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Quantum Monte Carlo methods

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Path integrals in quantum statistical mechanics
- example: hard-core bosons (equivalent to S=1/2 spins)
- seriex-expansion formulation

SSE algorithm for the S=1/2 Heisenberg model
- some details needed to make a simple but very efficient program
- essentially lattice-independent (bipartite) formulation

Examples: properties of 1D chains, ladders, and 2D 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 $T \to 0$). How to deal with the exponential operator?

"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

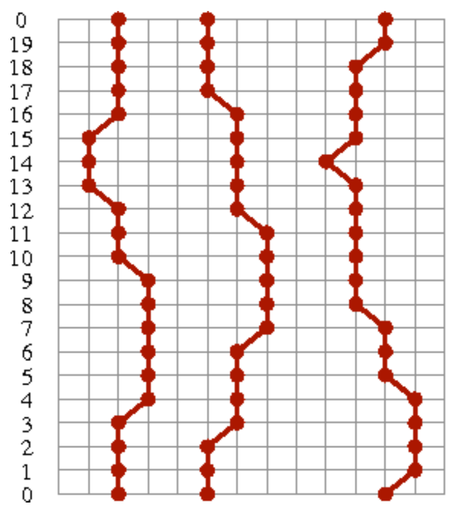
$$H = K = -\sum_{\langle i,j \rangle} K_{ij} = -\sum_{\langle i,j \rangle} (a_j^\dagger a_i + a_i^\dagger a_j) \qquad n_i = a_i^\dagger a_i \in \{0,1\}$$

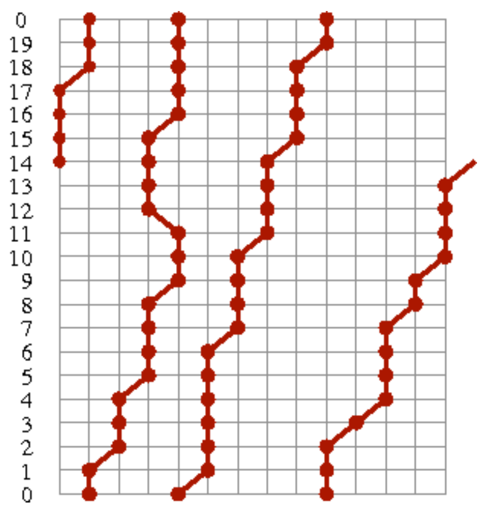
Equivalent to S=1/2 XY model

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

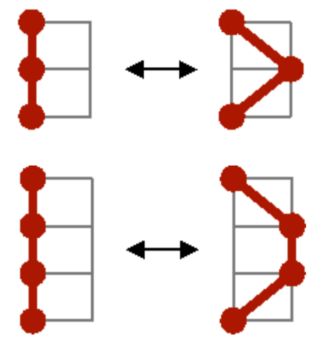
“World line” representation of

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





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

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

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

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

$$\begin{aligned} W(\{\alpha\}) &= \text{weight} \\ A(\{\alpha\}) &= \text{estimator} \end{aligned}$$

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

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

Average over all slices → count number of kinetic jumps

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

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

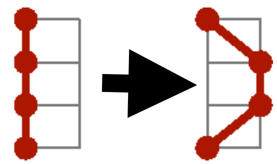
Including interactions

For any diagonal interaction V (Trotter, or split-operator, approximation)

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

Product over all times slices →

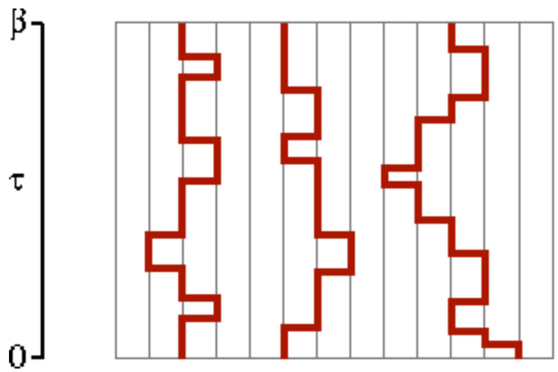
$$W(\{\alpha\}) = \Delta_\tau^{n_K} \exp\left(-\Delta_\tau \sum_{l=0}^{L-1} V_l \right)$$



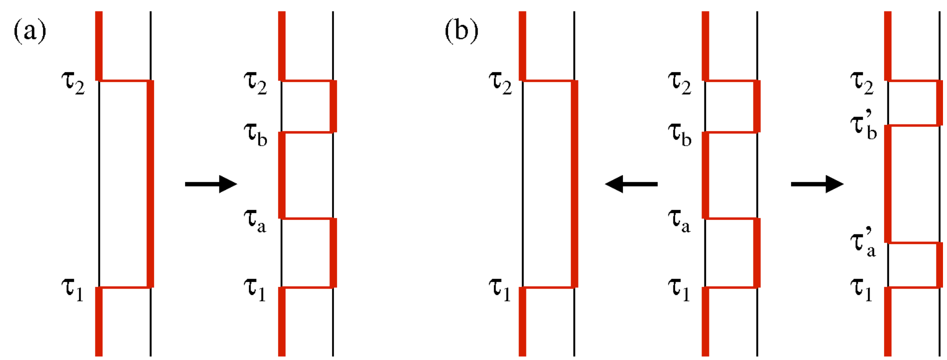
$$P_{\text{acc}} = \min \left[\Delta_\tau^2 \frac{V_{\text{new}}}{V_{\text{old}}}, 1 \right]$$

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 (problem when $\Delta_\tau \to 0$?)

- 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 $e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$ (approximation-free method from the outset)

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

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

this is the operator we "measure"

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

one more "slice" to sum over here

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

relabel terms to "get rid of" extra slice

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

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

Fixed-length scheme

- n fluctuating → varying size of the configurations
- the expansion can be truncated at some $n_{max}=L$ (exponentially small error)
- cutt-off at n=L, fill in operator string with unit operators $H_0=I$

n=10	H_4	H_7	H_1	H_6	H_2	H_1	H_8	H_3	H_3	H_5				
M=14	H_4	I	H_7	I	H_1	H_6	I	H_2	H_1	H_8	H_3	H_3	I	H_5

- conisider all possible locations in the sequence
- overcounting of actual (original) strings, correct by combinatorial factor:

$$\binom{L}{n}^{-1} = \frac{n!(L-n)!}{L!}$$

Here n is the number of H_i, i>0 instances in the sequence of L operators

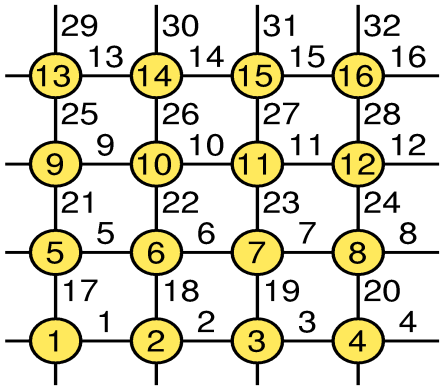
$$Z = \sum_{\{\alpha\}_L} \sum_{\{H_i\}} \frac{(-\beta)^n (L-n)!}{L!} \langle \alpha_0 | H_{i(L)} | \alpha_{L-1} \rangle \cdots \langle \alpha_2 | H_{i(2)} | \alpha_1 \rangle \langle \alpha_1 | H_{i(1)} | \alpha_0 \rangle$$

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

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

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

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

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

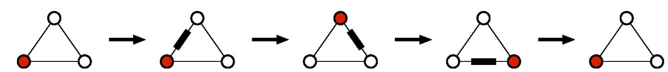
n_2 = number of a(i)=2 (off-diagonal operators) in the sequence

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

For fixed-length scheme

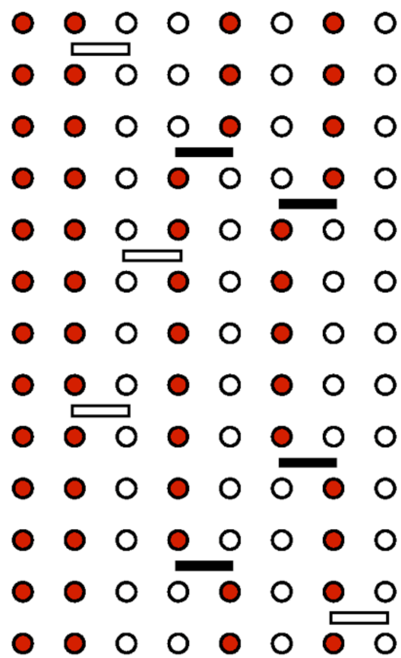
$$Z = \sum_{\alpha} \sum_{S_L} (-1)^{n_2} \frac{\beta^n (L-n)!}{L!} \left\langle \alpha \left| \prod_{p=0}^{L-1} H_{a(p),b(p)} \right| \alpha \right\rangle \qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$$

