DMRG in the Thermodynamic limit

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

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Outline

Method 1: quantize a classical state

Start from a *classical* (product) state

$$|\psi\rangle = |s^1\rangle\ |s^2\rangle\ |s^3\rangle\ |s^4\rangle\ \cdots$$

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

$$|s^i\rangle = a_i^x|x\rangle + a_i^y|y\rangle + a_i^z|z\rangle$$

Turn our (commuting) numeric coefficients into a matrix

$$|s^i\rangle_{jk} = A_{jk}^x|x\rangle + A_{jk}^y|y\rangle + A_{jk}^z|z\rangle$$

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

$$|\psi\rangle = \mathrm{Tr}\sum_{s_i} A^{s_1}A^{s_2}A^{s_3}A^{s_4}\cdots|s^1\rangle\ |s^2\rangle\ |s^3\rangle\ |s^4\rangle\cdots$$

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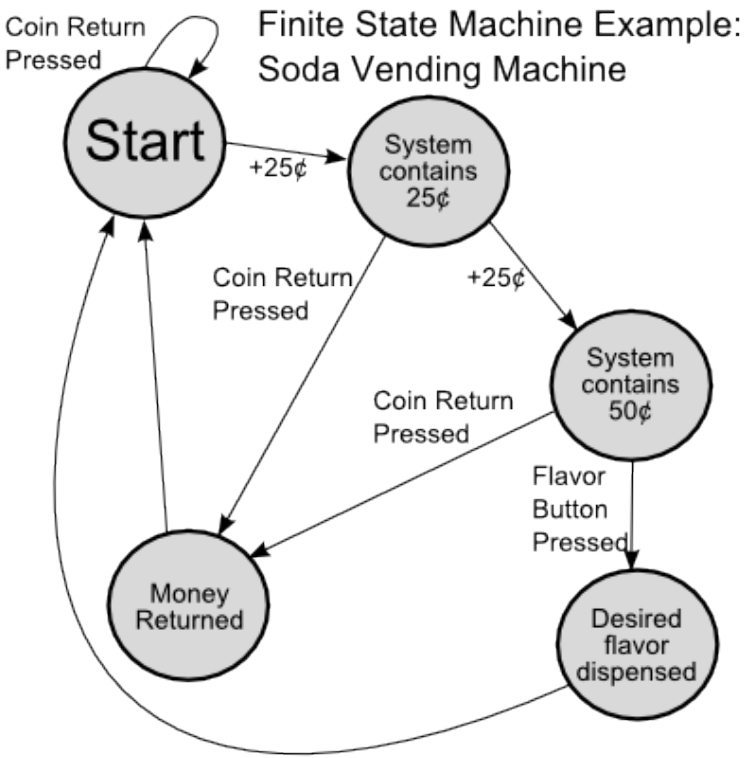
Method 2: quantum finite-state machines

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.



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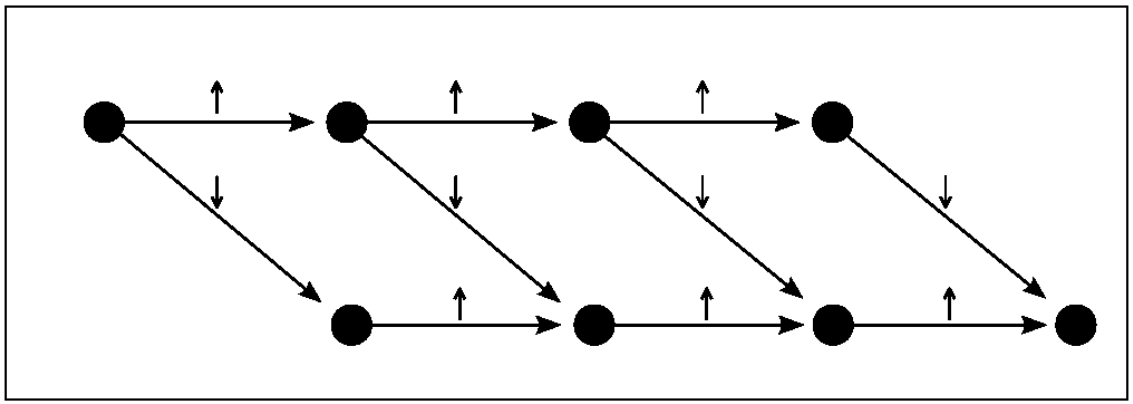
In a *quantum* finite-state machine, we choose every possible transition with some probability amplitude



(from Crosswhite and Bacon, Phys. Rev. A 78, 012356 (2008))

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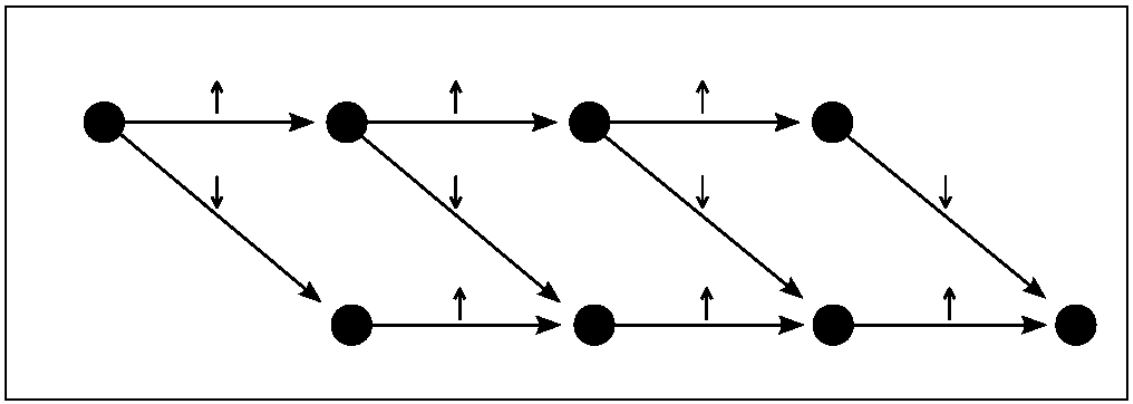

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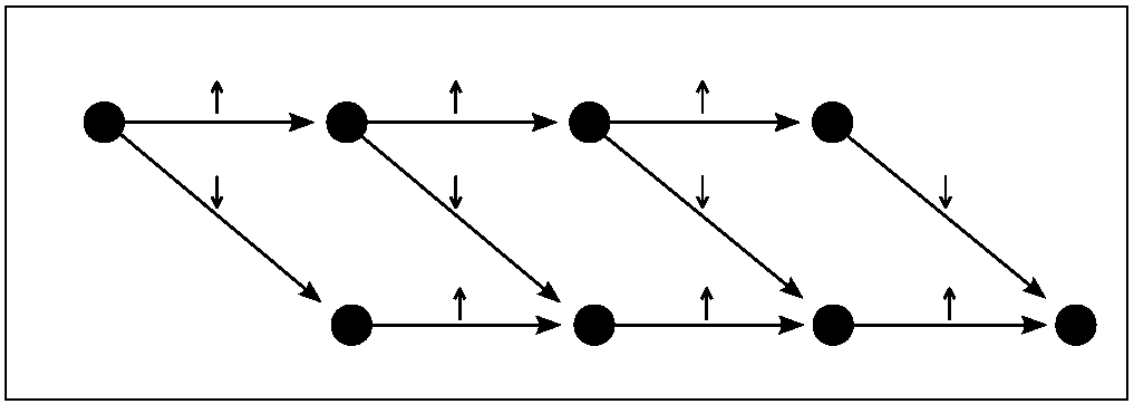

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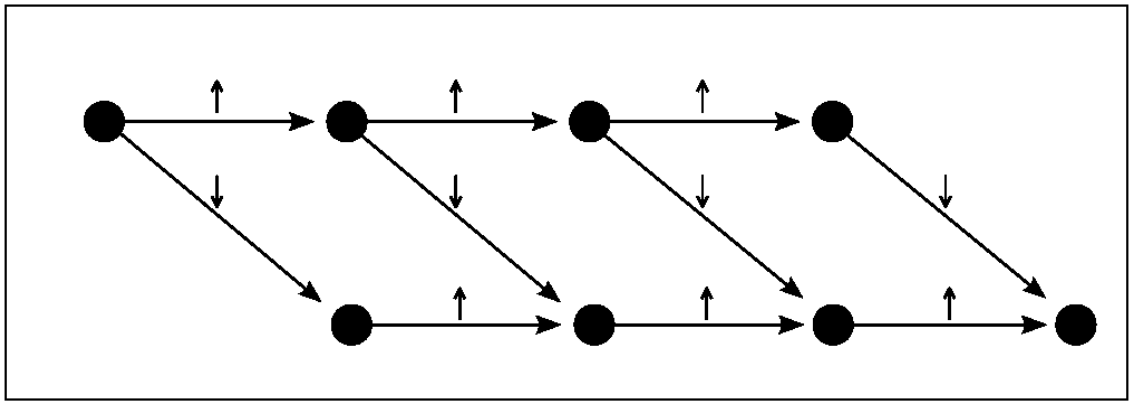

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Matrix Product States

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, $S = \ln 2$

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

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- AKLT state

$$A = \begin{pmatrix} \sqrt{1/3}|0\rangle & -sqrt2/3|+\rangle \\ \sqrt{2/3}|-\rangle & -\sqrt{1/3}|0\rangle \end{pmatrix}$$

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The Matrix Product Ansatz: beyond groundstates

The key advantage of MPS formulation: *arithmetic manipulations*
The sum (superposition) of two matrix product states is also a matrix product state

$$|C\rangle = |A\rangle + |B\rangle$$

$$C = \sum_{\{s_i\}} \mathrm{Tr}\ C^{s_1} C^{s_2} \dots C^{s_L} \ |s_1 s_2 \dots s_L\rangle$$

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:

$$O = O_1 \otimes O_2 \otimes \dots$$

$|C\rangle = O|A\rangle$ 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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Matrix Product Operators

IPM J. Stat. Mech. P10014 (2007), arXiv:0804.2509

- 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 $H = \sum_{<i,j>} S_i^z S_j^z + \lambda \sum_i S_i^x$, 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:

$$\underbrace{\begin{pmatrix} H & S^z & I \end{pmatrix}'}_{\text{new block operators}} = \underbrace{\begin{pmatrix} H & S^z & I \end{pmatrix}}_{\text{old block operators}} \times \underbrace{\begin{pmatrix} I & & \\ S^z & & \\ \lambda S^x & S^z & I \end{pmatrix}}_{\text{local}}$$

Matrix Product Operators

This form can represent many operators

- fermionic $c^\dagger_{k=0}$: $W_{c^\dagger_{k=0}} = \begin{pmatrix} I & \\ c^\dagger & P \end{pmatrix}$, $P = (-1)^N$, J-W string
- finite momentum $b^\dagger_k$: $W_{b^\dagger_k} = \begin{pmatrix} I & \\ b^\dagger & e^{ik} I \end{pmatrix}$

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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Symmetry and Invariance

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 $[U_a, U_b] \neq 0$?

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

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Symmetry and Invariance

Suppose we have an Abelian symmetry, for example conservation of z-component of spin.

$$H = \sum_{<i,j>} S_i^z S_j^z + \left(S_i^+ S_j^- + S_i^- S_j^+\right)/2$$

We have $[S^z, H] = 0$, therefore also

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

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 *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:

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

The representation label n tells us how the outgoing quantum number relates to the incoming quantum number.

