_H = \begin{pmatrix} I & 0 \\ X & I \end{pmatrix}$ Boundary vectors $\begin{pmatrix} 0 & I \end{pmatrix}$ and $\begin{pmatrix} I \\ 0 \end{pmatrix}$

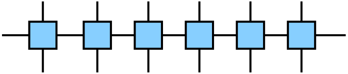
Expand the product W^N:

$$\begin{aligned} & X \otimes I \otimes I \otimes I \otimes I \cdots \\ + \; & I \otimes X \otimes I \otimes I \otimes I \cdots \\ + \; & I \otimes I \otimes X \otimes I \otimes I \cdots \end{aligned}$$

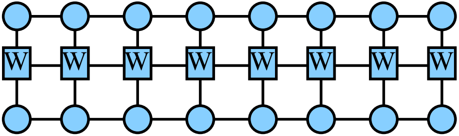
Matrix representation of the Hamiltonian

I P McCulloch, J. Stat. Mech. P10014 (2007)

Convenient representation: the Hamiltonian operator as a 4-index *MPO*



DMRG cast as variational optimization of a tensor network for the energy



Some examples:

Sum of local terms $H = \sum_i X_i$

$$W_H = \begin{pmatrix} I & 0 \\ X & I \end{pmatrix}$$

Boundary vectors $\begin{pmatrix} 0 & I \end{pmatrix}$ and $\begin{pmatrix} I \\ 0 \end{pmatrix}$

Expand the product W^N:

$$\begin{array}{cl} & X \otimes I \otimes I \otimes I \otimes I \otimes I \cdots \\ + & I \otimes X \otimes I \otimes I \otimes I \otimes I \cdots \\ + & I \otimes I \otimes X \otimes I \otimes I \otimes I \cdots \end{array}$$

Matrix Product Operators

Sum of nearest-neighbor terms $H = \sum_i X_i Y_{i+1}$

$$W_H = \begin{pmatrix} I & 0 & 0 \\ Y & 0 & 0 \\ 0 & X & I \end{pmatrix}$$

Ising model in a transverse field

$$H = \sum_i \sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^x$$

$$W_H = \begin{pmatrix} I & 0 & 0 \\ \sigma^z & 0 & 0 \\ \lambda\sigma^x & \sigma^z & I \end{pmatrix}$$

Also:

- fermionic operators
- string operators
- operators at finite momenta, $c_k^\dagger$, N_k, $\ldots$

Operator arithmetic

The principal advantage of the MPO representation is that it allows arithmetic operations on the operators

$$\text{sum:} \quad X = Y + Z \quad \rightarrow \quad W_X = W_Y \oplus W_Z$$

Dimension increases: $\dim_X \leq \dim_Y + \dim_Z$

$$\text{product:} \quad X = YZ \quad \rightarrow \quad W_X = W_Y \otimes W_Z$$

Dimension increases: $\dim_X \leq \dim_Y \times \dim_Z$

Calculating observables of 'complicated' operators is often easy

- example, variance of an observable

$$\sigma_O^2 = \langle (O - \langle O \rangle)^2 \rangle = \langle O^2 \rangle - \langle O \rangle^2$$

Operator arithmetic

The principal advantage of the MPO representation is that it allows arithmetic operations on the operators

$$\text{sum:} \quad X = Y + Z \quad \to \quad W_X = W_Y \oplus W_Z$$

Dimension increases: $\dim_X \leq \dim_Y + \dim_Z$

$$\text{product:} \quad X = YZ \quad \to \quad W_X = W_Y \otimes W_Z$$

Dimension increases: $\dim_X \leq \dim_Y \times \dim_Z$

Calculating observables of ‘complicated’ operators is often easy

- example, variance of an observable

$$\sigma_O^2 = \langle (O - \langle O \rangle)^2 \rangle = \langle O^2 \rangle - \langle O \rangle^2$$

DMRG in the infinite size limit (arxiv:0804.2509)

