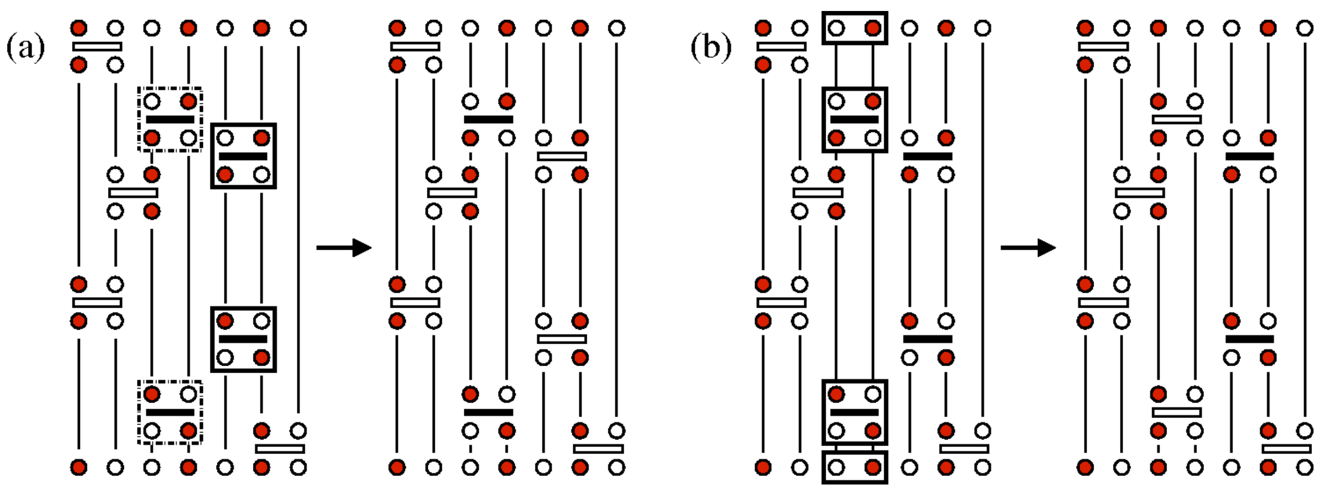
Diagonal update; pseudocode implementation

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

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

Local off-diagonal update

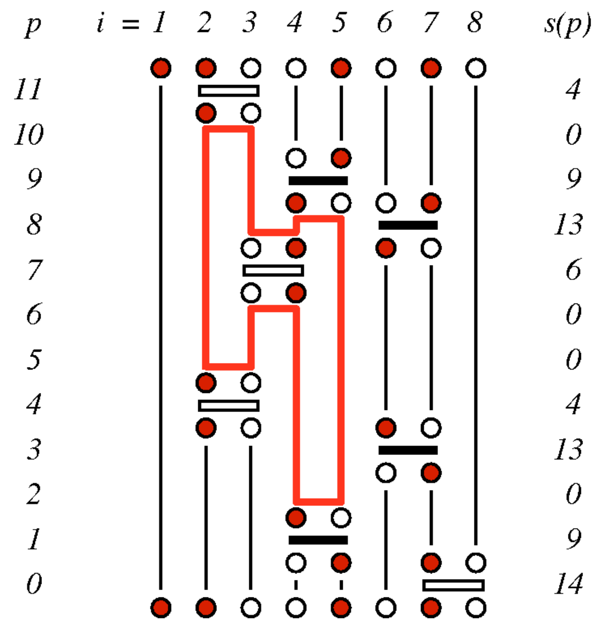


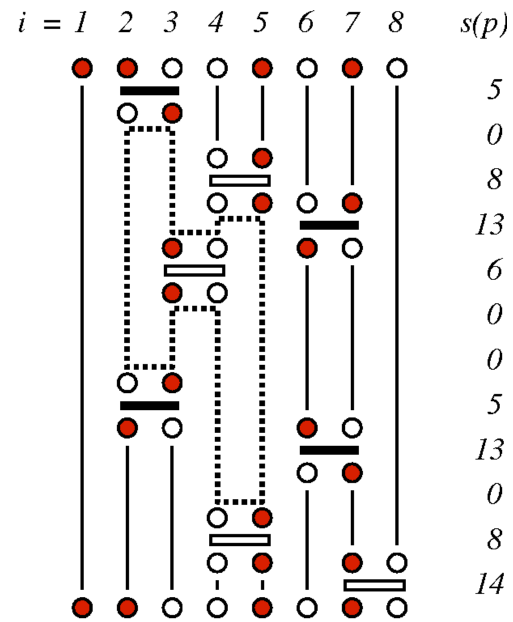
Switch the type (a=1 ↔ a=2) of two operators on the same spins

