Correlations and order parameters in infinite matrix product states

Ian McCulloch
Jason Pillay

University of Queensland
School of Mathematics and Physics

December 6, 2019

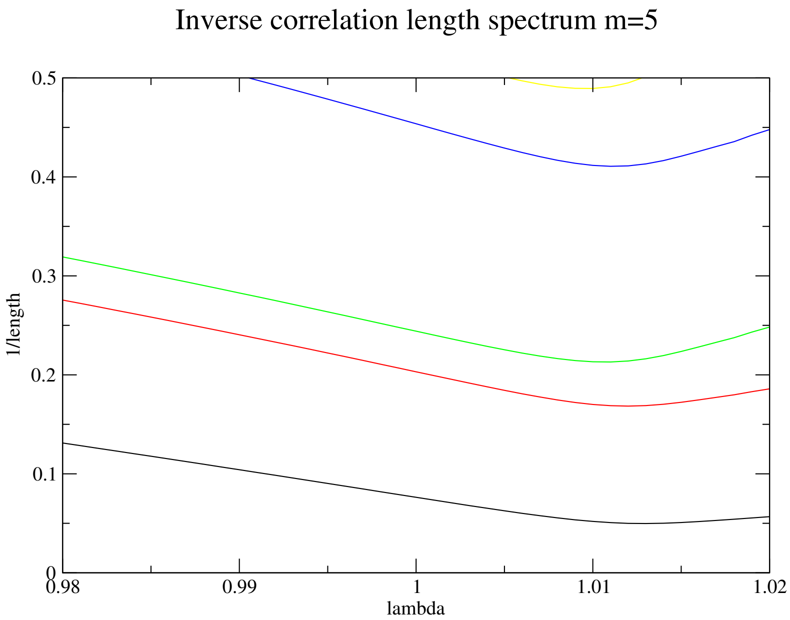
THE UNIVERSITY OF QUEENSLAND
AUSTRALIA

Australian Government
Australian Research Council

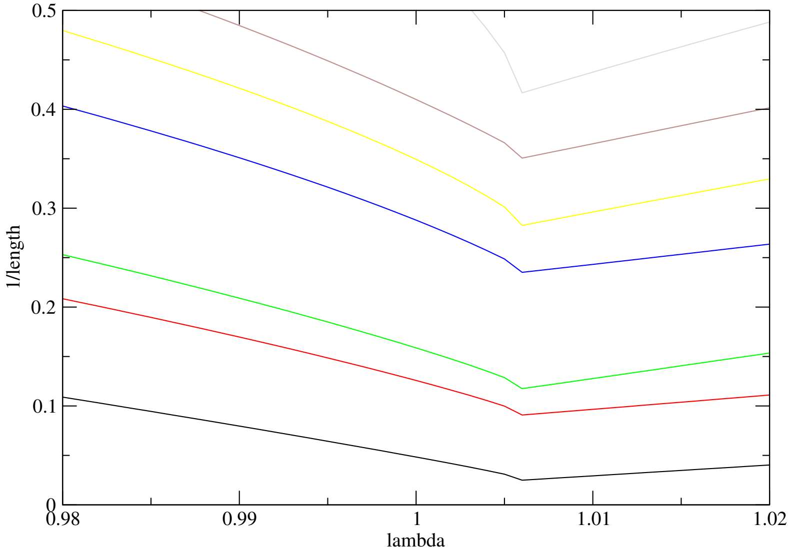
Outline

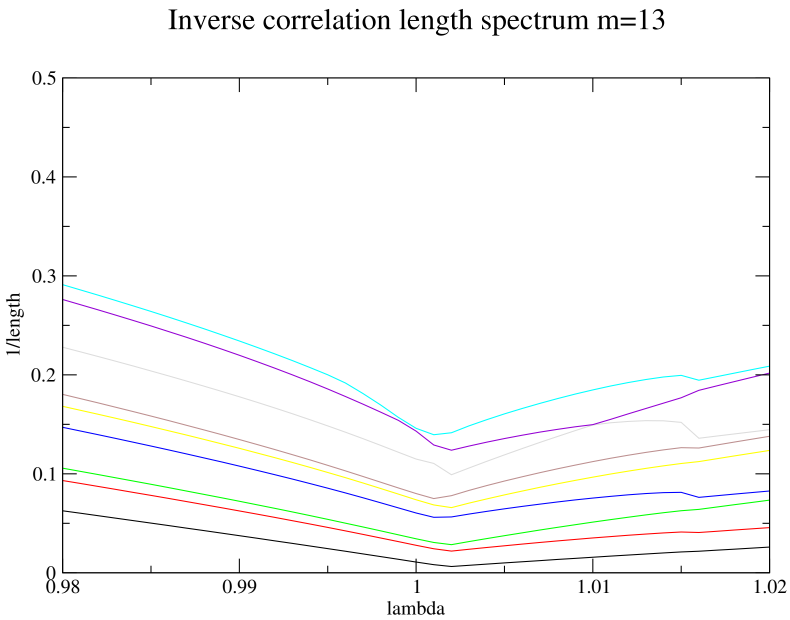
Approaches to detecting criticality

- Bipartite fluctuations
  - Bipartite entropy
  - Entanglement spectrum
  - Bipartite fluctuations in quantum numbers (eg J. Stat. Mech. (2014) P10005 from Karyn le Her's group; Kjall, Phys. Rev. B 87, 235106 (2013))
- Transfer matrix spectrum
  - Eigenvalues λ_i
  - $\lambda_0 = 1$ by construction (normalization condition)
  - Spectrum of correlation lengths $\xi_i = -\frac{1}{\ln \lambda_i}$
  - Or consider $\epsilon_i = -\ln \lambda_i = 1/\xi_i$
    – Behaves like an energy scale
  - Choice of which quantity to use as the scaling variable
    - Scaling with respect to the bond dimension
    - Scaling with respect to the correlation length – diverges at critical point
    - Scaling with respect to $\delta = \epsilon_2 - \epsilon_1$ *(or some other combination of ϵ_i)*
- Order parameter and order parameter fluctuations (higher moments)
  - Lots of history behind finite-size scaling, can be modified for finite-entanglement scaling
  - J. Pillay and IPM, arXiv:1906.03833 (to appear in PRB)


