XIV Training Course on Strongly Correlated Systems
Vietri Sul Mare, Salerno, Italy, October 5-16, 2009

Stochastic Series Expansion (quantum Monte Carlo)

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Introduction; path integrals and series representation

SSE algorithm for the S=1/2 Heisenberg model

- all details needed to make a simple butvery efficient program
- essentially lattice-independent (bipartite) formulation

Examples: properties of chains, ladders, planes

- critical state of the Heisenberg chain and odd number of coupled chains
- gapped (quantum diordered) state of even number of coupled chains
- long-range order in 2D

Path integrals in quantum statistical mechanics

We want to compute a thermal expectation value

$$\langle A \rangle = \frac{1}{Z}\mathrm{Tr}\{A\mathrm{e}^{-\beta H}\}$$

where $\beta=1/T$ (and possibly T→0)

"Time slicing" of the partition function

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \mathrm{Tr}\left\{\prod_{l=1}^{L}\mathrm{e}^{-\Delta_\tau H}\right\} \qquad \Delta_\tau = \beta/L$$

Choose a basis and insert complete sets of states;

$$Z = \sum_{\alpha_0}\sum_{\alpha_1}\cdots\sum_{\alpha_{L-1}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau H}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}|\alpha_0\rangle$$

Use approximation for imaginary time evolution operator. Simplest way

$$Z \approx \sum_{\{\alpha\}}\langle\alpha_0|1-\Delta_\tau H|\alpha_{L-1}\rangle\cdots\langle\alpha_2|1-\Delta_\tau H|\alpha_1\rangle\langle\alpha_1|1-\Delta_\tau H|\alpha_0\rangle$$

Leads to error $\propto \Delta_\tau$. Limit $\Delta_\tau \to 0$ can be taken

Example: hard-core bosons

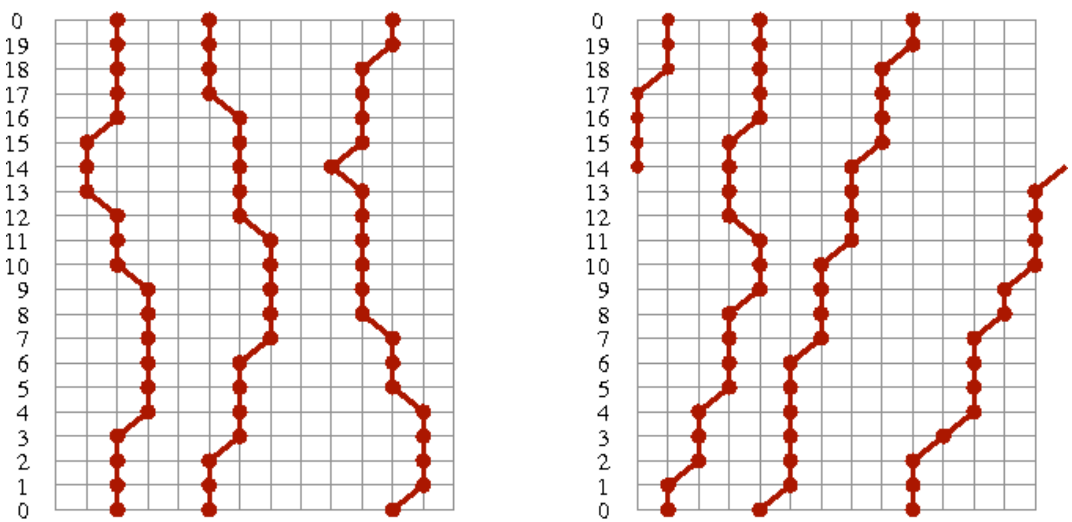
$$H = K = -\sum_{\langle i,j\rangle} K_{ij} = -\sum_{\langle i,j\rangle}(a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0,1\}$$

Equivalent to S=1/2 XY model

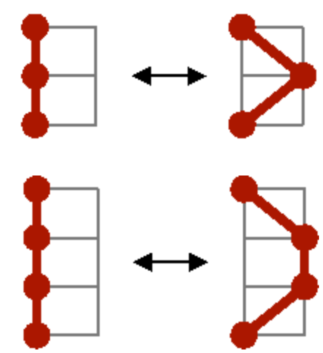
$$H = -2\sum_{\langle i,j\rangle}(S_i^x S_j^x + S_i^y S_j^y) = -\sum_{\langle i,j\rangle}(S_i^+ S_j^- + S_i^- S_j^+), \quad S^z = \pm\frac{1}{2} \sim n_i = 0,1$$

"World line" representation of

$$Z \approx \sum_{\{\alpha\}} \langle\alpha_0|1-\Delta_\tau H|\alpha_{L-1}\rangle \cdots \langle\alpha_2|1-\Delta_\tau H|\alpha_1\rangle\langle\alpha_1|1-\Delta_\tau H|\alpha_0\rangle$$



world line moves for Monte Carlo sampling



$$Z = \sum_{\{\alpha\}} W(\{\alpha\}), \quad W(\{\alpha\}) = \Delta_\tau^{n_K}$$

n_K = number of "jumps"

Expectation values

$$\langle A\rangle = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\mathrm{e}^{-\Delta_\tau}|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\mathrm{e}^{-\Delta_\tau H}|\alpha_1\rangle\langle\alpha_1|\mathrm{e}^{-\Delta_\tau H}A|\alpha_0\rangle$$

We want to write this in a form suitable for MC importance sampling

$$\langle A\rangle = \frac{\sum_{\{\alpha\}} A(\{\alpha\})W(\{\alpha\})}{\sum_{\{\alpha\}} W(\{\alpha\})} \longrightarrow \langle A\rangle = \langle A(\{\alpha\})\rangle_W$$

$$W(\{\alpha\}) = \text{weight}$$
$$A(\{\alpha\}) = \text{estimator}$$

For any quantity diagonal in the occupation numbers (spin z)

$$A(\{\alpha\}) = A(\alpha_n) \quad \text{or} \quad A(\{\alpha\}) = \frac{1}{L}\sum_{l=0}^{L-1} A(\alpha_l)$$

Kinetic energy (here full energy). Use

$$K\mathrm{e}^{-\Delta_\tau K} \approx K \qquad K_{ij}(\{\alpha\}) = \frac{\langle\alpha_1|K_{ij}|\alpha_0\rangle}{\langle\alpha_1|1-\Delta_\tau K|\alpha_0\rangle} \in \{0,1\}$$

Average over all slices → count number of kinetic jumps

$$\langle K_{ij}\rangle = \frac{\langle n_{ij}\rangle}{\beta}, \quad \langle K\rangle = \frac{\langle n_K\rangle}{\beta}, \qquad \langle K\rangle \propto N \to \langle n_K\rangle \propto \beta N$$

There should be of the order βN "jumps" (regardless of approximation used)

Including interactions

For any diagonal interaction V

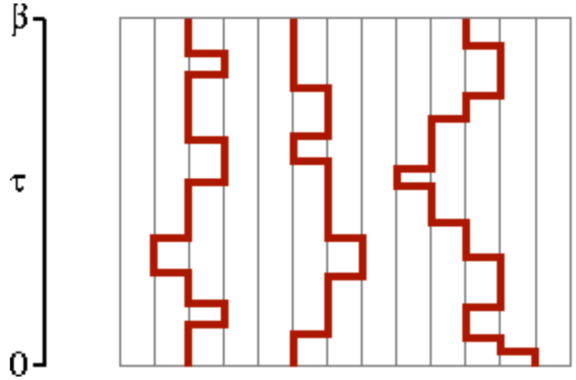
$$\mathrm{e}^{-\Delta_\tau H} = \mathrm{e}^{-\Delta_\tau K}\mathrm{e}^{-\Delta_\tau V} + \mathcal{O}(\Delta_\tau^2) \to \langle \alpha_{l+1}|\mathrm{e}^{-\Delta_\tau H}|\alpha_l\rangle \approx \mathrm{e}^{-\Delta_\tau V_l}\langle \alpha_{l+1}|\mathrm{e}^{-\Delta_\tau K}|\alpha_l\rangle$$

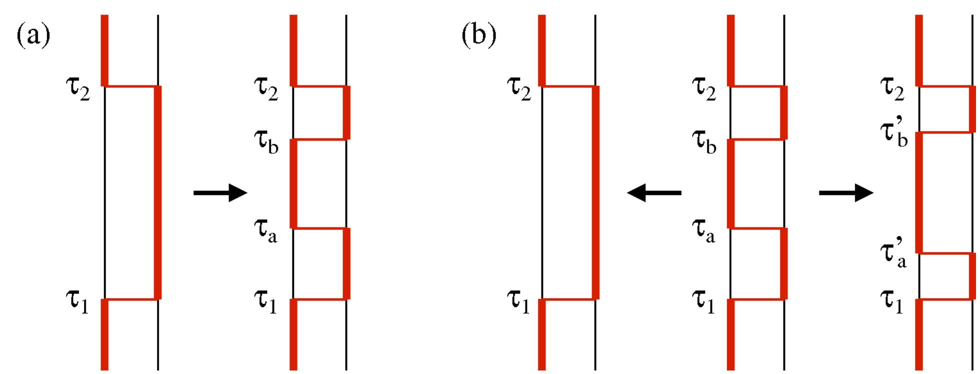
Product over all times slices →

$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l\right)$$

The continuous time limit

Limit $\Delta_\tau \to 0$: number of kinetic jumps remains finite, store events only