- 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
```

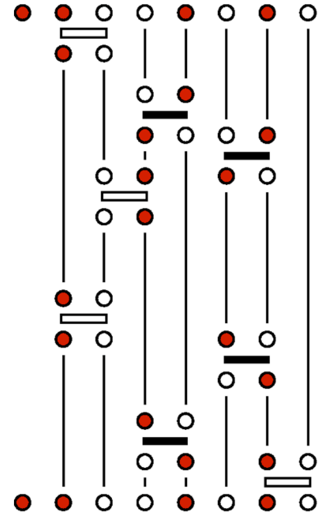
construct and flip a loop

```
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**



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

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

creating the last links across the “time” boundary

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

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

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

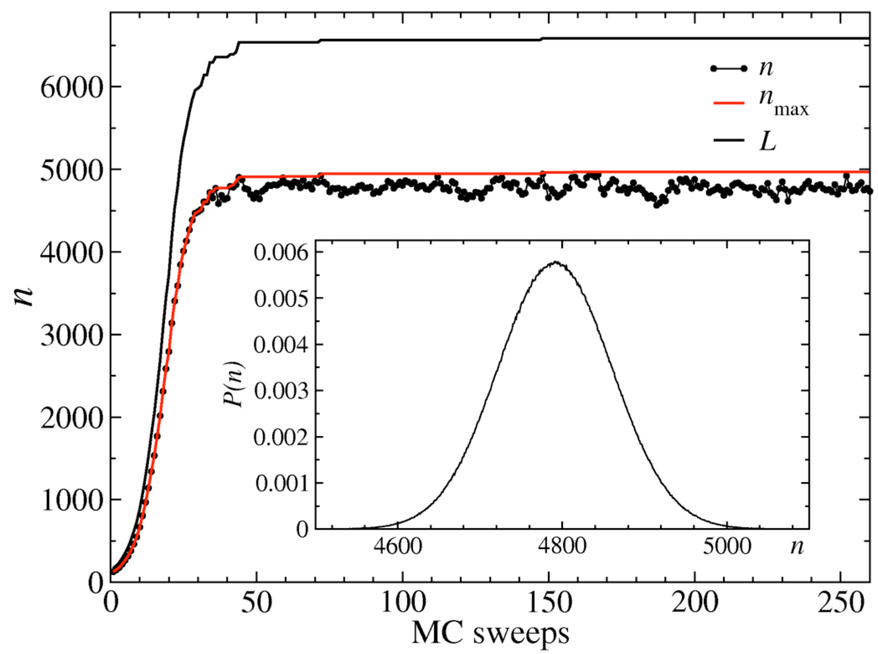
- adjust during equilibration
- start with arbitrary (small) n

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 ⇒

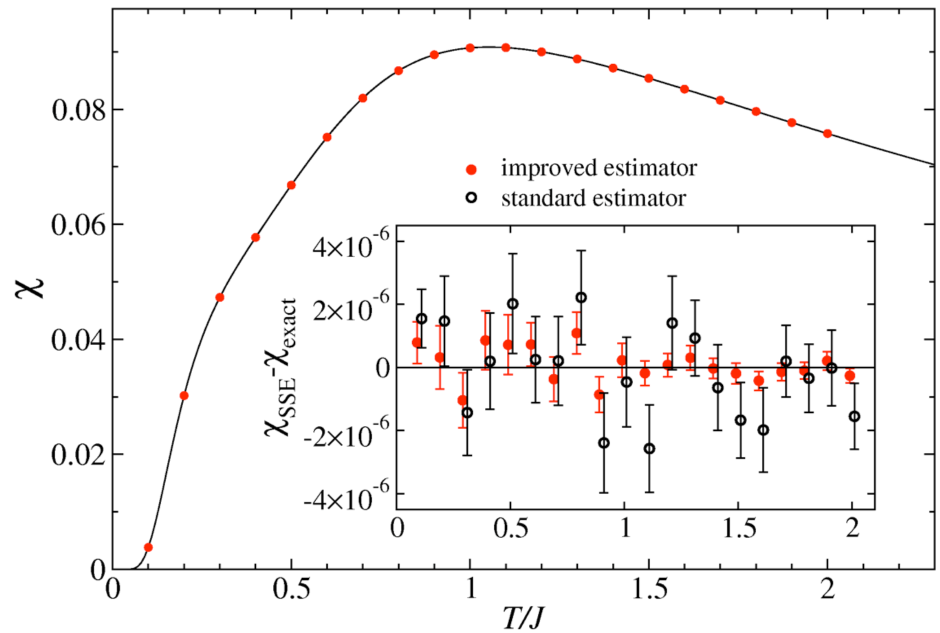
- evolution of L
- n distribution after equilibration
- truncation is no approximation



Does it work?