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



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

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



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

In a program:

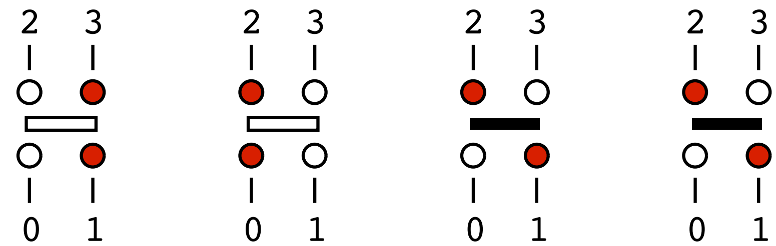
s(p) = operator-index string
- **s(p) = 2*b(p) + a(p)-1**
- diagonal; s(p) = even
- off-diagonal; s(p) = off

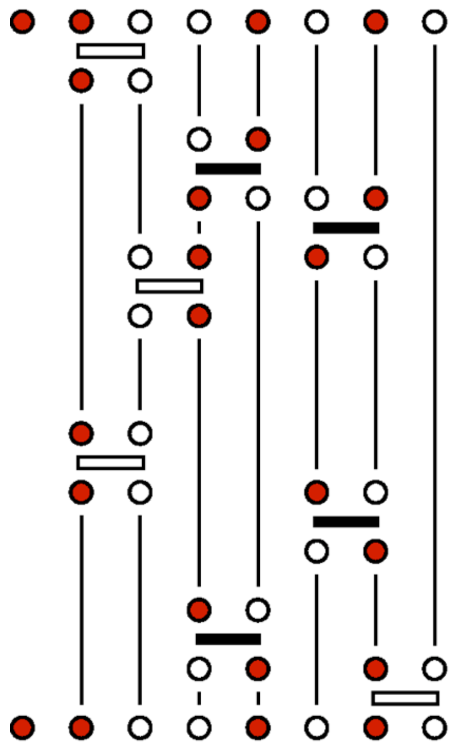
σ(i) = spin state, i=1,...,N
- only one has to be stored

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	X(v)	v	X(v)	v	X(v)	v	X(v)
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	33	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
	$l=0$		$l=1$		$l=2$		$l=3$	

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

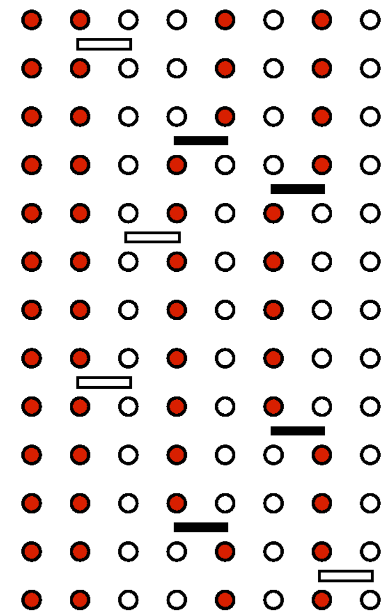
- network of linked vertices will be used for loop updates of vertices/operators

Monte Carlo sampling scheme

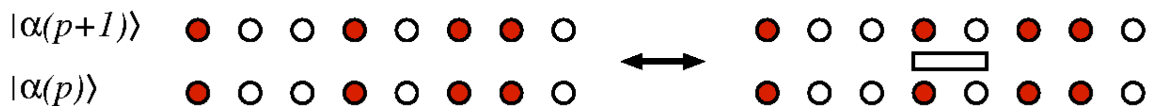
Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

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

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



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

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

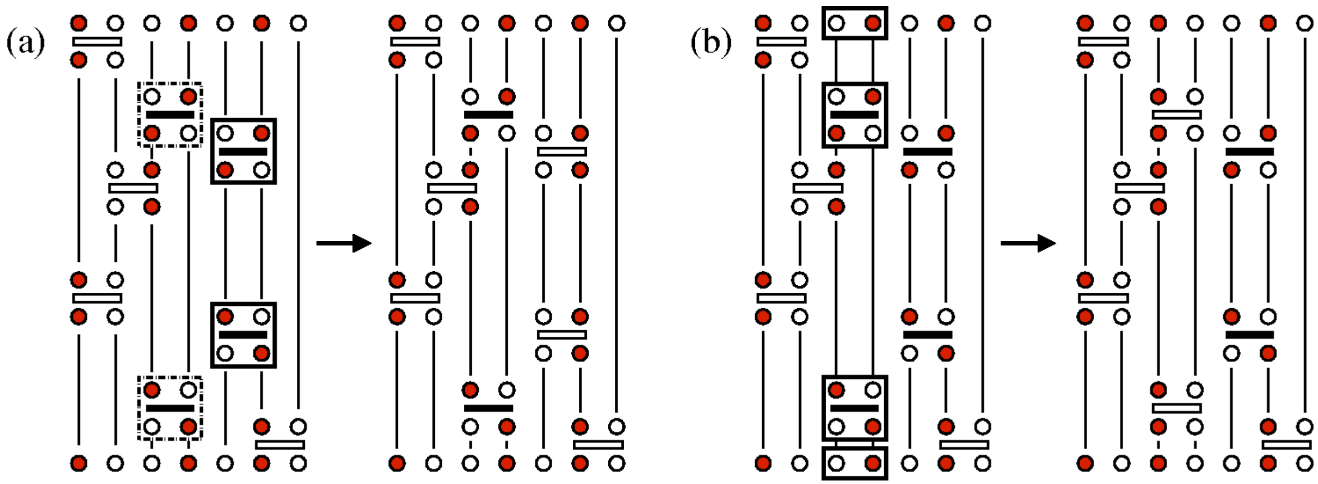
$$P_{\text{accept}}([1,b] \to [0,0]) = \min\left[\frac{2(L-n+1)}{\beta N_b}, 1\right]$$

Diagonal update; pseudocode implementation

$$
\begin{array}{l}
\textbf{do } p = 0 \textbf{ to } L-1 \\
\quad \textbf{if } (s(p)=0) \textbf{ then} \\
\quad\quad b = \textbf{random}[1,\ldots,N_b];\ \textbf{if } \ \sigma(i(b)) = \sigma(j(b)) \textbf{ cycle} \\
\quad\quad \textbf{if } (\textbf{random}[0-1] < P_{\text{insert}}(n)) \textbf{ then } s(p)=2b;\ n=n+1 \textbf{ endif} \\
\quad \textbf{elseif } (\textbf{mod}[s(p),2]=0) \textbf{ then} \\
\quad\quad \textbf{if } (\textbf{random}[0-1] < P_{\text{remove}}(n)) \textbf{ then } s(p)=0;\ n=n-1 \textbf{ endif} \\
\quad \textbf{else} \\
\quad\quad b = s(p)/2;\ \sigma(i(b)) = -\sigma(i(b));\ \sigma(j(b)) = -\sigma(j(b)) \\
\quad \textbf{endif} \\
\textbf{enddo}
\end{array}
$$

