Title: Nearly fractionalized excitations in 2D quantum antiferromagnets

Date: May 25, 2017 01:30 PM

URL: http://pirsa.org/17050086

Abstract: The 2D S = 1/2 square-lattice Heisenberg model is a keystone of theoretical studies of quantum magnetism. It also has very good realizations in several classes of layered insulators with localized electronic spins. While spin-wave theory provides a good understanding of the antiferromagnetic ground state and low-lying excitations of the Heisenberg model, an anomaly in the excitations at higher energy around wave-number q = (\pi, 0) has been diffi_cult to explain. At first sight, the anomaly is just a suppression of the excitation energy by a few percent, but it also represents a more dramatic shift of spectral weight in the dynamic spin structure factor from the single- magnon (spin wave) pole to a continuum. Recent neutron scattering experiments on the quasi-2D material Cu(DCOO)2_.4D2O (the best realization so far of the 2D Heisenberg model) were even interpreted as a complete lack of magnon pole at the anomaly; instead it was suggested that the excitations there are fractional (spinons) [1]. I will discuss recent quantum Monte Carlo and stochastic analytic continuation results pointing to the existence of fragile q~(\pi,0) magnon excitations in the Heisenberg model [2], which can be fractionalized by interactions competing with the nearest-neighbor exchange coupling. This phenomenon can be understood phenomenologically within a simple theory of magnon-spinon mixing.

Four Corners Symposium, May 25, 2017

BOSTON UNIVERSITY

Nearly Fractionalized Excitations in 2D Quantum Antiferromagnets

Anders W Sandvik, Boston University

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Collaborators

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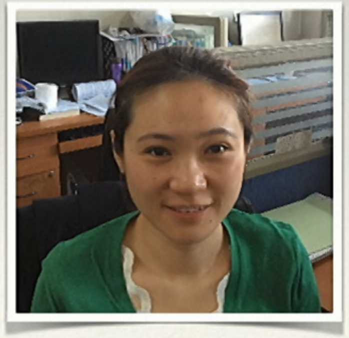

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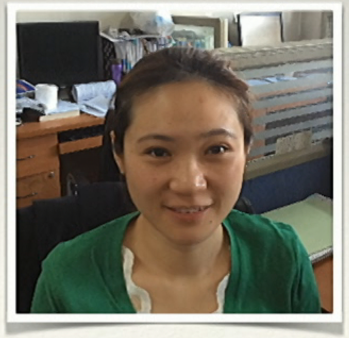

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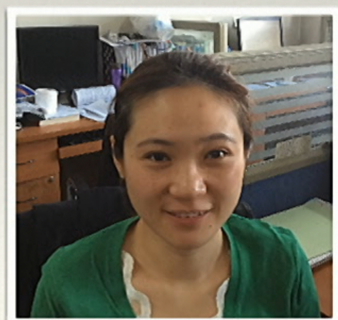


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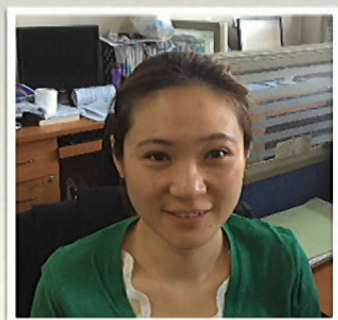


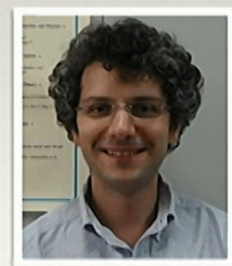


The S=1/2 Heisenberg antiferromagnet

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad \langle i,j \rangle = \text{nearest neighbors}$$

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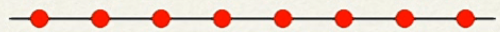

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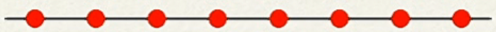

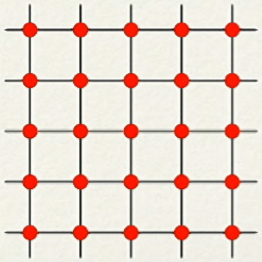

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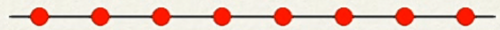

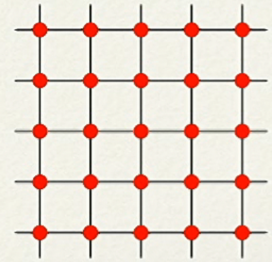

Ground state

- critical in 1D (spin correlations ~1/r)
- long-range ordered in 2D (order reduced by quantum fluctuations)

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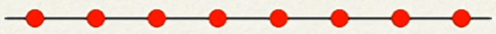

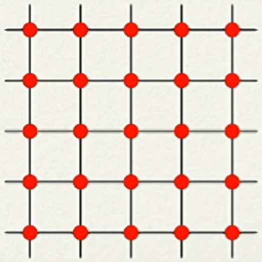

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1D
"spinons", carry spin S=1/2 (exactly from Bethe Ansatz)

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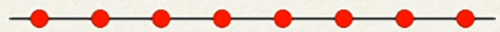

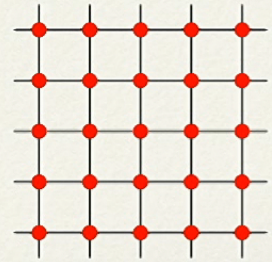

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Conventional wisdom (spin-wave theory etc): magnons, carry S^z=1

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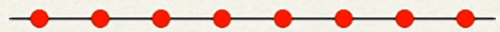

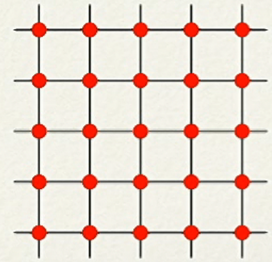

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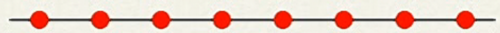

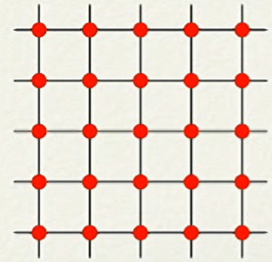

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This talk

QMC study of dynamic structure factor of 2D Heisenberg and J-Q models
- numerical analytic continuation of imaginary-time correlation functions
- comparisons with previous calculations and experiments
- theory of spinon-magnon mixing

Spinons in 1D

Ising picture

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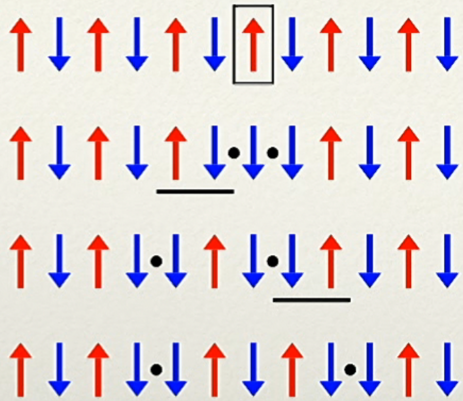

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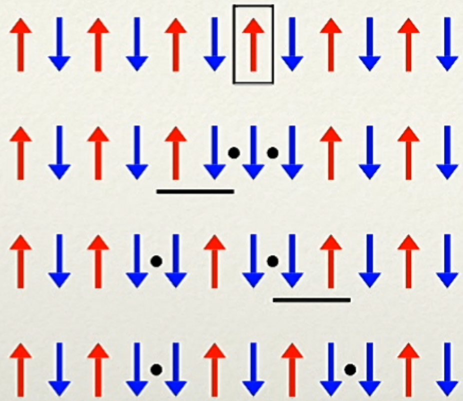

Spin-flip excitation breaks up into two domain walls - independently movable through quantum fluctuations

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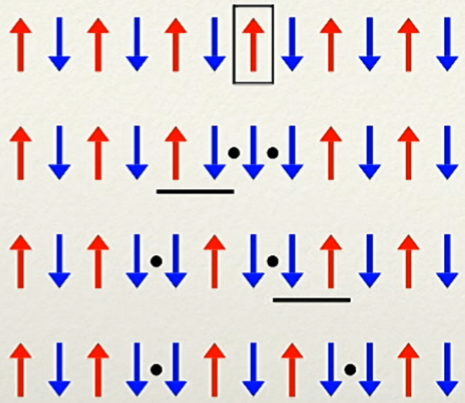

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Valence-bond picture

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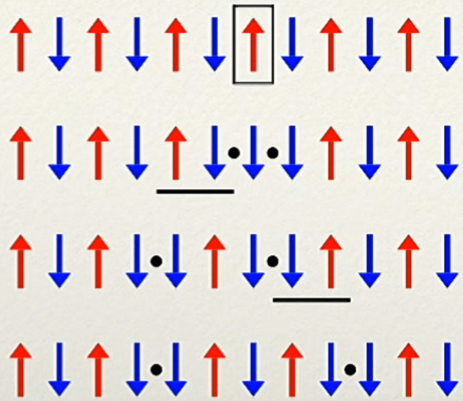

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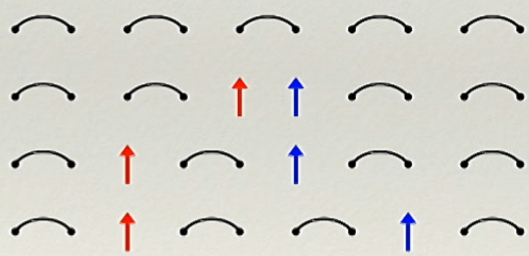

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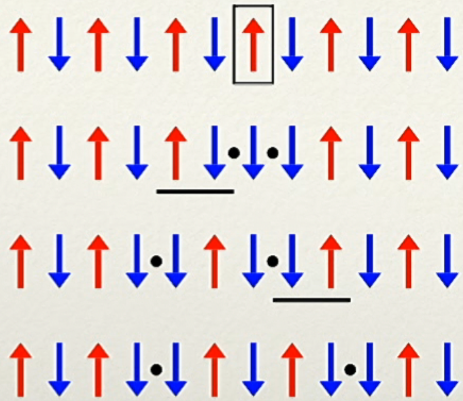

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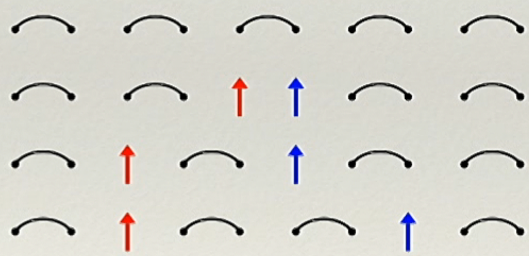

Valence-bond (singlet) breaks (into triplet) - unpaired spins propagate independently in singlet background

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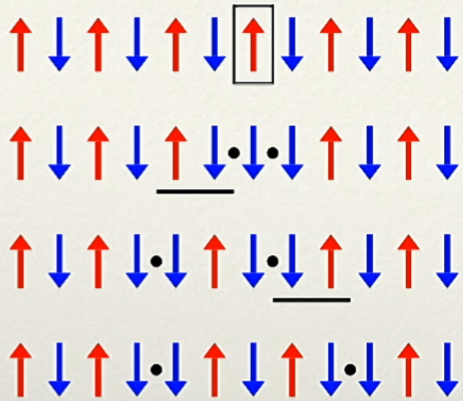

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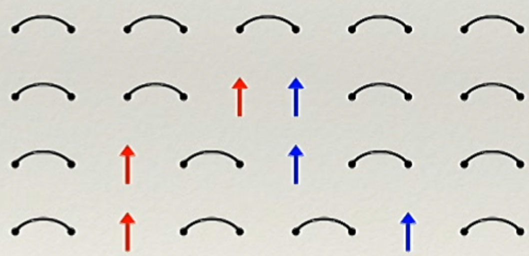

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The Heisenberg chain has aspects of both pictures
- Bethe Ansatz solution contains spinon excitations (critical domain walls)

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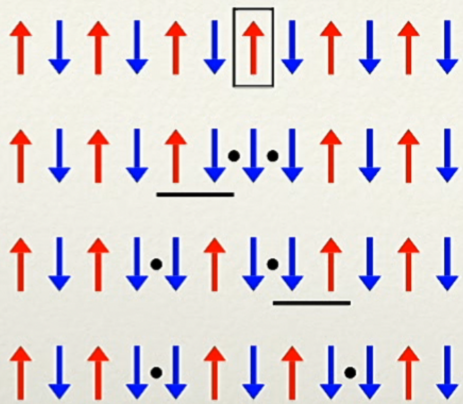

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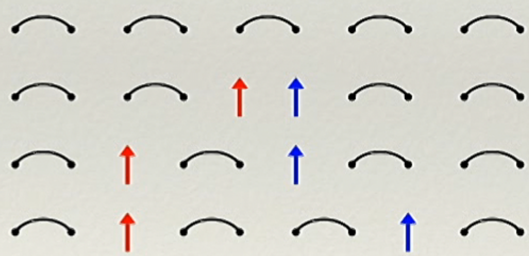

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2D: Simple pictures suggests confinement (correct?)

PRL 111, 137205 (2013) PHYSICAL REVIEW LETTERS week ending 27 SEPTEMBER 2013

Multispinon Continua at Zero and Finite Temperature in a Near-Ideal Heisenberg Chain

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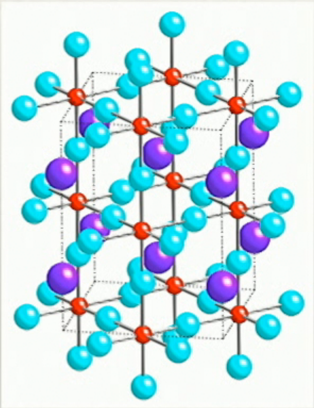

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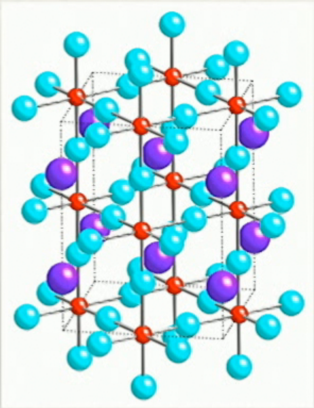
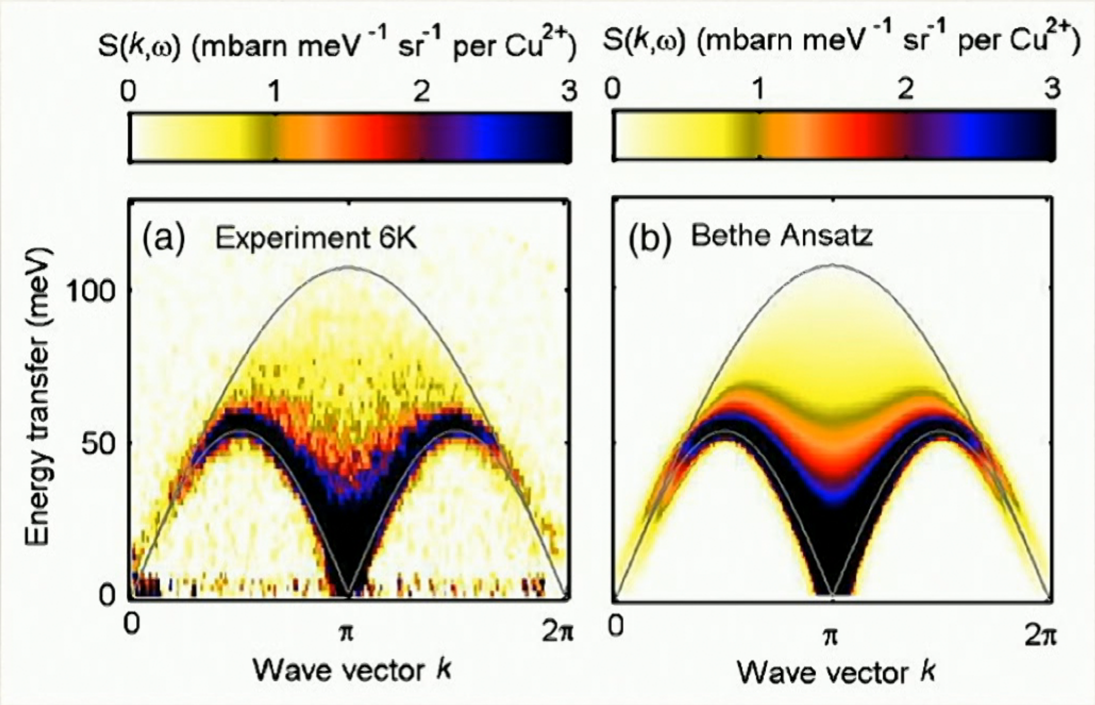


chain direction (anisotropic bonding)



Spin-wave theory of the 2D Heisenberg model

$$H_{ij} = J_{ij}(S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z) = J_{ij}[S_i^z S_j^z + \frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)]$$

