Correlations and order parameters in infinite matrix product states

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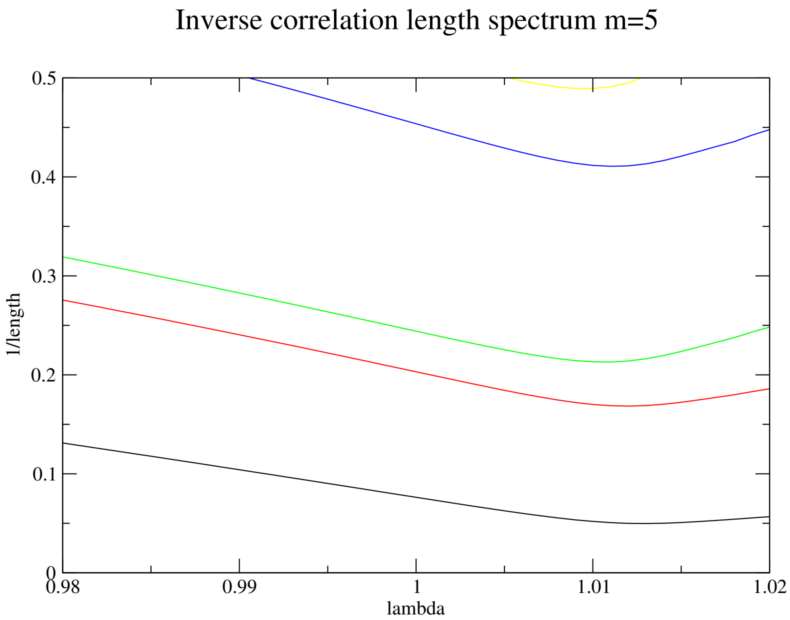
Outline

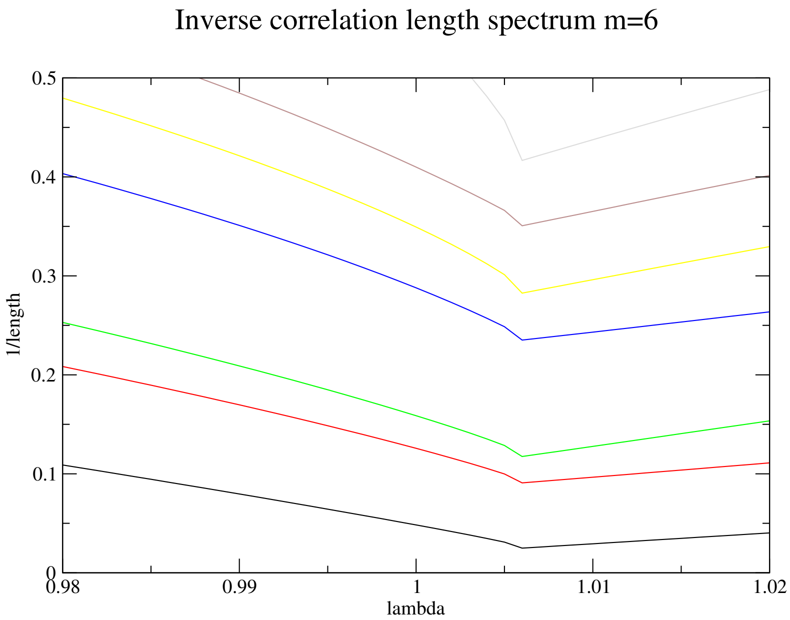
1. Approaches to detecting quantum criticality
2. Cumulants
3. Examples
   - Ising model
   - Potts model
4. Generalising beyond local order parameters
   - string order parameters
   - SPT and time reversal

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, Phys. Rev. B 100, 235140 (2019)