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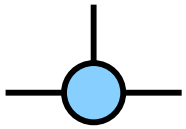
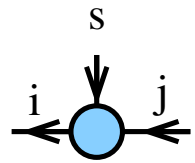
Symmetries in a tensor network

In a *symmetric tensor network*, we attach quantum numbers to every index

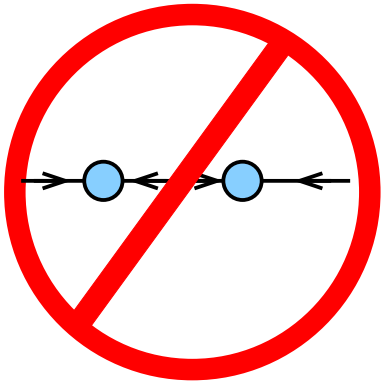
Absence of an index indicates a scalar, example: 
This is a scalar operator, with constraint $q_i = q_j$.
If we wanted to represent a non-scalar operator, we need another leg



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



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
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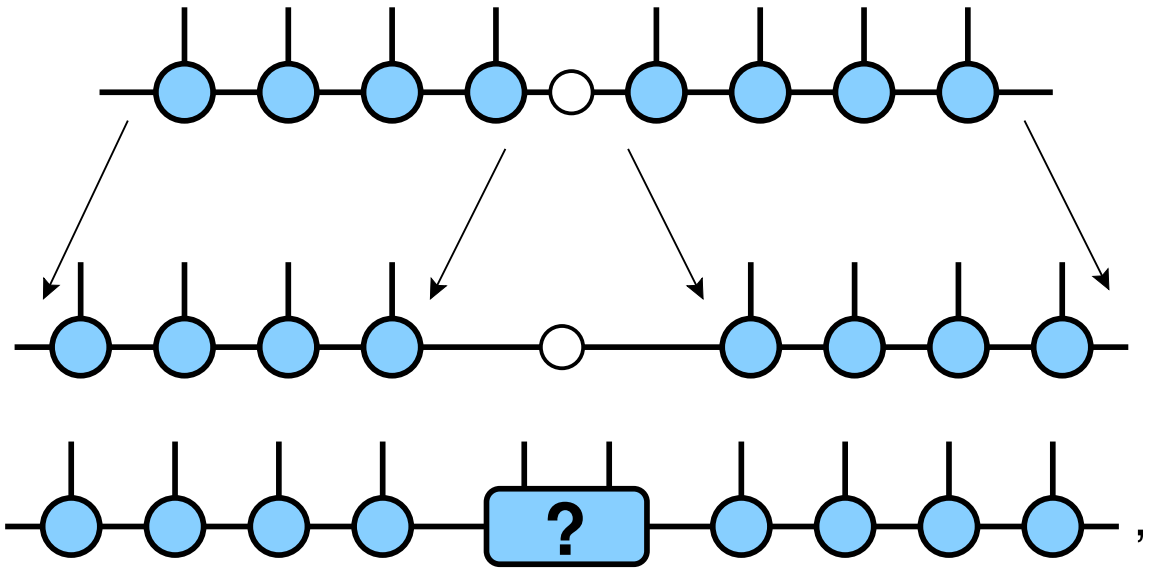
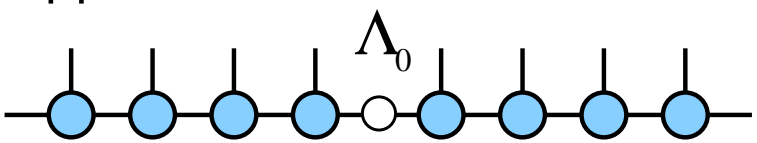
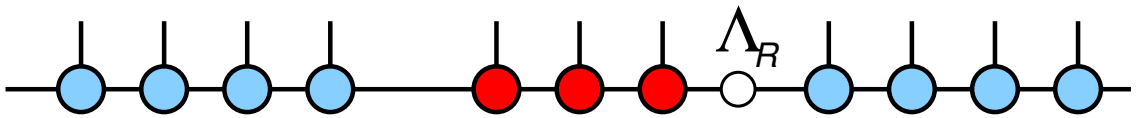


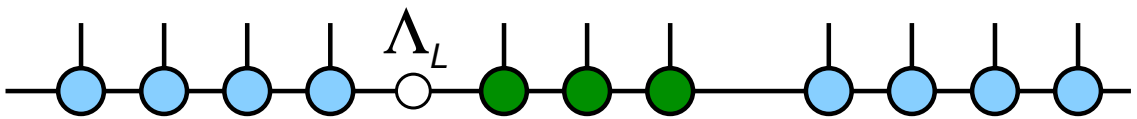
A recurrence relation for MPS

Suppose we have an initial state:



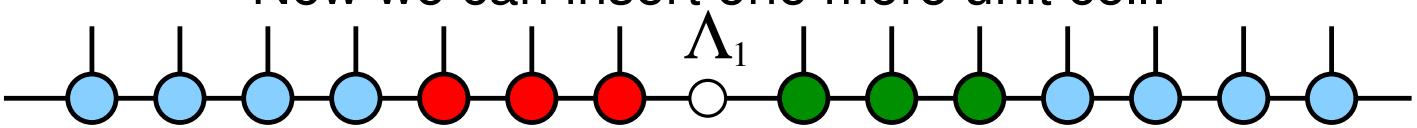
Suppose we also have the MPS enlarged with an extra unit cell:





Note: Λ_L and Λ_R are not necessarily diagonal

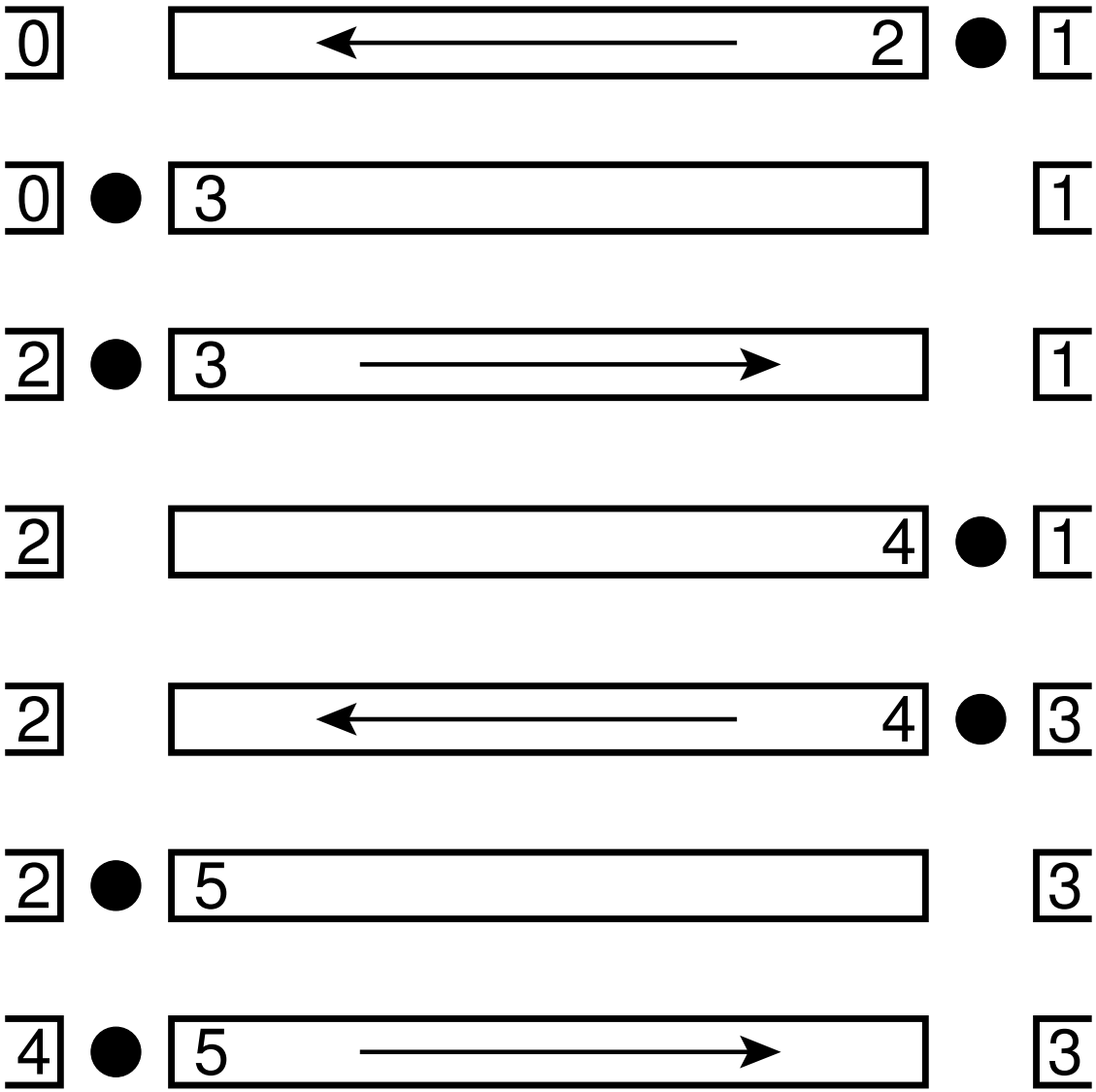
Now we can insert one more unit cell:



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

Variant of the finite system algorithm

- Different treatment of the boundaries



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 $\sim \exp(-L) \quad \to 0$
- 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
- 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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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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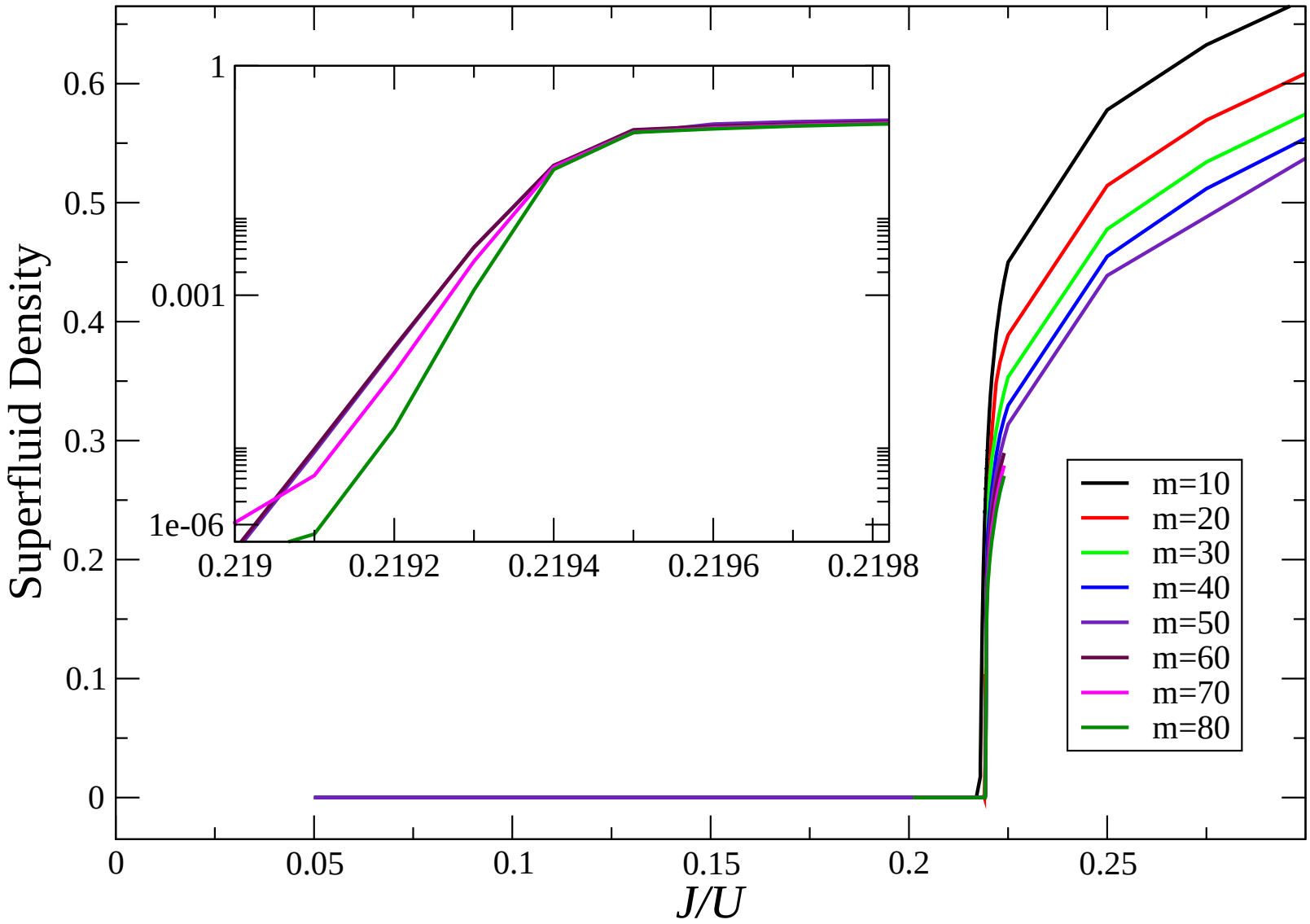
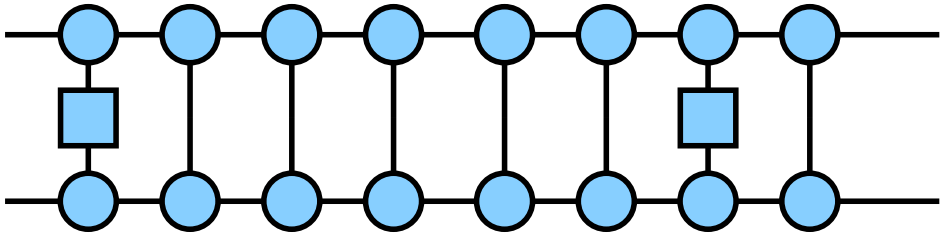
Bose-Hubbard Model Mott-Superfluid Transition