Inverse correlation length spectrum m=5
0.5
0.4
0.3
0.2
0.1
0
1/length
0.98
0.99
1
1.01
1.02
lambda

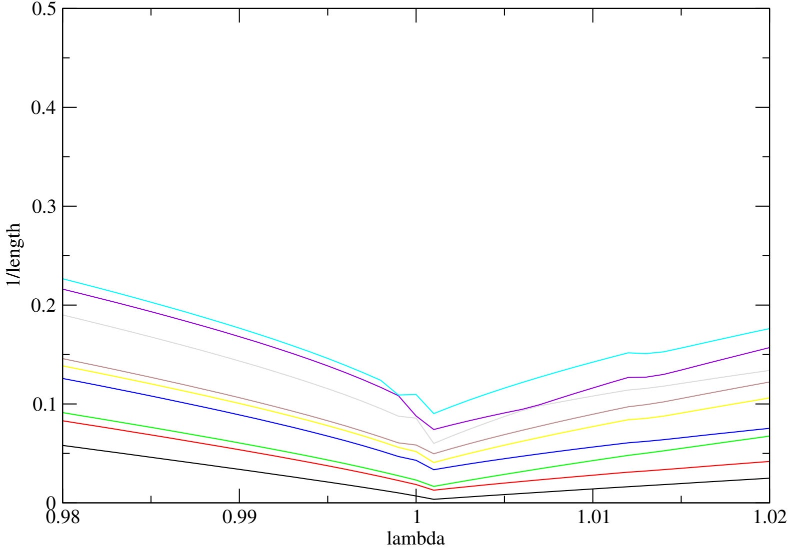
Inverse correlation length spectrum m=6

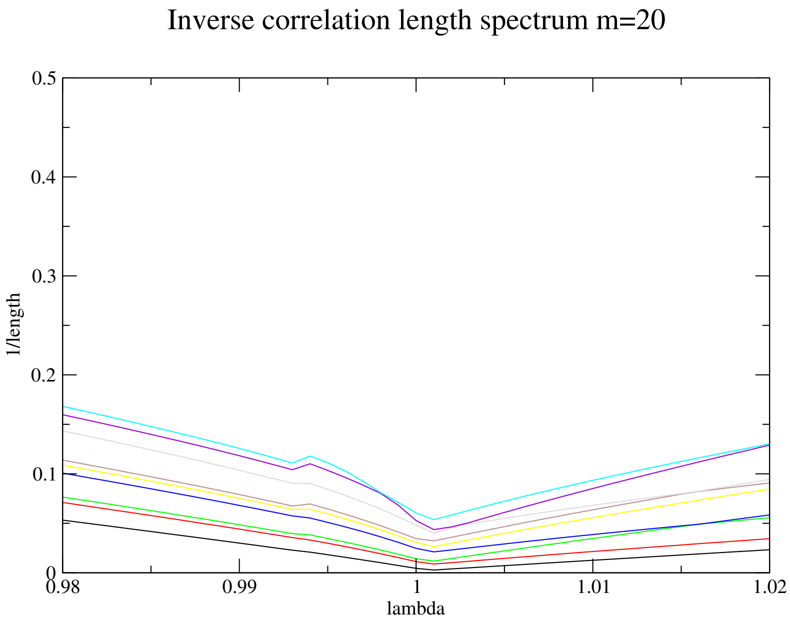


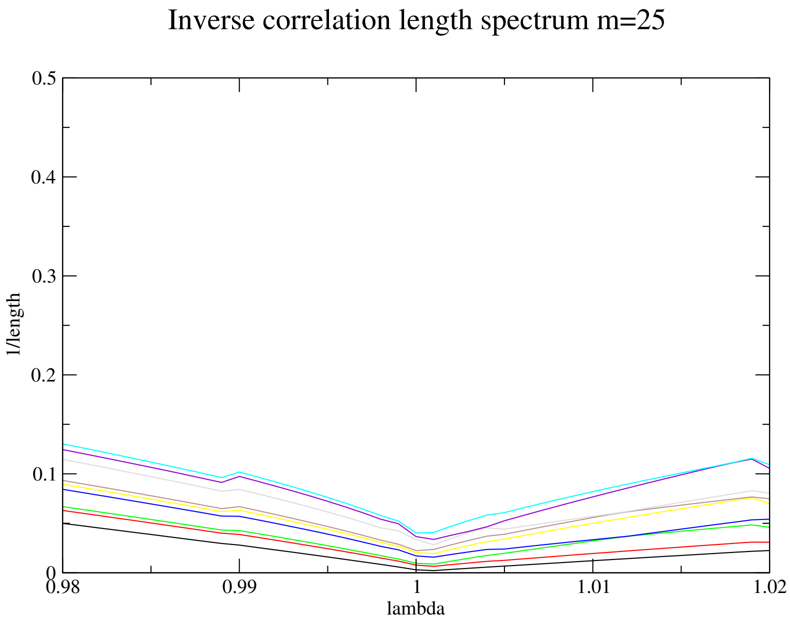


Inverse correlation length spectrum m=13
1/length
lambda
0.5
0.4
0.3
0.2
0.1
0
0.98
0.99
1
1.01
1.02

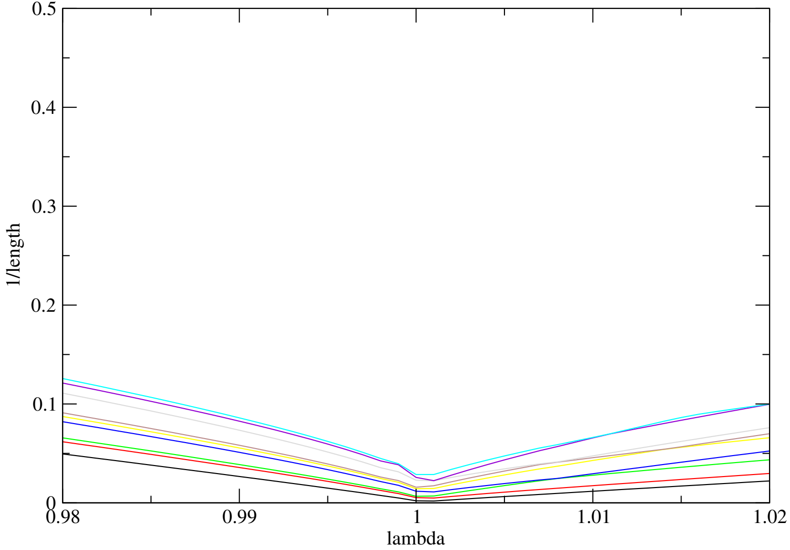
Inverse correlation length spectrum m=16

