Algorithms in Lattice Gauge Theory and Spin Systems
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Dynamics: Analytic Continuation

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Outline

QMC imaginary-time correlations and spectral functions
The Maximum-Entropy method
Stochastic analytic continuation
Progress on spectra with sharp features

SIMONS FOUNDATION

SSE calculations of imaginary-time correlations

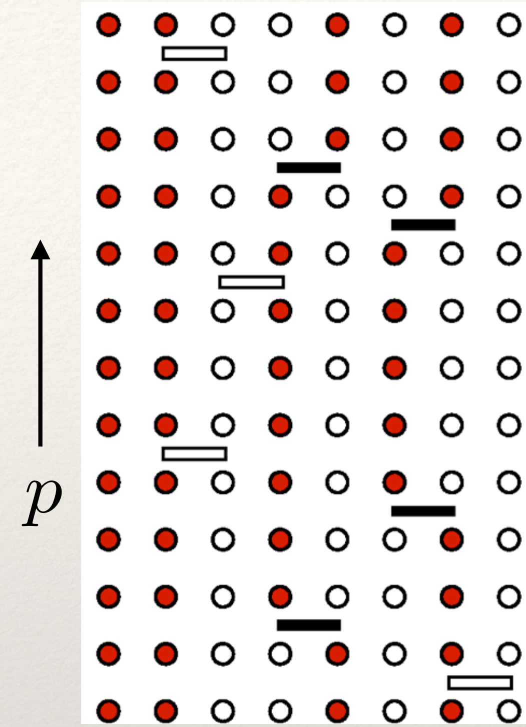
Time evolved operator: $A(\tau) = \mathrm{e}^{\tau H} A \mathrm{e}^{-\tau H}$

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

By Taylor expansion:

$F(m)$

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



F(m) 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 $\tau = i\Delta_\tau$ (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(τ) 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(τ) from QMC for some points τ_i, i=1,2,…,Nτ
- 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	$G(\tau)$	$\sigma(\tau)$ (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 $S(\omega)$ 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

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

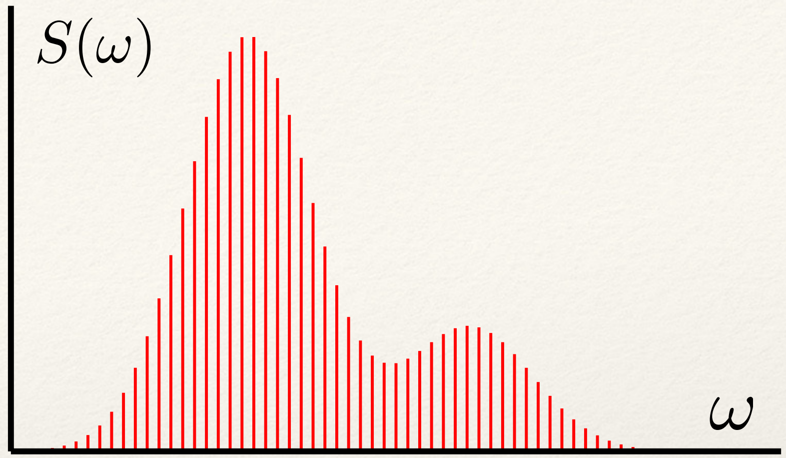
QMC statistical errors are correlated; use covariance matrix

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

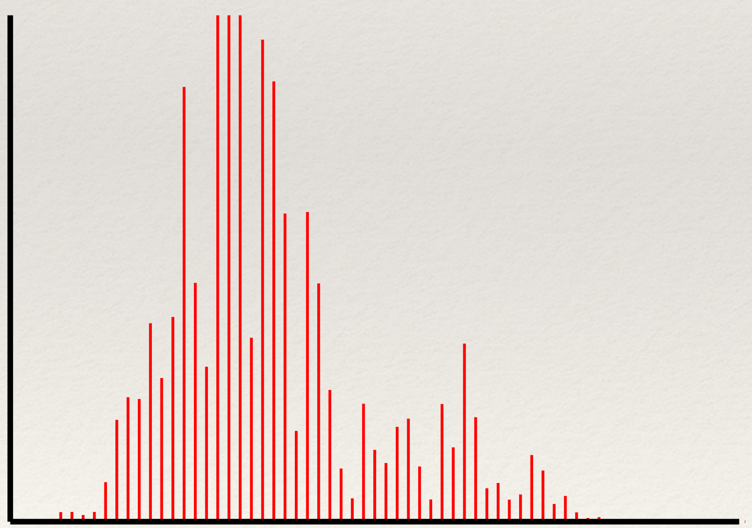
Parametrization and Regularization

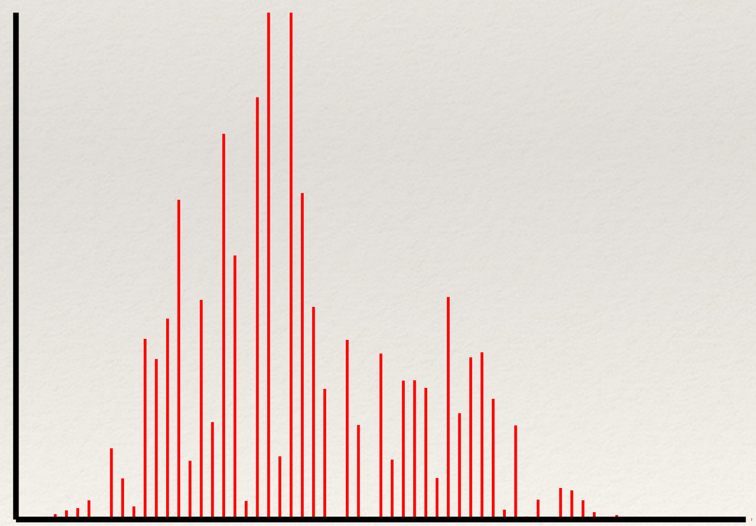
Represent the spectrum using
some suitable generic parametrization
- e.g., sum of many delta functions

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



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

The Maximum Entropy (MaxEnt) method

Silver, Sivia, Gubernatis, PRB 1990; Jarrell, Gubernatis, Phys. Rep. 1996

Bayes' Theorem: $P(S|G) \propto P(G|S)P(S)$ $\qquad P(G|S) \propto \exp(-\chi^2/2)$

Entropy quantifies amount of information (structure) in the spectrum

$$E = -\int d\omega S(\omega) \ln\left(\frac{S(\omega)}{D(\omega)}\right) \qquad P(S) \propto \exp\left(\alpha E\right)$$

D is a "default model"; result in the absence of data

$$P(S|G) \propto \exp(-\chi^2/2 + \alpha E)$$

Find S that maximizes P(S|G).

