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Selected Topics in Computational Quantum Physics

量子物理计算方法选讲

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Quantum Monte Carlo

- classical Monte Carlo

  importance sampling, Markov chain, detailed balance, Metropolis method

- quantum Monte Carlo for spin and bosonic systems

  world line QMC, continuous time limit, Stochastic Series Expansion (SSE)

- quantum Monte Carlo for fermonic systems

selected references:

A. W. Sandvik, arXiv:1101.3281.
http://physics.bu.edu/~sandvik/programs/ssebasic/ssebasic.html
http://physics.bu.edu/~sandvik/perimeter/programs/sse/index.html

Path integrals in quantum statistical mechanics

- we want to compute a thermal expectation value

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

where $\beta = 1/T$ and possibly $T \to 0$

- time slicing of the partition function

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

choose a basis and insert complete sets of states

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

- use approximation for imaginary time evolution operator

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

leads to error $\propto \Delta_\tau$, limit $\Delta_\tau \to 0$ can be taken

- we can compute the weights for the different time periodic paths

$$\alpha_0 \to \alpha_1 \to \cdots \to \alpha_{L-1} \to \alpha_0$$

these paths are importance sampled according to their weight

Boson path integral and world lines

- we consider the purely kinetic energy Hamiltonian for hard-core bosons

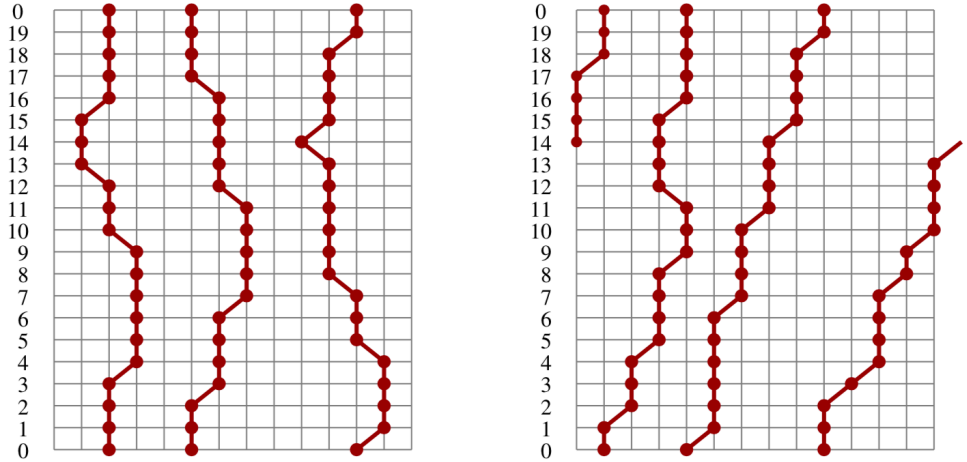
$$H = K = -\sum_{\langle i,j\rangle} K_{i,j} = -\sum_{\langle i,j\rangle} \left(a_i^\dagger a_j + a_j^\dagger a_i \right) \qquad n_i = a_i^\dagger a_i \in \{0,1\}$$

it is equivalent to $S = 1/2$ XY model

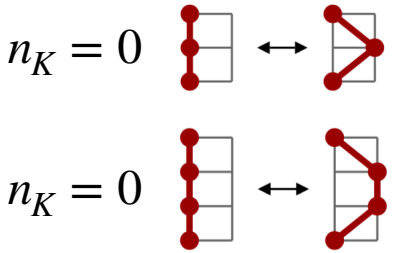
$$H = -2\sum_{\langle i,j\rangle} \left(S_i^x S_j^x + S_i^y S_j^y \right) = -\sum_{\langle i,j\rangle} \left(S_i^+ S_j^- + S_i^- S_j^+ \right) \qquad S^z = \pm\frac{1}{2} \sim n_i = 0,1$$

- 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



- the term $\langle \alpha_{l+1} | \, 1 + \Delta_\tau K_{ij} \, | \alpha_l \rangle$ is either $|\alpha_{l+1}\rangle = |\alpha_l\rangle$ or $|\alpha_{l+1}\rangle = \Delta_\tau K_{ij} |\alpha_l\rangle$

we have $Z = \sum_{\{\alpha\}} (\Delta_\tau)^{n_K} = \sum_{\{\alpha\}} W(\{\alpha\})$

