Techniques for translationally invariant matrix product states

Ian McCulloch

University of Queensland Centre for Engineered Quantum Systems (EQuS)

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Outline



- Expectation values of iMPO's
 - Higher moments
 - Binder cumulant
- Entanglement spectrum
 - Projective representations
- 5 Triangular Heisenberg model example
- 6 Binder ratio for symmetric states

Correlation Functions



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



- All eigenvalues ≤ 1
- One eigenvalue equal to 1, corresponding to the identity operator

Expansion in terms of eigenspectrum λ_i :

$$\langle O(x)O(y)\rangle = \sum_i a_i \lambda_i^{|y-x|}$$

Hubbard Model transfer matrix spectrum

Half-filling, U/t = 4





Critical scaling example

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



For a critial mode, the correlation length increases with number of states m as a power law,

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

[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,

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

[Pollmann et al, PRL 2009]

Note: in practice this usually isn't a good way to determine c – better to use entropy scaling

Scaling dimensions

(Vid Stojevic, IPM et al, Phys. Rev. B **91**, 035120 (2015)) 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 ξ_1 and ξ_2
- We expect: $\frac{O(\xi_2)}{O(\xi_1)} = \left(\frac{\xi_2}{\xi_1}\right)^{\Delta}$
- for *x* large, we have: $O(x) \simeq a \lambda^x$ (with $\xi = -1/\ln \lambda$)
- Prefactor *a* is overlap of operator *O* with next-leading eigenvector of transfer operator

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

This gives directly the operator scaling dimensions by direct fit

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Heisenberg model fit for the scaling dimension



Expectation values of MPO's - arxiv:0804.2509

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

$$\left(egin{array}{ccc} I & & \ S^z & & \ \lambda S^x & S^z & I \end{array}
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 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:

$$\left(egin{array}{ccc} I & & \ S^z & & \ \lambda S^x & S^z & I \end{array}
ight)$$

Eigentensor is $(E_1 \quad E_2 \quad E_3)$

• 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

$$\begin{aligned} E_1(L+1) &= T_I(E_1(L)) + T_{S^z}(E_2) + T_{\lambda S^z}(E_3) \\ &= T_I(E_1(L)) + C \end{aligned}$$

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 λ₁ = 1 by construction, this motivates decomposing into components parallel (e₁) and perpendicular (E'₁) to the identity:

$$E_1(L+1) = E'_1(L) + e_1(L) I$$

where $\operatorname{Tr} E_1'(L)\rho = 0$

• Component in the direction of the identity:

$$e_1(L+1) = e_1(L) + \operatorname{Tr} C\rho$$

Has the solution

$$e_1(L) = L \operatorname{Tr} C \rho$$

is the energy

• Component perpendicular to the identity:

$$E'_1(L+1) = T_I(E'_1(L)) + C'$$

where $C' = C - (\operatorname{Tr} C\rho) I$

$$E_1'(L+1)_n = \lambda_n E_1'(L)_n + C_n'$$

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:

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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

E_3	=	Ι	Identity operator
E_2	=	Sz	Sz block operator
$E_1(L)$	=	$E' + Le_1$	Hamiltonian operator + energy per site

Generalization to arbitrary triangular MPO's arXiv:1008.4667

At the *i*th iteration, we have



Basic idea:

• if $W_{ii} = 0$, then $E_i = C$

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

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 arXiv:1008.4667

At the *i*th iteration, we have

$$E_i(L+1) = T_{W_{ii}}(E_i(L)) + \underbrace{\sum_{j>i} T_{W_{ji}}(E_j(L))}_{= C(L)}$$

Basic idea:

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

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
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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

$$\langle H^2 \rangle_L - \langle H \rangle_L^2 = \langle (H-E)^2 \rangle_L = L\sigma^2$$

A universal measure for the quality of a variational wavefunction
 lower bound for the energy: there is always an eigenstate within *σ* of *E* We can easily construct an MPO representation of *H*²



Ian McCulloch (UQ)

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Example 2 - momentum distribution

Momentum-dependent operators have a simple form,

$$b_{k}^{\dagger} = \sum_{x} e^{ikx} b_{x}^{\dagger}$$
$$W_{b_{k}^{\dagger}} = \begin{pmatrix} I \\ b^{\dagger} & e^{ik}I \end{pmatrix}$$

Momentum occupation:

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

- Broken U(1) symmetry: $\langle b^{\dagger} \rangle \neq 0$ 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



æ

It is straight forward 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



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

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

Express the *moments* m_i in terms of the *cumulants per site* κ_j ,

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

 κ_1 is the order parameter itself κ_2 is the variance (related to the susceptibility) κ_3 is the skewness κ_4 is the kurtosis

