Workshop on Diagrammatic Monte Carlo Methods for QFTs in Particle-, Nuclear-, and Condensed-Matter Physics, MITP, 18-29 September, 2017

Analytic Continuation with Optimized Features

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Outline

- Time correlations and spectral functions
- Recent developments of sampling methods (stochastic analytic continuation)
- Test results for known cases and synthetic data
- New results for excitations of 2D Heisenberg model

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Spectral functions and Imaginary time correlations

We want the spectral function of some operator

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

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):

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

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 (noisy) 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

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 minimize the "distance" to the QMC data points; mimimize

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

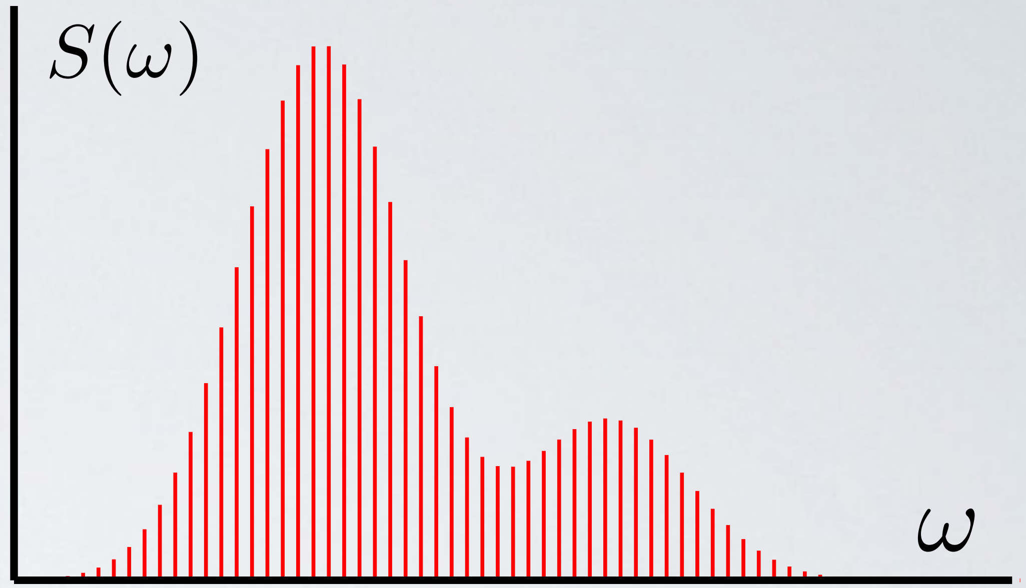
QMC statistical errors are correlated; actually has to use covariance matrix

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

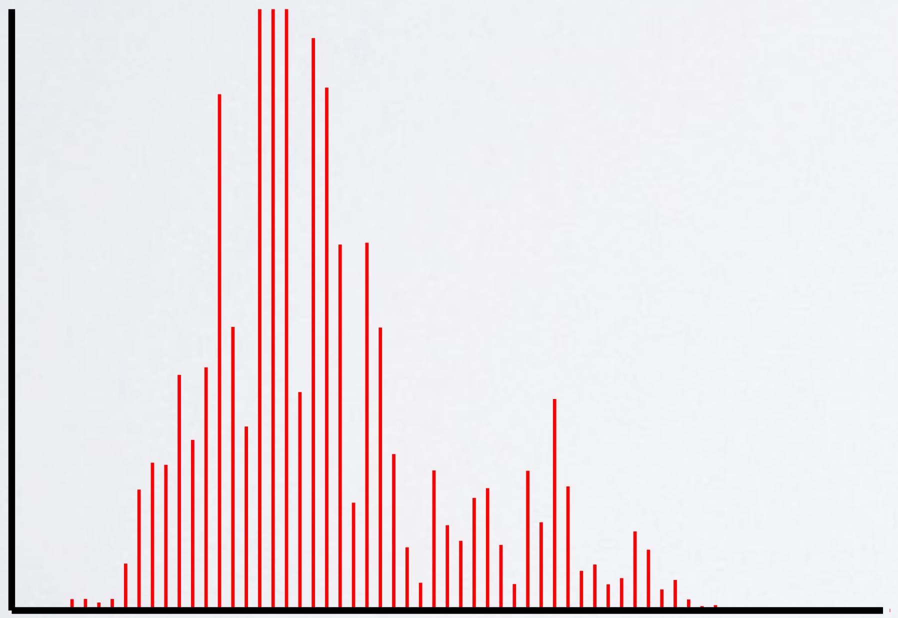
General analytic continuation procedure

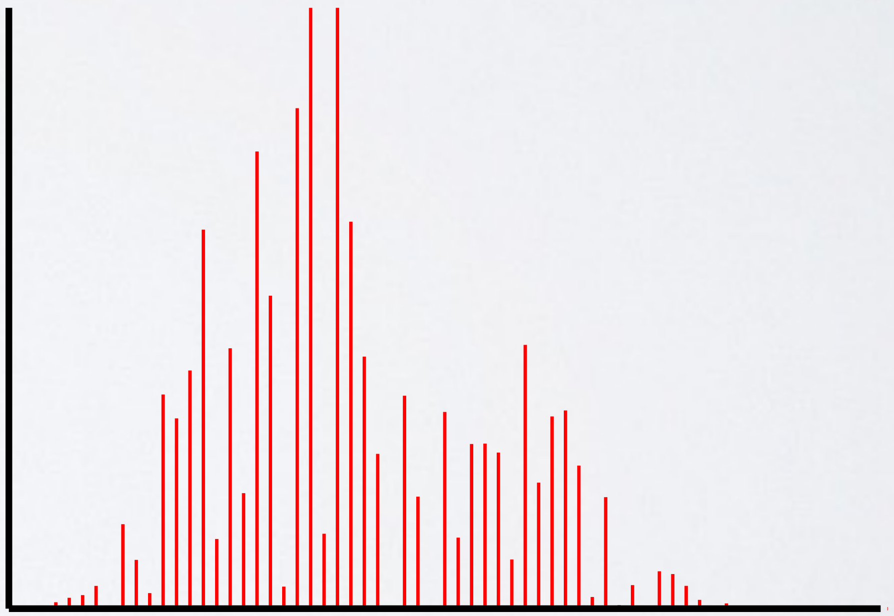
Represent the spectrum using
some suitable generic parametrization
- e.g., sum of many delta functions

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



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

Maximum entropy (MaxEnt) method

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

Use entropy to quantify amount of information 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), i.e., maximize

$$Q = \alpha E - \chi^2$$

E has a smoothing effect if α is not too small

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

Was for some time the standard approach

- still most widely used
- indications that E may bias the spectrum too much in some cases
- sharp features (edges, sharp peaks) cannot be resolved

Stochastic analytic continuation (SAC)

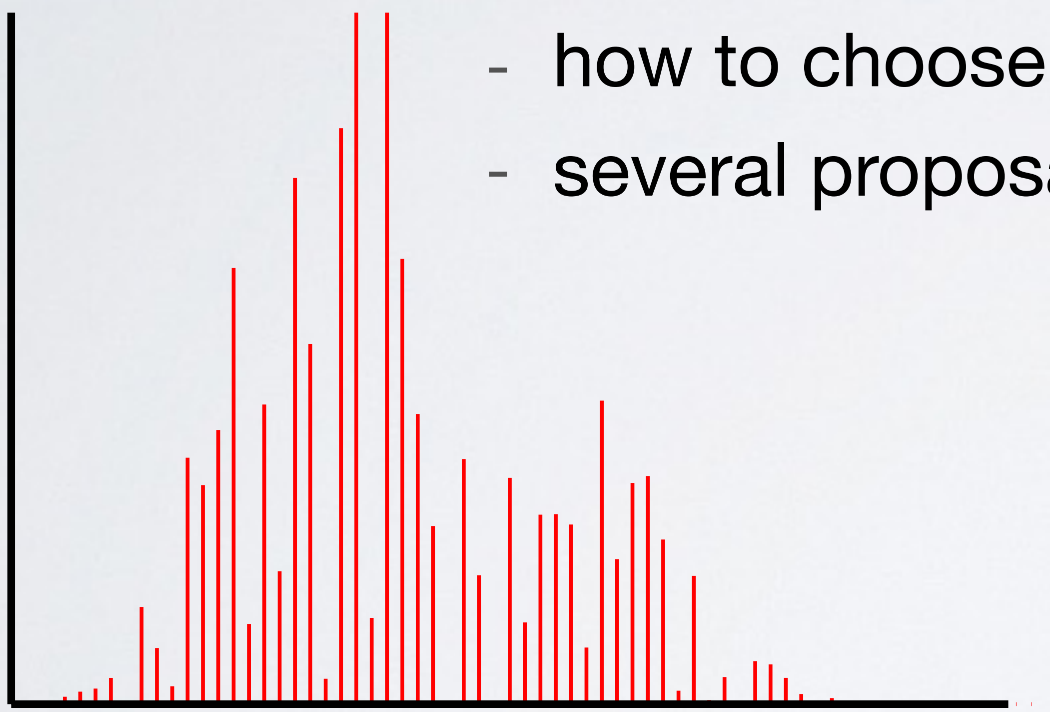
Sandvik, PRB 1998; Beach, arXiv 2004; Syljuåsen, PRE 2008; Sandvik, PRE 2016