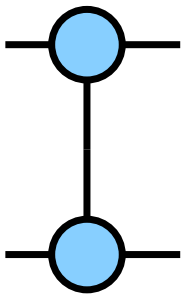
μ=0.25



Correlation Functions



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



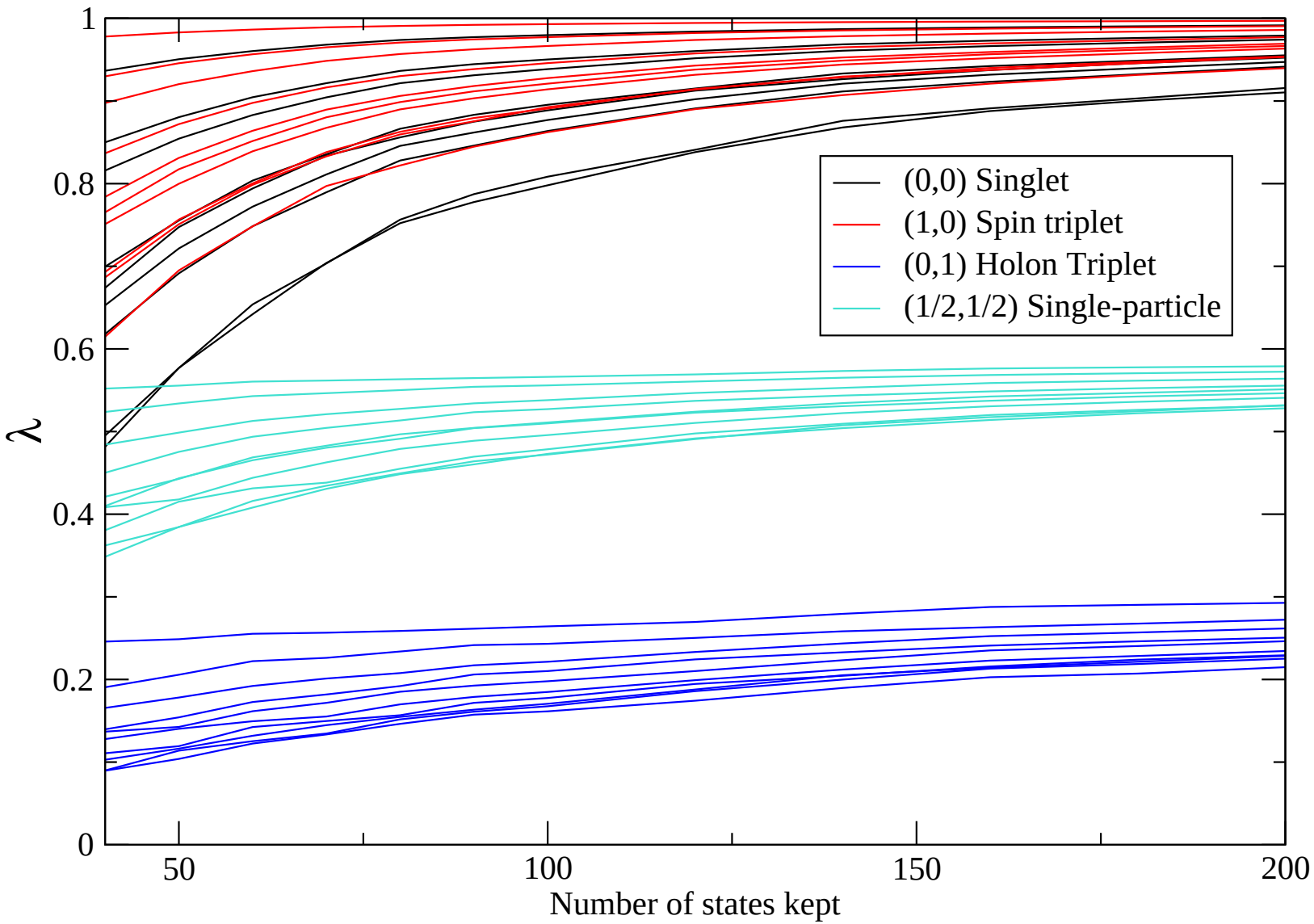
- All eigenvalues ≤ 1
- One eigenvalue equal to 1, corresponding to the identity operator

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



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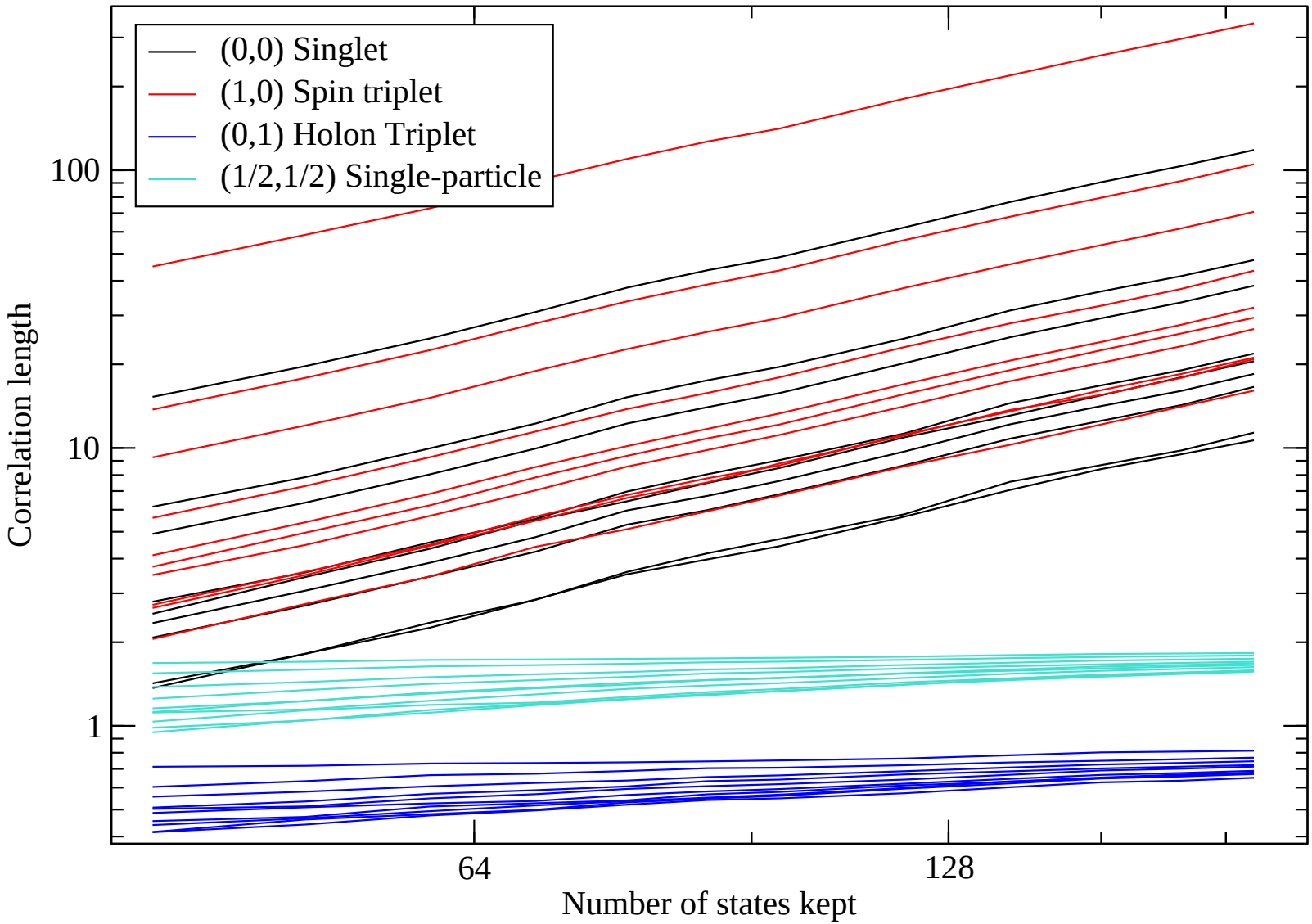
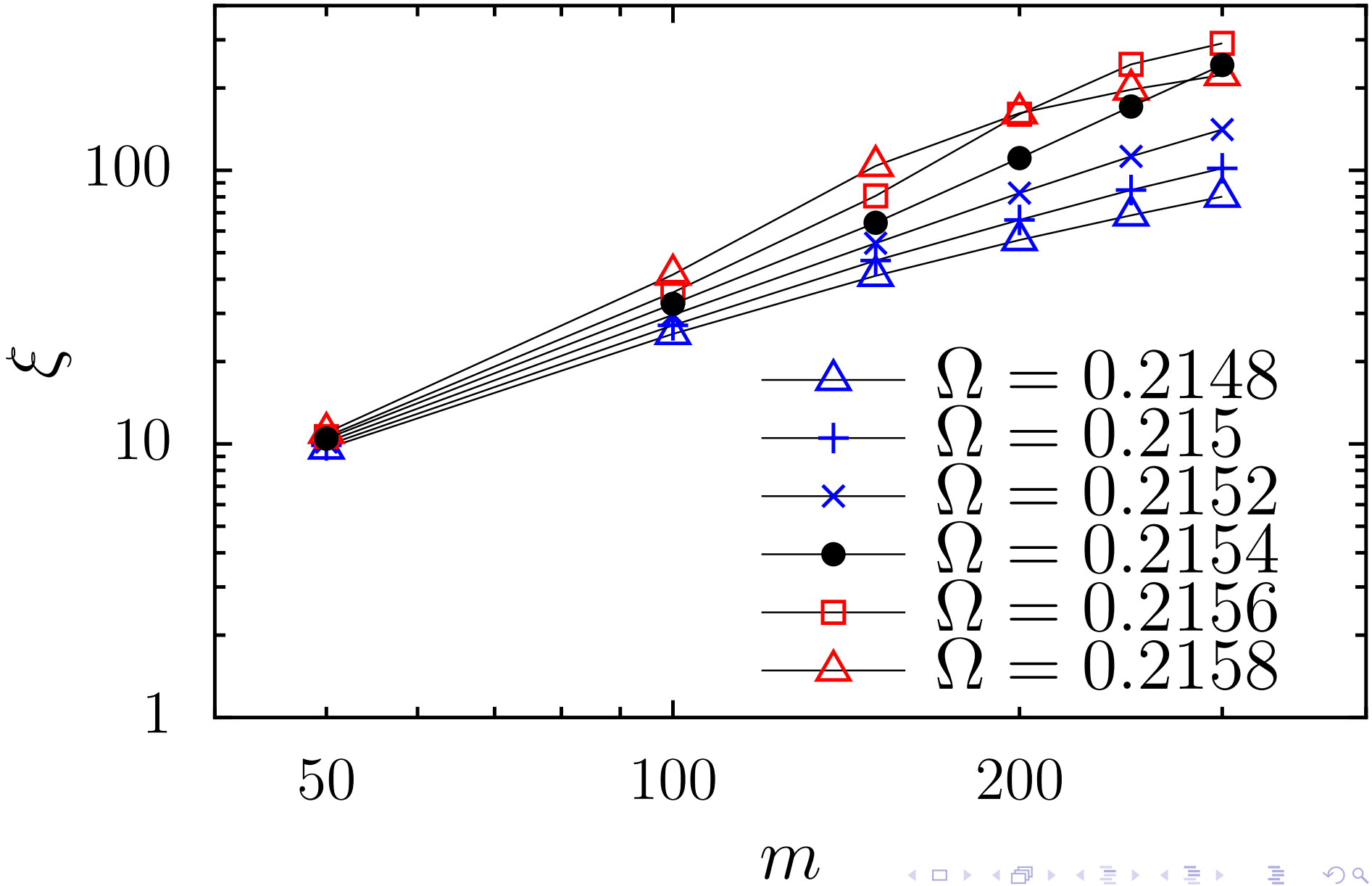


Critical scaling example

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



CFT Parameters

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]

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 ξ_1 and ξ_2
- We expect: $\dfrac{O(\xi_2)}{O(\xi_1)} = \left(\dfrac{\xi_2}{\xi_1}\right)^{\Delta}$
- 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
- $\cdots$ algebra $\cdots$