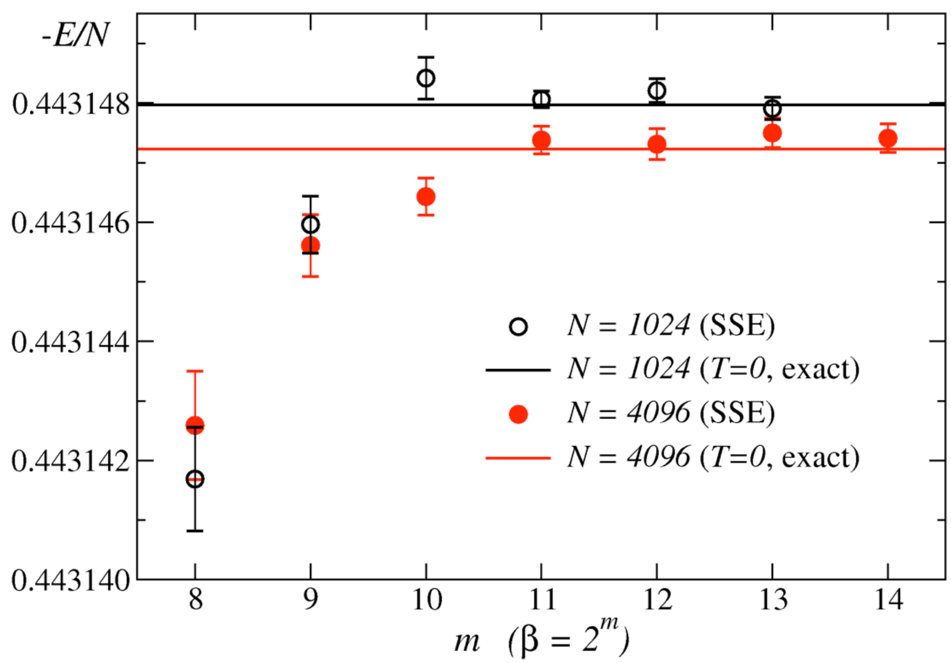
Compare with exact results

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



Susceptibility of the 4×4 lattice ⇒

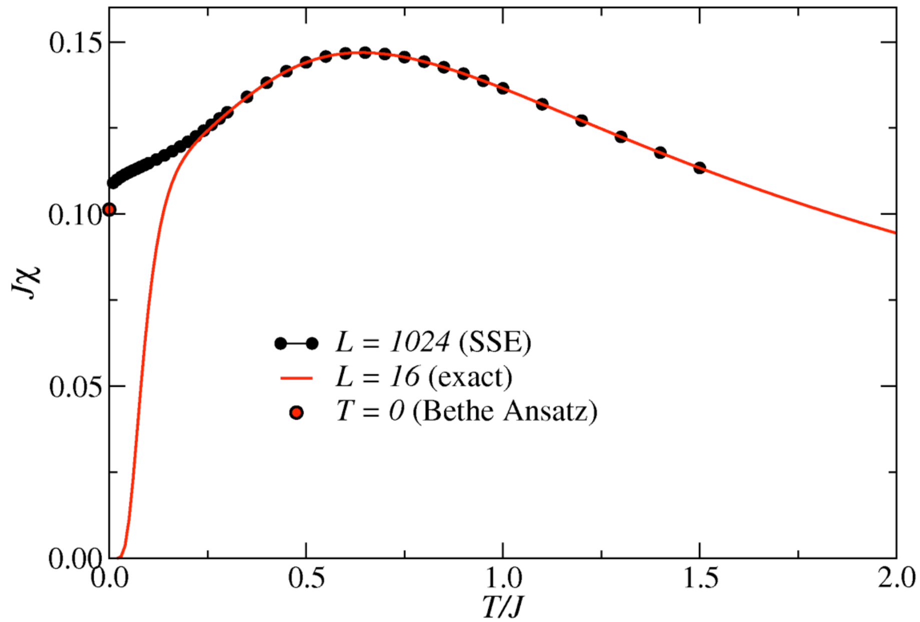
- SSE results from 10^{10} sweeps
- improved estimator gives smaller error bars at high T (where the number of loops is larger)