Expectation values

- the expectation value of the operator O is

$$\langle O\rangle = \frac{1}{Z}\mathrm{Tr}\left\{Oe^{-\beta H}\right\} = \frac{1}{Z}\sum_{\{\alpha\}}\langle\alpha_0|\, e^{-\Delta_\tau H}\,|\alpha_{L-1}\rangle\cdots\langle\alpha_2|\, e^{-\Delta_\tau H}\,|\alpha_1\rangle\,\langle\alpha_1|\, e^{-\Delta_\tau H}O\,|\alpha_0\rangle$$

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

$$\langle O\rangle = \frac{\sum_{\{\alpha\}} O\left(\{\alpha\}\right) W\left(\{\alpha\}\right)}{\sum_{\{\alpha\}} W\left(\{\alpha\}\right)} \rightarrow \langle O\rangle = \langle O\left(\{\alpha\}\right)\rangle_W$$

where $W\left(\{\alpha\}\right)$ = weight, and $O\left(\{\alpha\}\right)$ = estimator

- the estimator for a specific kinetic operator $K_{i,j}$, using $Ke^{-\Delta_\tau K} \simeq K$

$$K_{i,j}\left(\{\alpha\}\right) = \frac{\langle\alpha_1|\, K_{i,j}\,|\alpha_0\rangle}{\langle\alpha_1|\, 1-\Delta_\tau K\,|\alpha_0\rangle} = \begin{cases} 0 & \text{no jump} \\ \frac{1}{\Delta_\tau} = \frac{L}{\beta} & \text{jump between } i \text{ and } j \end{cases}$$

average over all slices → count number of kinetic jumps

$$\langle K_{i,j}\rangle = \langle n_{i,j}\rangle/\beta \qquad \langle K\rangle = -\langle n_K\rangle/\beta \qquad \langle n_K\rangle = -\langle K\rangle\beta \sim N\beta$$

there should be of the order $N\beta$ jumps

- diagonal operators, O can be inserted anywhere in the time slice

$$O\,|\alpha_l\rangle = O\left(\alpha_l\right)|\alpha_l\rangle$$

one can average over all time slices $O\left(\{\alpha\}\right) = \frac{1}{L}\sum_{l=0}^{L-1} O\left(\alpha_l\right)$

Including interactions

- for any diagonal interaction V

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

product over all time slices

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

Continuous time limit

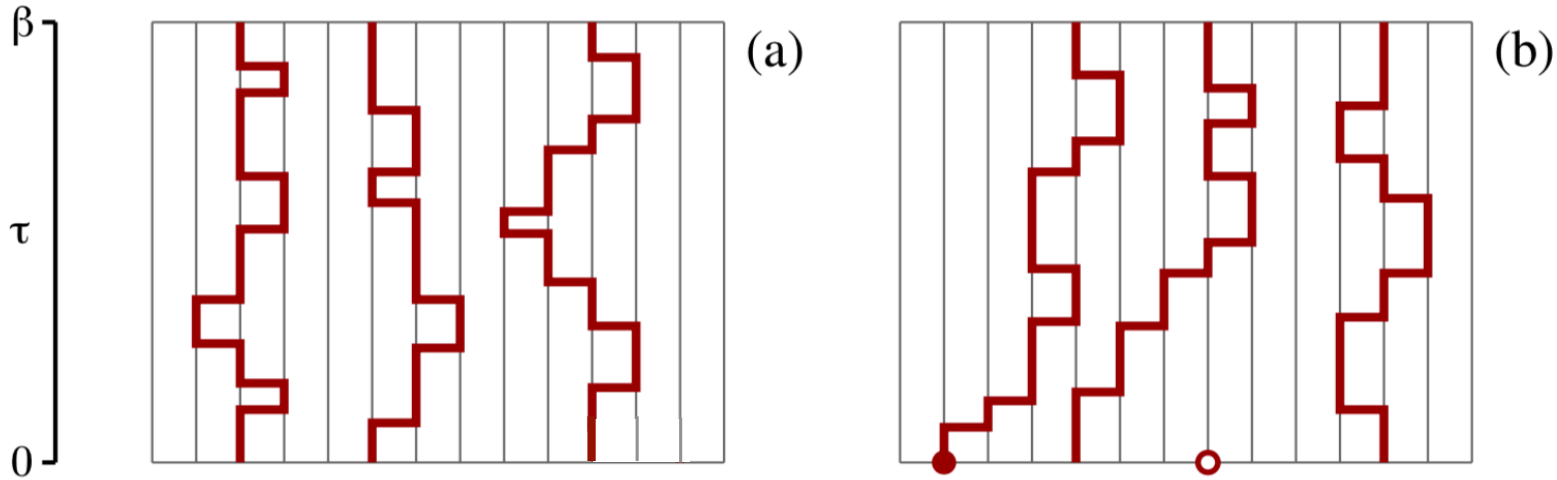


FIGURE 52. Continuous-time world line configurations. Here the kinetic events (jumps) occur at arbitrary imaginary times $0 \leq \tau < \beta$. Configuration (a) contributes to the partition function, whereas (b) includes a pair of creation (solid circle) and annihilation (open circle) operators separated by more than one lattice spacing and does not contribute to Z or diagonal expectation values. Such a configuration instead contributes to an off-diagonal expectation value $\langle a_i^+ a_j \rangle$.