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Minimize classical (zz) energy, map deviations (spin flips) to bosons

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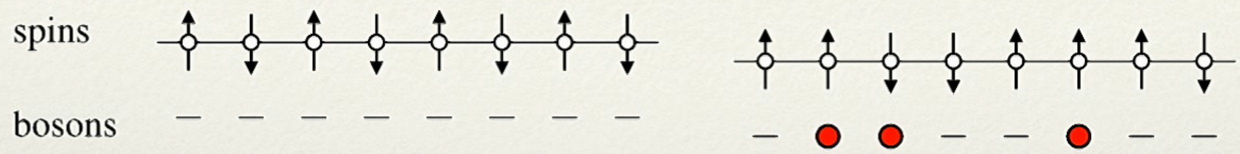

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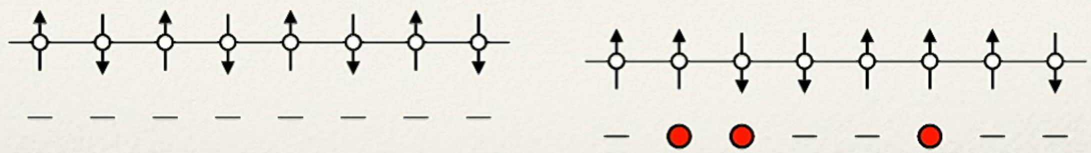
spins

bosons



$\underline{i \in \text{sublattice A}}$

$$S_i^z = S - n_i$$
$$n_i = a_i^+ a_i$$
$$S_i^+ = (2S - n_i)^{1/2} a_i$$
$$S_i^- = a_i^+ (2S - n_i)^{1/2}$$

$\underline{j \in \text{sublattice B}}$

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$$n_j = b_j^+ b_j$$
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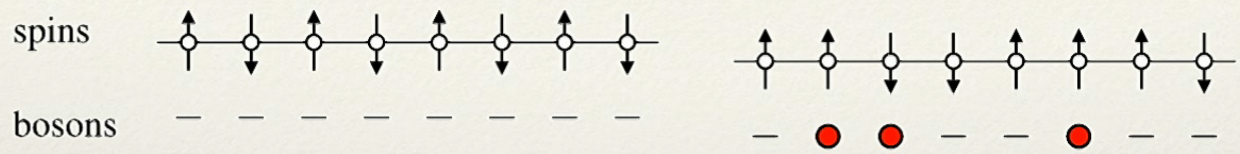

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Lowest order in 1/S (linear spin-wave theory):

$$H_{\mathrm{LSW}} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} [\alpha_{\mathbf{k}}^+ \alpha_{\mathbf{k}} + \beta_{\mathbf{k}}^+ \beta_{\mathbf{k}}]$$

$$\omega(\mathbf{k}) = 4SJ\sqrt{1 - \gamma_{\mathbf{k}}^2} \qquad \gamma_{\mathbf{k}} = \frac{1}{2}[\cos(k_x) + \cos(k_y)]$$

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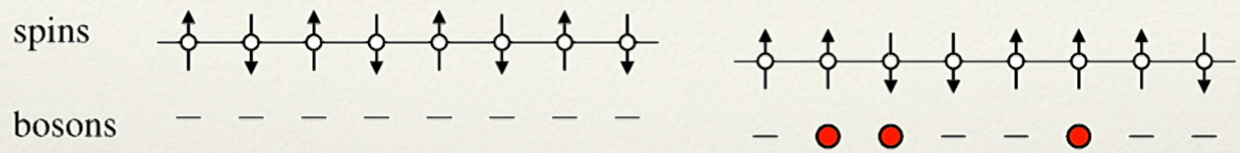

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Order parameter (sublattice magnetization)

$$m_s = S - \frac{1}{N}\sum_{\mathbf{k}}\left(\frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1\right)$$

For S=1/2: m_s=0.3034 (0.3069 up to order $1/S^2$)

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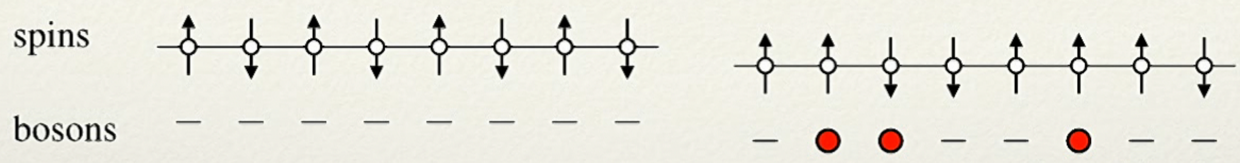
Minimize classical (zz) energy, map deviations (spin flips) to bosons



Lowest order in 1/S (linear spin-wave theory):

$$H_{\rm LSW} = \sum_{\mathbf{k}} \omega_{\mathbf{k}} [\alpha^+_{\mathbf{k}} \alpha_{\mathbf{k}} + \beta^+_{\mathbf{k}} \beta_{\mathbf{k}}]$$

$$\omega(\mathbf{k}) = 4SJ\sqrt{1-\gamma_{\mathbf{k}}^2} \qquad \gamma_{\mathbf{k}} = \frac{1}{2}[\cos(k_x) + \cos(k_y)]$$

$i \in$ sublattice A

$$S_i^z = S - n_i$$
$$n_i = a_i^+ a_i$$
$$S_i^+ = (2S - n_i)^{1/2} a_i$$
$$S_i^- = a_i^+ (2S - n_i)^{1/2}$$

$j \in$ sublattice B

$$S_j^z = -S + n_j$$
$$n_j = b_j^+ b_j$$
$$S_j^+ = b_j^+ (2S - n_j)^{1/2}$$
$$S_j^- = (2S - n_j)^{1/2} b_j.$$

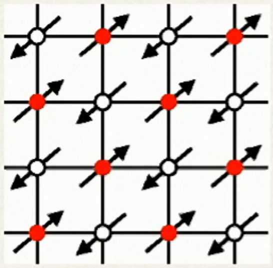
Order parameter (sublattice magnetization)

$$m_s = S - \frac{1}{N}\sum_{\mathbf{k}} \left(\frac{1}{\sqrt{1-\gamma_{\mathbf{k}}^2}} - 1 \right)$$

For S=1/2: m_s=0.3034 (0.3069 up to order $1/S^2$)

Is this correct?

QMC calculations of antiferromagnetic order



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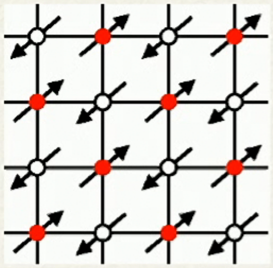
Sublattice magnetization

$$\vec{m}_s = \frac{1}{N}\sum_{i=1}^{N} \phi_i \vec{S}_i, \qquad \phi_i = (-1)^{x_i+y_i} \quad \text{(2D square lattice)}$$



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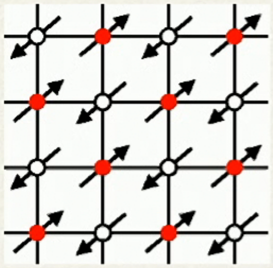

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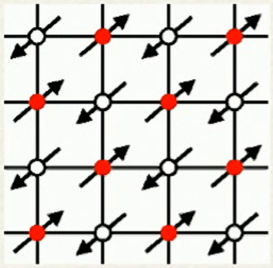

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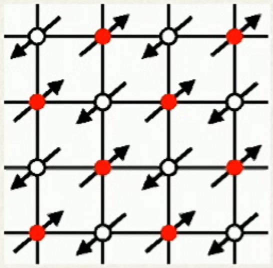

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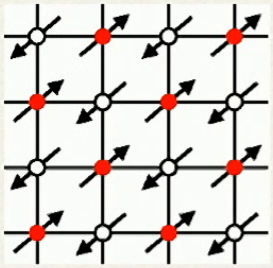

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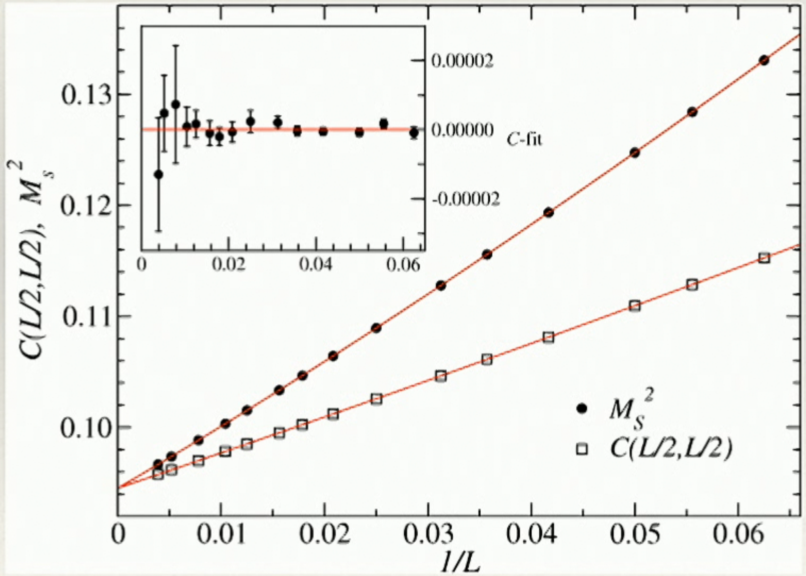
L×L lattices up to 256×256, T=0



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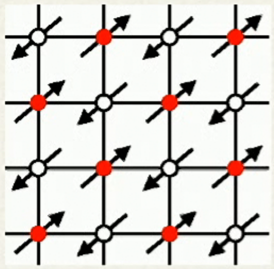

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Spin-wave theory describes the ground state very well

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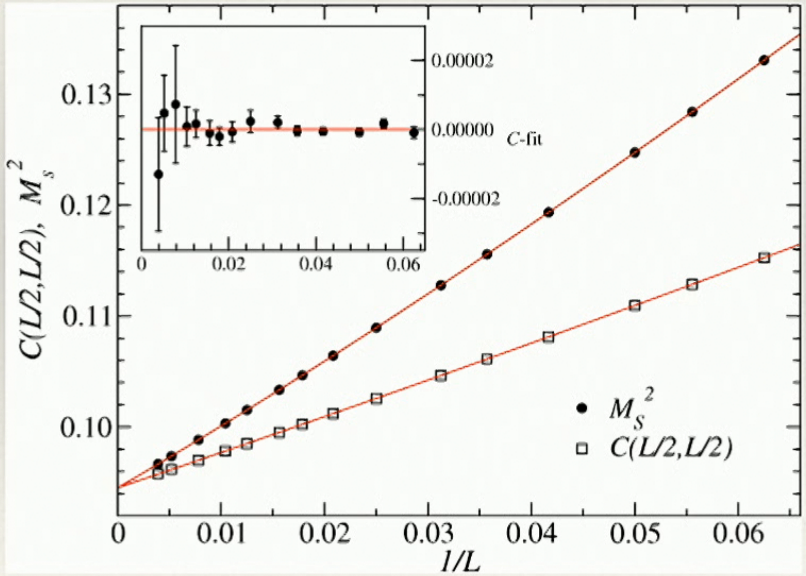
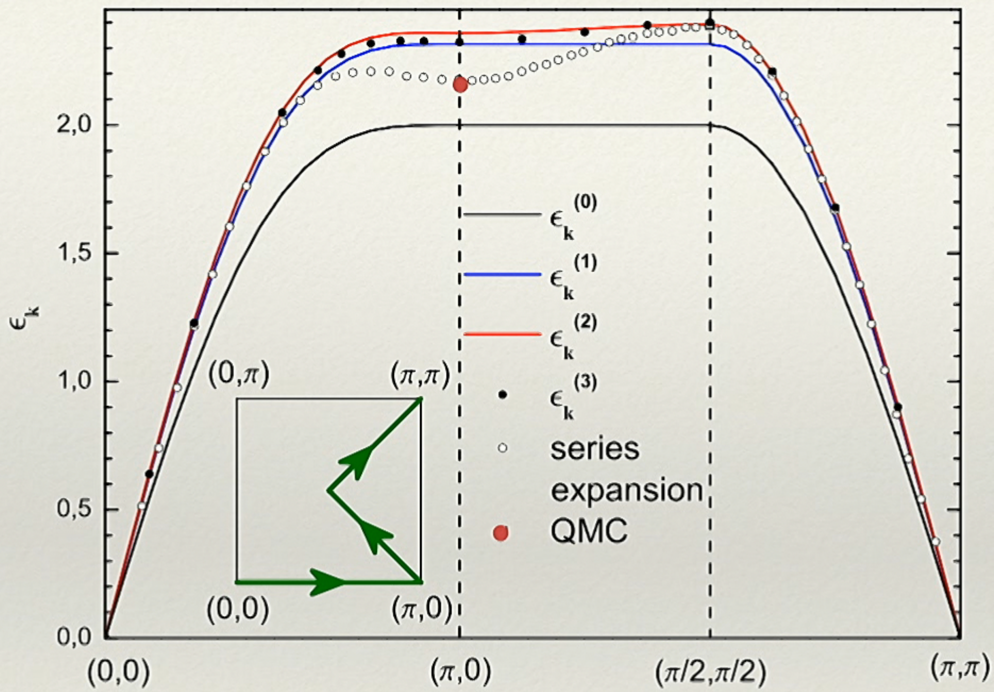


Dispersion relation beyond linear spin-wave theory

High-order spin-wave theory appears to fail close to q = $(\pi,0)$



Graph: A. Syromyatnikov, J. Phys. Cond. Mat (2010)

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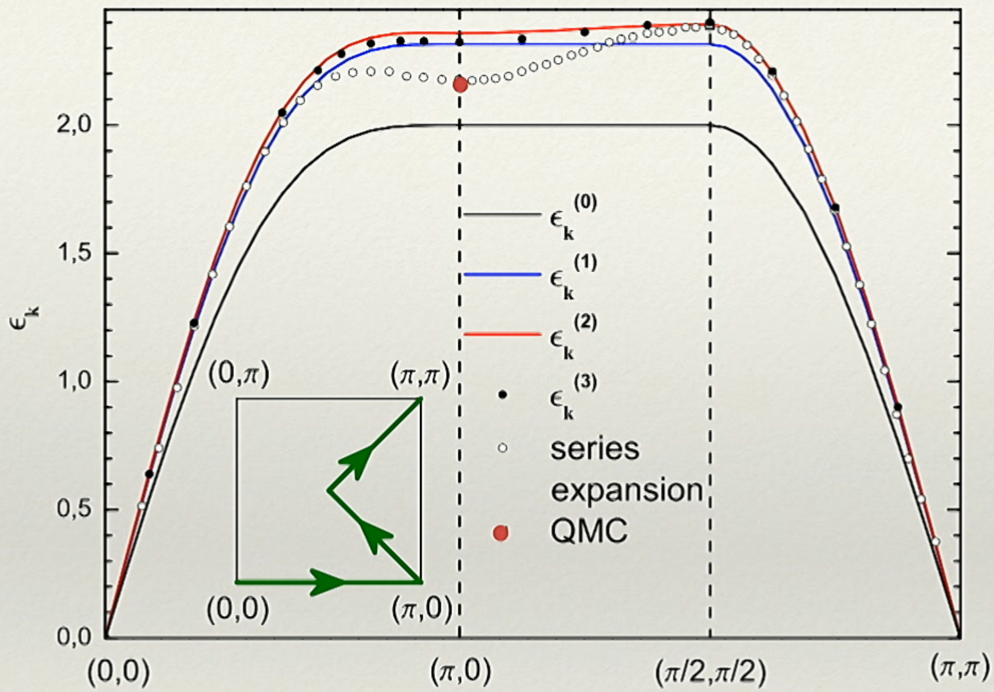

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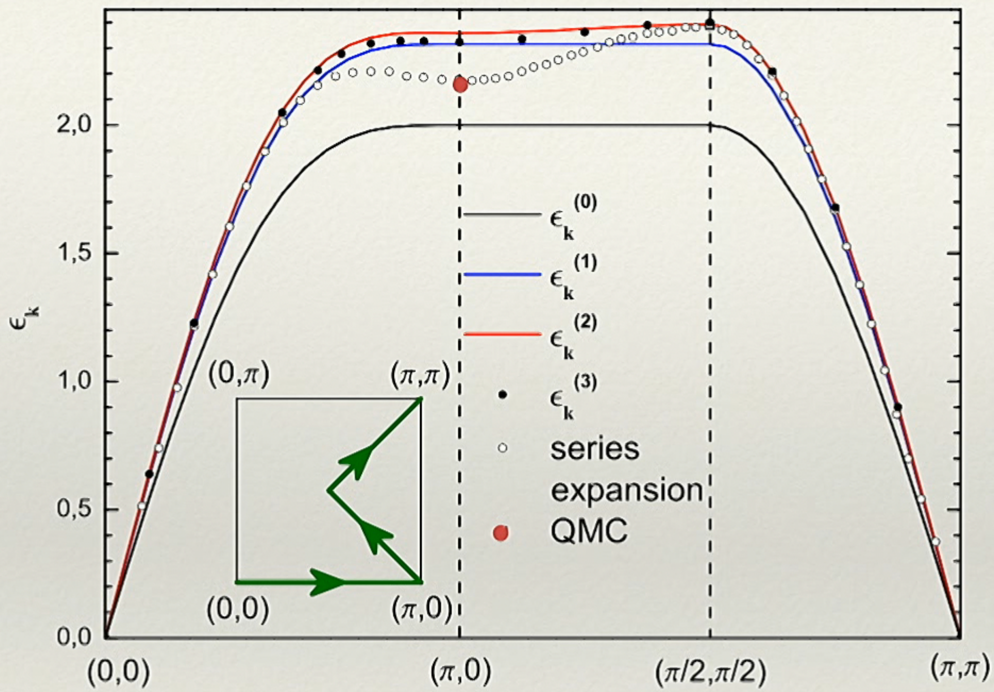