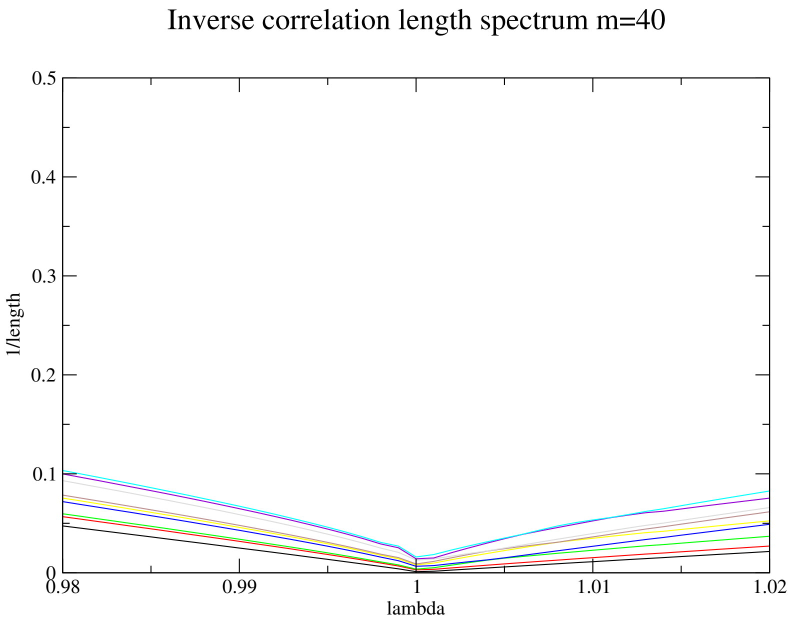



Inverse correlation length spectrum m=20
1/length
lambda
0
0.1
0.2
0.3
0.4
0.5
0.98
0.99
1
1.01
1.02


Inverse correlation length spectrum m=25
1/length
0
0.1
0.2
0.3
0.4
0.5
0.98
0.99
1
1.01
1.02
lambda

Inverse correlation length spectrum m=30




Inverse correlation length spectrum m=40
0.5
0.4
0.3
0.2
0.1
0
1/length
0.98
0.99
1
1.01
1.02
lambda

Higher moments

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.

Cumulant expansions

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

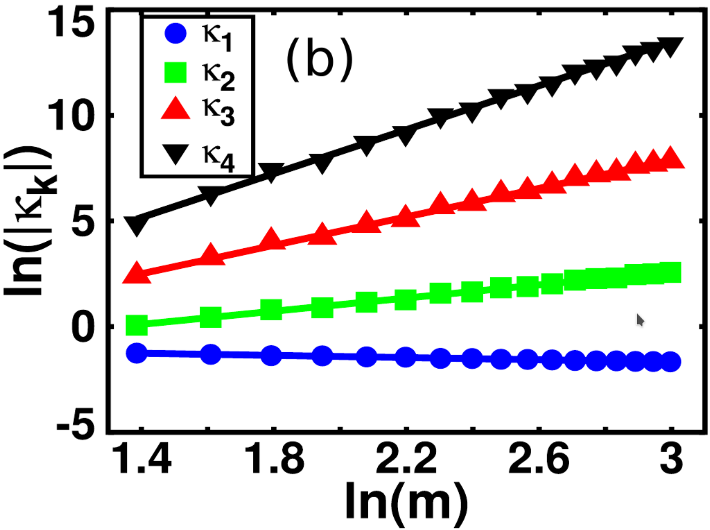
$$
\begin{aligned}
m_1(L) &= \kappa_1 L \\
m_2(L) &= \kappa_1^2 L^2 + \kappa_2 L \\
m_3(L) &= \kappa_1^3 L^3 + 3\kappa_1\kappa_2 L^2 + \kappa_3 L \\
m_4(L) &= \kappa_1^4 L^4 + 6\kappa_1^2\kappa_2 L^3 + (3\kappa_2^2 + 4\kappa_1\kappa_3) L^2 + \kappa_4 L
\end{aligned}
$$

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 a translationally invariant iMPS
- The moments (and hence cumulants) can be obtained *directly* as a polynomial-valued expectation value (arXiv:1008.4667)

(I don't know of a good way to calculate the cumulants per site for a finite system!)

The cumulants have power-law scaling at a critical point, $\kappa_i \propto m^{\alpha_i}$



Ising model example

Scaling functions

For finite systems, scale with respect to system size L
Control parameter $h \equiv \frac{\lambda - \lambda_c}{\lambda_c}$

Critical exponents

Exponent	relation
ν	$\xi \propto \|h\|^{-\nu}$
β	$\langle M \rangle \propto (-h)^{\beta}$
γ	$\sigma^2 = \langle M^2 \rangle - \langle M \rangle^2 \propto \|h\|^{\gamma}$

Scaling relation $2\beta + \gamma = \nu d$

Note: no fluctuation-dissipation theorem: γ is not related to dM/dH.

Finite-size scaling functions

$$
\begin{aligned}
\xi &= L\, \mathcal{X}(h\, L^{1/\nu}) \\
\langle M \rangle &= L^{-\beta/\nu}\, \mathcal{M}(h\, L^{1/\nu}) \\
\sigma^2 &= L^{\gamma/\nu}\, \mathcal{G}(h\, L^{1/\nu}) \\
U_L &= \mathcal{U}(h\, L^{1/\nu}) \qquad \text{(Binder ratio)}
\end{aligned}
$$

Finite entanglement

Effective 'system size' $L \to m^\kappa$

New scaling functions that scale with $t\, m^{\kappa/\nu}$.