i(b),j(b) sites on bond b

Local off-diagonal update

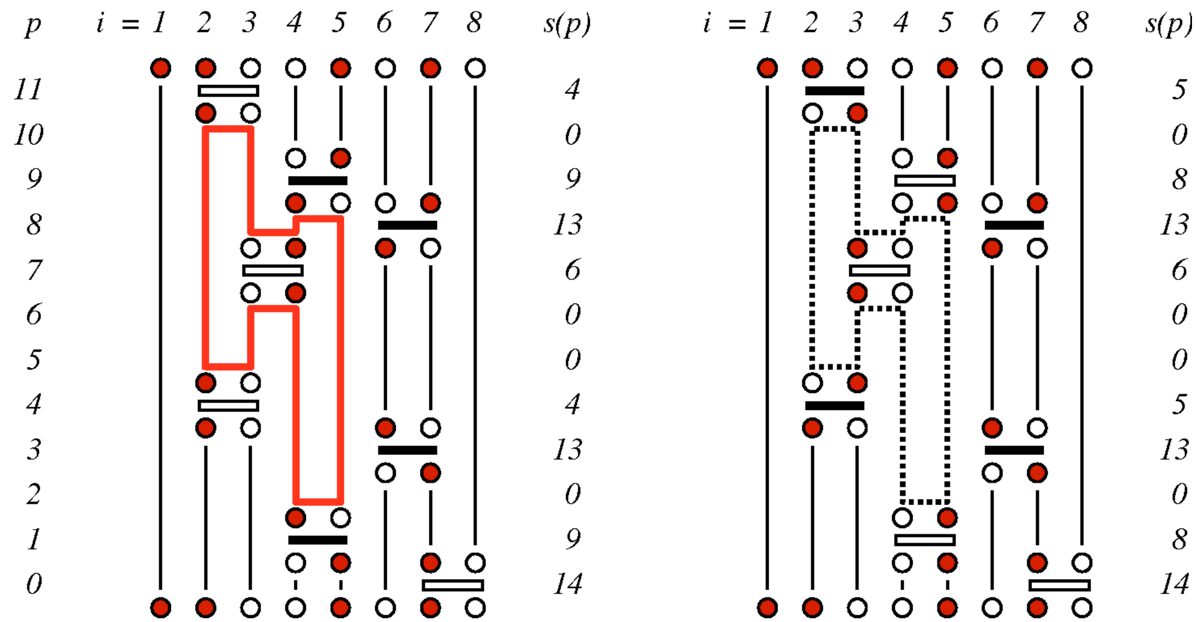


Switch the type (a=1 ↔ a=2) of two operators on the same spins

- 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
```

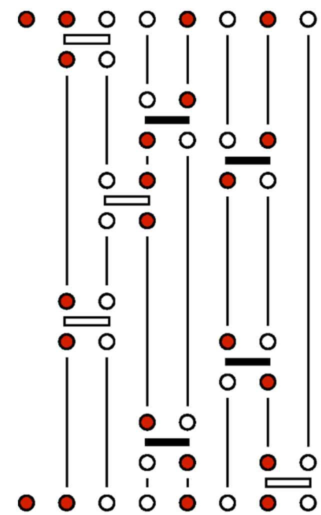
Constructing the linked vertex list

Traverse operator list *s(p)*, *p*=0,...,*L*−1

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

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

- ***V***
- $V_{\text{first}}(i)$ = 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



p	v	X(v)	v	X(v)	v	X(v)	v	X(v)
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	33	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
	l=0		l=1		l=2		l=3	

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

creating the last links across the “time” boundary

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

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