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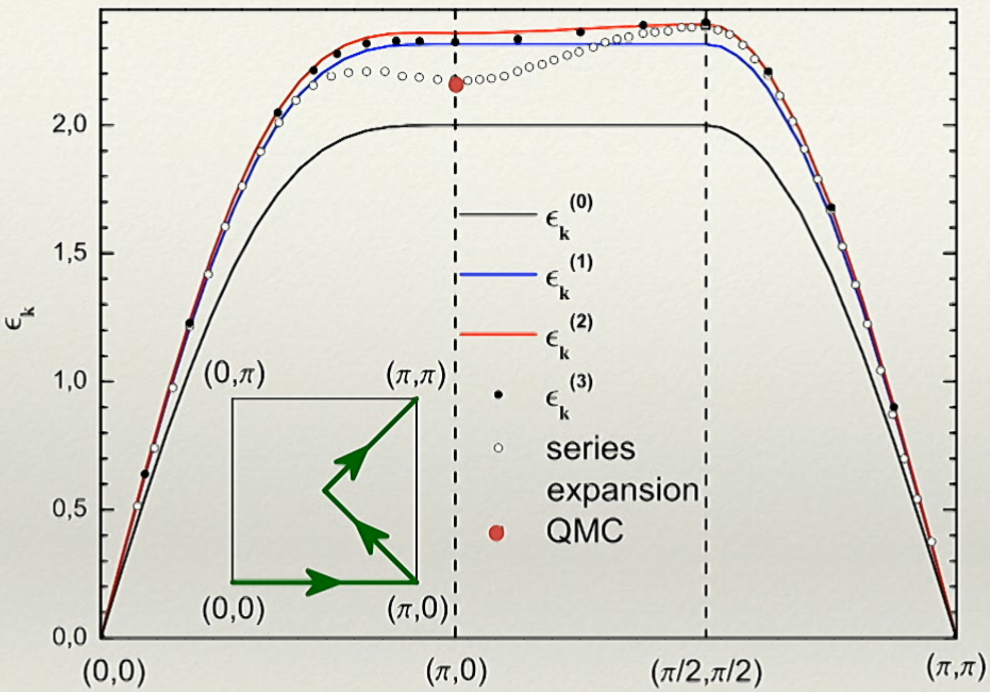

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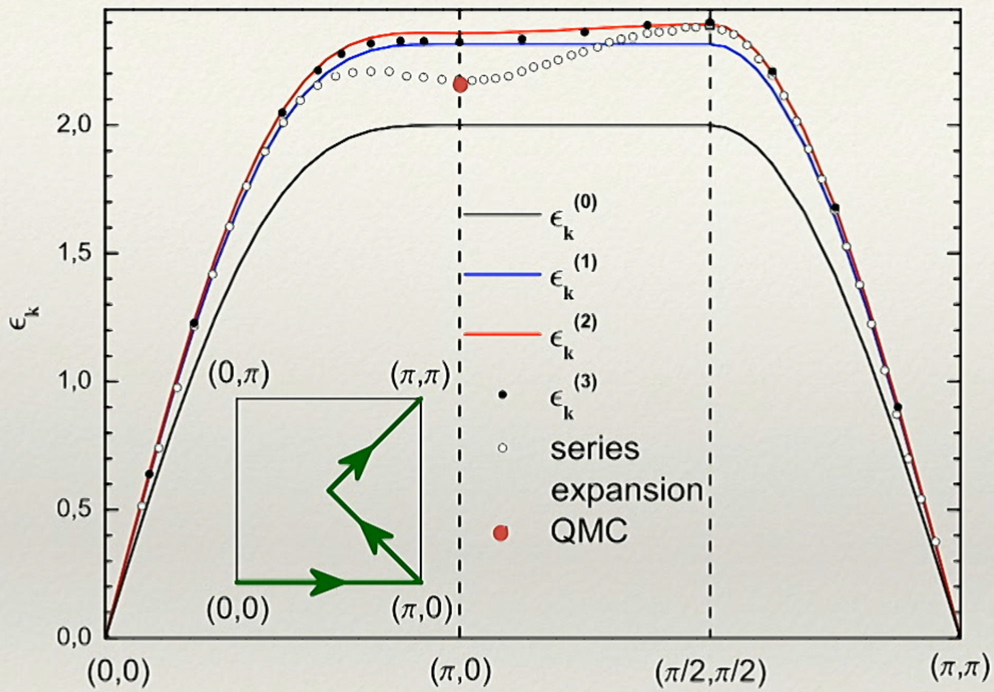

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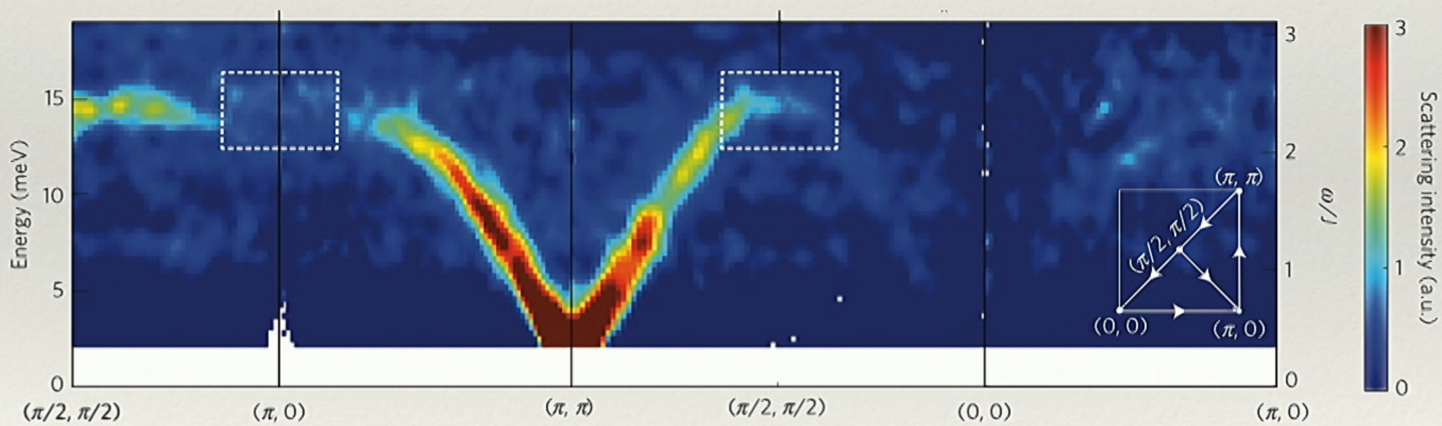
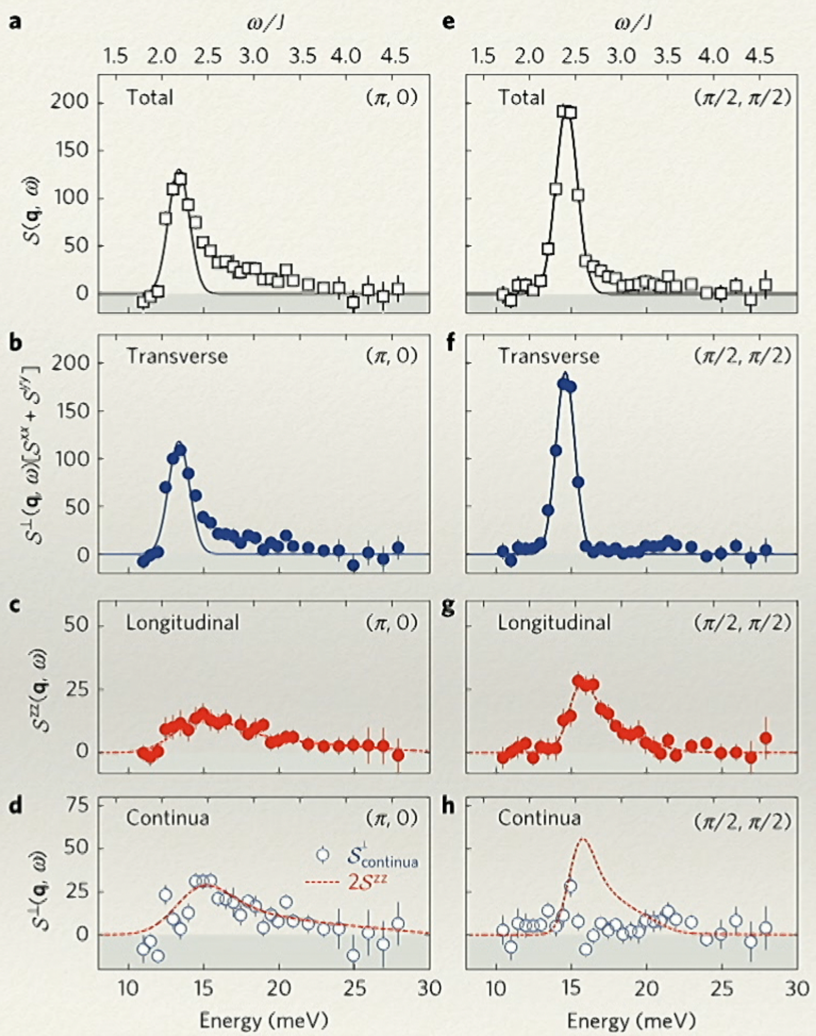
ARTICLES
PUBLISHED ONLINE: 23 DECEMBER 2014 | DOI: 10.1038/NPHYS3172
nature physics

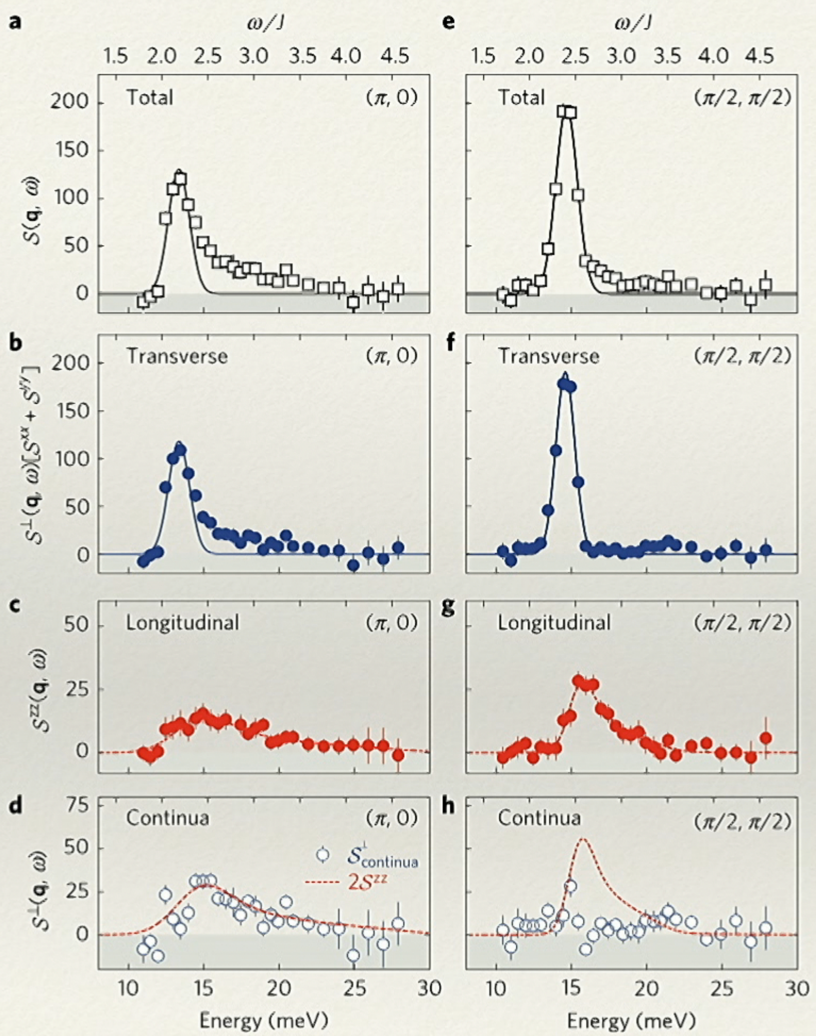
Fractional excitations in the square-lattice quantum antiferromagnet $Cu(DCOO)_2 \cdot 4D_2O$

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]





Polarized neutrons:
transversal (spin-wave)
and longitudinal (amplitude)
modes separated



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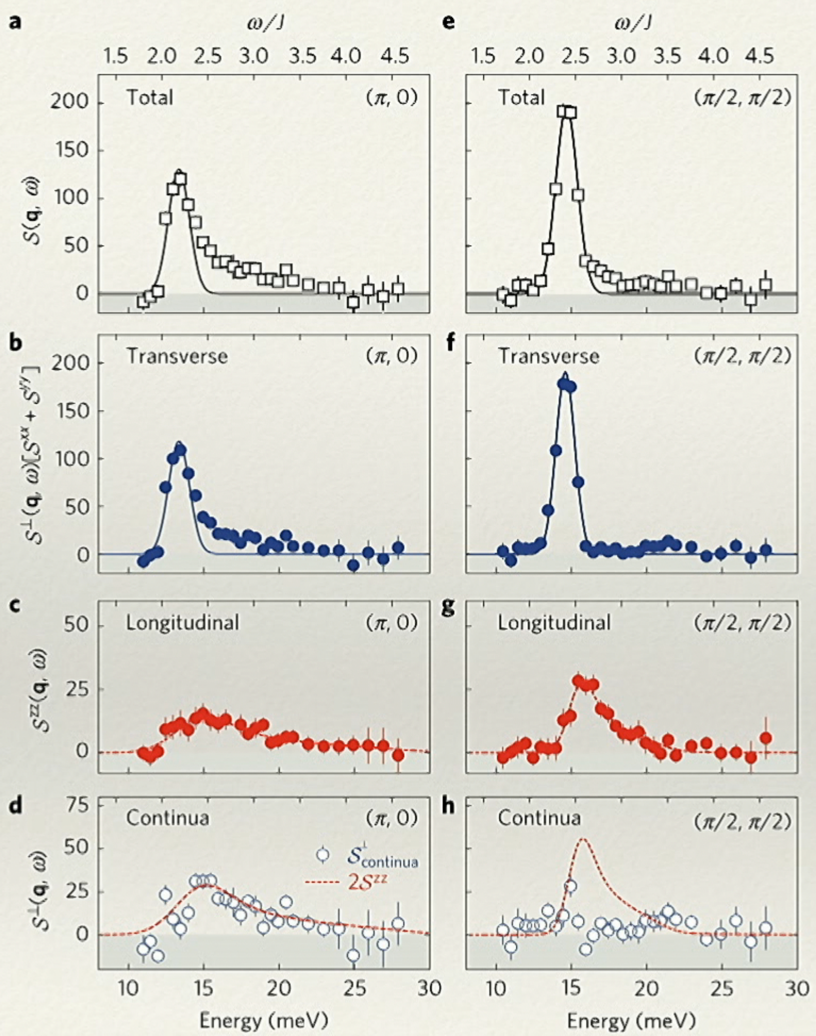
Claim:
Spinons at q=(π,0)