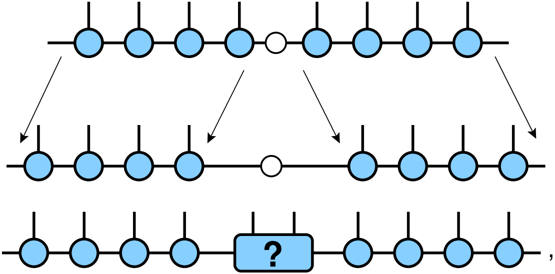
Infinite-size translationally invariant MPS

- The “infinite size” DMRG algorithm has existed since the start (1992)
- It doesn’t produce a translationally invariant MPS fixed point
- No prescription for constructing the initial wavefunction at next iteration
- Rarely used in the literature, and often incorrectly
- iTEBD produces a translationally invariant MPS, but for groundstates imaginary time evolution is not so fast

DMRG in the infinite size limit (arxiv:0804.2509)

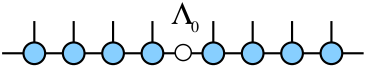
Infinite-size translationally invariant MPS

- The “infinite size” DMRG algorithm has existed since the start (1992)
- It doesn’t produce a translationally invariant MPS fixed point
- No prescription for constructing the initial wavefunction at next iteration
- Rarely used in the literature, and often incorrectly
- iTEBD produces a translationally invariant MPS, but for groundstates imaginary time evolution is not so fast

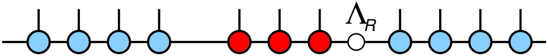


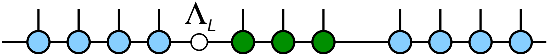
A recurrence relation for MPS

Suppose we can an initial state:



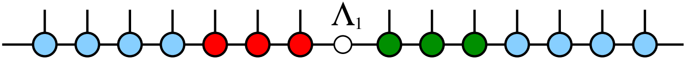
Suppose we also have the MPS enlarged with an extra unit cell:





Note: Λ_L and Λ_R are not necessarily diagonal

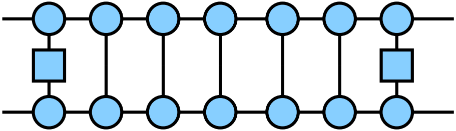
Now we can insert one more unit cell:



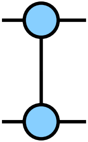
$$\Lambda_1 = \Lambda_R \, \Lambda_0^{-1} \, \Lambda_L$$

Expectation Values

Correlation functions



The form of correlation functions are determined by the eigenvalues of the *transfer operator*

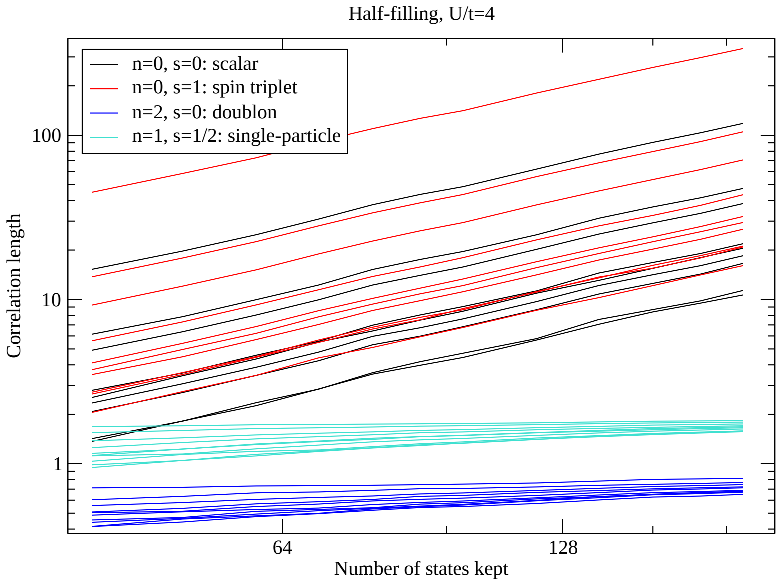


- All eigenvalues $|\lambda| \leq 1$
- One eigenvalue equal to 1, corresponding to the identity operator

