Stochastic Series Expansion

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- Series representation of quantum stat mech
- Stochastic series expansion (SSE) QMC
  - Example: 2D S=1/2 Heisenberg antiferromagnets
- Real-material application:
  - inelastic neutron scattering; compare with experiments

References:

- School book (chapter 16)
- AIP Conf. Proc. **1297**,135 (2010); arXiv:1101.3281
- PRE **68**, 056701 (2003)
- PRX **7**, 041072 (2017)

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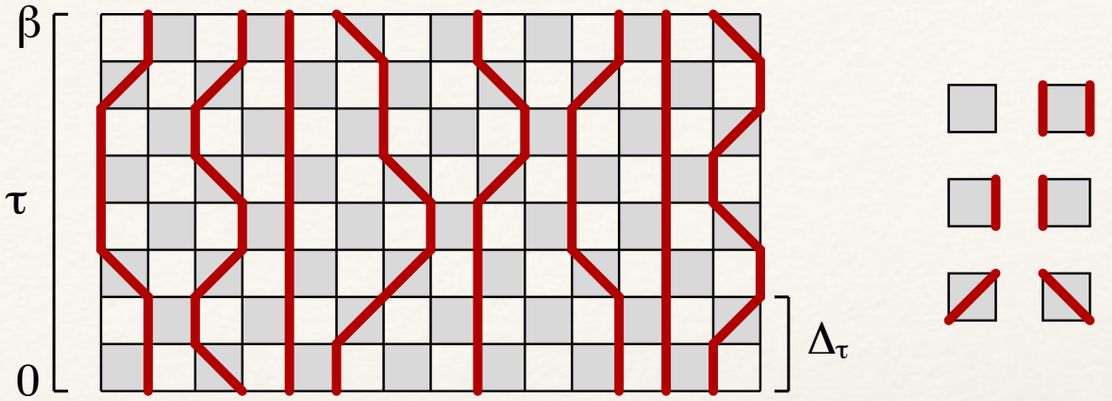
QMC algorithms for quantum spins (and bosons)

From operators to numbers

$$\langle A \rangle = \frac{\mathrm{Tr}\{A e^{-\beta H}\}}{\mathrm{Tr}\{e^{-\beta H}\}} \rightarrow \frac{\sum_c A_c W_c}{\sum W_c}$$



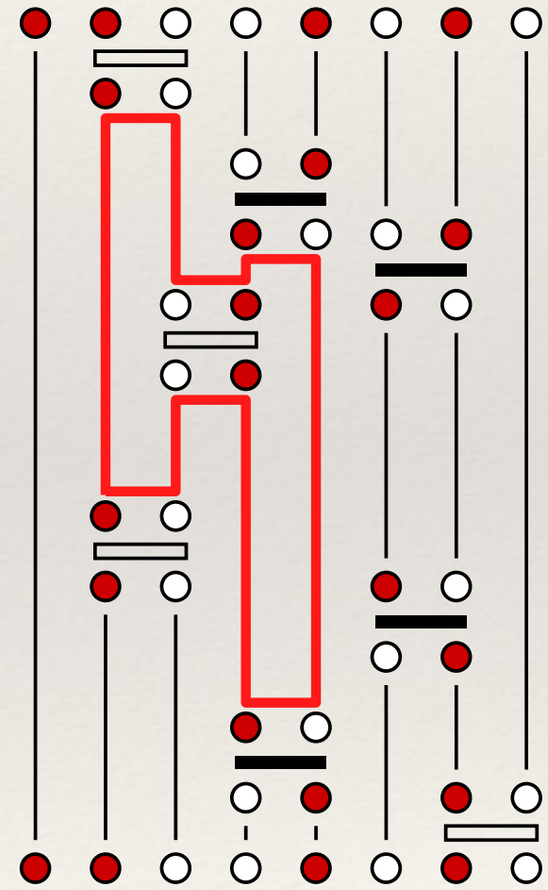
"sign problem" if W_c not positive-definite
- consider sign-free models

- **Trotter slicing;** discrete imaginary time; world line methods (Suzuki 1971,...)

- **Taylor expansion;** stochastic series expansion (SSE) (Handscomb -61,… Sandvik, Kurkijärvi -91,…)

- **Continuous time;** take $\Delta_\tau \rightarrow 0$ limit before programming (Beard, Wiese, -96, Prokof'ev et al. -96,…)

- From local updates to **loops, worms, directed loops....** (Evertz et al. -93, Beard, Wiese, -96, Prokof'ev et al. -96, Sandvik -99, Sandvik, Syljuåsen -02)



Related: ground-state projection

$$|\Psi_\beta\rangle \sim \mathrm{e}^{-\beta H}|\Psi_0\rangle \qquad |\Psi_\beta\rangle \rightarrow |0\rangle \quad \text{when} \quad \beta \rightarrow \infty$$

- Differs only in time boundary condition (open vs periodic)

Series expansion representation of quantum stat mech

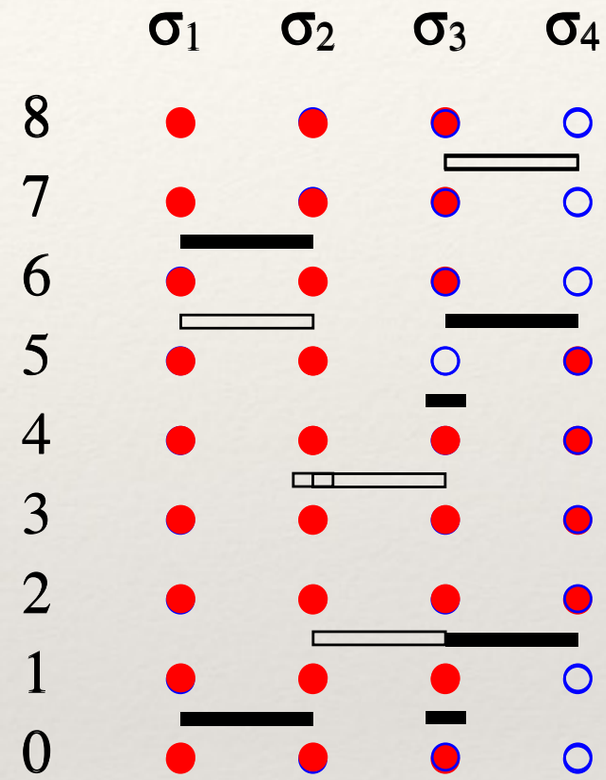
Start from the **Taylor expansion** (no approximation)

$$Z = \mathrm{Tr}\{\mathrm{e}^{-\beta H}\} = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\alpha_0} \langle \alpha_0 | H^n | \alpha_0 \rangle$$

Index sequence (string) referring to terms of H

$$H = \sum_{i=1}^{m} H_i \qquad S_n = (a_1, a_2, \ldots, a_n)$$

$$a_i \in \{1, \ldots, m\}$$



Break up H^n into strings:

$$Z = \sum_{n=0}^{\infty} \frac{(-\beta)^n}{n!} \sum_{\alpha_0} \sum_{S_n} \langle \alpha_0 | H_{a_n} \cdots H_{a_2} H_{a_1} | \alpha_0 \rangle$$

We should have (always possible): $H_i |\alpha_j\rangle \propto |\alpha_k\rangle$

- **no branching** during propagation with operator string
- some strings not allowed (illegal operations)

Path weight: $W(S_n, \alpha_0) = \frac{(-\beta)^n}{n!} \prod_{p=1}^{n} \langle \alpha_p | H_{a_p} | \alpha_{p-1} \rangle$

Easy to calculate

- use as MC sampling weight

Expectation values

$$\langle A\rangle = \frac{1}{Z}\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\sum_{\alpha_0}\langle\alpha_0|H^n A|\alpha_0\rangle$$

Simplest case: Operator A **diagonal** in the chosen basis:

$$\langle A\rangle = \sum_{n=0}^{\infty}\sum_{\alpha_0}\sum_{S_n} W(S_n,\alpha_0)A(\alpha_0) \qquad A(\alpha_0)\to\frac{1}{n}\sum_{p=0}^{n-1}A(\alpha_p)$$

Energy: $$\langle H\rangle = \frac{1}{Z}\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\sum_{\alpha_0}\langle\alpha_0|H^n H|\alpha_0\rangle$$

Relabel terms of n-sum: replace n+1 by n

$$\langle H\rangle = -\frac{1}{Z}\sum_{n=1}^{\infty}\frac{(-\beta)^n}{n!}\frac{n}{\beta}\sum_{\alpha_0}\langle\alpha_0|H^n|\alpha_0\rangle$$

we can extend the sum to include n=0, because that term vanishes

Therefore the energy is: $E = -\langle n\rangle/\beta$

Can also derive specific heat: $C = \langle n^2\rangle - \langle n\rangle^2 - \langle n\rangle$

Follows: $\langle n\rangle \propto \beta N, \quad \sigma_n \propto \sqrt{\beta N}$

Fixed string-length scheme

- n fluctuating → varying size of the sampled configurations
- the expansion can be truncated at some n_{max}=L
  (exponentially small error if large enough)
- 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 | ⟹

L=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 original strings, correct by $\binom{L}{n}^{-1} = \frac{n!(L-n)!}{L!}$

$$Z = \sum_{\alpha_0} \sum_{S_L} \frac{(-\beta)^n (L-n)!}{L!} \langle \alpha_0 | H_{a_m} \cdots H_{a_2} H_{a_1} | \alpha_0 \rangle$$

Here n is the number of H_i, i>0 instances in the sequence of L ops
- the summation over n is now implicit

L can be chosen automatically by the simulation (shown later)

Relation to the expansion in interaction representation

For ***H=D+V***, diagonal *D*, off-diagonal *V*

Sandvik, Singh, Campbell (PRB 1997)

$$Z=\sum_{n=0}^{\infty}(-1)^n\int_0^{\beta}d\tau_1\int_0^{\tau_1}d\tau_2\cdots\int_0^{\tau_{n-1}}d\tau_n\ \mathrm{Tr}\{e^{-\beta\hat{D}}\hat{V}(\tau_1)V(\tau_2)\cdots V(\tau_n)\}$$

Proceed as in SSE, only off-diagonal operators in diagrams

$$Z=\sum_{\alpha}\sum_{n=0}^{\infty}\sum_{T_n}\int_0^{\beta}d\tau_1\int_0^{\tau_1}d\tau_2\cdots\int_0^{\tau_{n-1}}d\tau_n W(\alpha,T_n,\{\tau\})$$

What is better, SSE or interaction rep?

