DMRG in the Thermodynamic limit
Workshop and Symposium on DMRG Technique for Strongly Correlated Systems in Physics and Chemistry

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23/6/2015
Outline

1. Constructing Matrix Product States - alternative views
   - From classical to quantum states
   - Sequential generation

2. Matrix Product Operators

3. Symmetries

4. Infinite size DMRG

5. Broken symmetries

6. Scaling relations in the thermodynamic limit

7. Expectation values of iMPO's
   - Higher moments
   - Binder cumulant

8. Infinite Boundary Conditions

9. 2D
Method 1: quantize a classical state

Start from a \textit{classical} (product) state

\[ |\psi\rangle = |s^1\rangle |s^2\rangle |s^3\rangle |s^4\rangle \ldots \]

Each \(|s^i\rangle\) is a classical vector, with real (or c-number) coefficients in some basis

\[ |s^i\rangle = a^x_i |x\rangle + a^y_i |y\rangle + a^z_i |z\rangle \]

Turn our (commuting) numeric coefficients into a matrix

\[ |s^i\rangle_{jk} = A^x_{jk} |x\rangle + A^y_{jk} |y\rangle + A^z_{jk} |z\rangle \]

We can recover an amplitude at the end by taking the trace, or arranging that the boundary matrices are \(1 \times D\) and \(D \times 1\).

\[ |\psi\rangle = \text{Tr} \sum_{s_i} A^{s_1} A^{s_2} A^{s_3} A^{s_4} \ldots |s^1\rangle |s^2\rangle |s^3\rangle |s^4\rangle \ldots \]
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Method 2: quantum finite-state machines

What is a Matrix Product State?

- Another way to visualizing them (from Greg Crosswhite)

A finite-state machine is a model of a system that can transition between a finite number of states.
A classical finite-state machine is always in one discrete state.

In a *quantum* finite-state machine, we choose every possible transition with some probability amplitude

$$|\psi\rangle = \left\{ \begin{array}{c} |\uparrow\rangle \\ |\downarrow\rangle \end{array} \right\}$$

(from Crosswhite and Bacon, Phys. Rev. A 78, 012356 (2008))
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\[
|\psi\rangle = \begin{cases} 
|\uparrow\uparrow\uparrow\rangle \\
|\downarrow\uparrow\uparrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\uparrow\uparrow\downarrow\rangle 
\end{cases}
\]

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Matrix Product States

This quantum finite-state machine has a transition matrix associated with it:

- **W-state**

  \[ |\psi\rangle = \frac{1}{\sqrt{N}} (|\downarrow\uparrow\uparrow\uparrow \ldots \rangle + |\uparrow\downarrow\uparrow\uparrow \ldots \rangle + |\uparrow\uparrow\downarrow\uparrow \ldots \rangle + \ldots) \]

  \[ A = \begin{pmatrix} |\uparrow\rangle & 0 \\ |\downarrow\rangle & |\uparrow\rangle \end{pmatrix} \]

- Practically all prototype wavefunctions studied in quantum information have a low-dimensional MPS representation:

  - **GHZ state** – long-range entangled, \( S = \ln 2 \)

    \[ |\psi\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\uparrow \ldots \rangle + |\downarrow\downarrow\downarrow \ldots \rangle) \]

    \[ A = \begin{pmatrix} |\uparrow\rangle & 0 \\ 0 & |\downarrow\rangle \end{pmatrix} \]

  - **AKLT state**

    \[ A = \begin{pmatrix} \sqrt{1/3} |0\rangle & -\sqrt{2/3} |+\rangle \\ \sqrt{2/3} |\downarrow\rangle & -\sqrt{1/3} |0\rangle \end{pmatrix} \]
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|\psi\rangle = \frac{1}{\sqrt{N}}(|↓↑↑↑\ldots⟩ + |↑↓↑↑\ldots⟩ + |↑↑↓↑\ldots⟩ + \ldots)
\]

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\end{pmatrix}
\]
The Matrix Product Ansatz: beyond groundstates

