Scattering Neutrons from Magnons, Spinons, Solitons, and Breathers

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Johns Hopkins University and NIST Center for Neutron Research

- Neutron Scattering and 1D magnetism
- Spin-1 chains
- Toward Quantum Criticality
  - strongly interacting dimers (PHCC)
  - Quantum critical spin-1/2 chain
- Field Effects at Criticality
  - $H>0$: Extended Critical phase
  - $h_s>0$: From spinons to solitons
- Conclusions

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M. M. Turnbull	Clarke University
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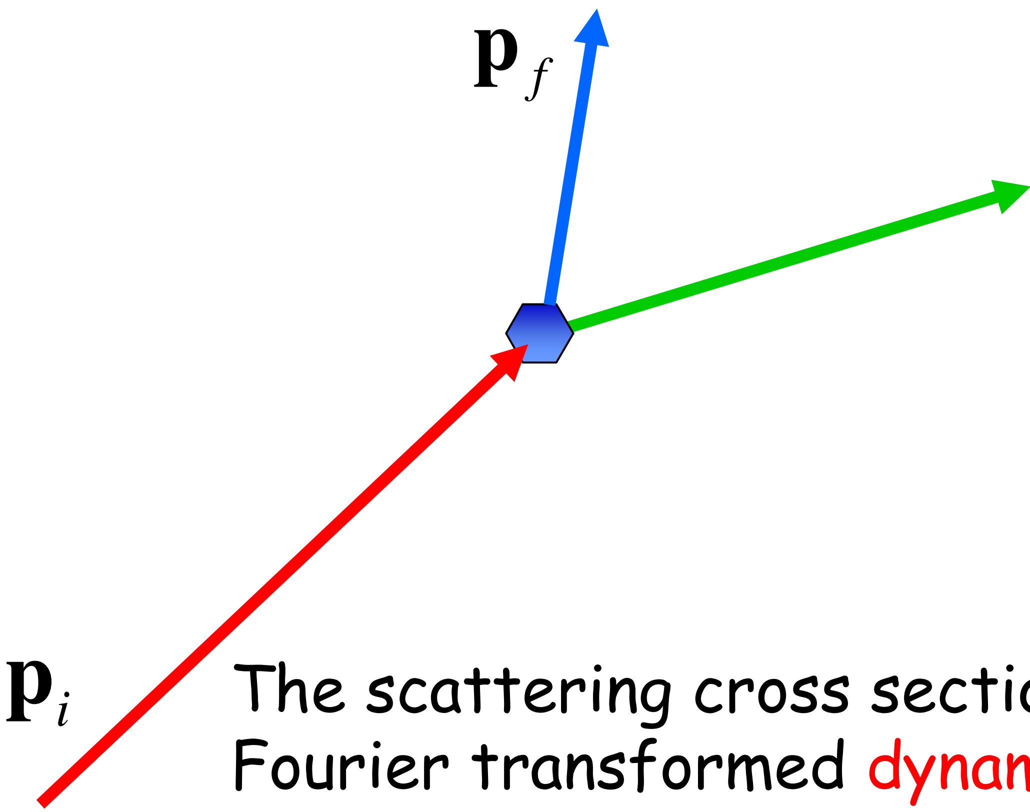
Neutron Scattering and 1D Magnetism