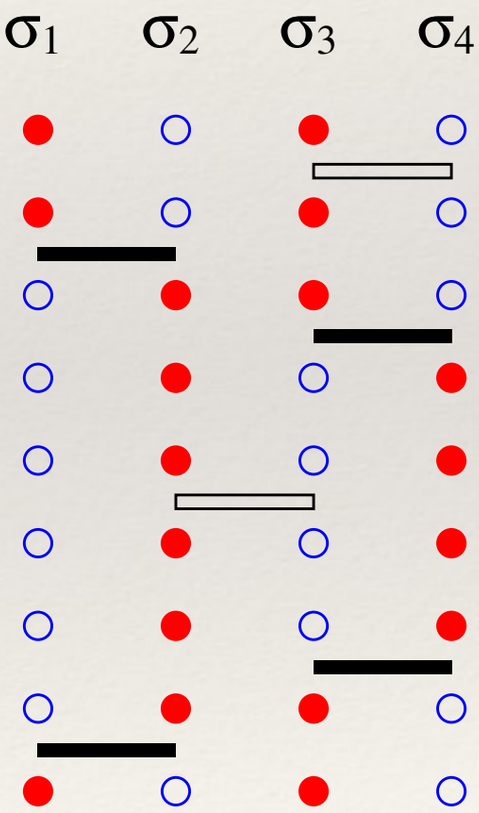
- depends on balance of diagonal and off-diagonal energy
- Interaction rep better if diagonal energy dominates
- SSE better if that is not the case

Extreme case: Only off-diagonal operators

- for example, XY model in z basis

Time integrals in interaction rep give $\beta^n/n!$

- configurations identical to SSE
- SSE avoids time integrals

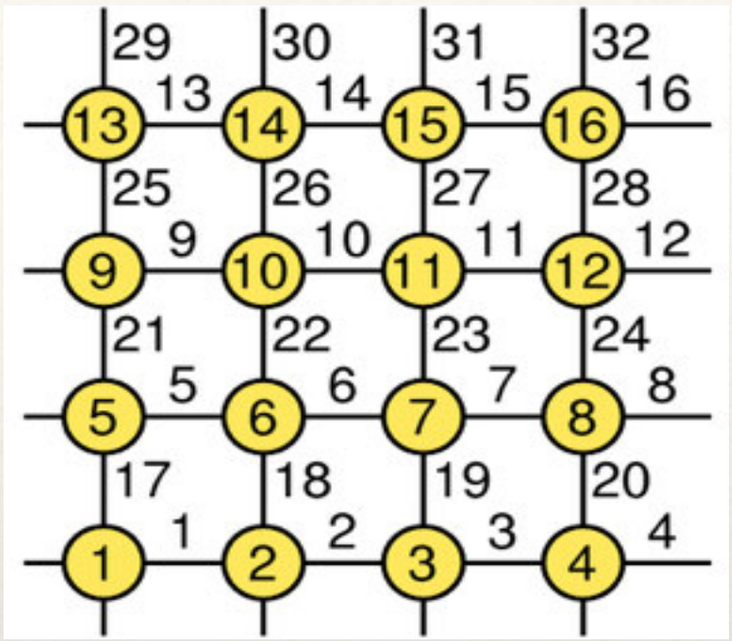


Stochastic Series expansion (SSE): S=1/2 Heisenberg model

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

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

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

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

Four non-zero matrix elements

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

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

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

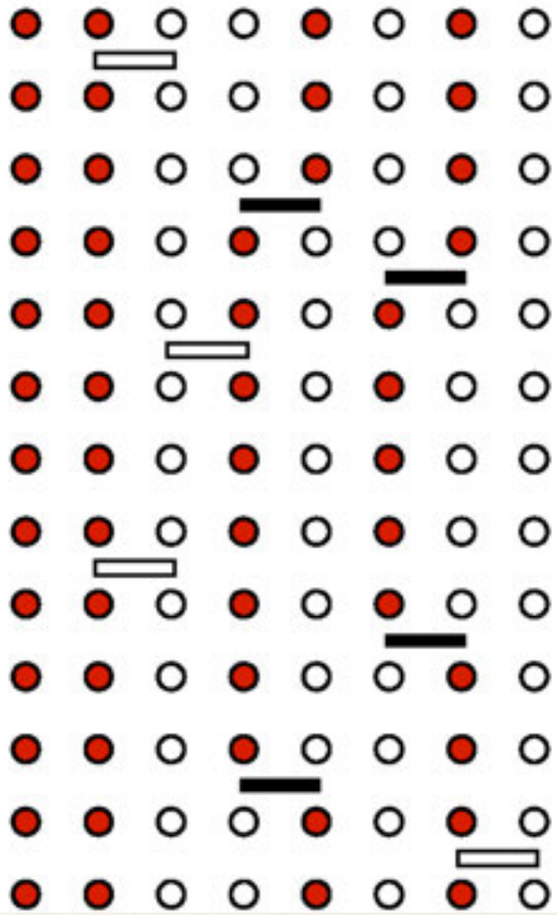
For fixed-length scheme

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

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	$a(p)$	$b(p)$	$s(p)$
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

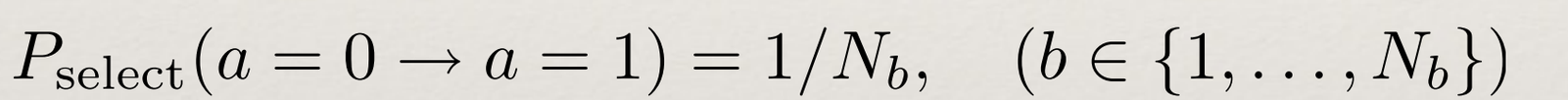
Monte Carlo sampling scheme

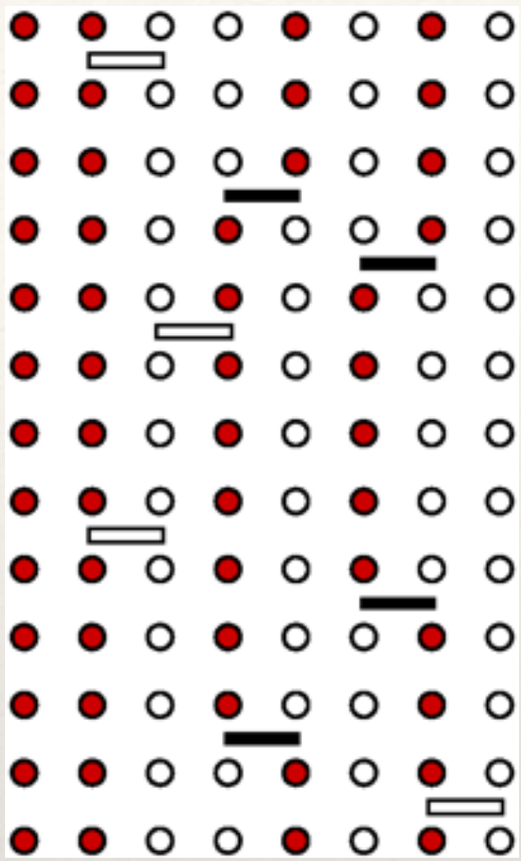
Change the configuration; $(\alpha, S_L) \to (\alpha', S'_L)$

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

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

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

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

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

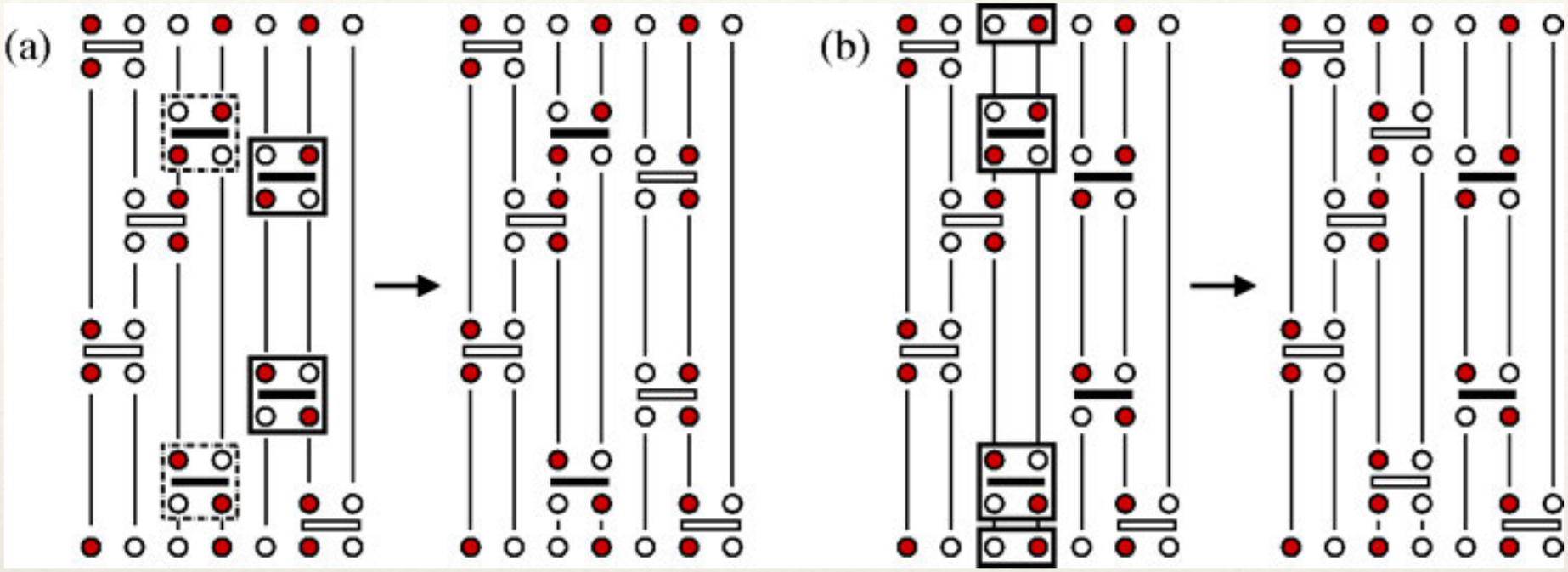
Pseudocode: Sweep of diagonal updates

```
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
```

Code explanation:

- To insert operator, bond b generated at random among 1,...,N_b
  - can be done only if connected spins i(b),j(b) are anti-parallel
  - if so, do it with probability $P_{insert}(n)$
- Existing diagonal operator can always be removed
  - do it with probability $P_{remove}(n)$
- If off-diagonal operator, advance the state
  - extract bond b, flip spins at i(b),j(b)