Continuous time limit

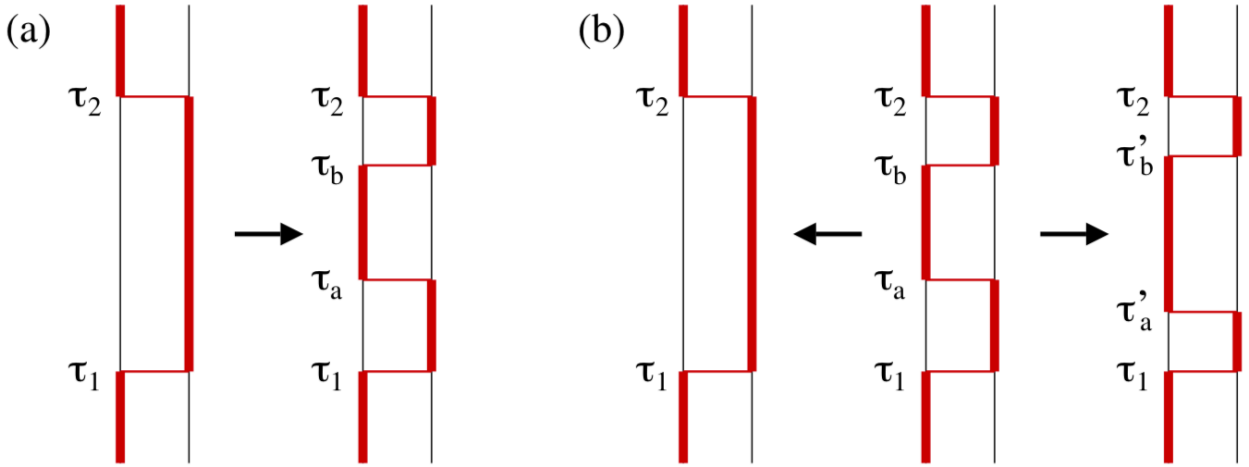


FIGURE 53. Local world line moves in continuous time. In (a), two opposite kinetic jumps are inserted at randomly chosen times τ_a and τ_b between two existing jumps at τ_1 and τ_2. In (b), two opposite jumps are either removed ($\leftarrow$) or the times of the two events are randomly changed to new arbitrary times τ'_a and τ'_b between τ_1 and τ_2 ($\rightarrow$).

- consider a line segment $\tau_2 = \tau_1 + m\Delta_\tau$

  there are totally $m\left(m-1\right)/2$ different ways of inserting events

  gives a total relative weight $\Delta_\tau^2 m\left(m-1\right)/2$, versus 1 for removing events

  in the continuum limit $\Delta_\tau^2 m\left(m-1\right)/2 \rightarrow \left(\tau_2-\tau_1\right)^2/2$

- acceptance probabilities for insertion and removal are

$$P_{\text{insert}} = \frac{\left(\tau_2-\tau_1\right)^2/2}{1+\left(\tau_2-\tau_1\right)^2/2} \qquad P_{\text{remove}} = \frac{1}{1+\left(\tau_2-\tau_1\right)^2/2}$$

Series expansion representation

- Taylor expansion of the Boltzmann operator $e^{-\beta H} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} H^n$

  Choosing a basis, the partition function can be written as

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

- for any model, the energy is

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

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

  from this, $\langle n \rangle \propto N\beta$

- fixed length scheme: cut-off at $n = L$, fill in with unit operators I

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

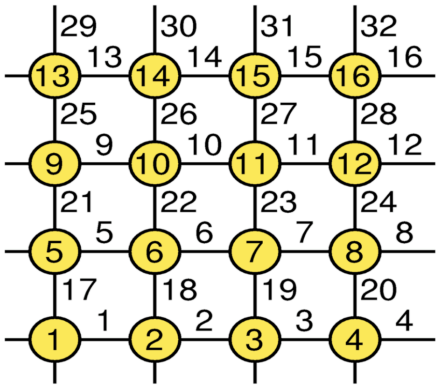
  here n is the number of $S_i = H$ instances in the sequence S