The key advantage of MPS formulation: *arithmetical manipulations*

The sum (superposition) of two matrix product states is also a matrix product state

\[ |C\rangle = |A\rangle + |B\rangle \]

\[ C = \sum_{\{s_i\}} \text{Tr} \ C^{s_1} C^{s_2} \ldots C^{s_L} |s_1 s_2 \ldots s_L\rangle \]

where

\[ C^{s_i} = A^{s_i} \oplus B^{s_i} \]

The dimension of the matrices increases: \( \dim(C) = \dim(A) + \dim(B) \)

Action of an operator on a state: if the operator is a product of local terms:

\[ O = O_1 \otimes O_2 \otimes \ldots \]

|C\rangle = O|A\rangle is a Matrix Product State, with

\[ C^{s_i} = \sum_{s'_i} O_{i}^{s_i, s'_i} A^{s'_i} \]
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\[ C^{s_i} = \sum_{s_i'} O_{i}^{s_i, s_i'} A^{s_i'} \]
At each iteration we have a set of **block operators**, acting on the \( m \)-dimensional auxiliary space.

It is natural to use a Matrix Product approach to constructing the block operators used in DMRG.

**Ising model** \( H = \sum_{<i,j>} S^z_i S^z_j + \lambda \sum_i S^x_i \), adding a site to the block:

- (identity operator) \( I \rightarrow I \otimes I_{\text{local}} \)
- (z-spin acting on right-most site) \( S^z \rightarrow I \otimes S^z_{\text{local}} \)
- (block Hamiltonian) \( H \rightarrow \lambda I \otimes S^x_{\text{local}} + S^z \otimes S^z_{\text{local}} + H \otimes I_{\text{local}} \)

In matrix form:

\[
\begin{pmatrix}
H & S^z & I
\end{pmatrix}' = \begin{pmatrix}
H & S^z & I
\end{pmatrix} \times \begin{pmatrix}
I & S^z & \lambda S^x & S^z & I
\end{pmatrix}_{\text{local}}
\]
Matrix Product Operators

This form can represent many operators

- fermionic $c_{k=0}^{\dagger}$: $W_{c_{k=0}^{\dagger}} = \begin{pmatrix} I & P \\ c_{k=0}^{\dagger} & P \end{pmatrix}$, $P = (-1)^N$, J-W string

- finite momentum $b_{k}^{\dagger}$: $W_{b_{k}^{\dagger}} = \begin{pmatrix} I & e^{ik}I \\ b_{k}^{\dagger} & I \end{pmatrix}$

Advantages of the MPO representation: *arithmetic operations!*

- $H_1 + H_2$ direct sum of the MPO representations
- $H_1 \times H_2$ direct product of the MPO representations

also derivatives, etc

This preserves the lower triangular form.

Can we evaluate an expectation value of an MPO in the thermodynamic limit?

$$\langle A \rangle_L = \text{polynomial function of } L$$

Examples:

- Energy: $\langle H \rangle_L = L E_0$
- Hamiltonian block operator matrix elements to restart a calculation
- Single-mode approximation: $\langle S_k^- H S_k^+ \rangle_L / \langle S_k^- S_k^+ \rangle_L$
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Suppose the Hamiltonian is invariant under some set of unitary transformations,

\[ [H, U_i] = 0 \]

Two classes:

- **discrete**: \( U_i \) are members of a group algebra
- **continuous**: \( U_i = \exp[i\theta J_i] \), where \( J_i \) define a Lie algebra

The case where all \( U_i \) commute is straightforward: use a basis in which the \( U_i \) are diagonal and label the Hilbert space by the set of eigenvalues \( u_i \).