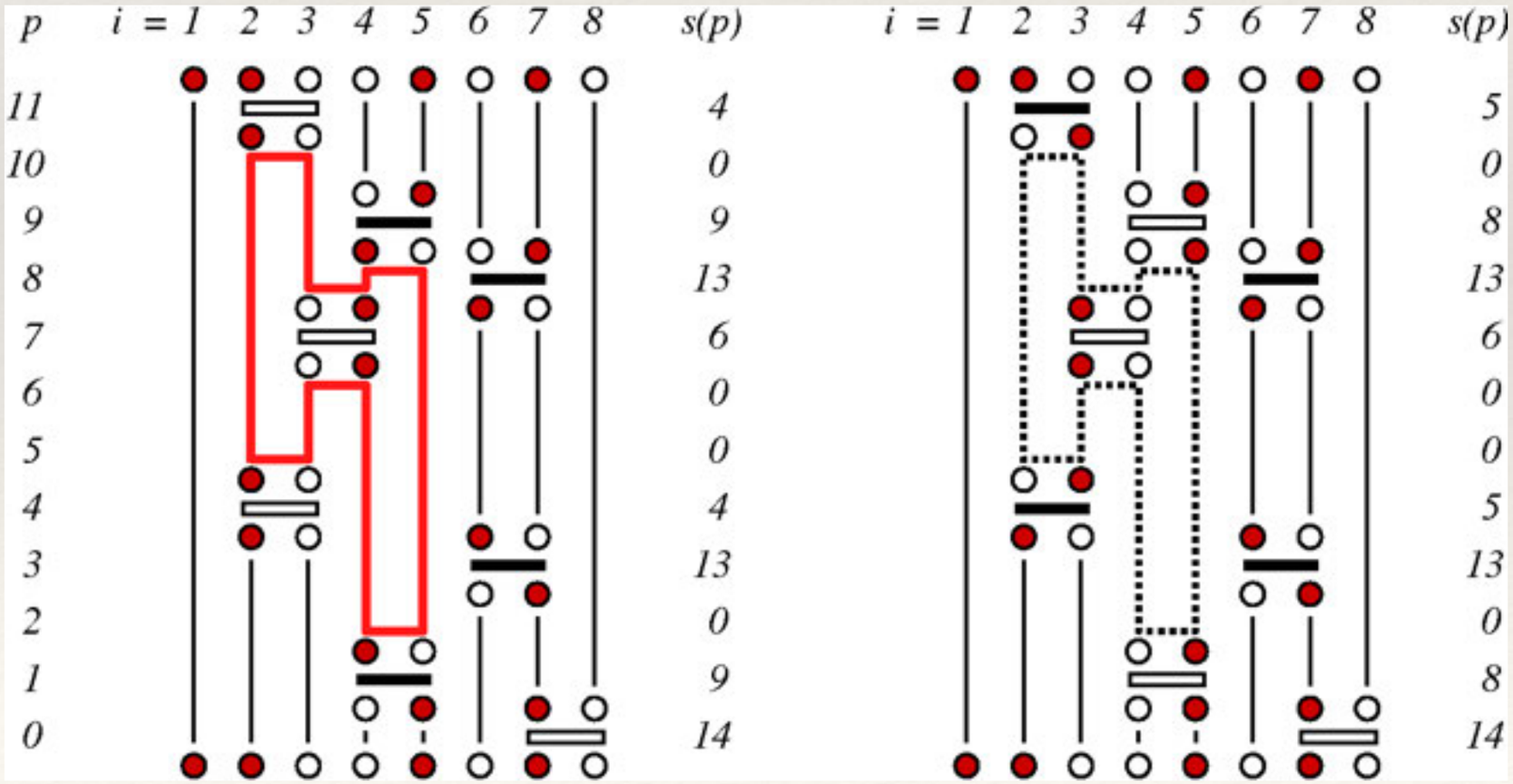
Off-diagonal updates



Local update

Change the type of two operators

- constraints
- inefficient
- cannot change winding numbers

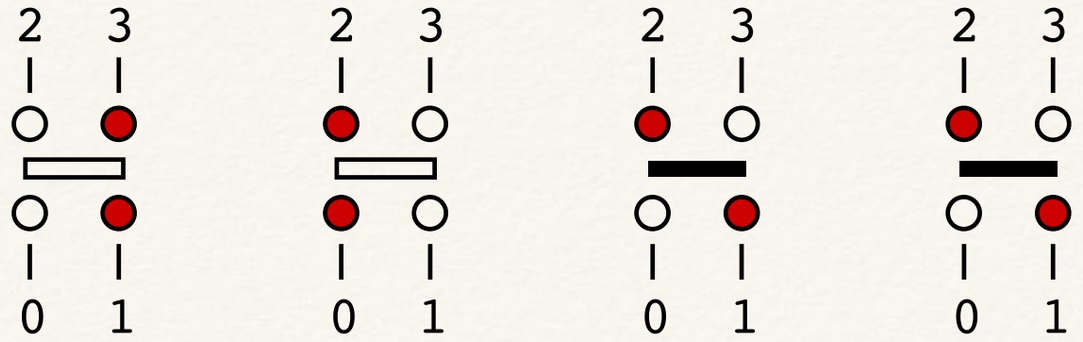


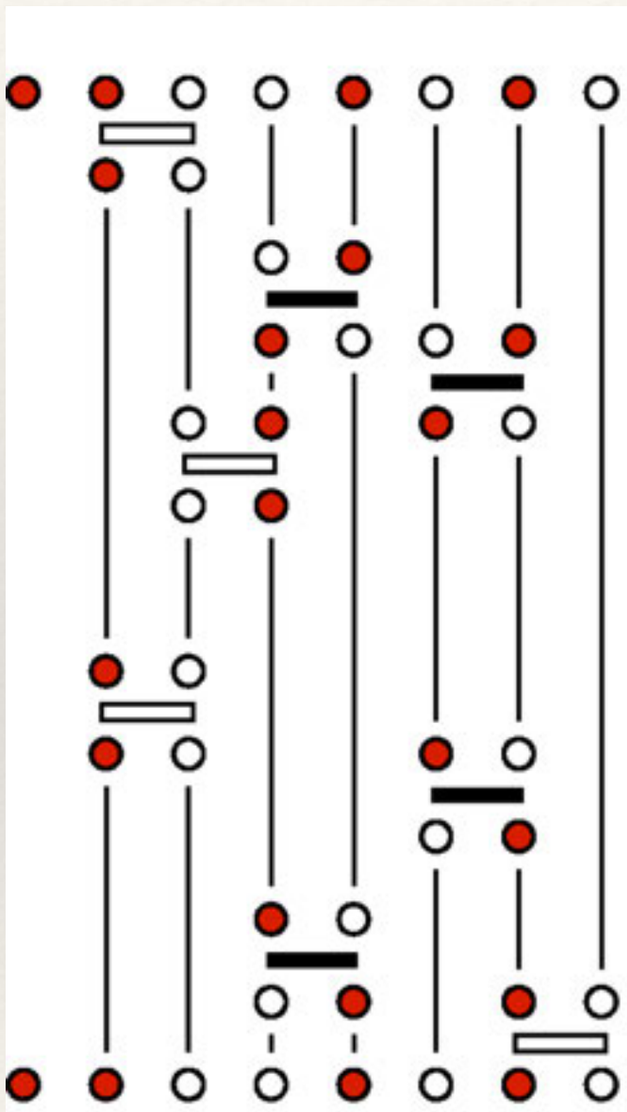
Operator-loop update

- Many spins and operators can be changed simultaneously
- can change winding numbers

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

Pseudocode: Sweep of loop updates

constructing all loops, flip probability 1/2

```
do v_0 = 0 to 4L − 1 step 2
    if (X(v_0) < 0) cycle
    v = v_0
    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
```

- visited vertices are no longer needed and we set them to a negative value -1 or -2, to indicate that the loop has been visited (-1) or visited and flipped (-2)

construct and flip a loop

```
v = v_0
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 = v_0) exit
enddo
```

- p is the location of the operator in the original length-L list of operatotors
- by flipping bit 0 of s(p), the operator changes from diagonal to off-diagonal, or vice versa
- moving on the vertex to the adjacent spin is also done with a bit flip

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

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

$v=V_{\text{first}}(i)$ is the location of the first vertex leg on site i

- flip the spin if X(v)=–2
- (do not flip it if X(v)=–1)
- no operation on i if $v_{\text{first}}(i)=-1$; then it is flipped with probability 1/2

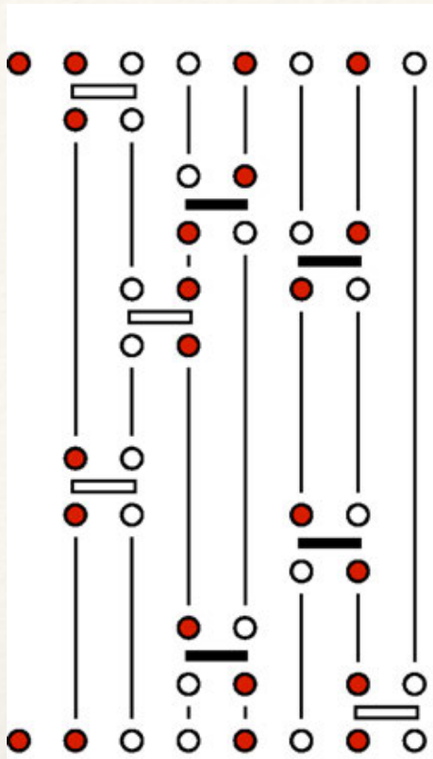
Constructing the linked vertex list

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

- $V_{first}(i)$ = location v of first leg on site i
- $V_{last}(i)$ = 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	

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

creating the last links across the “time” boundary

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

Determination of the cut-off L

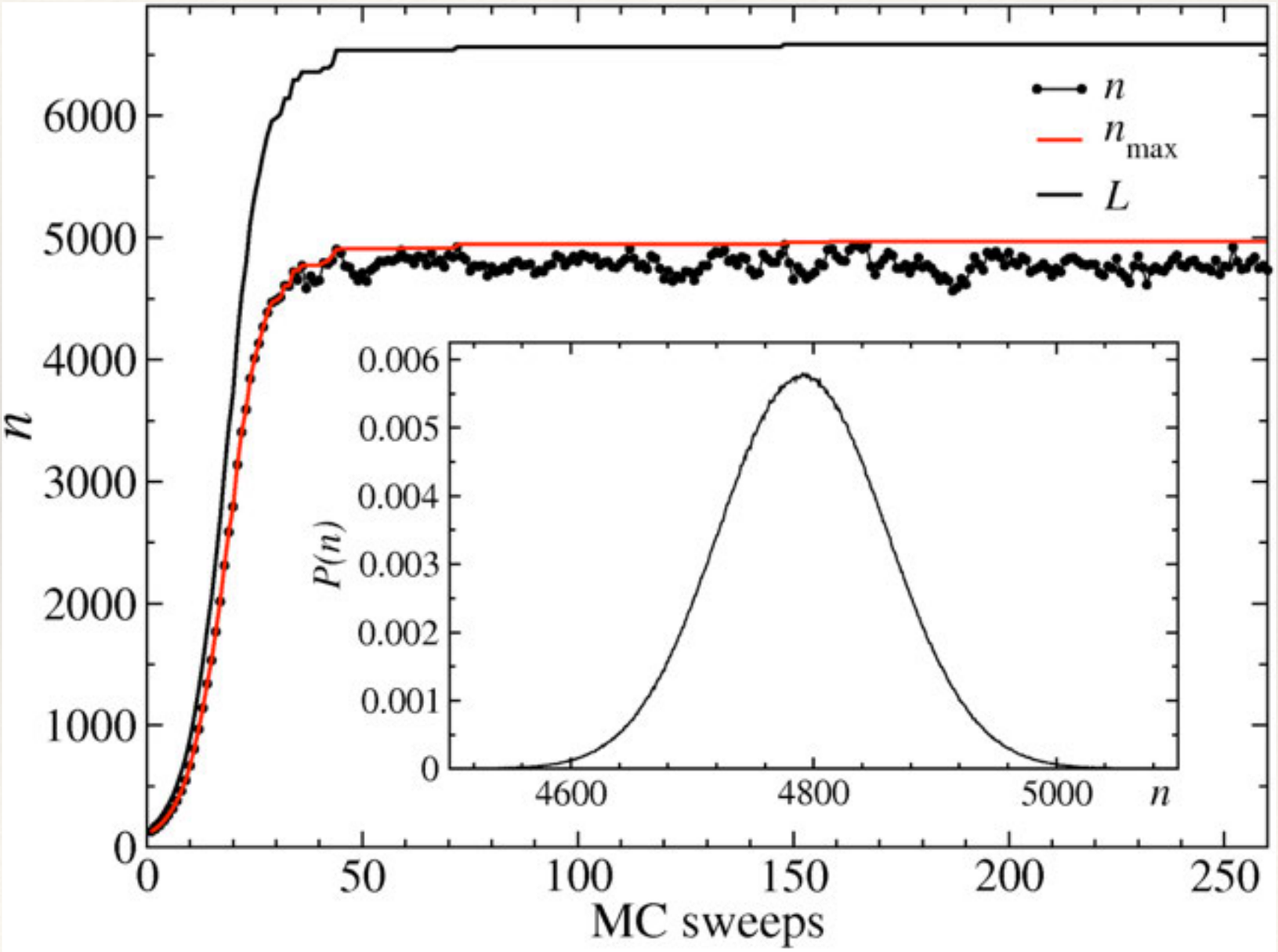
- adjust during equilibration
- start with arbitrary (small) n