[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

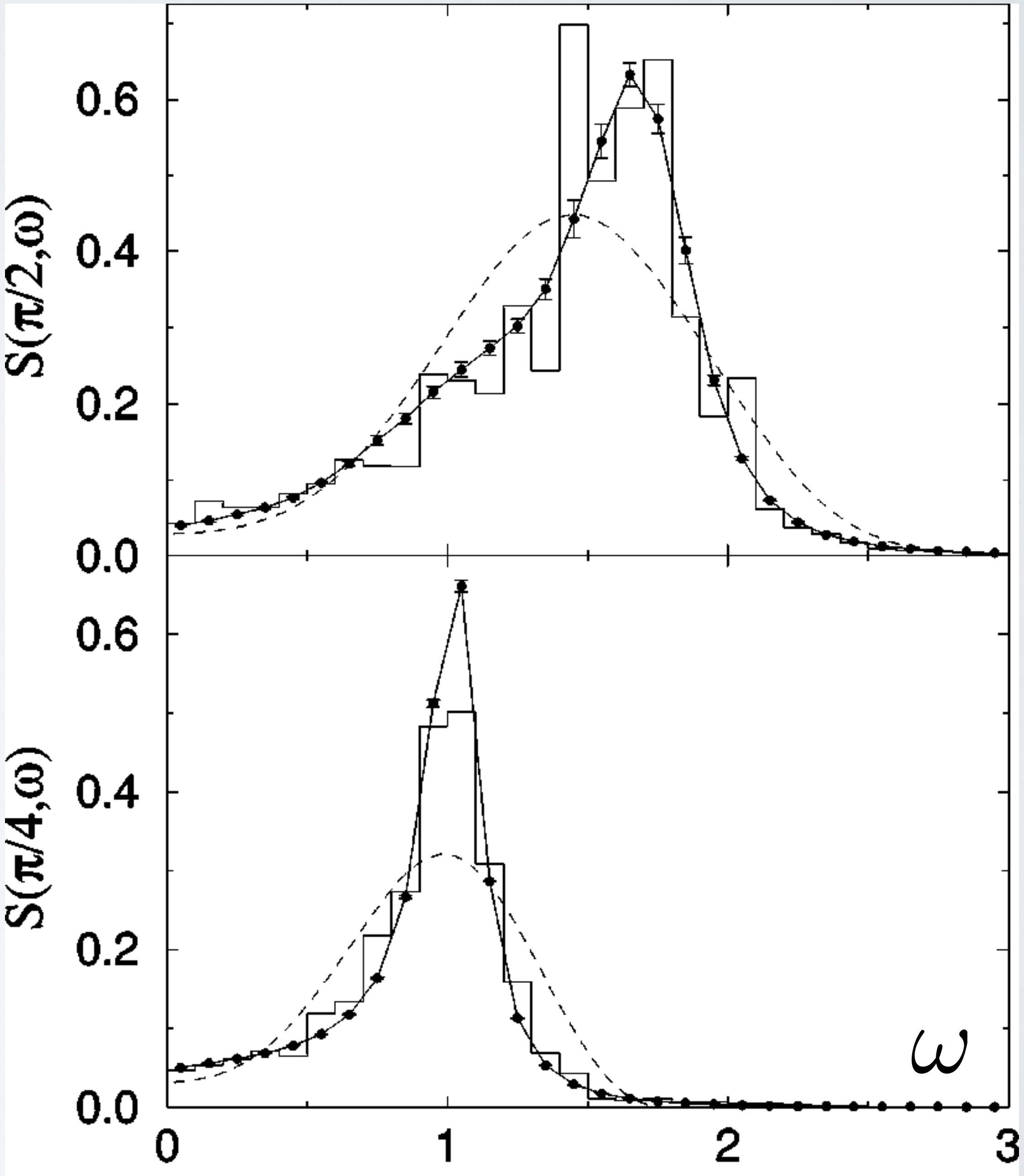


- how to choose θ
- several proposals

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

- average <S(ω)> is smooth

Heisenberg chain, T=J/2 (PRB 1998)
- SAC better than MaxEnt



SAC and entropic pressure

Syljuåsen (PRE 2008)

- just use θ=1

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

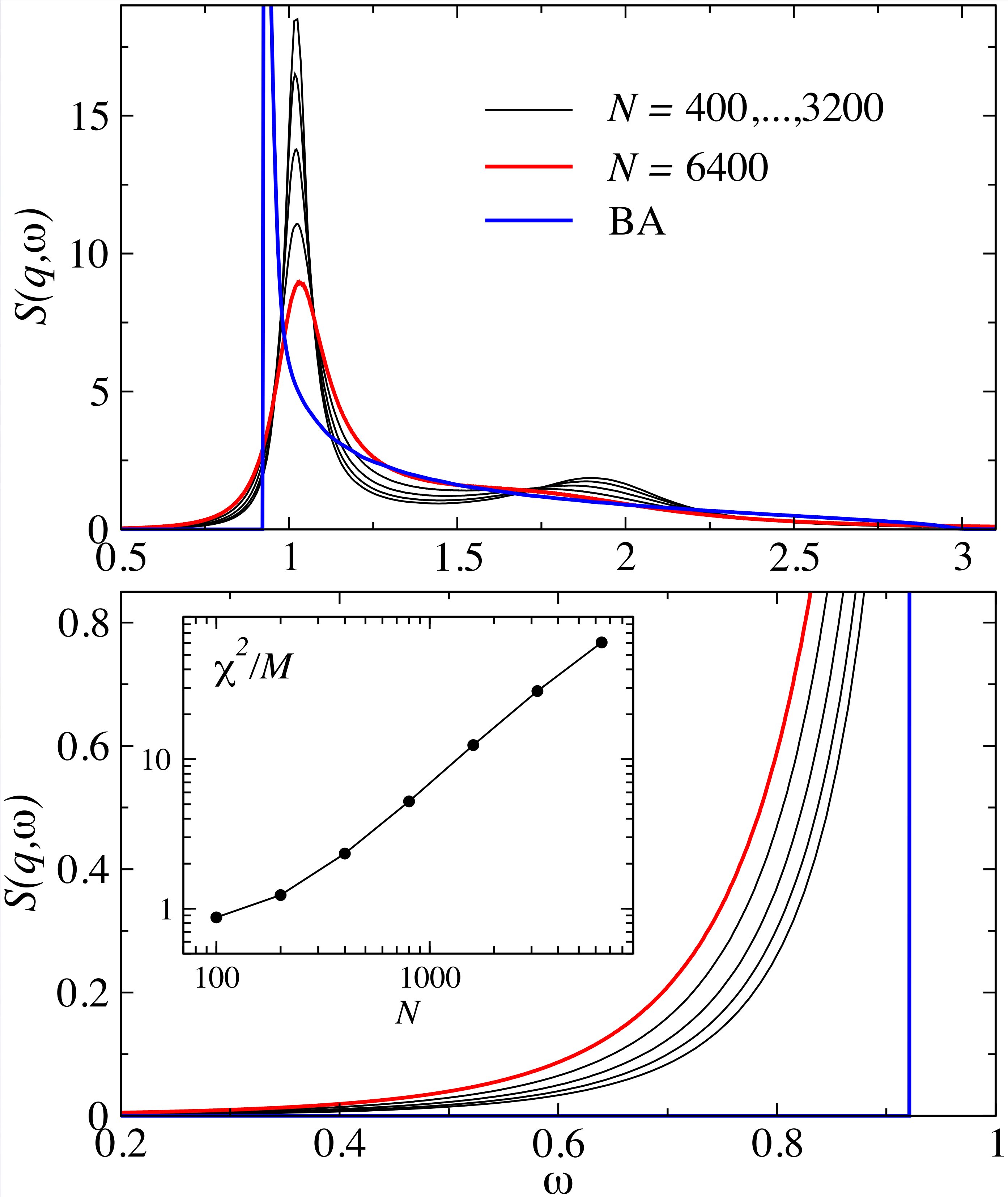
Leads to a problem
(Sandvik, PRE 2016)

when N_ω is large

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

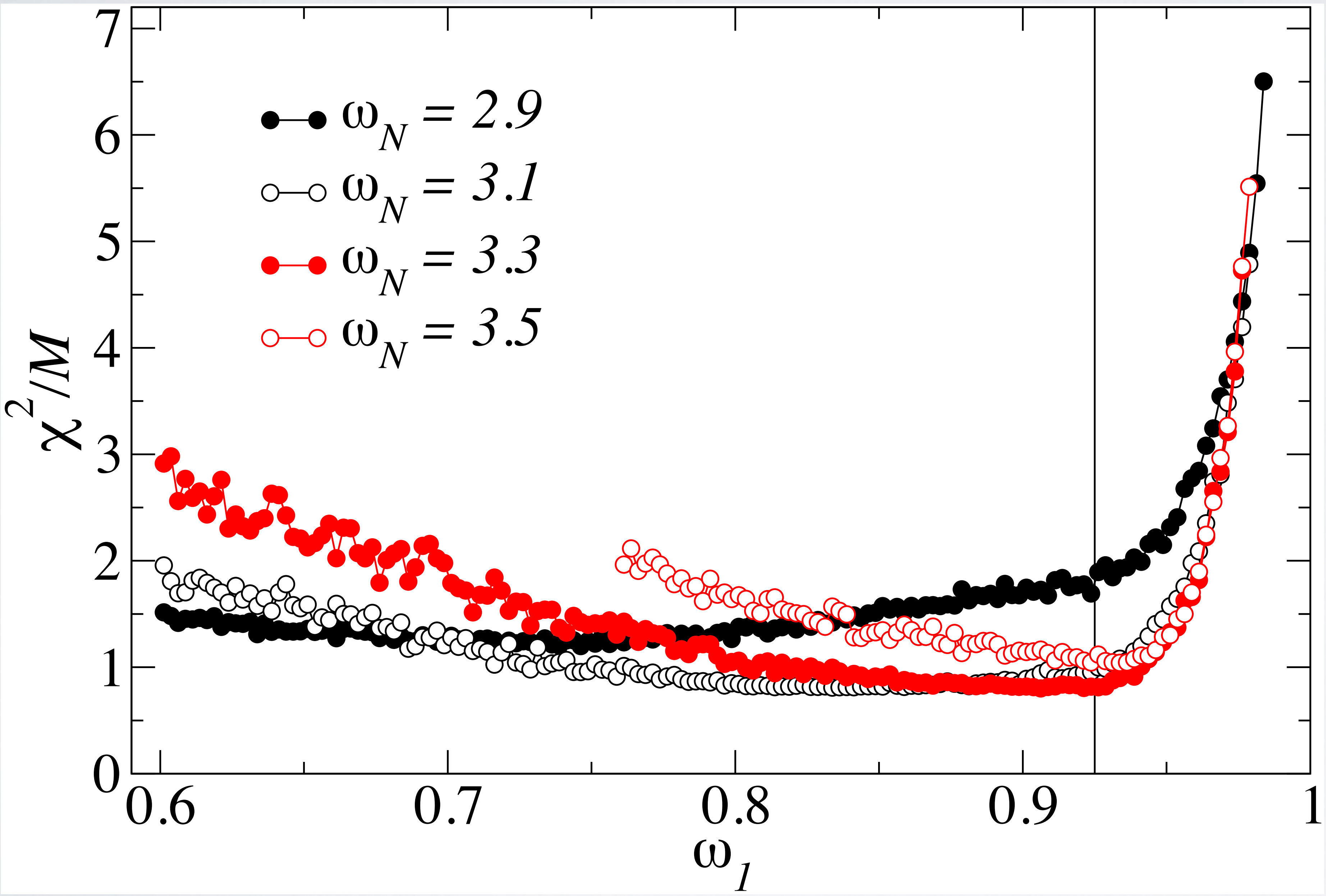
Test case:
Dynamic structure factor of 1D Heisenberg chain at T=0 (q=0.8π), L=500

Compare with:
Bethe Ansatz
(Sebastian Caux)