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

This gives directly the operator scaling dimensions by direct fit

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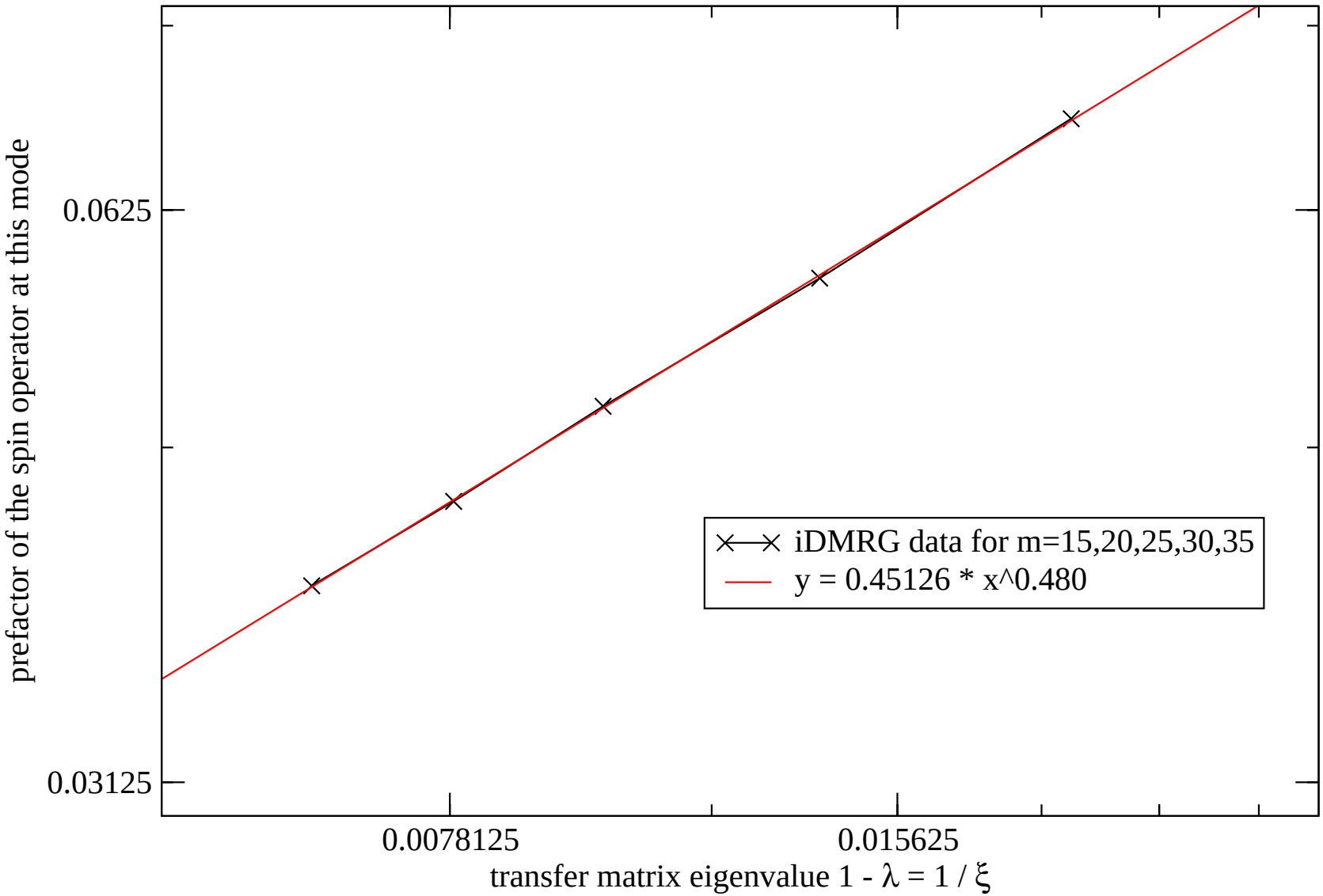
Heisenberg model fit for the scaling dimension



Generalized Scaling

Alternative viewpoint (Vid Stojevic et al, Phys. Rev. B **91**, 035120 (2015))

Scaling relation for large s:

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

So we obtain Δ 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: $O(s\xi) \simeq a\lambda^{s\xi}$ only for $s \gg 1$

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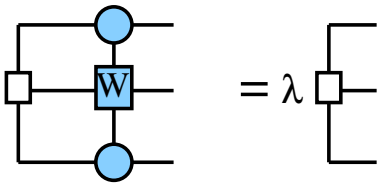
Expectation values of MPO's - arxiv:0804.2509

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

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

- index by index, each component is a function only of the previously calculated terms

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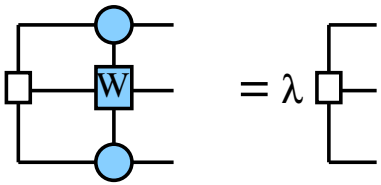

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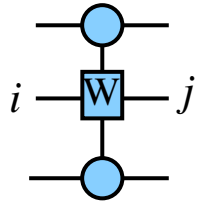

Choose bond indices i, j of W_{ij}, and denote $T_{W_{ij}}$
Example:

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

Eigentensor is $\begin{pmatrix} E_1 & E_2 & E_3 \end{pmatrix}$

- 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

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

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

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

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

- Component in the direction of the identity:

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

Has the solution

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

is the energy

- Component perpendicular to the identity:

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

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

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

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'

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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

$$
\begin{array}{lcll}
E_3 & = & I & \text{Identity operator} \\
E_2 & = & Sz & \text{Sz block operator} \\
E_1(L) & = & E' + Le_1 & \text{Hamiltonian operator + energy per site}
\end{array}
$$

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
- If any eigenvalues are complex, then expand also in fourier modes

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Examples 1 - Variance

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

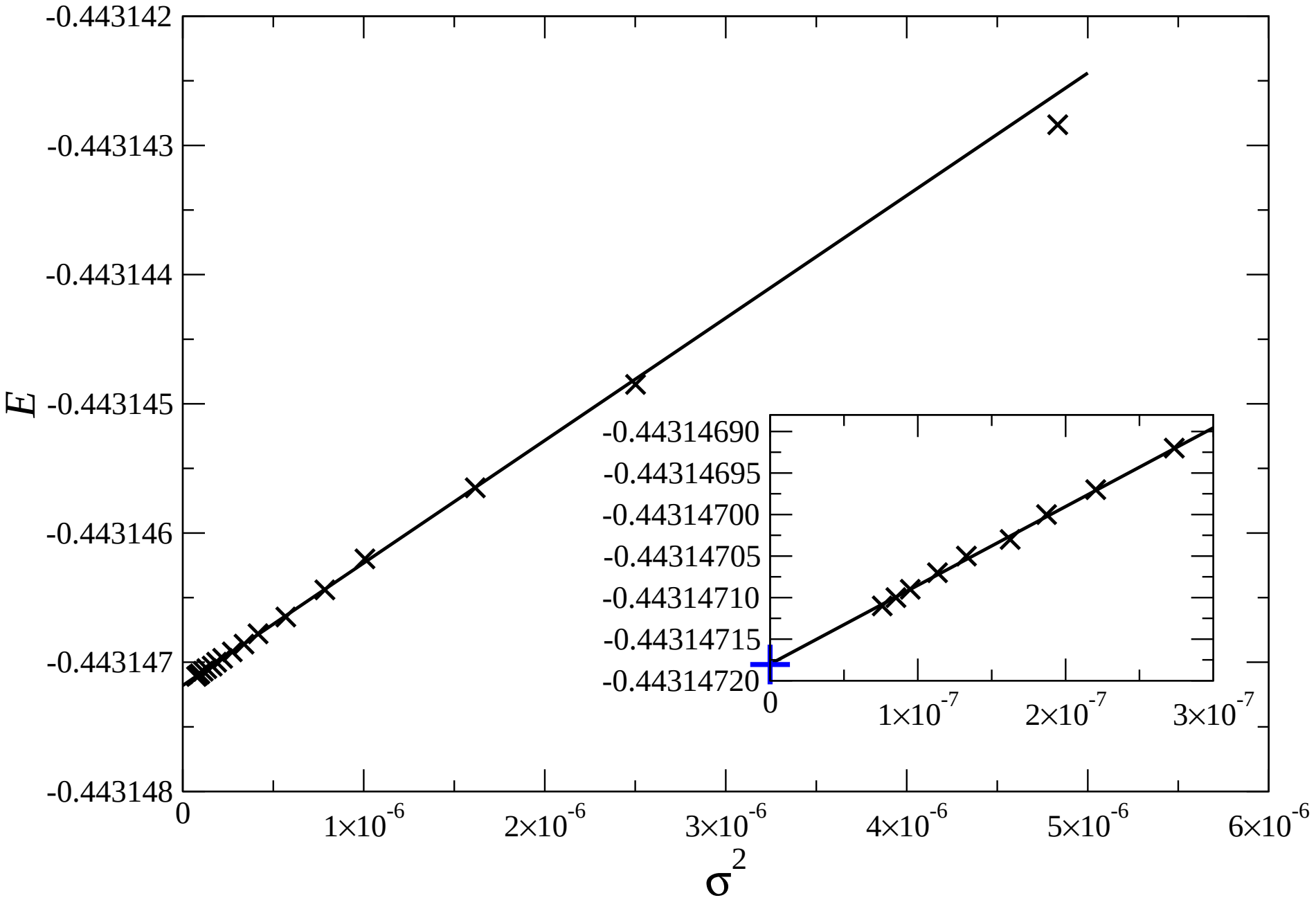
$$\langle H^2 \rangle_L - \langle H \rangle_L^2 = \langle (H - E)^2 \rangle_L = L\sigma^2$$

- 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

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,

$$b_k^\dagger = \sum_x e^{ikx} b_x^\dagger$$

$$W_{b_k^\dagger} = \begin{pmatrix} I & \\ b^\dagger & e^{ik} I \end{pmatrix}$$

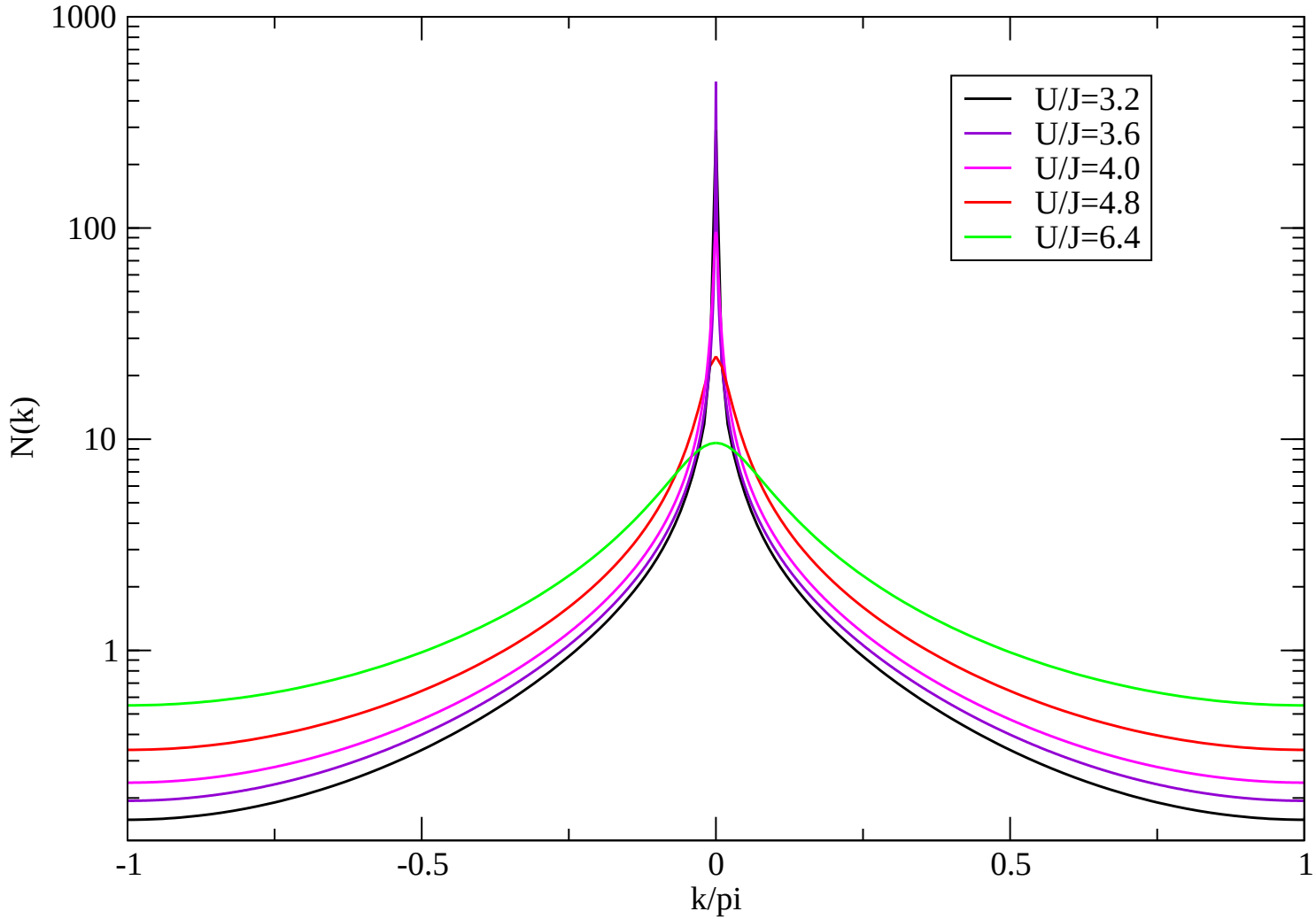
Momentum occupation:

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

- 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



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

$$\langle M^2 \rangle = m_2(L)$$

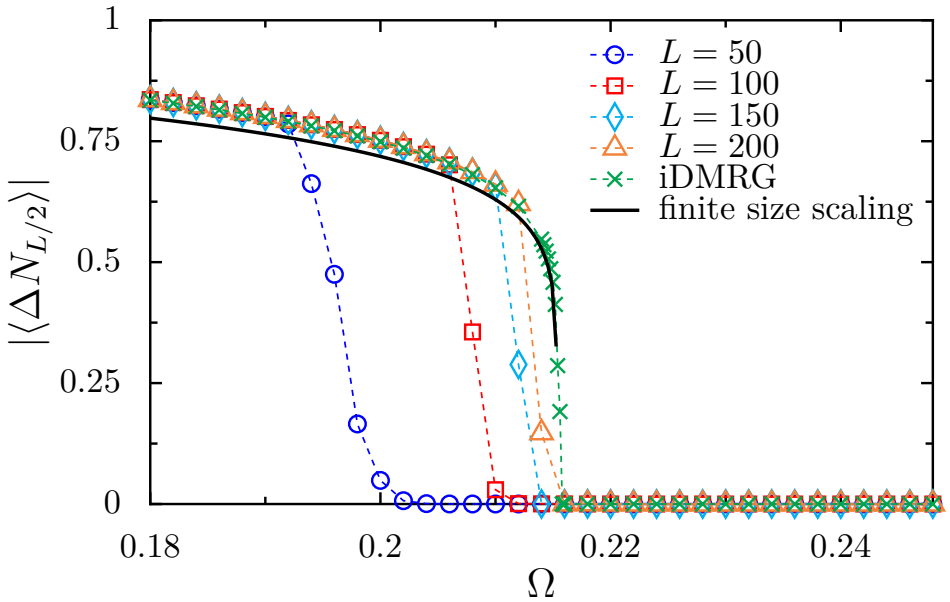
or generally

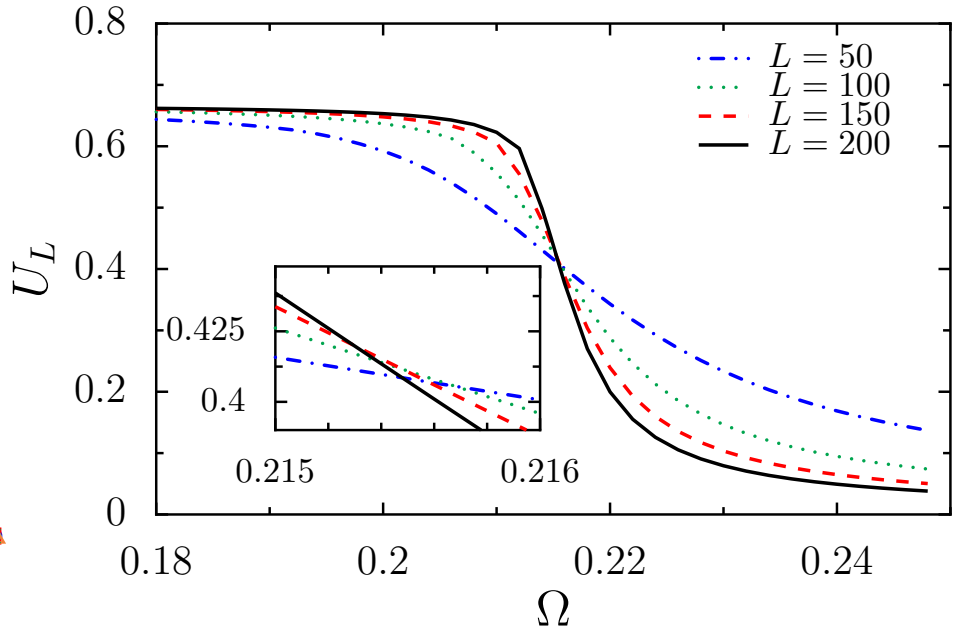
$$\langle M^k \rangle = m_k(L)$$

These are polynomial functions in the system size L.

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 Ω) to miscible (large Ω).

$$H = \sum_{<i,j>,\sigma} b^\dagger_{i,\sigma} b_{j,\sigma} + \text{H.c.} + U \sum_{i,\sigma} n_\sigma (n_\sigma - 1) + U_{12} \sum_i n_\uparrow n_\downarrow + \Omega \sum_{<i,j>} b^\dagger_{i,\uparrow} b_{j,\downarrow} + \text{H.c.}$$

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

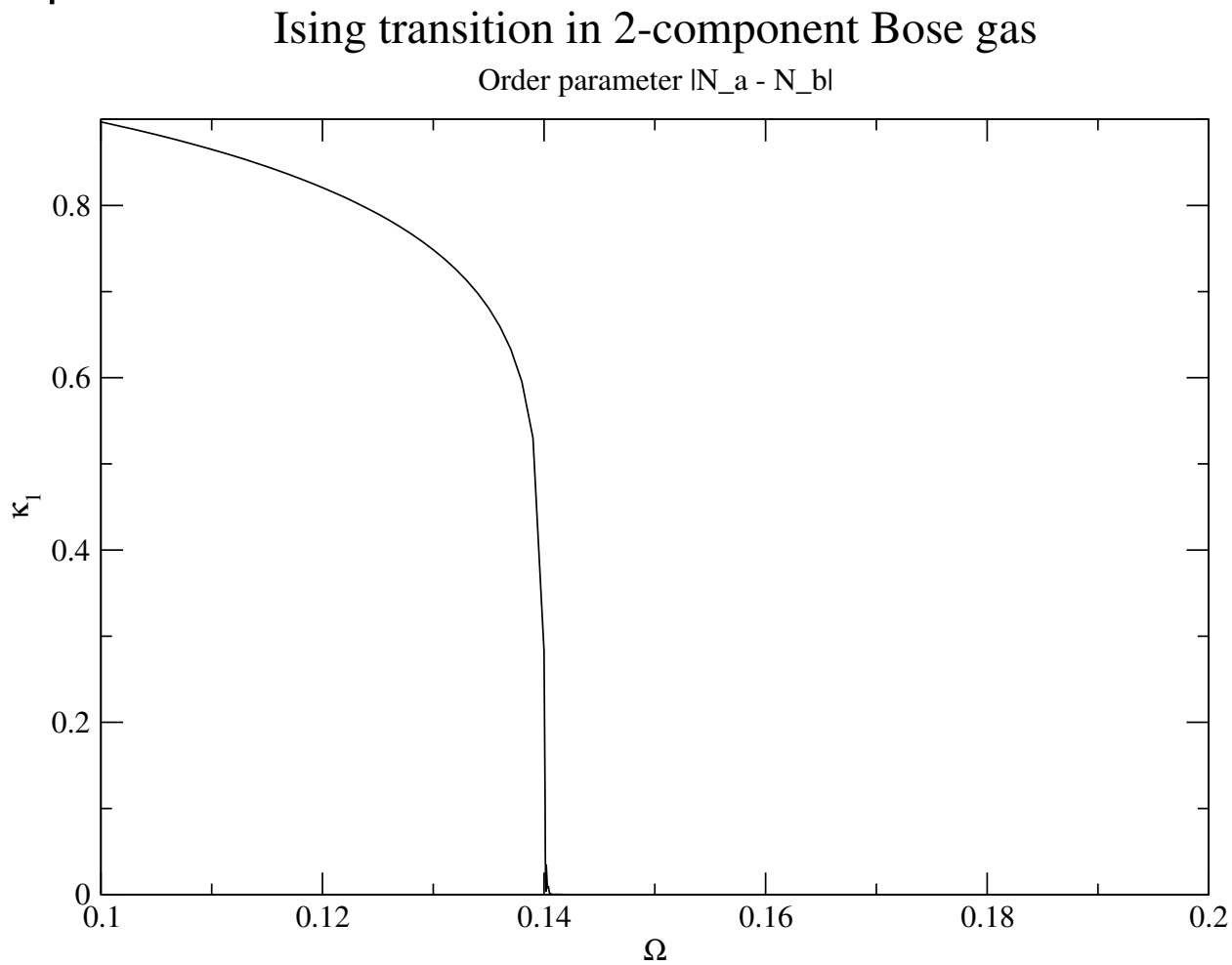
The cumulants per site κ_k are well-defined for an iMPS

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

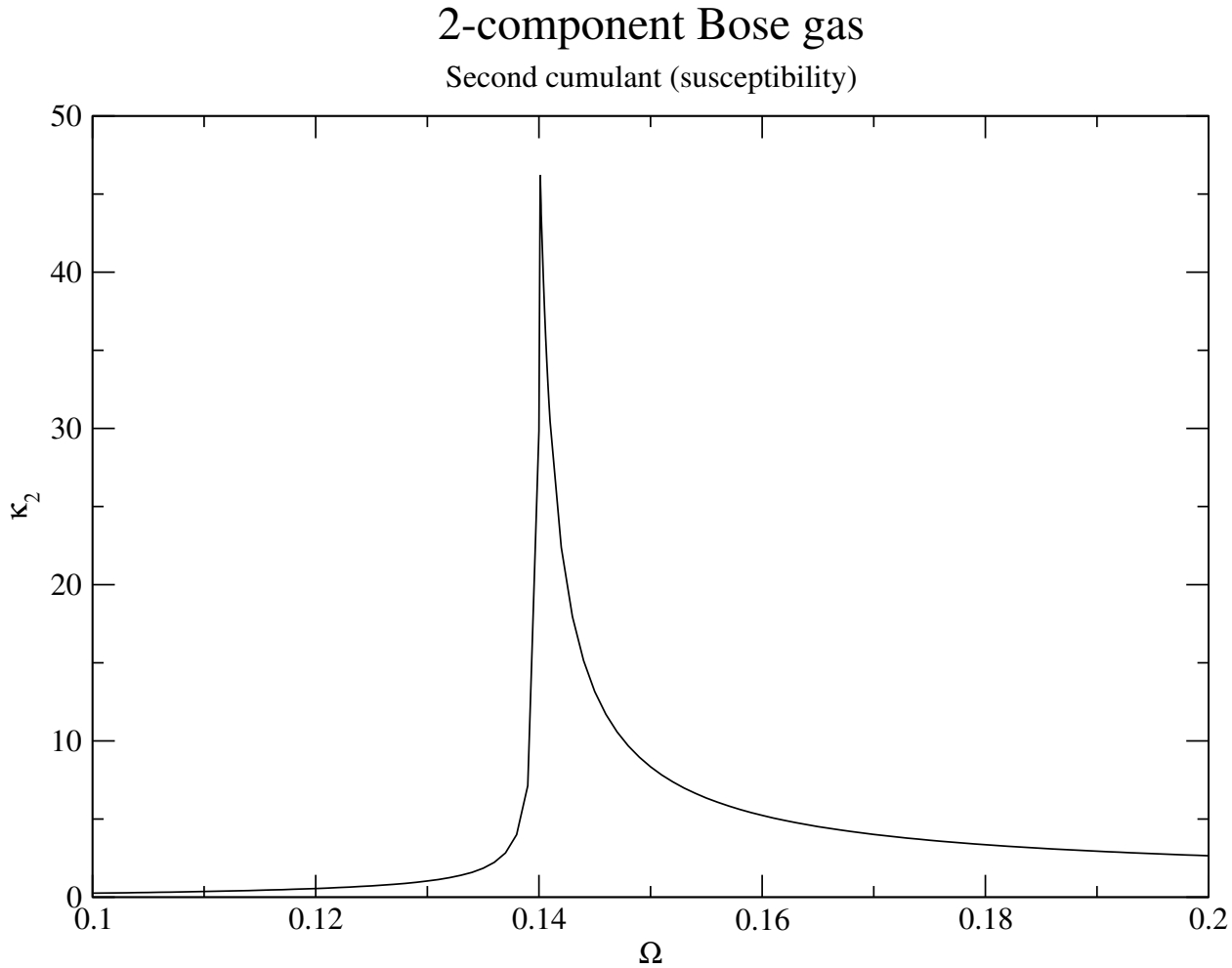
iMPS for two-component bose gas

The cumulant expansion already gives a lot of information

κ_1 is the order parameter itself

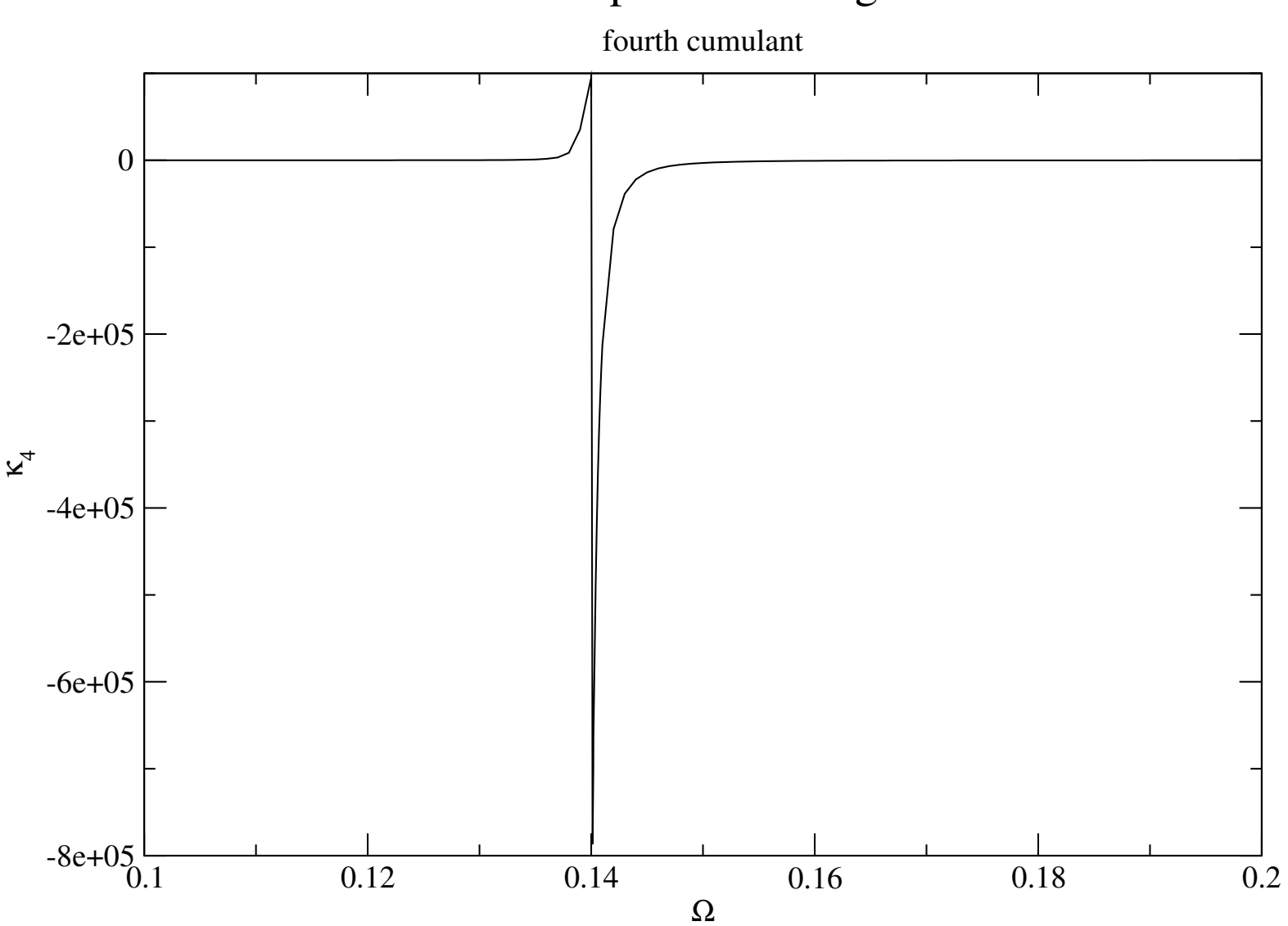


The second cumulant gives the susceptibility



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.