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

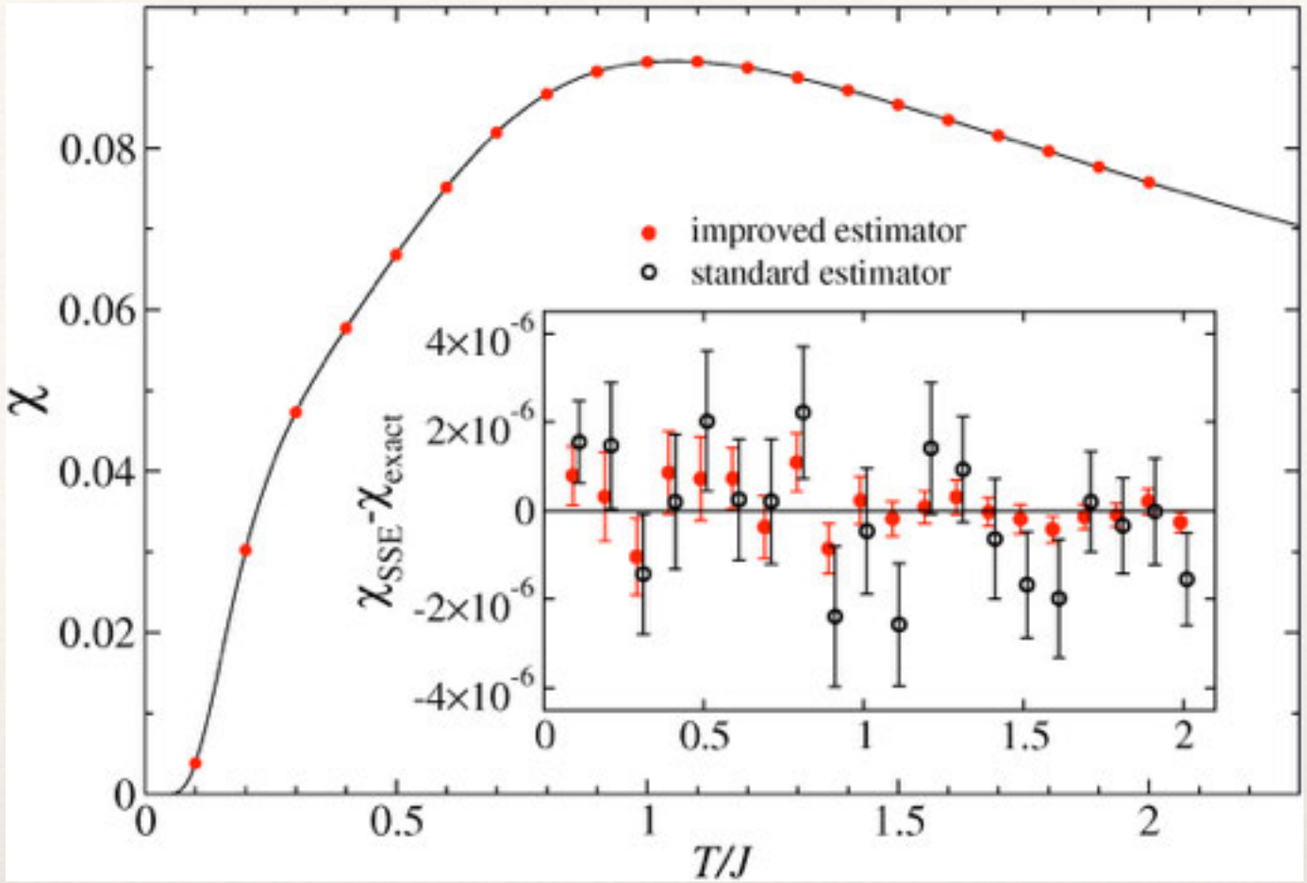


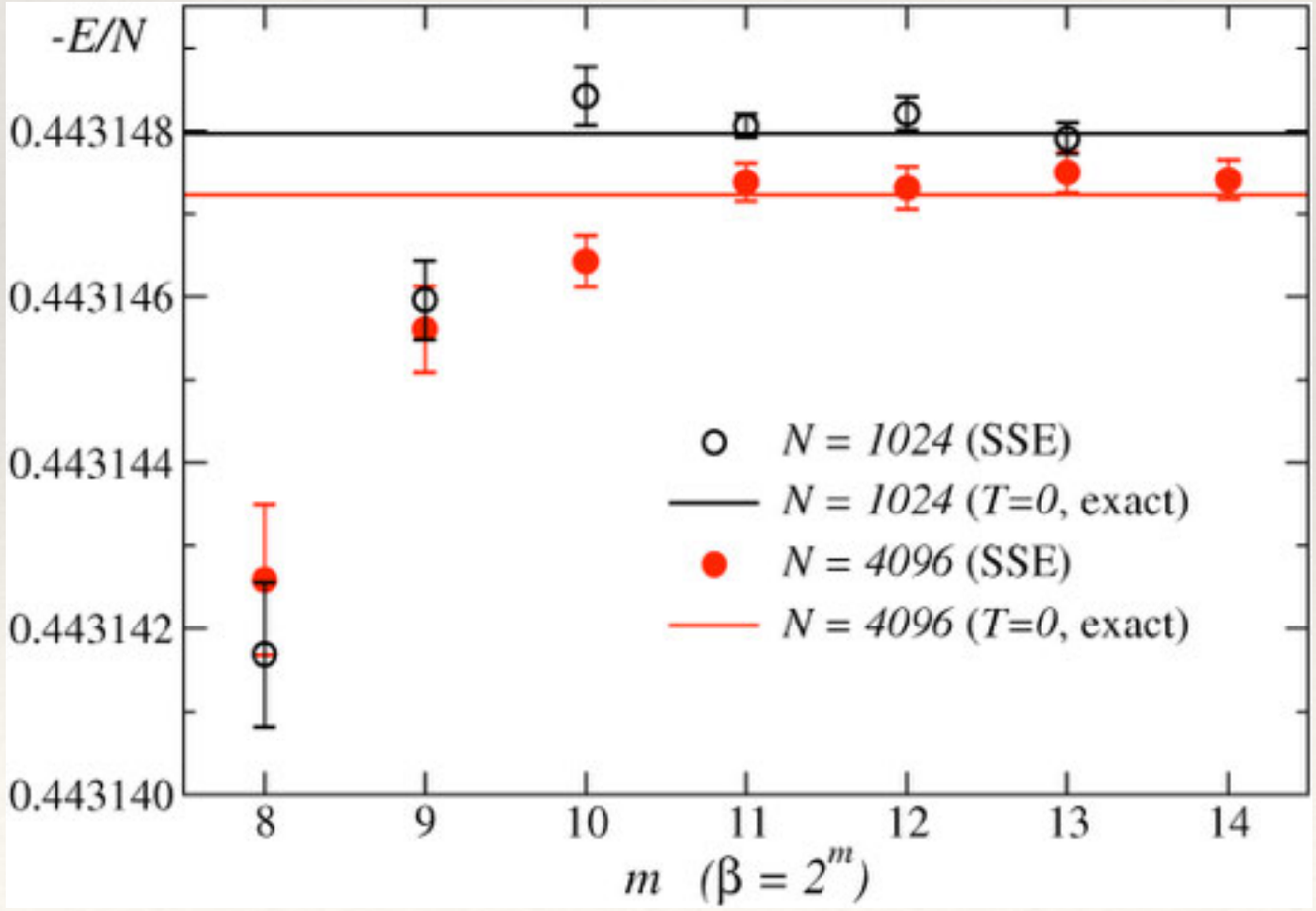
Does it work?
Compare with exact results

- 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)



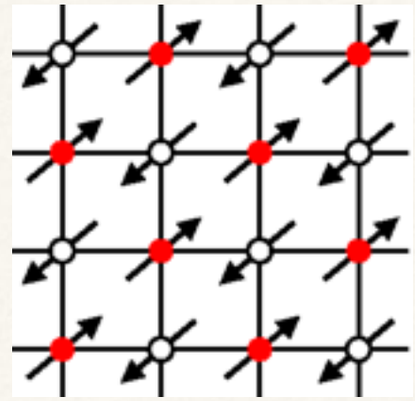


⇐ Energy for long 1D chains

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

Results for 2D Heisenberg model

$$\mathbf{H} = \mathbf{J} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \mathbf{S_i} \cdot \mathbf{S_j}$$



Sublattice magnetization

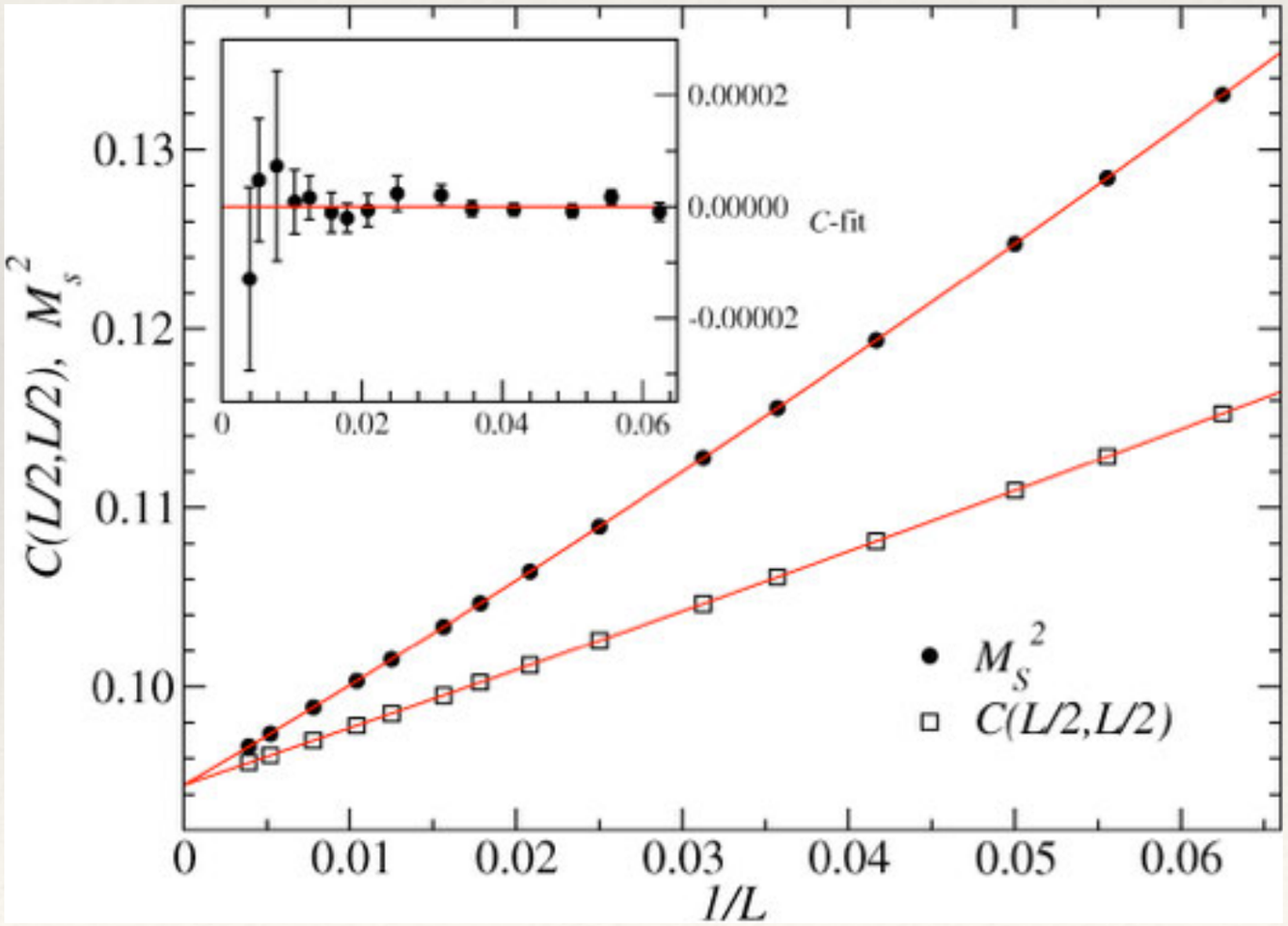
$$\vec{m}_s = \frac{1}{N} \sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i + y_i}$$

Long-range order: **$\langle m_s^2 \rangle > 0$ for $N \to \infty$**

Quantum Monte Carlo

- finite-size calculations
- no approximations
- extrapolation to infinite size

L×L lattices up to 256×256, T→0



Reger & Young (world-line) 1988

$$m_s = 0.30(2)$$

$$\approx 60\ \%\ \text{of classical value}$$

AWS & HG Evertz 2010

$$m_s = 0.30743(1)$$

SSE calculations of imaginary-time correlations

Time evolved operator: $A(\tau) = \mathrm{e}^{\tau H} A \mathrm{e}^{-\tau H}$

How is τ related to the SSE "propagation" dimension?