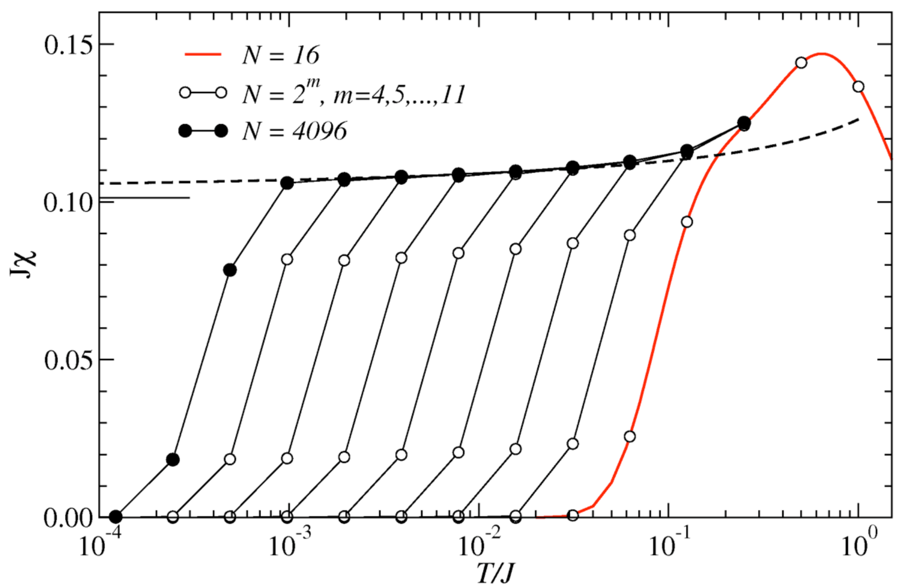


⇐ Energy for long 1D chains

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

Properties of the Heisenberg chain; large-scale SSE results





<u>Magnetic susceptibility</u>

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)

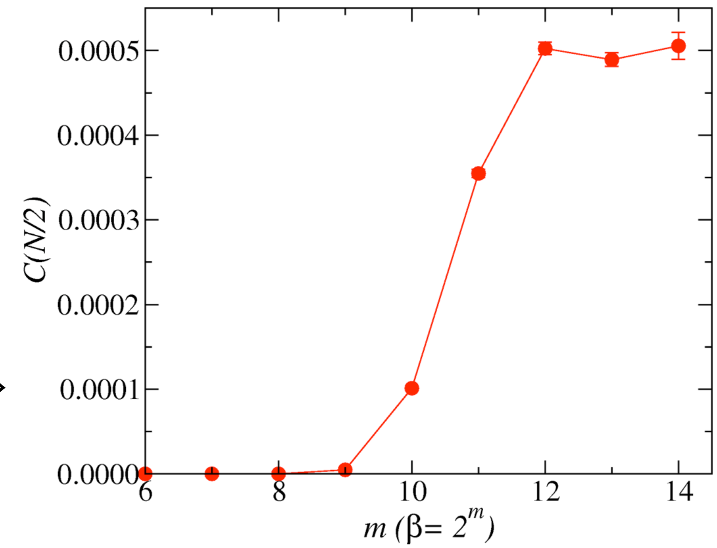
T=0 spin correlations

Low-energy field theory prediction

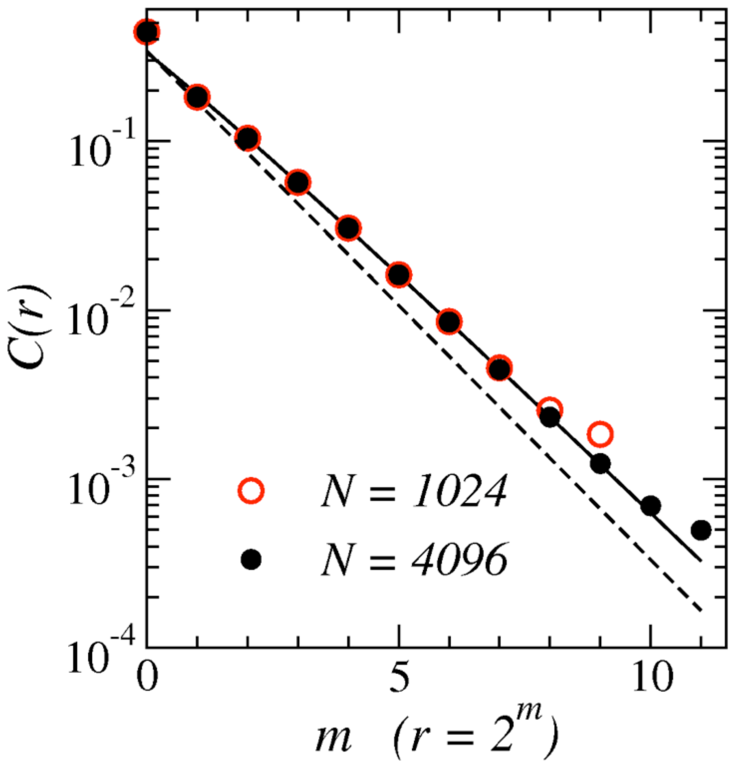
$$C(r) = A\frac{(-1)^r}{r}\ln\left(\frac{r}{r_0}\right)^{1/2}$$