Finite-entanglement scaling functions

$$\begin{aligned}
\xi &= m^\kappa\, \mathcal{X}(h\, m^{\kappa/\nu}) \\
\langle M \rangle &= m^{-\beta\kappa/\nu}\, \mathcal{M}(h\, m^{\kappa/\nu}) \\
\sigma^2 &= m^{\gamma\kappa/\nu}\, \mathcal{G}(h\, m^{\kappa/\nu}) \\
U_L &= \mathcal{U}(h\, m^{\kappa/\nu})
\end{aligned}$$

Cumulant exponent relation

Following V. Privman and M.E. Fisher, Phys. Rev. B 30, 322 (1984)

Singular part of the free energy:

$$f \simeq L^{-d} \, Y\left(C_1 t L^{1/\nu}, C_2 h L^{(\beta+\gamma)/\nu}\right)$$

Finite-entanglement version:

$$f \simeq m^{-\kappa d} \, Y\left(C_1 t m^{\kappa/\nu}, C_2 h L^{(\beta+\gamma)\kappa/\nu}\right)$$

Order parameter:

$$\kappa_1 = -\frac{\partial f}{\partial h} = C_2 m^{-\beta\kappa/\nu} Y'\left(C_1 t m^{\kappa/\nu}, C_2 h L^{(\beta+\gamma)\kappa/\nu}\right)$$

Higher cumulants:

$$\kappa_n = -\frac{\partial^n f}{\partial h^n} = C_2^n m^{((n-2)\beta+(n-1)\gamma)\kappa/\nu}$$

Cumulant exponent relation

This gives relation for *all* of the exponents (recall $\kappa_n \sim m^{\alpha_n}$)

$$\alpha_n = \left[(n-2)\beta + (n-1)\gamma\right]\frac{\kappa}{\nu}$$

$$\alpha_1 = -\beta$$

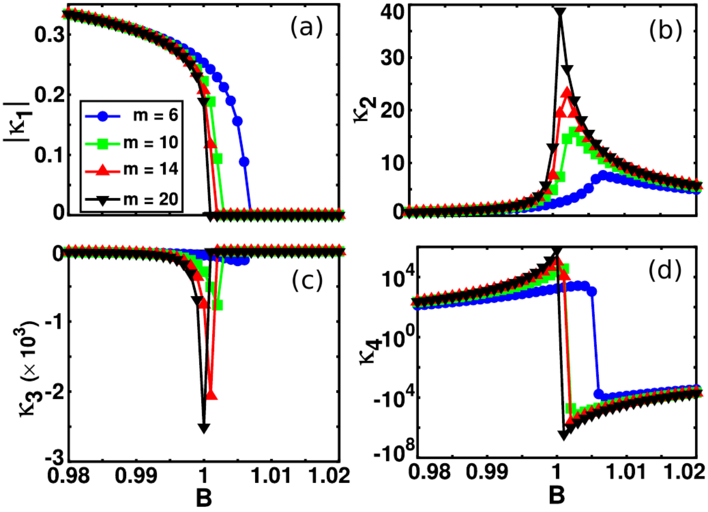
$$\alpha_2 = \gamma$$

This also works for $\alpha_0 = -(2\beta + \gamma)\kappa/\nu = d\kappa$
which is the correlation length exponent!

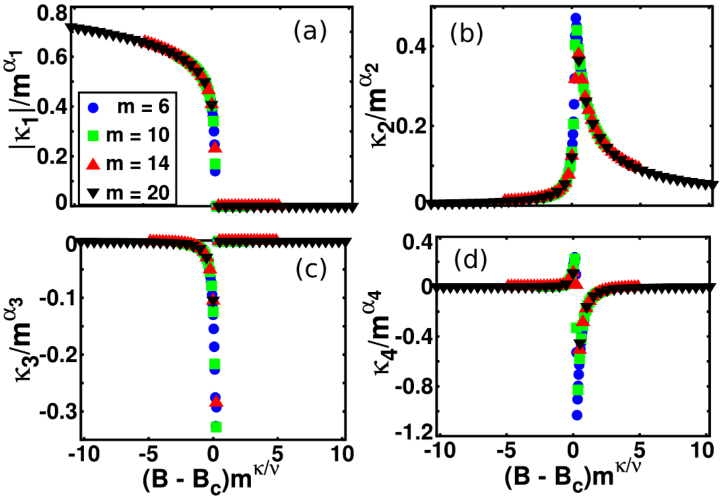
Alternative self-contained expression

$$\alpha_n = -(n-2)\alpha_1 + (n-1)\alpha_2$$

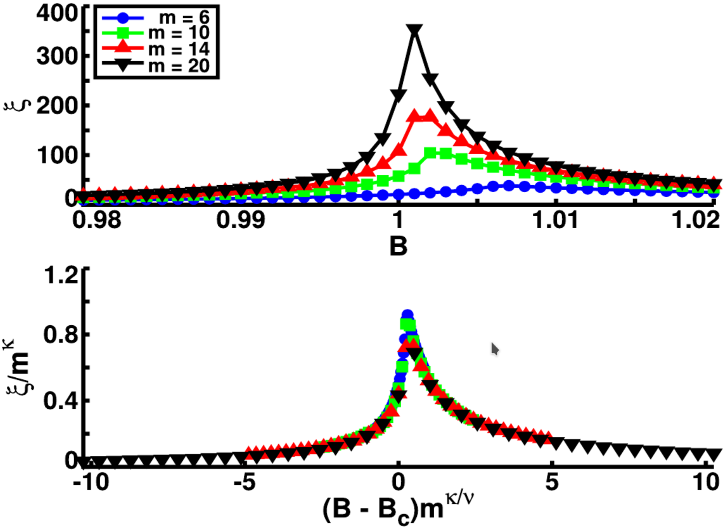
Ising model example



Ising model cumulant scaling functions



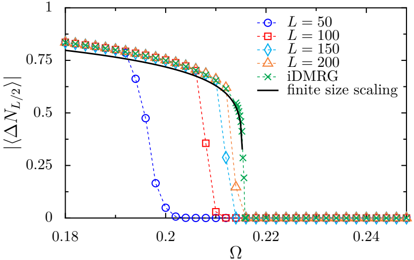
Ising model correlation length scaling function

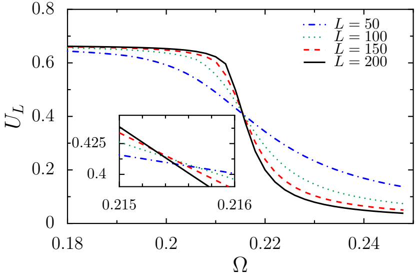


Binder cumulant scaling

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 immersible (small Ω) to miscible (large Ω).