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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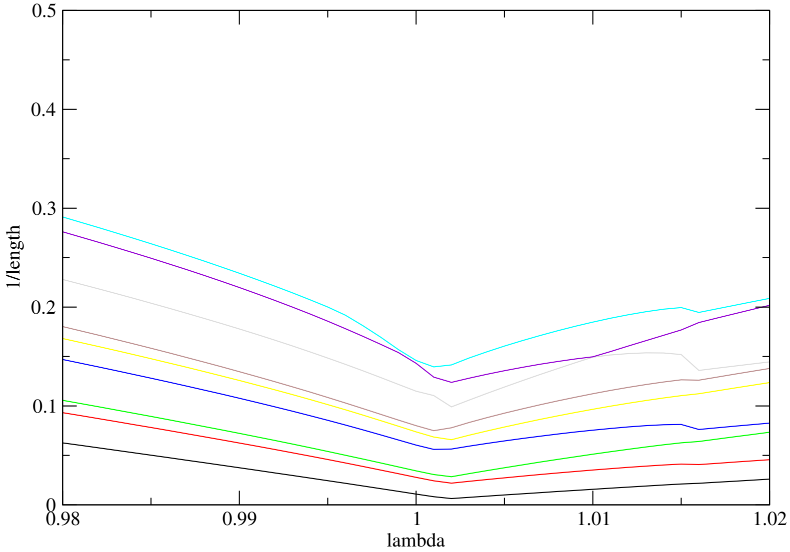
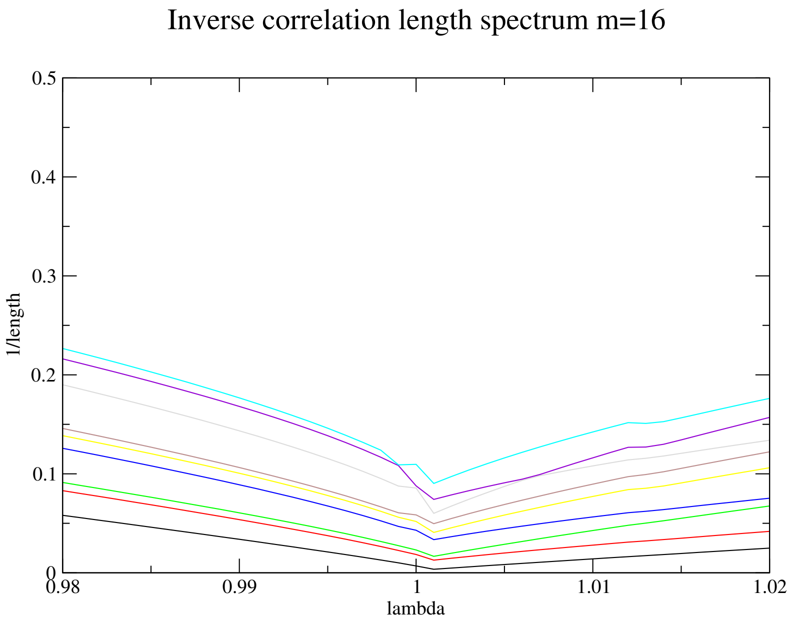
0.1
0
1/length
0.98
0.99
1
1.01
1.02
lambda

Inverse correlation length spectrum m=13

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0
1/length
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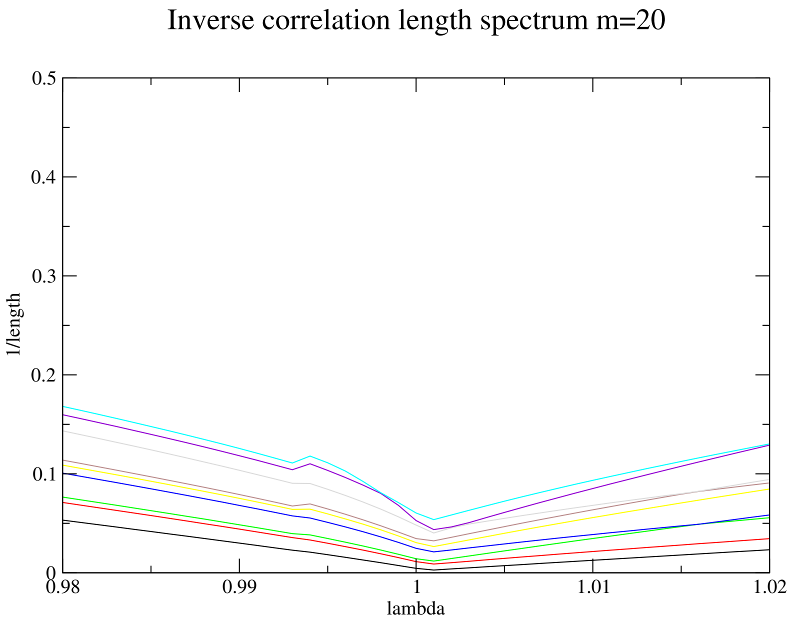
0.99
1
1.01
1.02
lambda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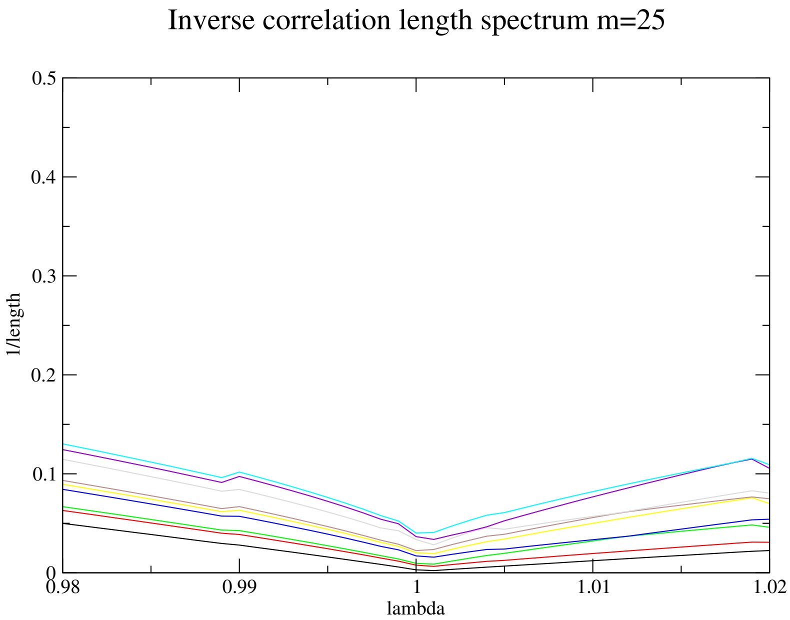
0.99
1
1.01
1.02
lambda