What happens if \( [U_a, U_b] \neq 0 \)?

\[ SU(2) \text{ example: } [J_i, J_j] = i\epsilon^{ijk}J_k \]

(I leave this as a homework problem - I won’t cover this case today)
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Suppose we have an Abelian symmetry, for example conservation of \( z \)-component of spin.

\[
H = \sum_{<i,j>} S^z_i S^z_j + (S^+_i S^-_j + S^-_i S^+_j)/2
\]

We have \([S^z, H] = 0\), therefore also

\[
[U, H] = 0, \quad \text{where} \quad U = \exp(i\theta S^z)
\]

That is, we can do unitary rotations around the \( z \)-axis, without changing any physics.

According to group representation theory, we can decompose all states and operators according to how they transform under this rotation.

The different classes of transformations are labelled by a set of \textit{quantum numbers}, in this case the eigenstates of \( S^z \).
Examples:
\( S^z \) transforms as a scalar (invariant): \([S^z, S^z] = 0\)
\( S^+ \) transforms as a +1 operator: \([S^z, S^+] = +1 \times S^+\)
\( S^- \) transforms as a –1 operator: \([S^z, S^-] = -1 \times S^-\)
\( S^+_i \) transforms as a +1 operator: \([S^z, S^+_i] = +1 \times S^+_i\)
\( S^+_i S^-_j \) transforms as a scalar: no calculation required because \( +1 - 1 = 0 \).

An arbitrary operator can be decomposed as a sum of irreducible operators

\[
O = \sum_n O^{[n]}
\]

where

\([S^z, O^{[n]}] = nO^{[n]}\)

The \( n \) is the representation label, or quantum number.

The matrix elements of an irreducible operator satisfy a sum rule:

\[
\langle s' | O^{[n]} | s \rangle \neq 0, \text{ only if } s' = s + n
\]

The representation label \( n \) tells us how the outgoing quantum number relates to the incoming quantum number.
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Symmetries in a tensor network

In a *symmetric tensor network*, we attach quantum numbers to every index. Absence of an index indicates a scalar, example: $\bullet$

This is a scalar operator, with constraint $q_i = q_j$.

If we wanted to represent a non-scalar operator, we need another leg:

Now we have $q_i = q_j + q_s$

Note: incoming and outgoing indices are different (bra vs ket!)

General rules: (1) sum of outgoing indices $=$ sum of incoming indices

(2) Contraction *must* respect the direction of arrows.
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
- iTEBD produces a translationally invariant MPS, but for groundstates imaginary time evolution is not so fast
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A recurrence relation for MPS

Suppose we have an initial state:

\[ \Lambda_0 \]

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

\[ \Lambda_R \Lambda_L \]

Note: \( \Lambda_L \) and \( \Lambda_R \) are not necessarily diagonal

Now we can insert one more unit cell:

\[ \Lambda_1 = \Lambda_R \Lambda_0^{-1} \Lambda_L \]
Variant of the finite system algorithm

- Different treatment of the boundaries

\[ \Lambda_{23} = \Lambda_{21} \Lambda_{01}^{-1} \Lambda_{03} \]

\[ \Lambda_{43} = \Lambda_{41} \Lambda_{21}^{-1} \Lambda_{23} \]

\[ \Lambda_{45} = \Lambda_{43} \Lambda_{23}^{-1} \Lambda_{25} \]
Broken symmetries

Finite size MPS: No broken symmetries (to $O(\text{truncation error})$)
Infinite size MPS: The Ansatz can break all symmetries

even continuous symmetries in one dimension

How to understand this?

- Matrix elements connecting symmetry sectors vanish as
  $\sim \exp(-L) \rightarrow 0$
- 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
- Alternatively: in order to get a finite correlation length we must perturb the
  Hamiltonian with a relevant perturbation. No reason why that perturbation
  should not break any (or all) symmetry.
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- Alternatively: in order to get a finite correlation length we must perturb the Hamiltonian with a *relevant* perturbation. No reason why that perturbation should not break any (or all) symmetry.
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 \( m = 1 \) infinite MPS (product state!)

\[ |\psi\rangle = (|0\rangle + a_1|1\rangle + a_2|2\rangle \ldots) \otimes^L \]

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- Imposing quantum number symmetries reduces the quality of the variational state (for fixed \( m \))
- But usually worth the cost in computational efficiency
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Bose-Hubbard Model Mott-Superfluid Transition

\( \mu = 0.25 \)
The form of correlation functions are determined by the eigenvalues of the transfer operator.