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

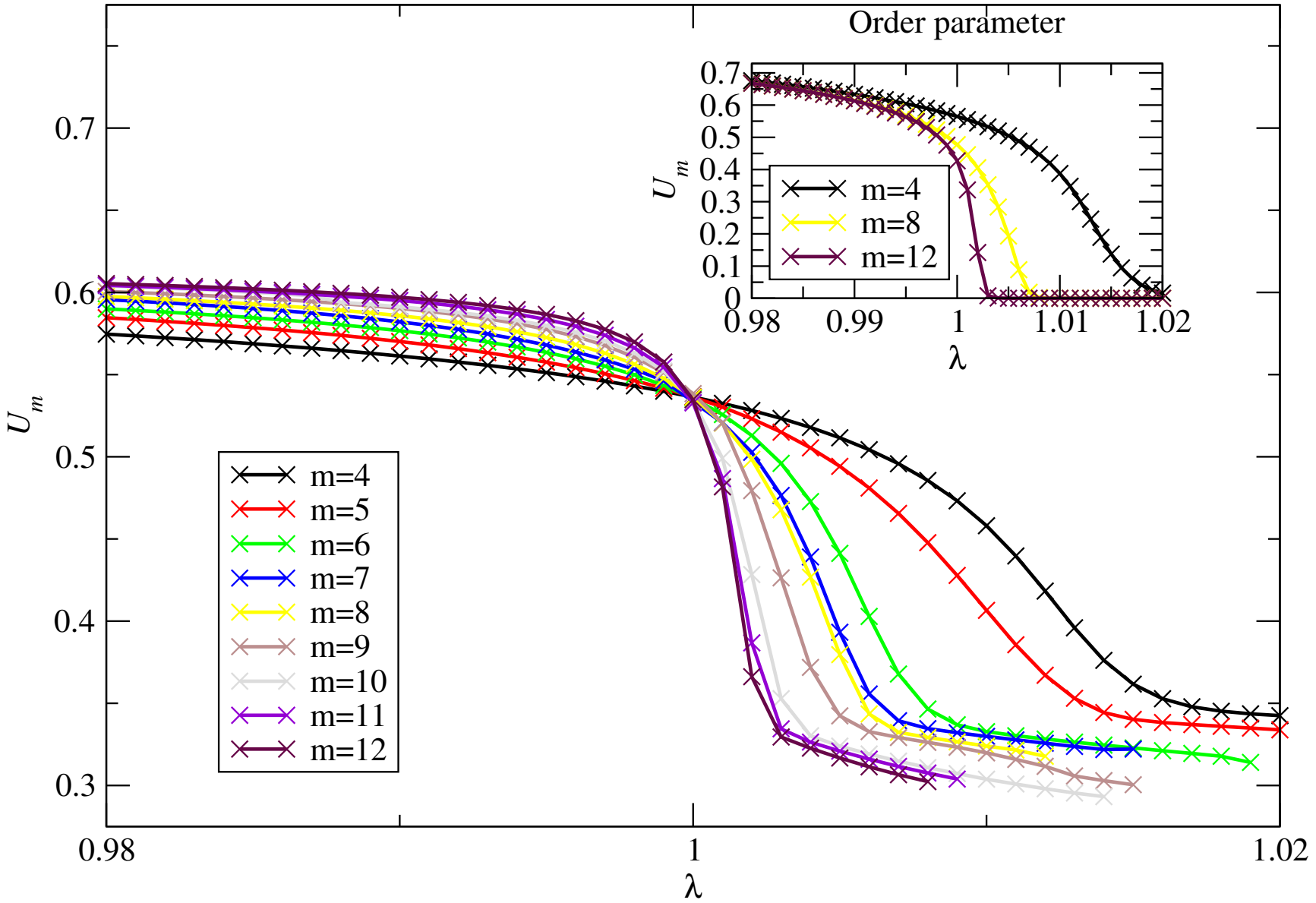
$$U_L = 1 - \frac{3k_2^2 L^2 + k_4 L}{3k_2^2 L^2} \to 0$$

- 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

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

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

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

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

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

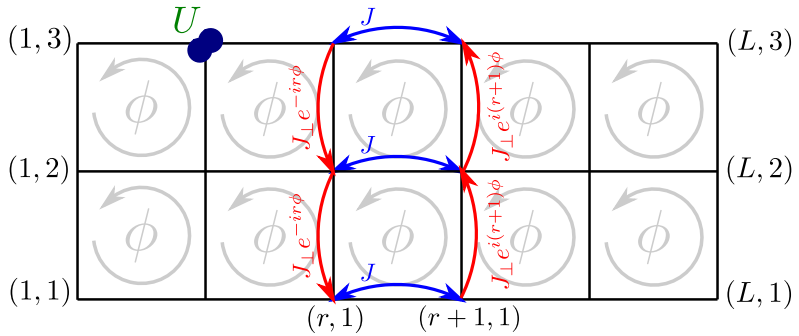
$$O_P^2 = \lim_{|j-i|\to\infty} \langle \, p_i \, p_j \, \rangle$$

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 $J_\perp$

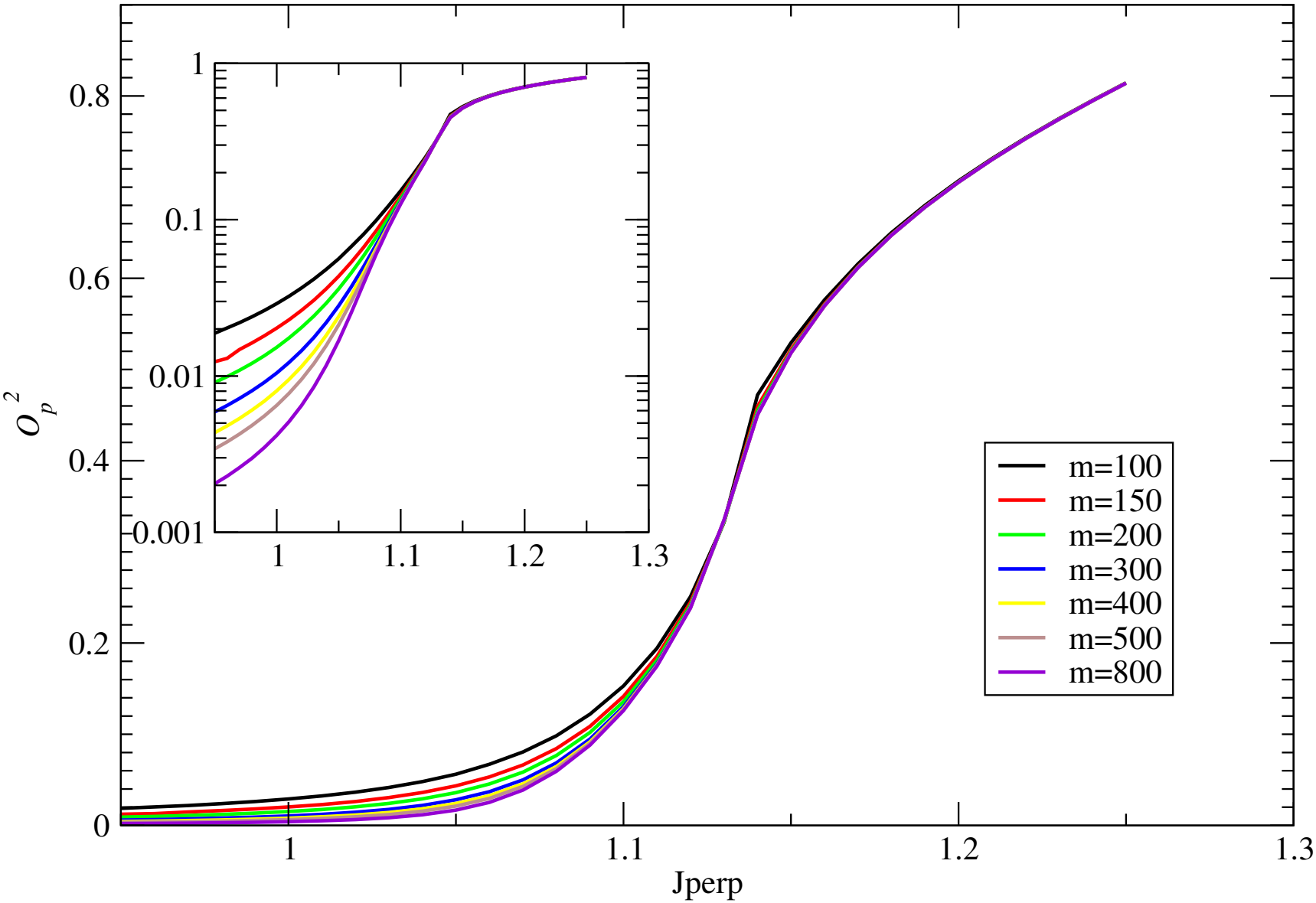
- P has a simple MPO representation

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

- Hence we can calculate higher moments of P.