Special methods (**loop and worm updates**) developed for efficient sampling of the paths in the continuum

local updates
consider probability of inserting/removing events within a time window

⇐ Evertz, Lana, Marcu (1993), Prokofev et al (1996)
Beard & Wiese (1996)

Series expansion representation

Start from the Taylor expansion $\mathrm{e}^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_n} \langle \alpha_0 | H | \alpha_{n-1} \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle$$

Very similar to the path integral; $1 - \Delta\tau H \rightarrow H$ and weight factor outside

For hard-core bosons the (allowed) path weight is $W(\{\alpha\}_n) = \beta^n / n!$

For any model, the energy is

$$\begin{aligned} E &= \frac{1}{Z} \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\{\alpha\}_{n+1}} \langle \alpha_0 | H | \alpha_{n+1} \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle \\ &= -\frac{1}{Z} \sum_{n=1}^{\infty} \frac{(-\beta)^n}{n!} \frac{n}{\beta} \sum_{\{\alpha\}_n} \langle \alpha_0 | H | \alpha_n \rangle \cdots \langle \alpha_2 | H | \alpha_1 \rangle \langle \alpha_1 | H | \alpha_0 \rangle = \frac{\langle n \rangle}{\beta} \end{aligned}$$

$$C = \langle n^2 \rangle - \langle n \rangle^2 - \langle n \rangle$$

From this follows: narrow n-distribution with $\langle n \rangle \propto N\beta, \quad \sigma_n \propto \sqrt{N\beta}$

Fixed-length scheme: cut-off at N=L, fill in with unit operators I

$$Z = \sum_S \frac{(-\beta)^n (L-n)!}{L!} \sum_{\{\alpha\}_L} \sum_{\{S_i\}} \langle \alpha_0 | S_L | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | S_2 | \alpha_1 \rangle \langle \alpha_1 | S_1 | \alpha_0 \rangle, \quad S_i \in \{0, H\}$$

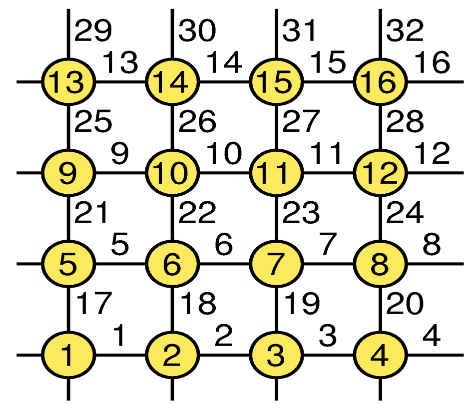
Here n is the number of S_i=H instances in the sequence $S_1,\ldots,S_L$

Stochastic Series expansion (SSE): S=1/2 Heisenberg model

Write H as a bond sum for arbitrary lattice

$$H = J \sum_{b=1}^{N_b} \mathbf{S}_{i(b)} \cdot \mathbf{S}_{j(b)},$$

2D square lattice
bond and site labels



Diagonal (1) and off-diagonal (2) bond operators

$$H_{1,b} = \tfrac{1}{4} - S^z_{i(b)} S^z_{j(b)},$$
$$H_{2,b} = \tfrac{1}{2}(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}).$$

$$H = -J \sum_{b=1}^{N_b} (H_{1,b} - H_{2,b}) + \frac{JN_b}{4}$$

Four non-zero matrix elements

$$\langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{1,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \tfrac{1}{2} \qquad \langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{2,b} | \uparrow_{i(b)} \downarrow_{j(b)} \rangle = \tfrac{1}{2}$$
$$\langle \downarrow_{i(b)} \uparrow_{j(b)} | H_{1,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \tfrac{1}{2} \qquad \langle \uparrow_{i(b)} \downarrow_{j(b)} | H_{2,b} | \downarrow_{i(b)} \uparrow_{j(b)} \rangle = \tfrac{1}{2}$$

Partition function

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} (-1)^{n_2} \frac{\beta^n}{n!} \sum_{S_n} \left\langle \alpha \left| \prod_{p=0}^{n-1} H_{a(p),b(p)} \right| \alpha \right\rangle$$

n_2 = number of a(i)=2
(off-diagonal operators)
in the sequence

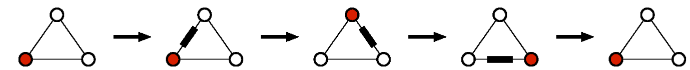
Index sequence: $S_n = [a(0), b(0)], [a(1), b(1)], \ldots, [a(n-1), b(n-1)]$

For fixed-length scheme

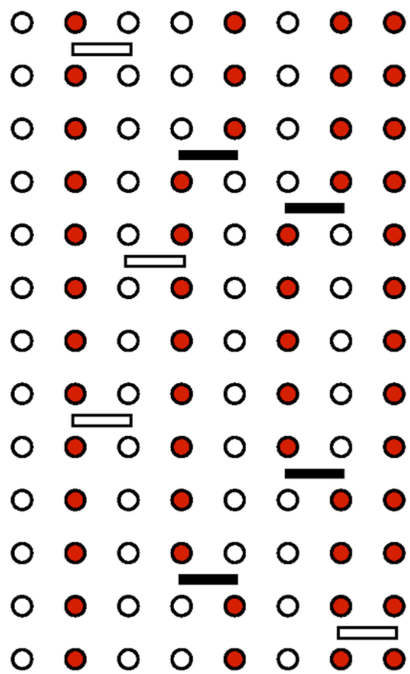
$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \sum_{S_L} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

Propagated states: $|\alpha(p)\rangle \propto \prod_{i=0}^{p-1} H_{a(i),b(i)} |\alpha\rangle$

W>0 (n_2 even) for bipartite lattice
Frustration leads to **sign problem**



i	1	2	3	4	5	6	7	8
$\sigma(i)$	-1	+1	-1	-1	+1	-1	+1	+1



p	$a(p)$	$b(p)$	$s(p)$
12	1	2	4
11	0	0	0
10	2	4	9
9	2	6	13
8	1	3	6
7	0	0	0
6	0	0	0
5	1	2	4
4	2	6	13
3	0	0	0
2	2	4	9
1	1	7	14

In a program:

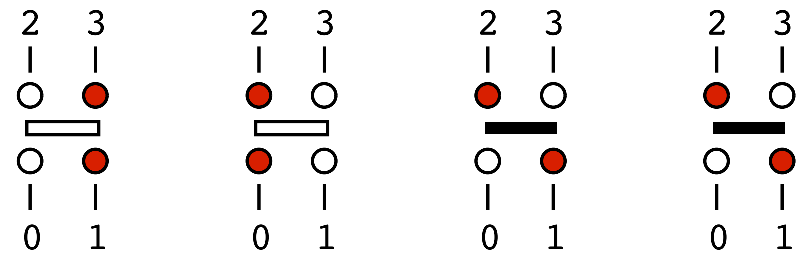
s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

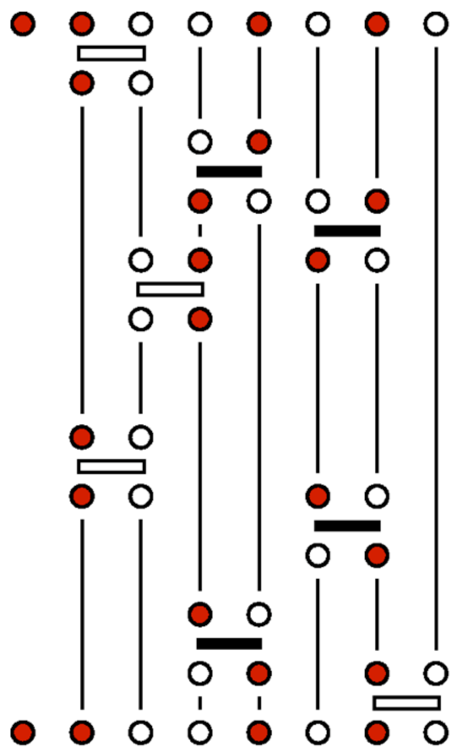
σ(i) = spin state, i=1,...,N
- only one has to be stored

SSE effectively provides a discrete representation of the time continuum
- computational advantage; only integer operations in sampling