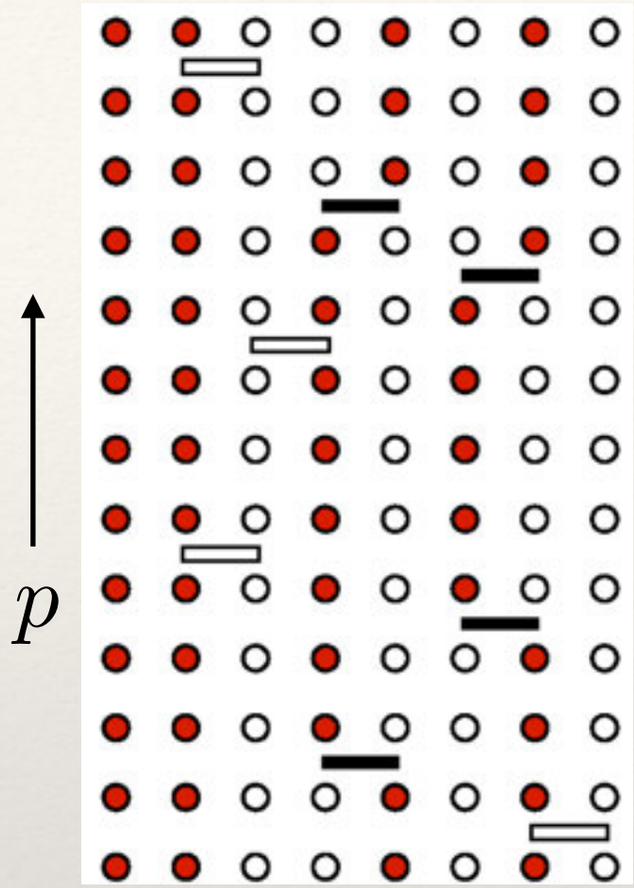
By Taylor expansion:

$$\langle \hat{A}_2(\tau)\hat{A}_1(0)\rangle = \frac{1}{Z}\sum_{\alpha}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{(\tau-\beta)^n(-\tau)^m}{n!m!}\langle\alpha|\hat{H}^n\hat{A}_2\hat{H}^m\hat{A}_1|\alpha\rangle$$

$F(m)$

F(m) weighted correlations between states separated by m operations with H; sharply peaked distribution

- dominated by **m ~ (τ/β)n_0**, n_0=n+m (expansion order)



Easy for diagonal (and some off-diagonal) operators

Alternative way: SSE with time-slicing

$$\mathrm{e}^{-\beta H} = \prod_{i=1}^{\Lambda}\mathrm{e}^{-\Delta_\tau H}, \quad \Delta_\tau = \beta/\Lambda$$

Each exponential is formally expanded individually

- only changes acceptance probability in diagonal updates
- n(i) Hamiltonian operators in slice i, n(i) ≤ l (l adjusted)

Time correlations easy to measure for τ=i$\Delta\tau$ (states at slice boundaries)

Spectral functions and Imaginary-time correlations

We want the spectral function of some operator

$$S(\omega) = \frac{1}{Z}\sum_{m,n} \mathrm{e}^{-\beta E_n} |\langle m|\hat{O}|n\rangle|^2 \delta[\omega - (E_m - E_n)]$$

Example:

$$O = S^z_q = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} \mathrm{e}^{ir_j\cdot q} S^z_j$$

With QMC we can compute the imaginary-time correlator

$$G(\tau) = \langle O^\dagger(\tau) O(0)\rangle = \langle \mathrm{e}^{\tau H} O^\dagger \mathrm{e}^{-\tau H} O\rangle \qquad \tau \in [0,\beta], \quad \beta = T^{-1}$$

Relationship between G($\boldsymbol{\tau}$) and S(ω):

$$G(\tau) = \int_{-\infty}^{\infty} d\omega S(\omega) \mathrm{e}^{-\tau\omega}$$

But we are faced with the difficult inverse problem:

- know G($\boldsymbol{\tau}$) from QMC for some points $\boldsymbol{\tau}_i$, i=1,2,…,N$\boldsymbol{\tau}$
- statistical errors are always present

Solution S(ω) is not unique given incomplete QMC data

- the numerical analytic continuation problem
- difficult to resolve fine-structure of S(ω)

QMC Data may look like this:

τ	G(τ)	$\sigma(\tau)$ (error)
0.100000000	0.785372902099492	0.000025785921025
0.200000000	0.617745252224320	0.000024110978744
0.300000000	0.486570613927804	0.000022858341732
0.400000000	0.383735739475007	0.000022201962003
0.600000000	0.239426314549321	0.000021230286782
0.900000000	0.118831597893045	0.000021304530787
1.200000000	0.059351045039398	0.000020983919497
1.600000000	0.023755763120921	0.000020963449347
2.000000000	0.009567293481952	0.000021147137686
2.500000000	0.003071962229791	0.000020315351879
3.000000000	0.001017989765629	0.000020635751833
3.600000000	0.000255665406091	0.000020493781188

Typical $\sigma(\tau)$ when G(0)=1;
as small as ~10^{-5} - 10^{-6}
in good QMC data

From a given "guess" of the spectrum S(ω) we can compute

$$G_S(\tau) = \int_{-\infty}^{\infty} \mathrm{e}^{-\tau\omega} S(\omega)\, d\tau$$

We want to have a good fit to the QMC data, quantified by

$$\chi^2 = \sum_j \frac{1}{\sigma_j^2} [G_S(\tau_j) - G(\tau_j)]^2$$

QMC statistical errors are correlated; use covariance matrix

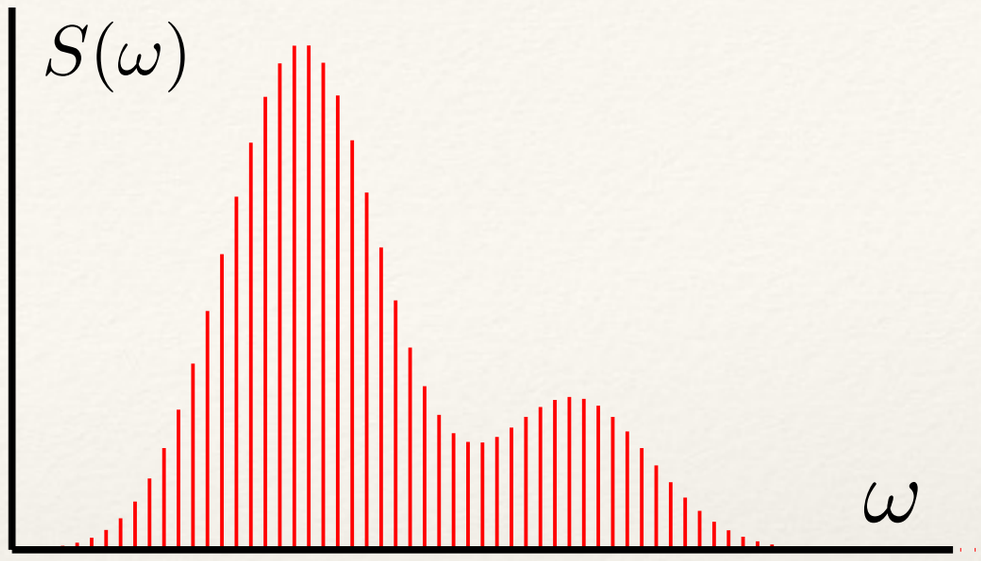
$$\chi^2 = \sum_i \sum_j [G_S(\tau_i) - G(\tau_i)] C_{ij}^{-1} [G_S(\tau_j) - G(\tau_j)]$$

Parametrization and Regularization

Represent the spectrum using some suitable generic parametrization

- e.g., sum of many delta functions

$$S(\omega) = \sum_{i=1}^{N_\omega} A_i \delta(\omega - \omega_i)$$



Manifestation of ill-posed analytic continuation problem:

- many spectra have almost same goodness-of-fit (close to best χ^2)

Need some way to regularize the spectrum, without loss of information

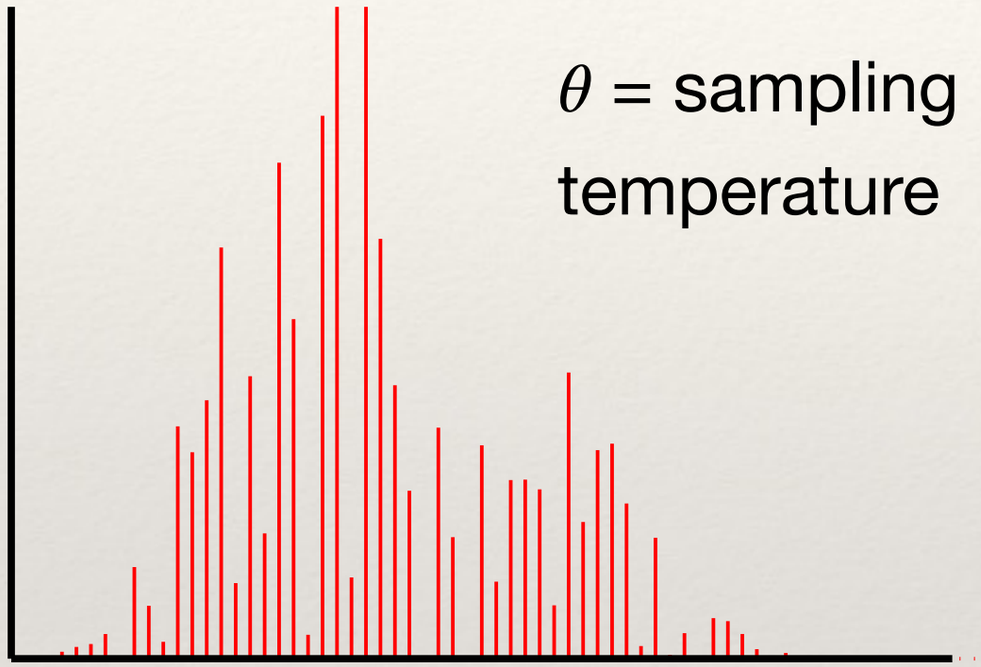
Stochastic analytic continuation (SAC)

White 1991, Sandvik 1998; Beach 2004; Syljuåsen 2008; Sandvik 2016,….

[slightly different approach: Mishchenko, Prokofev, Svistunov,… papers 2000-]

Sample the spectrum, using

$$P(S|G) \propto \exp\left(-\frac{\chi^2}{2\Theta}\right)$$



θ = sampling temperature

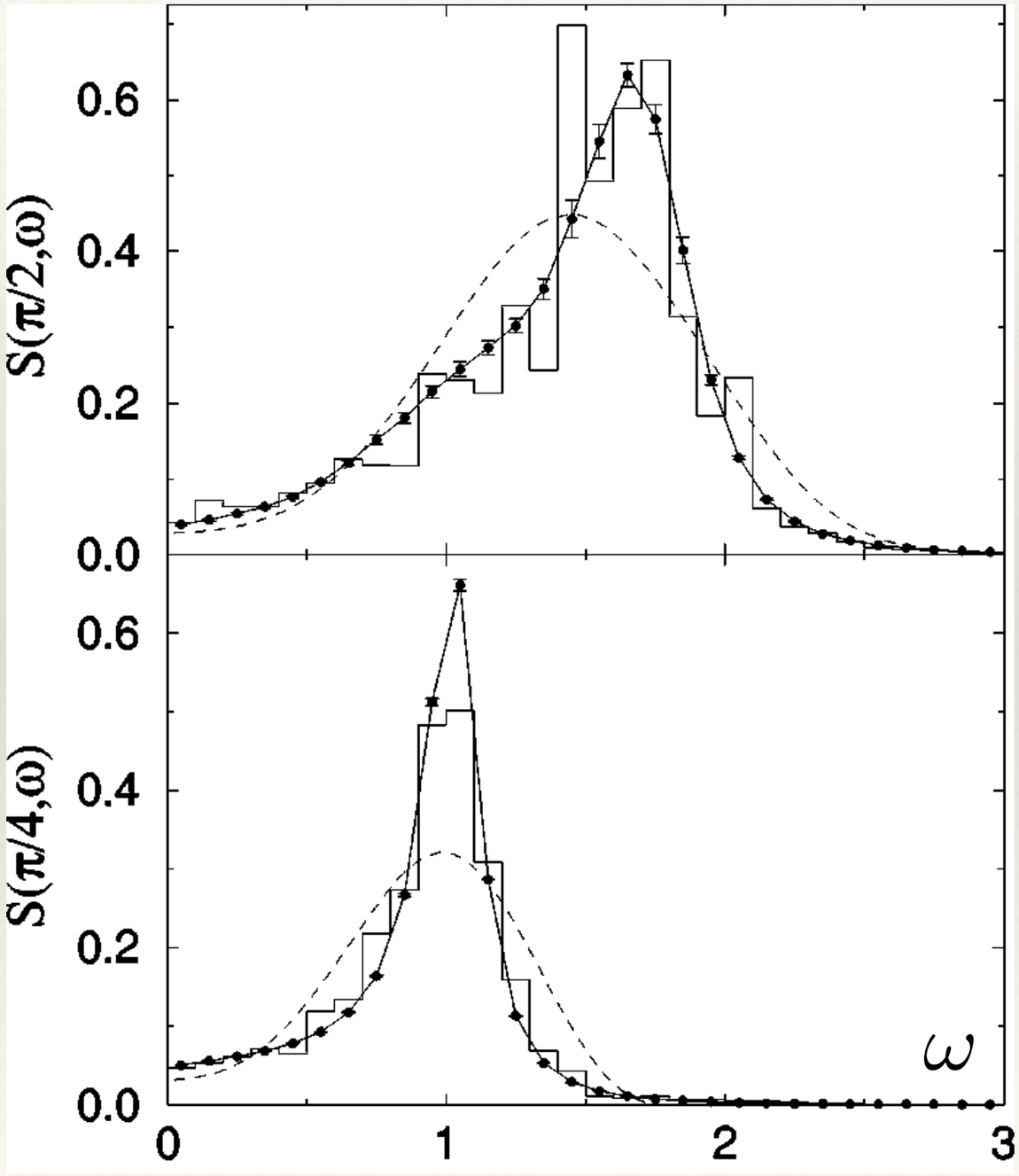
Monte Carlo sampling in space of delta functions (or other space)