Expansion in terms of eigenspectrum λ_i:

$$\langle O(x) O(y) \rangle = \sum_i a_i \, \lambda_i^{|y-x|} \qquad \xi_i = -\frac{1}{\ln |\lambda_i|}$$

Hubbard model transfer matrix spectrum



CFT Parameters

For a gapless groundstate with critical fluctuations, the correlation length increases with number of states D as a power law,

$$\xi \sim D^{\kappa}$$

[T. Nishino, K. Okunishi, M. Kikuchi, Phys. Lett. A **213**, 69 (1996)
M. Andersson, M. Boman, S. Östlund, Phys. Rev. B **59**, 10493 (1999)
L. Tagliacozzo, Thiago. R. de Oliveira, S. Iblisdir, J. I. Latorre, Phys. Rev. B **78**, 024410 (2008)]

This exponent is a function *only* of the central charge,

$$\kappa =\simeq \frac{6}{\sqrt{12c} + c}$$

[Pollmann et al, PRL 2009]

The spectrum already gives information about the critical scaling.

Can we go further and obtain scaling functions and exponents?

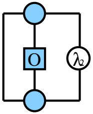
Scaling exponents

Suppose we have a two-point correlator that has a power-law at large distances

$$\langle O(x)O(y)\rangle = |y - x|^{-2\Delta}$$

As we increase the number of states kept D the correlation length increases, so the region of validity of the power law increases.

- Prefactor a is overlap of operator O with next-leading eigenvector of transfer operator

$a =$ 

- For power law behaviour, a must scale inversely with the corresponding correlation length ξ

$$a \propto \xi^{-\Delta}$$

This gives directly the operator scaling dimensions by direct fit

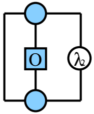
Scaling exponents

Suppose we have a two-point correlator that has a power-law at large distances

$$\langle O(x)O(y)\rangle = |y-x|^{-2\Delta}$$

As we increase the number of states kept D the correlation length increases, so the region of validity of the power law increases.

- Prefactor a is overlap of operator O with next-leading eigenvector of transfer operator

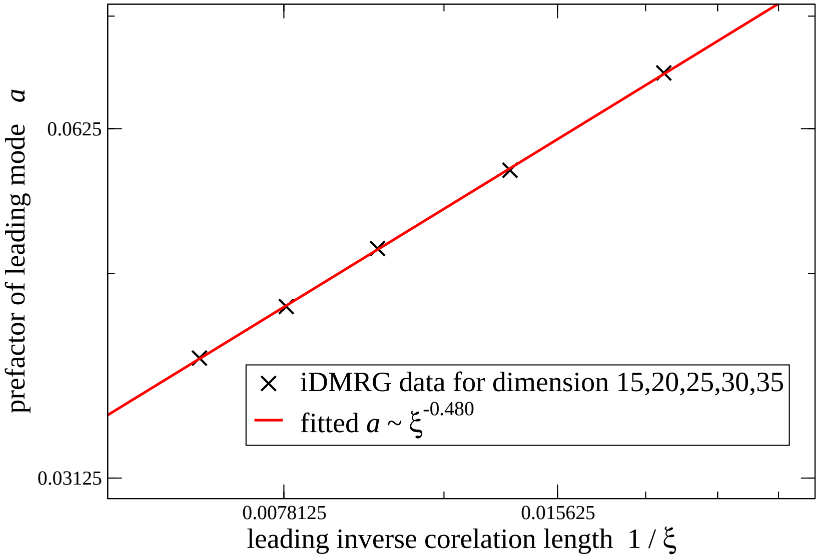
$a =$ 

- For power law behaviour, a must scale inversely with the corresponding correlation length ξ

$$a \propto \xi^{-\Delta}$$

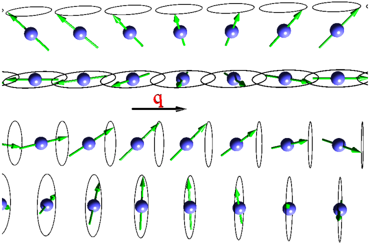
This gives directly the operator scaling dimensions by direct fit