Magnetic Neutron Scattering



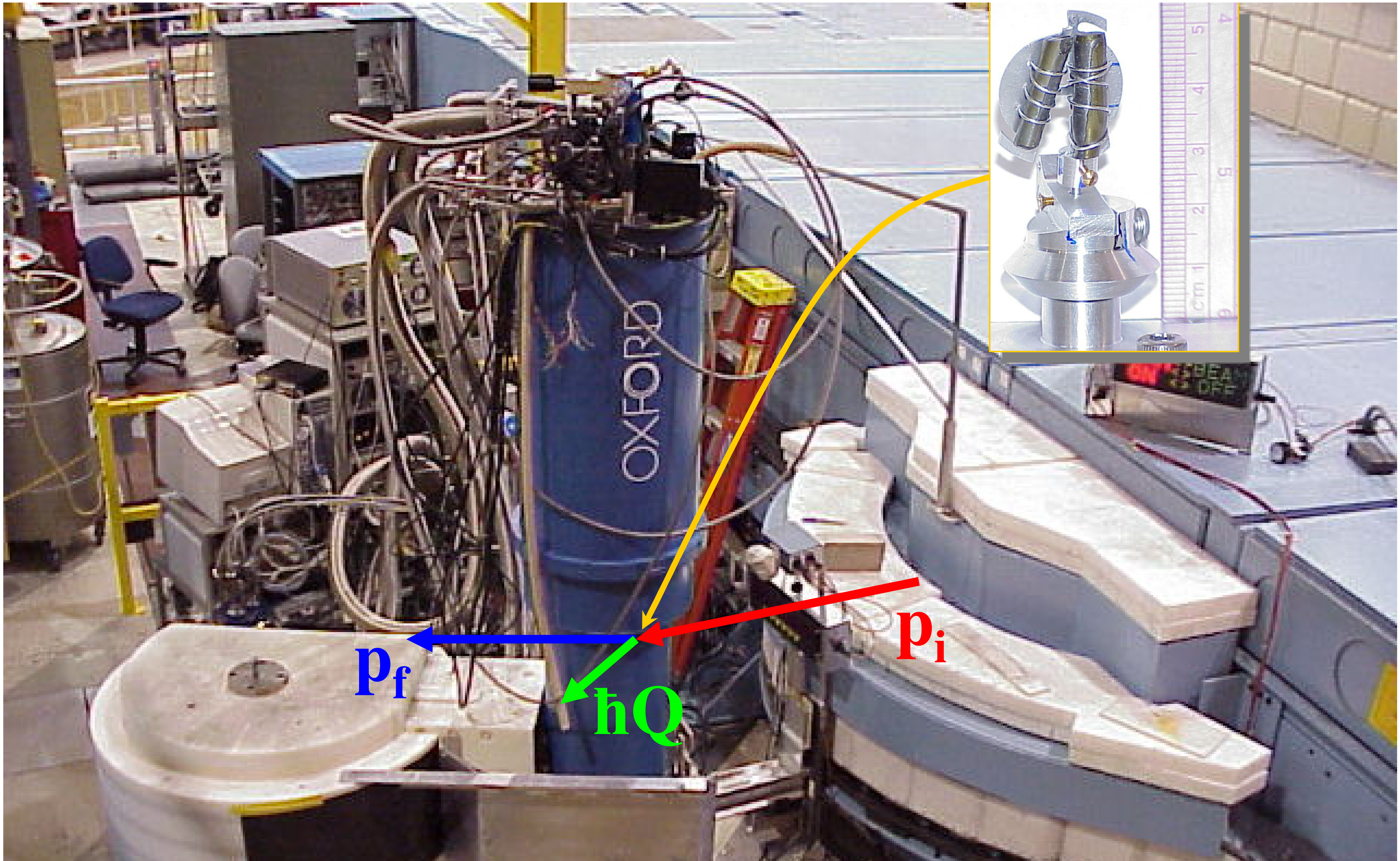
$$\hbar \mathbf{Q} = \mathbf{p}_i - \mathbf{p}_f$$

$$\hbar \omega = E_i - E_f$$

The scattering cross section is proportional to the Fourier transformed dynamic spin correlation function