Stochastic Series expansion (SSE)

- spin-1/2 Heisenberg model, write H as a bond sum for arbitrary lattice

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

2D square lattice
bond and site labels



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

$$H_{1,b} = \frac{1}{4} - S^z_{i(b)} S^z_{j(b)}$$

$$H_{2,b} = \frac{1}{2}\left(S^+_{i(b)} S^-_{j(b)} + S^-_{i(b)} S^+_{j(b)}\right)$$

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

- all operations on parallel spins destroy the states, the non-zero elements are

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

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

- partition function

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

n_2 = number of off-diagonal operators in the sequence

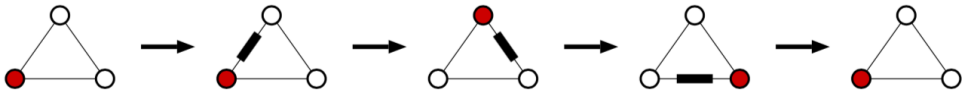
index sequence $S_n = [a(0), b(0)], [a(1), b(1)], \cdots, [a(n-1), b(n-1)]$

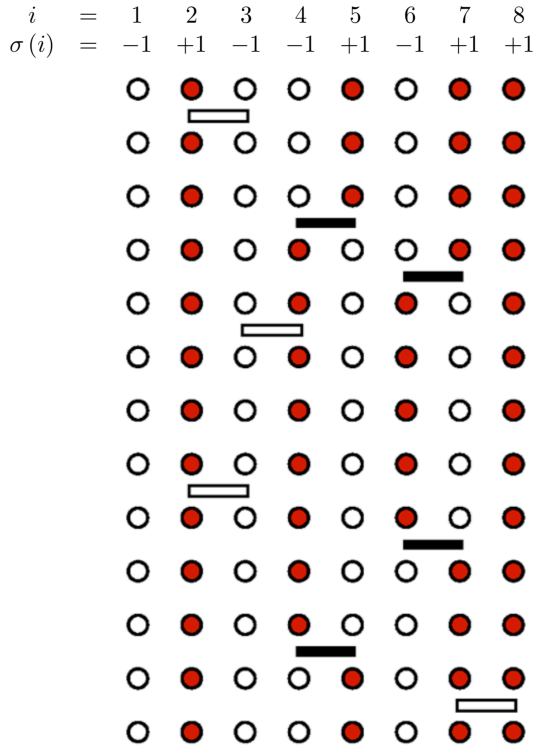
Stochastic Series expansion (SSE)

- for fixed length scheme

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

- frustrated systems have sign problem





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

- propagated states

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

- in a program

  $s(p)$ = operator index string

  $s(p) = 2*b(p) + a(p) - 1$

  diagonal: $s(p)$ = even

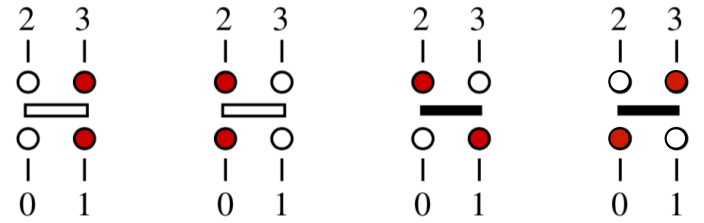
  off-diagonal: $s(p)$ = odd

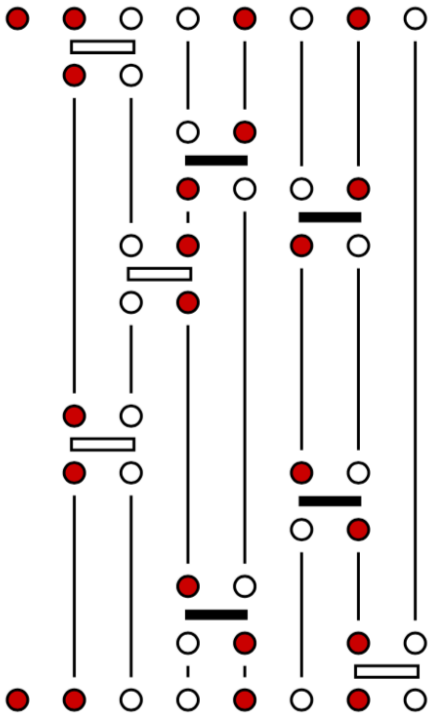
- SSE effectively provides a discrete representation of the time continuum