Heisenberg model fit for the scaling dimension



Time-reversal symmetry breaking

Several materials exhibit unusual phase transitions with quasi-1D magnetic ordering.
Bulk 3D material: broken rotational symmetry allows a *helical* state



Helical order: $\langle \vec{S}(0) \times \vec{S}(x) \rangle \sim \vec{a} \sin x$
This kind of symmetry breaking cannot occur in 1D

- No spontaneously broken *continuous* symmetries in exact 1D
- the corresponding Goldstone modes would destroy the long range order completely
- But can break a discrete subgroup

Chiral symmetry breaking

In 1D, the helical order is absent because we cannot spontaneously break $SU(2)$.
In a magnetic field or with finite anisotropy, the $SU(2)$ is broken down to $U(1) \times$ discrete symmetries, including spin reflection.
This allows a *rementant* of helical order to survive: *chiral order*.

$$\langle \vec{S}(0) \times \vec{S}(1) \cdot \vec{S}(n) \times \vec{S}(n+1) \rangle = \kappa^2$$

Define

$$\begin{aligned}
\vec{\kappa}(x) &= \vec{S}(n) \times \vec{S}(n+1) \\
\kappa^z(x) &= \frac{S^-(n)\, S^+(n+1) - S^+(n)\, S^-(n+1)}{2i}
\end{aligned}$$

In the usual computational basis, the matrix elements of this operator are pure imaginary.
Sign of κ determines choice of left/right chiral degenerate groundstates

CPT symmetry in lattice models

Most lattice models are CPT symmetric:

Charge symmetry: interchange particle $\leftrightarrow$ hole (up $\leftrightarrow$ down spins)

Parity symmetry: exchange $x \leftrightarrow -x$, $p \leftrightarrow -p$

Time-reversal symmetry: anti-unitary. complex conjugation plus spin inversion. $x \leftrightarrow x$, $p \leftrightarrow -p$

Combining time reversal with a spin rotation, we can construct an operator that (in our computational basis) is a pure complex conjugation $= CT$

CPT invariance implies that if P transforms one groundstate into another, then CT will have the same effect.

$$CT = P$$

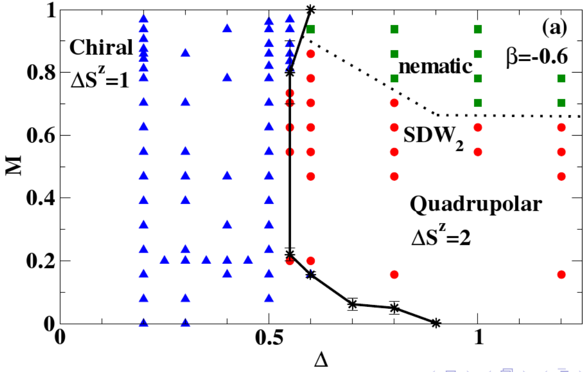
This implies that the chiral groundstate wavefunctions must have complex coefficients.

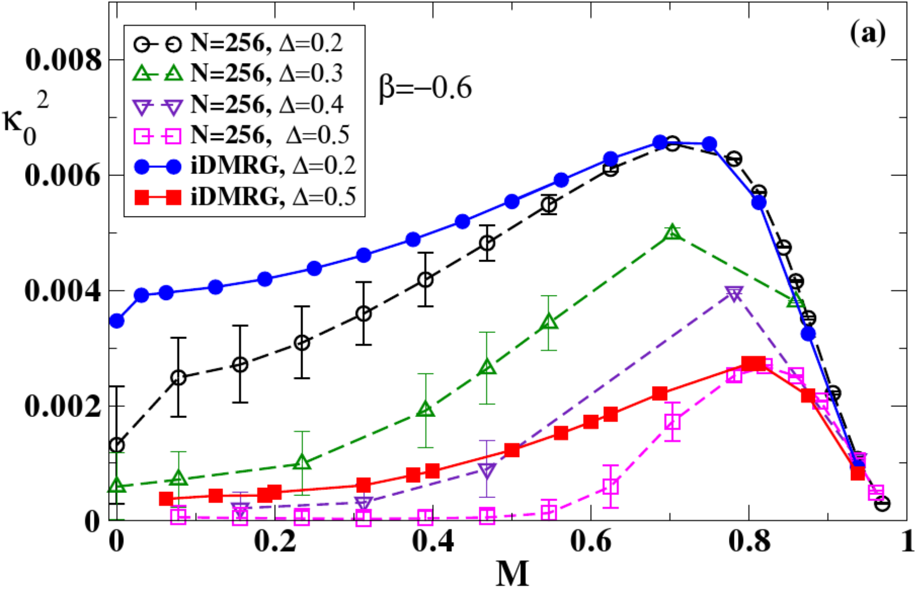
Chiral symmetry breaking in zig-zag chains