```
do i = 1 to N
    v = V_first(i)
    if (v = -1) then
        if (random[0-1] < 1/2) σ(i) = -σ(i)
    else
        if (X(v) = -2) σ(i) = -σ(i)
    endif
enddo
```

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

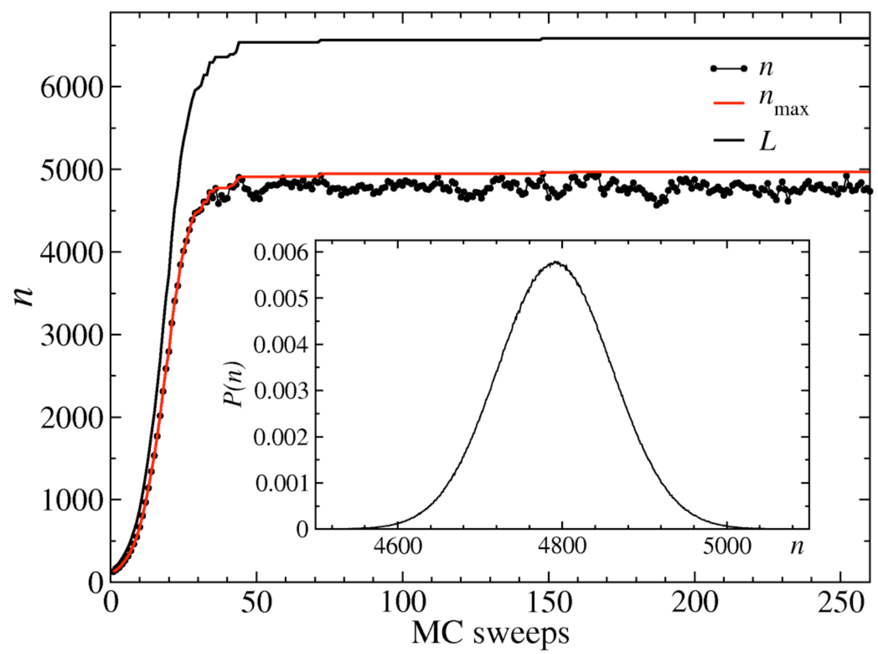
- adjust during equilibration
- start with arbitrary (small) n

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

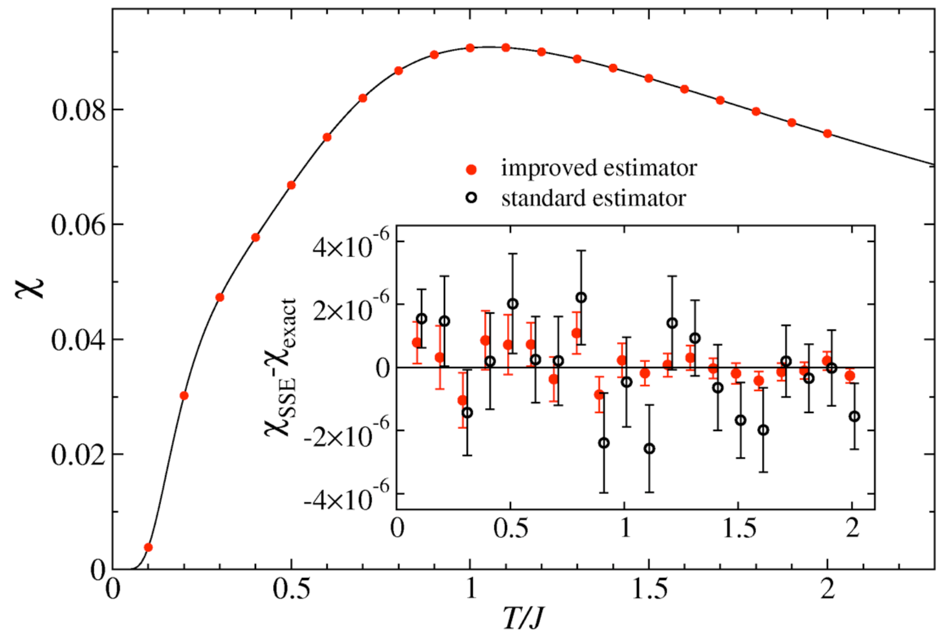


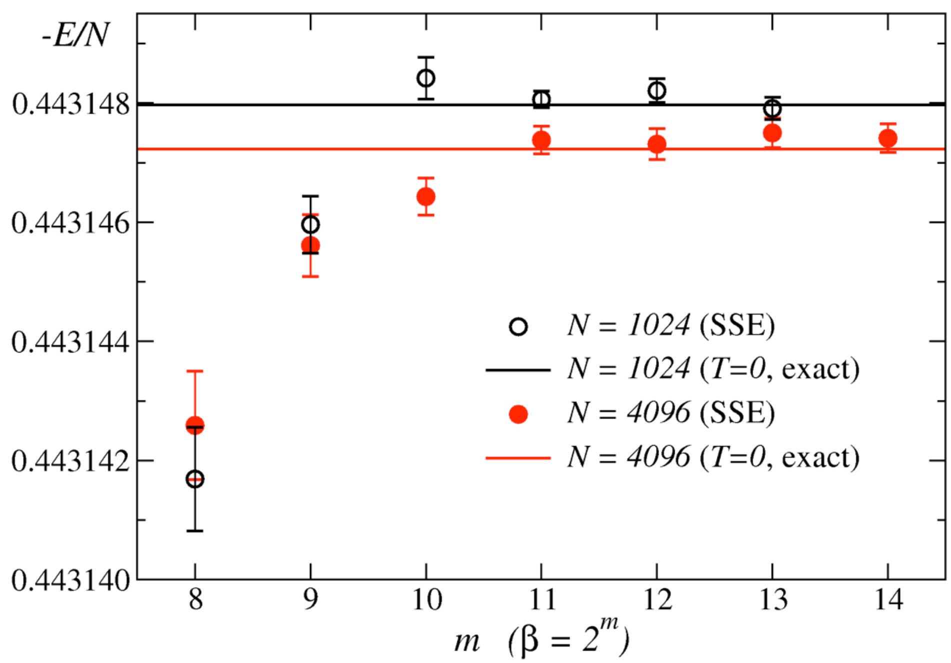
Does it work?
Compare with exact results

- 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)

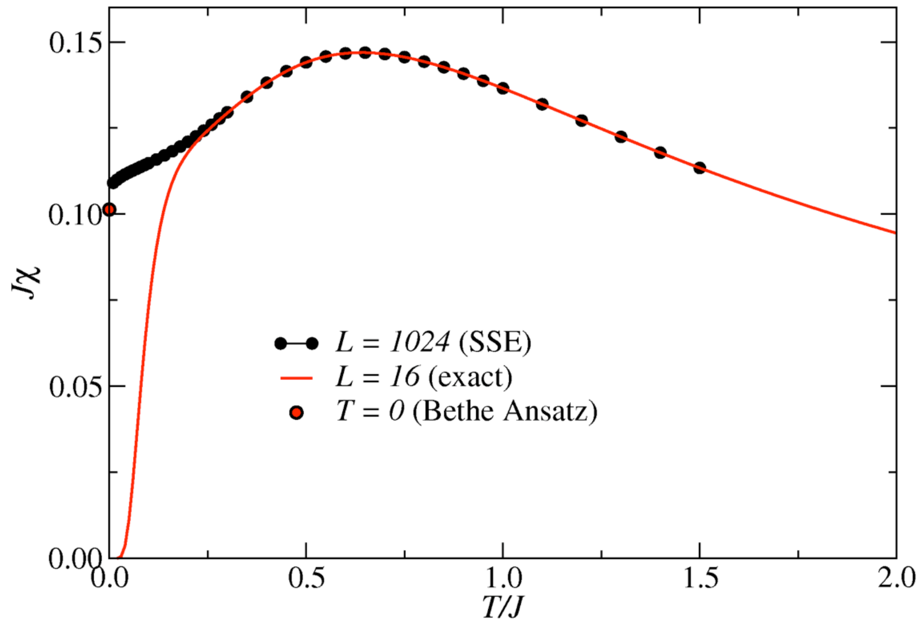


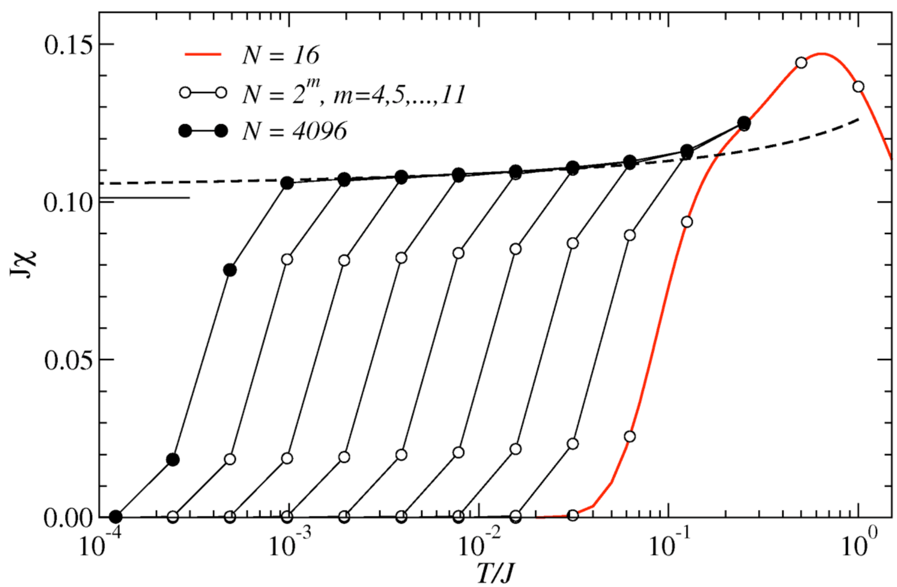


⇐ Energy for long 1D chains

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

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)

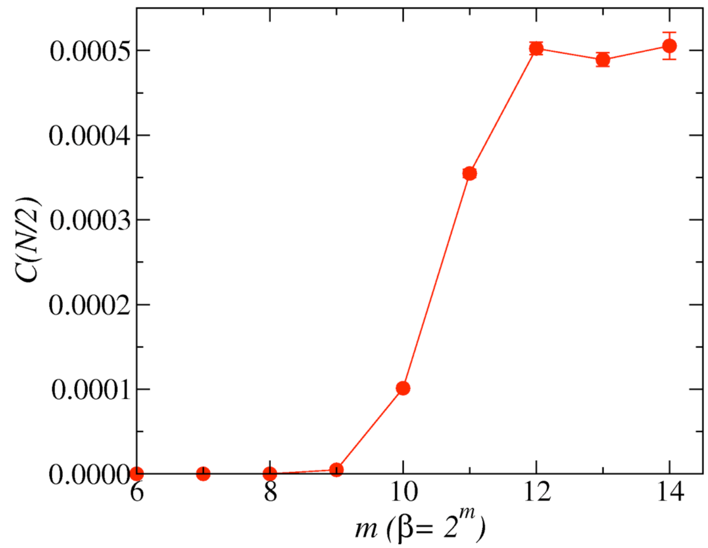
T=0 spin correlations

Low-energy field theory prediction

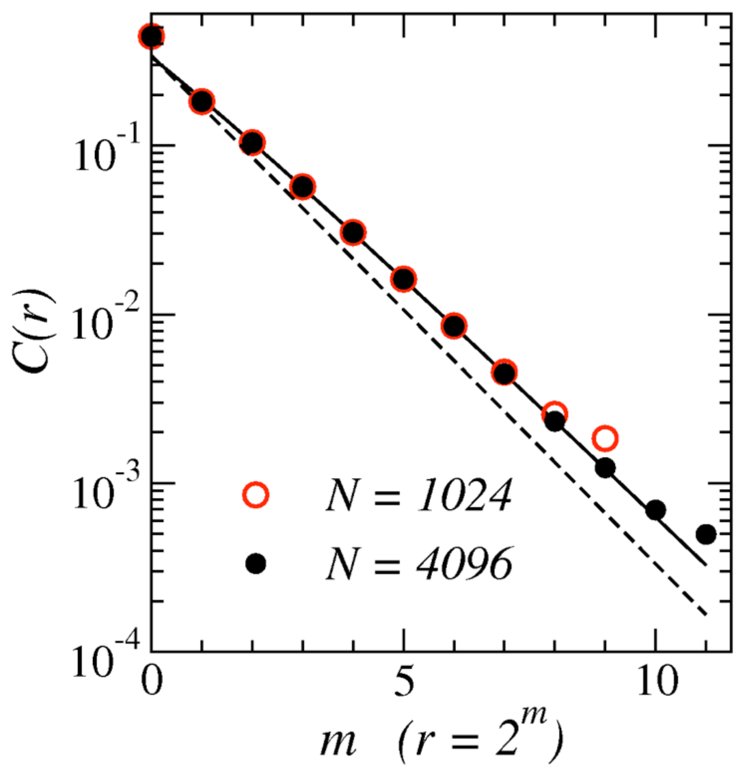
$$C(r) = A\frac{(-1)^r}{r}\ln\left(\frac{r}{r_0}\right)^{1/2}$$

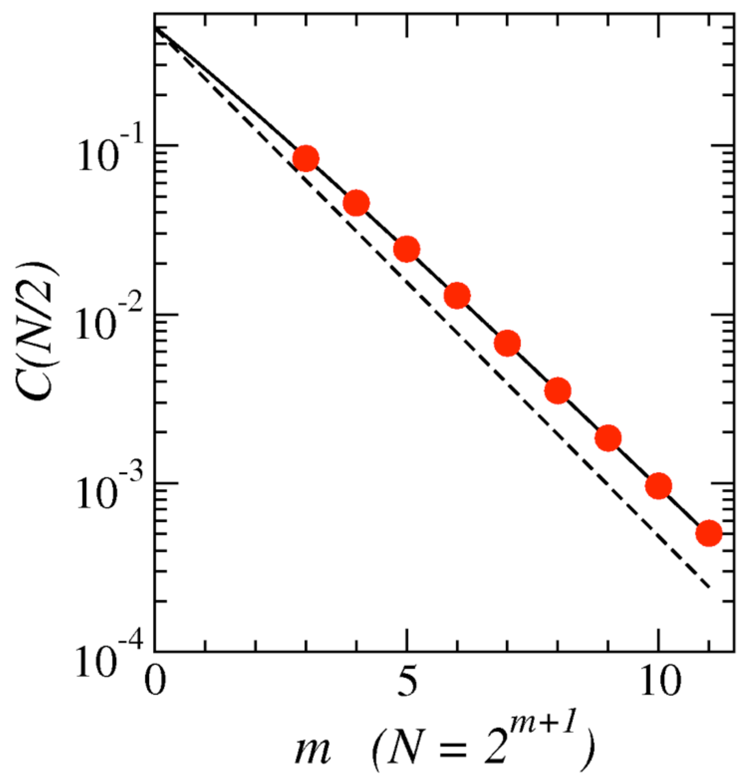
SSE: converge to T=0 limit

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



A=0.21, r_0=0.08





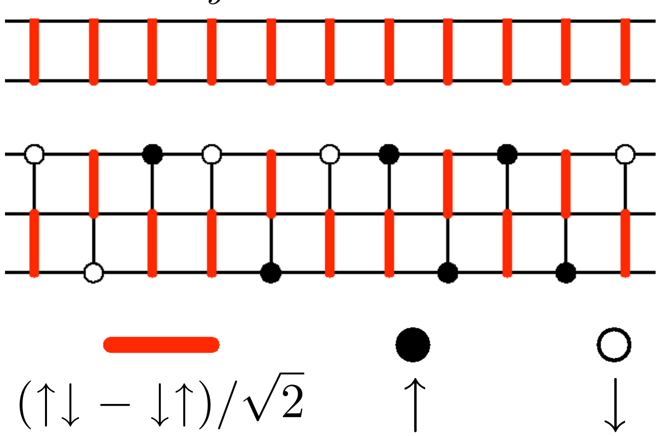
Ladder systems

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

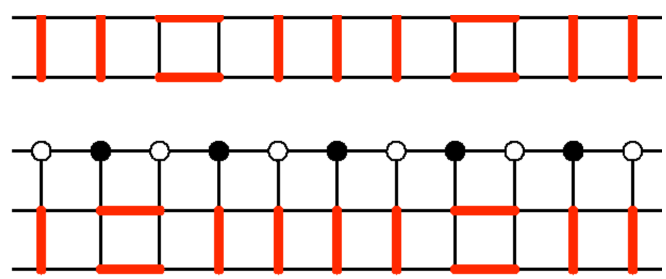