Binder Cumulant for iMPS

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

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

$$U_L = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2} \to \frac{2}{3}$$

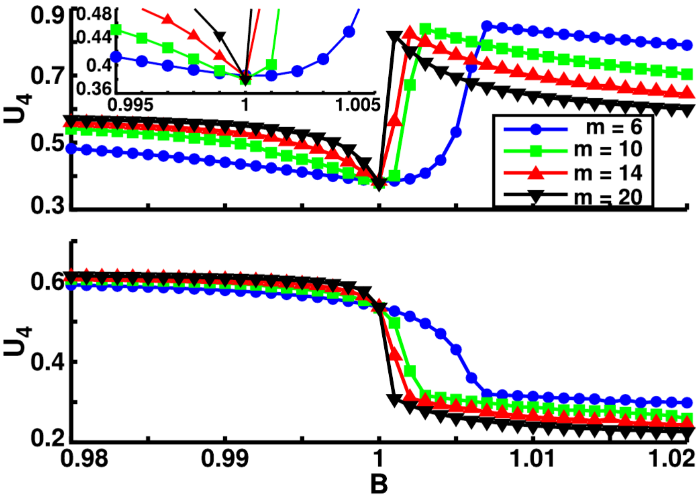
- if $\kappa_1 = 0$, then $m_4(L) = 3k_2^2 L^2 + k_4 L$
  Hence

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

- 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

Choice of scaling parameter $L = s\xi$ is important!



$s = 2$ (top) and $s = s^* = 5.31$ (bottom) chosen by optimisation

For Ising model the point of intersection doesn't depend so much on s, but important in other models!

String parameters
Order parameters do not have to be local

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’,

$$p_i = \Pi_{k<i} \ (-1)^{n_k - 1}$$

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

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

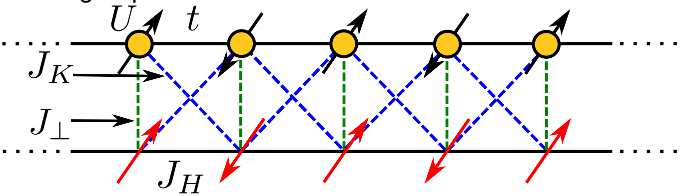
Or as an order parameter:

$$P = \sum_i p_i \qquad \text{MPO: } P = \begin{pmatrix} (-1)^{n-1} & I \\ 0 & I \end{pmatrix}$$

Then $O_p^2 = \frac{1}{L^2} \langle P^2 \rangle$

Example: Kondo lattice J Pillay, IPM, Phys. Rev. B 97, 205133 (2018), arXiv:1906.03833 (PRB)

Simplified model of topological Kondo insulators suggested by Piers Coleman's group M. Dzero, K. Sun, V. Galitski, and P. Coleman, Phys. Rev. Lett. 104, 106408 (2010)



Kondo lattice with local + topological couplings, $n = 1$ particle per site

$$H_{\perp} = J_{\perp} \sum_j \vec{S}_j \cdot \vec{s}_j \qquad H_K = J_K \sum_j \vec{S}_j \cdot \vec{\pi}_j$$

where $\vec{\pi}$ is a vector of non-local spins,

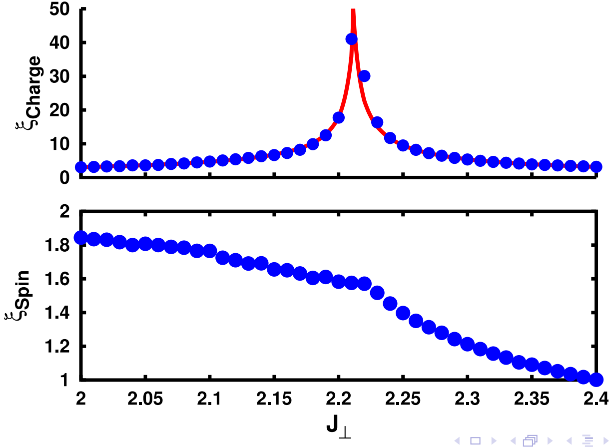
$$\vec{\pi}_j = \frac{1}{2} \sum_{\alpha,\beta} p^{\dagger}_{j,\alpha} \vec{\sigma}_{\alpha,\beta} p_{j,\beta}$$

$$p_{j,\sigma} = \frac{1}{\sqrt{2}} \left(c_{j+1,\sigma} - c_{j-1,\sigma} \right)$$

Topological Kondo chain

- $J_\perp/J_K$ large: topologically trivial insulator, Kondo singlet formation
- $J_K/J_\perp$ large: SPT protected by *spatial reflection*

Phase transition between these two limits:
charge gap vanishes but spin gap remains finite



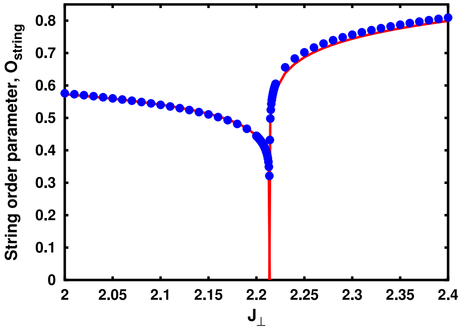
Order parameter for the insulating phases

The kink operators measure charge fluctuations crossing the boundary
In this case, need to use

$$p_i = \Pi_{k<i} (-1)^{\frac{n_k - 1}{2}}$$

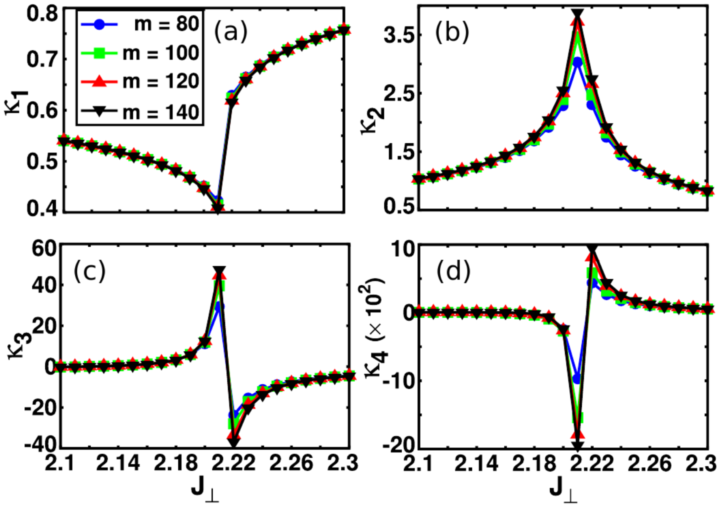
to capture (spinless) 2-particle fluctuations