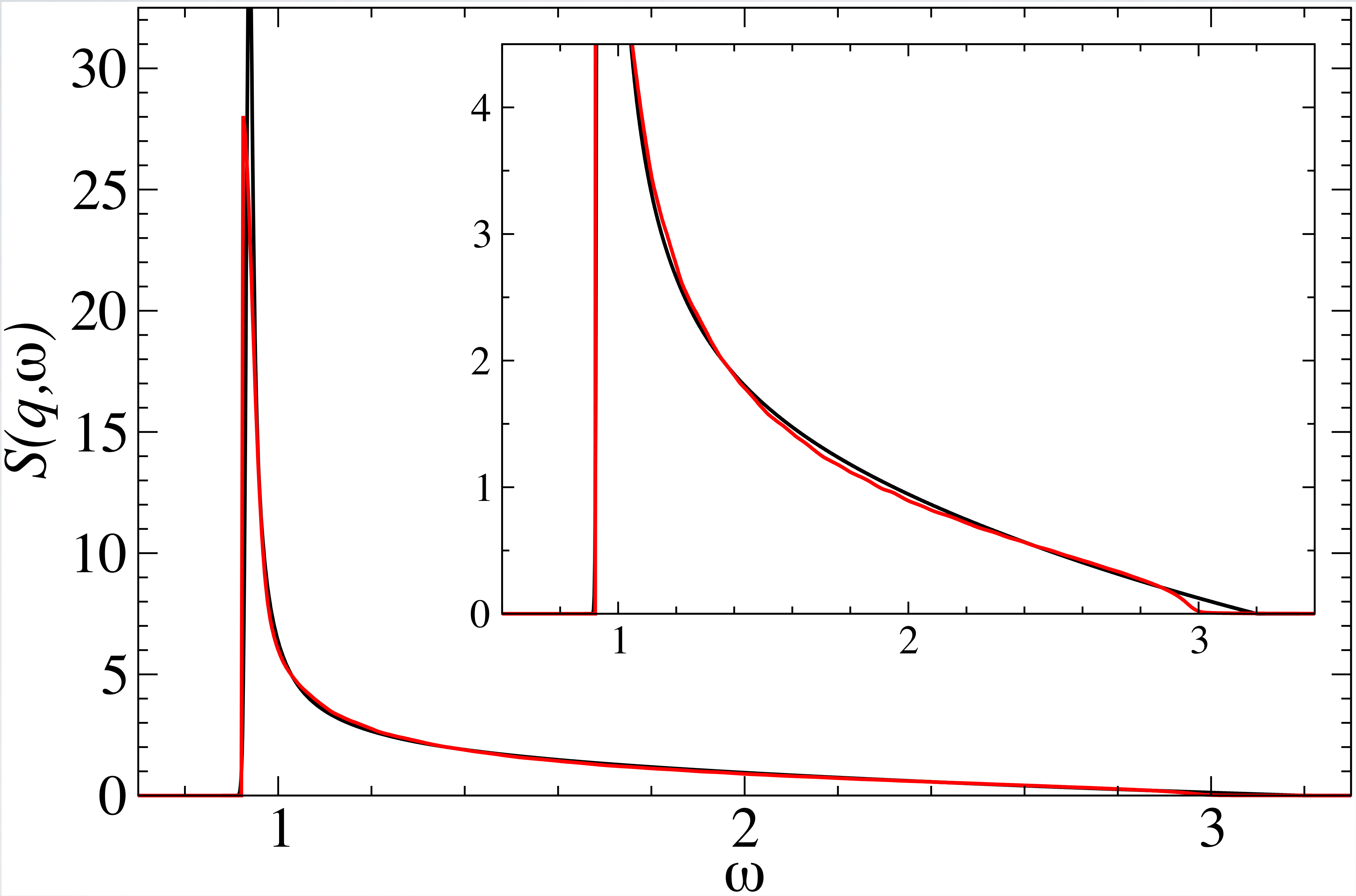


Diagnostics and input from entropy

Shift the lower and upper edges of the spectrum to avoid entropic distortions there
- entropy minimum signals actual edges of the spectrum



With the lower edge fixed the spectrum is very good
- important: **single maximum also imposed in sampling** (further reduces entropy)



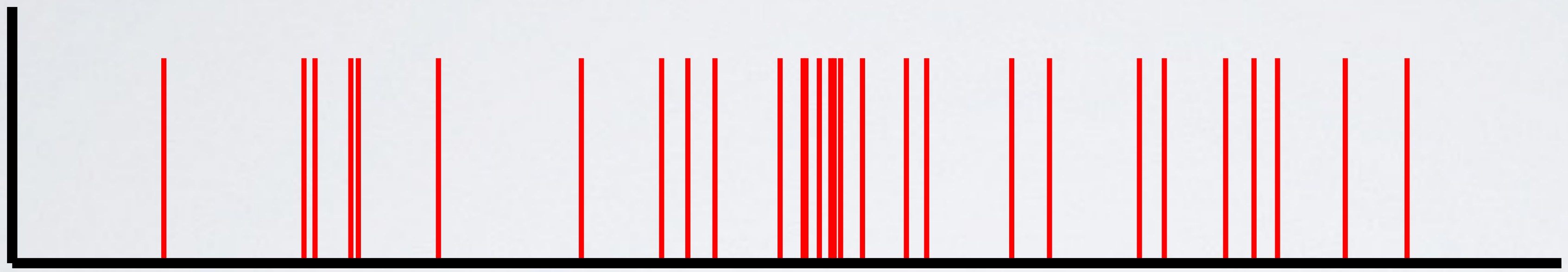
Referee comment:
"Of course if you know the answer you can cook up a method"

Improved SAC scheme

Hui Shao & A. Sandvik (work in progress)

Problem with all SAC schemes so far: slow sampling:
it can take several hours to find optimal sampling temp or optimal frequency bounds and obtain a final smooth average

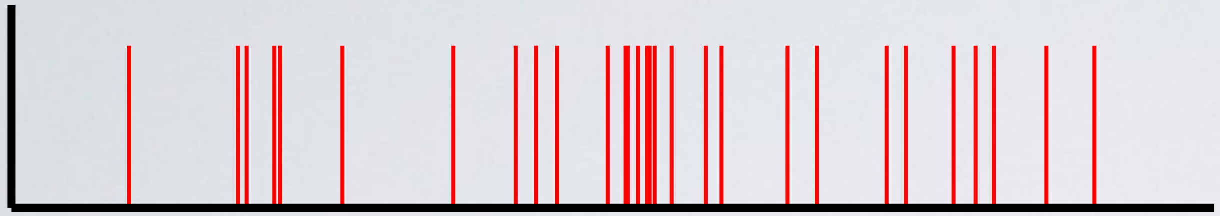
New parametrization: Delta-functions of equal amplitude in continuum
- use histogram to collect “hits”



Use monotonically increasing distances for an edge

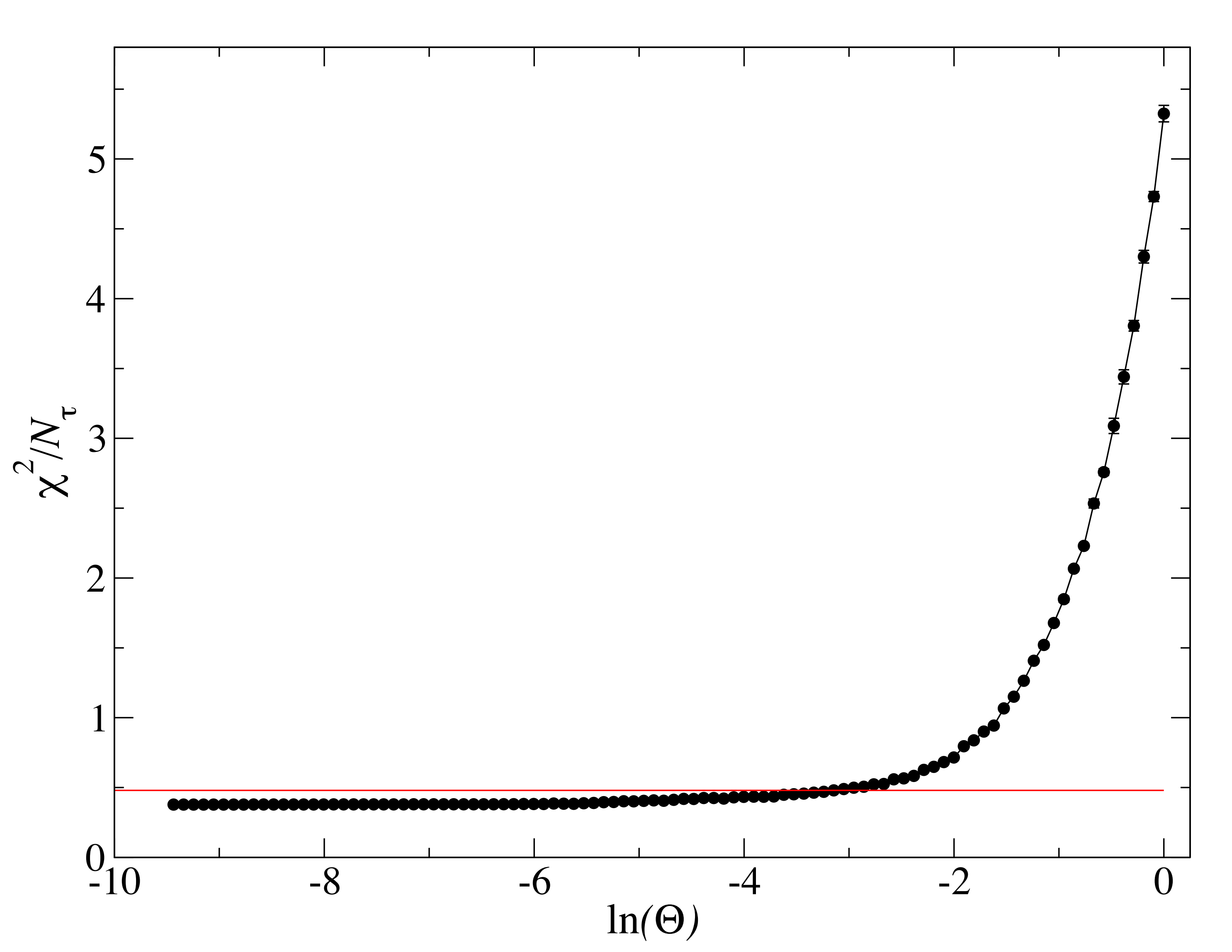
Can also build in “prominent feature”, e.g., dominant delta-fktn

Determination of sampling temperature



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

Use simulated annealing to find lowest chi-squared value
- the data is then overfitted



Raise the temperature such that χ^2 is above the minimum value by ~ one standard deviation of the χ^2 distribution

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

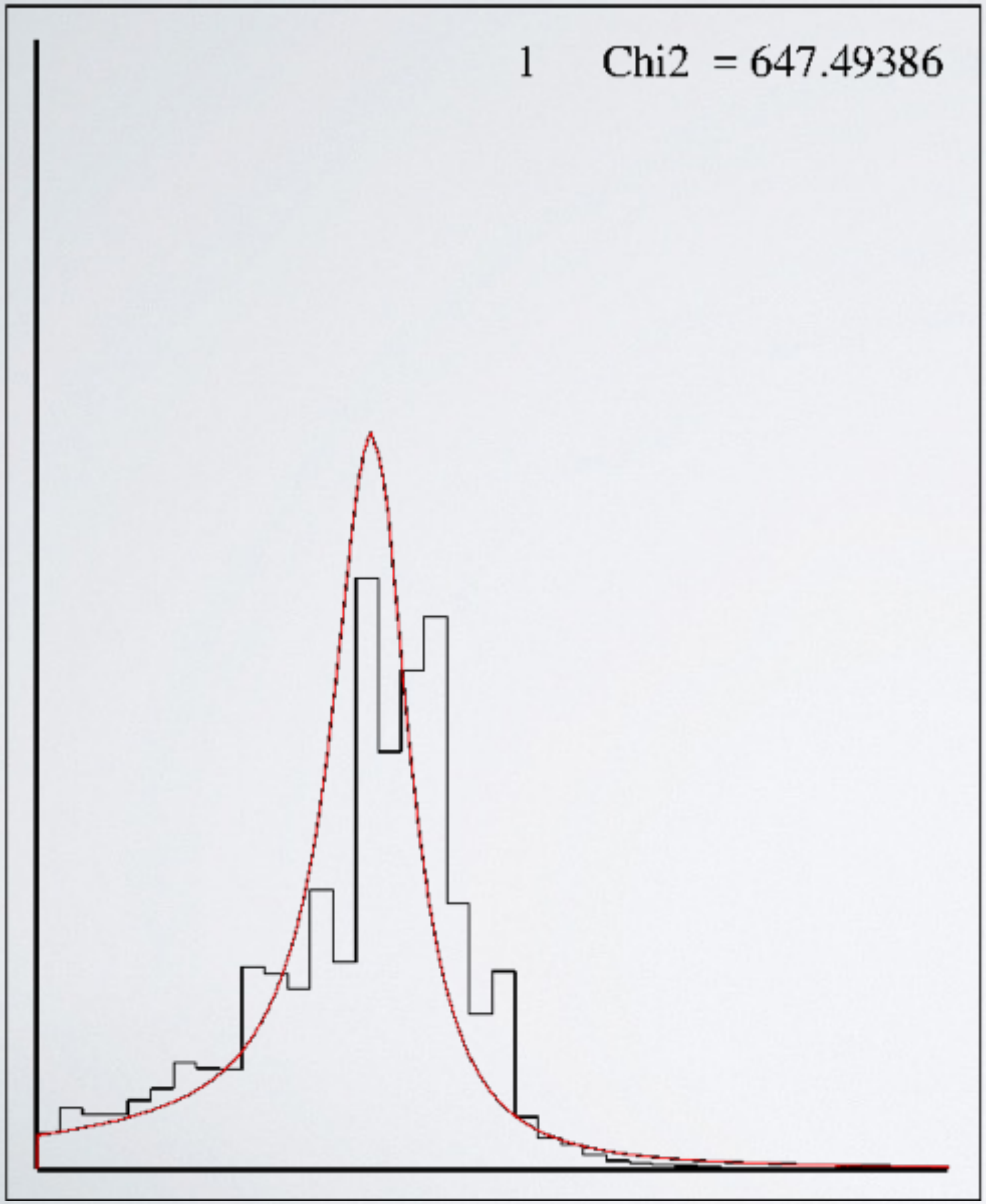
- the spectrum fluctuates and data not overfitted