Linked vertex storage

The “legs” of a vertex represents the spin states before (below) and after (above) an operator has acted





p	v (l=0)	X(v) (l=0)	v (l=1)	X(v) (l=1)	v (l=2)	X(v) (l=2)	v (l=3)	X(v) (l=3)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1

X( ) = vertex list
- operator at p→X(v)
  v=4p+l, l=0,1,2,3
- links to next and previous leg

Spin states between operations are redundant; represented by links
- network of linked vertices will be used for loop updates of vertices/operators

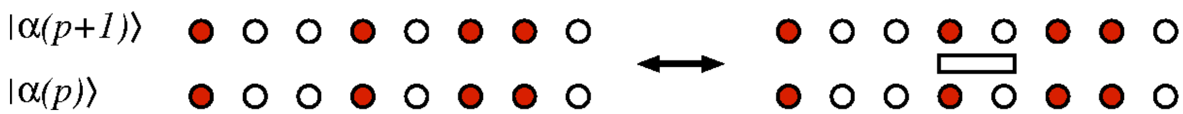
Monte Carlo sampling scheme

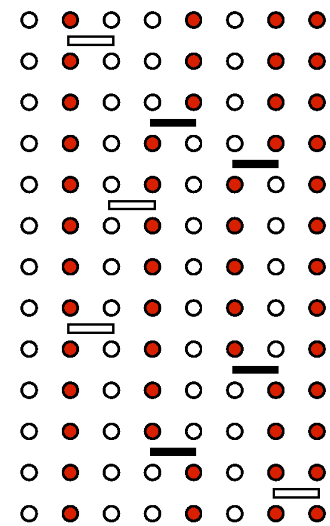
Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

$$W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

$$P_{\text{accept}} = \min\left[\frac{W(\alpha', S_L)}{W(\alpha, S_L)} \frac{P_{\text{select}}(\alpha', S'_L \to \alpha, S_L)}{P_{\text{select}}(\alpha, S_L \to \alpha', S'_L)}, 1\right]$$

Diagonal update: $[0,0]_p \leftrightarrow [1,b]_p$





Attempt at p=0,...,L-1. Need to know |α(p)>

- generate by flipping spins when off-diagonal operator

$$P_{\text{select}}(a=0 \to a=1) = 1/N_b, \quad (b \in \{1,\ldots,N_b\})$$

$$P_{\text{select}}(a=1 \to a=0) = 1$$

$$\frac{W(a=1)}{W(a=0)} = \frac{\beta/2}{L-n} \qquad \frac{W(a=0)}{W(a=1)} = \frac{L-n+1}{\beta/2}$$

n is the current power

- n → n+1 (a=0 → a=1)
- n → n-1 (a=1 → a=0)

Acceptance probabilities

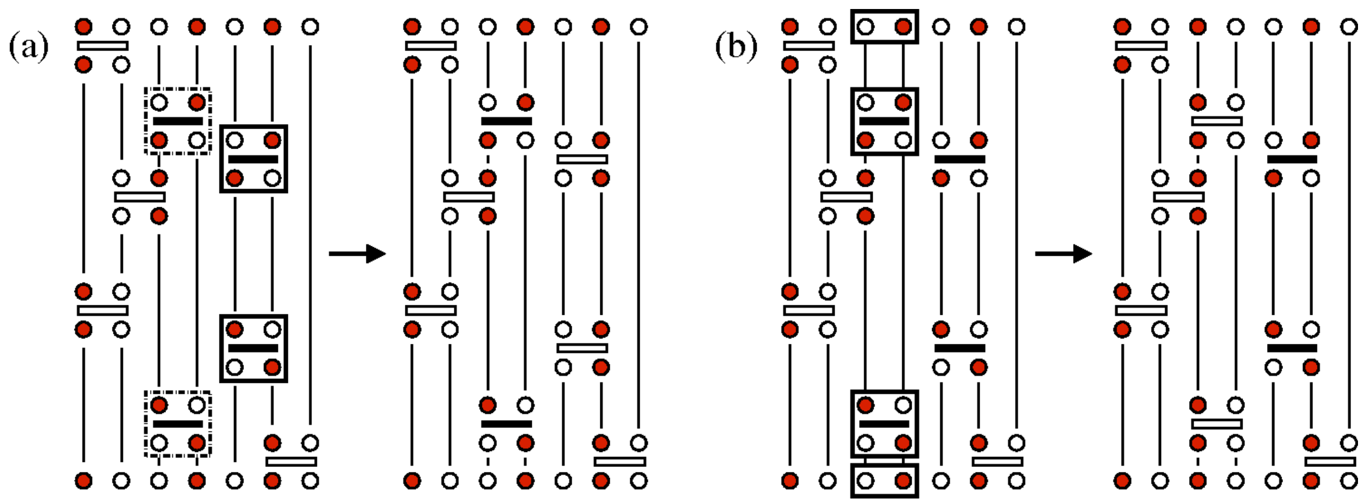
$$P_{\text{accept}}([0,0] \to [1,b]) = \min\left[\frac{\beta N_b}{2(L-n)}, 1\right]$$

$$P_{\text{accept}}([1,b] \to [0,0]) = \min\left[\frac{2(L-n+1)}{\beta N_b}, 1\right]$$

Diagonal update; pseudocode implementation

```
do p = 0 to L − 1
    if (s(p) = 0) then
        b = random[1, . . . , N_b]; if  σ(i(b)) = σ(j(b)) cycle
        if (random[0 − 1] < P_insert(n)) then s(p) = 2b; n = n + 1 endif
    elseif (mod[s(p), 2] = 0) then
        if (random[0 − 1] < P_remove(n)) then s(p) = 0; n = n − 1 endif
    else
        b = s(p)/2; σ(i(b)) = −σ(i(b)); σ(j(b)) = −σ(j(b))
    endif
enddo
```

Local off-diagonal update

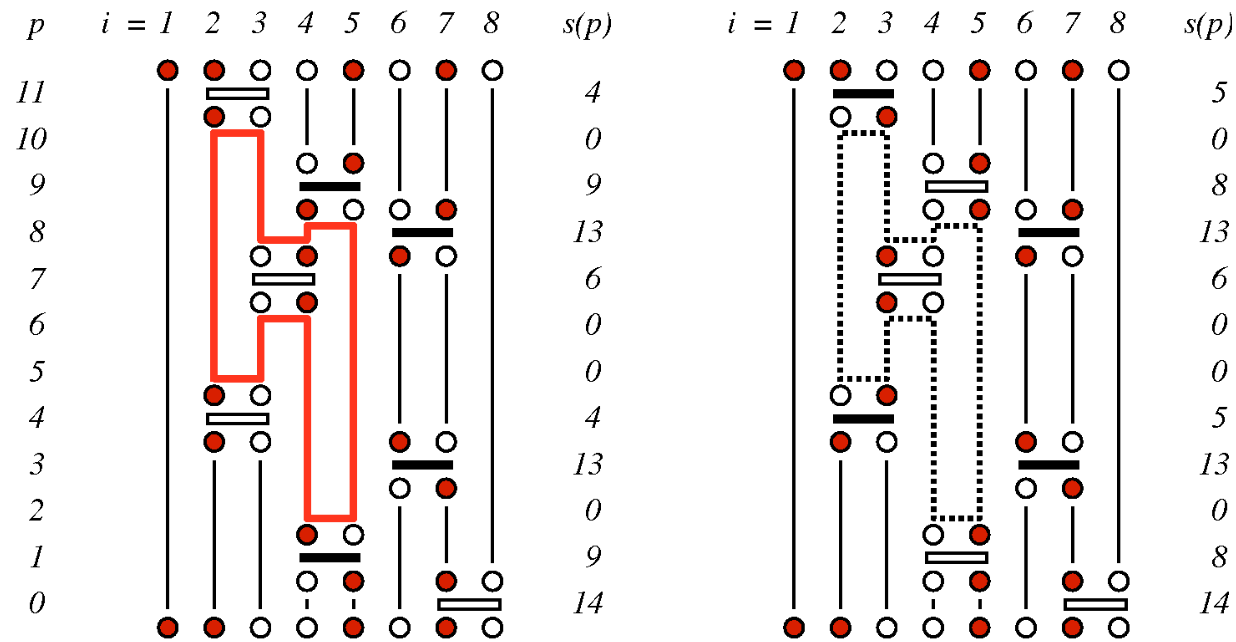


Switch the type (a=1 ↔ a=2) of two operators on the same spins

- constraints have to be satisfied
- inefficient, cannot change the winding number

Operator-loop update

Many spins and operators can be changed simultaneously



Pseudocode

moving horizontally in the list corresponds to changing v even↔odd

- **flipbit**(*v,0*) flips bit 0 of v

- a given loop is only constructed once
- vertices can be erased
- *X(v) < 0* = erased
- *X(v)* = *-1* not flipped loop
- *X(v)* = *-2* flipped loop

constructing all loops, flip probability 1/2

```
do v0 = 0 to 4L − 1 step 2
    if (X(v0) < 0) cycle
    v = v0
    if (random[0 − 1] < 1/2) then
        traverse the loop; for all v in loop, set X(v) = −1
    else
        traverse the loop; for all v in loop, set X(v) = −2
        flip the operators in the loop
    endif
enddo
```