$$O^2_{\text{string}} = \frac{1}{L^2} \langle P^2 \rangle$$

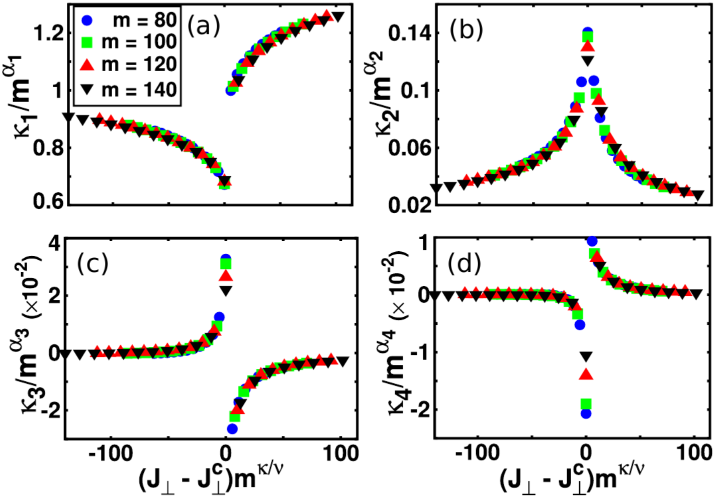


- gives scaling exponent β

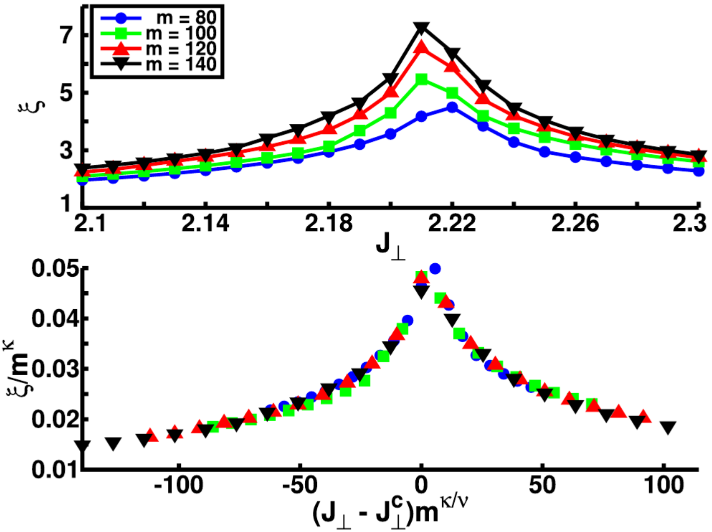
TKI cumulants



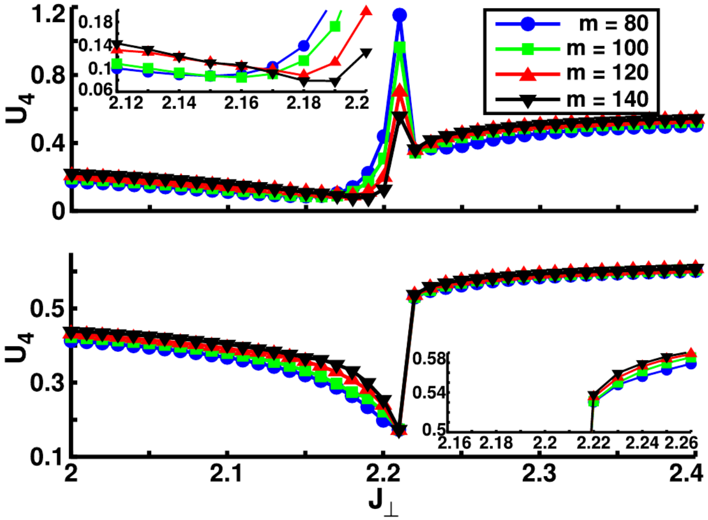
TKI cumulant scaling functions



TKI Correlation length scaling function



TKI Binder Cumulant



The Binder cumulant is more problematic. $s = 2$ (top), $s = s^* = 5.29$ (bottom)

SPT transitions

- Can use conventional string order parameter $\langle S^z(0) \prod_{j=1}^{x-1} (-1)^{S^z(x)} S^z(x) \rangle$
- Not universal – can deform state, string order parameter arbitrarily small
- Proper way to understand SPT: symmetry fractionalization

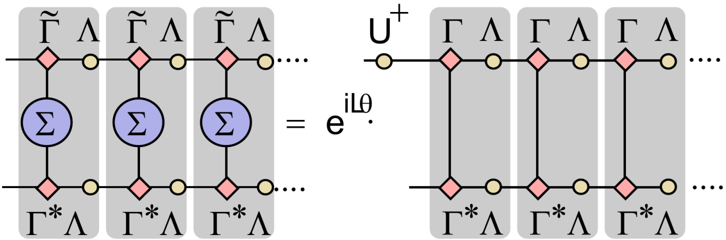


figure shamelessly stolen from Pollman and Turner, PRB 86, 125441 (2012)

- Dihedral: $U^x U^y = \pm U^y U^x$
- Time reversal: $U^\tau U^{\tau *} = \pm 1$
- Space refection: $U^R U^{R*} = \pm 1$

Requires entanglement spectrum spectroscopy – not observable from the physical degrees of freedom

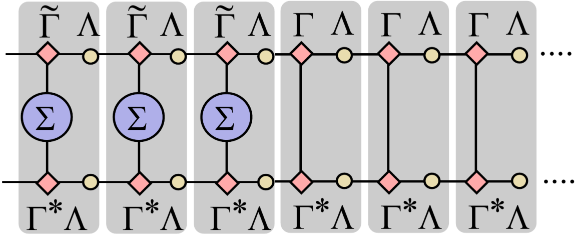
Kink operator for time reversal

Time reversal operator $\tau = UK$, $\tau s^\alpha \tau^{-1} = -s^\alpha$
$K =$ complex conjugation
$U =$ some basis-dependent unitary
Normal basis: $U = \exp i\pi S^y$