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

Expansion in terms of eigenspectrum $\lambda_i$:

$$\langle O(x)O(y) \rangle = \sum_i a_i \lambda_i^{y-x}$$
Hubbard Model transfer matrix spectrum

Half-filling, U/t = 4

Number of states kept: 0, 0.2, 0.4, 0.6, 0.8, 1

λ

(0,0) Singlet
(1,0) Spin triplet
(0,1) Holon Triplet
(1/2,1/2) Single-particle

Hubbard Model transfer matrix spectrum
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Half-filling, U/t=4

Correlation length

Number of states kept

Correlation length

Number of states kept
Critical scaling example

Two-species bose gas with linear tunneling $\Omega$, from F. Zhan et al, Phys. Rev. A 90, 023630 2014

Graph showing the scaling of $\xi$ with $m$ for different values of $\Omega$: $\Omega = 0.2148, 0.215, 0.2152, 0.2154, 0.2156, 0.2158$. The data points and lines are color-coded for each $\Omega$ value.
For a critical mode, the correlation length increases with number of states $m$ as a power law,

$$\xi \sim m^\kappa$$


This exponent is a function only of the central charge,

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

[Pollmann et al, PRL 2009]

Can we find an expression for the scaling dimension?
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 $m$ the correlation length increases, so the region of validity of the power law increases.

- Take two different calculations with $m_1$ and $m_2$
- Correlation lengths $\xi_1$ and $\xi_2$
- We expect: 
  $$\frac{O(\xi_2)}{O(\xi_1)} = \left( \frac{\xi_2}{\xi_1} \right)^\Delta$$
- for $x$ large, we have: $O(x) \sim a \lambda^x$ (with $\xi = -1/\ln \lambda$)
- Prefactor $a$ is overlap of operator $O$ with next-leading eigenvector of transfer operator
- ... algebra ...

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

This gives directly the operator scaling dimensions by direct fit
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Heisenberg model fit for the scaling dimension

\[ y = 0.45126 \times x^{0.480} \]

transfer matrix eigenvalue \( \lambda = 1 / \xi \)
Generalized Scaling


Scaling relation for large $s$:

$$O(s\xi) = a\lambda^{s\xi} = a\lambda^{-s/\ln \lambda} = ae^{-s}$$

So we obtain $\Delta$ by scaling $O(s\xi)$ versus $s\xi$

However, this also works for $s$ small, eg $s \ll 1$,

$$O(s\xi) \propto (s\xi)^{-\Delta}$$

because for $s \ll 1$, the correlation function is already (approximately) power-law.

the scaling relation works for any $0 < s < \infty$!

But: $O(s\xi) \sim a\lambda^{s\xi}$ only for $s \gg 1$
Generalized Scaling


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So we obtain $\Delta$ by scaling $O(s^\xi)$ versus $s^\xi$

However, this also works for $s$ small, eg $s \ll 1$,

$$O(s^\xi) \propto (s^\xi)^{-\Delta}$$

because for $s \ll 1$, the correlation function is already (approximately) power-law.

the scaling relation works for any $0 < s < \infty$!

But: $O(s^\xi) \sim a\lambda^{s^\xi}$ only for $s \gg 1$
Generalized Scaling


Scaling relation for large $s$:

$$O(s\xi) = a\lambda^{s\xi} = a\lambda^{-s/\ln \lambda} = ae^{-s}$$

So we obtain $\Delta$ by scaling $O(s\xi)$ versus $s\xi$

However, this also works for $s$ small, eg $s \ll 1$,

$$O(s\xi) \propto (s\xi)^{-\Delta}$$

because for $s \ll 1$, the correlation function is already (approximately) power-law.

the scaling relation works for any $0 < s < \infty$ !