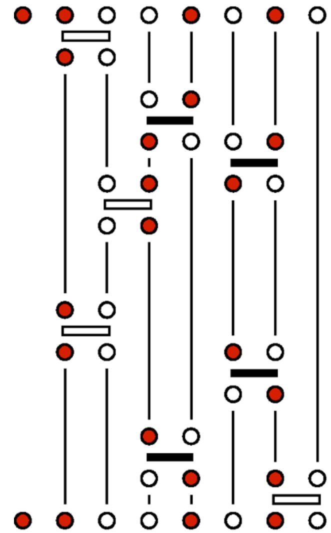
construct and flip a loop

```
v = v0
do
    X(v) = −2
    p = v/4; s(p) = flipbit(s(p), 0)
    v′ = flipbit(v, 0)
    v = X(v′); X(v′) = −2
    if (v = v0) exit
enddo
```

Constructing the linked vertex list

Traverse operator list $s(p)$, $p=0,\ldots,L-1$

- vertex legs **v=4p,4p+1,4p+2,4p+3**



p	v (l=0)	X(v) (l=0)	v (l=1)	X(v) (l=1)	v (l=2)	X(v) (l=2)	v (l=3)	X(v) (l=3)
11	44	18	45	30	46	16	47	17
10	40	-	41	-	42	-	43	-
9	36	31	37	7	38	4	39	5
8	32	14	31	15	34	12	35	0
7	28	19	29	6	30	45	31	36
6	24	-	25	-	26	-	27	-
5	20	-	21	-	22	-	23	-
4	16	46	17	47	18	44	19	28
3	12	34	13	2	14	32	15	33
2	8	-	9	-	10	-	11	-
1	4	38	5	39	6	29	7	37
0	0	35	1	3	2	13	3	1

Use arrays to keep track of the first and last (previous) vertex leg on a given spin

- $V_{\text{first}}(i)$ = location v of first leg on site i
- $V_{\text{last}}(i)$ = location v of last (currently) leg
- these are used to create the links
- initialize all elements to −1

$$
\begin{aligned}
&V_{\text{first}}(:) = -1;\ V_{\text{last}}(:) = -1\\
&\textbf{do } p = 0 \textbf{ to } L-1\\
&\quad \textbf{if } (s(p)=0) \textbf{ cycle}\\
&\quad v_0 = 4p;\ b = s(p)/2;\ s_1 = i(b);\ s_2 = j(b)\\
&\quad v_1 = V_{\text{last}}(s_1);\ v_2 = V_{\text{last}}(s_2)\\
&\quad \textbf{if } (v_1 \neq -1) \textbf{ then } X(v_1) = v_0;\ X(v_0) = v_1 \textbf{ else } V_{\text{first}}(s_1) = v_0 \textbf{ endif}\\
&\quad \textbf{if } (v_2 \neq -1) \textbf{ then } X(v_2) = v_0;\ X(v_0) = v_2 \textbf{ else } V_{\text{first}}(s_2) = v_0 + 1 \textbf{ endif}\\
&\quad V_{\text{last}}(s_1) = v_0 + 2;\ V_{\text{last}}(s_2) = v_0 + 3\\
&\textbf{enddo}
\end{aligned}
$$

creating the last links across the "time" boundary

$$
\begin{aligned}
&\textbf{do } i = 1 \textbf{ to } N\\
&\quad f = V_{\text{first}}(i)\\
&\quad \textbf{if } (f \neq -1) \textbf{ then } l = V_{\text{last}}(i);\ X(f) = l;\ X(l) = f \textbf{ endif}\\
&\textbf{enddo}
\end{aligned}
$$

We also have to modify the stored spin state after the loop update

- we can use the information in $V_{first}()$ and $X()$ to determine spins to be flipped
- spins with no operators, $V_{first}(i)=-1$, flipped with probability 1/2

$$
\begin{aligned}
&\textbf{do } i = 1 \textbf{ to } N \\
&\quad v = V_{\text{first}}(i) \\
&\quad \textbf{if } (v = -1) \textbf{ then} \\
&\qquad \textbf{if } (\textbf{random}[0\text{-}1] < 1/2)\ \sigma(i) = -\sigma(i) \\
&\quad \textbf{else} \\
&\qquad \textbf{if } (X(v) = -2)\ \sigma(i) = -\sigma(i) \\
&\quad \textbf{endif} \\
&\textbf{enddo}
\end{aligned}
$$

v is the location of the first vertex leg on spin i

- flip it if $X(v)=-2$
- (do not flip it if $X(v)=-1$)
- no operation on i if $v_{first}(i)=-1$

Determination of the cut-off L

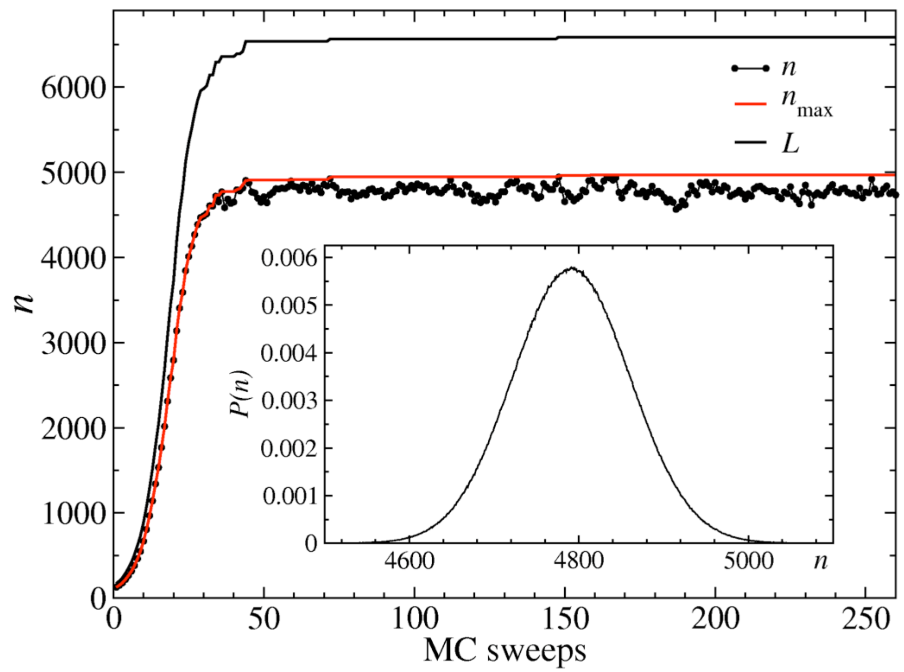
- adjust during equilibration
- start with arbitrary (small) n

Keep track of number of operators n

- increase L if n is close to current L
- e.g., ***L=n+n/3***

Example; 16×16 system, β=16 ⇒

- evolution of L
- n distribution after equilibration
- truncation is no approximation