  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	

- in a program

  $X(\ )$ = vertex list

  operator at $p \rightarrow X(v)$

  $v = 4p + l$, $l = 0,1,2,3$

  links to next and previous leg

- spin states between operators are redundant, represented by links

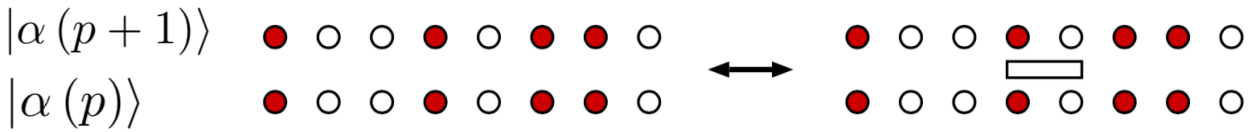
  network of linked vertices will be used for loop updates of vertices/operators

Monte Carlo sampling scheme

- change the configuration $(\alpha, S_L) \to (\alpha', S'_L)$ $\qquad W(\alpha, S_L) = \left(\frac{\beta}{2}\right)^n \frac{(L-n)!}{L!}$

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

- diagonal update $[0,0]_p \longleftrightarrow [1,b]_p$



attempt at $p = 0,1,\cdots,L-1$, need to know $|\alpha(p)\rangle$

- generate by selecting one bond

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

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

- 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

if the p^{th} operator

choose one of the bonds

parallel spins destroy the states this case is skipped

```
do p = 0 to L − 1
  if (s(p) = 0) then                                                          ← is identity
    b = random[1,...,N_b];  if σ(i(b)) = σ(j(b)) skip to next p
    if (random[0 − 1] < P_insert(n)) then s(p) = 2b;  n = n + 1 endif          → insert diagonal operator
  elseif (mod[s(p),2] = 0) then                                               ← is diagonal
    if (random[0 − 1] < P_remove(n)) then s(p) = 0;  n = n − 1 endif           → remove diagonal operator
  else                                                                        ← is off-diagonal
    b = s(p)/2; σ(i(b)) = −σ(i(b));  σ(j(b)) = −σ(j(b))
  endif
enddo
```

the spins belonging to bond b are flipped to update states

where $P_{\text{insert}} = \min\left[\frac{\beta N_b}{2(L-n)}, 1\right], P_{\text{remove}} = \min\left[\frac{2(L-n+1)}{\beta N_b}, 1\right]$