More delta-functions → lower temperature
- overcomes some of the entropy problems

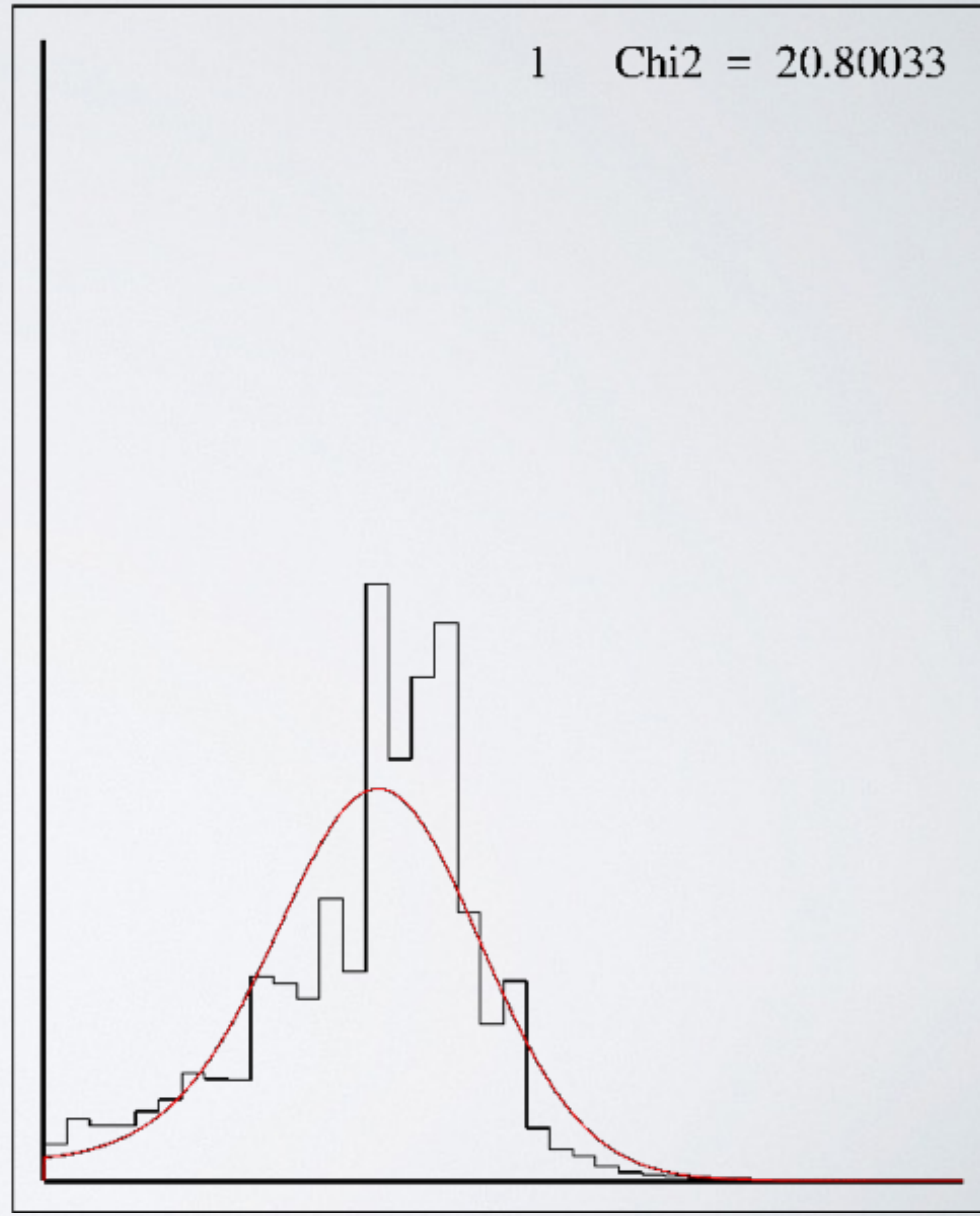
Dependence on the sampling temperature, $\Theta = 10 \times 1.1^{-n}$