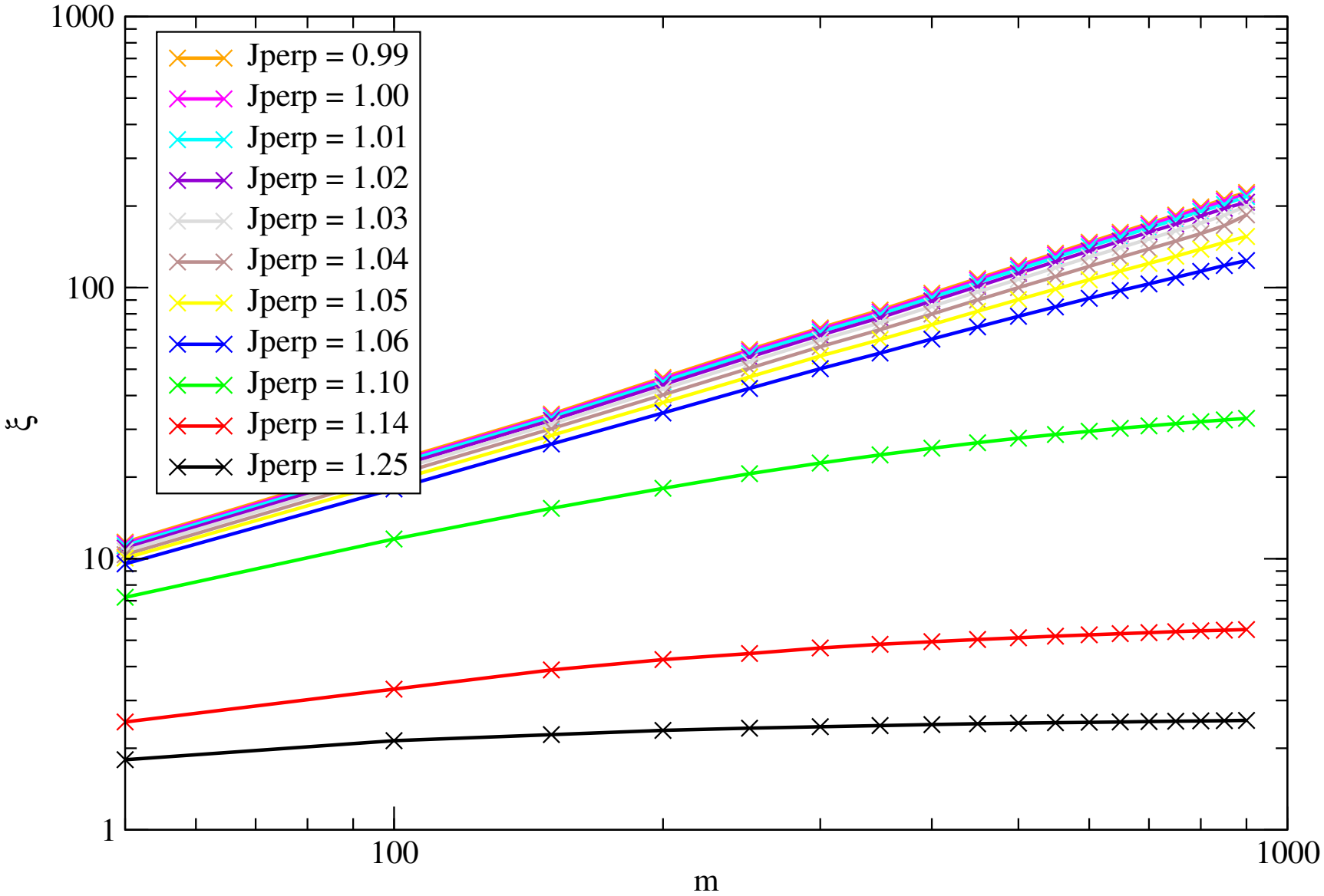
Bose-Hubbard Ladder

String order parameter



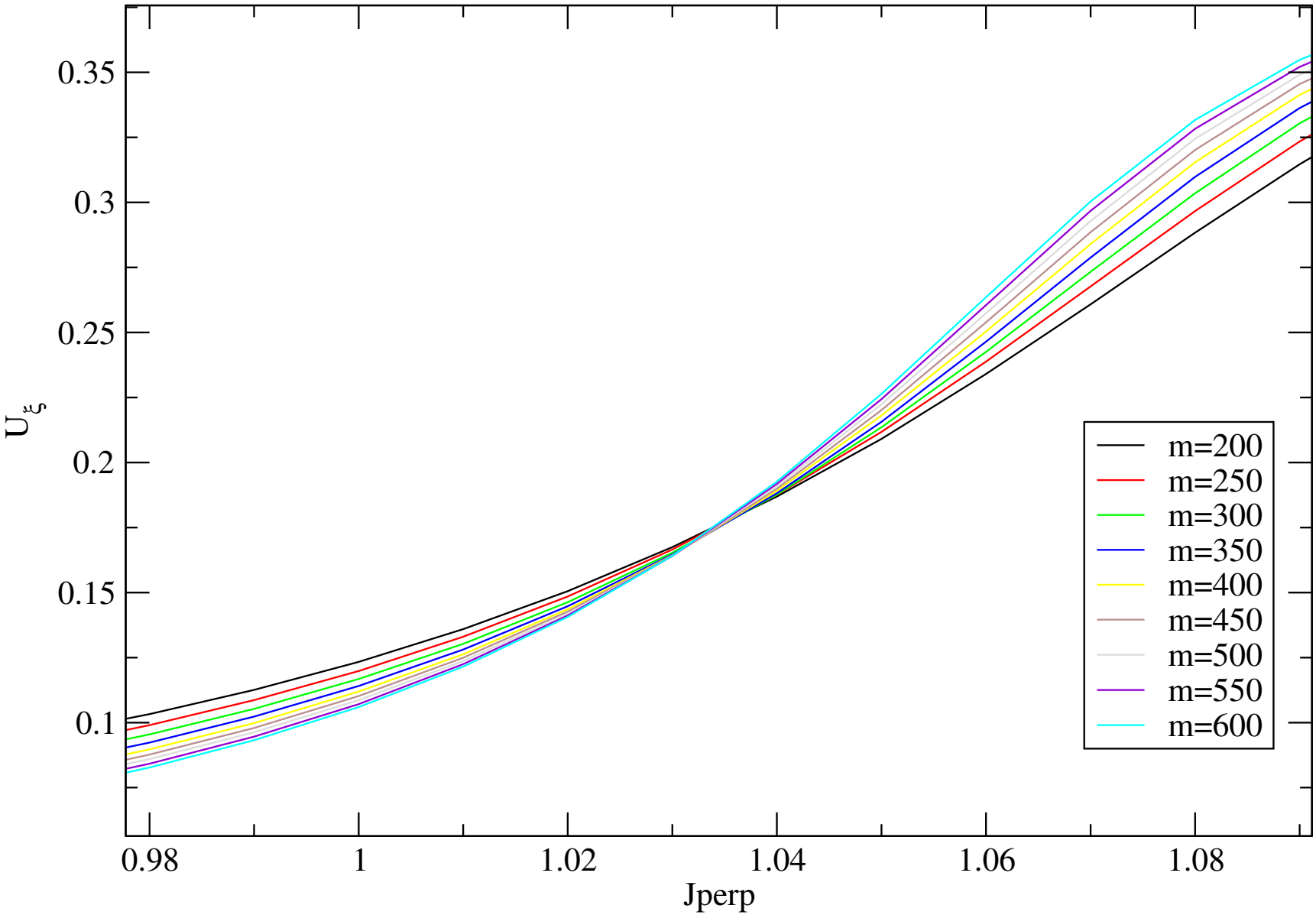
Bose=Hubbard Ladder

Scaling of correlation length



Bose-Hubbard Ladder

String parameter Binder cumulant

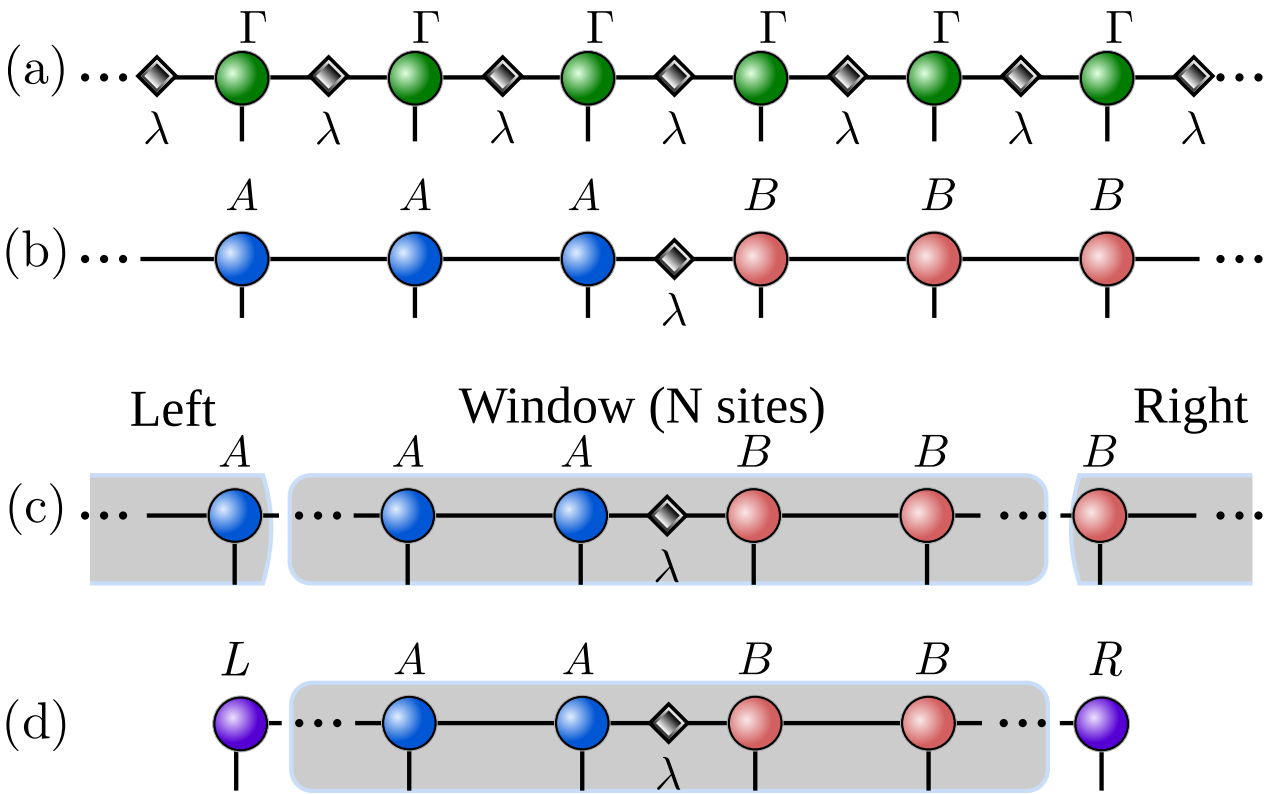


Infinite boundary conditions

H.N. Phien, G. Vidal, IPM, Phys. Rev. B 86, 245107 (2012), Phys. Rev. B 88, 035103 (2013)

(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

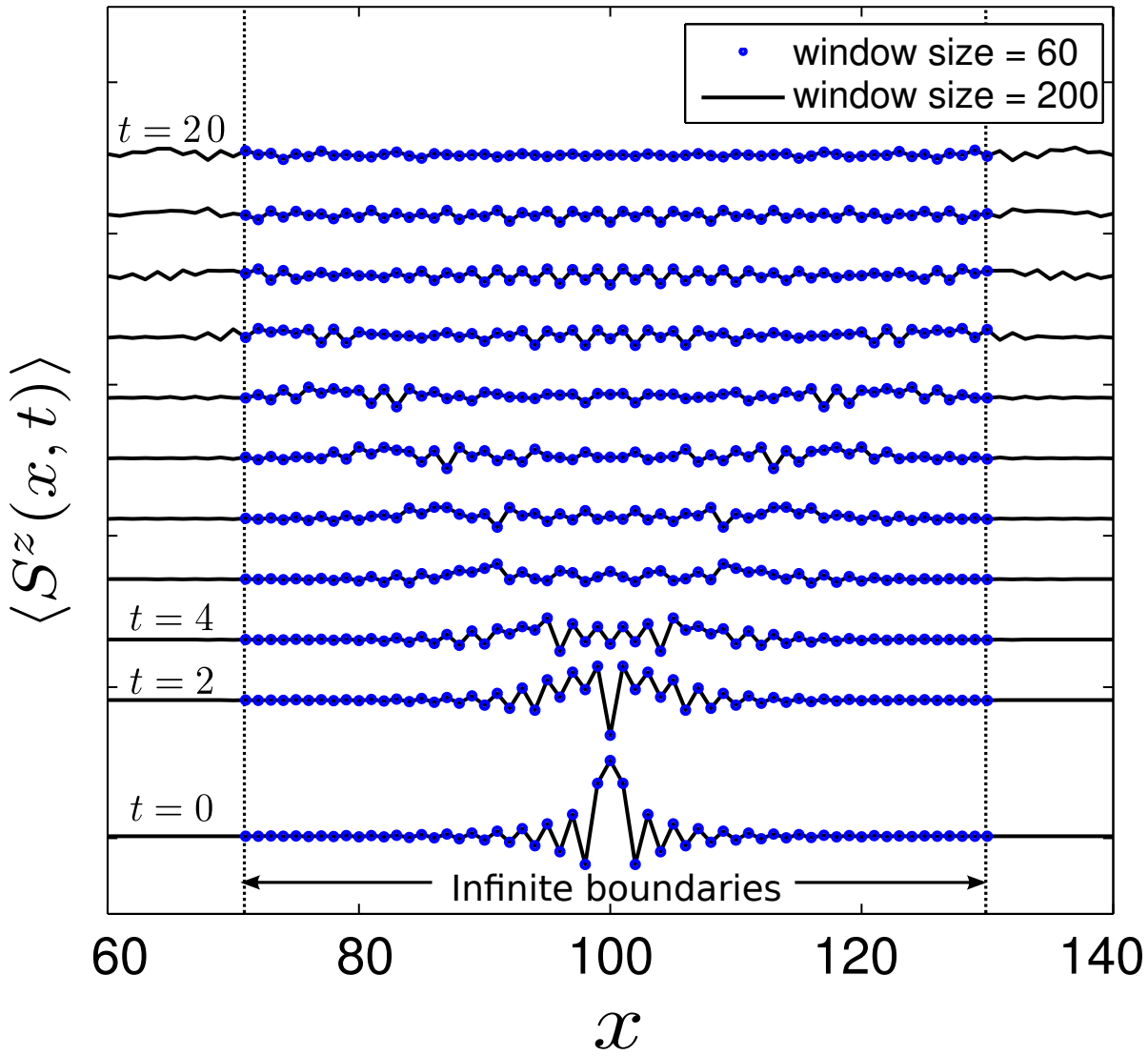
$$H = H_L + H_{LW} + H_W + H_{WR} + H_R$$