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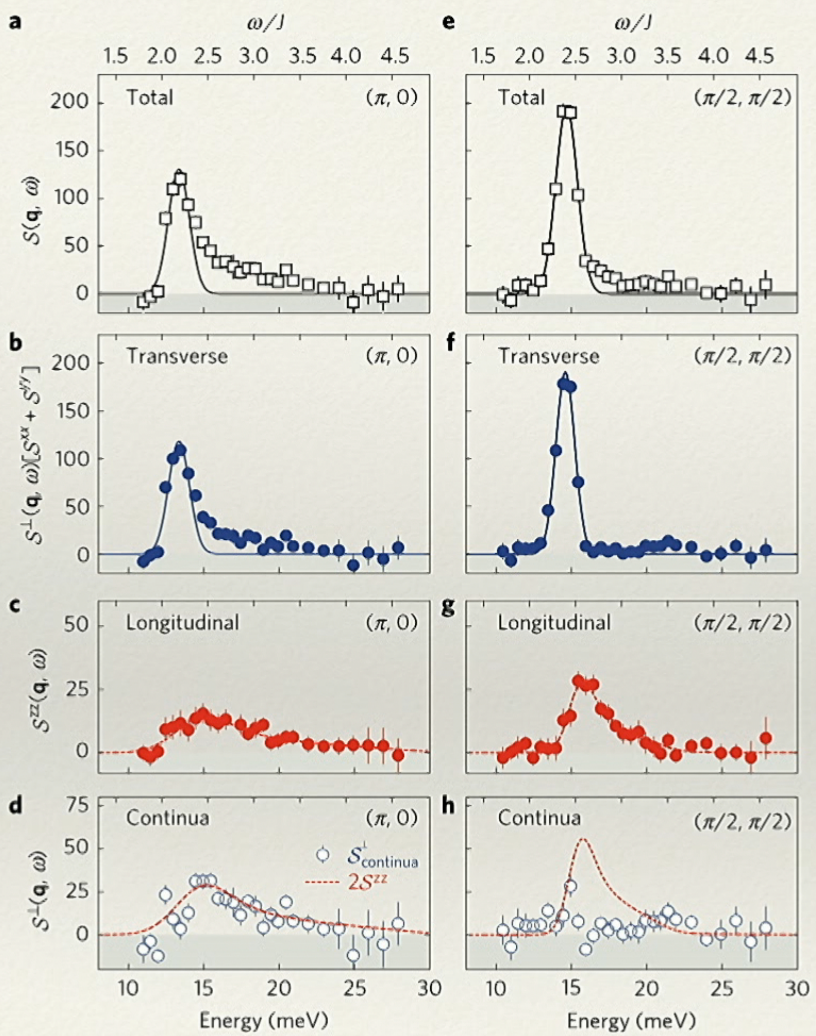

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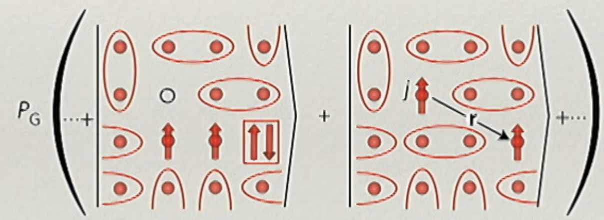

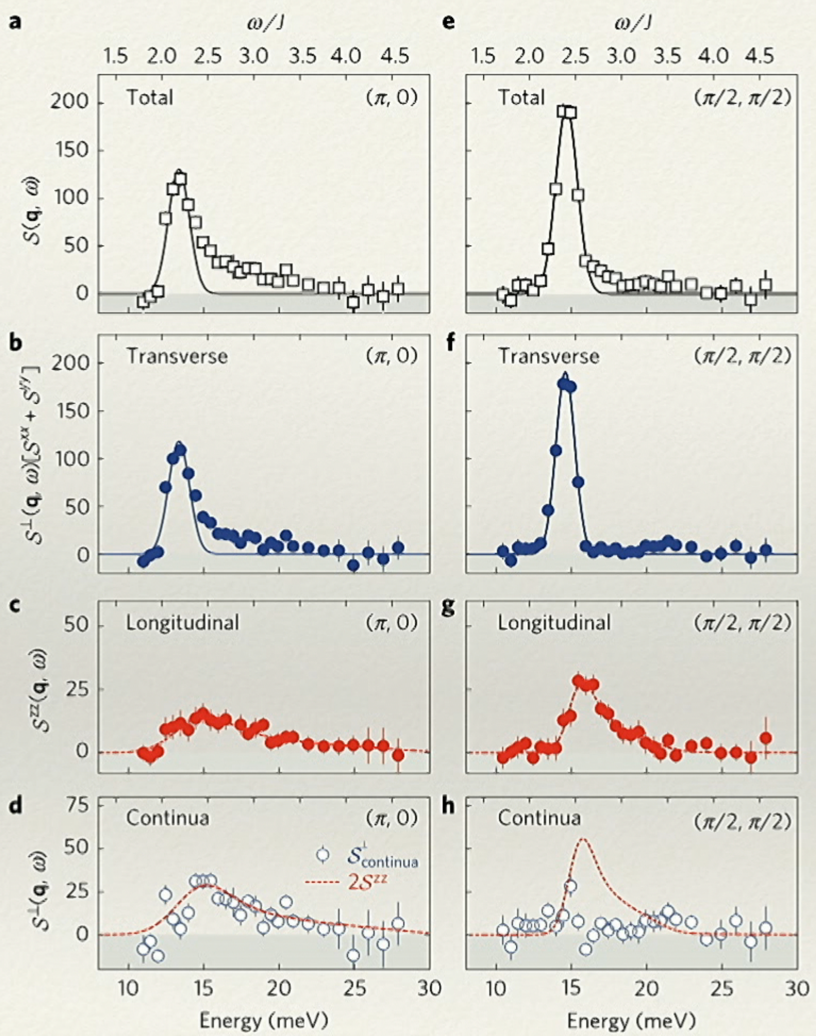

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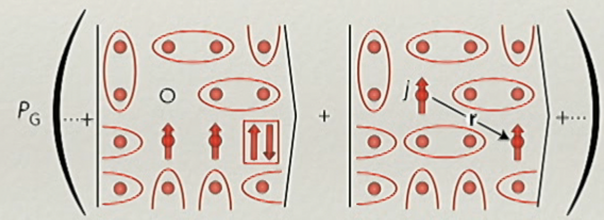

Dispersion and excitation
continuum match (approximately)
the experiments
- but wavefunction is that of
  a spin liquid….

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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

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

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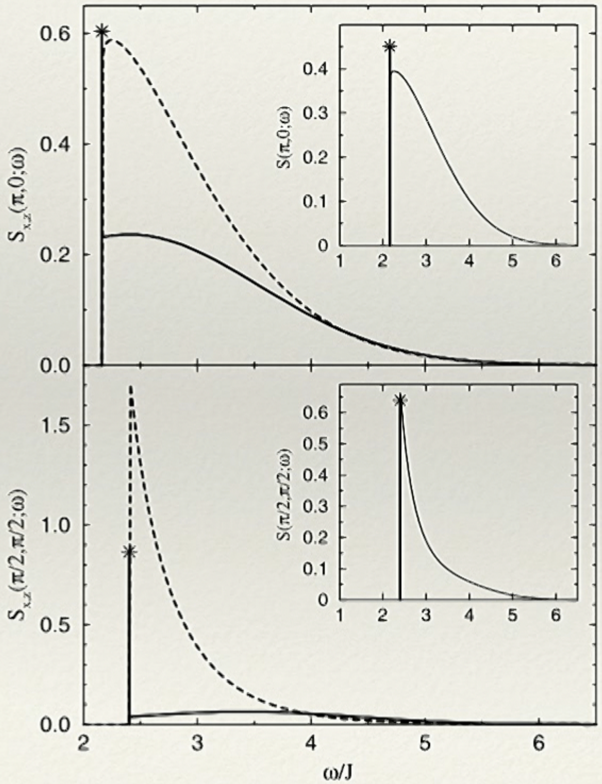

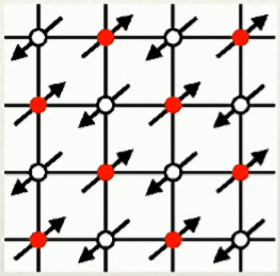

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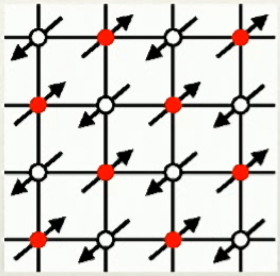

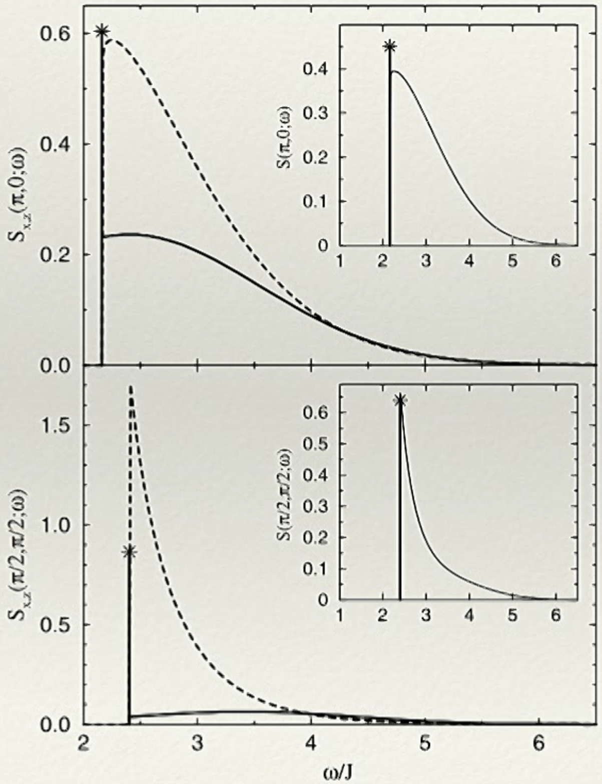

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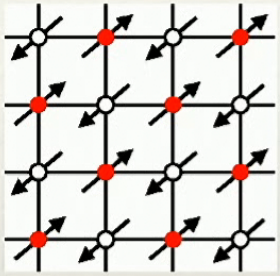

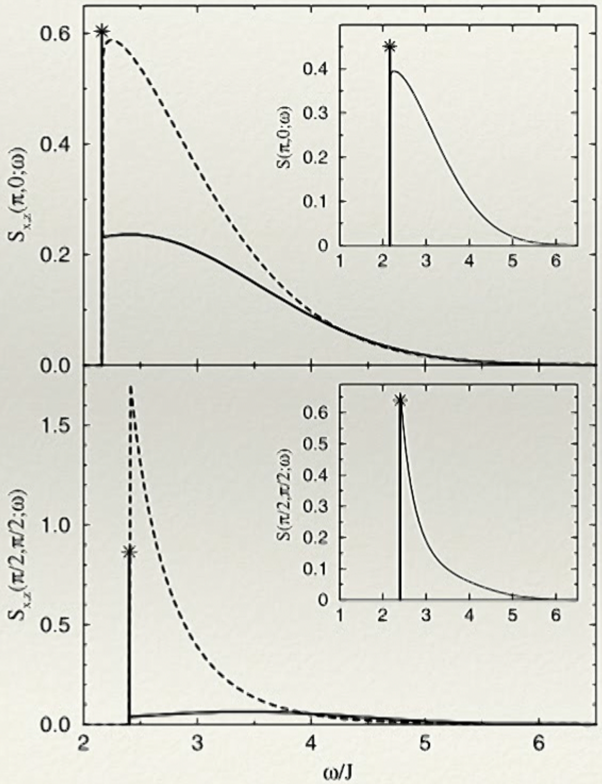

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General analytic continuation procedure

Represent the spectrum using
some suitable generic parametrization

- e.g., sum of many delta functions

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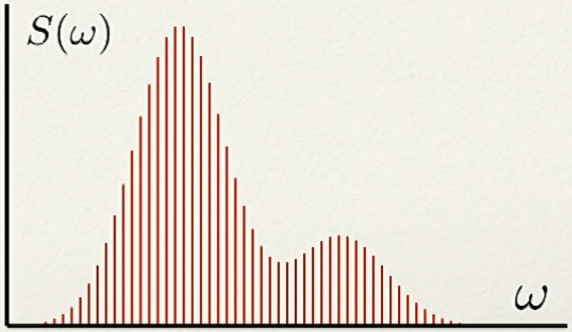

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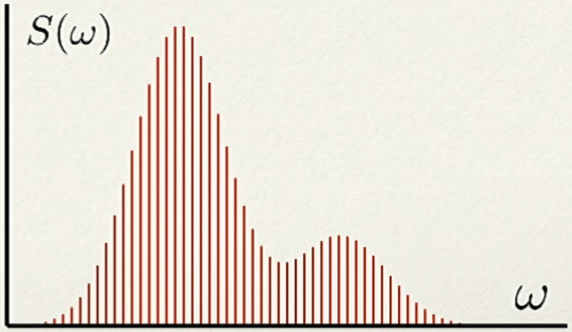

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- many spectra have almost same goodness-of-fit (close to best χ^2)

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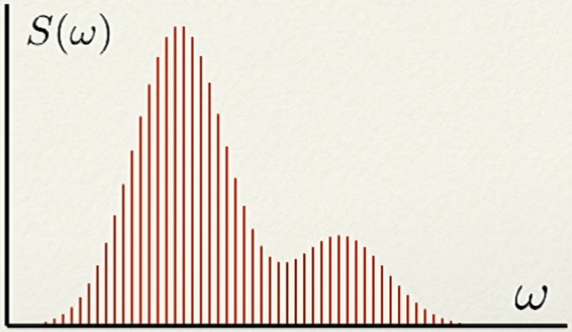

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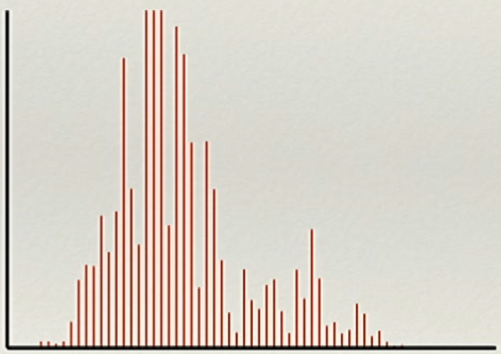

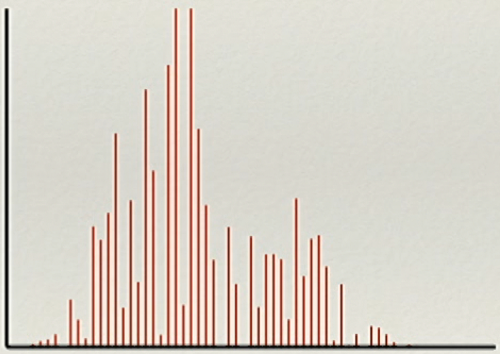

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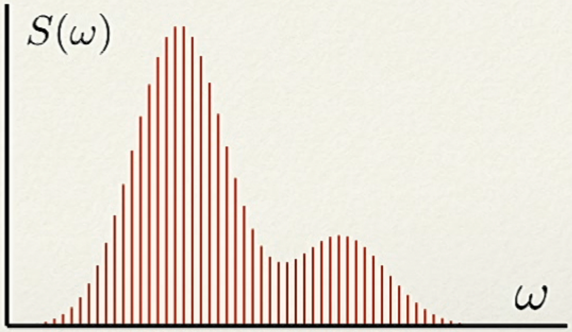

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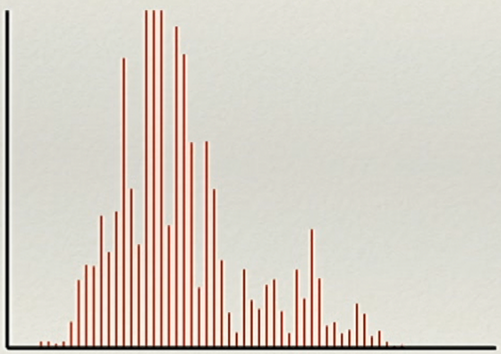

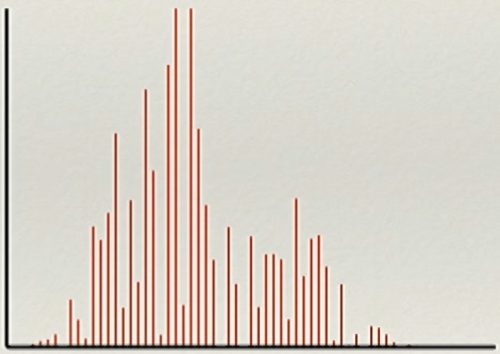

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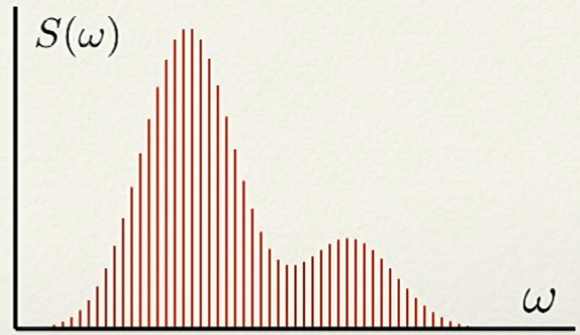