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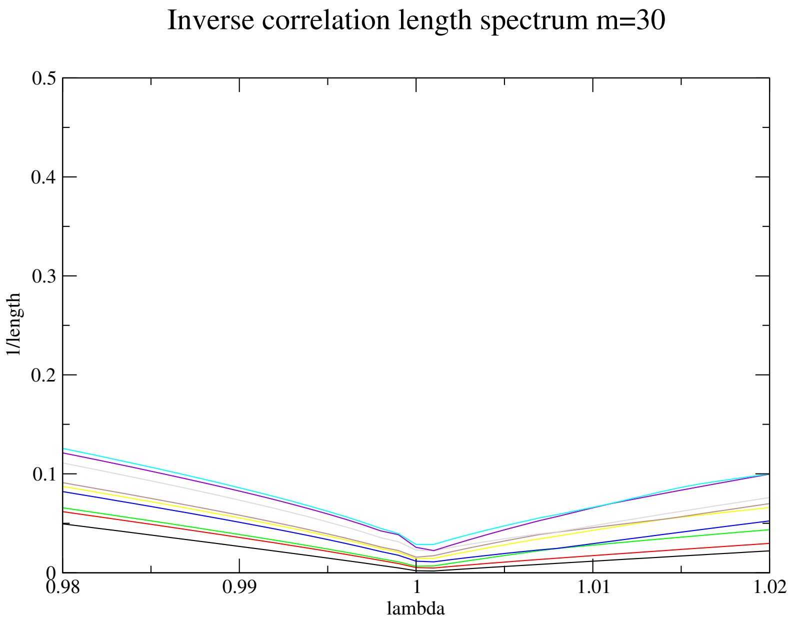
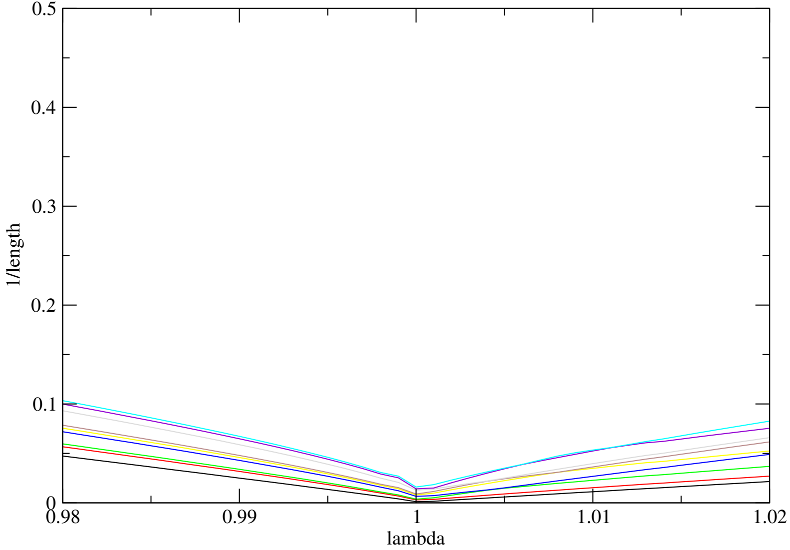
0.2
0.1
0
1/length
0.98
0.99
1
1.01
1.02
lambda



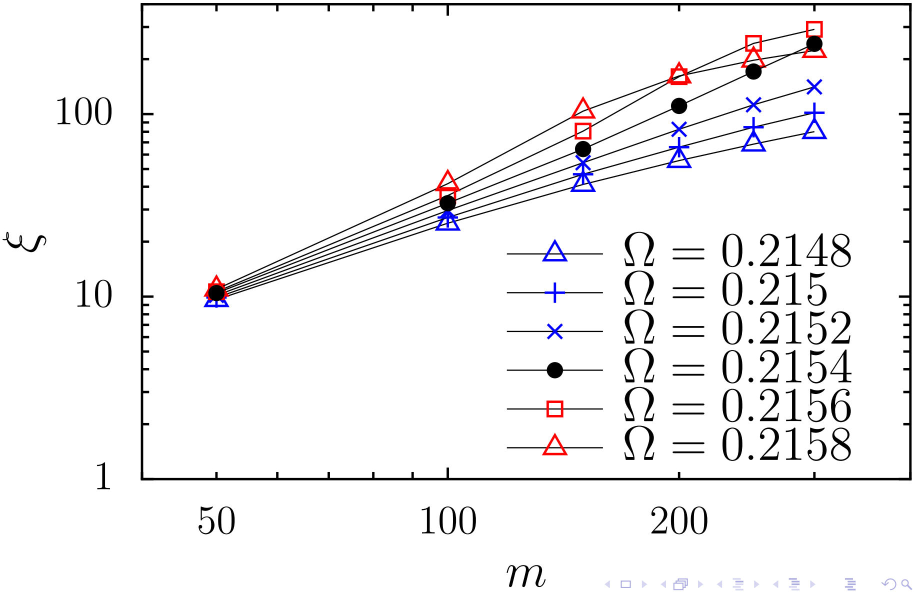
Inverse correlation length spectrum m=30
0.5
0.4
0.3
0.2
0.1
0
1/length
0.98
0.99
1
1.01
1.02
lambda

Inverse correlation length spectrum m=40



Critical scaling example

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



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.