But: $O(s\xi) \sim a\lambda^{s\xi}$ only for $s \gg 1$
We have seen that we can write many interesting operators in the form of a matrix product operator

- Can we evaluate the expectation value of an arbitrary MPO?

If the MPO has no Jordan structure, this is a simple eigenvalue problem

For a lower triangular MPO, this doesn’t work.

- But we can make use of the triangular structure

\[
\begin{pmatrix}
I & & \\
S^z & I & \\
\lambda S^x & S^z & I
\end{pmatrix}
\]

- Index by index, each component is a function only of the previously calculated terms
We have seen that we can write many interesting operators in the form of a matrix product operator

- Can we evaluate the expectation value of an arbitrary MPO?

If the MPO has no Jordan structure, this is a simple eigenvalue problem

$$W = \lambda W$$

For a lower triangular MPO, this doesn’t work.

- But we can make use of the triangular structure

$$\begin{pmatrix}
I \\
S_z \\
\lambda S_x & S_z & I
\end{pmatrix}$$

- Index by index, each component is a function only of the previously calculated terms
Choose bond indices $i, j$ of $W_{ij}$, and denote $T_{W_{ij}}$

Example:

$$
\begin{pmatrix}
I \\
S^z \\
\lambda S^x \\
S^z \\
I
\end{pmatrix}
$$

Eigentensor is $(E_1 \ E_2 \ E_3)$

- Starting from $E_3$:
  $$E_3 = T_I(E_3) = I$$
  is equivalent to the orthogonality condition - $E_3$ is just the identity

- $E_2$:
  $$E_2 = T_{S^z}(E_3) = T_{S^z}(I) = S^z$$

- $E_1$: doesn’t reach a fixed point, $E_1 = E_1(L)$ depends on the number of iterations $L$
  $$E_1(L + 1) = T_I(E_1(L)) + T_{S^z}(E_2) + T_{\lambda S^x}(E_3)$$
  $$= T_I(E_1(L)) + C$$

where $C$ is a constant matrix, $C = T_{S^z}(S^z) + \lambda S^x$
Fixed point equations for $E_1$:

$$E_1(L + 1) = T_I(E_1(L)) + C$$

Eigenmatrix expansion of $T_I$:

$$T_I = \sum_{n=1}^{m^2} \lambda_n |\lambda \rangle \langle \lambda|$$

giving

$$E_1^{(n)}(L + 1) = \lambda_n E_1^{(n)}(L) + C^{(n)}$$

- Since $\lambda_1 = 1$ by construction, this motivates decomposing into components parallel and perpendicular to the identity:

$$E_1(L) = E_1'(L) + e_1(L)I$$

where $\text{Tr} E_1'(L) \rho = 0$
Component in the direction of the identity:
\[ e_1(L + 1) = e_1(L) + \text{Tr } C\rho \]

Has the solution
\[ e_1(L) = L \cdot \text{Tr } C\rho \]
is the energy

Component perpendicular to the identity:
\[ E'_1(L + 1) = T_I(E'_1(L)) + C' \]
where \( C' = C - (\text{Tr } C\rho) I \)
\[ E'_1(L + 1)_n = \lambda_n E'_1(L)_n + C'_n \]

Since all \( |\lambda_n| < 1 \) here, this is a geometric series that converges to a fixed point (independent of \( L \)),
\[ (1 - T_I)(E'_1) = C' \]

*Linear solver for the unknown matrix \( E'_1 \)*
Component in the direction of the identity:

\[ e_1(L + 1) = e_1(L) + \text{Tr} \, C \rho \]

Has the solution

\[ e_1(L) = L \, \text{Tr} \, C \rho \]

is the energy

Component perpendicular to the identity:

\[ E'_1(L + 1) = T_I(E'_1(L)) + C' \]

where \( C' = C - (\text{Tr} \, C \rho) \, I \)

\[ E'_1(L + 1)_n = \lambda_n E'_1(L)_n + C'_n \]