- For an MPS, we can treat this as a *local* action
- $\tau(A^s) = \sum_t \langle s \,|\, U \,|\, t \rangle A^{*t}$

Kink operator for time evolution:

$$p_\tau(x) = \prod_{j<x} \tau(j)$$



String correlator $\langle p_\tau(0) p_\tau(x) \rangle$

- Trivial phase: symmetric under time reversal, $\langle p_\tau(0) p\tau(x) \rangle \neq 0$
- SPT phase: antisymmetric under time reversal, $\langle p_\tau(0) p\tau(x) \rangle = 0$

Order parameter: $P_\tau = \sum_x p_\tau(x)$ has MPO form $P_\tau = \begin{bmatrix} e^{i\pi S^y} K & I \\ 0 & I \end{bmatrix}$

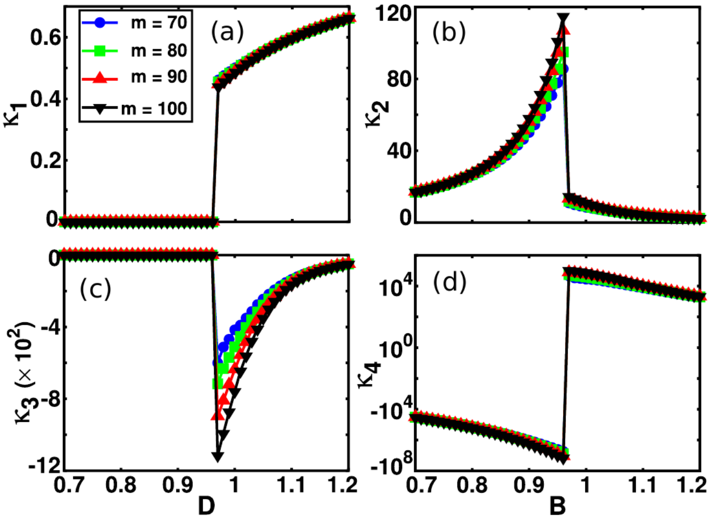
Can calculate $\langle P_\tau^2 \rangle$ straightforwardly, and higher moments, $\langle P_\tau^4 \rangle$, etc

Example: $S = 1$ chain with single-ion anisotropy

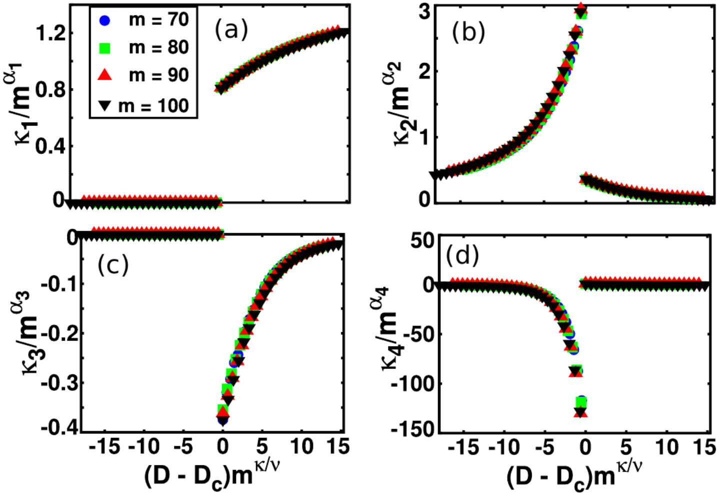
$$H = J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j + D \sum_i (S_i^z)^2$$

Transition from Haldane SPT to trivial phase at $D \simeq 0.96845(8)$ Hu, Normand, Wang, Yu, PRB 84, 220402 (2011)

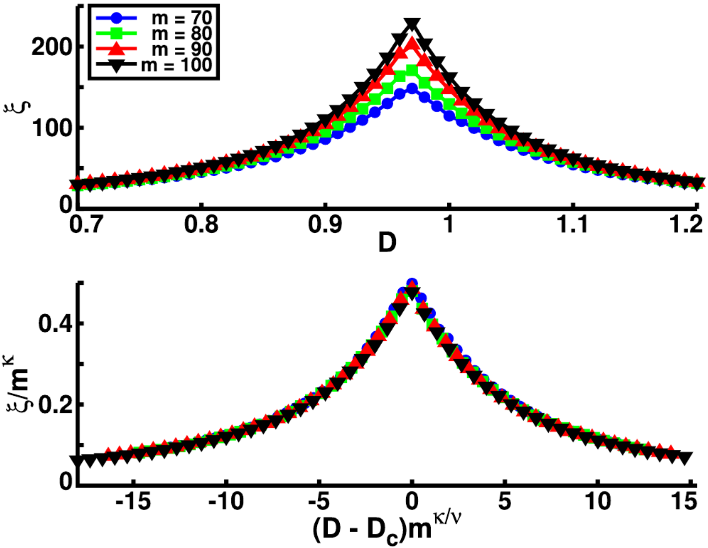
$S = 1$ chain time-reversal order parameter cumulants



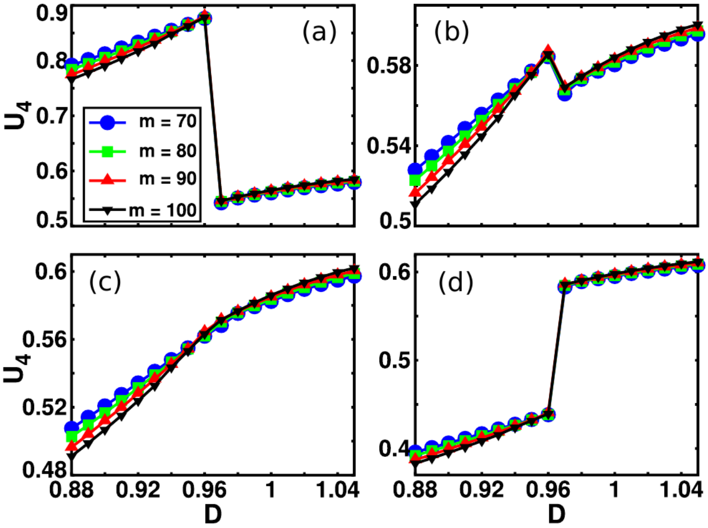
$S = 1$ chain time-reversal cumulant scaling functions