Local off-diagonal update

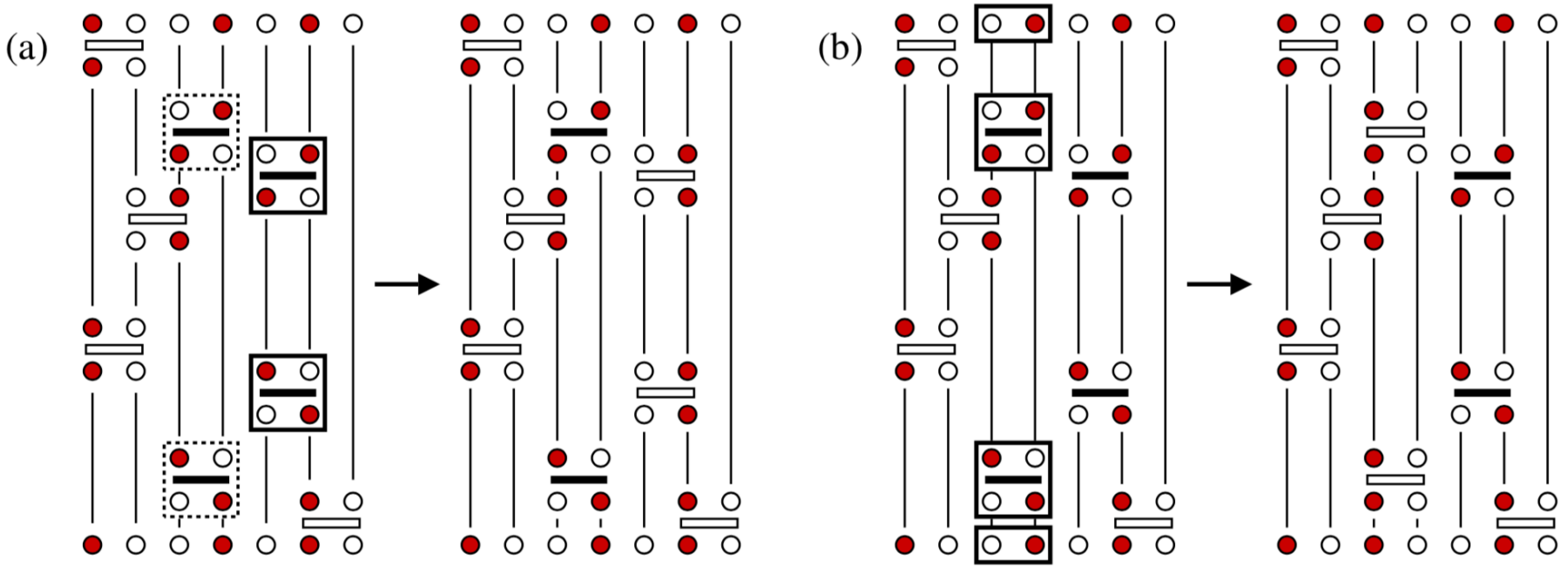


FIGURE 59. (a) A pair of off-diagonal operators, indicated by solid-line boxes, which can be replaced by diagonal ones if the spins between the two operators are flipped as well. Such an update cannot be done with the operators enclosed by dashed boxes, because of the illegal spin configuration (a vertex with all four legs in the same spin state) that would result at the operator acting between the two boxed vertices on their left spin. However, as shown in (b), this operator pair can be changed if instead the spins on the opposite sides of the operators are flipped. This also forces a change in the stored state $|\alpha\rangle$.

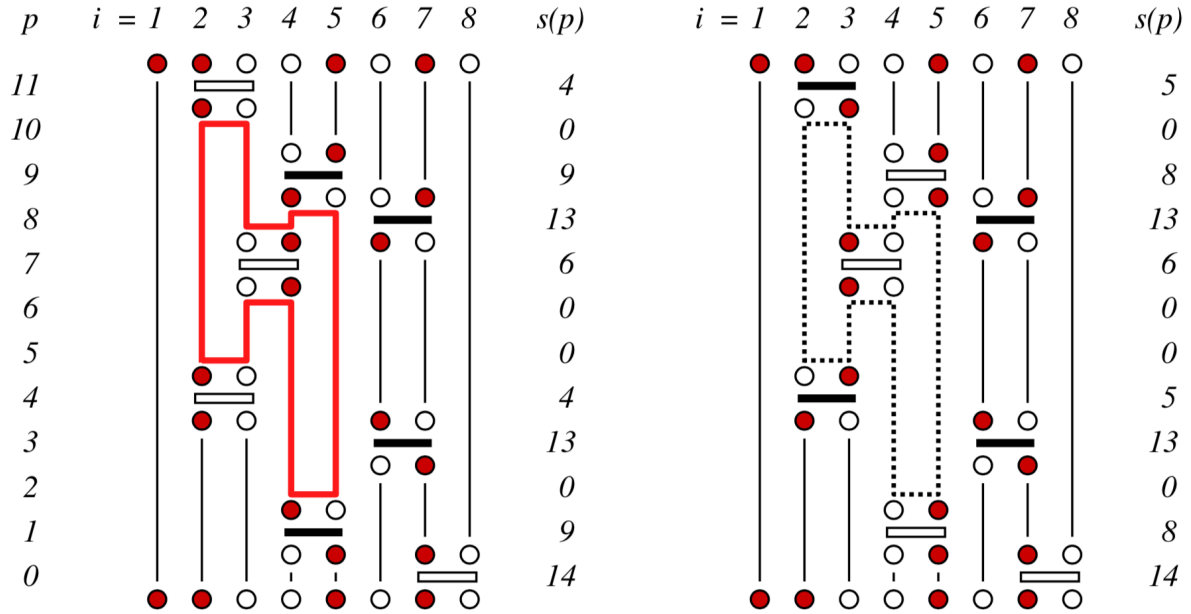
- switch the type ($a = 1 \longleftrightarrow a = 2$) of two operators on the same spins

  constraints have to be satisfied

  inefficient, cannot change the winding number

Operator loop update

- many spins and operators can be changed simultaneously



- in a program

  a given loop is only constructed once

  $X(v) < 0 \rightarrow$ visited loop

  $X(v) = -1 \rightarrow$ not flipped loop

  $X(v) = -2 \rightarrow$ flipped loop

- constructing all loops, flip probability 1/2

do $v_0 = 0$ **to** $4L-1$ **step** 2 ⟶ check each vertex, step 2 because v_0 and v_0+1 always in the same loop
  if $(X(v_0) < 0)$ **skip** to next v_0 ⟶ if this vertex is already visited, will not visit it again
  $v = v_0$
  if (**random**$[0-1] < 1/2$) **then**
    • traverse the loop; for all v in loop, set $X(v) = -1$ ⟶ only visit these loops, but not flip them
  else
    • traverse the loop; for all v in loop, set $X(v) = -2$ ⟶ visit and flip these loops
    • flip the loop (change operator types $s(p = v/4)$ while loop is traversed)
  endif
enddo