F. Heidrich-Meisner, I. P. McCulloch, A. K. Kolezhuk, Phys. Rev. B **80**, 144417 (2009)

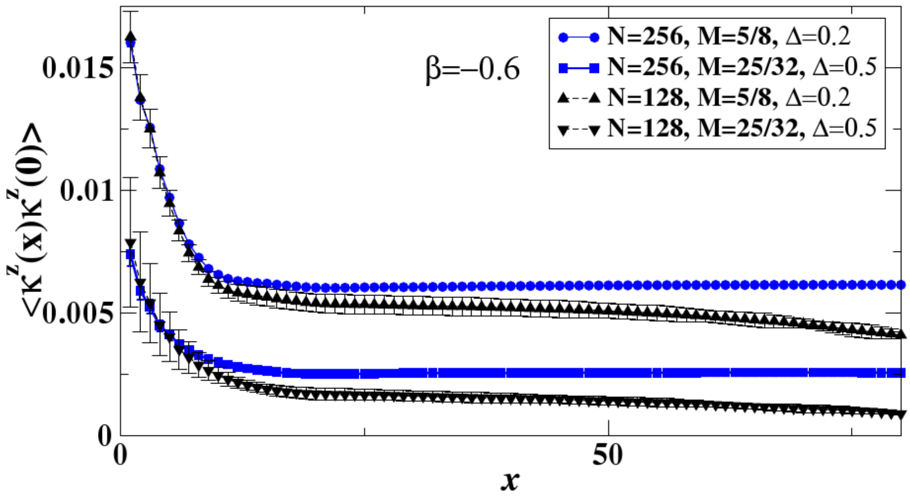
- J_1 - J_2 zig-zag chain, $J_1 < 0$, $J_2 > 0$
- Anisotropic spin-spin interaction $(\vec{S}_i \cdot \vec{S}_i)_\Delta = S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z$

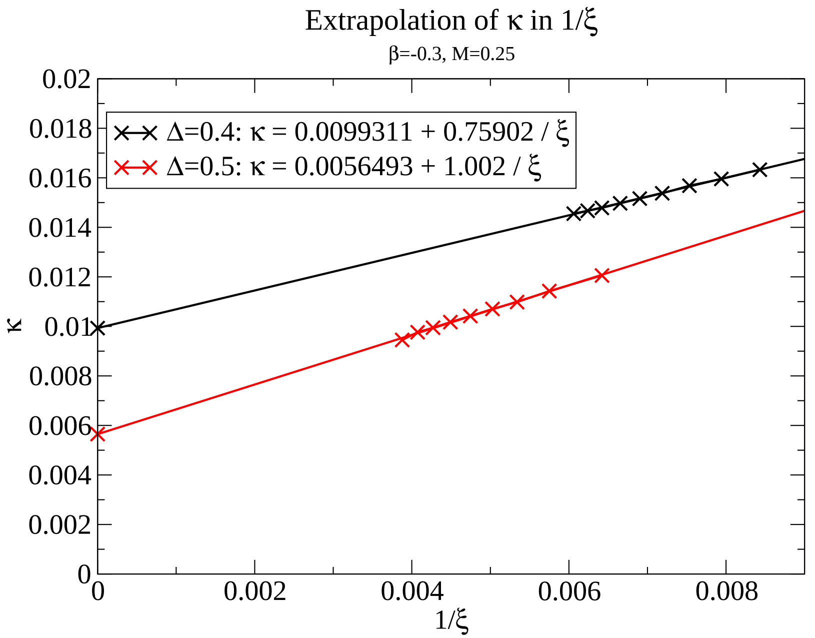
$$H = \sum_i \left\{ J_1 (\vec{S}_i \cdot \vec{S}_{i+1})_\Delta + J_2 (\vec{S}_i \cdot \vec{S}_{i+2})_\Delta - h S_i^z \right\}$$