Cumulant expansions

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

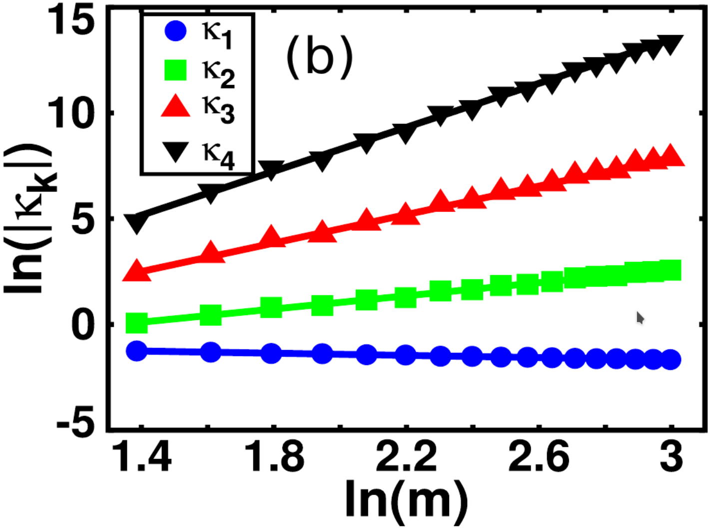
$$\begin{aligned} m_1(L) &= \kappa_1 L \\ m_2(L) &= \kappa_1^2 L^2 + \kappa_2 L \\ m_3(L) &= \kappa_1^3 L^3 + 3\kappa_1\kappa_2 L^2 + \kappa_3 L \\ m_4(L) &= \kappa_1^4 L^4 + 6\kappa_1^2\kappa_2 L^3 + (3\kappa_2^2 + 4\kappa_1\kappa_3)L^2 + \kappa_4 L \end{aligned}$$

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 $t \equiv \frac{\lambda - \lambda_c}{\lambda_c}$ h (external field)

Critical exponents

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

Scaling relation $2\beta + \gamma^* = \nu$

Note: no fluctuation-dissipation theorem: $\gamma^* \neq \gamma$ is different to dM/dH.
In $d = 2$ classical systems, $2\beta + \gamma = \nu d$

Finite-size scaling functions

$$\begin{aligned} \xi &= L\, \mathcal{X}(t\, L^{1/\nu}) \\ \langle M \rangle &= L^{-\beta/\nu}\, \mathcal{M}(t\, L^{1/\nu}) \\ \sigma^2 &= L^{\gamma^*/\nu}\, \mathcal{G}(t\, L^{1/\nu}) \end{aligned}$$

Finite entanglement

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

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

Finite-entanglement scaling functions

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

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:

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

Order parameter:

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

Higher cumulants:

$$\kappa_n = -\frac{\partial^n f}{\partial h^n} = C_2^n m^{((n-2)\beta+(n-1)\gamma)\kappa/\nu} Y^{(n)}\left(C_1 t m^{\kappa/\nu}, C_2 h m^{(\beta+\gamma)\kappa/\nu}\right)$$

Cumulant exponent relation

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

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

$$\alpha_1 = -\frac{\beta\kappa}{\nu}$$

$$\alpha_2 = \frac{\gamma^*\kappa}{\nu}$$

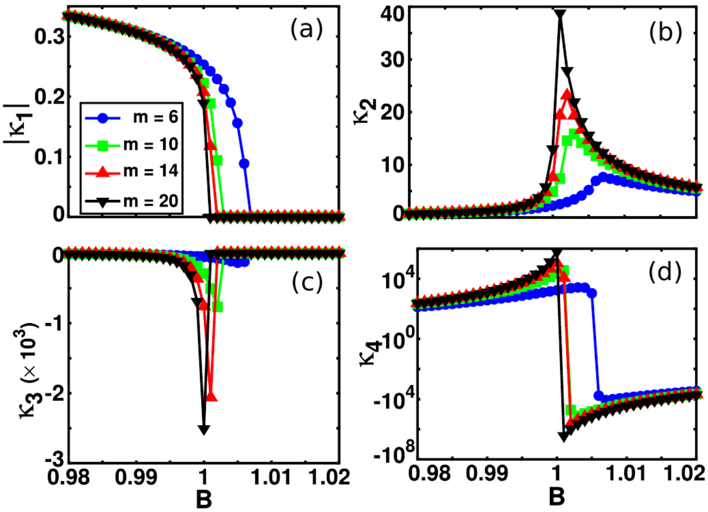
This also works for $\alpha_0 = -(2\beta + \gamma)\kappa/\nu = -\kappa$
which is the correlation length exponent!
Hence include $\kappa_0 \equiv \xi$ as the 0^{th} order cumulant $\quad \xi \sim m^\kappa \to \kappa_0 \sim m^{-\alpha_0}$