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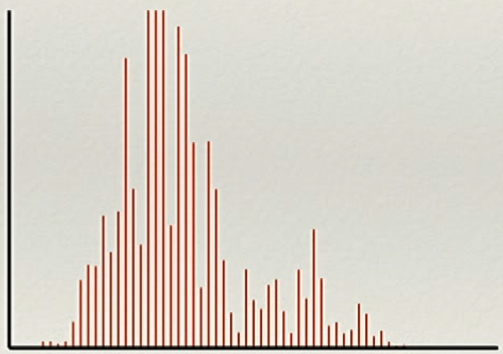

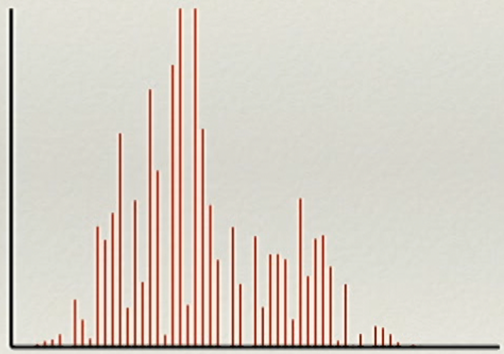

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Standard way: Maximum-Entropy method
- balance between high entropy (smooth spectrum) and good χ^2 fit

Stochastic analytic continuation

Hui Shao & A. Sandvik (in progress)

Sandvik, PRB 1998; Beach, arXiv 2004; Syljuåsen, PRE 2008; Sandvik, PRE 2016
[slightly different approach: Mishchenko, Prokofev, Svistunov,… papers 2000-]

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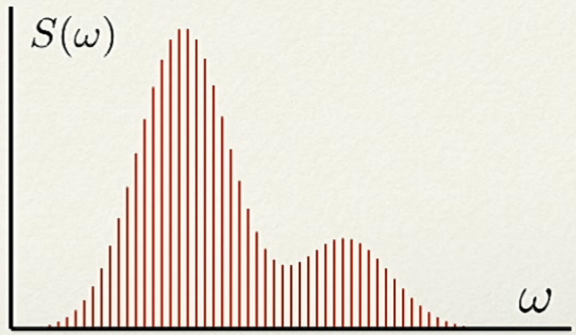

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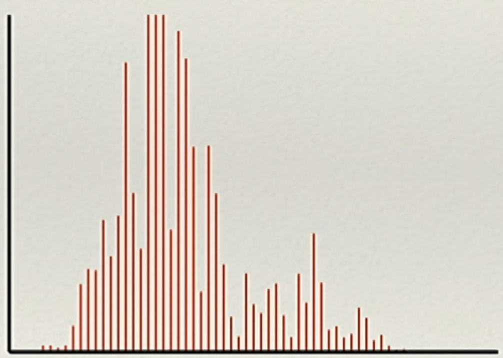

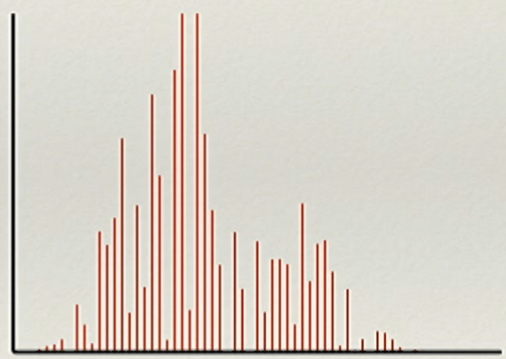

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- several proposals
- balance between good fit and overfitting (fitting to noise)

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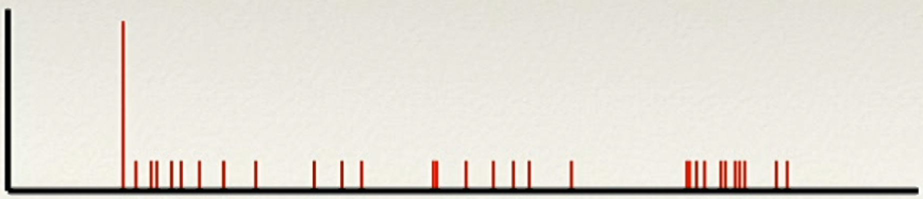
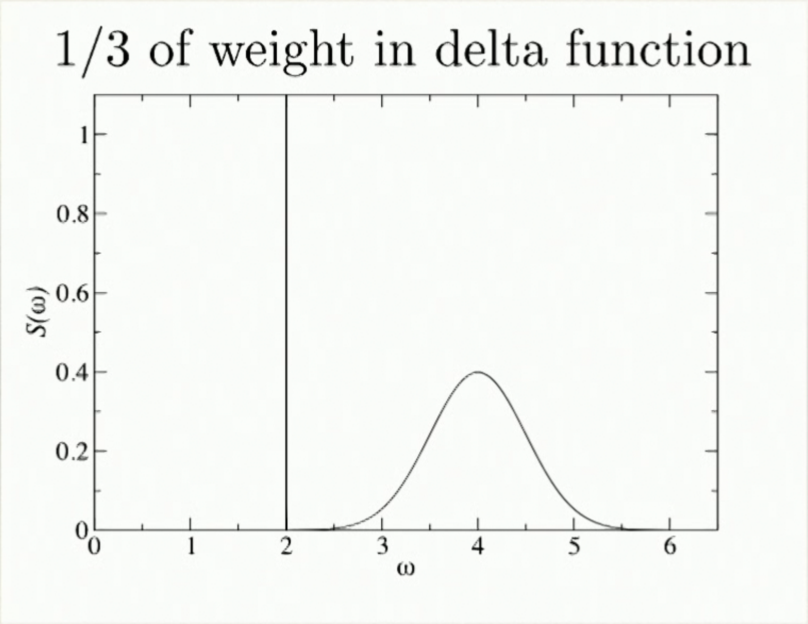
Can also build in “prominent feature”, e.g., dominant delta-fktn



Delta-function and continuum, test with synthetic data

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



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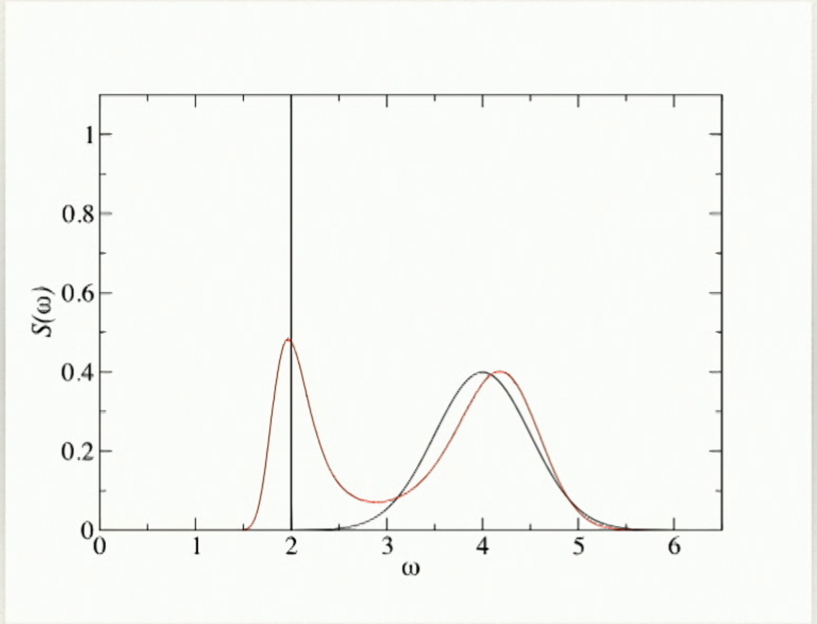

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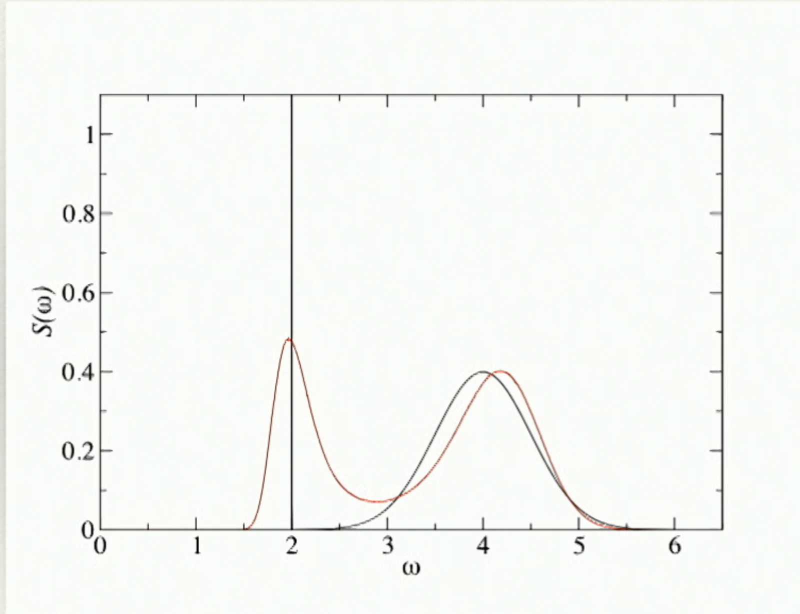

Unrestricted sampling cannot resolve the delta function very well

- high-energy peak is also distorted

Special treatment of delta-fktn at the edge
- optimize amplitude, but sample location

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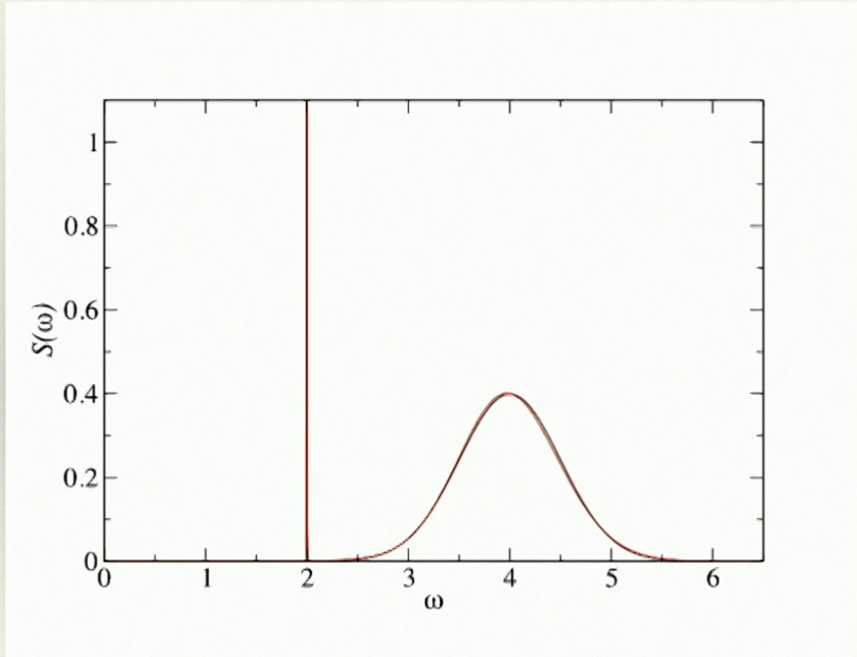
- optimize amplitude, but sample location



The entire spectrum is very well reproduced!

More challenging case: continuum touches delta-fktn

Synthetic spectrum with

- $\omega_0 = 0.4$
- $a_0 = 1.0$

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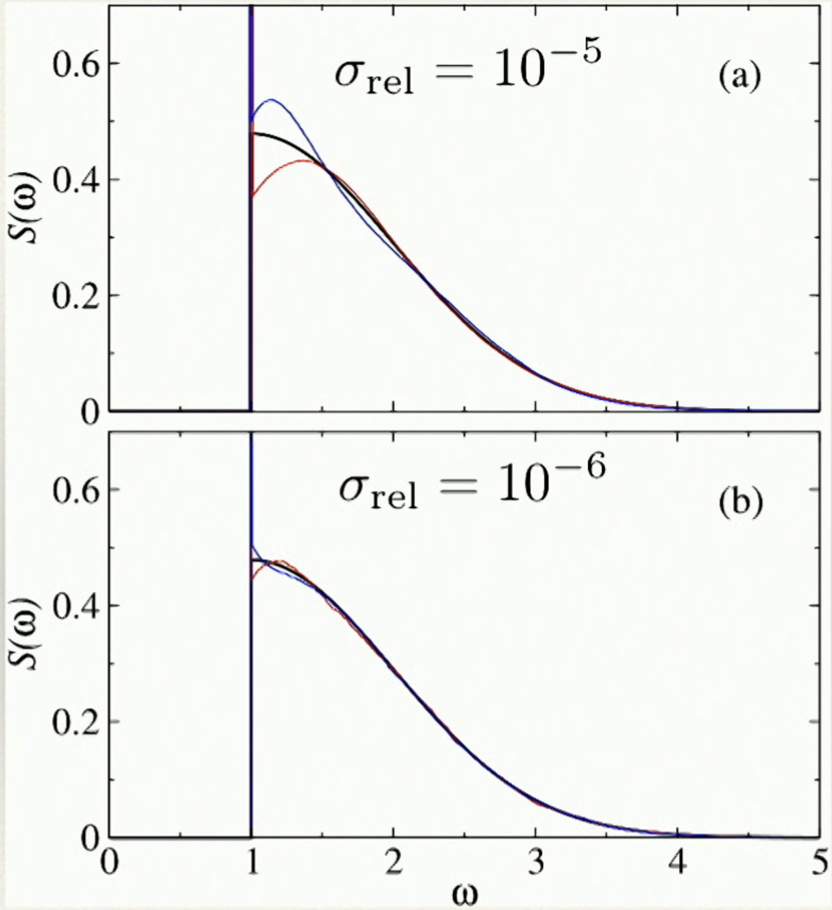

Dynamic structure factor of 2D S=1/2 Heisenberg model

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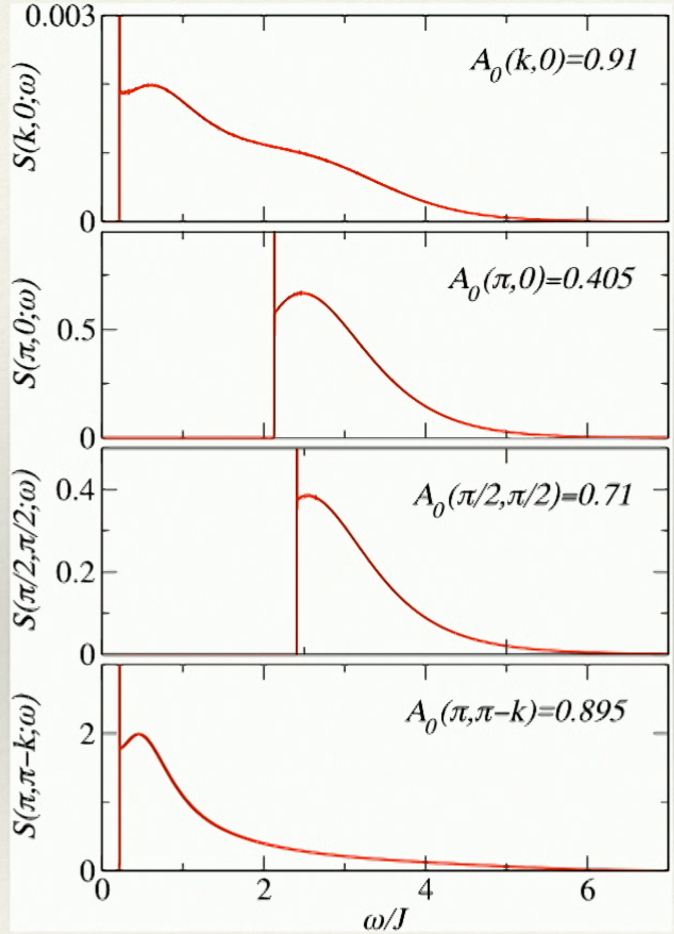
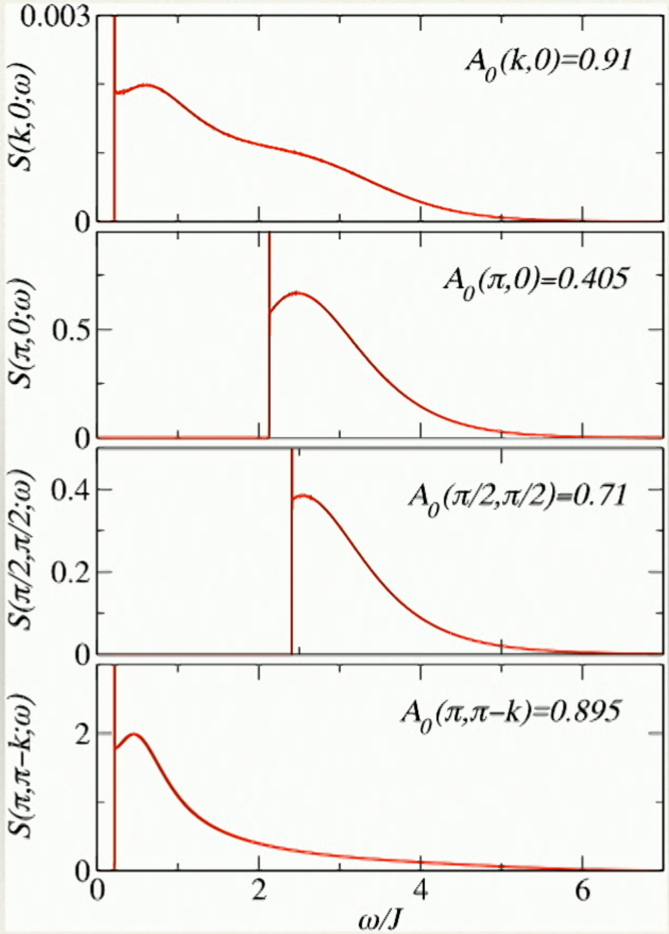