Coupled Heisenberg chains; $L_x \times L_y$ spins, $L_y \to \infty$, L_x finite
- systems with even and odd L_y have qualitatively different properties
  - spin gap $\Delta>0$ for L_y even, $\Delta \to 0$ when $L_x \to \infty$
  - critical state, similar to single chain, for odd L_y
  - the 2D limit 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

$J_y = 1, J_x = 0$



$0 < J_x/J_y \ll 1$



L_y =2,4,... : $\Delta = J_y$ for $J_x=0$
- gap persists for $J_x>0$

L_y =3,5,... : $\Delta=0$ 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)

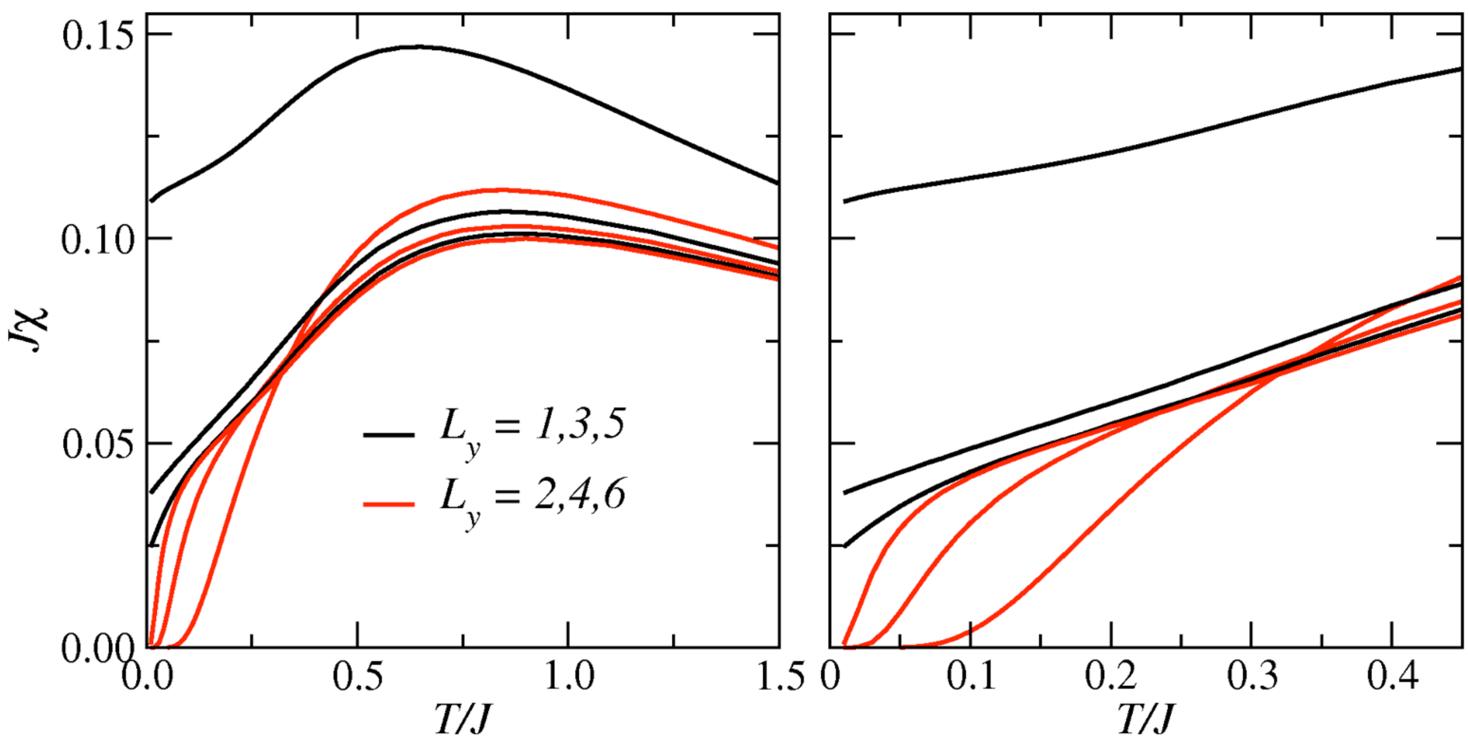
$$\chi(T) = \frac{1}{2\pi c} + \frac{1}{4\pi c \ln(T_0/T)}$$

Even L_y: from large J_y/J_x expansion

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

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

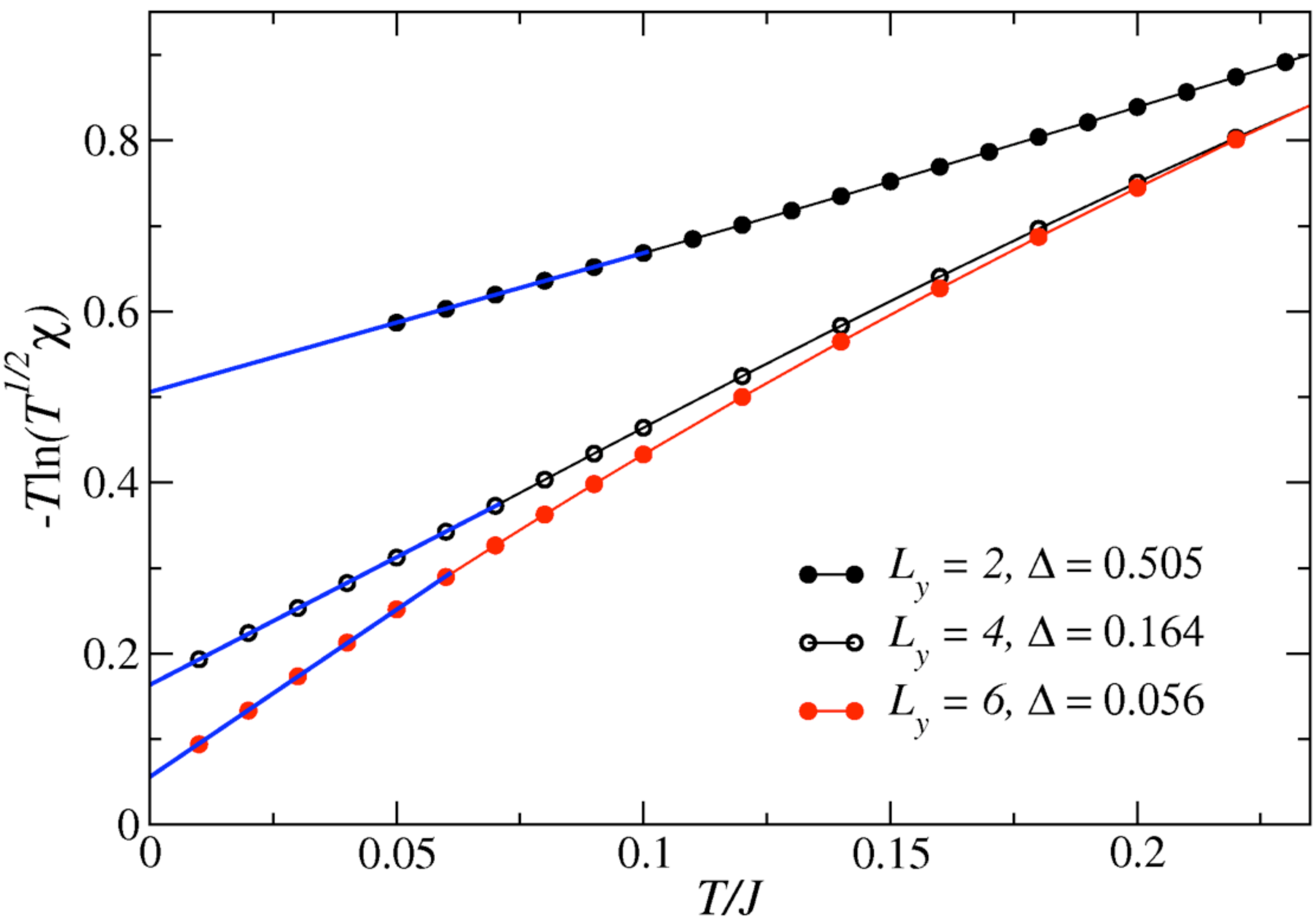
SSE results for large L_x (up to 4096, giving $L_x \to \infty$ limit for T shown);



Extracting the gap for evel-L_y systems

From the low-T susceptibility form:

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

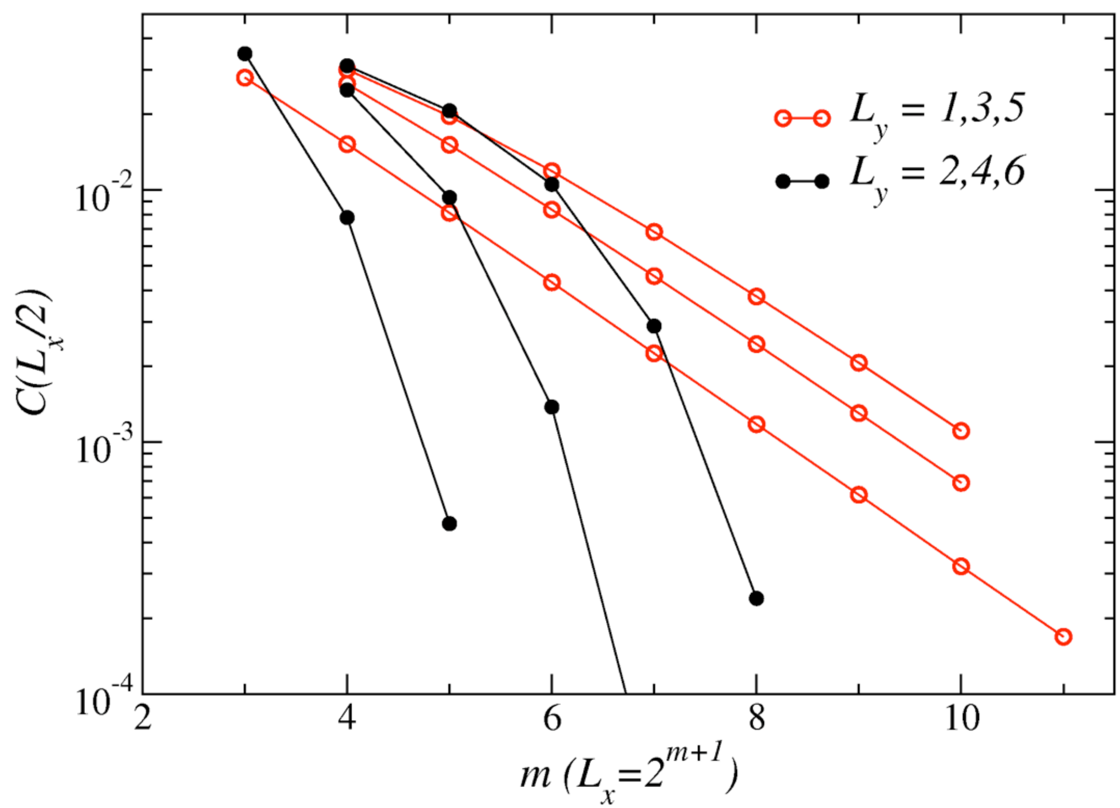


T=0 spin correlations of ladders

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 $r<L_y$

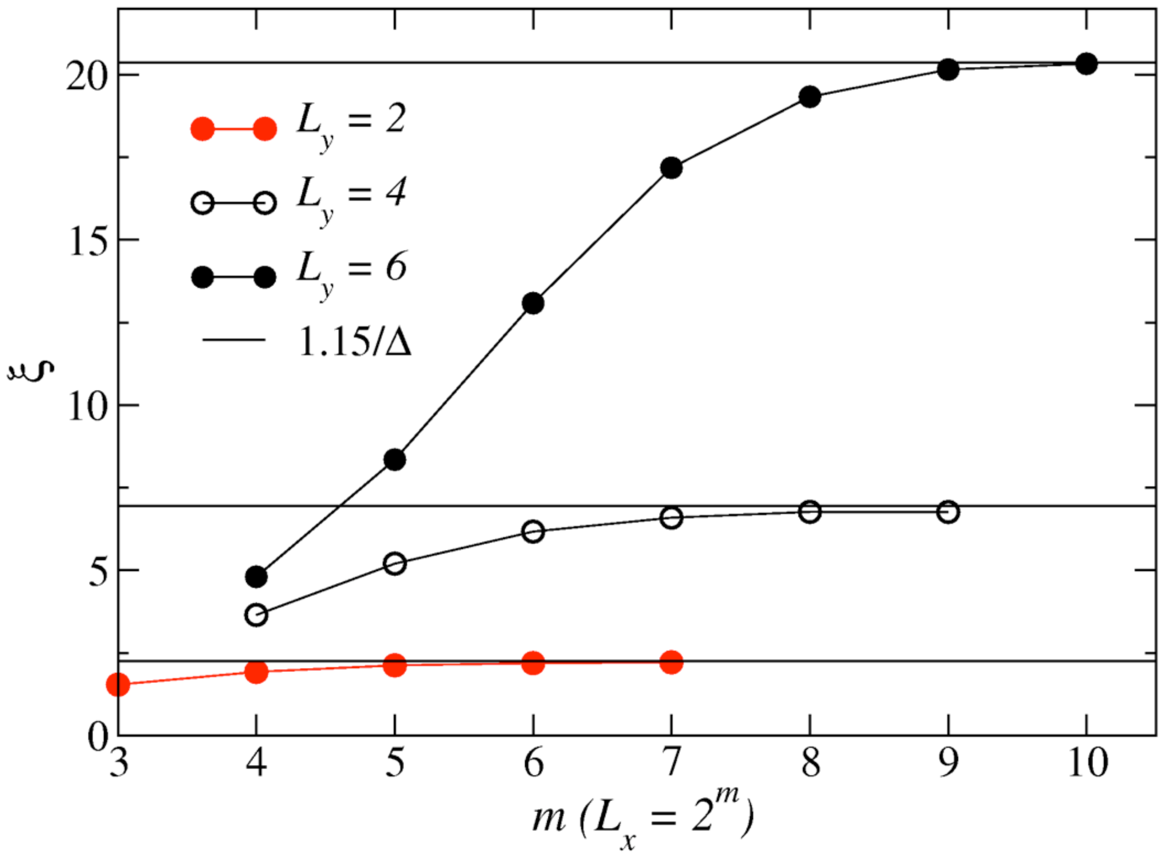
- L×L lattices used to study 2D case