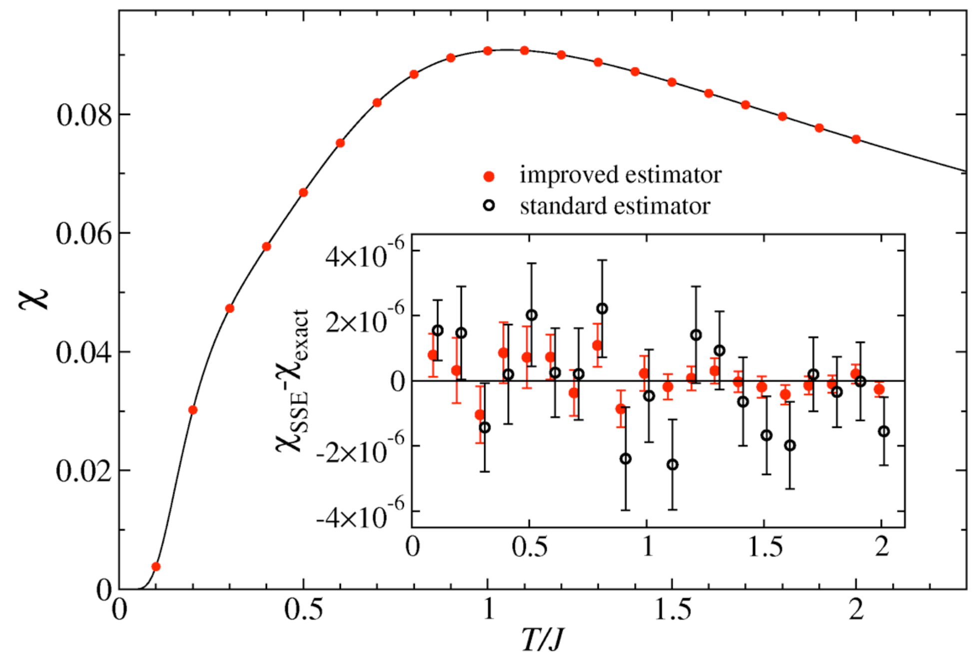


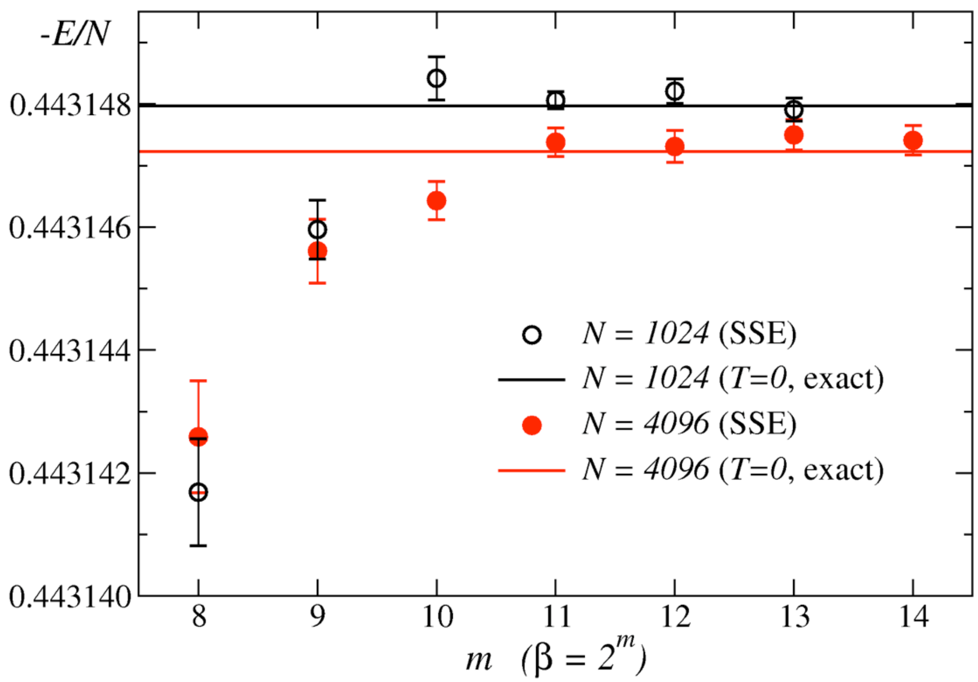
Does it work?
Compare with exact results

- 4×4 exact diagonalization
- Bethe Ansatz; long chains

Susceptibility of the 4×4 lattice ⇒

- SSE results from 10^{10} sweeps
- improved estimator gives smaller error bars at high T (where the number of loops is larger)





⇐ Energy for long 1D chains

- SSE results for 10^6 sweeps
- Bethe Ansatz ground state E/N
- SSE can achieve the ground state limit (T→0)

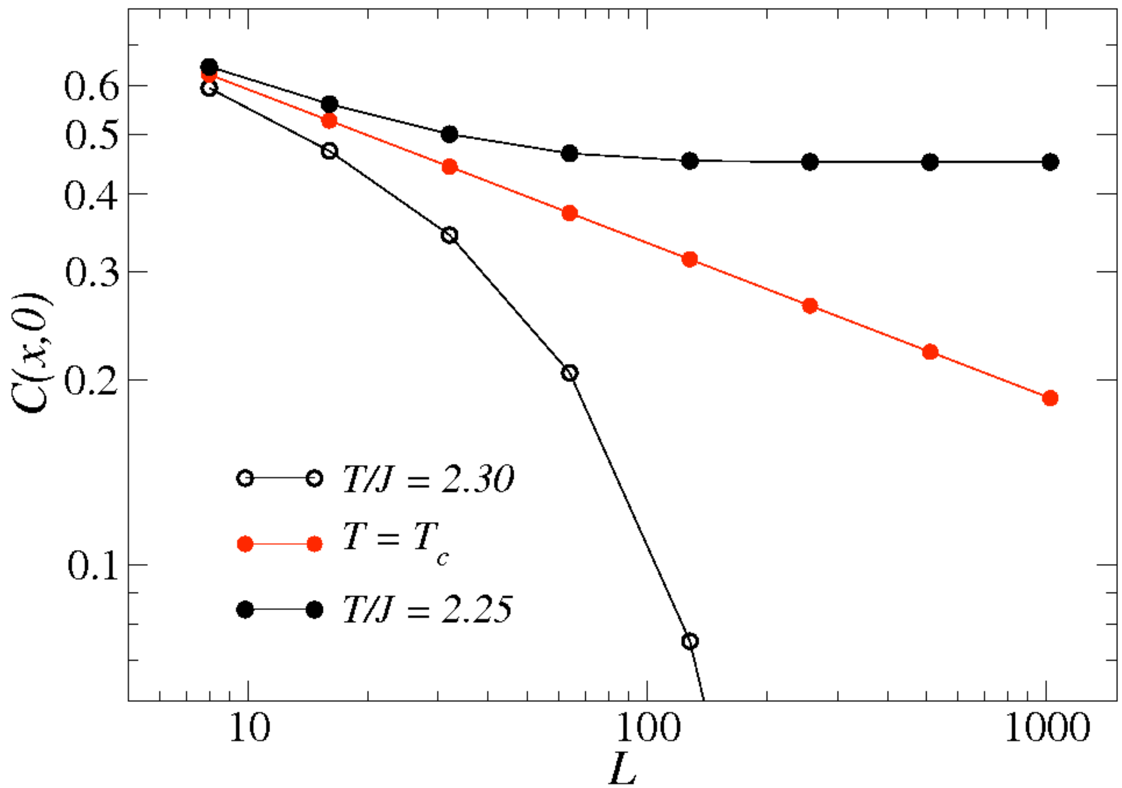
Correlations, criticality and long-range order

Example: 2D Ising model. Correlation function $C(r_{ij}) = \langle \sigma_i \sigma_j \rangle$

Three different behaviors

$$C(r) = \begin{cases} e^{-r/\xi}, & T > T_c \\ r^{-(2-D+\eta)}, & T = T_c \\ m^2 + e^{-r/\xi}, & T < T_c \end{cases} \qquad \eta = 1/8$$

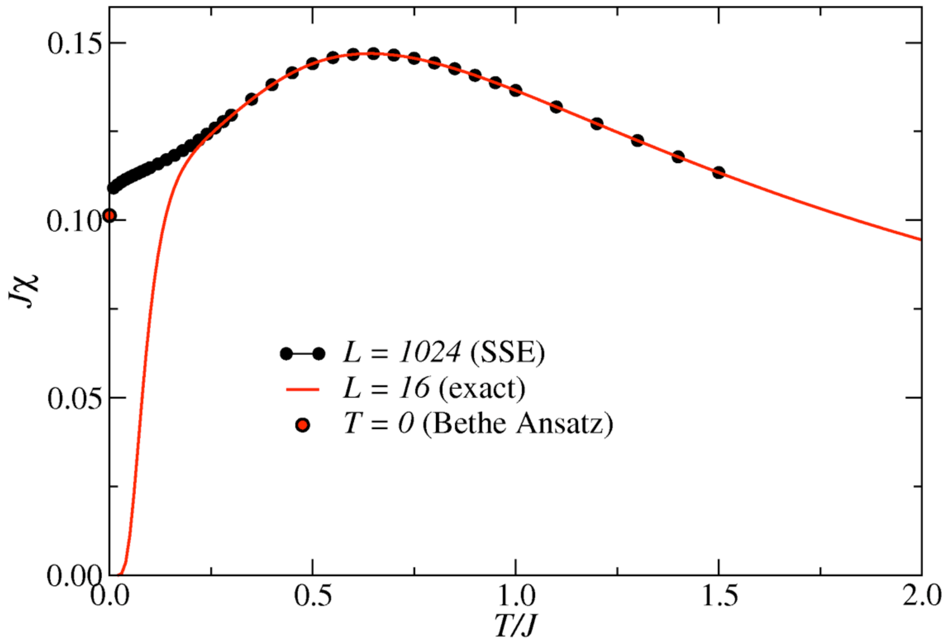
The correlation length diverges at T_c: $\xi \sim |T - T_c|^{-\nu}$