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

uniform grid

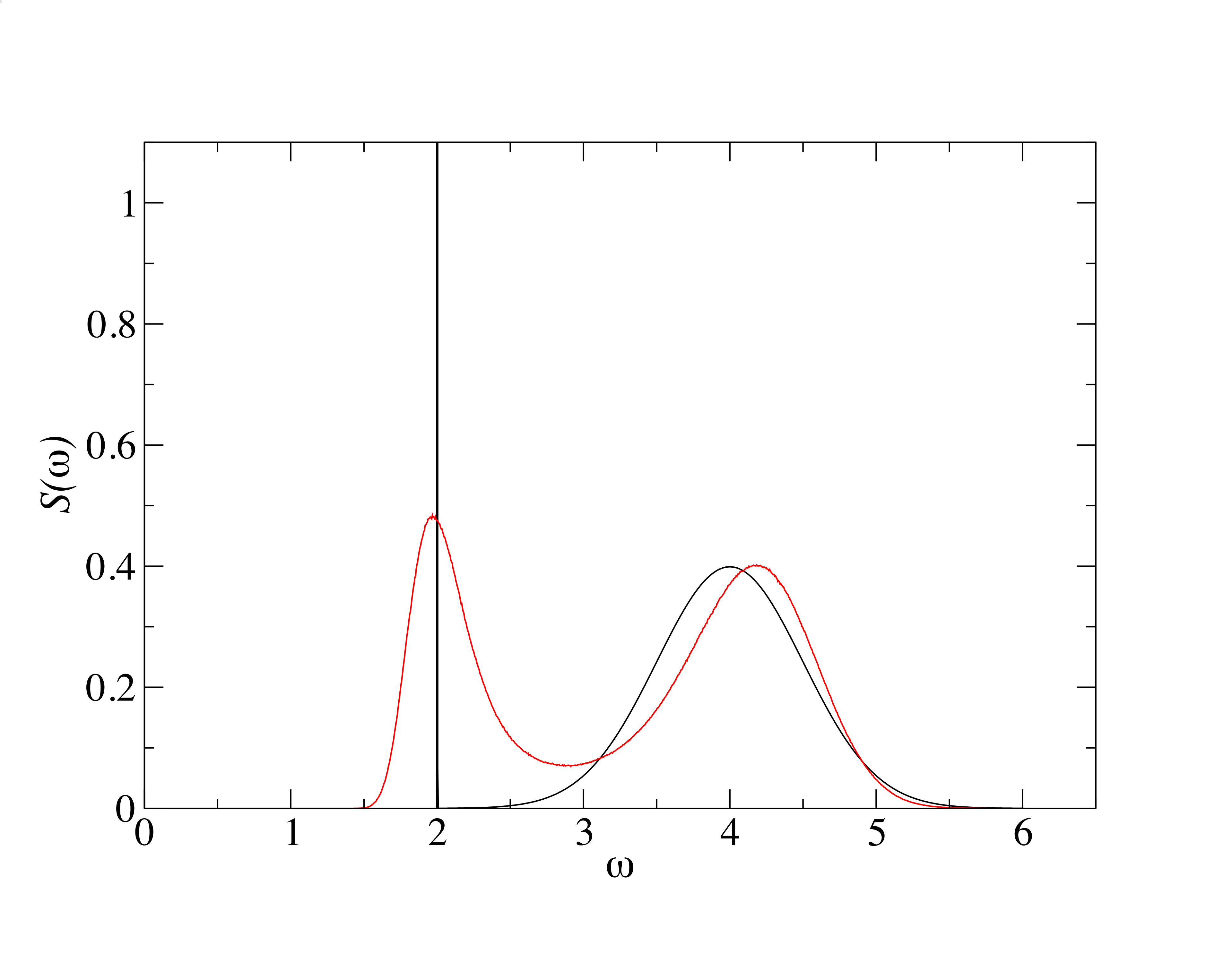


no grid



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

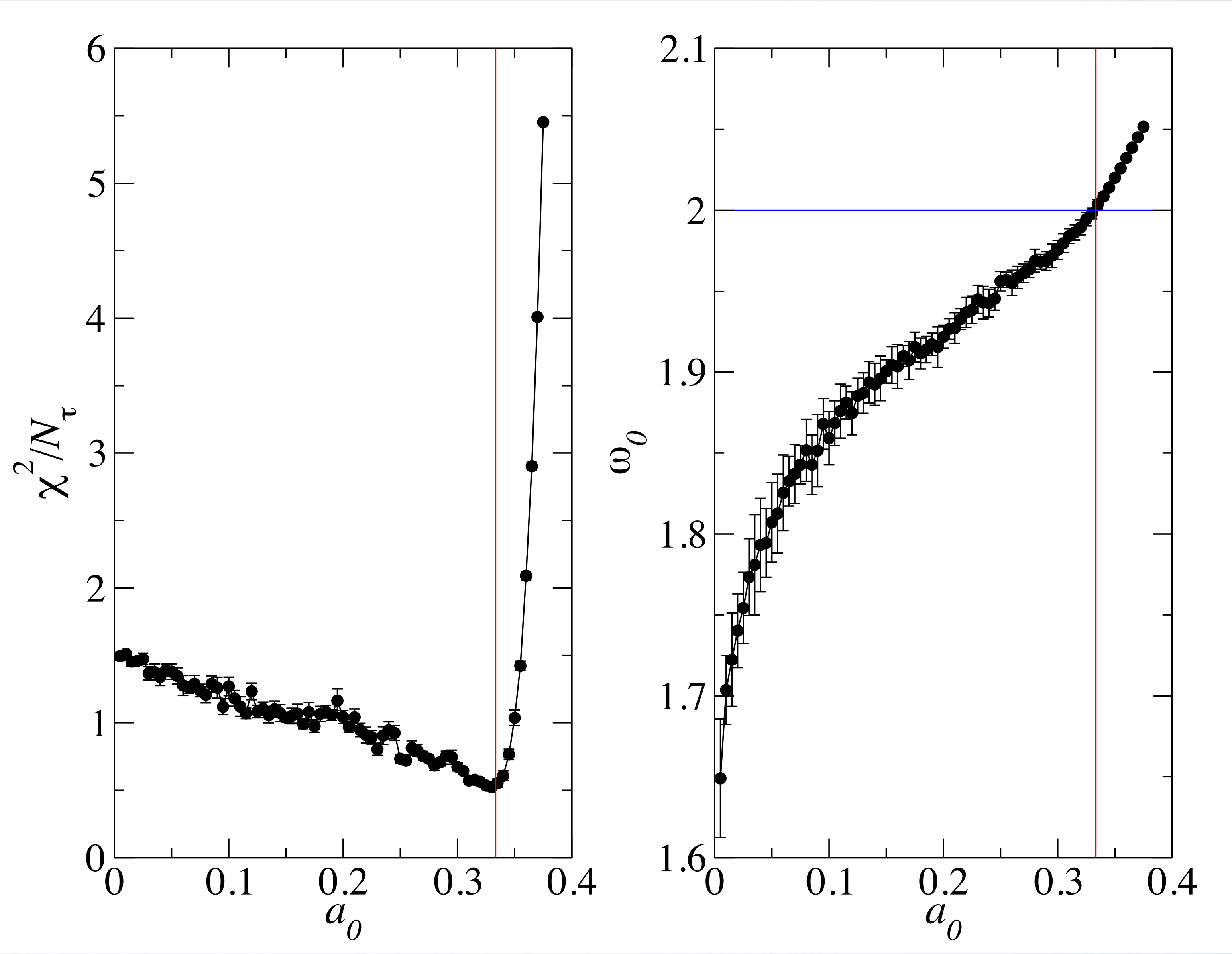
Delta function as prominent feature

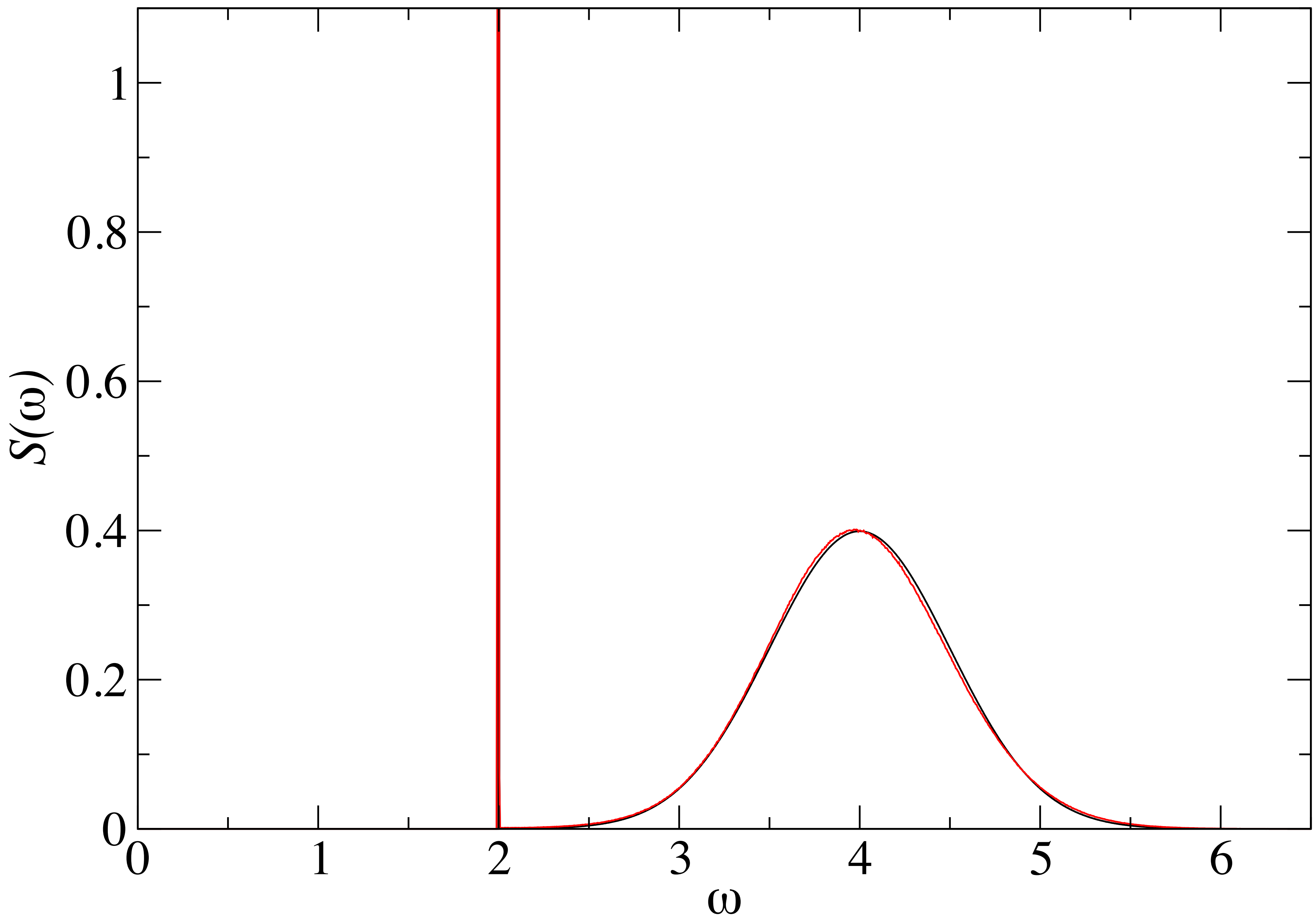
- use one main delta function with adjustable weight a_0
- other delta functions can not go below its energy ω_0

Motivation: Moving weight into the main delta function reduces the entropy; detected in χ^2 vs amplitude a_0

Results for previous synthetic test data
- 1+500 delta-fktns
Gives the correct weight and location of the delta function

Fix a slightly higher sampling temperature than in free sampling, to see the χ^2 minimum appears more clearly





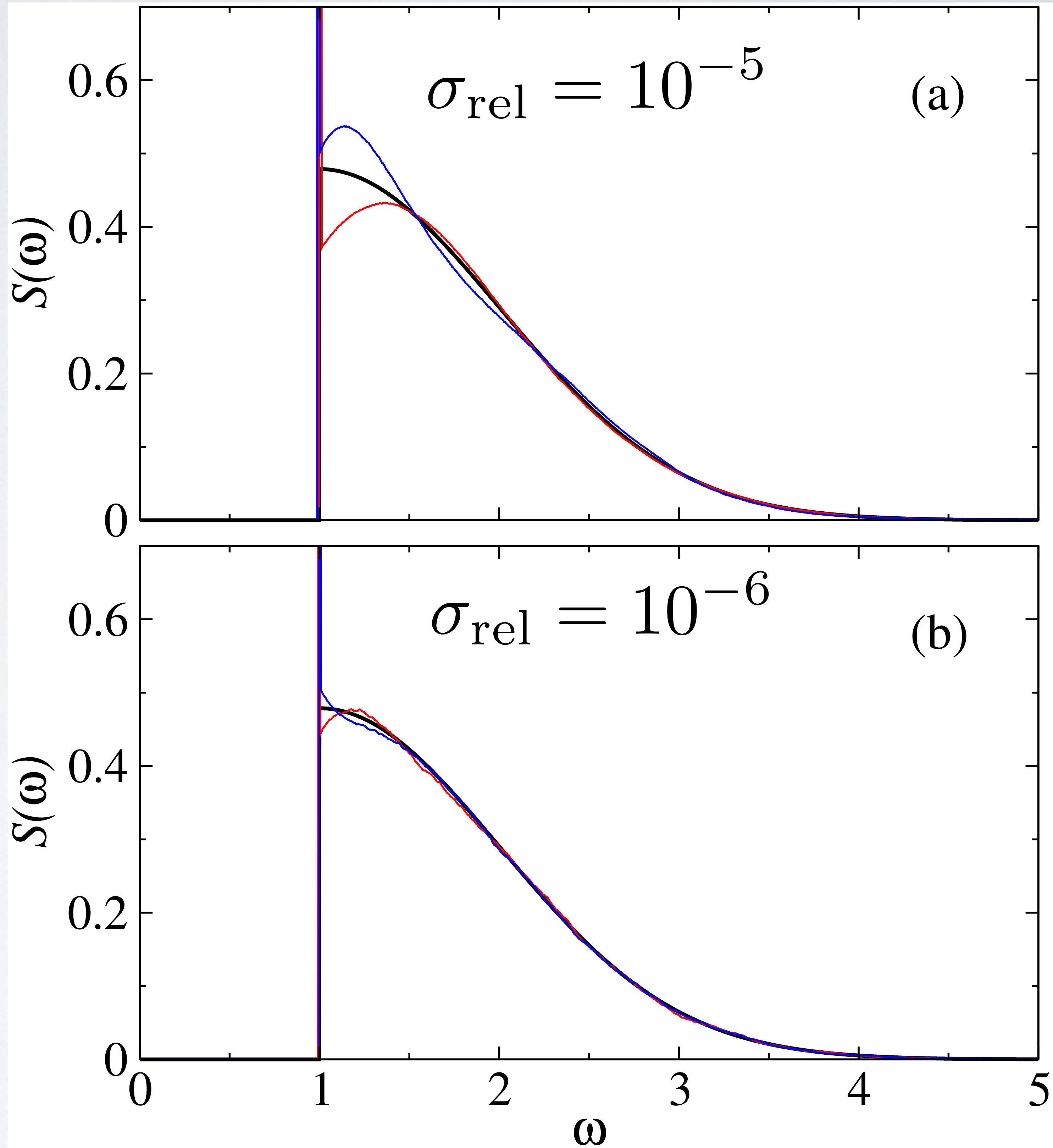
The entire spectrum is very well reproduced!