(a)
β=–0.6
N=256, Δ=0.2
N=256, Δ=0.3
N=256, Δ=0.4
N=256, Δ=0.5
iDMRG, Δ=0.2
iDMRG, Δ=0.5
κ_0^2
0.008
0.006
0.004
0.002
0
0.2
0.4
0.6
0.8
1
M


0.015
0.01
0.005
0
0
50
x
$<\kappa^z(x)\kappa^z(0)>$
β=−0.6
N=256, M=5/8, Δ=0.2
N=256, M=25/32, Δ=0.5
N=128, M=5/8, Δ=0.2
N=128, M=25/32, Δ=0.5


Extrapolation of κ in 1/ξ
β=-0.3, M=0.25
Δ=0.4: κ = 0.0099311 + 0.75902 / ξ
Δ=0.5: κ = 0.0056493 + 1.002 / ξ
κ
1/ξ
0.02
0.018
0.016
0.014
0.012
0.01
0.008
0.006
0.004
0.002
0
0
0.002
0.004
0.006
0.008

Continuous symmetries

If you take no action to preserve exactly a symmetry, an infinite MPS can break it

even continuous symmetries in one dimension

How to understand this?

- Matrix elements connecting symmetry sectors vanish as $\sim \exp(-N) \quad \rightarrow 0$
- Continuous symmetries cannot break in *exact* 1D because the associated goldstone modes would destroy the order parameter completely (percolation threshold!)
- But if the goldstone modes are gapped due to finite basis size, the symmetry can break

Continuous symmetries

If you take no action to preserve exactly a symmetry, an infinite MPS can break it

even continuous symmetries in one dimension

How to understand this?

- Matrix elements connecting symmetry sectors vanish as $\sim \exp(-N) \quad \rightarrow 0$
- Continuous symmetries cannot break in *exact* 1D because the associated goldstone modes would destroy the order parameter completely (percolation threshold!)
- But if the goldstone modes are gapped due to finite basis size, the symmetry can break

Continuous symmetries

If you take no action to preserve exactly a symmetry, an infinite MPS can break it

even continuous symmetries in one dimension

How to understand this?

- Matrix elements connecting symmetry sectors vanish as $\sim \exp(-N) \quad \to 0$
- Continuous symmetries cannot break in *exact* 1D because the associated goldstone modes would destroy the order parameter completely (percolation threshold!)
- But if the goldstone modes are gapped due to finite basis size, the symmetry can break

Prototypical example: Mean field

$$H = \frac{U}{2}\sum_i N_i(N_i - 1) - J \sum_{<i,j>} b_i^\dagger b_j + b_j^\dagger b_i - \mu N$$

Bose-Hubbard model

$$H_{\text{MF}} = \sum_i \frac{N_i(N_i - 1)}{2} - J\alpha(b_i^\dagger + b_i) - \mu N_i$$

Mean field Hamiltonian breaks $U(1)$ particle number conservation
Groundstate is an $D = 1$ infinite MPS (product state!)

$$|\psi\rangle = (|0\rangle + a_1|1\rangle + a_2|2\rangle \ldots)^{\otimes L}$$

- An iMPS with no symmetries reduces to mean-field like
- Imposing quantum number symmetries reduces the quality of the variational state (for fixed D)
- But usually worth the cost in computational efficiency

Prototypical example: Mean field

$$H = \frac{U}{2}\sum_i N_i(N_i - 1) - J\sum_{<i,j>} b_i^\dagger b_j + b_j^\dagger b_i - \mu N$$