Cumulant relation

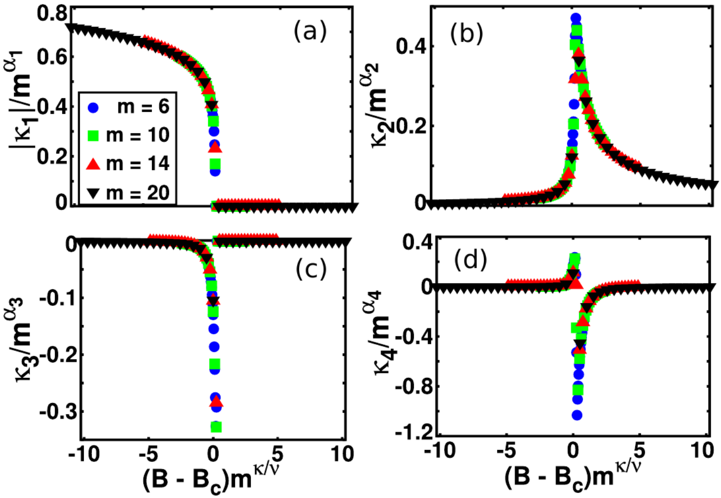
$$\begin{aligned} \alpha_n &= (n-1)\alpha_2 + (2-n)\alpha_1 \\ &= n\alpha_1 + (1-n)\alpha_0 \end{aligned}$$

Ising model example

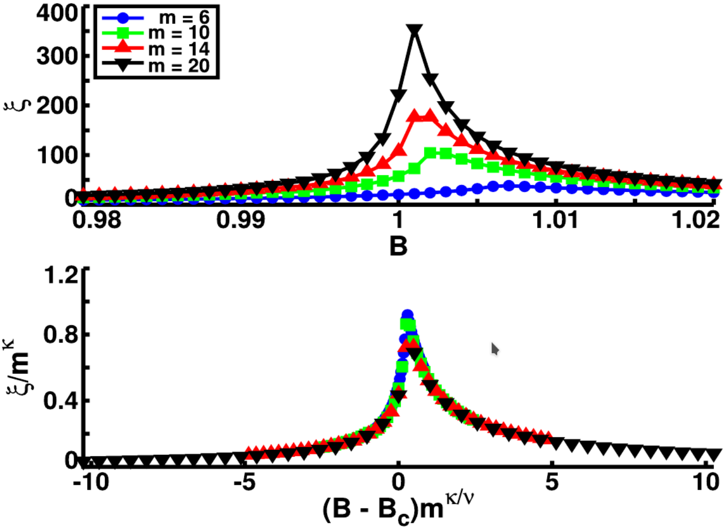
(from J. Pillay, IPM, Phys. Rev. B 100, 235140 (2019))



Ising model cumulant scaling functions



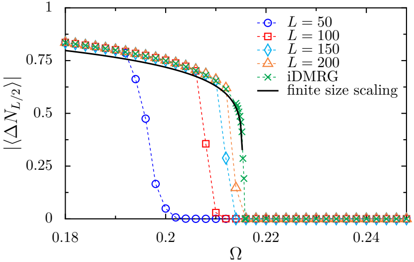
Ising model correlation length scaling function

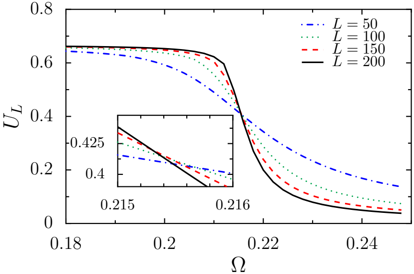


Binder cumulant scaling

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

2019 approach: Evaluate the moment polynomial using $L \propto$ correlation length
Better approach: Find a combination of cumulants such that the bond dimension cancels

- Products of cumulants $\kappa_0^{a_0}\kappa_1^{a_1}\kappa_2^{a_2}\ldots$ scales as $m^{a_0\alpha_0+a_1\alpha_1+a_2\alpha_2+\ldots}$
- Find a combination such that $a_0\alpha_0 + a_1\alpha_1 + a_2\alpha_2 + \ldots = 0$
- This quantity is independent of basis size at the critical point
- Simplest case:

$$C_2 = \frac{\kappa_2}{\kappa_1^2\kappa_0} = \frac{\sigma^2}{\langle m\rangle^2\xi}$$

Closely related to the 2nd order cumulant $\frac{\langle m^2\rangle}{\langle m\rangle^2}$