Since all \(|\lambda_n| < 1\) here, this is a geometric series that converges to a fixed point (independent of \(L\)),

\[ (1 - T_I)(E'_1) = C' \]

*Linear solver for the unknown matrix \( E'_1 \)*
Summary:

- Decompose eigentensor into components parallel and perpendicular to the identity
- The component parallel to the identity is the energy per site
- The perpendicular components reach a fixed point and give the Hamiltonian matrix elements

\[
\begin{align*}
E_3 &= I & \text{Identity operator} \\
E_2 &= S_z & \text{Sz block operator} \\
E_1(L) &= E' + Le_1 & \text{Hamiltonian operator + energy per site}
\end{align*}
\]
At the $i^{th}$ iteration, we have

$$E_i(L + 1) = TW_{ii}(E_i(L)) + \sum_{j > i} TW_{ji}(E_j(L))$$

$$\Rightarrow = C(L)$$

Basic idea:

- if $W_{ii} = 0$, then $E_i = C$
- if $W_{ii} \neq 0$, then solve $(1 - TW_{ii})(E_i) = C$

The result will be a polynomial function of $L$

- solve separately for the coefficient of the $k$-th power of $n$
- If the diagonal element is unitary, then obtain the eigenvalues of magnitude 1
- If any eigenvalues are complex, then expand also in fourier modes
Generalization to arbitrary triangular MPO’s

At the \(i\)th iteration, we have

\[ E_i(L + 1) = T_{Wii}(E_i(L)) + \sum_{j>i} T_{Wji}(E_j(L)) = C(L) \]

Basic idea:

- if \(W_{ii} = 0\), then \(E_i = C\)
- if \(W_{ii} \neq 0\), then solve \((1 - T_{Wii})(E_i) = C\)

The result will be a polynomial function of \(L\)

- solve separately for the coefficient of the \(k\)-th power of \(n\)
- If the diagonal element is unitary, then obtain the eigenvalues of magnitude 1
- If any eigenvalues are complex, then expand also in fourier modes
How close is a variational state to an eigenstate of the Hamiltonian?

- Sometimes there is an algorithmic measure, often not.

The square of the Hamiltonian operator determines the energy variance

\[ \langle H^2 \rangle_L - \langle H \rangle^2_L = \langle (H - E)^2 \rangle_L = L\sigma^2 \]

- A universal measure for the quality of a variational wavefunction
- lower bound for the energy: there is always an eigenstate within \( \sigma \) of \( E \)

We can easily construct an MPO representation of \( H^2 \)
Spin 1/2 Heisenberg Model

Energy per site scaling with variance (exact energy = \(-\ln 2 + 0.25 = -0.44314718056\))
Momentum distribution

Momentum-dependent operators have a simple form,

\[ b_k^\dagger = \sum_x e^{ikx} b_x^\dagger \]

\[ W_{b_k^\dagger} = \begin{pmatrix} I \\ b_k^\dagger \\ e^{ik} I \end{pmatrix} \]

Momentum occupation:

\[ n(k) = \frac{1}{L} b_k^\dagger b_k \]

- Broken \( U(1) \) symmetry: \( \langle b_k^\dagger \rangle \neq 0 \) hence \( n(k = 0) \propto L \) (extensive)
- With \( U(1) \) symmetry: \( n(k = 0) \) is finite, but diverges with \( m \) in superfluid phase
Bose-Hubbard Model $N(k)$

Infinite 1D, one particle per site

$N(k)$

$U/J = 3.2$

$U/J = 3.6$

$U/J = 4.0$

$U/J = 4.8$

$U/J = 6.4$

Bose-Hubbard Model $N(k)$

Infinite 1D, one particle per site
Higher moments

It is straightforward to evaluate a local order parameter, eg

\[ M = \sum_i M_i \]

The first moment of this operator gives the order parameter,

\[ \langle M \rangle = m_1(L) \]

It is also useful to calculate higher moments, eg

\[ \langle M^2 \rangle = m_2(L) \]

or generally

\[ \langle M^k \rangle = m_k(L) \]