E has a smoothing effect if α is not too small

- how to choose α?
- different variants of the method use different criteria

MaxEnt method is widely used, many successes, but

- indications that E may smoothen the spectrum too much in some cases
- sharp features (edges, sharp peaks) cannot be resolved

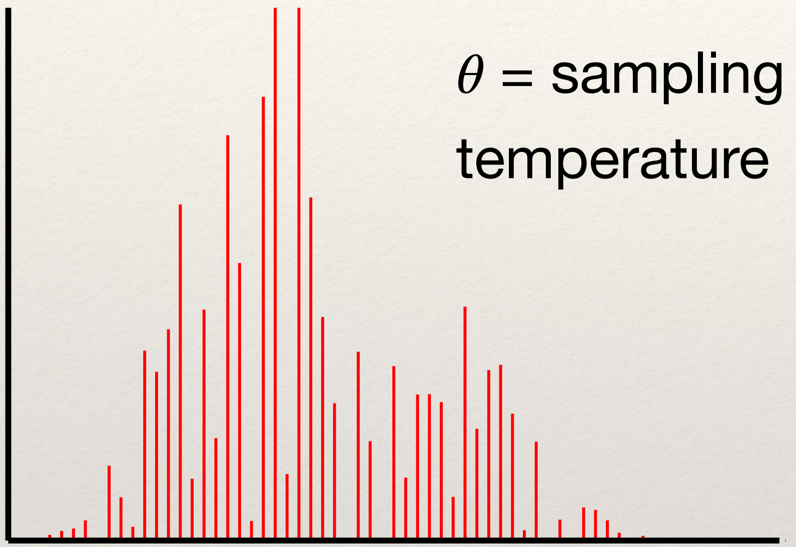
➔ Explore alternative methods

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

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



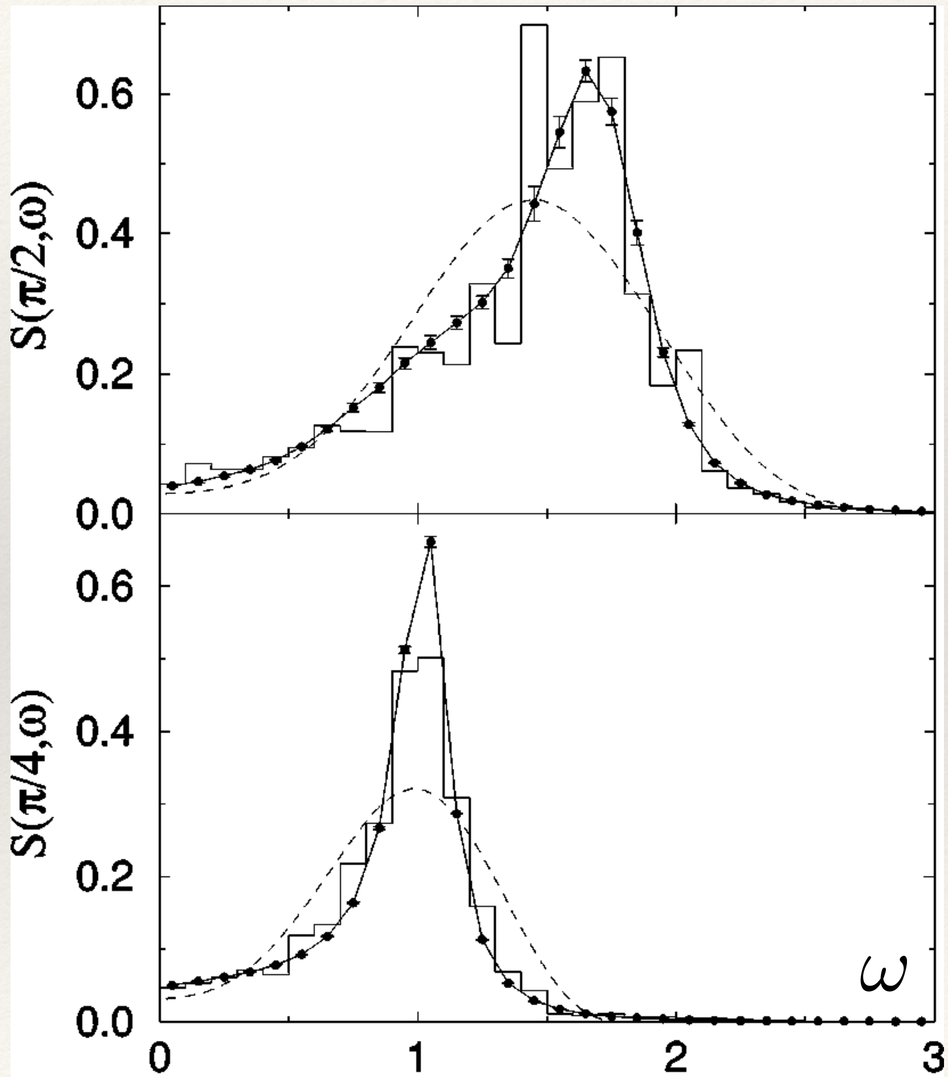
θ = sampling temperature

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



SAC and entropic pressure

How to choose θ?

White 1991, Syljuåsen 2008:

- just use θ=1

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

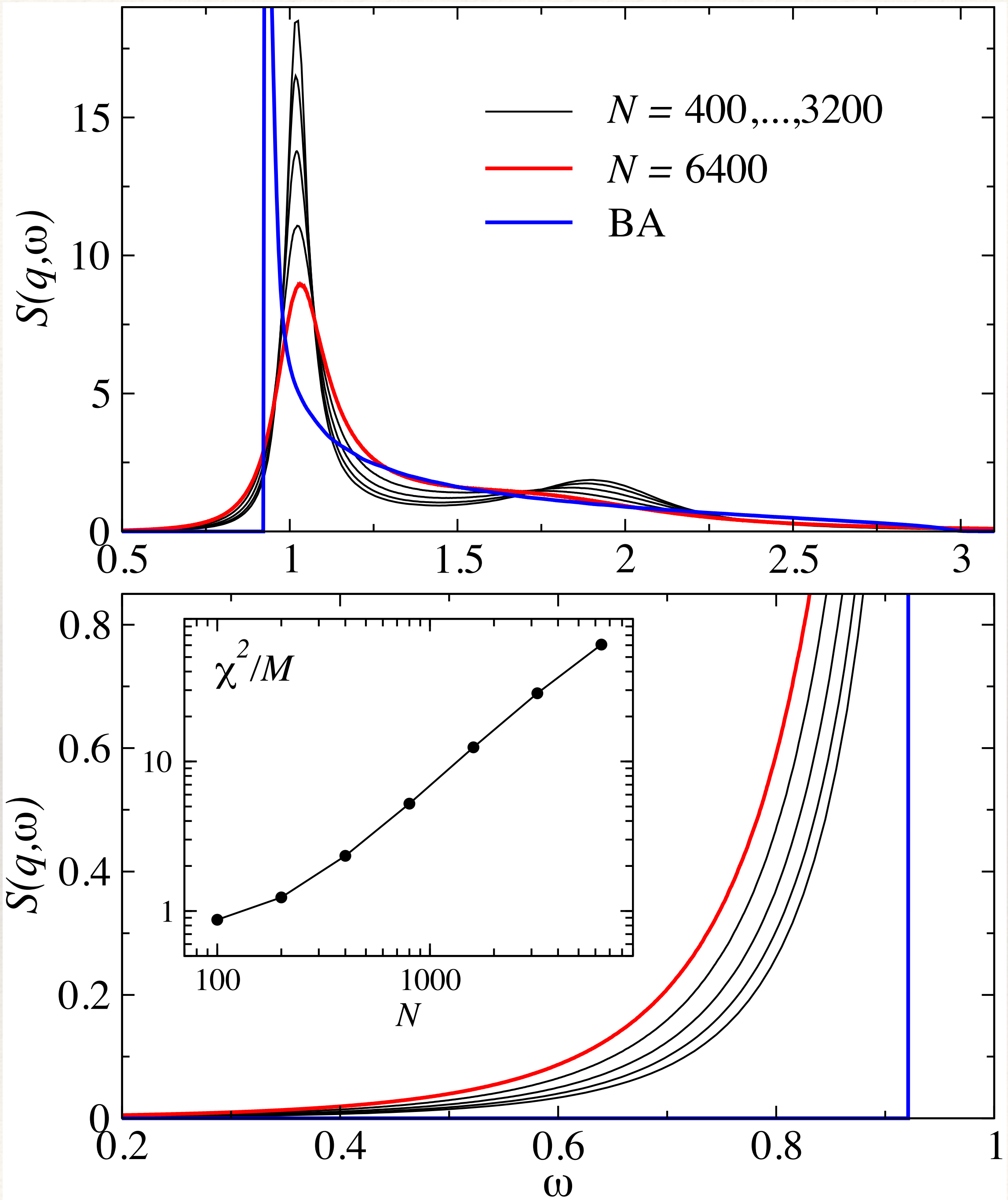
Leads to a problem
(Sandvik 2016)

when N$_\omega$ is large

- sampling become dominated by configurational entropy
- quality of fit deteriorates

Test case:
Dynamic structure factor of Heisenberg chain at T=0 (q=0.8π), L=500

Compare with:
Bethe Ansatz (almost exact)
(Sebastian Caux)



Reducing entropic pressures by constraints

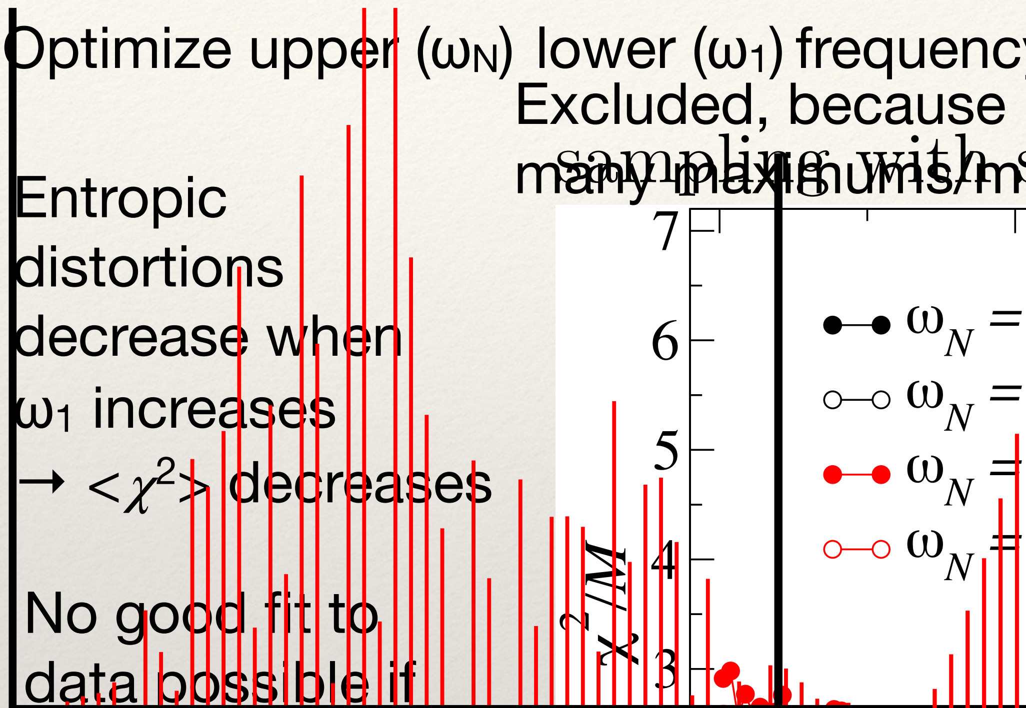
Sampling under constraint of fixed number of peaks in weights $A(\omega_i)$