- Higher order cumulants are possible,

$$C_4 = \frac{\kappa_4}{\kappa_2^2\kappa_0}$$

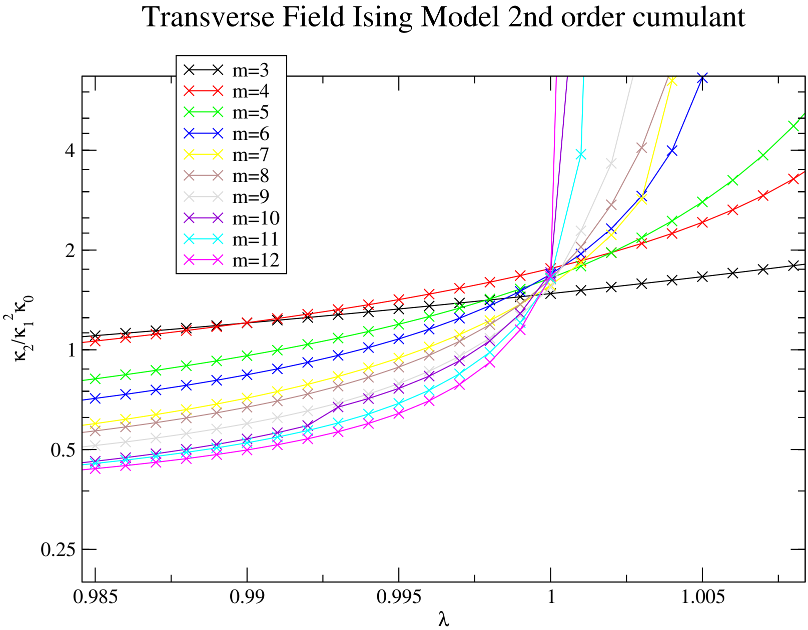
(Closely related to the Binder cumulant)

$$C_4^{(3)} = \frac{\kappa_4\kappa_1^2}{\kappa_2^3}$$

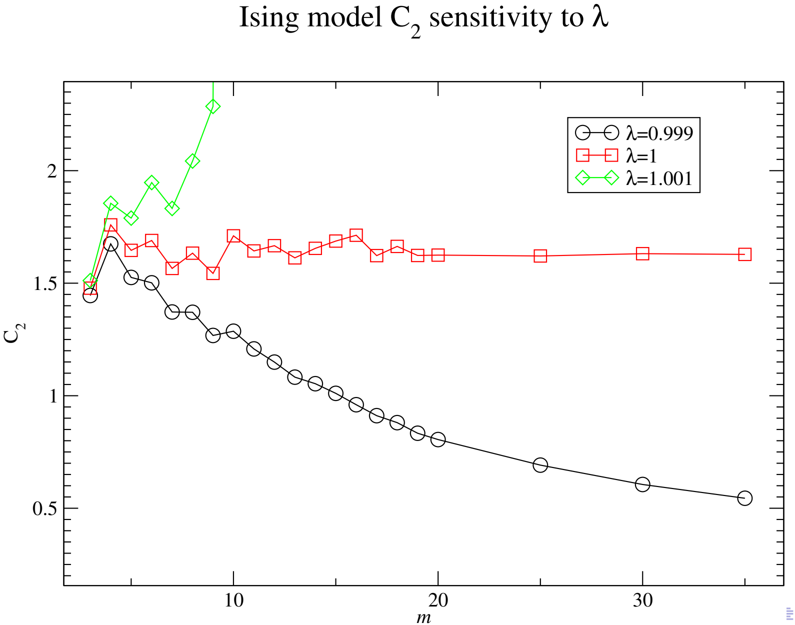
(Avoids using the correlation length κ_0)

In cases I've tried so far, C_2 works best.