Dynamic structure factor of 2D S=1/2 Heisenberg model

Presence of magnon pole detected for all momenta q



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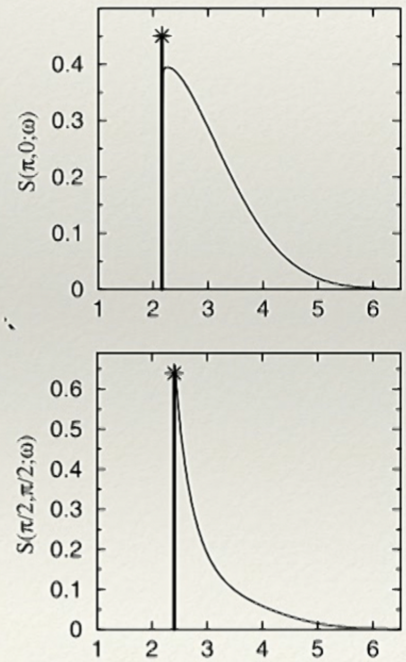
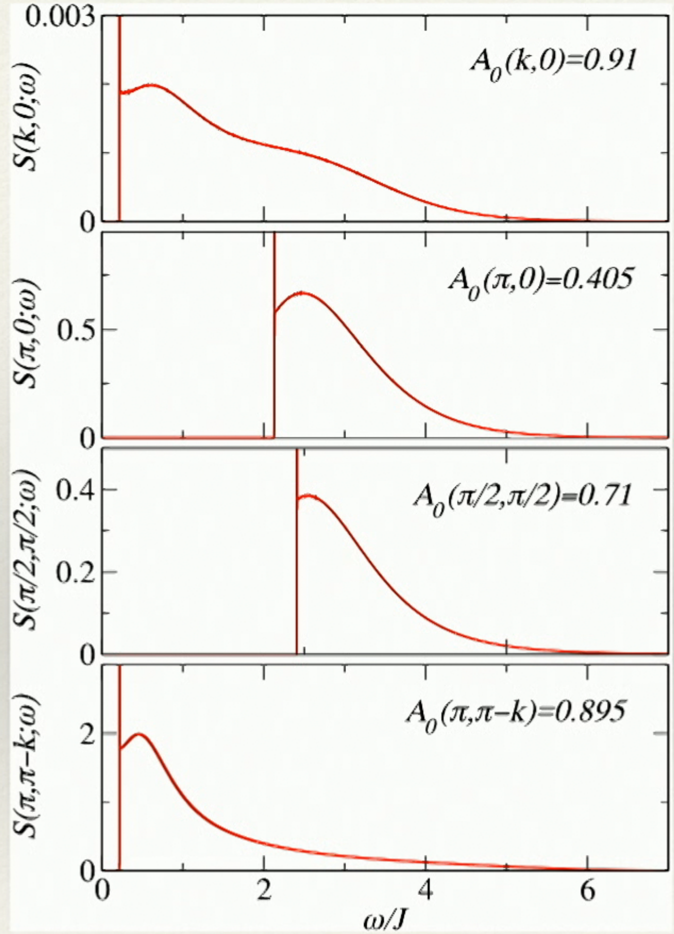
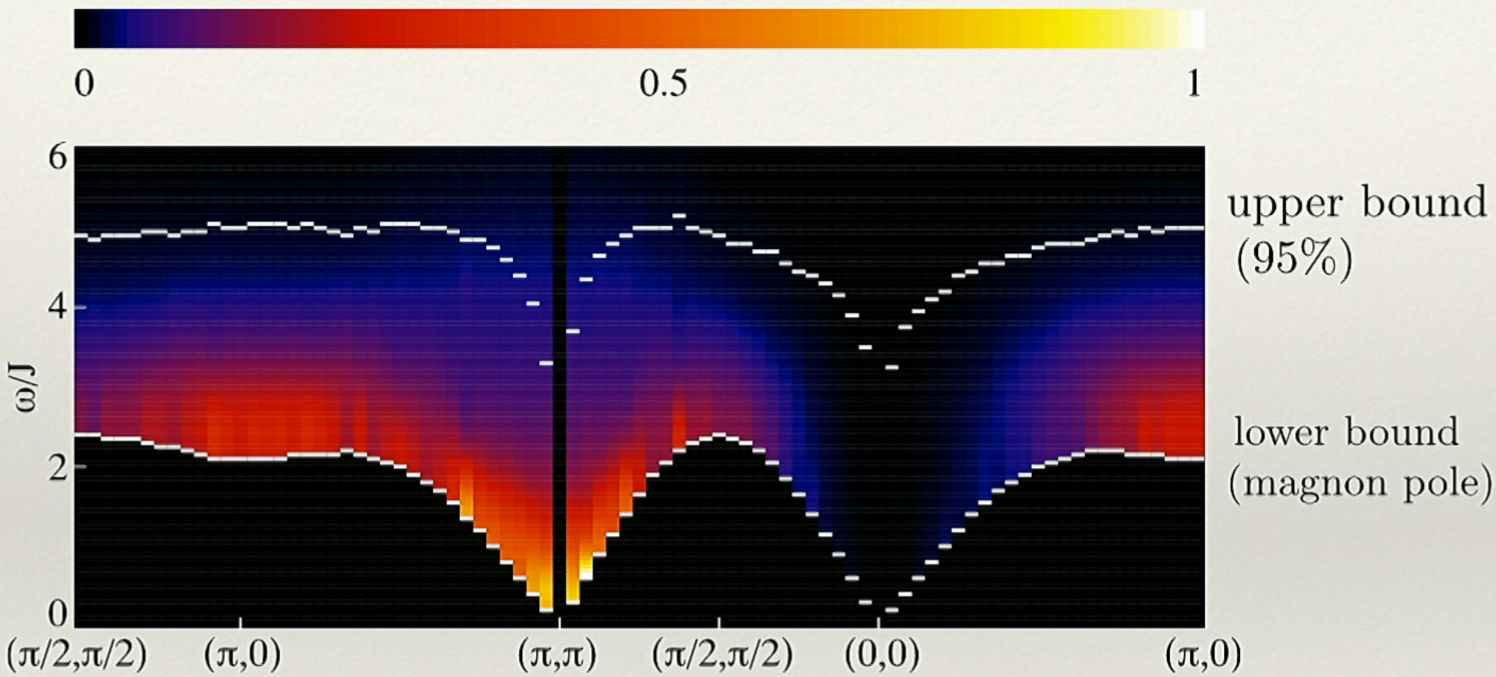
Compare with previous results (Sandvik, Sing, 2001):





QMC + SAC, L=48


0
0.5
1
6
4
2
0
ω/J
upper bound
(95%)
lower bound
(magnon pole)
(π/2,π/2)
(π,0)
(π,π)
(π/2,π/2)
(0,0)
(π,0)

Finite-size effects

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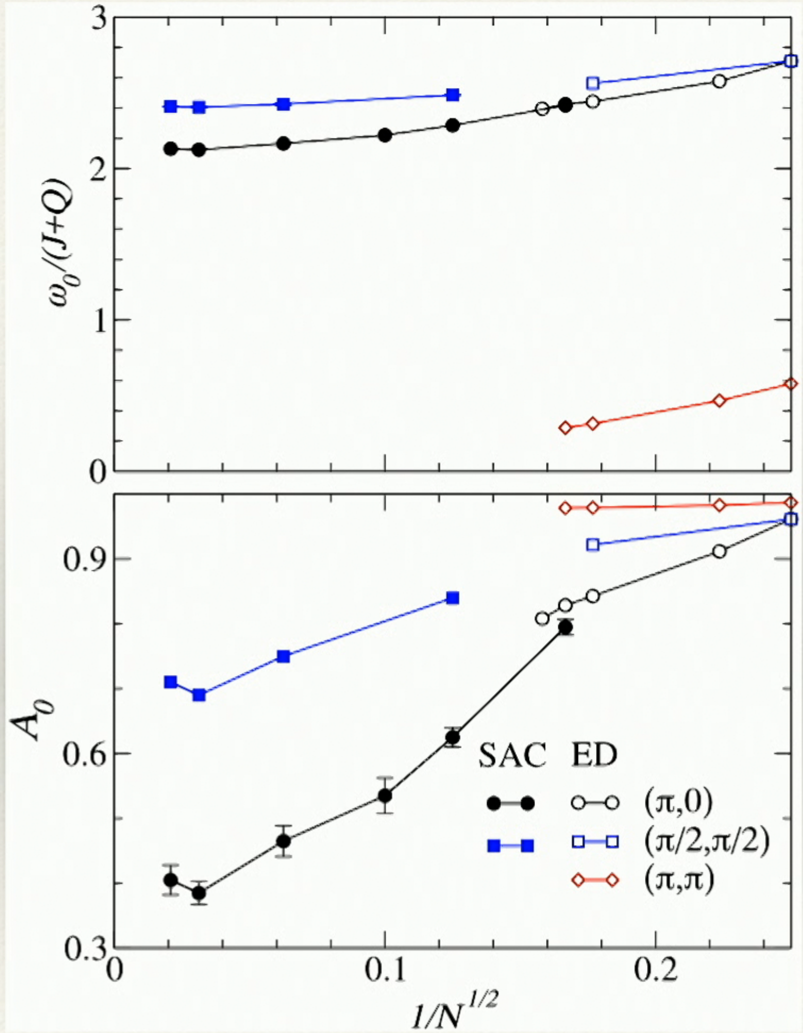

Comparison with neutron scattering experiments

$Cu(DCOO)_2 \cdot 4D_2O$

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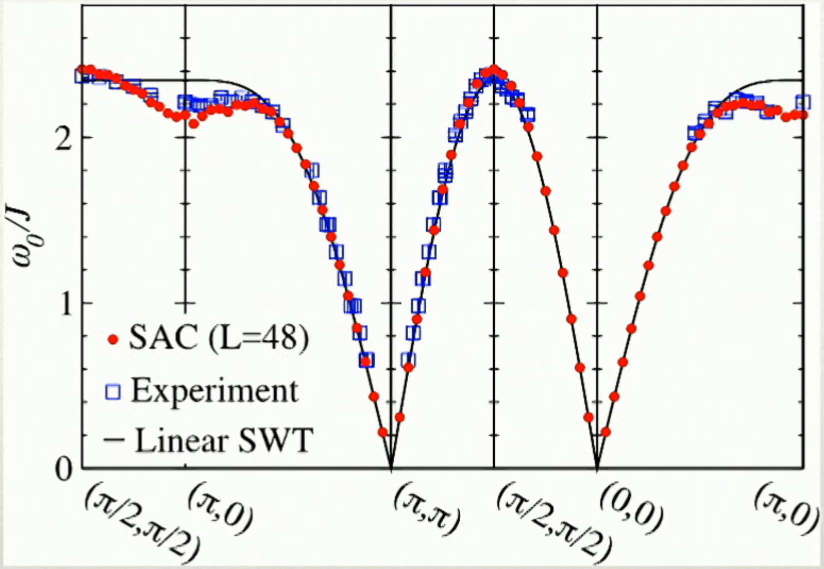

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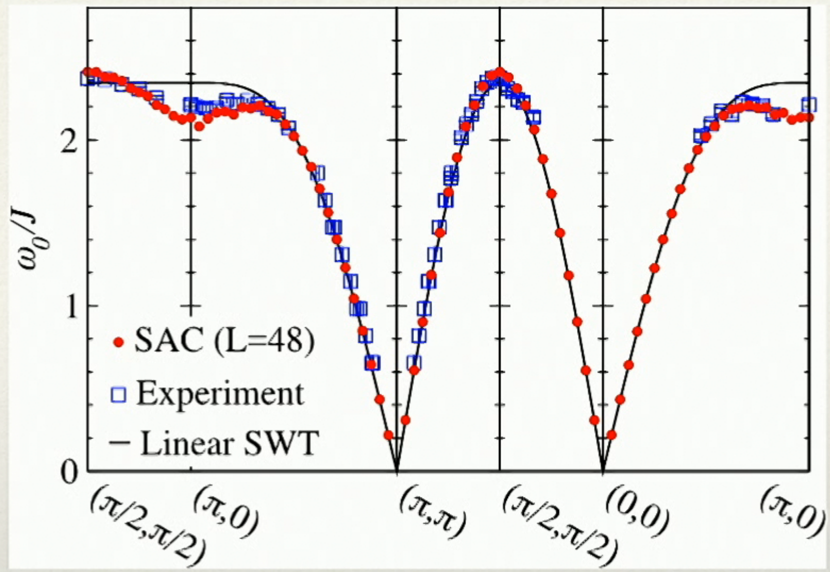

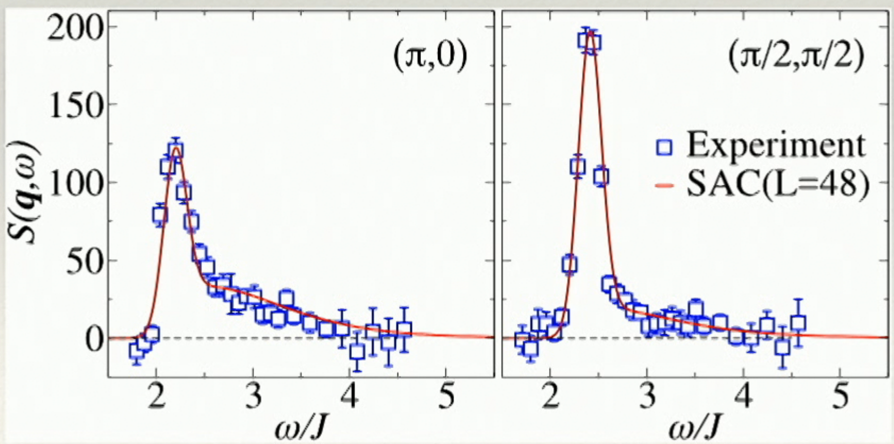

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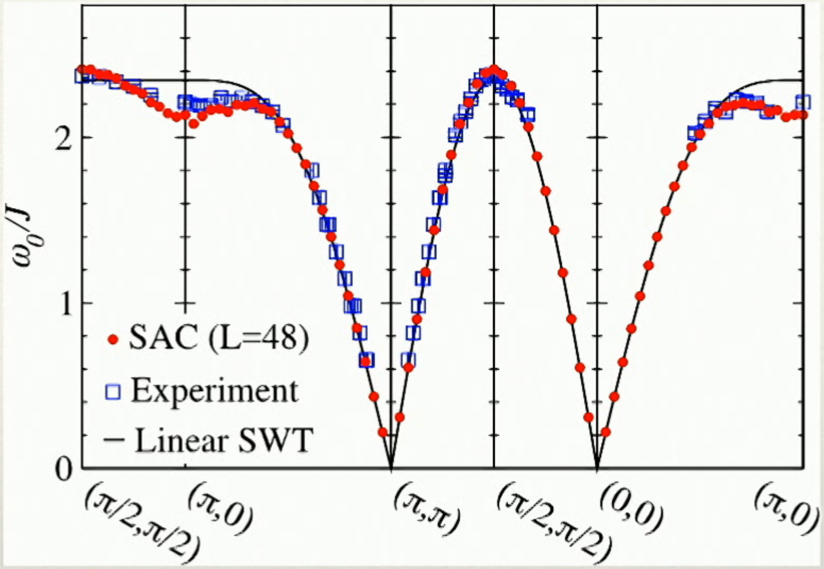

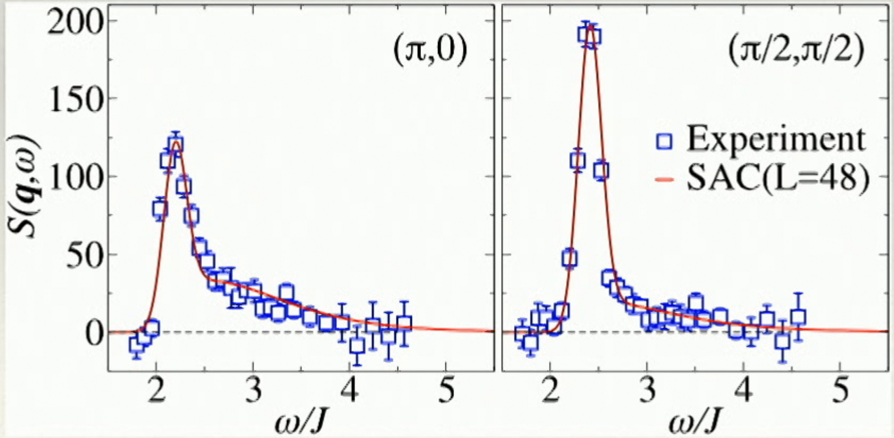

SAC result broadened
- same for both q
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Conclusion: Excitations are magnons for all q