- use the minimum number of peaks for which $\langle\chi^2\rangle$ is good

Optimize upper (ω_N) lower (ω_1) frequency bounds of the spectrum

Excluded, because many maximums/minimums

OK for 2-peak spectrum



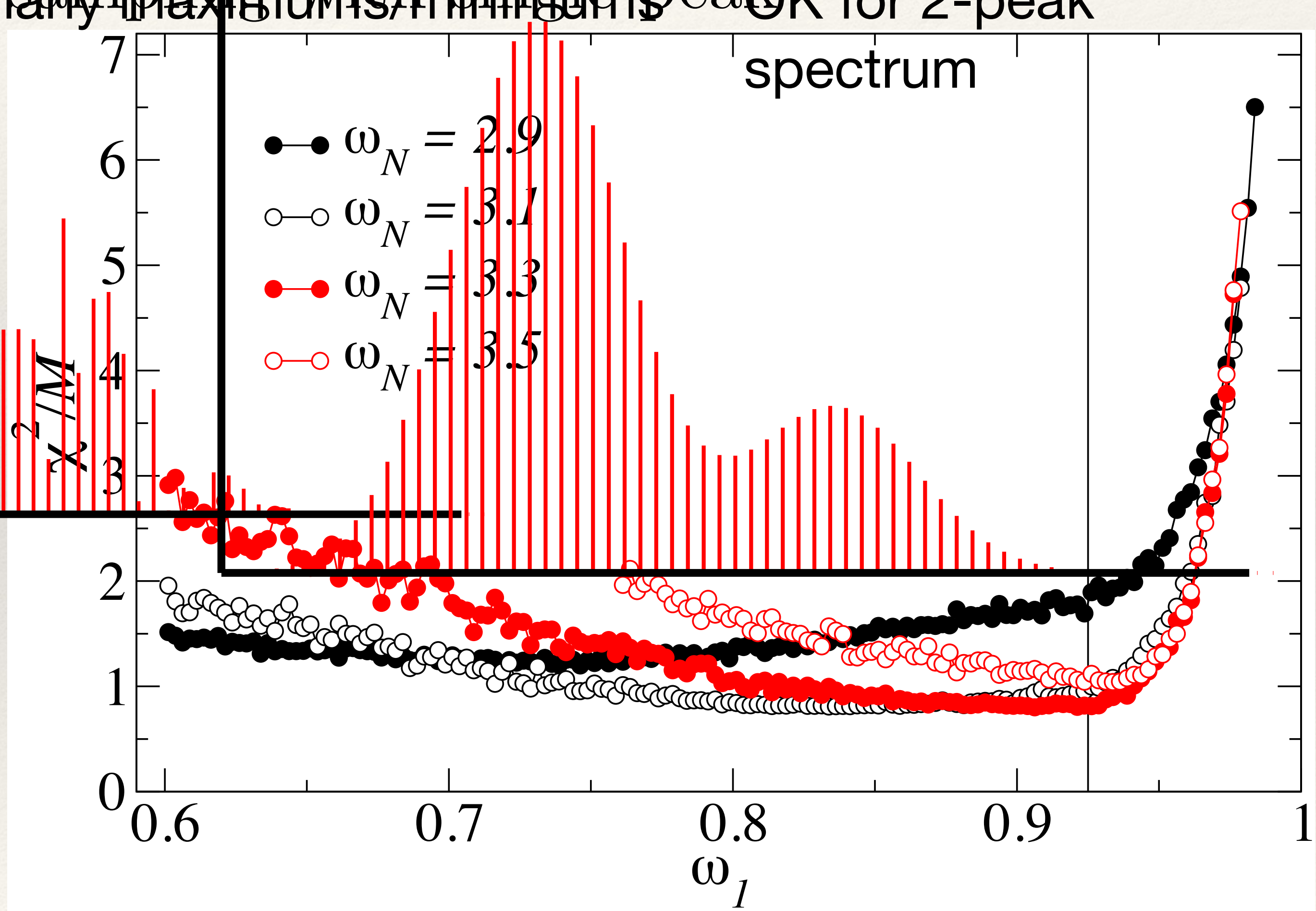
Entropic distortions decrease when ω_1 increases

→ $\langle\chi^2\rangle$ decreases

No good fit to data possible if ω_1 exceeds true lower bound

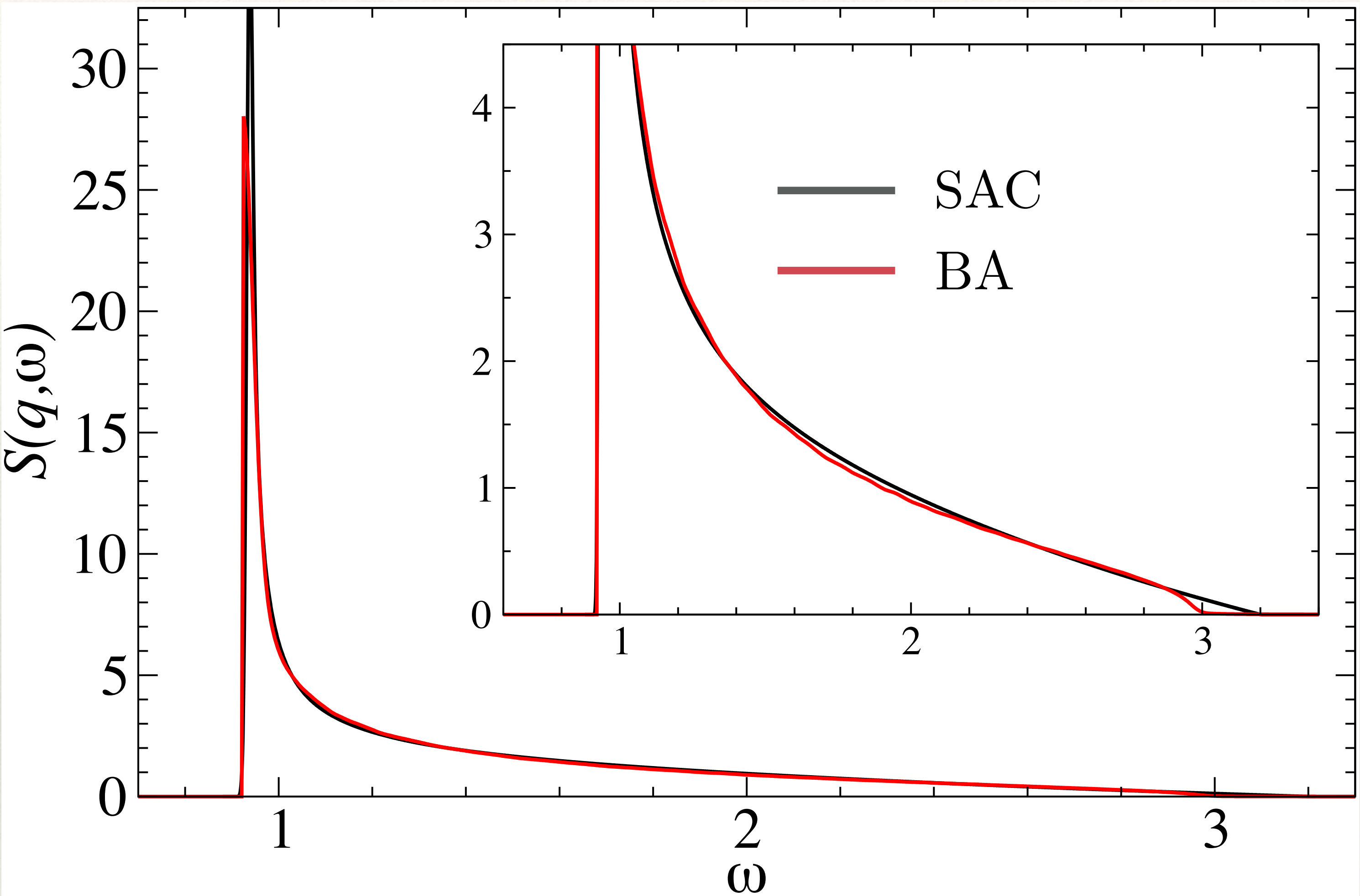
→ $\langle\chi^2\rangle$ increases

$\langle\chi^2\rangle$ minimum for best bounds



Heisenberg chain, $S(q=0.8\pi,\omega)$, L=500 (T→0)

Heisenberg chain, S(q=0.8π,ω), L=500, SAC and BA

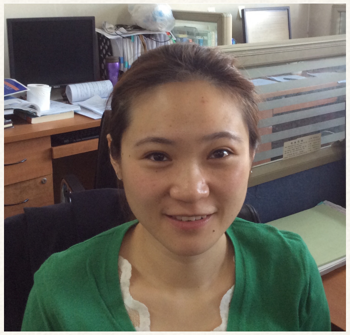


MaxEnt cannot produce a sharp edge with power-law singularity, even if the correct bounds are imposed (unless, perhaps, a singular default model is used).