$S = 1$ chain time-reversal correlation length scaling function



$S = 1$ chain time-reversal Binder cumulant



(a) $s = 2$, (b) $s = 3$, (c) $s = s^* = 3.12$, (d) $s = 4$

Bose-Hubbard model BKT transition

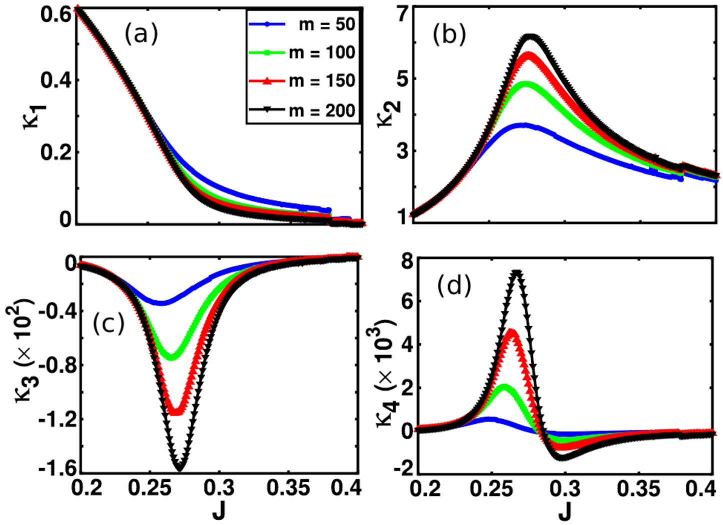
In 1D, there is no superfluid order, so the transition is from an ordered state (Mott insulator) to a critical region.
String order parameter for the Mott transition:

$$O^2_{\text{Mott}} = \lim_{|j-k|\to\infty} \left\langle \mathbb{1}_j \, \text{exp} \left[i\pi \sum_{l=j}^{k} (\hat{n}_l - 1) \right] \mathbb{1}_k \right\rangle ,$$

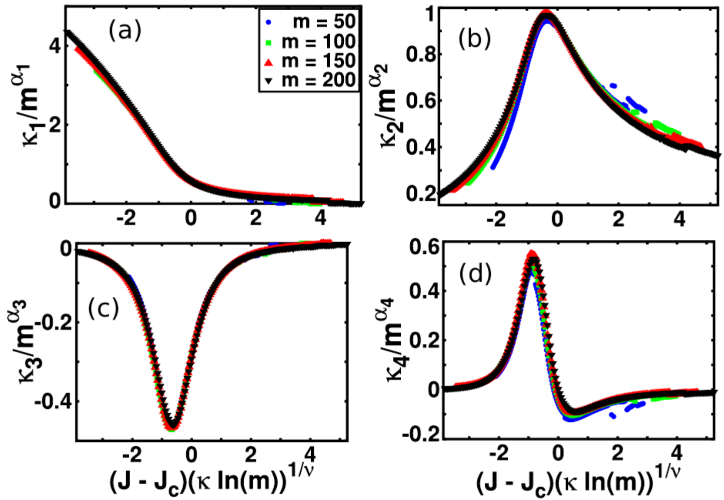
In the insulating phase, fluctuations in the density are short-ranged and $O^2_{\text{Mott}} \neq 0$
In the superfluid phase, there are long-range (power-law) density fluctuations which drives $O^2_{\text{Mott}} \to 0$ (but not exactly zero for an MPS because correlation length is finite! – we preserve $U(1)$ particle number)
At the BKT transition, the correlation length diverges more strongly than power-law

$$\xi \sim \exp\left(\frac{1}{|J - J_c|^\nu} \right)$$

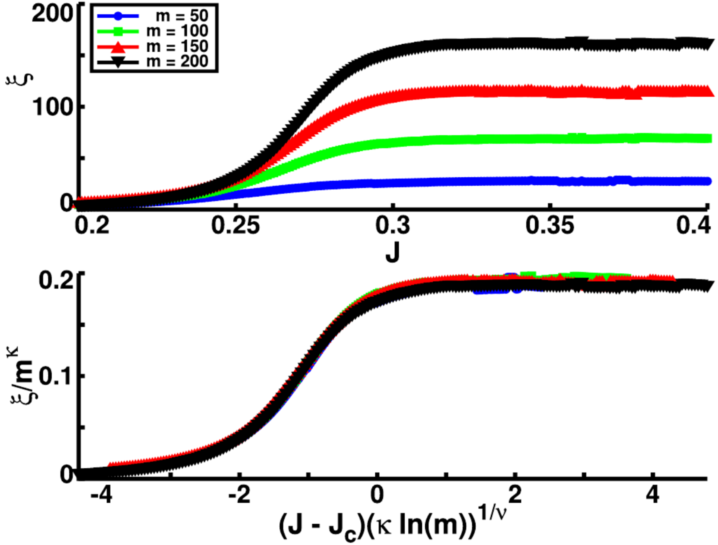
Bose-Hubbard model cumulants



Bose-Hubbard model cumulant scaling functions



Bose-Hubbard model correlation length scaling function



Bose-Hubbard model BKT transition

Scaling function collapse of the Mott string order parameter predicts

$$
\begin{aligned}
J_c &= 0.2850 \pm 0.0005 & (1)\\
\kappa &= 1.275 \pm 0.001 & (2)\\
\beta &= 0.375 \pm 0.001 & (3)\\
\gamma &= 0.350 \pm 0.005 & (4)
\end{aligned}
$$

The obtained κ differs from the expected $c = 1$ result by $\sim 5.1\%$.
J_c differs quite significantly from other recent works, eg $J_c = 0.3048(3)$ obtained by Rams et al with $m = 4000$ states and ϵ scaling.

Summary

- MPO techniques for higher moments
- Scaling functions work very well for detecting critical points
- Correlation length scaling function is simplest case, perhaps easiest
- Binder cumulant – not as easy to use as we hoped
- String order parameters – same scaling properties as local order parameters
- Time reversal as a string order parameter
- Spatial reflection can be considered in a similar way
- Our approach still involves scaling with respect to bond dimension – want to avoid this!

Postdoc and PhD positions available to start 2020

Quantum-Inspired Machine Learning.
This project aims to develop new machine learning techniques based around the close correspondence between neural networks used in deep learning, and tensor networks used in quantum physics.