More challenging case: continuum touches delta-fktn

Synthetic spectrum with

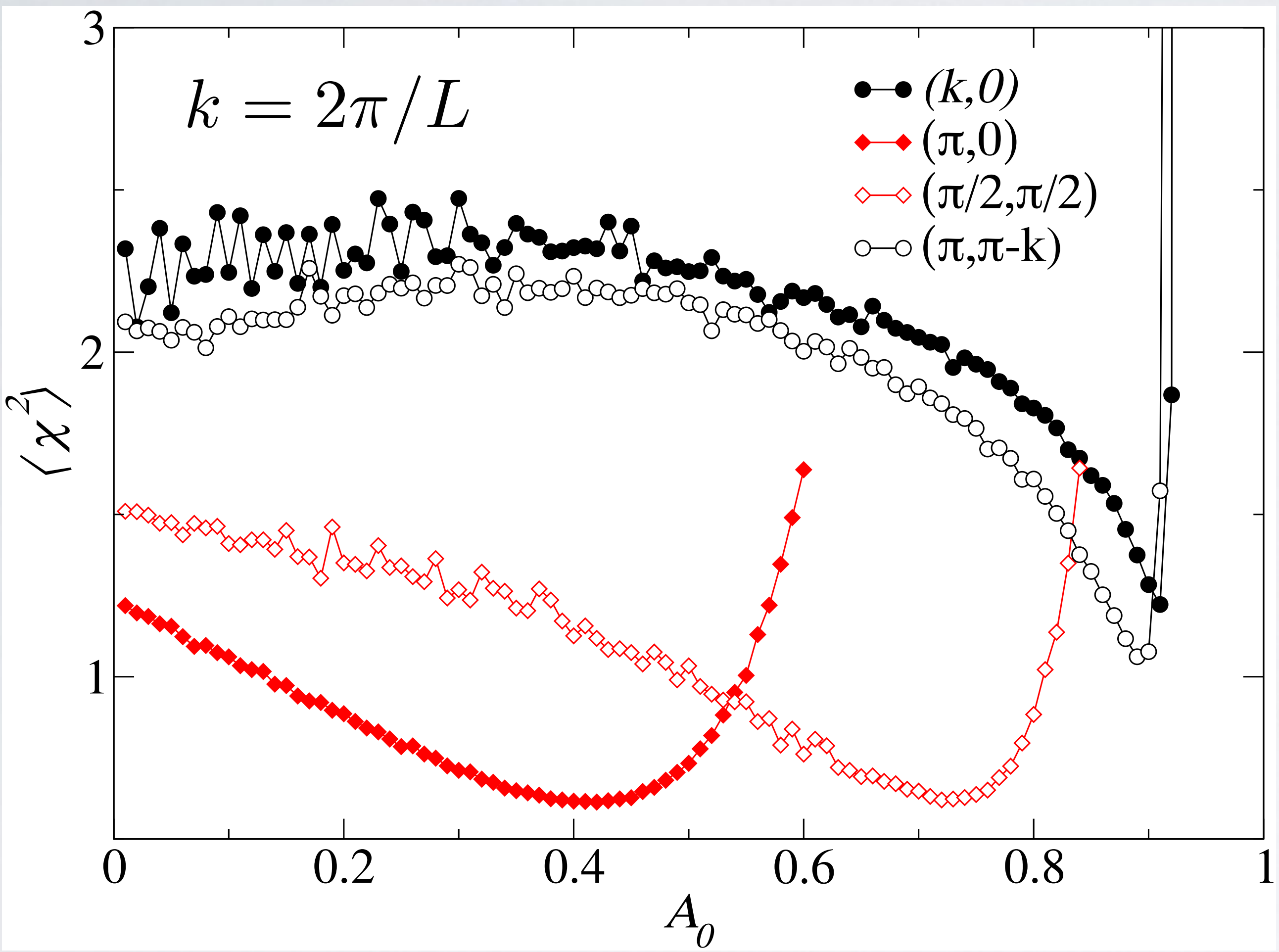
- ω_0 = 0.4
- a_0 = 1.0

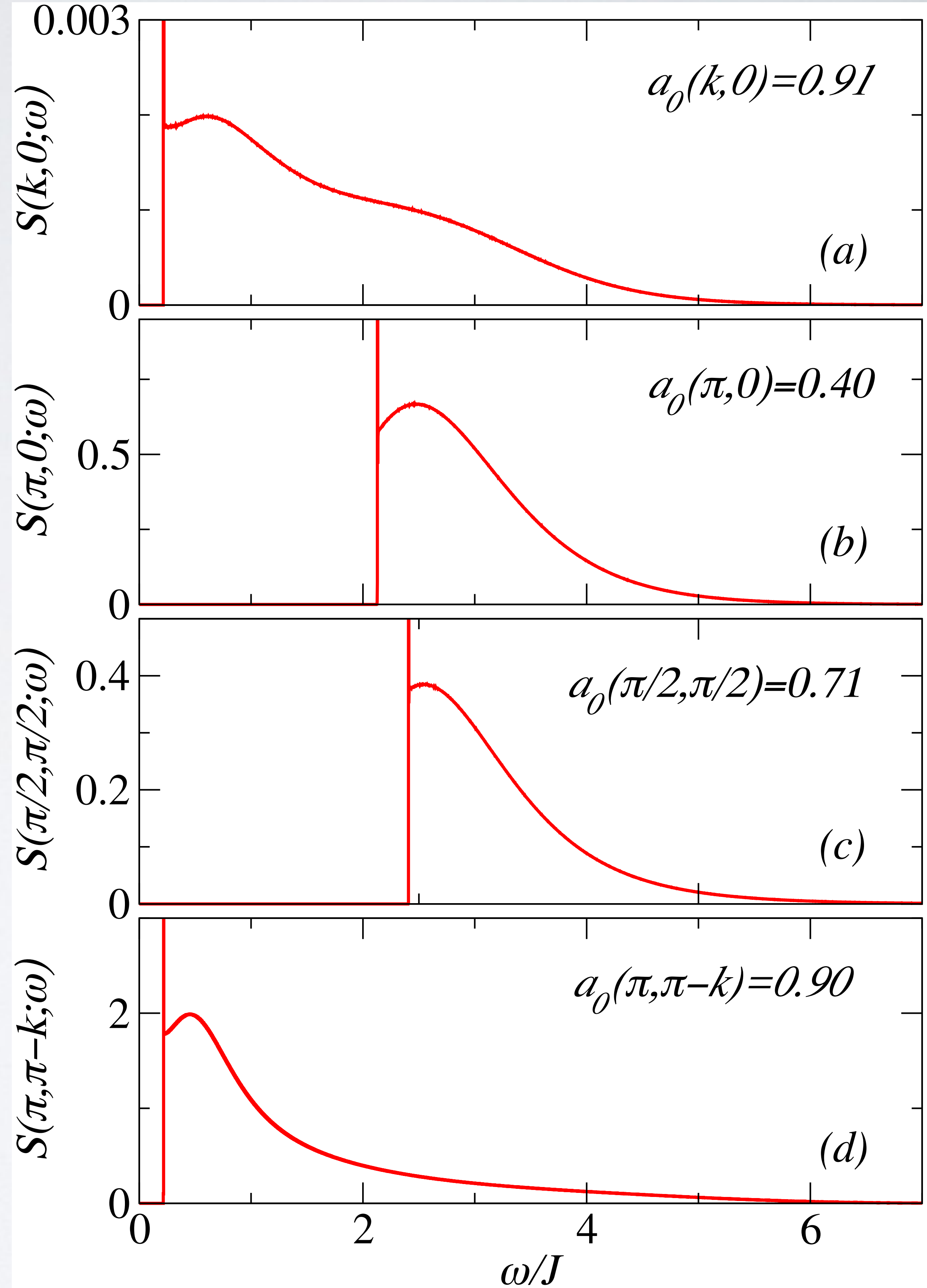
QMC data can reach error level 10^{-6}



Dynamic structure factor of 2D S=1/2 Heisenberg model

H. Shao, Y. Q Qin, S. Capponi, S Chesi, Z. Y. Meng, A. W. Sandvik, arXiv:1708.03232





Presence of magnon pole detected for all momenta q

Small pole at $(\pi,0)$ related to almost deconfined spinons (from study of J-Q model)