SAC gave the above result without any prior knowledge except for the single-peak assumption!

Improved SAC scheme

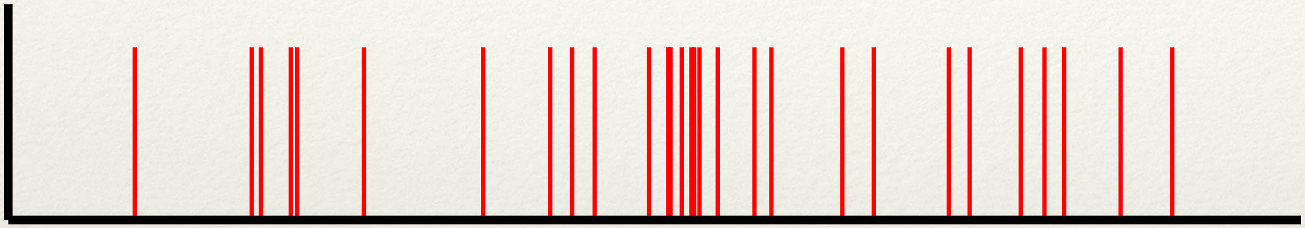
H. Shao & A. Sandvik - work in progress
(some applications published)



New parametrization:

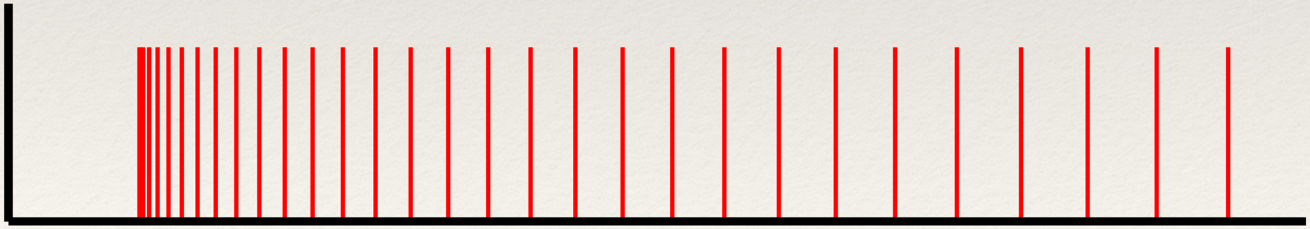
N_ω δ-functions of equal amplitude in continuum

- 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

Back to fighting entropy with temperature: $P(S) \propto \exp(-\chi^2/2\theta)$

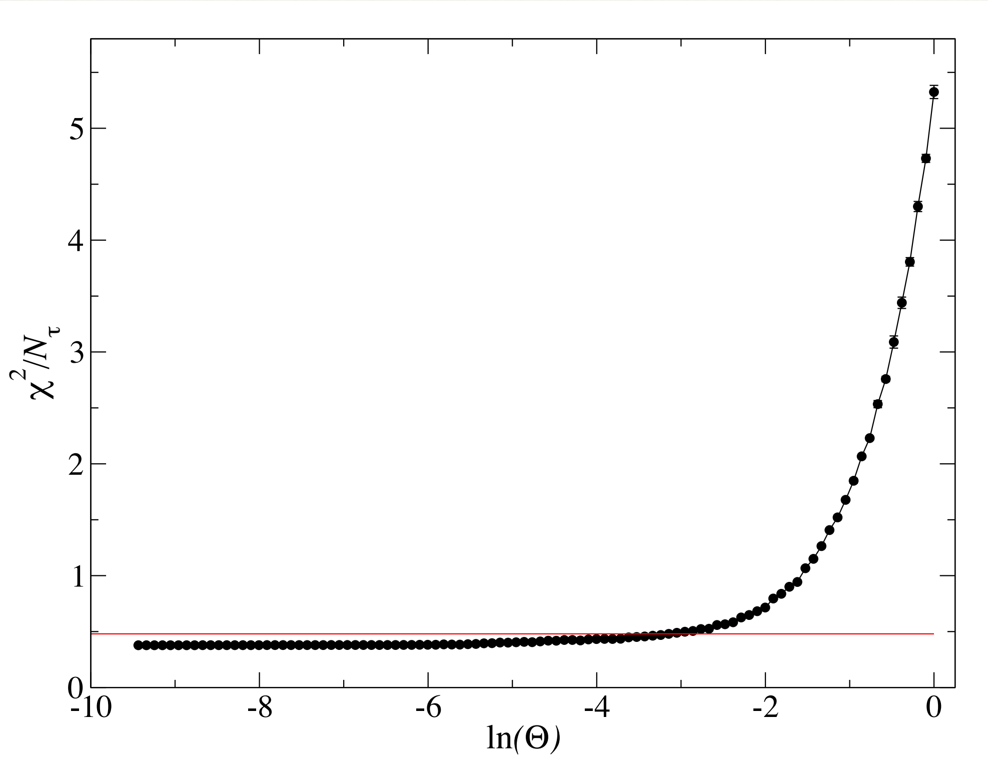
Example: L=16 Heisenberg chain, S(π/2,ω), T/J=0.5