Correlation length for even-L_y

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

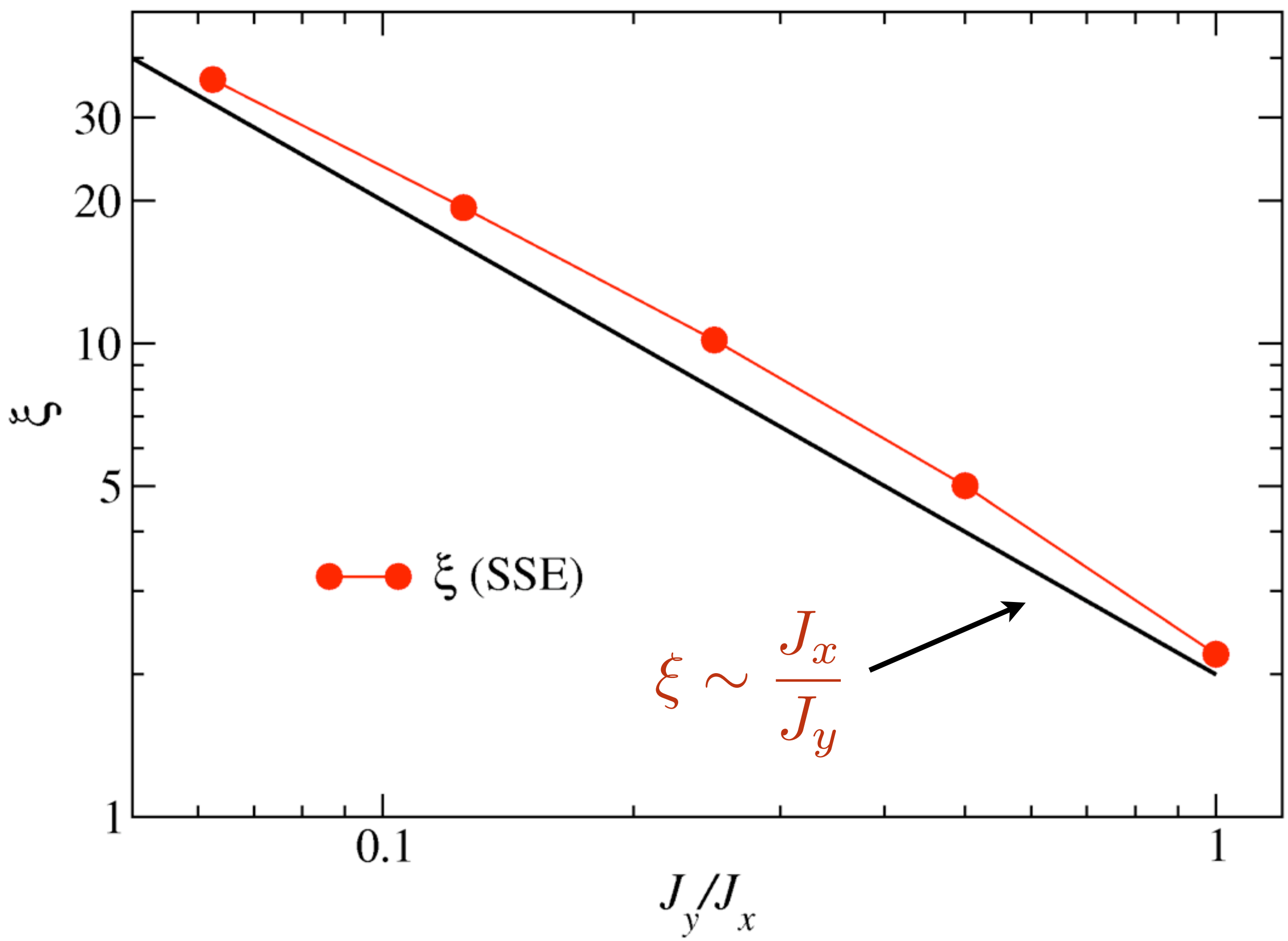
We need system lengths $L_x \gg \xi$ to compute ξ reliably. Use:

$$\xi^2 = \frac{1}{q^2}\left(\frac{S(\pi,\pi)}{S(\pi-q,\pi)} - 1\right) \qquad\qquad S(\mathbf{q}) = \sum_{\mathbf{r}} \mathrm{e}^{-i\mathbf{q}\cdot\mathbf{r}} C(\mathbf{r})$$



Correlation length versus J_y/J_x for L_y=2

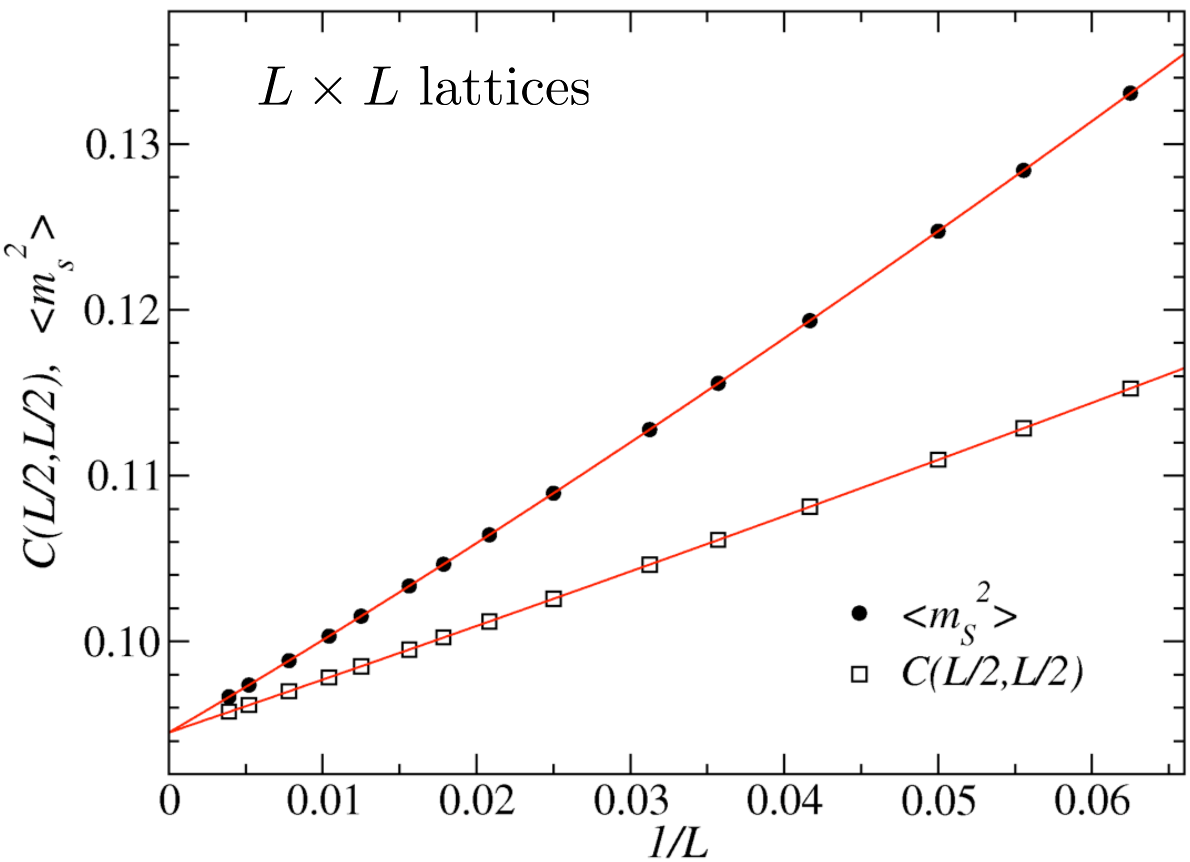
the single chain is critical (1/r correlations) → ξ diverges as J_y/J_x → 0



2D Heisenberg model; long-range order at T=0

Spin-wave theory shows large sublattice magnetization; m_s=0.3034

- including up to $1/S^2$ corrections gives m_s=0.3070
- large-scale QMC (SSE, valence-bond projector) gives m_s=0.3074

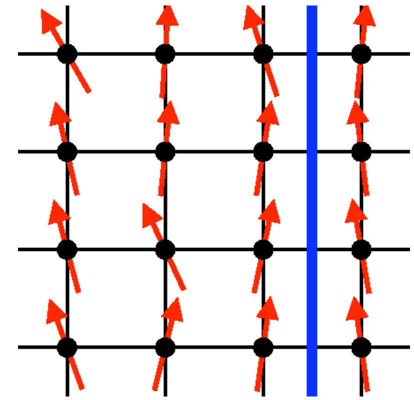


comparing results of

- m_s averaged over all sites (then squared)
- the spin correlation function C(L/2,L/2) at the longest distance

Linear size correction predicted from spin wave theory (and also more general symmetry arguments)

The spin stiffness (helicity modulus)



Corresponds to an Young's modulus of an elastic medium

- an important ground-state parameter of a spin system
- finite for an ordered state
- equivalent to the superfluid stiffness in boson language