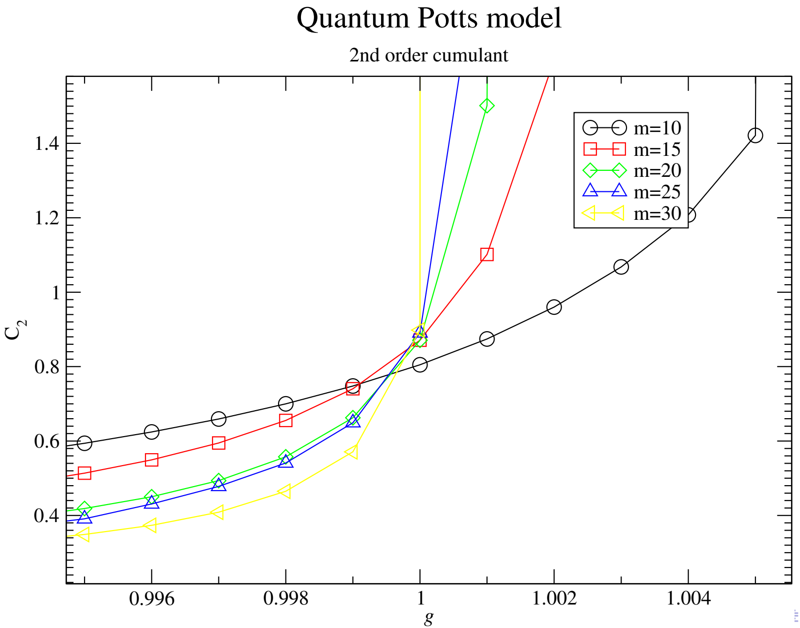
Ising model example



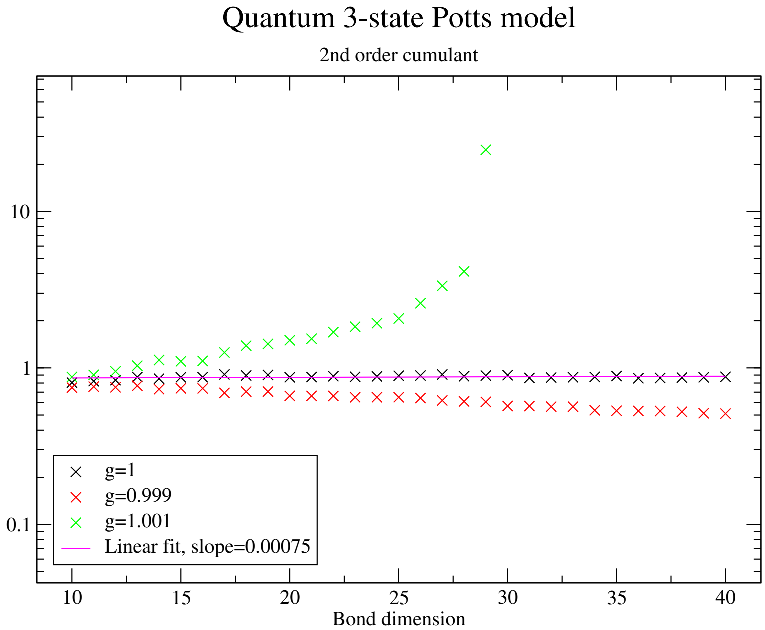
Ising model example



Quantum 3-state Potts model example



Quantum 3-state Potts model example



Critical exponents

Once we know the critical point, there are several approaches to determining the exponents

- Direct fit as a function of g
- Scaling function collapse – choice of scaling parameter
  - bond dimension scaling – J. Pillay, IPM, Phys. Rev. B 100, 235140 (2019)
  - $\delta = \epsilon_i - \epsilon_j$ scaling – Vanhecke, Haegeman, et al, Phys. Rev. Lett. 123, 250604 (2019)
- Correlation length scaling at the critical point

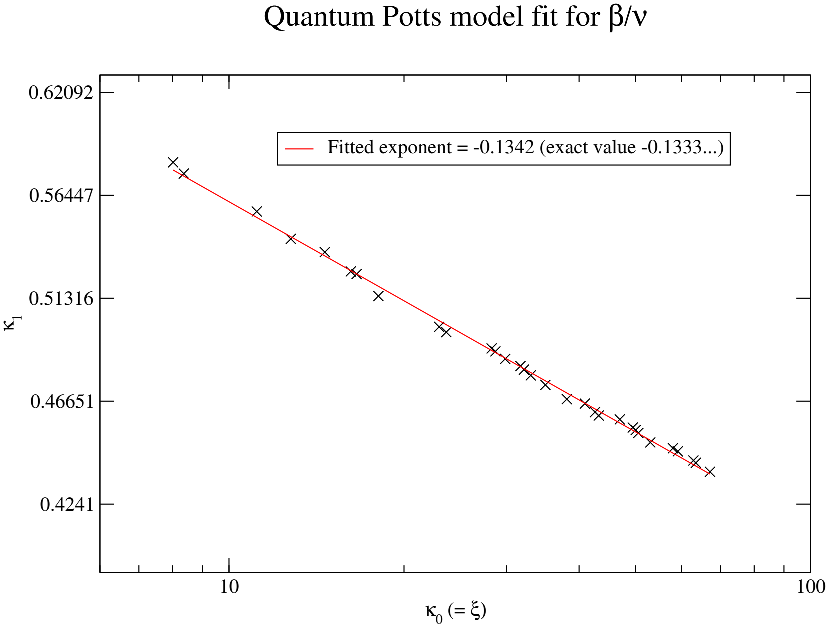
The exponents of the order parameter and 2nd cumulant are