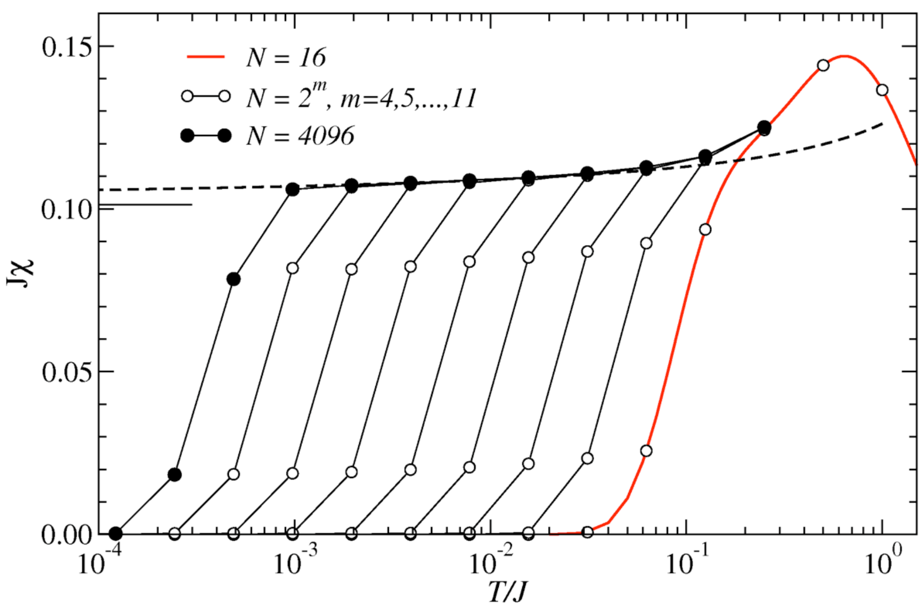


In **quantum system** we can have ordered, disordered, and critical ground states

- **quantum phase transitions** versus some parameter
- nature of the ground state reflected in finite-T properties

Properties of the Heisenberg chain; large-scale SSE results





Magnetic susceptibility

anomalous behavior as T→0

- low-T results seem to disagree with known T=0 value obtained using the Bethe Ansatz method
- Reason: logarithmic correction at low T>0

Eggert, Affleck, Takahashi, PRL 73, 332 (1994)

$$\chi(T) = \frac{1}{2\pi c} + \frac{1}{4\pi c \ln(T_0/T)}$$

- Low-T form expected based on low-energy field theory
- For the standard chain

$$c = \pi J/2, \;\; T_0 \approx 7.7$$

- Other interactions → same form, different parameters

Long chains needed for studying low-T behavior (T < finite-size gap)

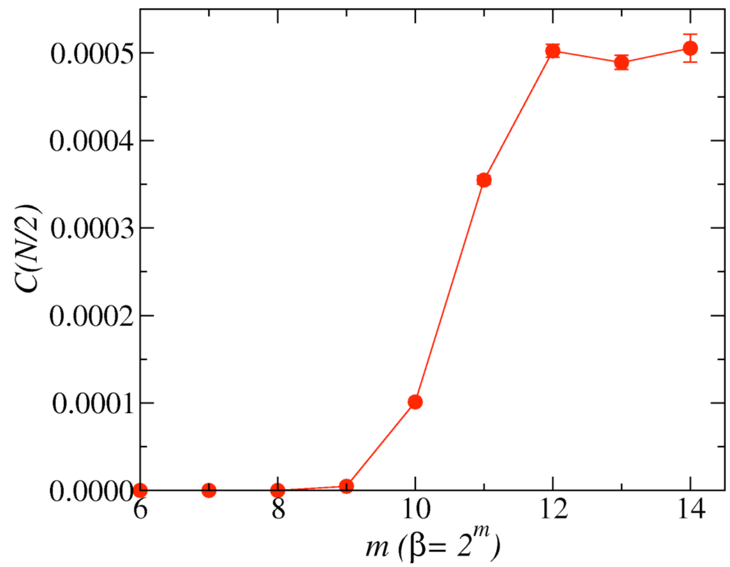
T=0 spin correlations

Low-energy field theory prediction

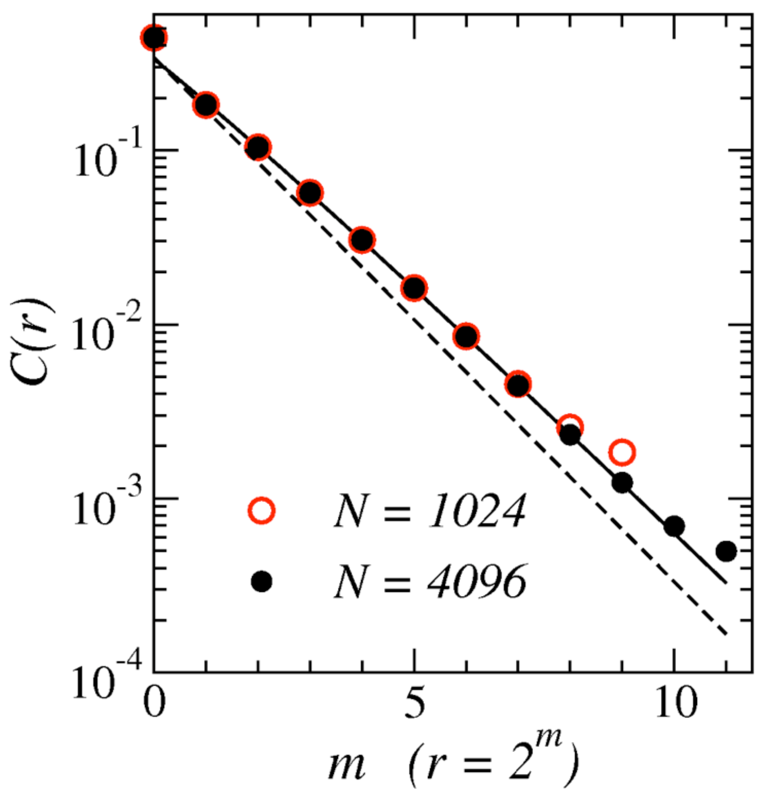
$$C(r) = A\frac{(-1)^r}{r}\ln\left(\frac{r}{r_0}\right)^{1/2}$$

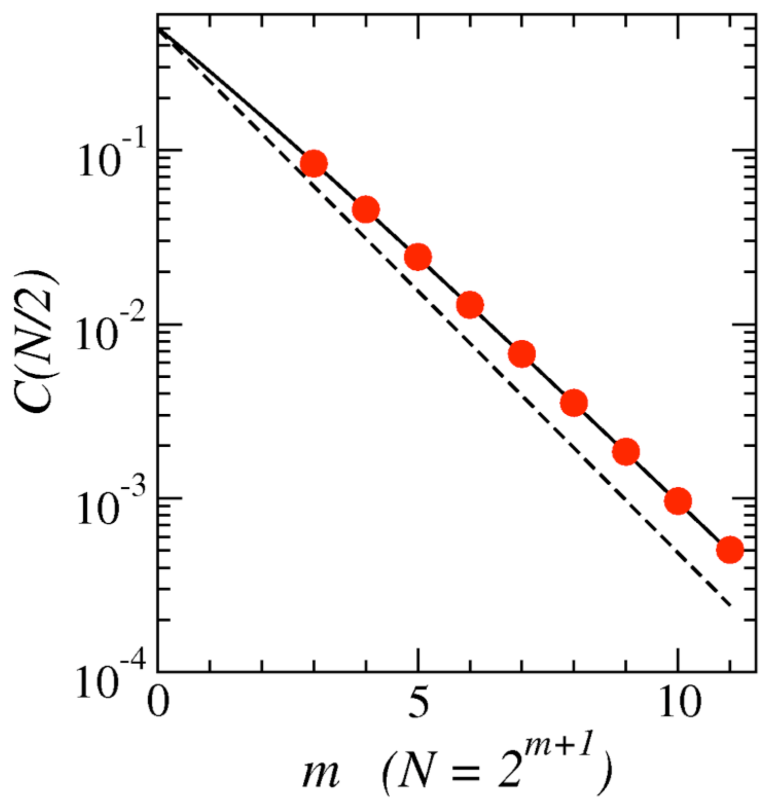
SSE: converge to T=0 limit

- β dependence of *C(N/2)*, *N* = 4096 ⇒
- C(r) vs r and and r=N/2 ⇓



A=0.21, r_0=0.08





Ladder systems

E. Dagotto and T. M. Rice, Science 271, 618 (1996)

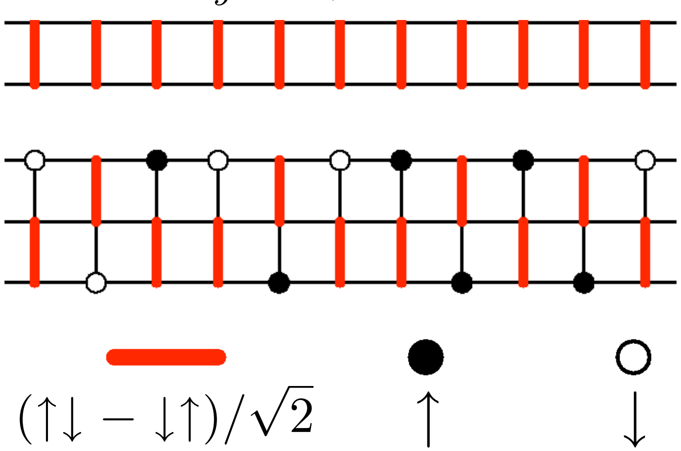
Coupled Heisenberg chains; $L_x \times L_y$ spins, $L_y \to \infty$, L_x finite