These are polynomial functions in the system size \( L \).
For finite systems, the Binder cumulant of the order parameter cancels the leading-order finite size effects

\[ U_L = 1 - \frac{\langle m^4 \rangle}{3 \langle m^2 \rangle^2} \]

The 2-component Bose-Hubbard model, with a linear coupling between components, has an Ising-like transition from immiscible (small \( \Omega \)) to miscible (large \( \Omega \)).

\[
H = \sum_{\langle i,j \rangle, \sigma} b_{i,\sigma}^{\dagger} b_{j,\sigma} + \text{H.c.} + U \sum_{i,\sigma} n_{\sigma}(n_{\sigma} - 1) + U_{12} \sum_{i} n_{\uparrow} n_{\downarrow} + \Omega \sum_{\langle i,j \rangle} b_{i,\uparrow}^{\dagger} b_{j,\downarrow} + \text{H.c.}
\]
Cumulant expansions

Express the moments $m_i$ in terms of the cumulants per site $\kappa_j$,

$$
\begin{align*}
    m_1(L) &= \kappa_1 L \\
    m_2(L) &= \kappa_1^2 L^2 + \kappa_2 L \\
    m_3(L) &= \kappa_1^3 L^3 + 3\kappa_1\kappa_2 L^2 + \kappa_3 L \\
    m_4(L) &= \kappa_1^4 L^4 + 6\kappa_1^2\kappa_2 L^3 + (3\kappa_2^2 + 4\kappa_1\kappa_3)L^2 + \kappa_4 L \\
\end{align*}
$$

$\kappa_1$ is the order parameter itself
$\kappa_2$ is the variance (related to the susceptibility)
$\kappa_3$ is the skewness
$\kappa_4$ is the kurtosis

The cumulants per site $\kappa_k$ are well-defined for an iMPS

Note: the cumulants are normally written such that they are extensive quantities $\rightarrow L\kappa_k$. 
The cumulant expansion already gives a lot of information

$\kappa_1$ is the order parameter itself

Ising transition in 2-component Bose gas

Order parameter $|N_a - N_b|$
The second cumulant gives the susceptibility

Different to a finite-size scaling, the susceptibility exactly diverges at the critical point.
Sufficiently close to the critical point, it looks mean-field-like (so will generally give the wrong exponent!)

2-component Bose gas
Second cumulant (susceptibility)
The fourth cumulant changes sign at the transition.

2-component Bose gas

The fourth cumulant
Naively taking the limit $L \to \infty$ for the Binder cumulant doesn’t produce anything useful:

- if the order parameter $\kappa_1 \neq 0$,
  $$U_L = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle^2_L} \to \frac{2}{3}$$

- if $\kappa_1 = 0$, then $m_4(L) = 3k_2^2L^2 + k_4L$
  Hence
  $$U_L = 1 - \frac{3k_2^2L^2 + k_4L}{3k_2^2L^2} \to 0$$

Finally, a step function that detects whether the order parameter is non-zero

Better approach, in the spirit of finite-entanglement scaling: Evaluate the moment polynomial using $L \propto$ correlation length
Transverse field Ising model

Binder cumulant, scale factor $s=5$
String parameters
Order parameters do not have to be local

Mott insulator string order parameter

\[ O_P^2 = \lim_{|j-i| \to \infty} \langle \prod_{k=i}^{j} (-1)^{n_k} \rangle \]

We can write this as a correlation function of ‘kink operators’,

\[ p_i = \prod_{k<i} (-1)^{n_k} \]

This turns the string order into a 2-point correlation function:

\[ O_P^2 = \lim_{|j-i| \to \infty} \langle p_i p_j \rangle \]

Or as an order parameter:

\[ P = \sum_i p_i \]

Then \[ O_P^2 = \frac{1}{L^2} \langle P^2 \rangle \]
Real example: 3-leg Bose-Hubbard model with flux phase (F. Kolley, M. Piraud, IPM, U. Schollwoeck, F. Heidrich-Meisner, *in preparation*)