Sensitivity of the ground-state energy (free energy at T>0) to "twisting" the spins along a boundary column

$$\rho_s^\gamma = \frac{1}{L}\frac{d^2\langle H(\phi)\rangle}{d\phi^2}, \qquad \phi = \text{"twist" at boundary in } \gamma \text{ direction}$$

Twist imposed by changing the Heisenberg interaction at the boundary

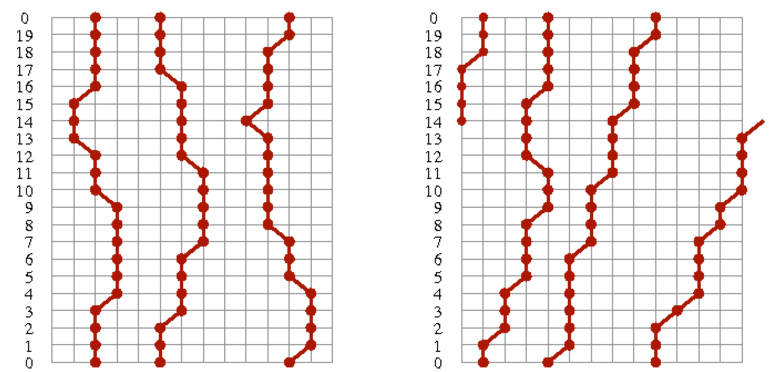
$$\mathbf{S}_i \cdot \mathbf{S}_j \to \mathbf{S}_i \cdot R\mathbf{S}_j, \qquad R = \begin{pmatrix} \cos(\phi) & -\sin(\phi) & 0 \\ \sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

One can show that the
stiffness is related to the winding number fluctuations

$$\rho_s^\gamma = \frac{3}{2}\frac{1}{\beta}\langle W_\gamma^2\rangle, \qquad \gamma = x, y$$

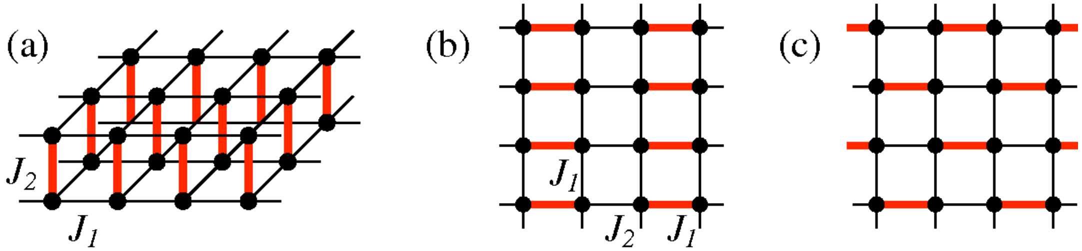
In SSE we have to count spin flip "events"

$$W_\gamma = \frac{1}{L}\sum_{p=0}^{n-1} J_\gamma, \quad J_\gamma = \pm 1 \quad \text{(currents)}$$

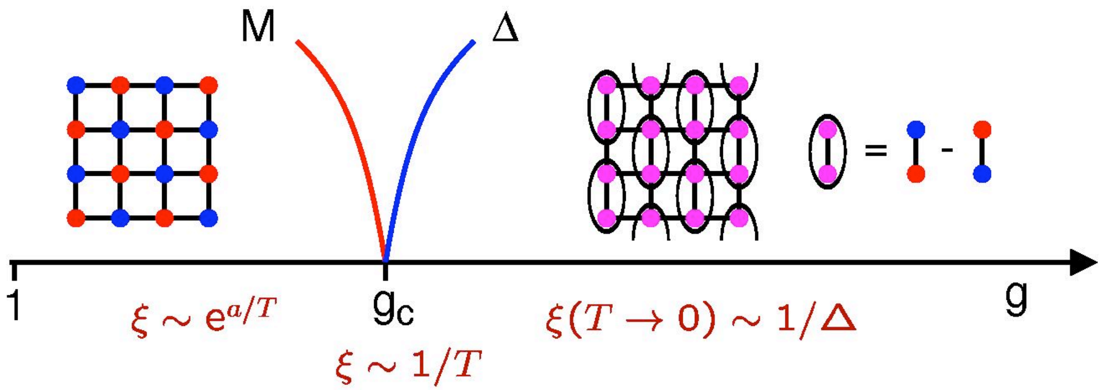


2D quantum-criticality (T=0 transition)

Examples: bilayer, dimerized single layer



Singlet formation on strong bonds ➙ Neel - disordered transition



2D quantum spins map onto (2+1)D classical spins (Haldane)

- Continuum field theory: nonlinear σ-model (Chakravarty, Halperin, Nelson)

⇒3D classical Heisenberg (O3) universality class expected