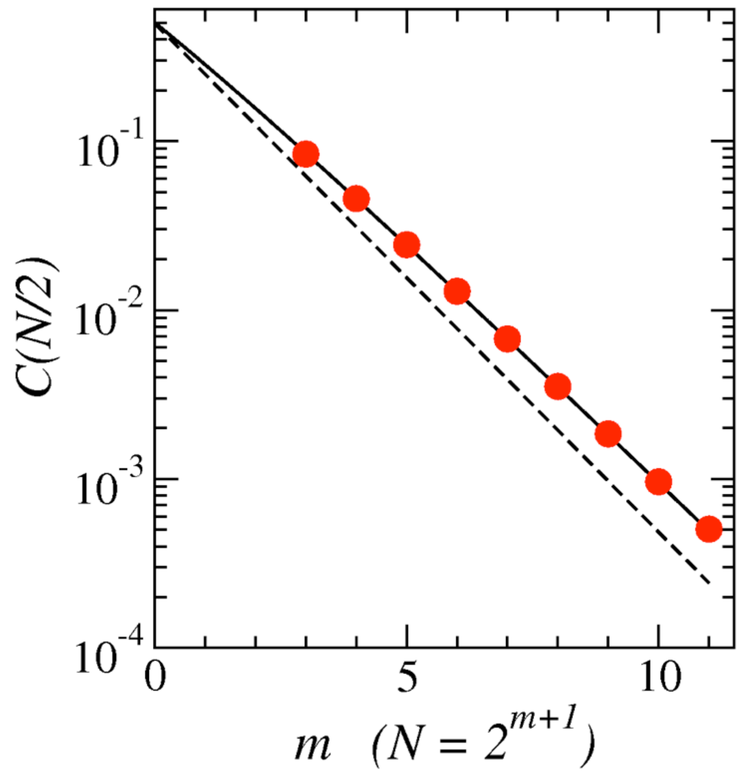
SSE: converge to T=0 limit

- 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)

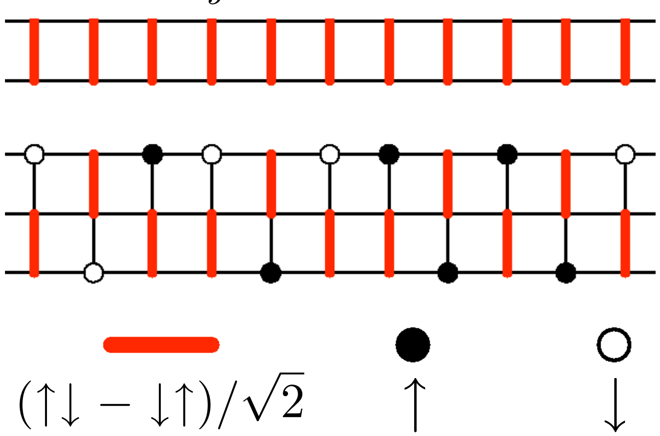
Coupled Heisenberg chains; $L_x \times L_y$ spins, $L_y \to \infty$, L_x finite

- 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

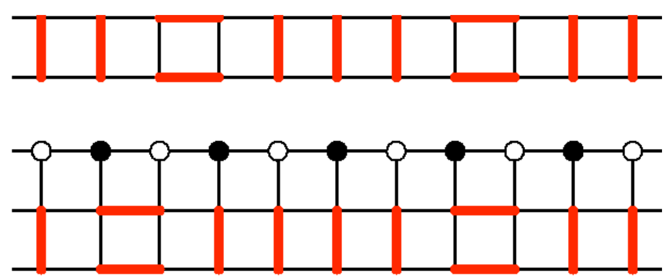
Consider anisotropic couplings; J_x and J_y

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

$J_y = 1, J_x = 0$



$0 < J_x/J_y \ll 1$



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

- gap persists for $J_x > 0$

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

- critical state for $J_x > 0$