- systems with even and odd L_y have qualitatively different properties
  - spin gap $\Delta > 0$ for L_y even, $\Delta \to 0$ when $L_x \to \infty$
  - critical state, similar to single chain, for odd L_y
  - the 2D limit is approached in different ways

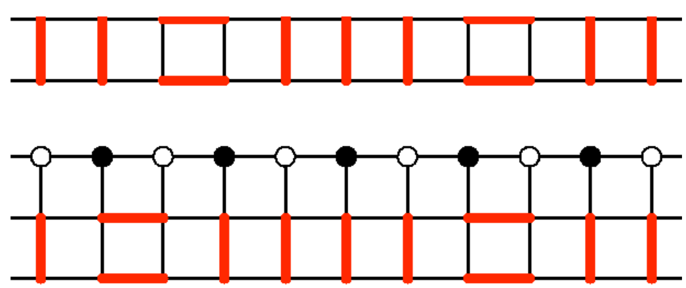
Consider anisotropic couplings; J_x and J_y

- the correct physics for all J_y/J_x can be understood based on large J_y/J_x
- short-range valence bond states (more later)

$J_y = 1, J_x = 0$



$0 < J_x/J_y \ll 1$



$L_y = 2,4,\ldots$: $\Delta = J_y$ for $J_x = 0$

- gap persists for $J_x > 0$

$L_y = 3,5,\ldots$: $\Delta = 0$ for $J_x = 0$

- critical state for $J_x > 0$

Properties of Heisenberg ladders; large-scale SSE results

Magnetic susceptibility   Low-T theoretical forms:

Odd L_y: from nonlinear -sigma model

Eggert, Affleck, Takahashi, PRL 73, 332 (1994)

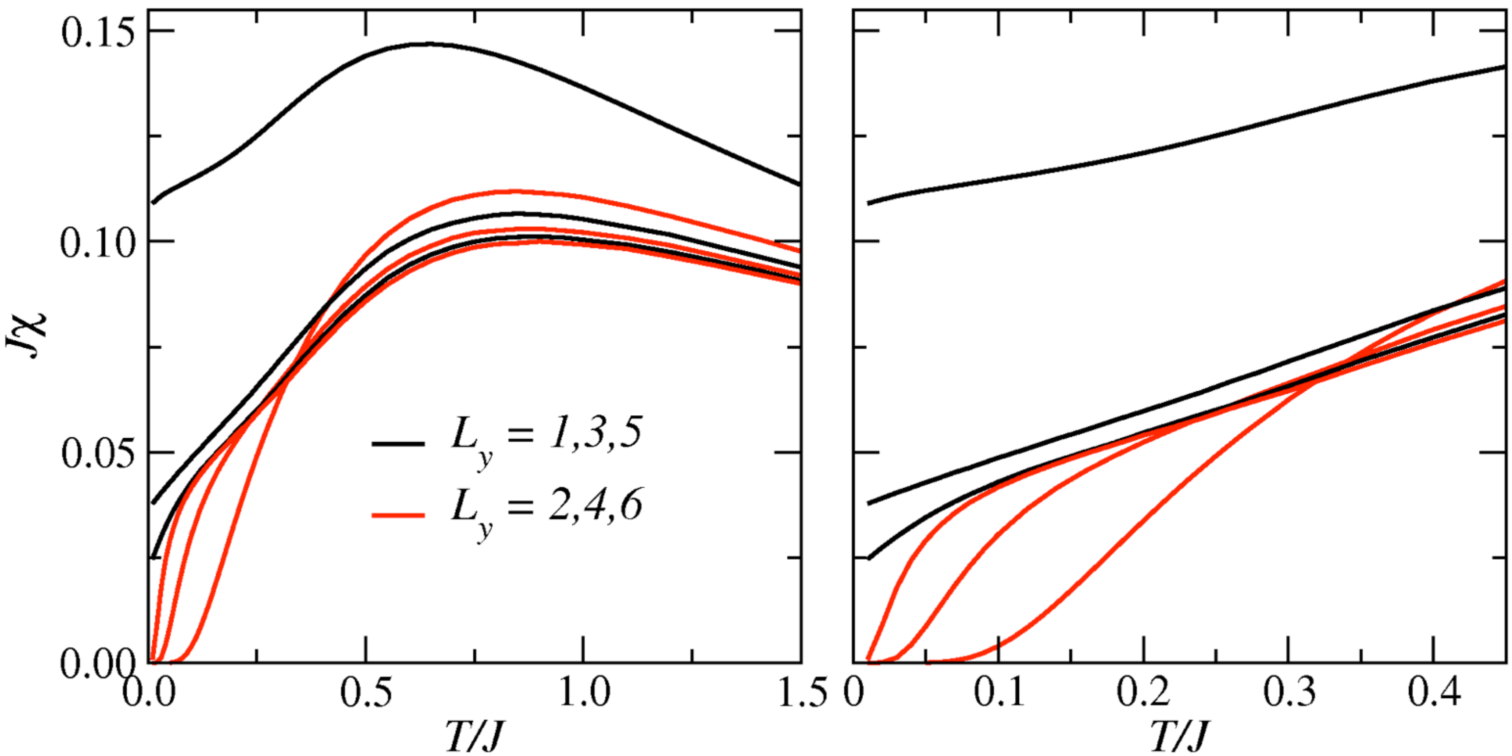
$$\chi(T) = \frac{1}{2\pi c} + \frac{1}{4\pi c \ln(T_0/T)}$$

Even L_y: from large J_y/J_x expansion

Troyer, Tsunetsugu, Wurz, PRB 50, 13515 (1994)

$$\chi(T) = \frac{a}{\sqrt{T}} \mathrm{e}^{-\Delta/T}$$

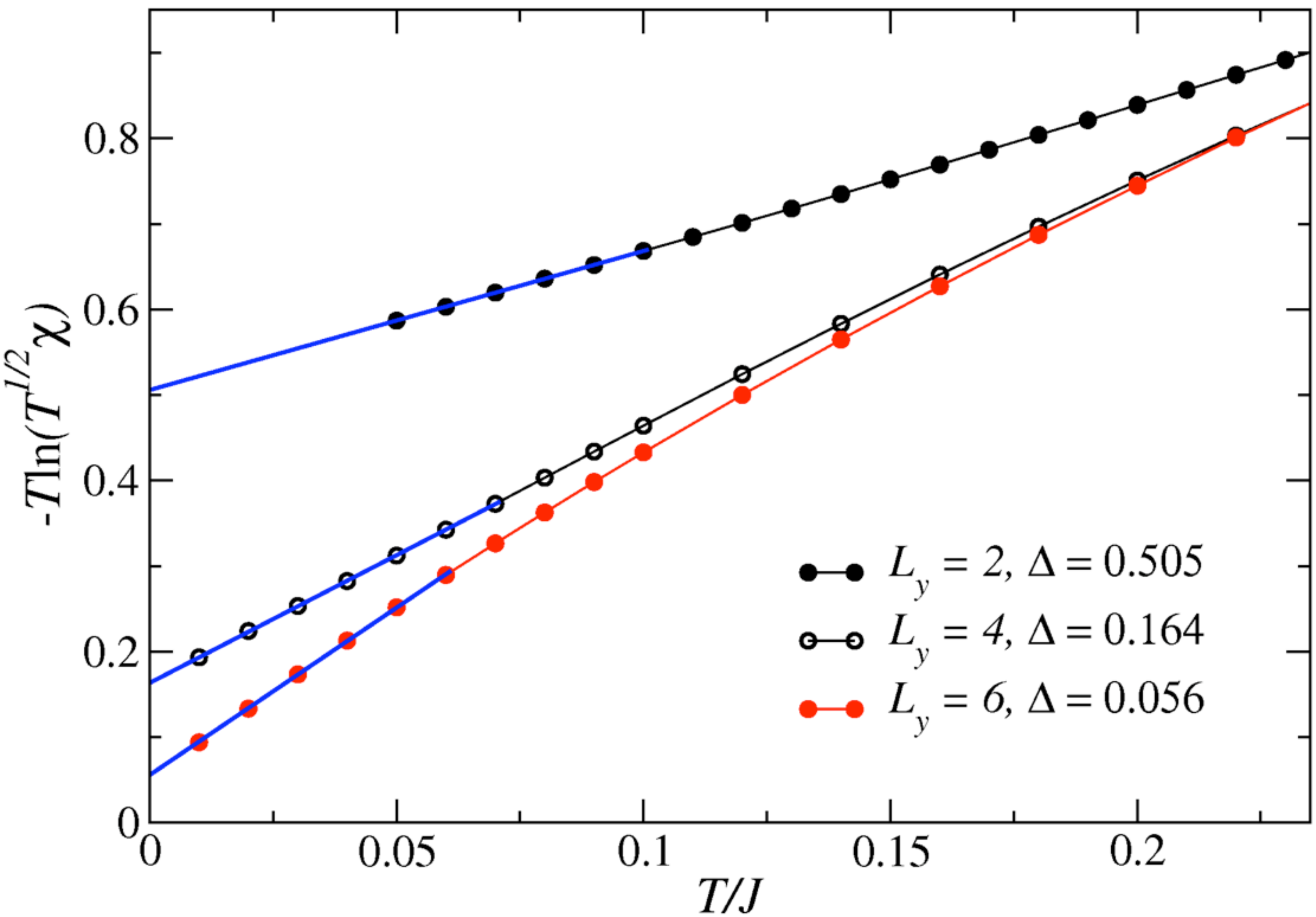
SSE results for large L_x (up to 4096, giving $L_x \to \infty$ limit for T shown);