Comparison with neutron scattering experiments

$Cu(DCOO)_2 \cdot 4D_2O$

ARTICLES
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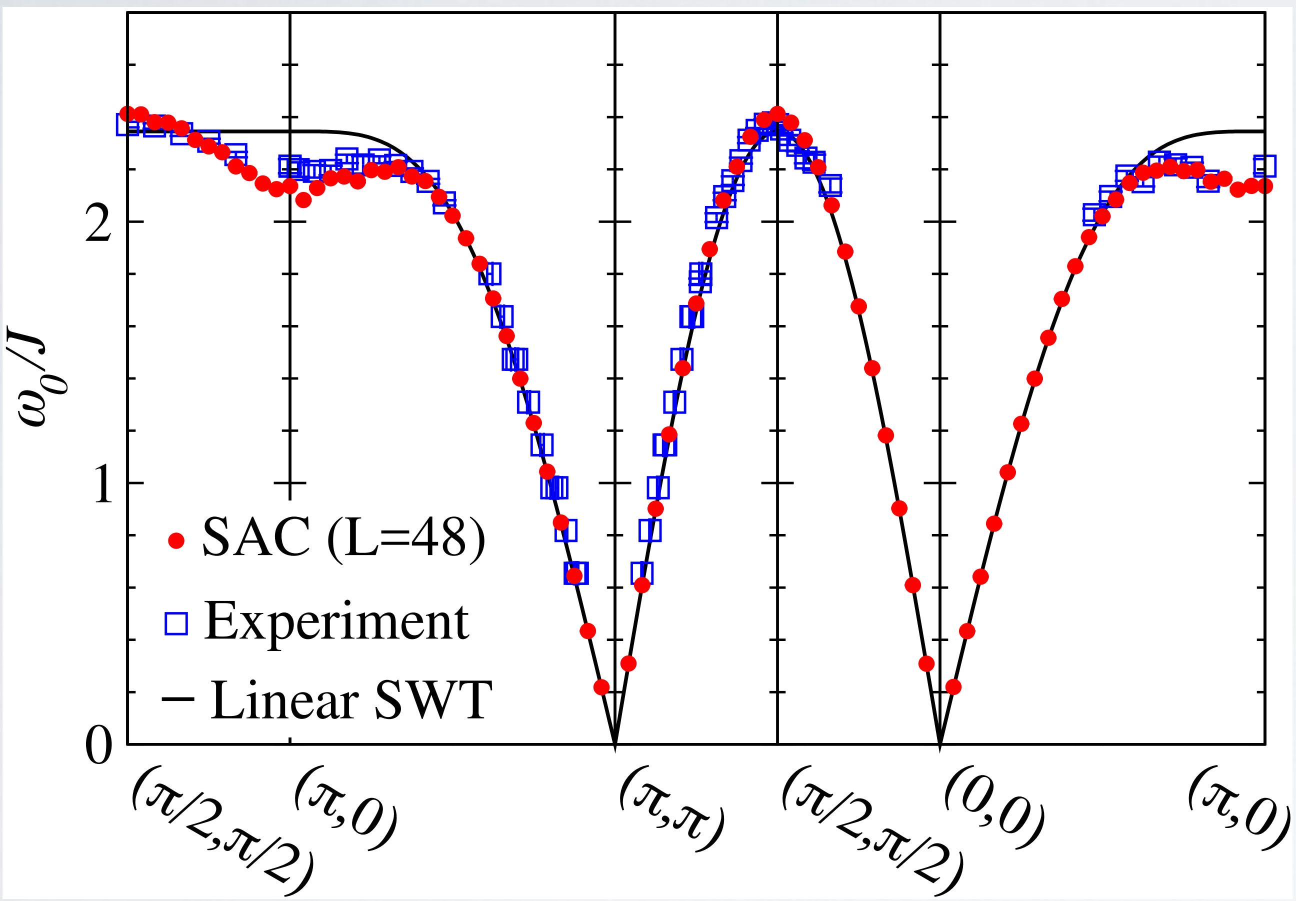
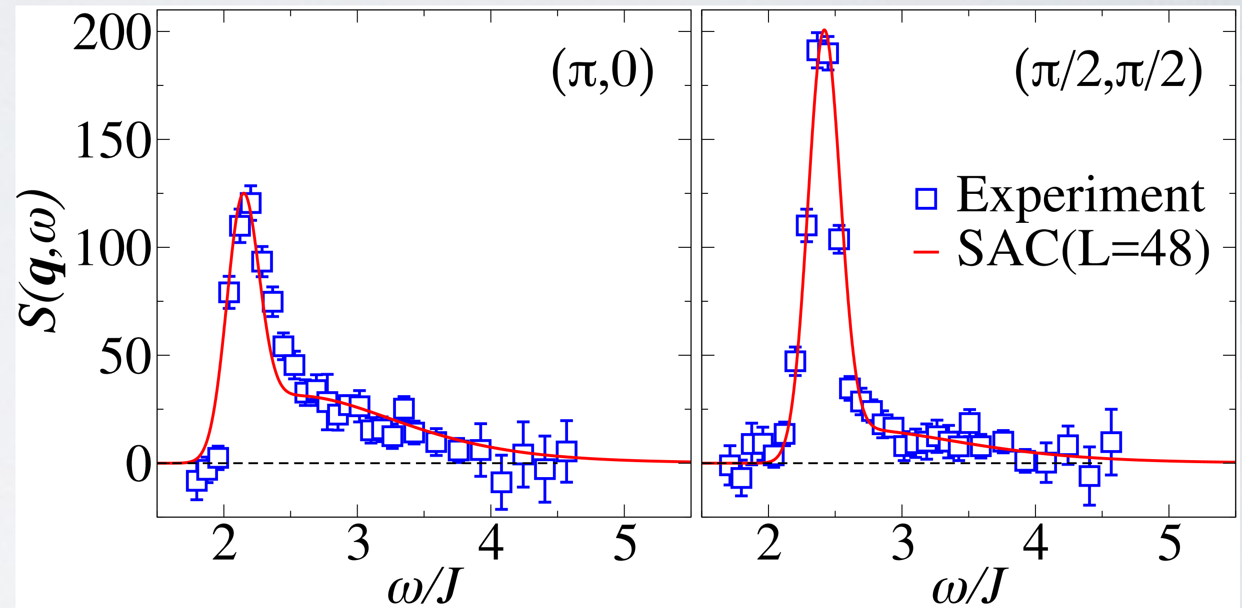
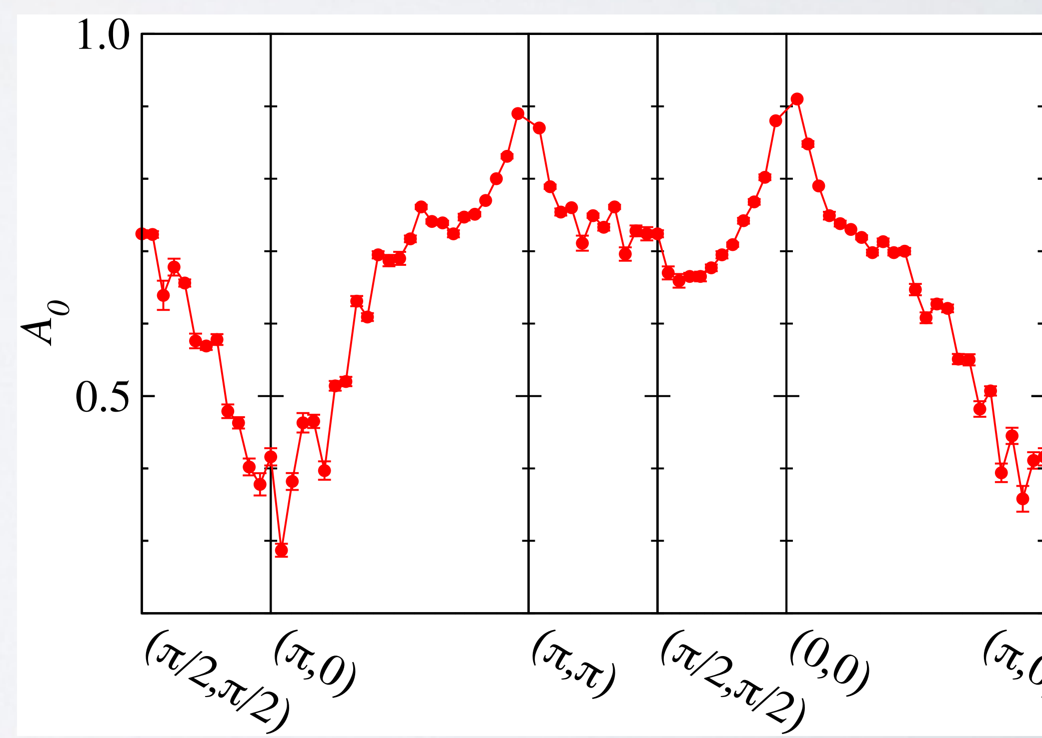
nature physics

Fractional excitations in the square-lattice quantum antiferromagnet

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]





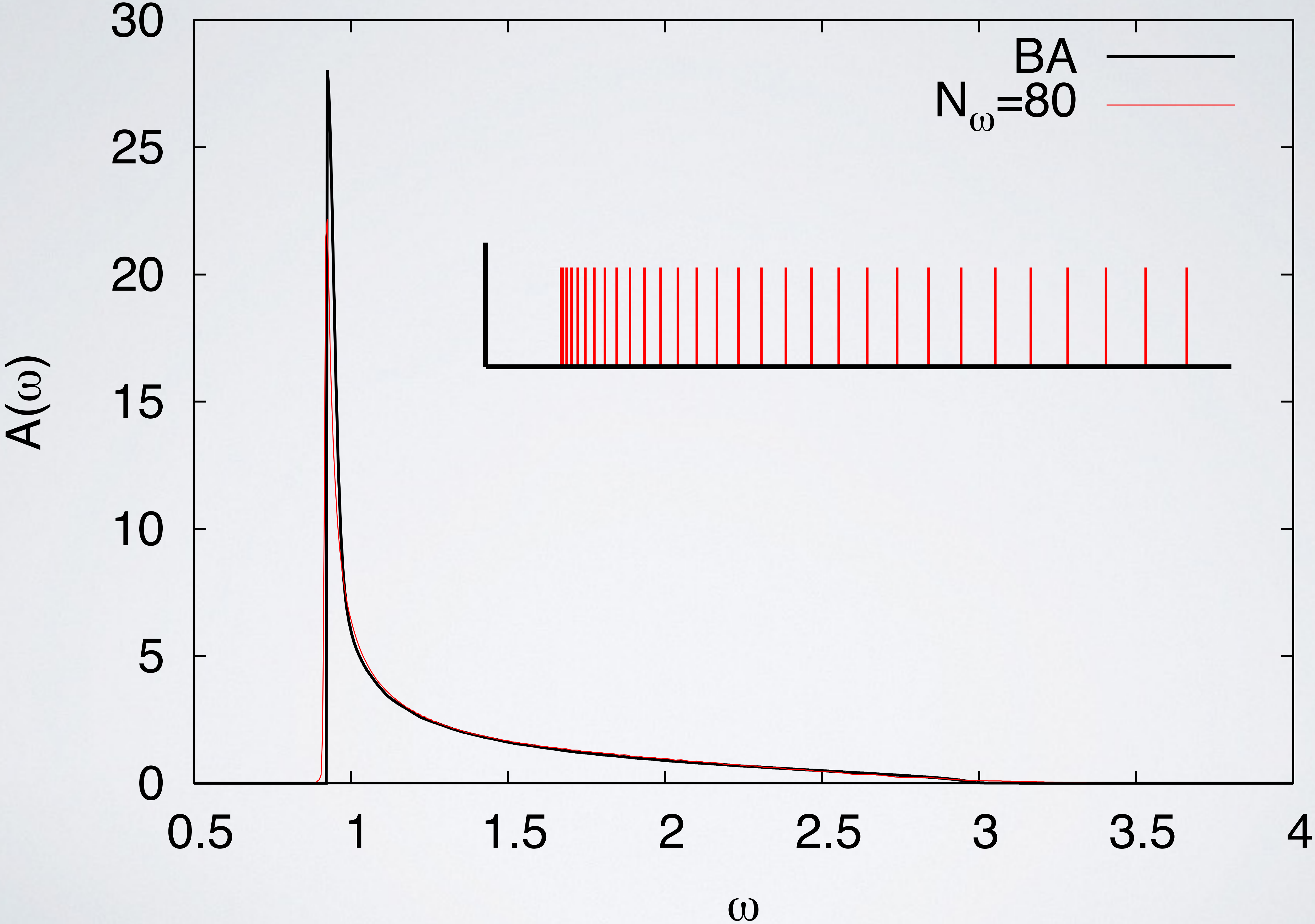


Our picture: Nearly deconfined spinons

- small but non-zero $(\pi,0)$ magnon pole
- deconfinement at $(\pi,0)$ when weak multi-spin interactions added

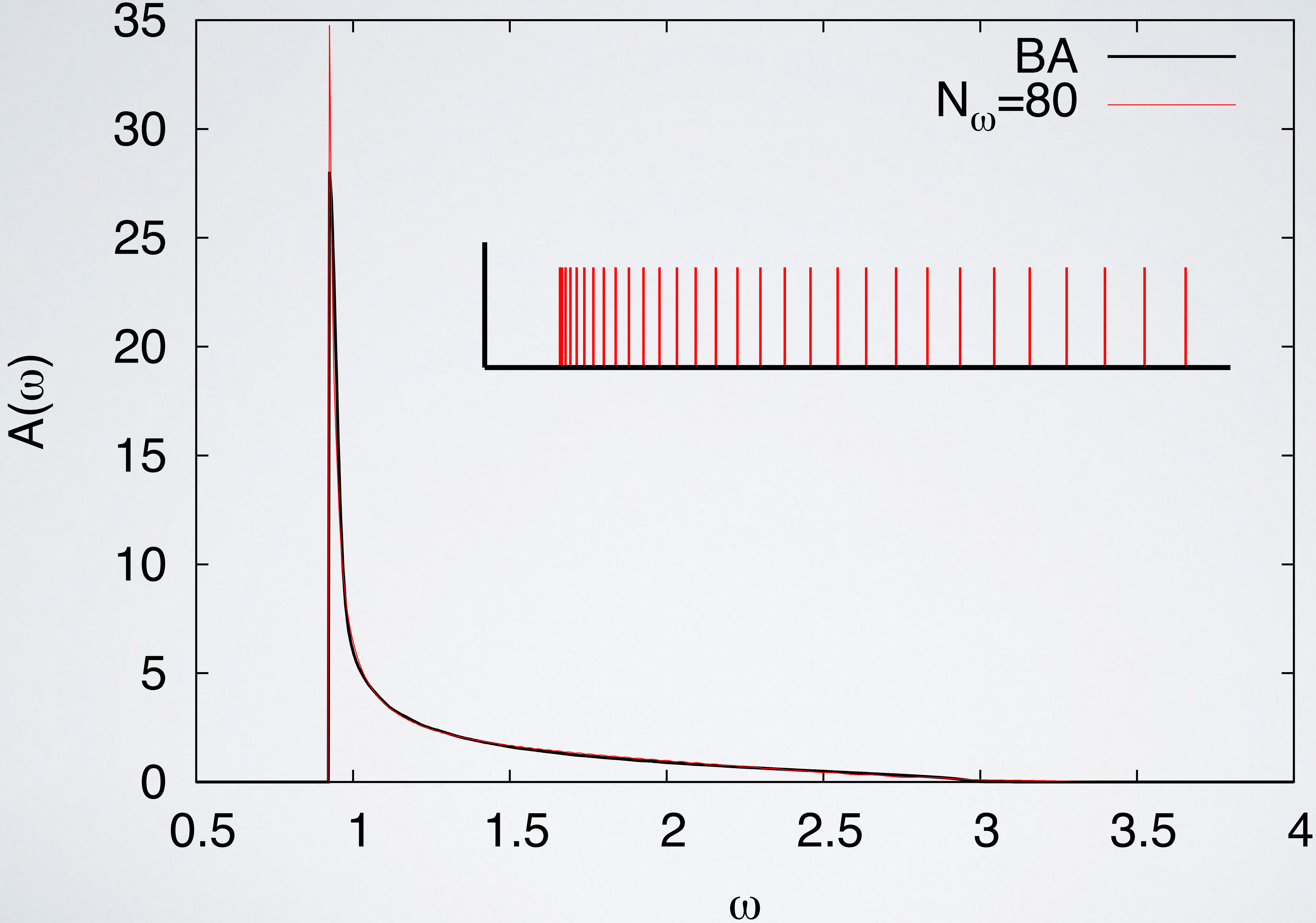
1D Heisenberg chain, $A(\omega)=S(0.8\pi,\omega)$