$$\kappa_1 \sim m^{-\beta\kappa/\nu}$$

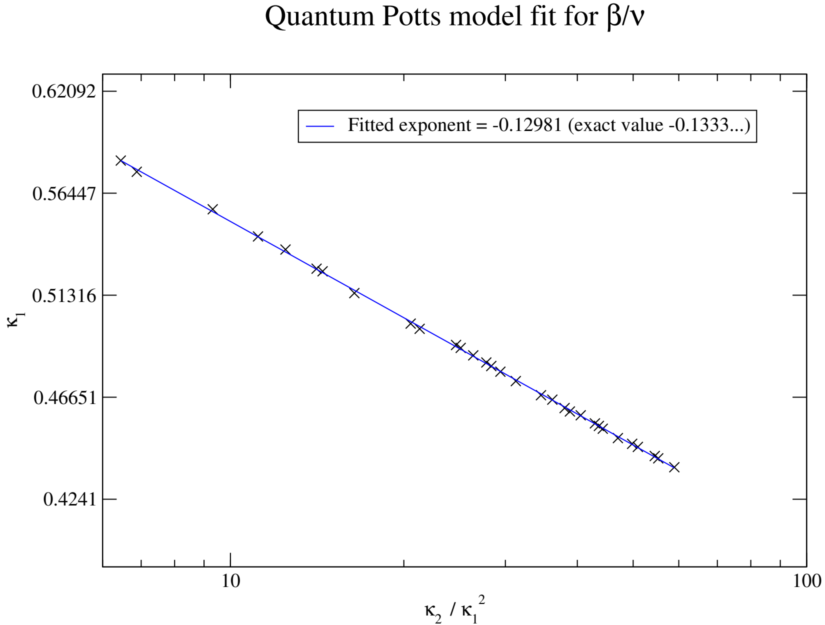
$$\kappa_2 \sim m^{\gamma\kappa/\nu}$$

And recall $\kappa_0 \sim m^{\kappa}$. So at the critical point, $\kappa_1 = \kappa_0^{-\beta/\nu}$ and $\kappa_2 = \kappa_0^{\gamma/\nu}$.

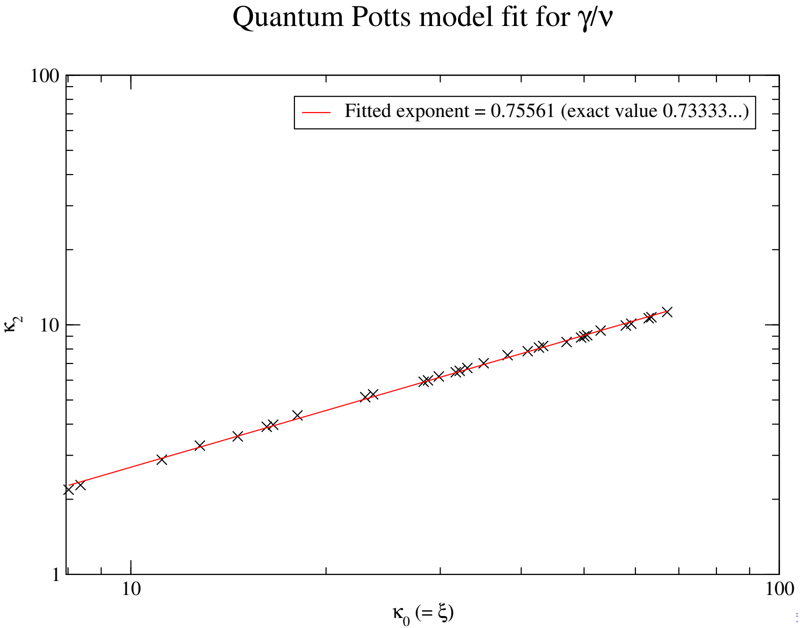
Quantum 3-state Potts model example



Alternative scaling variable – κ_2/κ_1^2



Quantum 3-state Potts model example – exponent γ



Generalising beyond local order parameters

- The approach of calculating moments of the order parameter doesn't require that the order parameter is strictly local.
- Example: Mott insulator at integer filling $n = 1$ particles everywhere, with only short-range fluctuations. String order parameter:

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

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 $O_p^2 = \frac{1}{L^2} \langle P^2 \rangle$
(see J. Pillay and IPM, Phys. Rev. B 100, 235140 (2019) for examples)

SPT transitions

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

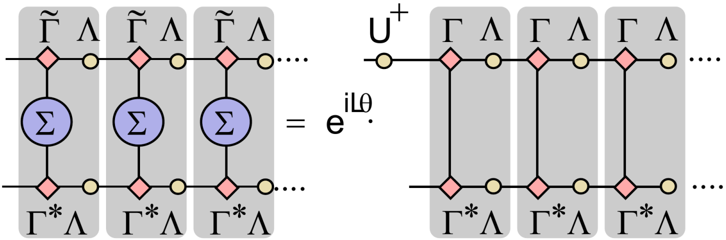


figure shamelessly stolen from Pollman and Turner, PRB 86, 125441 (2012)

- 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

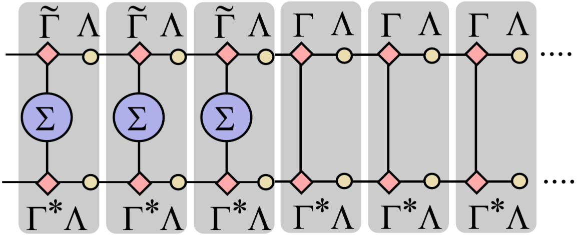
Kink operator for time reversal

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:

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



Kink operator for time reversal

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

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

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

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

- In principle the same scheme applies to spatial reflection too – the MPO contains the R operator that transposes an A-matrix. But no examples yet!

Conclusions

- MPO techniques for higher moments
- Bond-dimension scaling is inaccurate – explore methods that are insensitive to convergence of the MPS
- Higher cumulants are effective for calculating critical phenomena
- Second order cumulant $\kappa_2/\kappa_1^2\kappa_0$ is very effective for locating critical points with minimal effort.
- Generalising order parameters to strings, time reversal, ...
- Spatial reflection can be considered in a similar way

Future directions:

- 2D – some (confusing) results already for 2D cylinders (S.N. Saadatmand and IPM, Phys. Rev. B 96, 075117 (2017))
- Field-induced fluctuations