Operator loop update

- construct and flip a loop

change the operator code $s(p)$ from $2b$ (diagonal operator) to $2b$+1 (off-diagonal operator) or vice versa

get the position of the operator

get the adjacent leg

move to the next vertex

$v = v_0$
do
$p = v/4;\quad s(p) = \textbf{flipbit}(s(p),0);\quad X(v) = -2$ — labeled as flipped
$v = \textbf{flipbit}(v,0);\quad X(v) = -2$ — labeled as flipped
$v = X(v);\quad \textbf{if}\ (v = v_0)\ \textbf{exit}$ — complete a full loop
enddo

- update the spins in the stored state

there is no operator acting on spin i

the loop passing i has been flipped

flip with probability 1/2 any spin that has no loop connected to it

flip the spin i

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

Determination of the cut-off L

- adjust during the equilibration, start with arbitrary small n

  keep track of the number of operators n, increase L if n is close to the current L, e.g., $L = 4n/3$

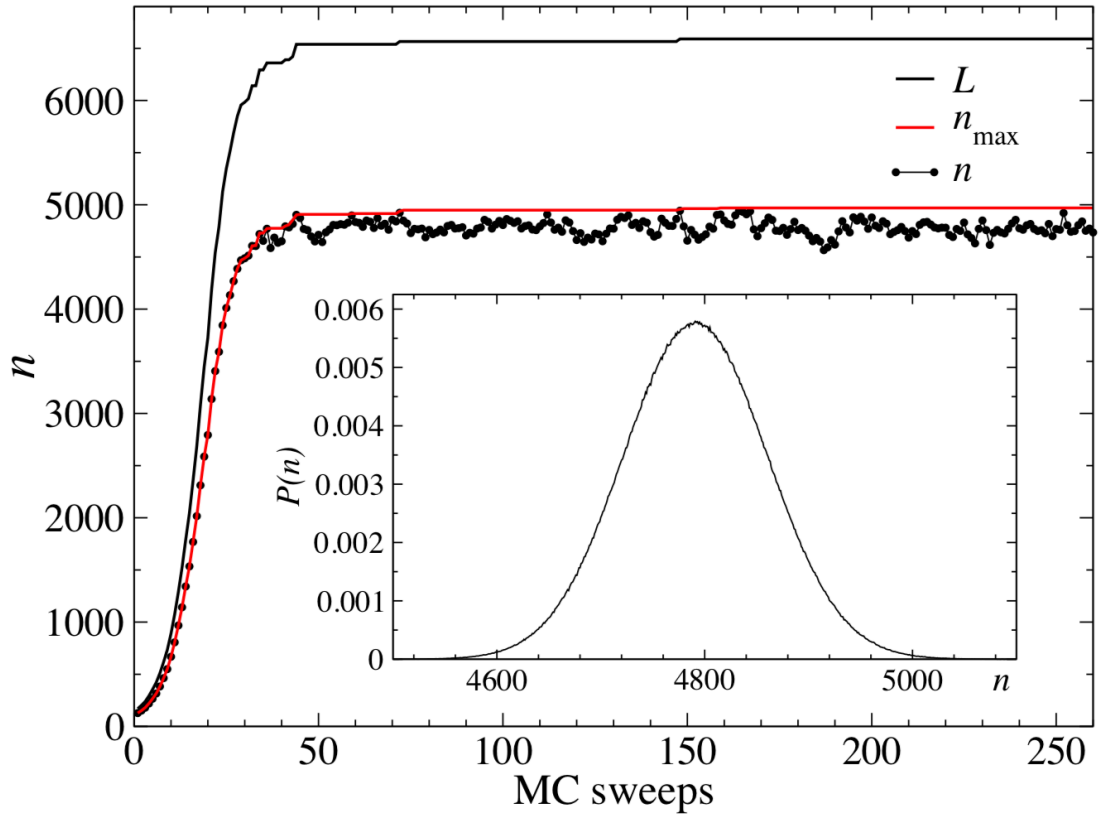
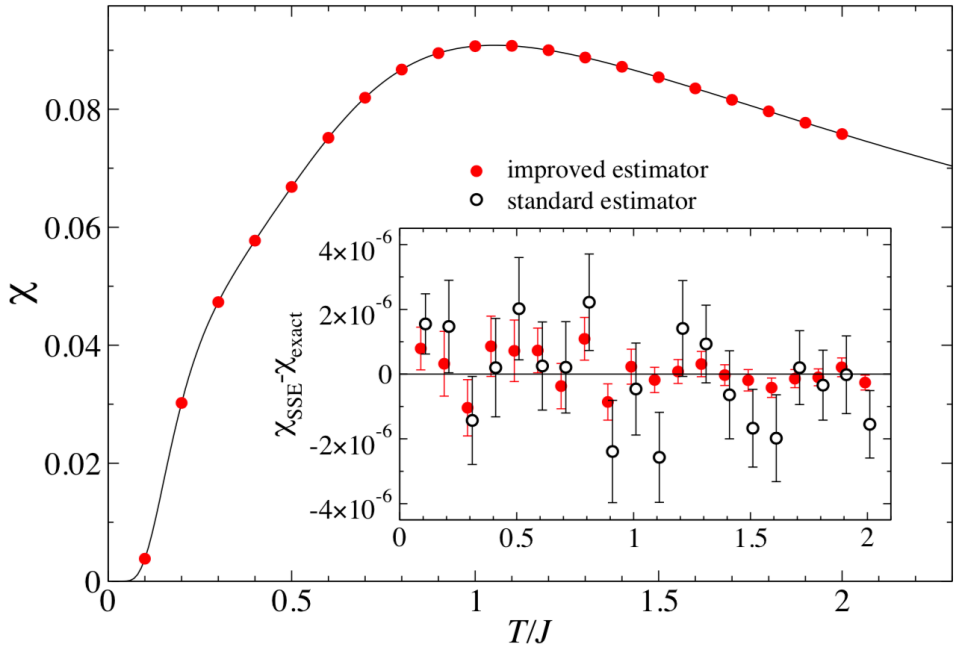