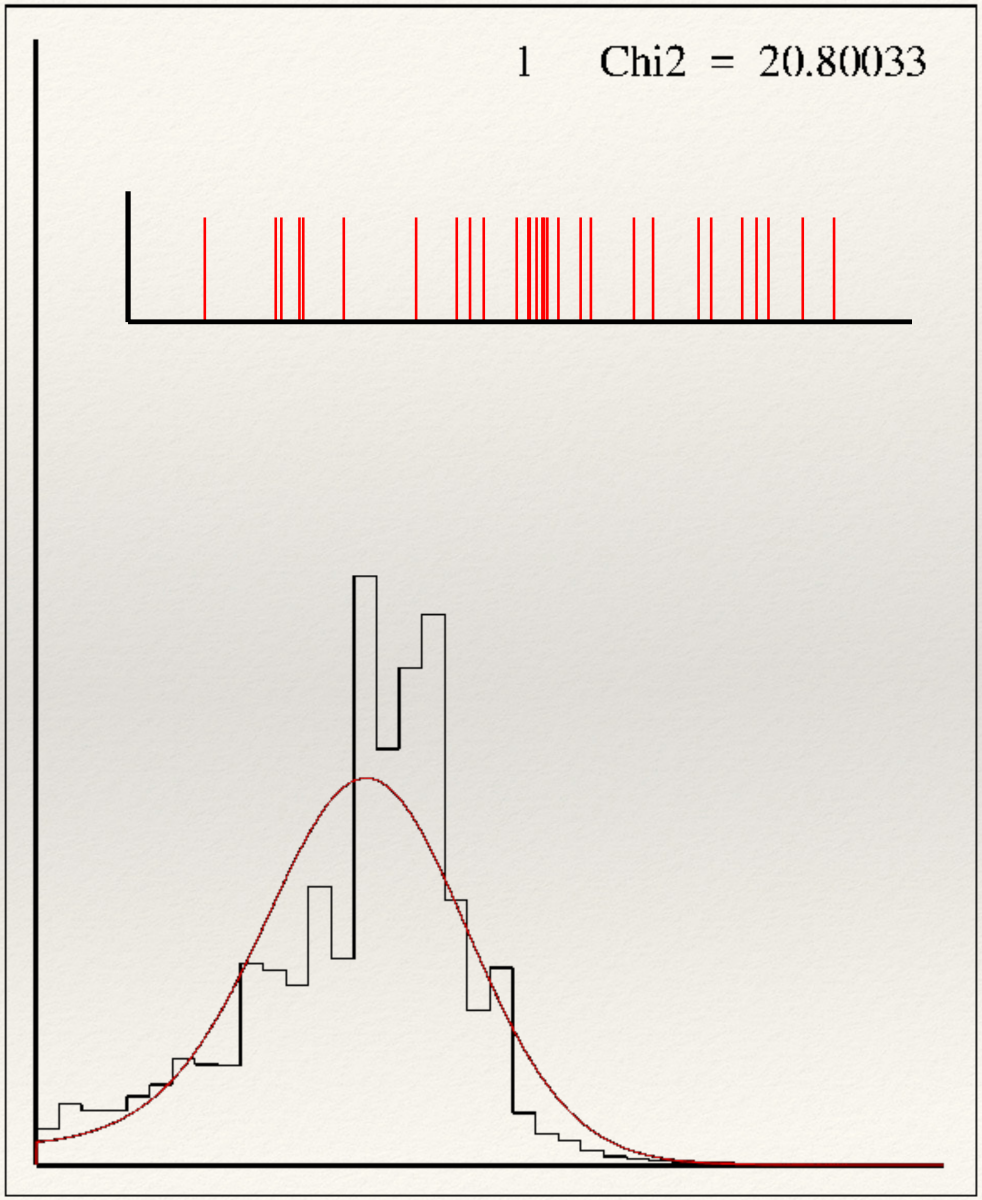
Dependence on the sampling temperature, θ = 10/1.1^n, n=0,1,2,…