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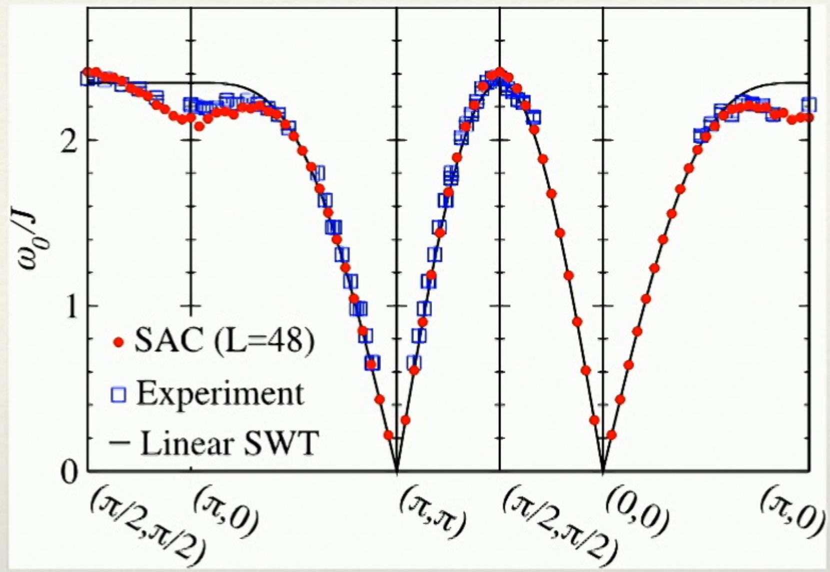

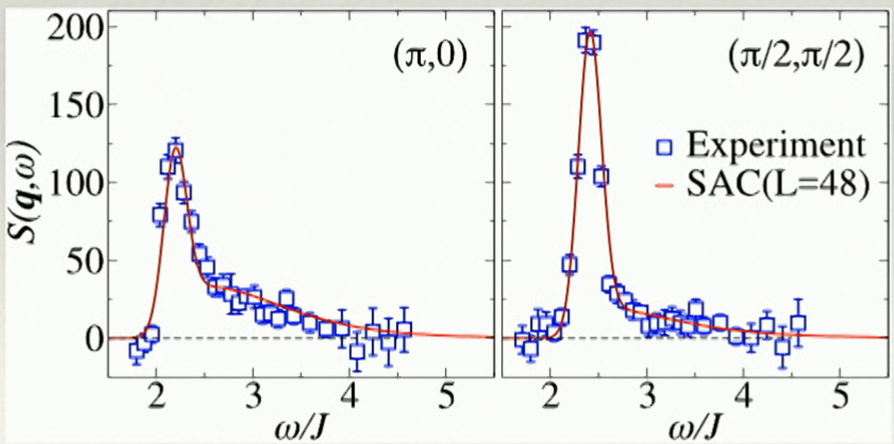

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Could spinons still be of some relevance?

The J-Q model and deconfined quantum-criticality

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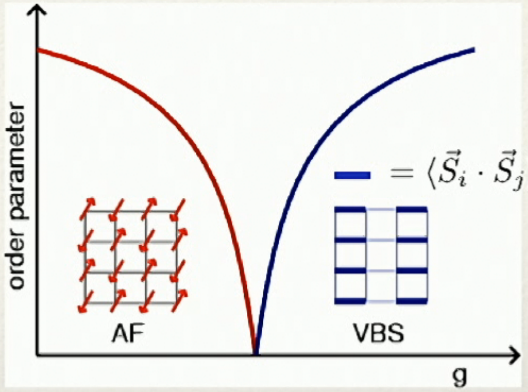
Proposed generic continuous quantum phase transition between the Néel state and VB solid (Senthil et al., Science 2004)
- spinons deconfined at the critical point



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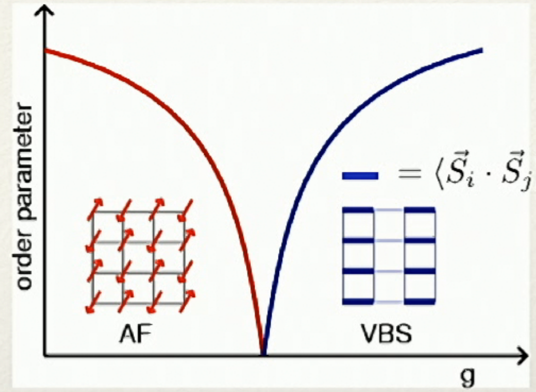
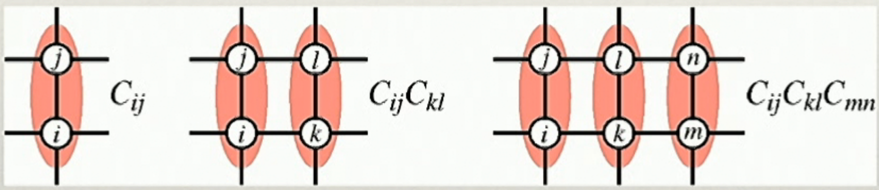


J-Q Hamiltonian based on singlet-projector

$$C_{ij} = \frac{1}{4} - \vec{S}_i \cdot \vec{S}_j$$



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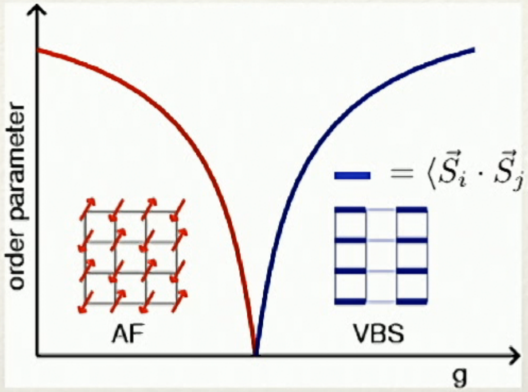

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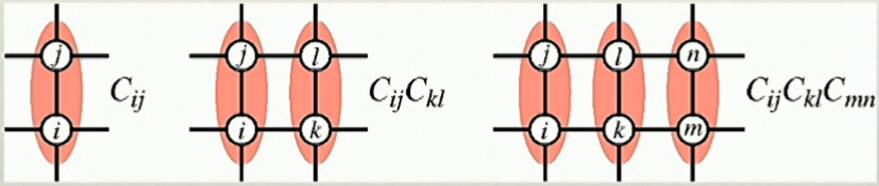

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The "J-Q" model with two projectors is (Sandvik 2007)

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$

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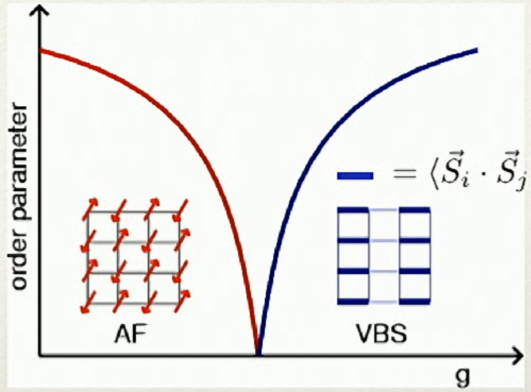

J-Q Hamiltonian based on singlet-projector

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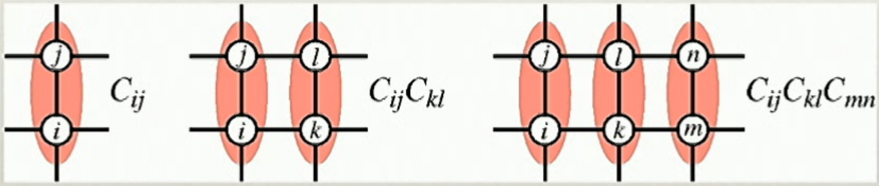

+ all translations and rotations

The "J-Q" model with two projectors is (Sandvik 2007)

$$H = -J \sum_{\langle ij \rangle} C_{ij} - Q \sum_{\langle ijkl \rangle} C_{ij} C_{kl}$$

- Correlated singlets reduce Néel order
- Néel-VBS transition appears to be continuous
- Not a realistic microscopic model for materials
- "Designer Hamiltonian" for VBS physics and Néel-VBS transition

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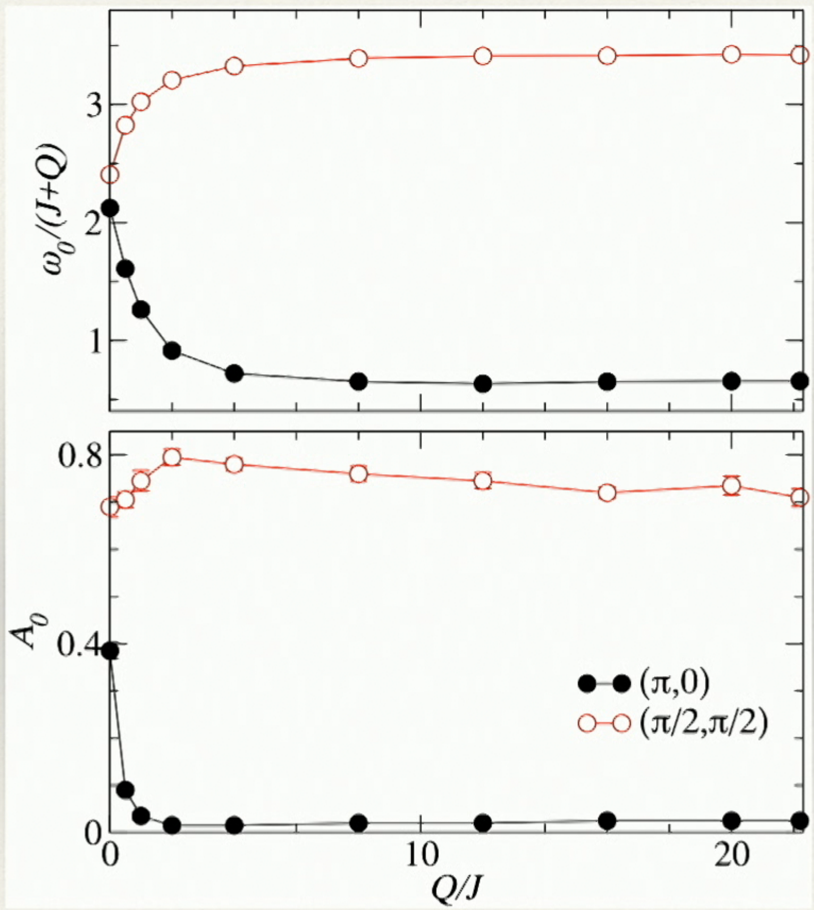

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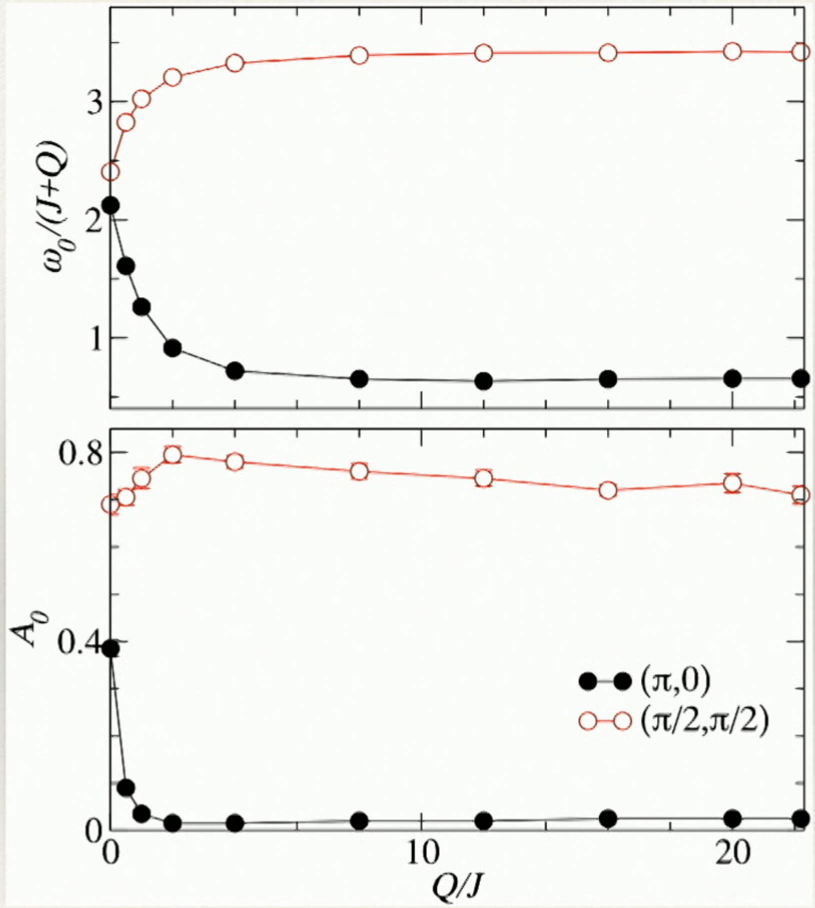

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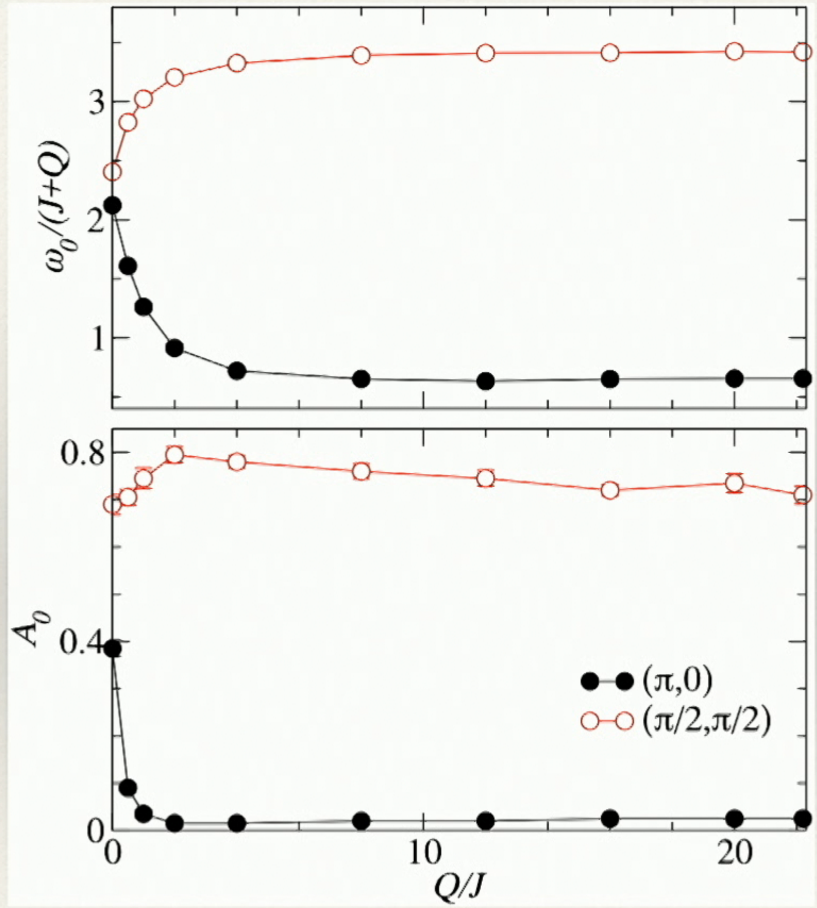