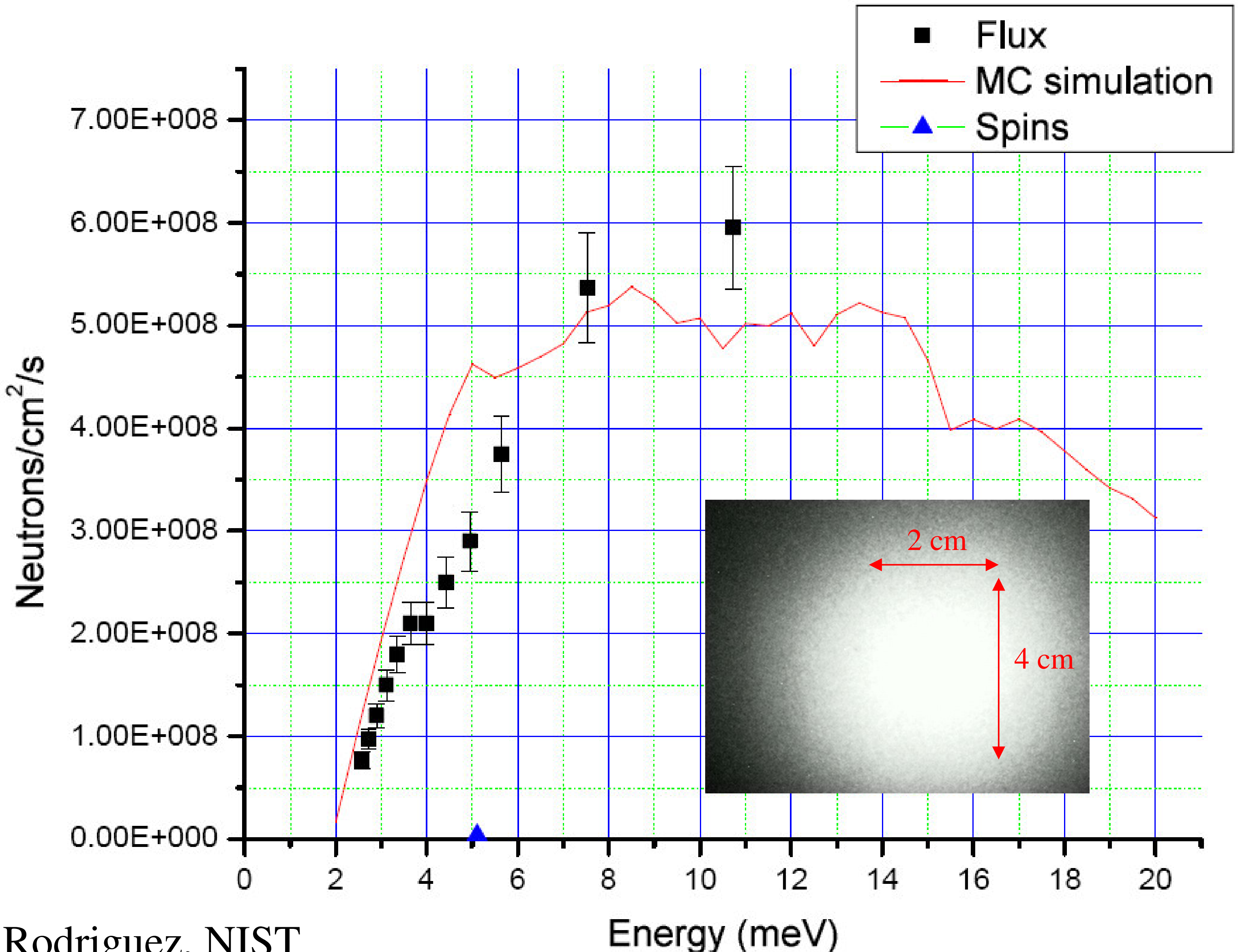
$$\mathbf{S}^{\alpha\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\ e^{-i\omega t}\ \frac{1}{N}\sum_{\mathbf{RR'}} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R'})} < S^{\alpha}_{\mathbf{R}}(t) S^{\beta}_{\mathbf{R'}}(0) >$$