- average <S(ω)> is smooth

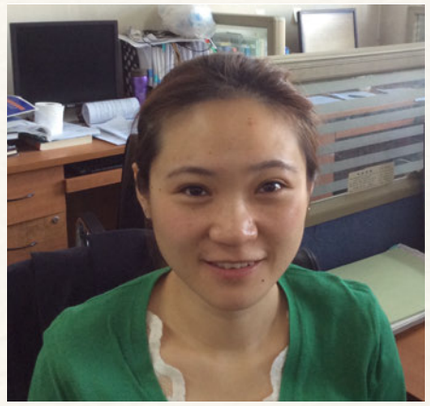
MaxEnt method can be regarded as mean-field version of SAC (Beach 2004)

Heisenberg chain, T=J/2 (PRB 1998)

- SAC seems better than MaxEnt



Improved SAC scheme



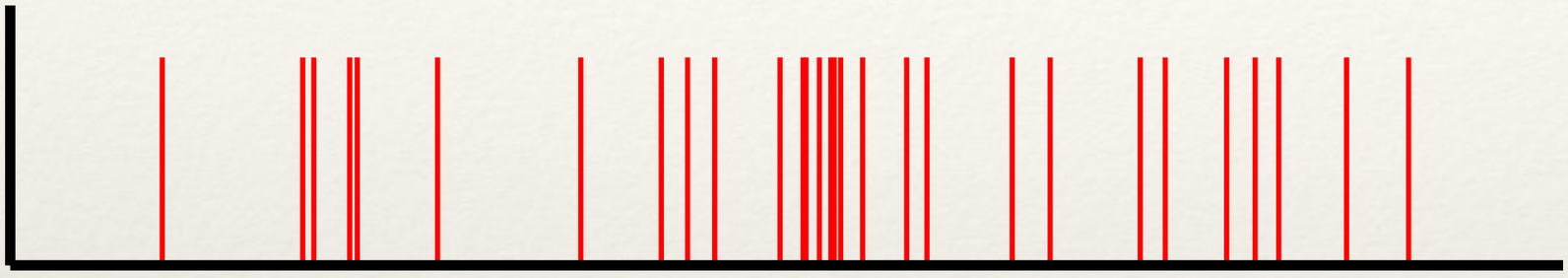
H. Shao & A. Sandvik

PHYSICAL REVIEW X **7,** 041072 (2017) + work in progress

New parametrization:

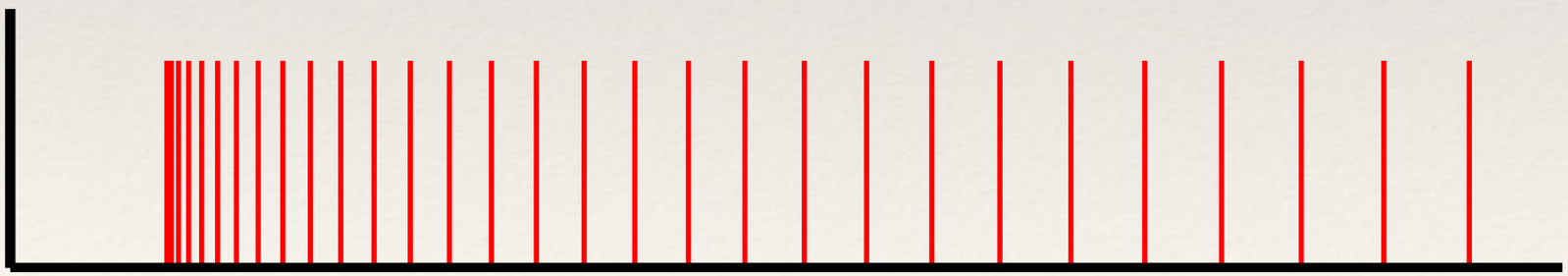
Nω δ-functions of equal amplitude in continuum

- use histogram to collect “hits”



Can build in “prominent features”, e.g., δ-fktn at the edge

Use monotonically increasing distances for a single peak at edge



Generalization possible for peak at arbitrary location
or set number of more than one peak

Determining the sampling temperature

$$P(S) \propto \exp(-\chi^2/2\theta)$$

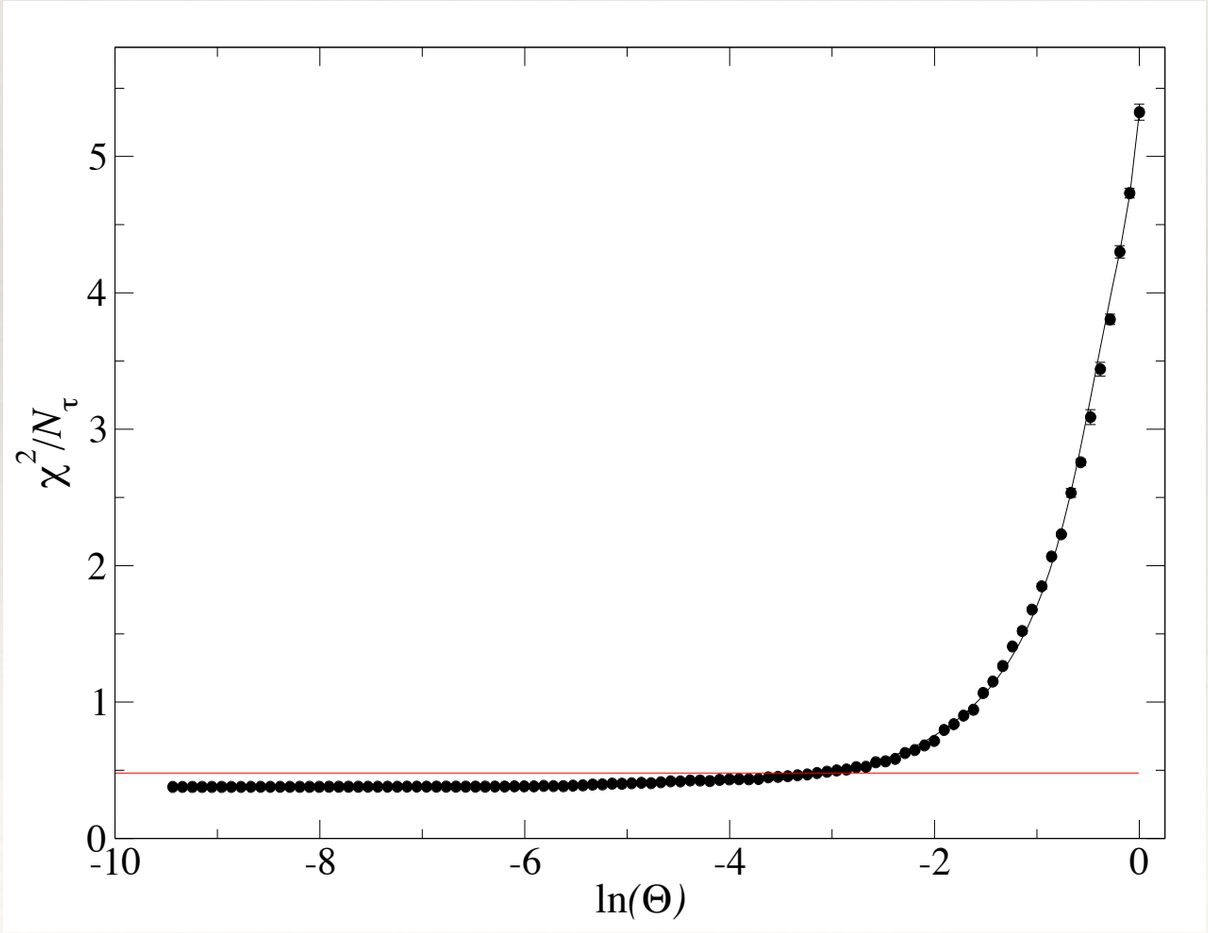
Example: L=16 Heisenberg chain, S(π/2,ω), T/J=0.5

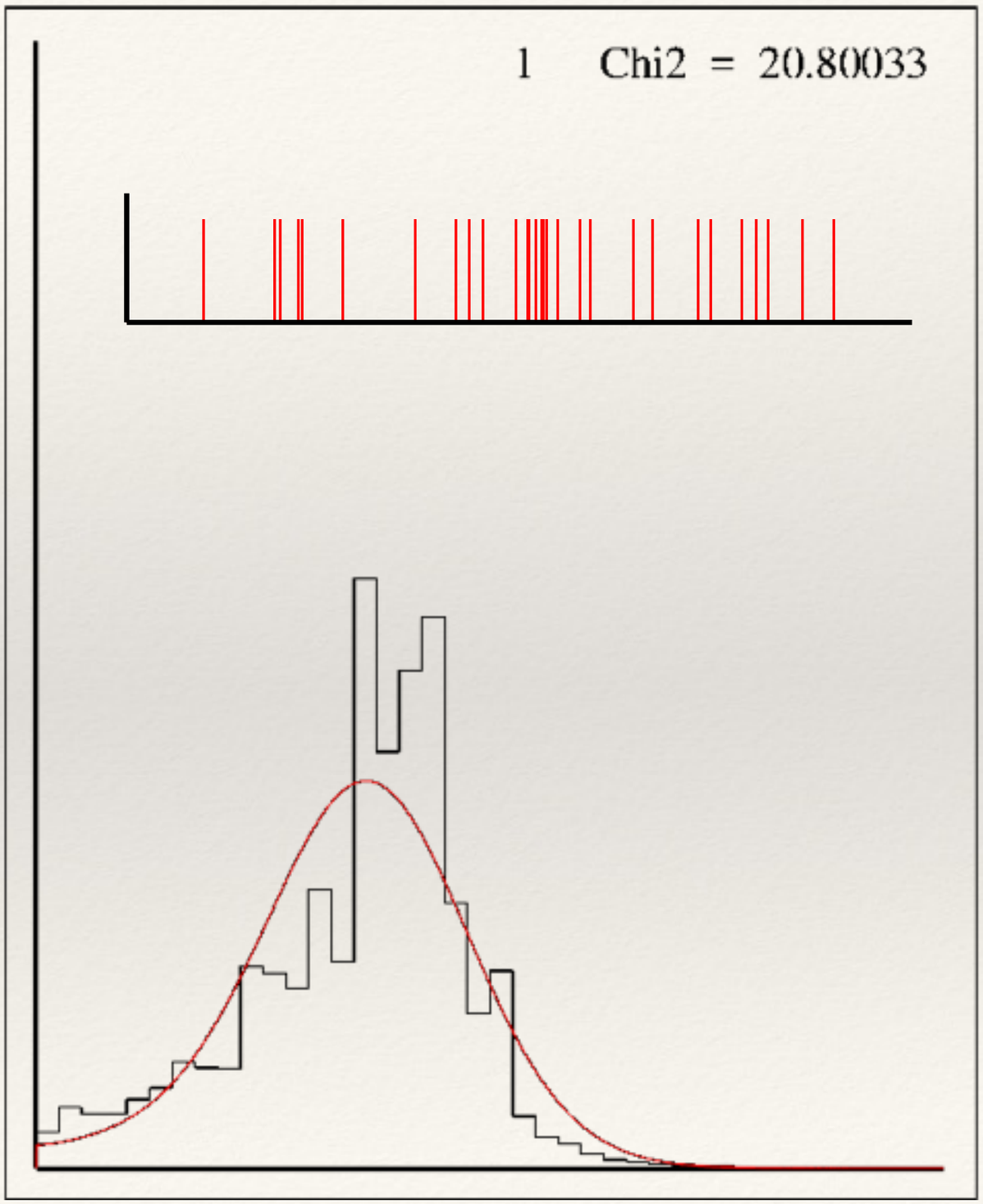
Dependence on the sampling temperature, θ = 10/1.1^n, n=0,1,2,…