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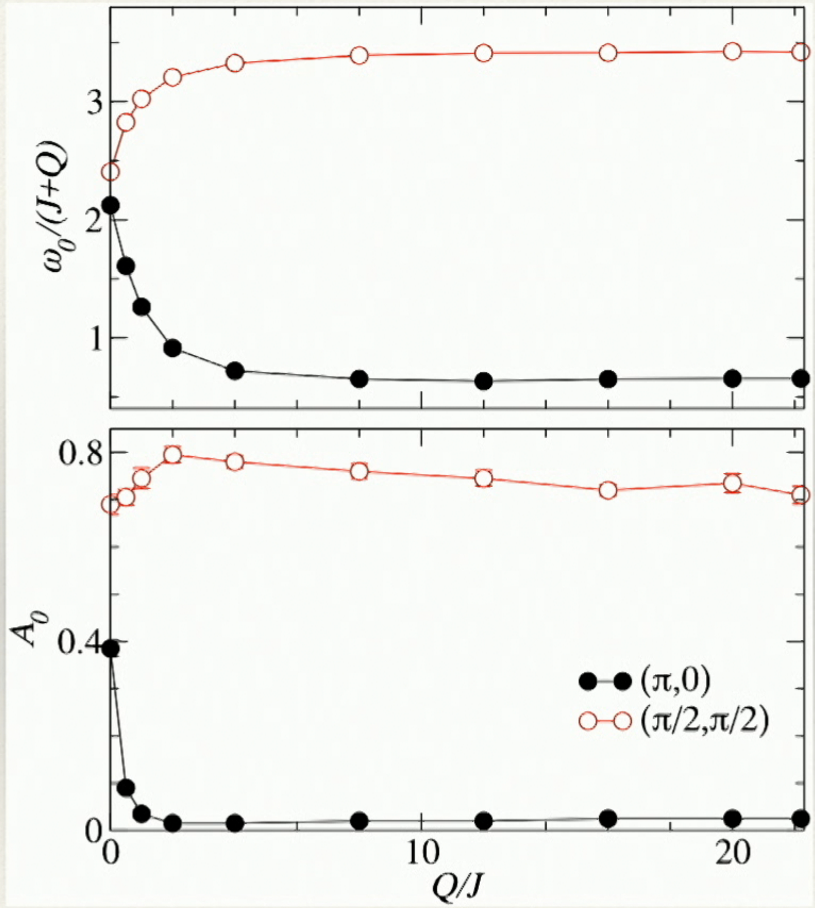
Suggests picture of nearly deconfined spinons around $(\pi,0)$ in the Heisenberg model



Effective spinon-magnon mixing model

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$$\omega^{\rm m}(\mathbf{q}) = \sqrt{2}c^{\rm m}\sqrt{1 - \frac{1}{4}\left[\cos(q_x) + \cos(q_y)\right]^2}$$

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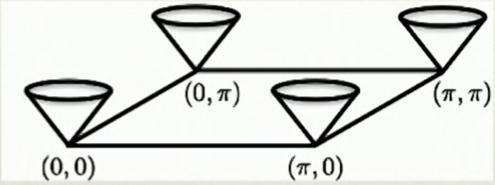

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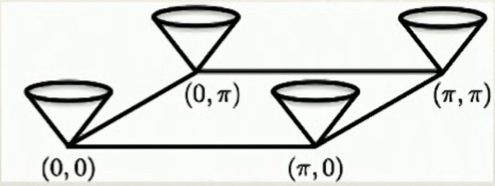

Magnon can break up into two virtual spinons - add binding energy to H

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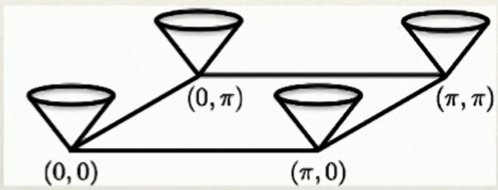

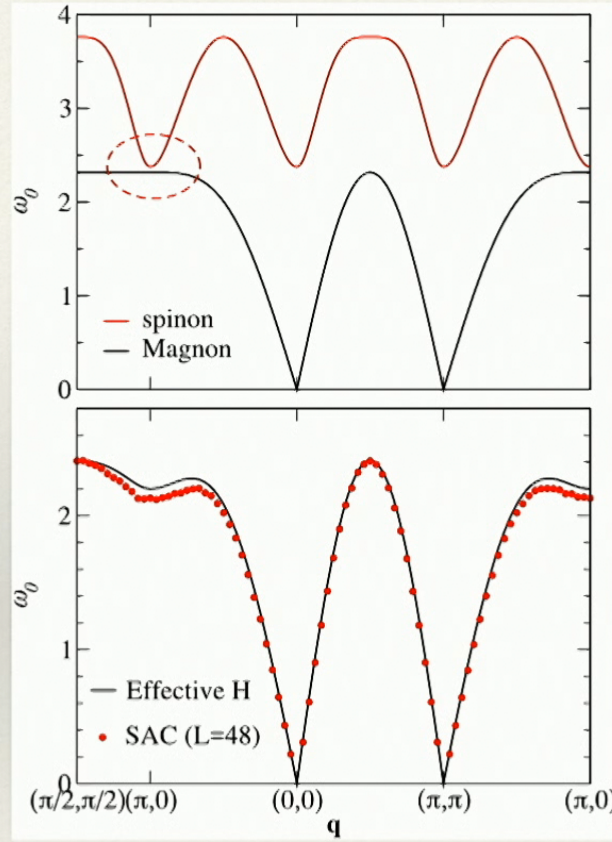

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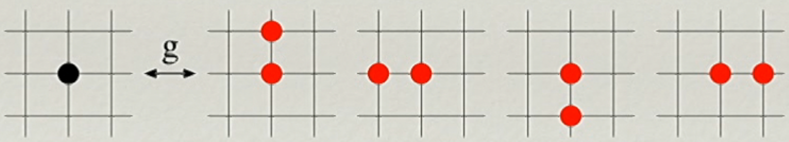
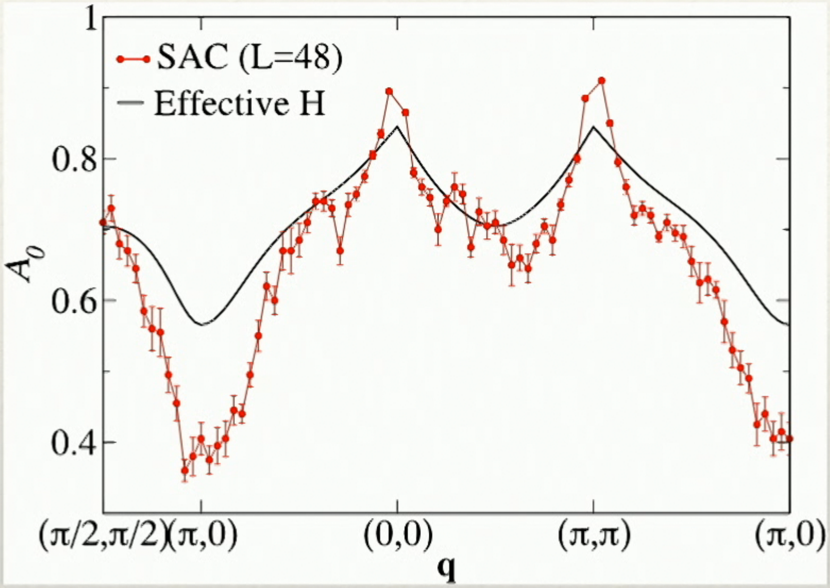


$$H^{\mathrm{I}} = \sum_{\mathbf{q},\mathbf{p}} I(\mathbf{p}) c^{\dagger}_{\mathbf{p}} c^{\dagger}_{\mathbf{q}-\mathbf{p}} d_{\mathbf{q}} + h.c.$$

$$I(\mathbf{p}) = g\sqrt{\frac{2}{N}}(\cos p_x + \cos p_y)$$

Qualitatively reproduces also the magnon amplitude



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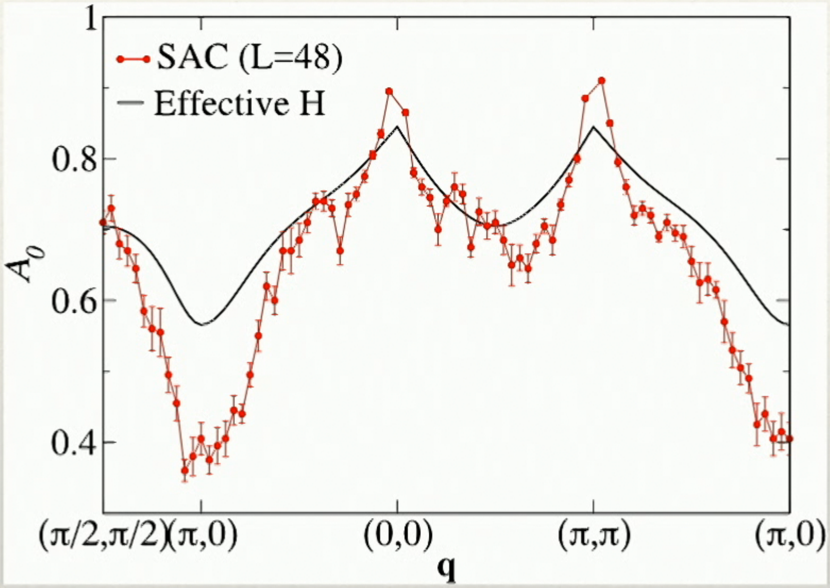
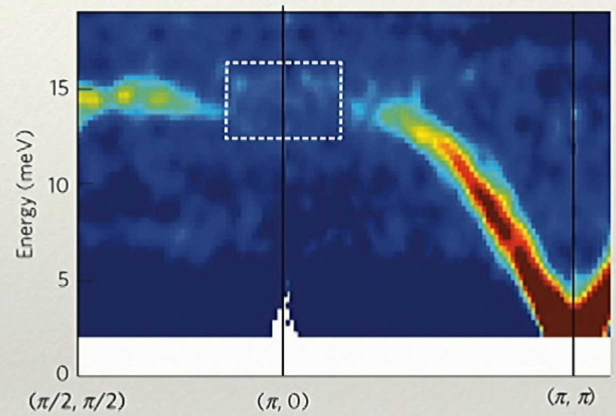


Compare with sharp drop in coherent weight in the experiments close to q = (π,0)



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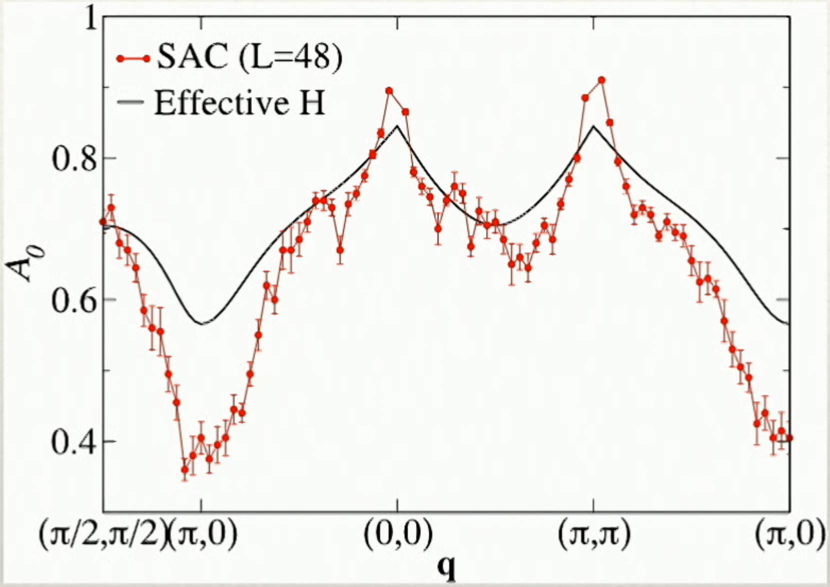

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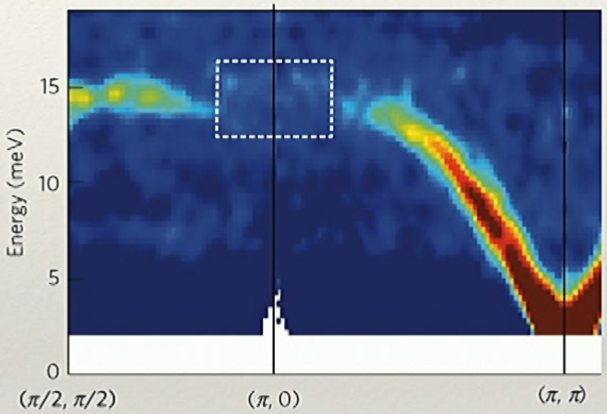

By adjusting the binding energy, the magnons close to (π,0) can deconfine

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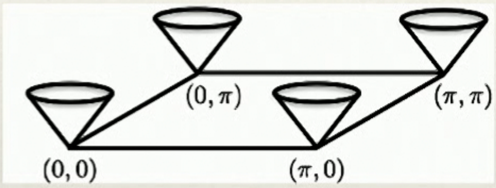

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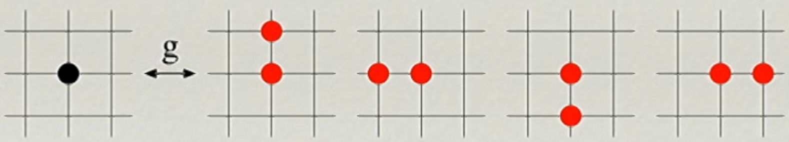

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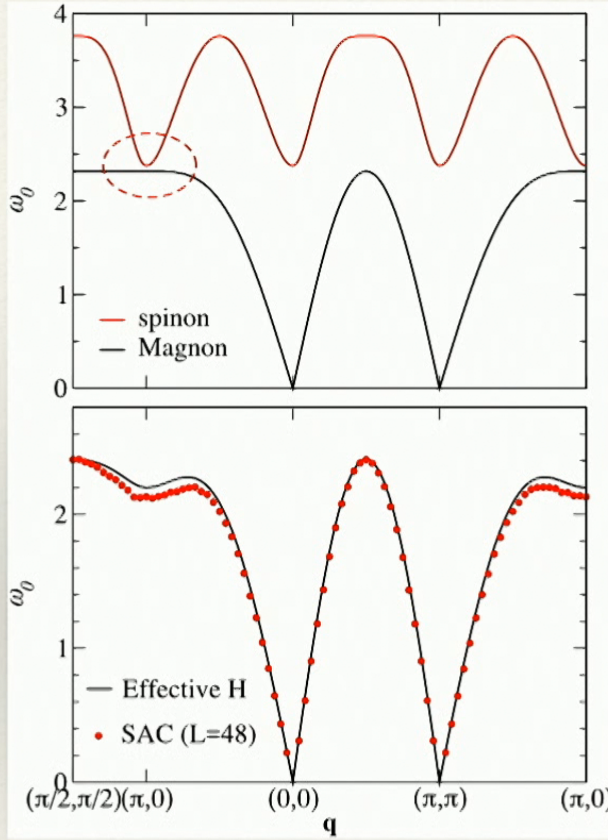
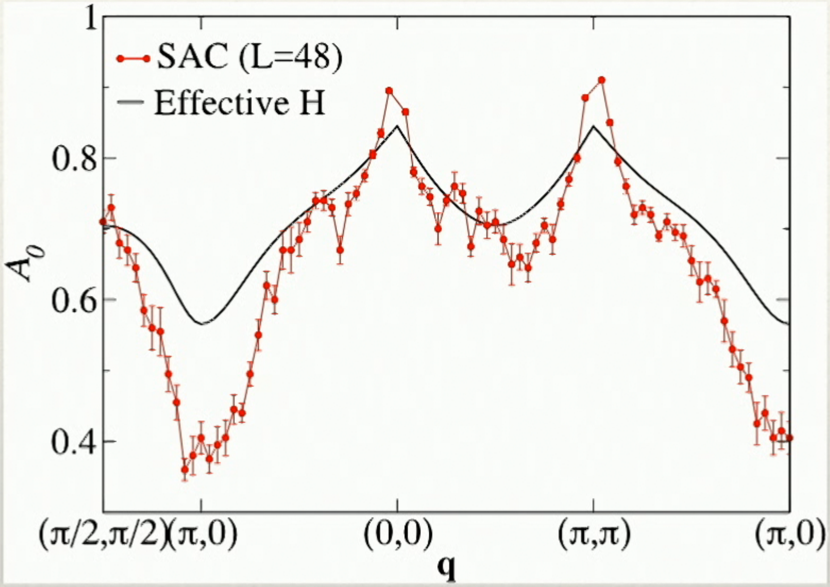


Magnon-spinon mixing strongest at q= (π,0); leads to observed anomaly

Qualitatively reproduces also the magnon amplitude



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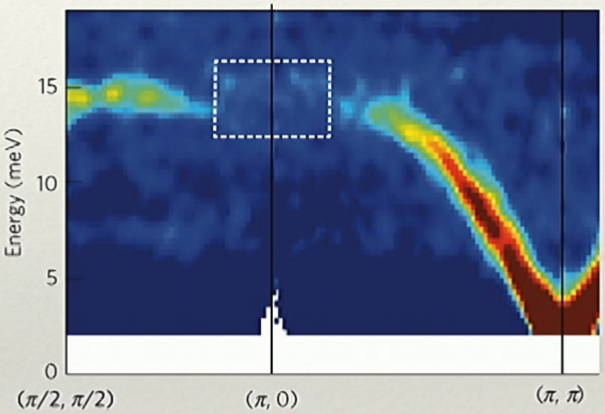

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Simple phenomenological model for nearly deconfined spinons