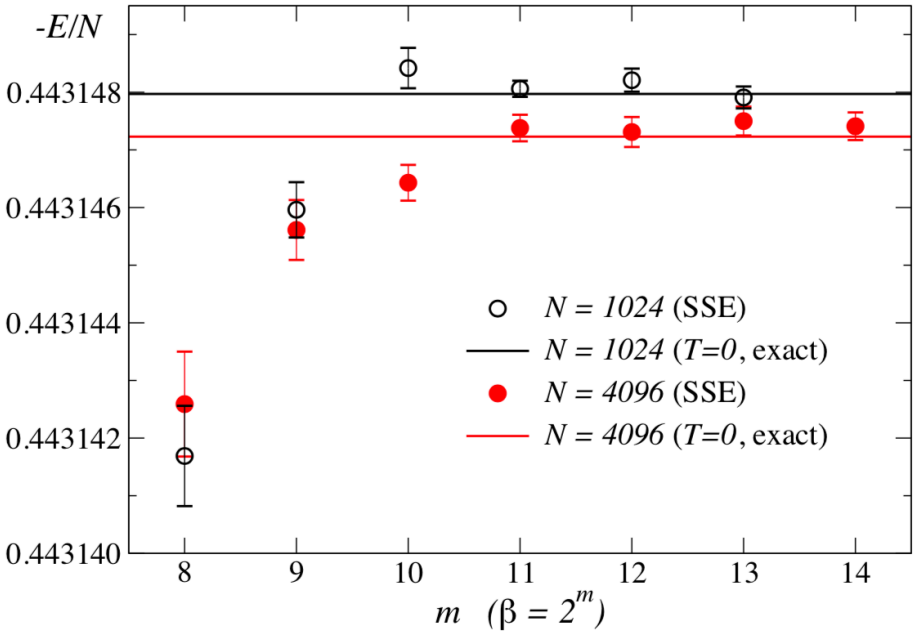
FIGURE 62. Evolution of the expansion cut-off L at the initial stage of an equilibration run of a 16×16 Heisenberg system at $\beta = 16$. The number of operators n in the string after each Monte Carlo sweep is also shown, along with the maximum n reached so far. The final cut-off after 5000 sweeps was $L = 6764$. The inset shows the distribution of n in a subsequent run of 10^7 MC sweeps.

Results

- compare with exact results

  4×4 exact diagonalization, Bethe Ansatz for long chains





- susceptibility of the 4×4 lattice

  SSE results from 10^{10} sweeps

  improved estimator gives smaller error bars at high T

- energy for long 1D chains

  SSE results for 10^6 sweeps

  Bethe Ansatz ground state E/N

  SSE can achieve the ground state limit