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

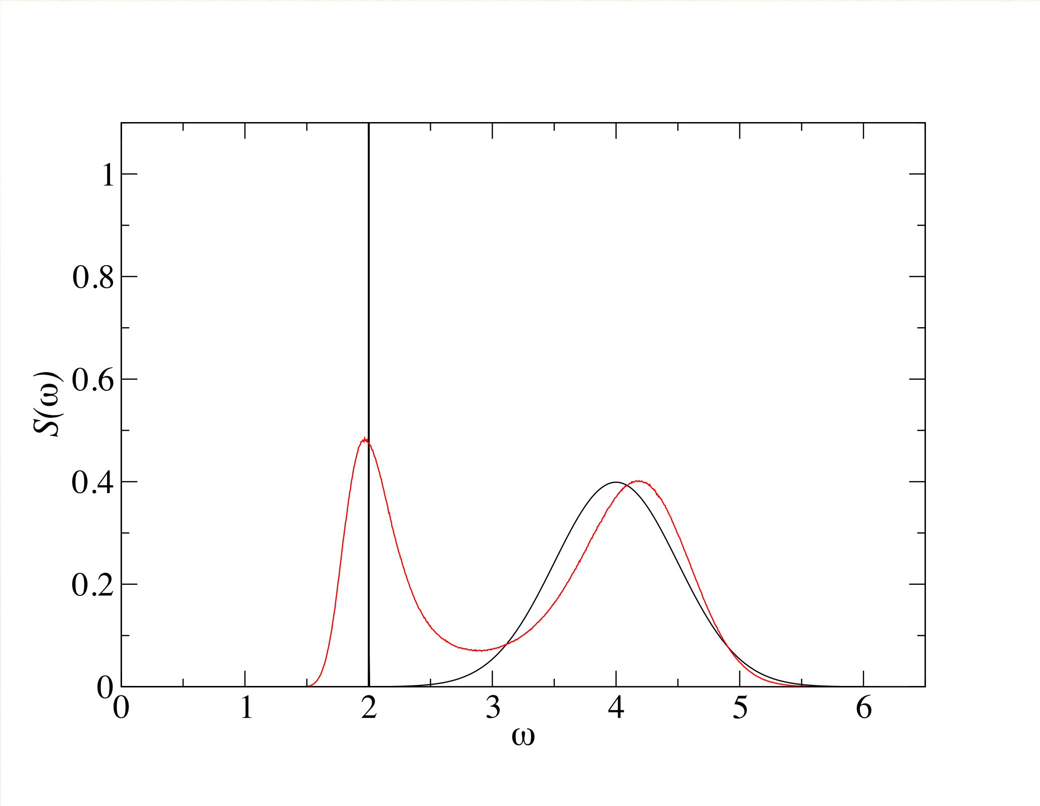




Spectra with sharp features

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

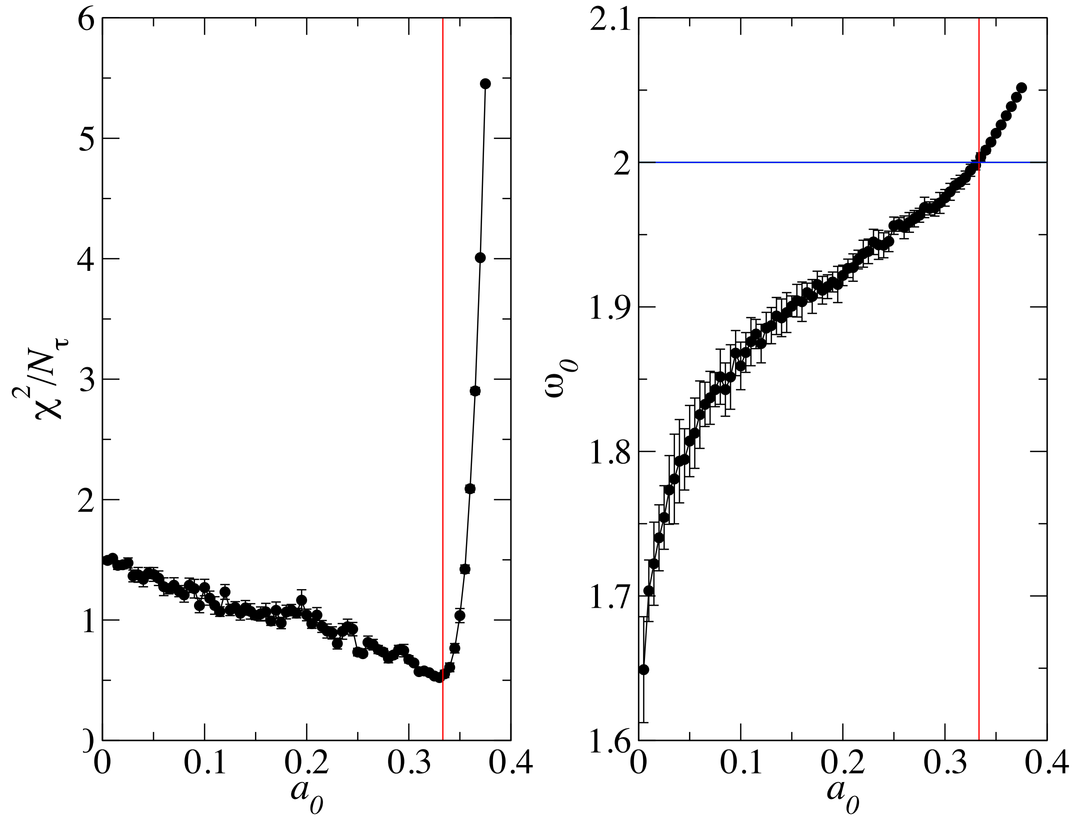
Moving weight to the main delta function affects the sampling entropy

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

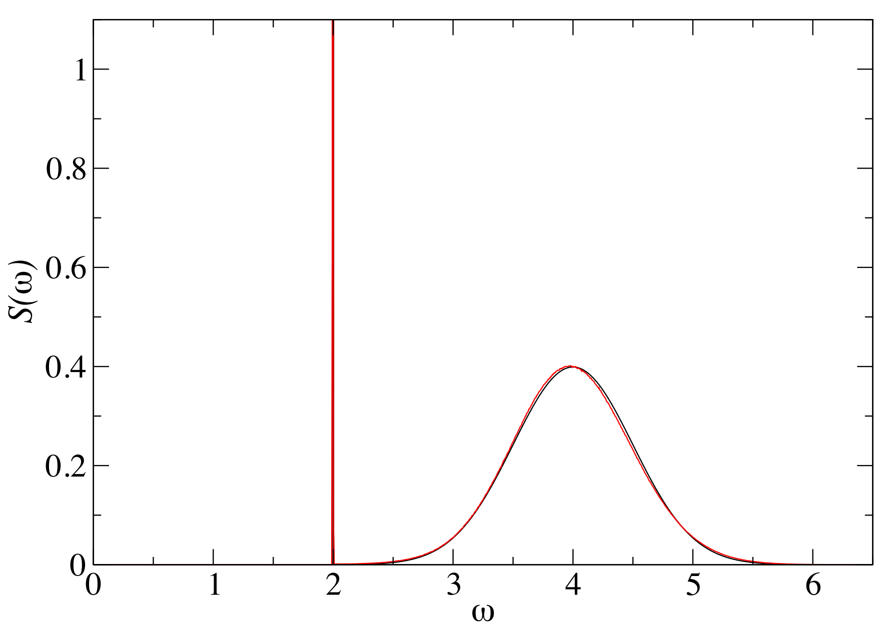
Results with 1+500 δ fktns

$<\chi^2>$ 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

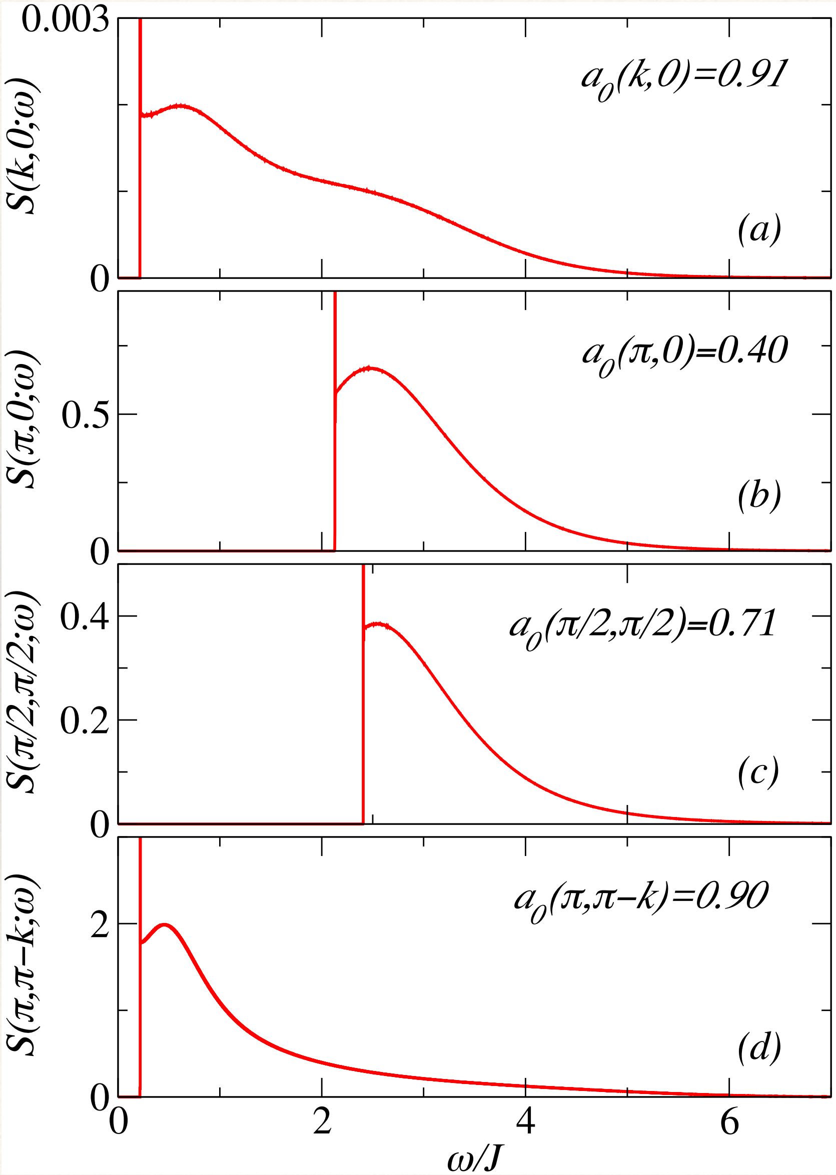
Success here isn't surprising:

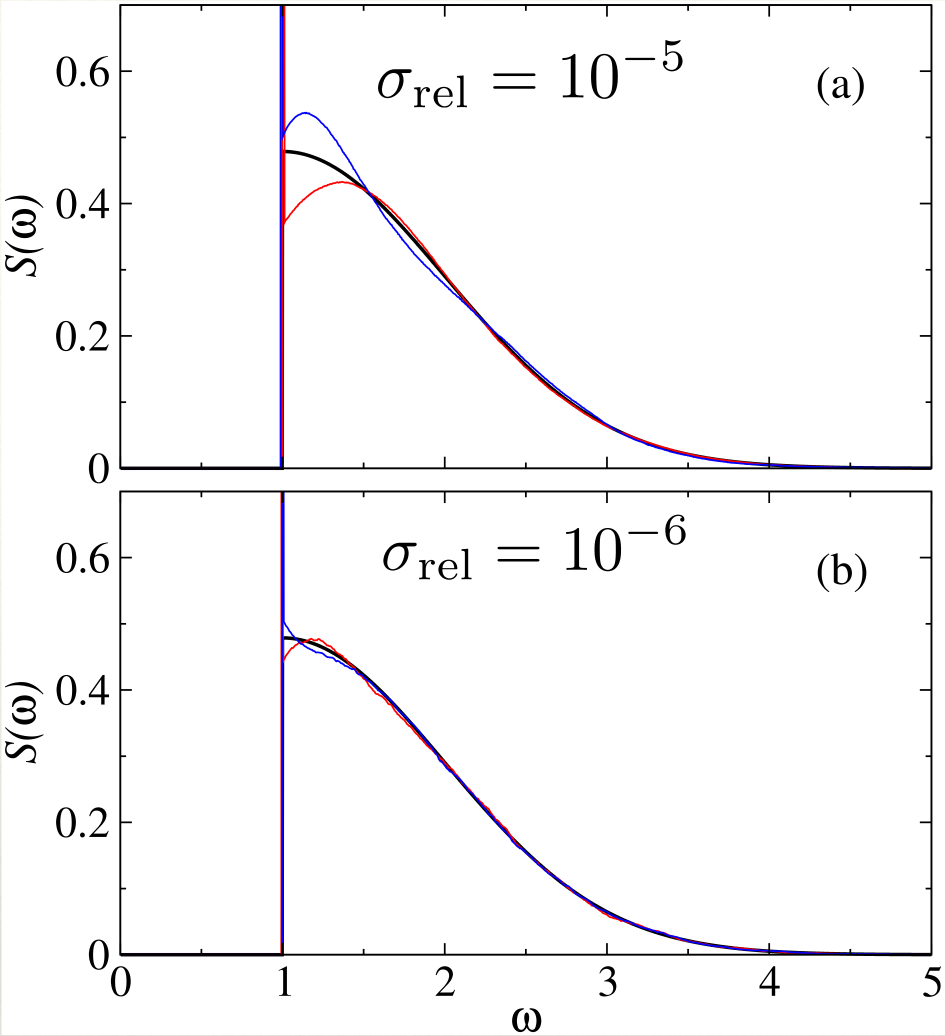
- clear separation of δ-fktn and continuum

More challenging case:

continuum touches δ-fktn

Synthetic spectrum, a_0 = 0.4, ω_0 = 1





2D Heisenberg model

Shao, Qin, Capponi, Chesi, Meng, Sandvik, PRX 2018

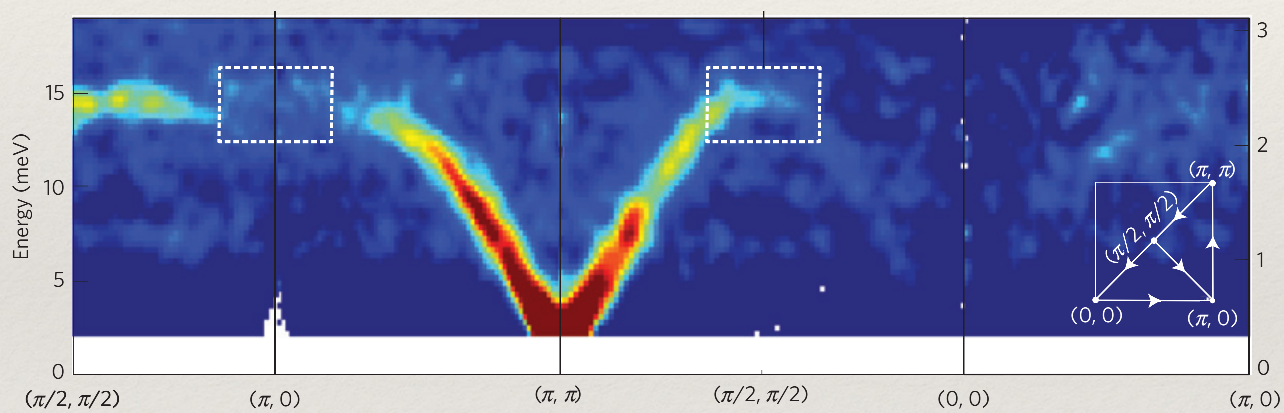
- nearly deconfined spinons at q≈(π,0)

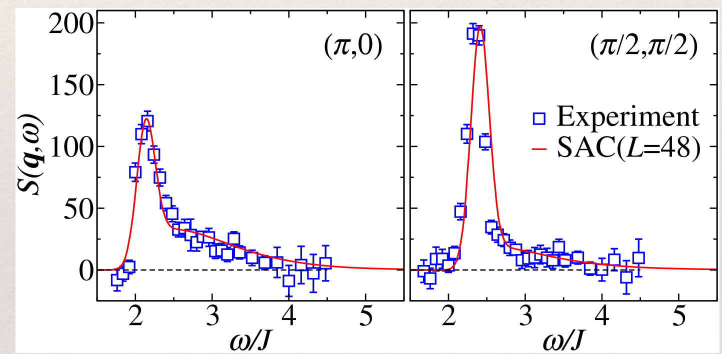
ARTICLES
PUBLISHED ONLINE: 23 DECEMBER 2014 | DOI: 10.1038/NPHYS3172
nature physics

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,‡]

QMC/SAC results agree well with experiments
- J-Q model demonstrates **mechanism of deconfinement**