Choose θ such that

$$\langle \chi^2 \rangle = \chi^2_{\min} + a\sqrt{\chi^2_{\min}},\ a \approx 1$$

- statistically motivated
- the spectrum fluctuates and data not overfitted

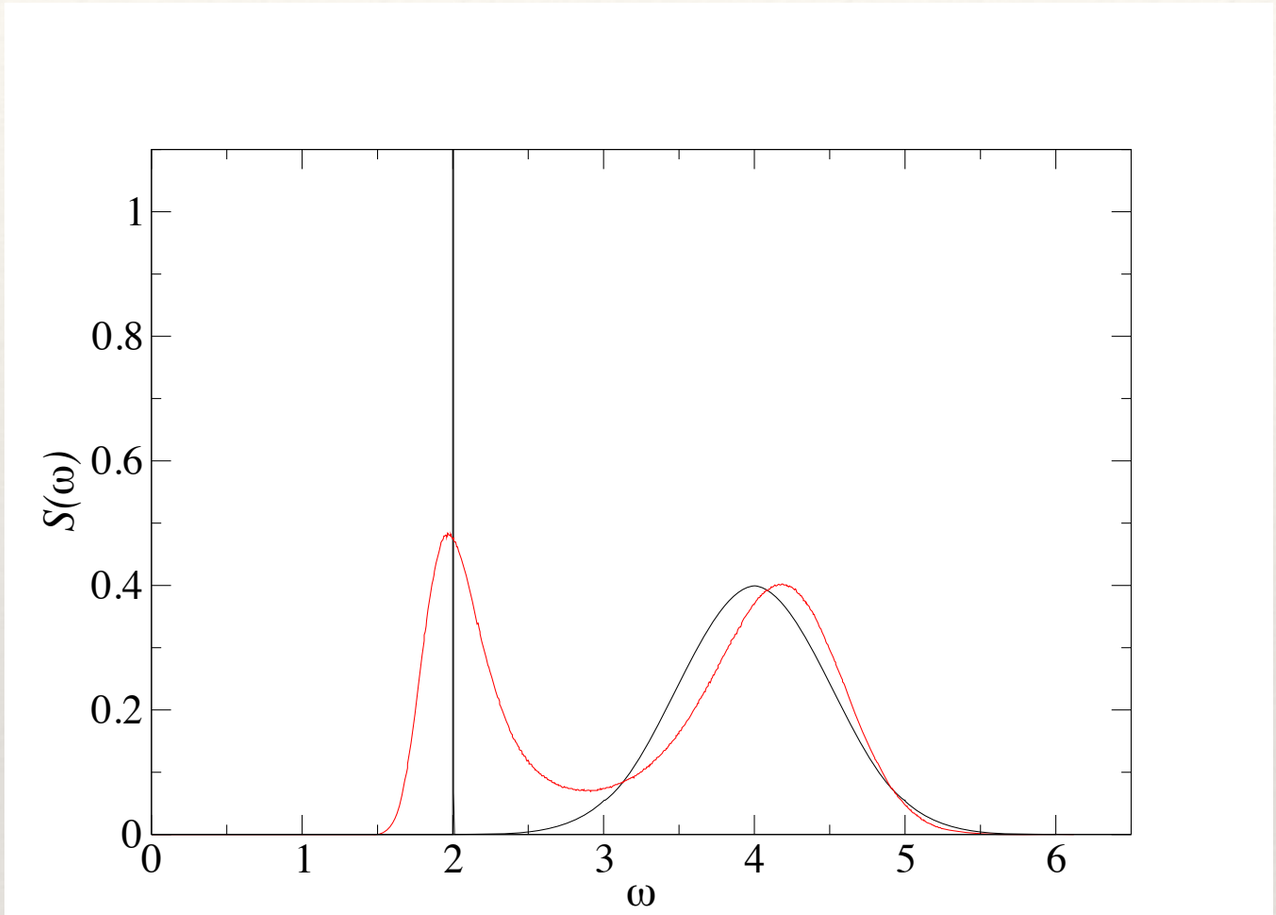




Spectra with sharp features

Example: Delta-function and continuum, test with synthetic data

- noise level $2*10^{-5}$ (20 τ points, $\Delta\tau$=0.1)



Free sampling cannot resolve the delta function very well

- high-energy peak is also distorted

Solution:

use one special δ-function,

- adjustable weight a_0 at ω_0
- other delta-functions can not go below ω_0

Moving weight to the main delta function affects the sampling entropy

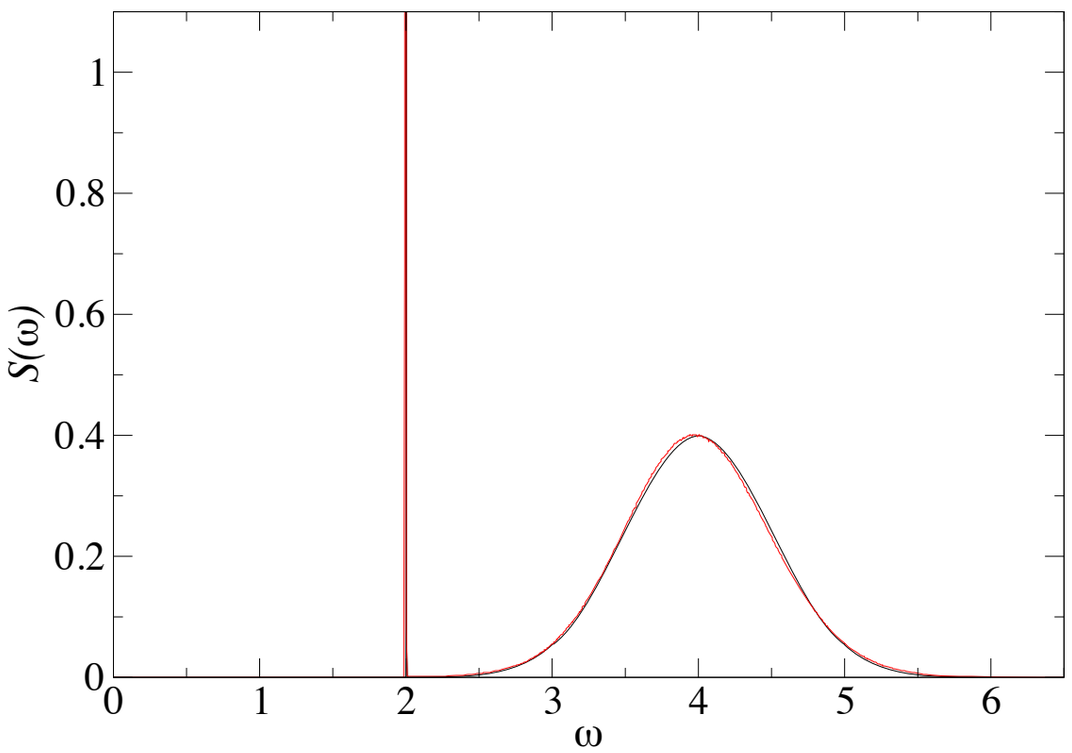
- detected in $<\chi^2>$ vs a_0

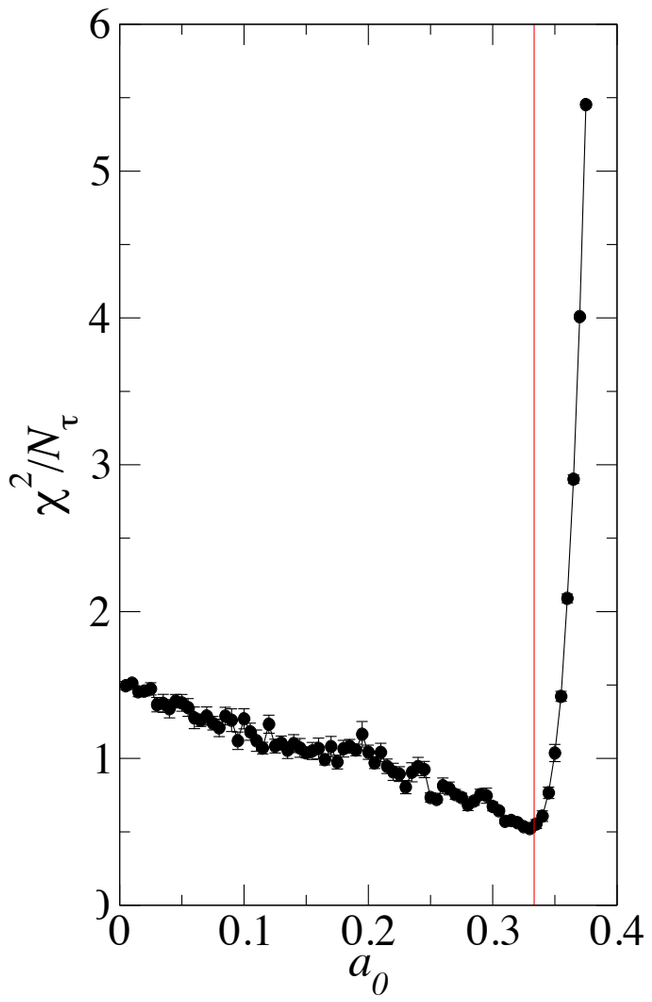
Results with 1+500 δ fktns

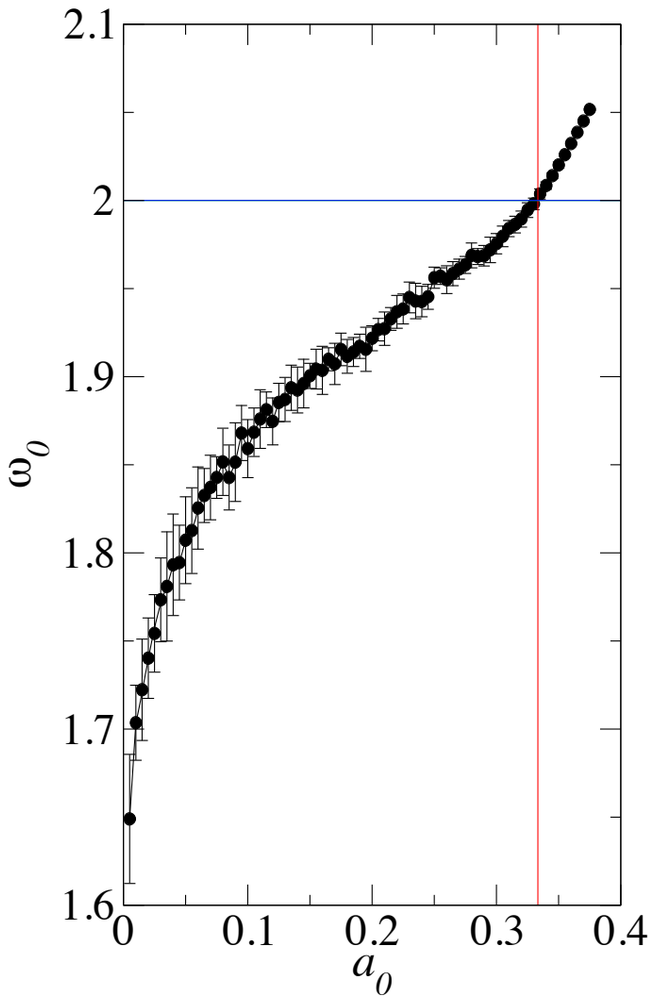
$<\chi^2>$ minimum observed

- gives the correct weight and location of the δ-function

The entire spectrum is very well reproduced







Fix a slightly higher sampling temperature to see minimum more clearly

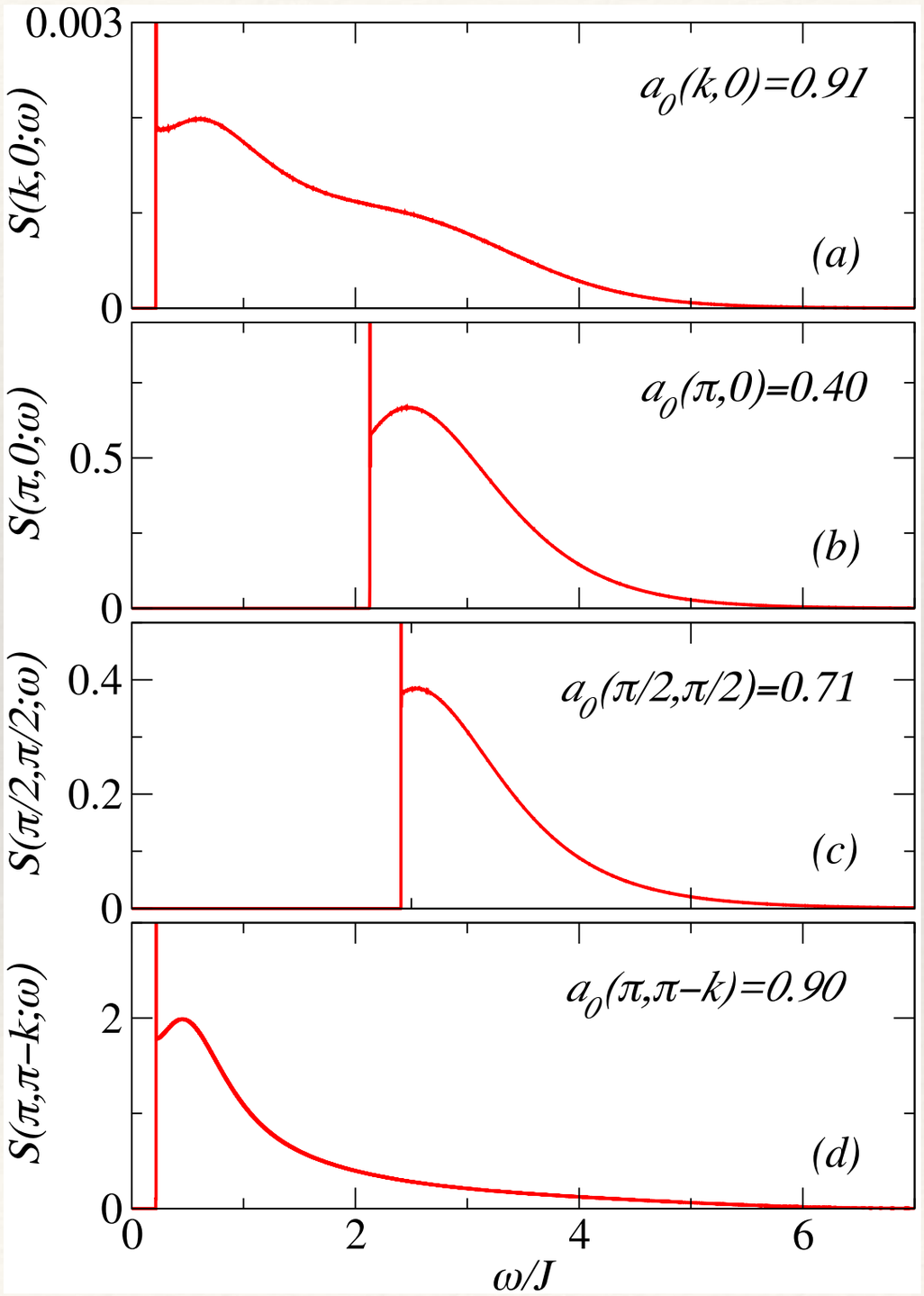
Success here isn't surprising:

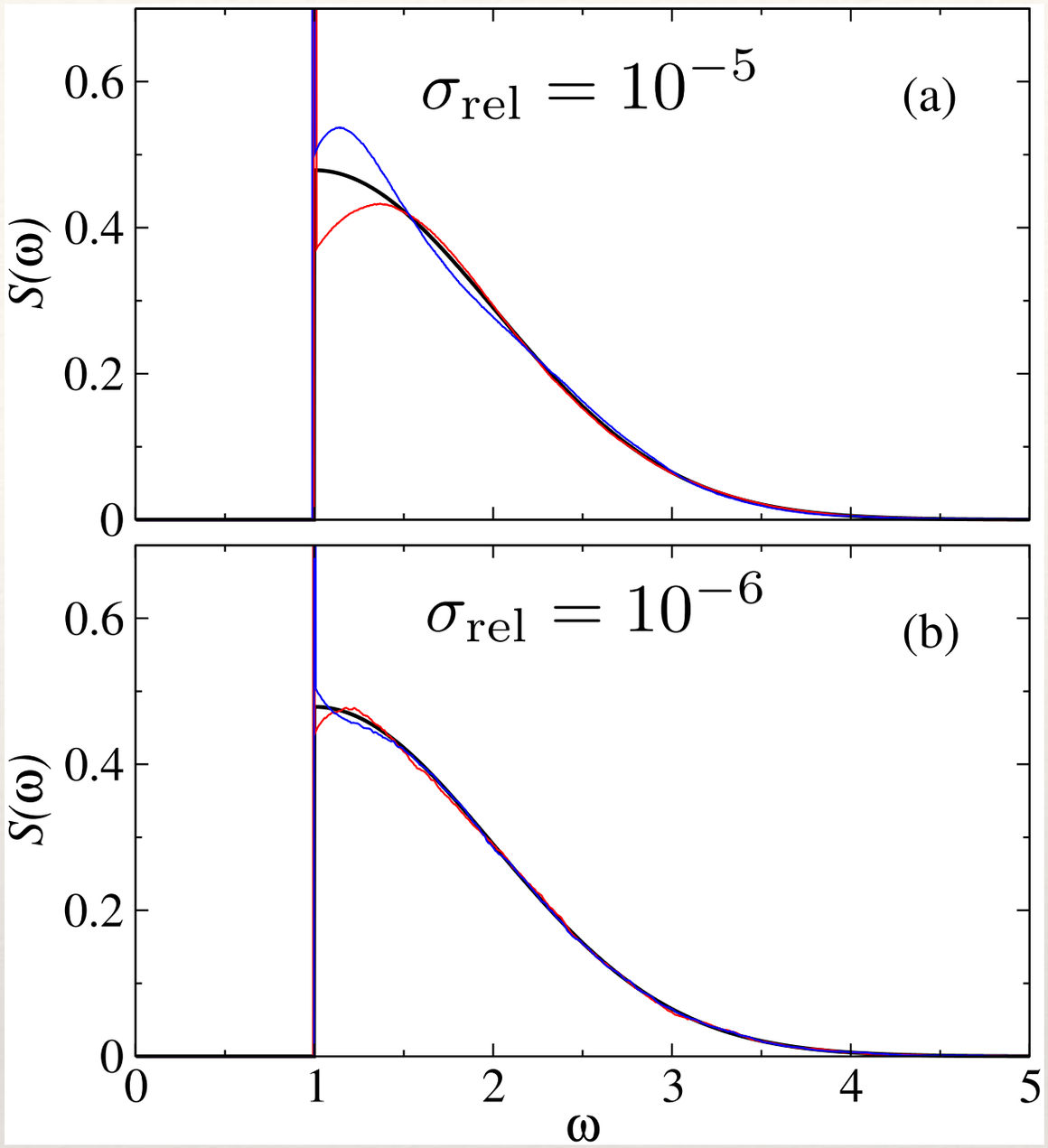
- clear separation of δ-fktn and continuum

More challenging case:

continuum touches δ-fktn

Synthetic spectrum, $a_0 = 0.4$, $\omega_0 = 1$





2D Heisenberg model

Shao, Qin, Capponi, Chesi, Meng, Sandvik, PRX 2017

- nearly deconfined spinons at q≈(π,0)

ARTICLES
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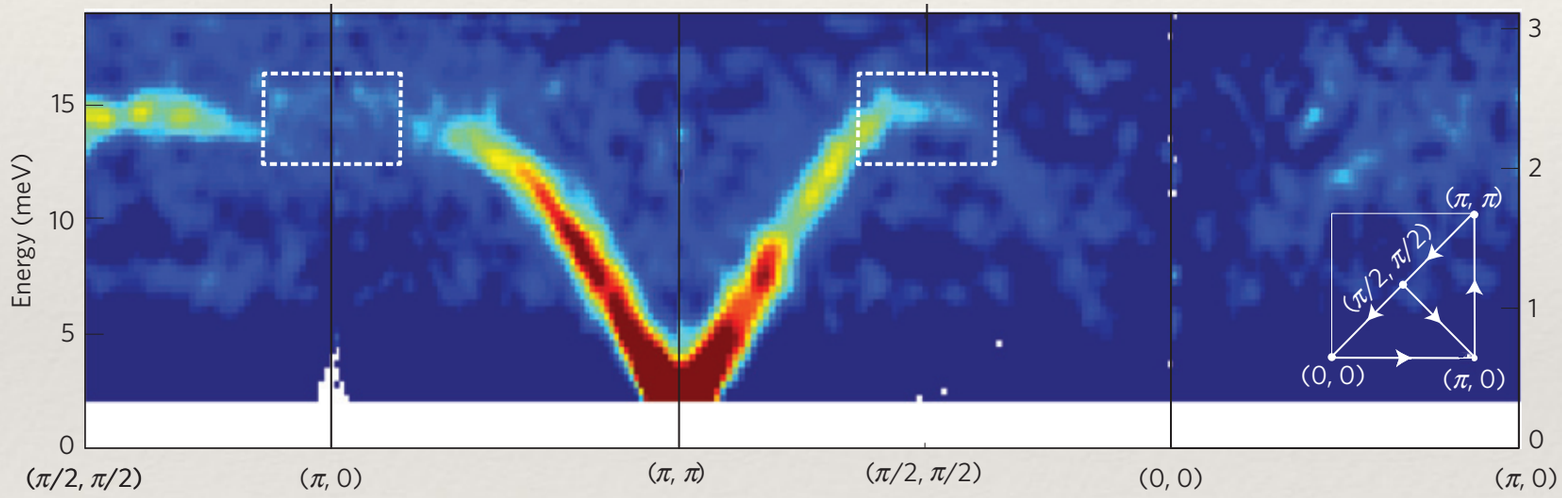
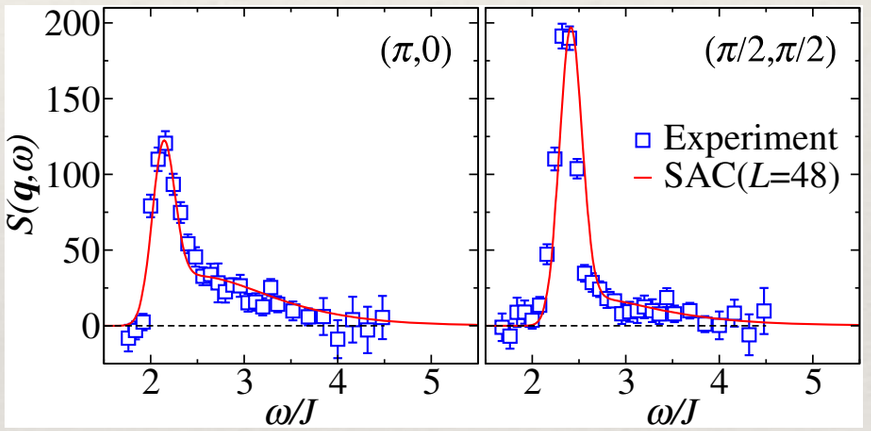
nature physics

Fractional excitations in the square-lattice quantum antiferromagnet $Cu(DCOO)_2 \cdot 4D_2O$

B. Dalla Piazza[1]*, M. Mourigal[1,2,3]*, N. B. Christensen[4,5], G. J. Nilsen[1,6], P. Tregenna-Piggott[5], T. G. Perring[7], M. Enderle[2], D. F. McMorrow[8], D. A. Ivanov[9,10] and H. M. Rønnow[1,11]

High-energy (~J) excitations are non-trivial: **signs of spinon deconfinement**





PHYSICAL REVIEW X **7,** 041072 (2017) **Nearly Deconfined Spinon Excitations in the Square-Lattice Spin-1/2 Heisenberg Antiferromagnet**

Hui Shao,[1,2,*] Yan Qi Qin,[3,4] Sylvain Capponi,[6,2] Stefano Chesi,[1] Zi Yang Meng,[3,5,†] and Anders W. Sandvik[2,1,‡]

Results agree well with experiments
- J-Q model demonstrates **mechanism of deconfinement**