- sampling with edge built in (location not fixed)

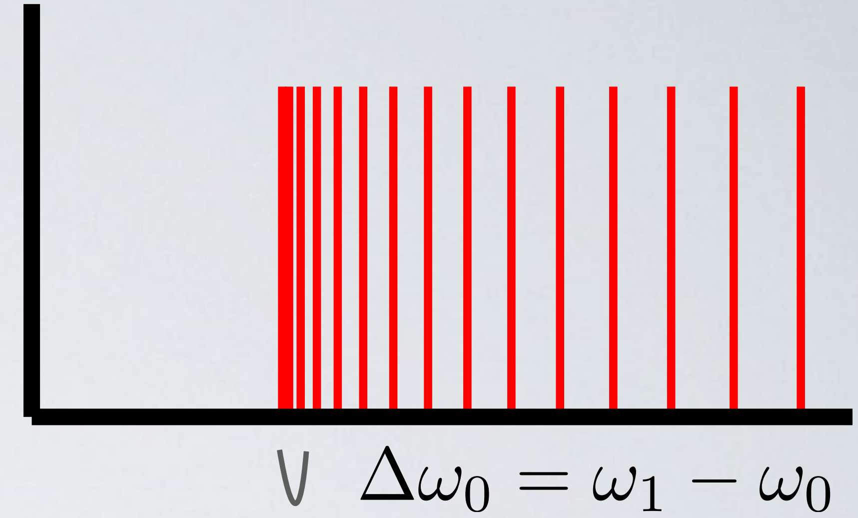


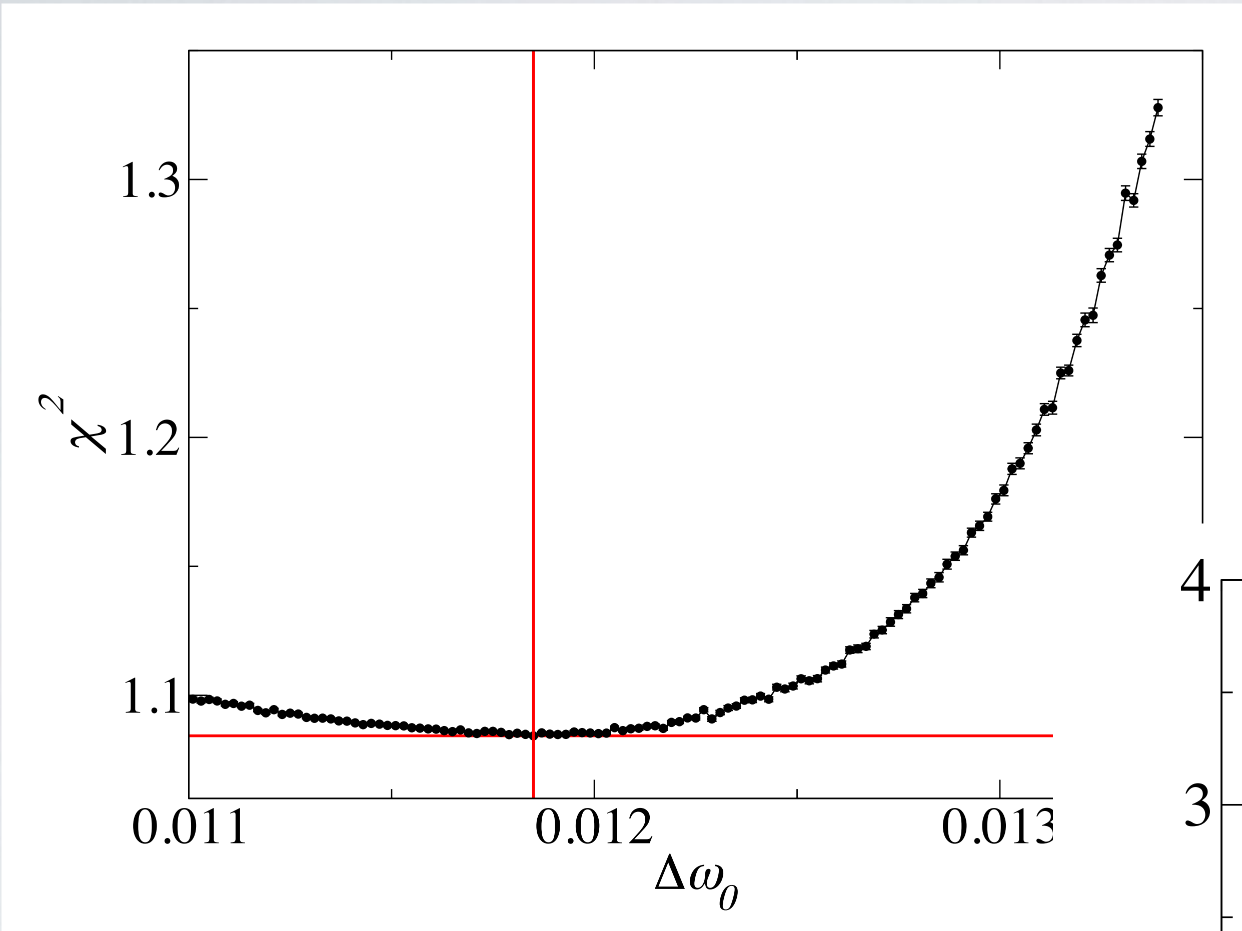
1D Heisenberg chain, $A(\omega)=S(0.8\pi,\omega)$

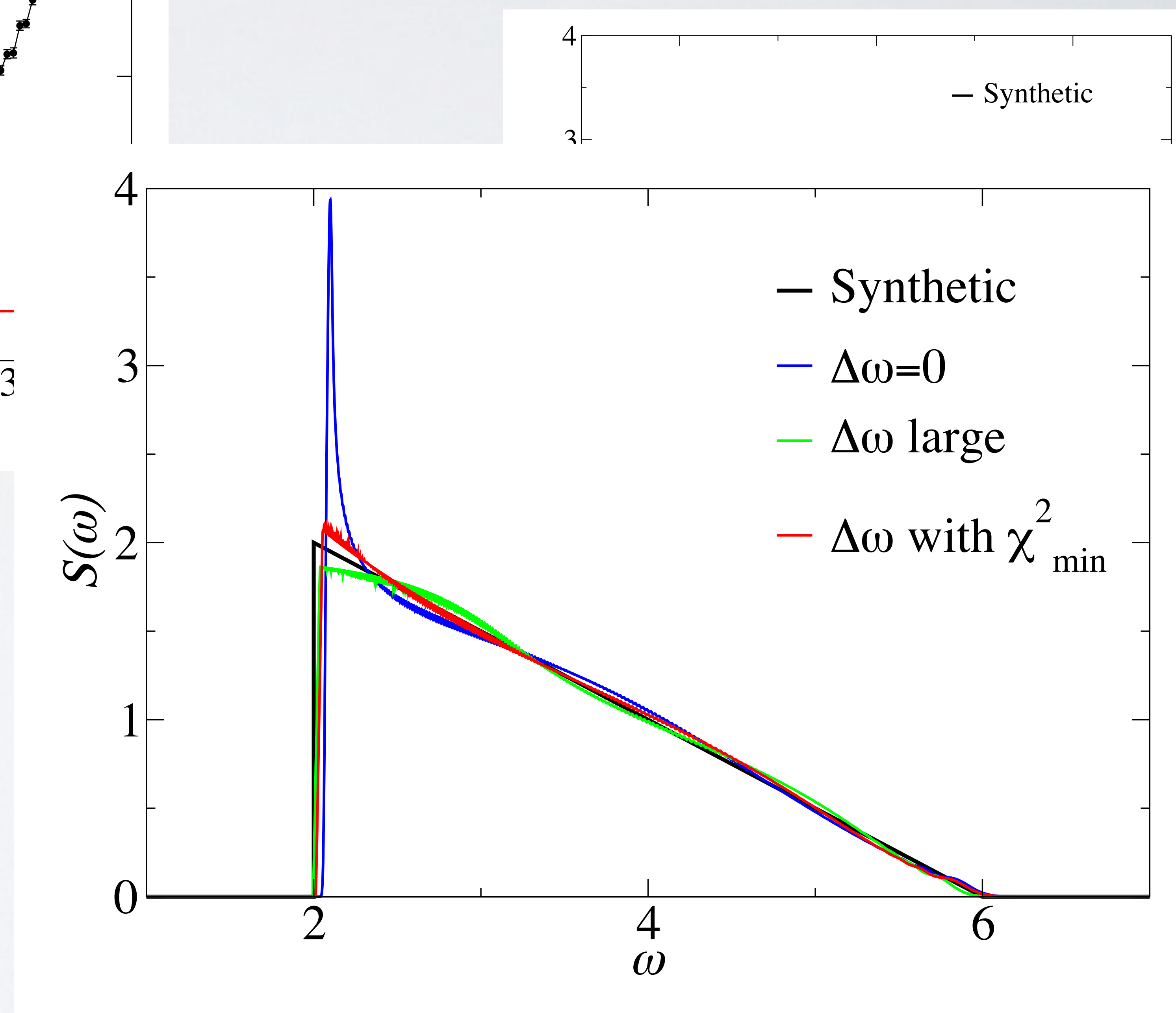
- sampling with edge built in (location fixed at known frequency)



Suppress peak entropy by imposing fixed distance between two lowest deltas







In principle one can optimize any feature within some parametrization, and also extend to more than one feature.

Conclusions

Further developments of stochastic analytic continuation method

Good parameterizations of the spectrum can
- reduce detrimental entropic pressures
- produce better results

One or more parameters (“features”) can be optimized by using entropy-related signal.

Some of these insights can also be used with Max-Ent

Lower-edge delta-function (magnon pole) confirmed for 2D Heisenberg
- good agreement with experiments
- calculations + theory suggest nearly deconfined spinons