Bose-Hubbard model

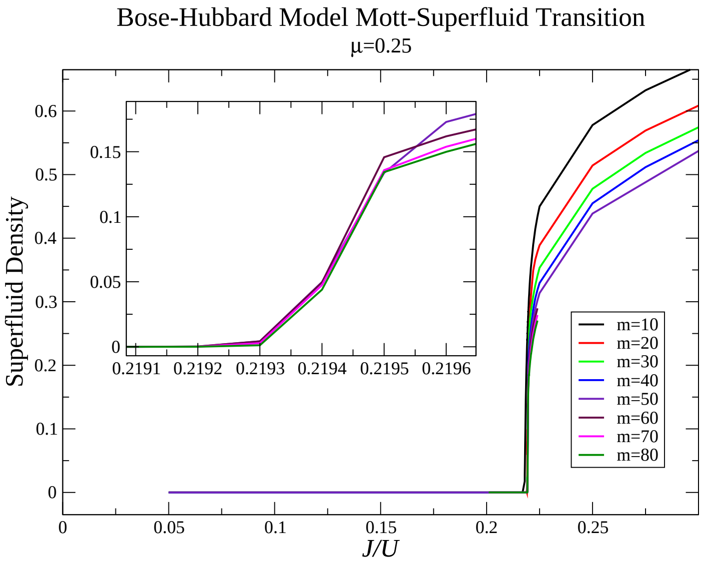
$$H_{\text{MF}} = \sum_i \frac{N_i(N_i - 1)}{2} - J\alpha(b_i^\dagger + b_i) - \mu N_i$$

Mean field Hamiltonian breaks $U(1)$ particle number conservation
Groundstate is an $D = 1$ infinite MPS (product state!)

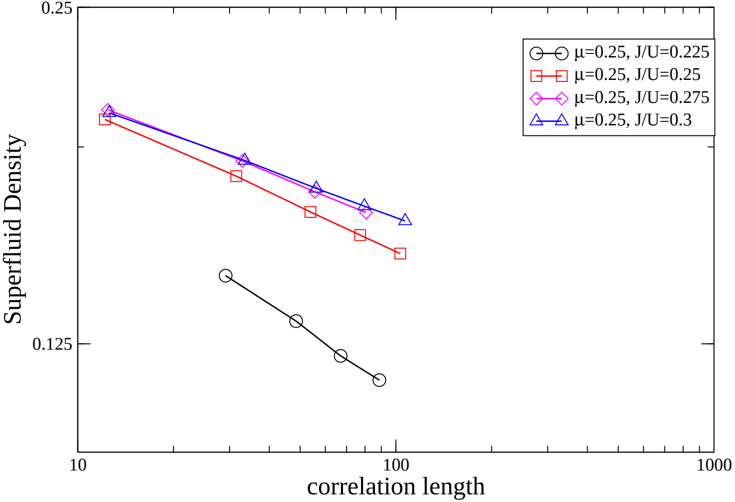
$$|\psi\rangle = (|0\rangle + a_1|1\rangle + a_2|2\rangle \ldots)^{\otimes L}$$

- An iMPS with no symmetries reduces to mean-field like
- Imposing quantum number symmetries reduces the quality of the variational state (for fixed D)
- But usually worth the cost in computational efficiency

Bose-Hubbard Superfluid Density



Bose-Hubbard Superfluid Density



Conclusions & Outlook

Matrix product states - more powerful than just DMRG algorithm

- iDMRG is a very efficient method to construct translationally invariant thermodynamic states
- All expectation values can be expressed in terms of the eigenmodes of the transfer matrix
- Scaling with respect to D can give power laws
- Transfer matrix gives detailed information about scaling and order parameters
- Other talks will show that entropy, fidelity, etc can determine phase boundaries without knowledge of the order parameter
- if the order parameter is known, then it is better to calculate the order parameter scaling
- generic way to determine order parameter: correlation density matrices (Henley, Münder, Läuchli, . . .)