The cumulants per site κ_k are well-defined for an iMPS

Note: the cumulants are normally written such that they are extensive quantities $\rightarrow L\kappa_k$.

iMPS for two-component bose gas

The cumulant expansion already gives a lot of information

 κ_1 is the order parameter itself





The second cumulant gives the susceptibility 2-component Bose gas

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!*)



The fourth cumulant changes sign at the transition. 2-component Bose gas

Binder Cumulant for iMPS

Naively taking the limit $L \rightarrow \infty$ for the Binder cumulant doesn't produce anything useful:

• if the order parameter $\kappa_1 \neq 0$,

$$U_L = 1 - rac{\langle m^4
angle_L}{3 \langle m^2
angle_L^2} o rac{2}{3}$$

• if
$$\kappa_1 = 0$$
, then $m_4(L) = 3k_2^2L^2 + k_4L$
Hence

$$U_L = 1 - \frac{3k_2^2 L^2 + k_4 L}{3k_2^2 L^2} \to 0$$

 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



Scaling functions

Critical exponents

Exponent	r	elati	on
ν	ξ	\propto	$ t ^{-\nu}$
β	$\langle M angle$	\propto	$(-t)^{\beta}$
α	С	\propto	$ t ^{\alpha}$
γ	χ	\propto	$ t ^{\gamma}$

Finite-size scaling functions

$$U_L = \mathcal{U}^0(t L^{1/\nu})$$

$$\langle M \rangle = L^{-\beta/\nu} \mathcal{M}^0(t L^{1/\nu})$$

Finite-entanglement scaling functions

$$U_m = \mathcal{U}^0(t \, m^{\kappa/\nu}) \langle M \rangle = m^{-\beta \kappa/\nu} \mathcal{M}^0(t \, m^{\kappa/\nu})$$

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Binder Cumulant scaling function collapse



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Mott insulator string order parameter

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

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:

$$O_P^2 = \lim_{|j-i| o \infty} \langle \ p_i \ p_j \
angle$$

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, New J. Phys. 17 (2015) 092001)



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

$$P = \left(\begin{array}{cc} I \\ I \end{array} \right)$$

• Hence we can calculate higher moments of P.

Bose-Hubbard Ladder

String order parameter



Bose=Hubbard Ladder

Scaling of correlation length



Bose-Hubbard Ladder

String parameter Binder cumulant



Entanglement spectrum spectroscopy



- Bipartite cut reduced density matrix ρ
- Entanglement Hamiltonian $H = -\ln \rho$
- Reduced dimension the entanglement Hamiltonian lives on the boundary
- Label states by global symmetries spin, transverse momentum
- Degeneracy structure provides information about symmetries

For SU(2) symmetry broken states:

- If the symmetry is allowed to break: bulk gap
- unbroken *SU*(2): Goldstone mode, separated band of excitations below the bulk gap

Symmetries

Infinite cylinder of circumference Ly





Map onto one-dimensional chain:

Global symmetries

Preserved in the MPS structure:

• internal symmetries, such as particle number, spin, ...

Broken by the real-space structure:

 spatial symmetries, such as translation, reflection of the cylinder



Symmetry-resolved density matrix



Eigenvalues of ρ' are $\lambda_i e^{i\theta_i}$

- λ_i are the density matrix eigenvalues
- θ_i is the corresponding symmetry angle up to a global phase

Allowed symmetries of the ES

Let U be a global symmetry of the wavefunction

 $U|\psi
angle = e^{i heta}|\psi
angle$

What is the action of U on the reduced density matrix ρ ?

Bipartition:

$$egin{array}{rcl} |\psi
angle &=& \sum_{ab}\psi_{ab} & |a
angle\otimes |b
angle \ U &=& U_A\otimes U_B \end{array}$$

Action on ρ is $U_A \rho U_A^{\dagger}$

- U_A is distinguishable only up to a global phase
- U_A is a projective representation of the symmetry

Projective representations

Physical states are rays in Hilbert space

• $a|\psi\rangle$, for $a \in \mathbb{C}$ represents the same physical state

Symmetry transformations that are ambiguous up to some scalar are *projective representations*

Assuming a unitary representation, only the phase is unknown: $a = e^{i\theta}$. A projective representation is defined by:

$$U_x U_y = e^{i\theta(x,y)} U_{xy}$$

The function $\theta(x, y)$ defines the representation Example:

- Z₂ has no non-trivial (unitary) projective representations
- $Z_2 \times Z_2$ has has two projective representations

$$egin{array}{rcl} U_x^2&=&I\ U_y^2&=&I\ U_xU_y&=&\pm U_yU_x \end{array}$$

Triangular lattice – frustration

Frustrated lattice – suppress ordering



- But ordering may be possible
- Groundstate widely established as SU(2)-broken 120° order