- 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

$$\exp itH_L \sim I$$

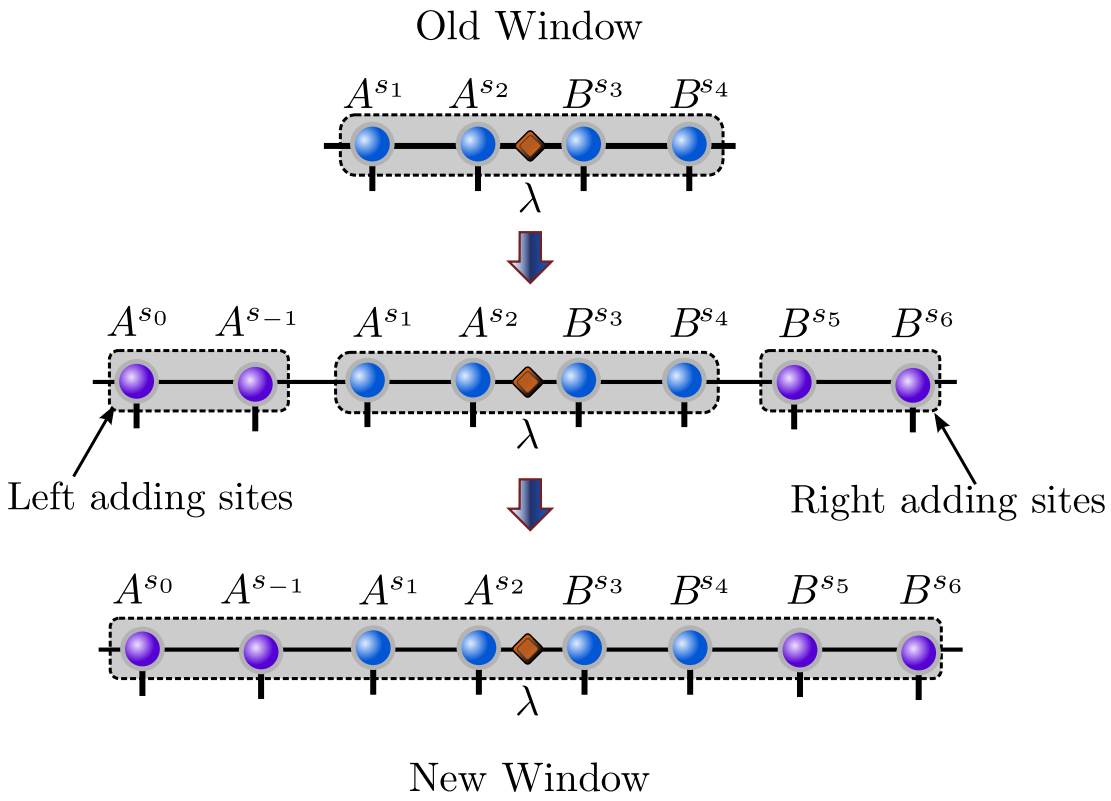
and we don't leave the Hilbert space of the semi-infinite strip

Spin-1 Heisenberg chain, S^+ initial perturbation

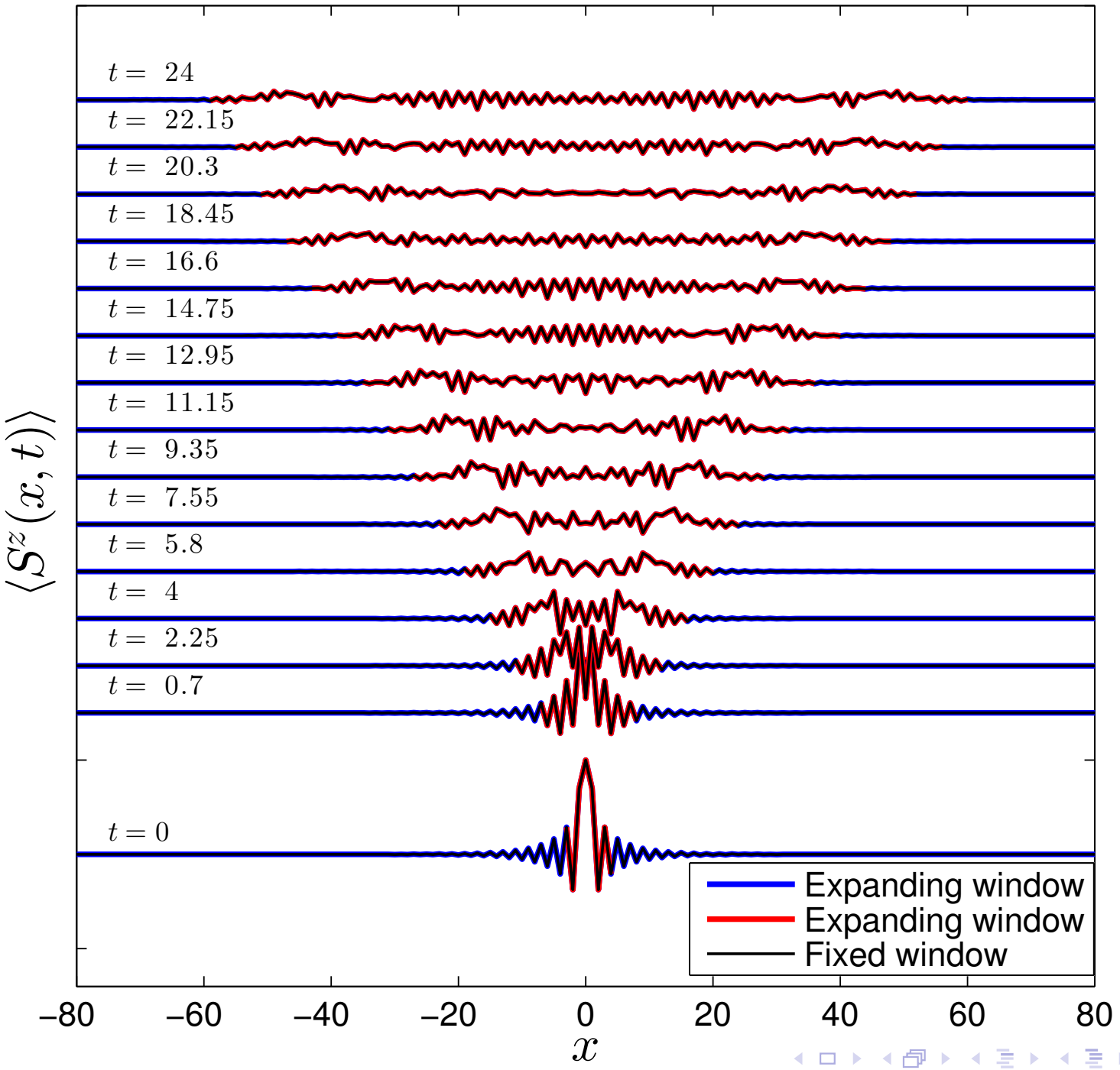


Resize the window

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

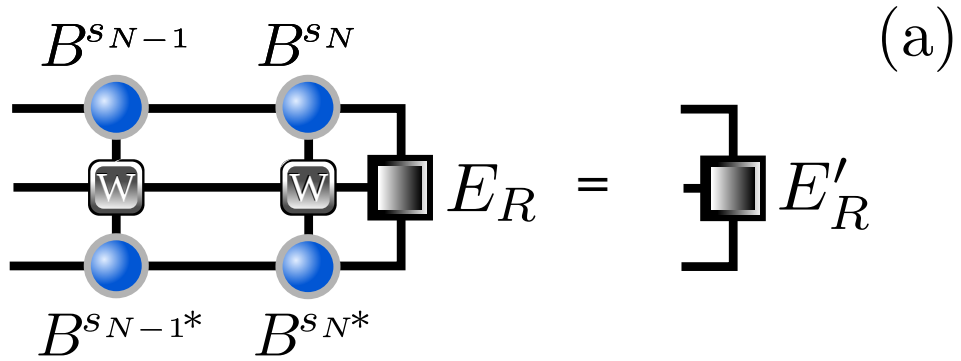


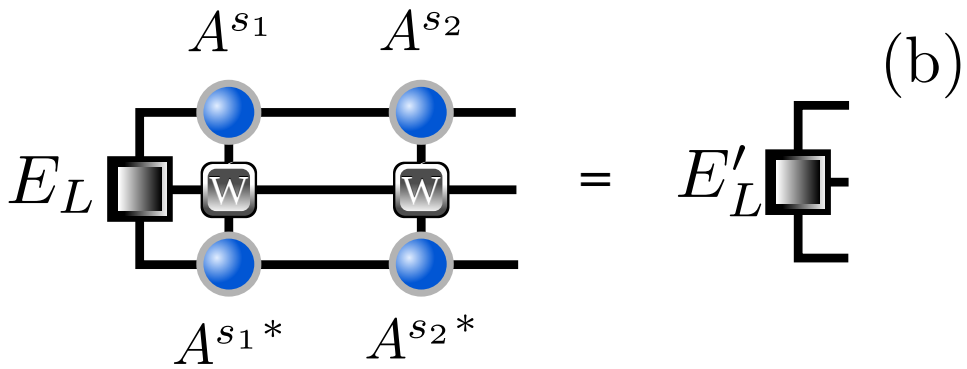
Criteria for expanding: is the wavefront near the boundary?
(Calculate from the fidelity of the wavefunction at the boundary)


$t = 24$
$t = 22.15$
$t = 20.3$
$t = 18.45$
$t = 16.6$
$t = 14.75$
$t = 12.95$
$t = 11.15$
$t = 9.35$
$t = 7.55$
$t = 5.8$
$t = 4$
$t = 2.25$
$t = 0.7$
$t = 0$
$\langle S^z(x,t)\rangle$
Expanding window
Expanding window
Fixed window
−80
−60
−40
−20
0
20
40
60
80
x

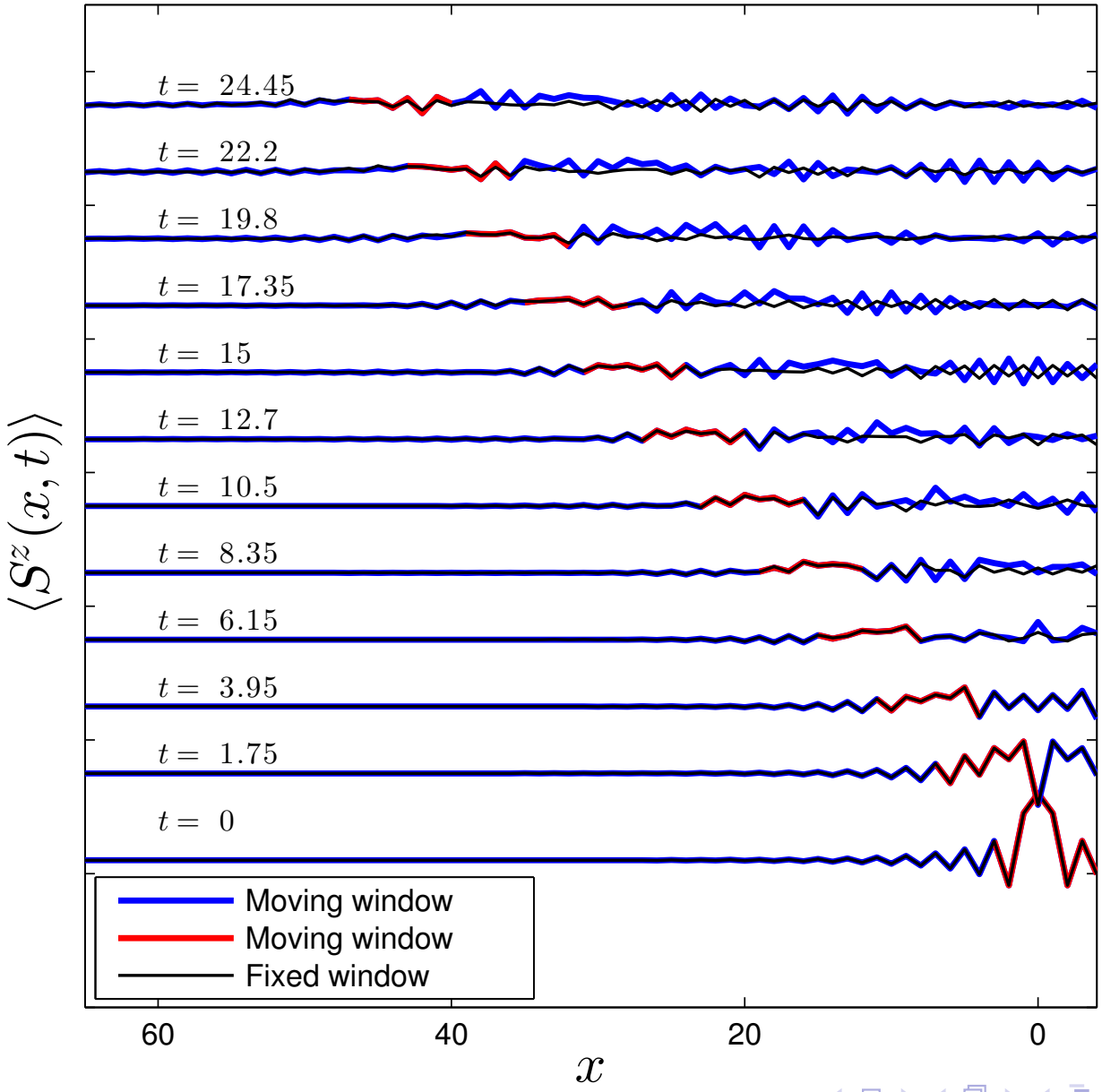
Window contraction

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





Follow the wavefront



Summary

- iDMRG – efficient algorithm for obtaining translationally invariant iMPS
- Many quantities are natural for iMPS but difficult to calculate for finite systems (eg 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*...