Dynamic Exponent z

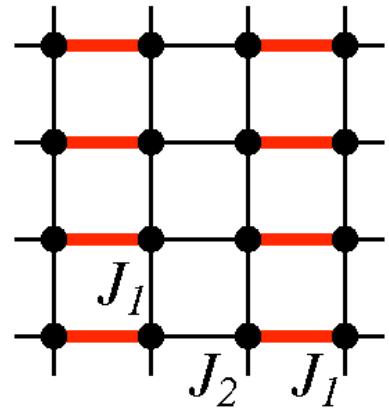
- relates space and time directions
- finite-size gap Δ scales as L^{-z}
- replace classical dimensionality d by d+z in scaling expressions

$$\xi_\tau \sim \xi_r^z, \qquad \Delta \sim L^{-z}$$

Analysis of the transition of dimerized (columnar) Heisenberg system

Two options of choosing the temperature in finite-lattice calculations

- get the ground state as T→0 limit
  - in practice **T<<Δ** (finite-size gap)
- use **1/T=β = aL^z** to analyze the transition
  - if z is known (or to test proposal)
  - the results should not depend on aspect ratio **a**



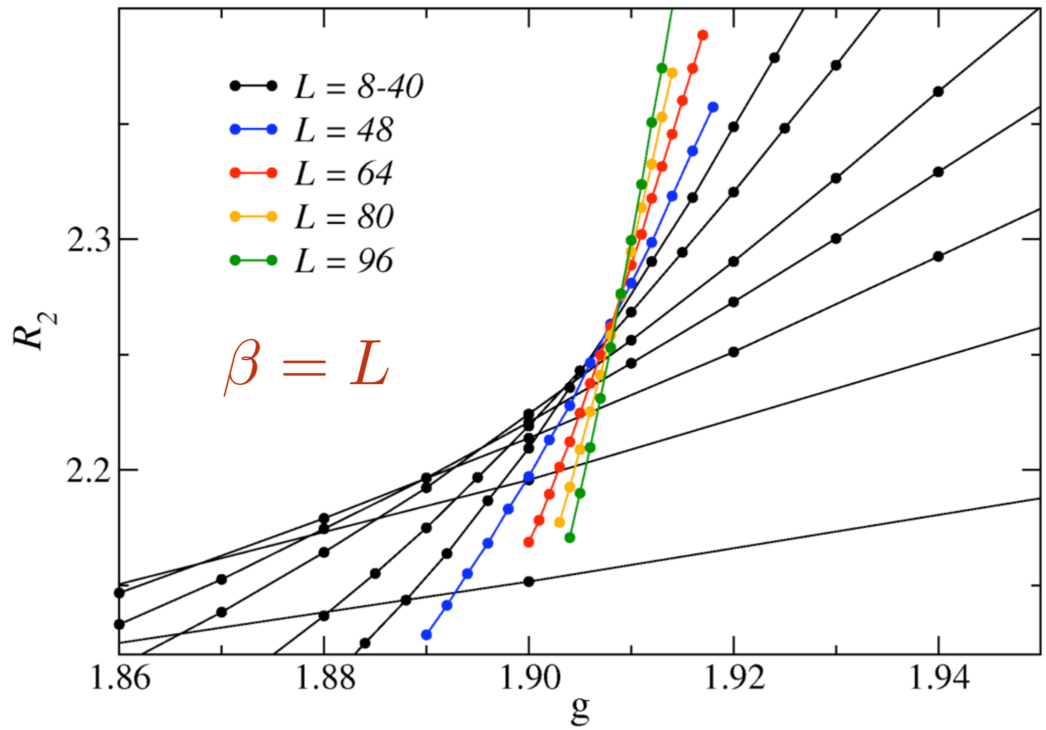
Use the Binder ratio

$$R_2 = \frac{\langle m_{sz}^4 \rangle}{\langle m_{sz}^2 \rangle^2}$$

to locate the critical coupling ratio g_c

Significant drifts in the crossing points, large lattices needed

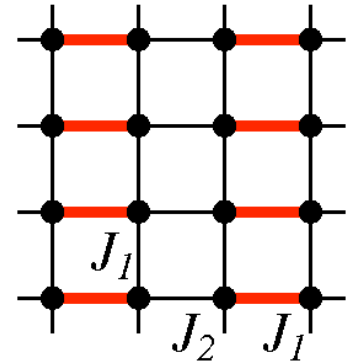
$$g_c \approx 1.91$$



The spin stiffness at criticality

For a quantum-critical point with dynamic exponent z:

$$\rho_s \sim L^{-(d+z-2)}$$



d=2, z=1 → plot $L\rho_s$ vs g for different L

- curves should cross (size independence) at g_c
- x- and y-stiffness different in this model

Finite-size scaling in agreement with z=1, $g_c \approx 1.9094$