For density \( n = 1/3 \) (one particle per rung), near flux \( \phi \sim \pi \), there is a transition from a Mott to critical as a function of \( J_\perp \)

- \( P \) has a simple MPO representation

\[
P = \begin{pmatrix}
I & (-1)^n \\
I & (-1)^n
\end{pmatrix}
\]

- Hence we can calculate higher moments of \( P \).
Bose-Hubbard Ladder
String order parameter

$O_p^2$ vs $J_{\text{perp}}$ for different $m$ values:
- $m=100$
- $m=150$
- $m=200$
- $m=300$
- $m=400$
- $m=500$
- $m=800$

Graph showing the relationship between the string order parameter and the transverse field $J_{\text{perp}}$ for various values of $m$. The inset graph provides a magnified view for a specific range of $J_{\text{perp}}$. The $y$-axis represents $O_p^2$ and the $x$-axis represents $J_{\text{perp}}$.
Bose=Hubbard Ladder
Scaling of correlation length

\[
\xi = \begin{cases} 
J_{\perp} = 0.99 \\
J_{\perp} = 1.00 \\
J_{\perp} = 1.01 \\
J_{\perp} = 1.02 \\
J_{\perp} = 1.03 \\
J_{\perp} = 1.04 \\
J_{\perp} = 1.05 \\
J_{\perp} = 1.06 \\
J_{\perp} = 1.10 \\
J_{\perp} = 1.14 \\
J_{\perp} = 1.25 
\end{cases}
\]
Infinite boundary conditions
(see also Zauner et al 1207.0862, Milsted et al Phys. Rev. B 155116 (2013))

Local perturbation to a translationally invariant state

Map infinite system onto a finite MPS, with an effective boundary
• Key point: Even if the perturbation is correlated at long range, only the tensors at the perturbation are modified

• Decompose the Hamiltonian

$$H = H_L + H_{LW} + H_W + H_{WR} + H_R$$

• We can calculate $H_L$ and $H_R$ by summing the infinite series of terms from the left and right

• Away from the perturbation the wavefunction is approximately an eigenstate, so

$$\exp itH_L \sim I$$

and we don’t leave the Hilbert space of the semi-infinite strip
Spin-1 Heisenberg chain, $S^+$ initial perturbation

\[ \langle S_z(x, t) \rangle \]

$t = 20$
$t = 4$
$t = 2$
$t = 0$

Infinite boundaries

window size = 60
window size = 200

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iDMRG
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Resize the window

We can do better - why keep the size of the window fixed?
Window expansion - incorporate sites from the translationally-invariant section into the window

Criteria for expanding: is the wavefront near the boundary? (Calculate from the fidelity of the wavefunction at the boundary)
Window contraction

Window contraction - incorporate tensors from the window into the boundary
Contract the MPS and Hamiltonian MPO

\[ \begin{align*}
B^{s_{N-1}} & \quad B^{s_N} \\
E_R & \quad (a) \\
B^{s_{N-1}^*} & \quad B^{s_N^*}
\end{align*} \]

\[ \begin{align*}
A^{s_1} & \quad A^{s_2} \\
E_L & \quad (b) \\
A^{s_1^*} & \quad A^{s_2^*}
\end{align*} \]

= 

= 

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Follow the wavefront

\[ \langle S_z(x, t) \rangle \]

Moving window

Fixed window

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Summary

- iDMRG – efficient algorithm for obtaining translationally invariant iMPS
- Many quantities are natural for iMPS but difficult to calculate for finite systems (e.g., correlation length)
- Finite-entanglement scaling – often easier than finite-size scaling
- Binder cumulant for detecting phase transitions
- Local perturbations – Infinite Boundary Conditions

Future:
- Equations for the moment expansion have the same structure as the equations for perturbations and excitations (see Frank’s talk!)

Thanks:
- Fei Zhan, Greg Crosswhite, Phien Ho, Guifre Vidal, lots more...