Extracting the gap for evel-L_y systems

From the low-T susceptibility form:

$$\chi(T) = \frac{a}{\sqrt{T}} \mathrm{e}^{-\Delta/T} \;\Rightarrow\; -T\ln\left(\sqrt{T}\chi\right) = \Delta - T\ln\left(a\right)$$

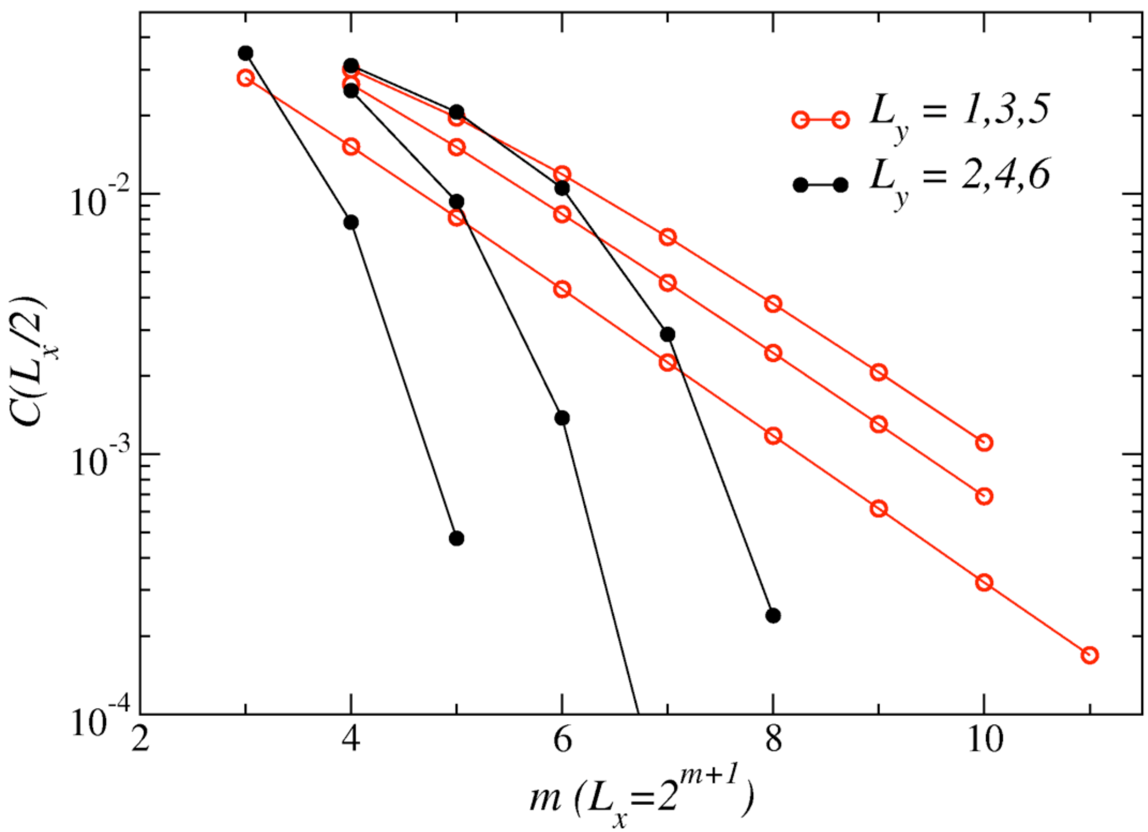


T=0 spin correlations of ladders

Expected **asymptotic** behaviors

$$C(r) = A\frac{(-1)^r}{r}\ln\left(\frac{r}{r_0}\right)^{1/2} \quad \text{(odd } L_y\text{)} \qquad C(r) = Ae^{-r/\xi} \quad \text{(even } L_y\text{)}$$

We also expect short-distance behavior reflecting 2D order for large L_y



short-long distance cross-over behavior starts to become visible, but larger L_y needed to see signs of 2D order for $r<L_y$

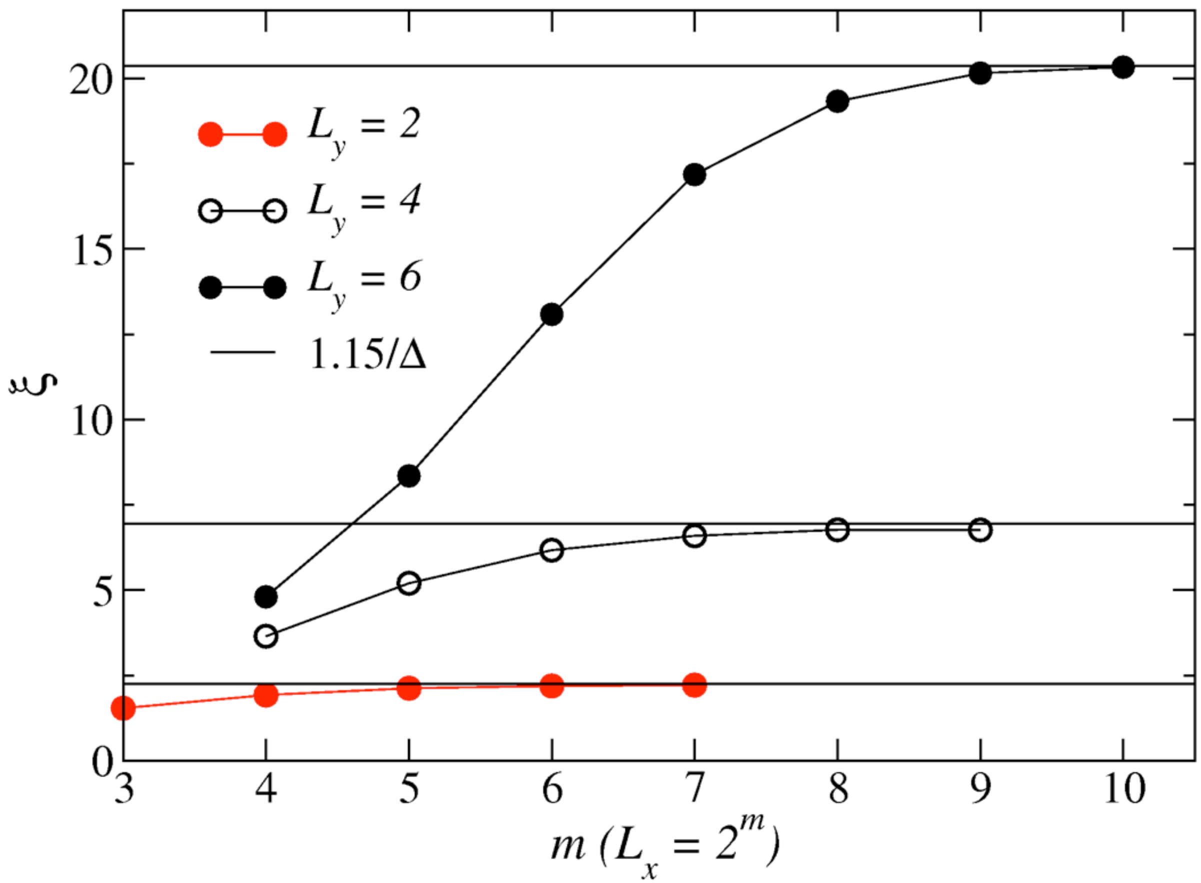
- L×L lattices used to study 2D case

Correlation length for even-L_y

$$C(r) \propto \mathrm{e}^{-r/\xi}, \qquad \xi \propto \frac{1}{\Delta}$$

We need system lengths $L_x >> \xi$ to compute ξ reliably. Use:

$$\xi^2 = \frac{1}{q^2}\left(\frac{S(\pi,\pi)}{S(\pi-q,\pi)} - 1\right)$$



Correlation length versus J_y/J_x for L_y=2

the single chain is critical (1/r correlations) → ξ diverges as J_y/J_x → 0