Beyond nearest neighbor: $H = J_1 \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j + J_2 \sum_{\langle \langle i,j \rangle \rangle} \vec{S}_i \vec{S}_j$

Z_2 spin liquid

- The simplest spin liquid that doesn't break time reversal symmetry
- Elementary excitations are spinons with non-trivial braiding statistics (anyons)
- Four anyon types:
 - 1 : vacuum
 - **b** : bosonic spinon (electric charge e)
 - V: vison

- (magnetic charge m)
- **f** : fermionic spinon (fermion ψ)
- Fusion rules for combining excitations:
 - $b \times b = 1$
 - $v \times v = 1$
 - $f \times f = 1$
 - $b \times v = f$
 - $b \times f = v$
 - $v \times f = b$

Anyonic statistics

R matrix: counter-clockwise exchange of particles

S matrix: intertwining two vacuum

 $\begin{array}{c} \stackrel{a}{\searrow} \stackrel{b}{\searrow} = R_c^{ab} \\
S^{ab} = \frac{1}{D} \underbrace{\bigcirc}_{c} \stackrel{a}{\longrightarrow} \\
S^{ab} = \frac{1}{D} \underbrace{\bigcirc}_{c} d_c \operatorname{Tr} \left(R_c^{ab} R_c^{ba} \right)
\end{array}$

$$R_1^{bb} = R_1^{vv} = 1$$

 $R_1^{ff} = (R_f^{vb})^2 = -1$

In basis (1, b, v, f):

excitations

- construct a vison or spinon that threads down the torus
- spinon flips between time-reversal symmetric and antisymmetric states
- vison inserts -1 flux antiperiodic boundary conditions
- Symmetry fractionalization these correspond to projective symmetries



How to construct these fluxes?

 translationally invariant infinite system and manipulate the boundary conditions



Antiperiodic boundary conditions

Dihedral group symmetries around the cut:

- T_y translation by one site around the cylinder
- R_y reflection about a site or bond

This forms the dihedral group $D_{2 \times L_y}$

$$T_y^{L_y} = R_y^2 = 1$$

 $R_y T_y^{L_y/2} R_y^{-1} = T_y^{L_y/2}$

(a π rotation commutes with a reflection)

The dihedral group has a non-trivial projective representation:

$$T_y^{L_y} = R_y^2 = 1$$
$$R_y T_y R_y^{-1} = -T_y^{-1}$$

(a π rotation anti-commutes with a reflection) This is the subgroup of $D_{2\times 2\times L_y}$ taking only the odd momenta (antiperiodic BC)

Antiperiodic boundary conditions

Nariman Saadatmand, IPM, Phys. Rev. B 94, 121111 (2016)

We see two (nearly) degenerate states

 smaller L_y: the groundstate has a 2-fold degenerate entanglement spectrum

• for larger L_y , we obtained a non-degenerate entanglement spectrum In the two-fold degenerate sector, we measure

$$\langle R_y T_y^{L_y/2} R_y^{\dagger} T_y^{L/2\dagger} \rangle = -0.9999970 \cdots$$



 $L_y = 6$ entanglement spectrum

Detecting ordered phases

120º ordor	topological	columnar	columnar order	columnar order J2	
120 01001	spin liquids	order	only for YC6: algebraic		2
0.10	5(5) 0.1-	40(5) 0.1	70(5) 0.2	00(5)	

Using SU(2) symmetry the magnetic order parameter is identically zero.

- can we see signatures of symmetry breaking in higher moments of the order parameter?
- Binder cumulant $U_4 = 1 \frac{\langle M^4 \rangle}{3 \langle M^2 \rangle}$

Cumulant expansion of the 4th moment:

$$\langle M^4 \rangle_L = \kappa_1^4 L^4 + 6\kappa_2\kappa_1^2 L^3 + (4\kappa_1\kappa_3 + 3\kappa_2^2)L^2 + \kappa_4 L^2$$

Symmetry implies all odd cumulants vanish

$$\langle M^4 \rangle_L = 3\kappa_2^2 L^2 + \kappa_4 L$$

Need *L* length scale – use correlation length ξ from transfer matrix Binder ratio

$$BR = \frac{\kappa_4}{\kappa_2^2 \xi}$$

Binder ratio -120° order



Binder ratio – staggered order



Binder ratio – staggered order YC6



Summary

Download the code: https://people.smp.uq.edu.au/lanMcCulloch/mptoolkit



- finite entanglement scaling
- higher moments
- Binder cumulant
- scaling functions
- symmetries of the entanglement spectrum
- Binder ratio for symmetric states

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