NIST Center for Neutron Research

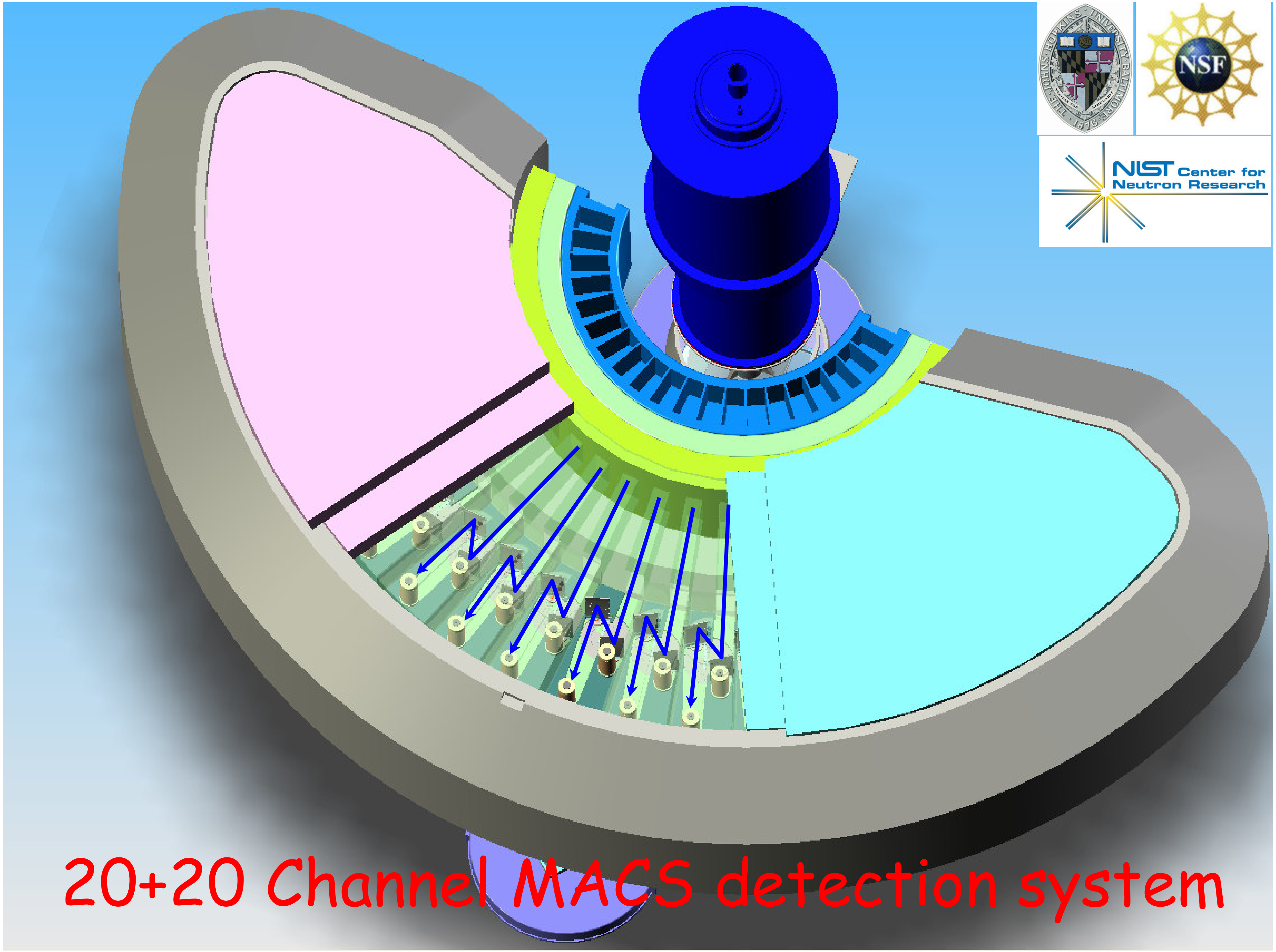


$$\mathbf{S}^{\alpha\beta}(\mathbf{Q},\omega)=\frac{1}{2\pi\hbar}\int dt\ e^{-i\omega t}\ \frac{1}{N}\sum_{\mathbf{RR'}}e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R'})}<S_{\mathbf{R}}^{\alpha}(t)\,S_{\mathbf{R'}}^{\beta}(0)>$$

Better Instrumentation at Existing Sources



Jose A. Rodriguez, NIST



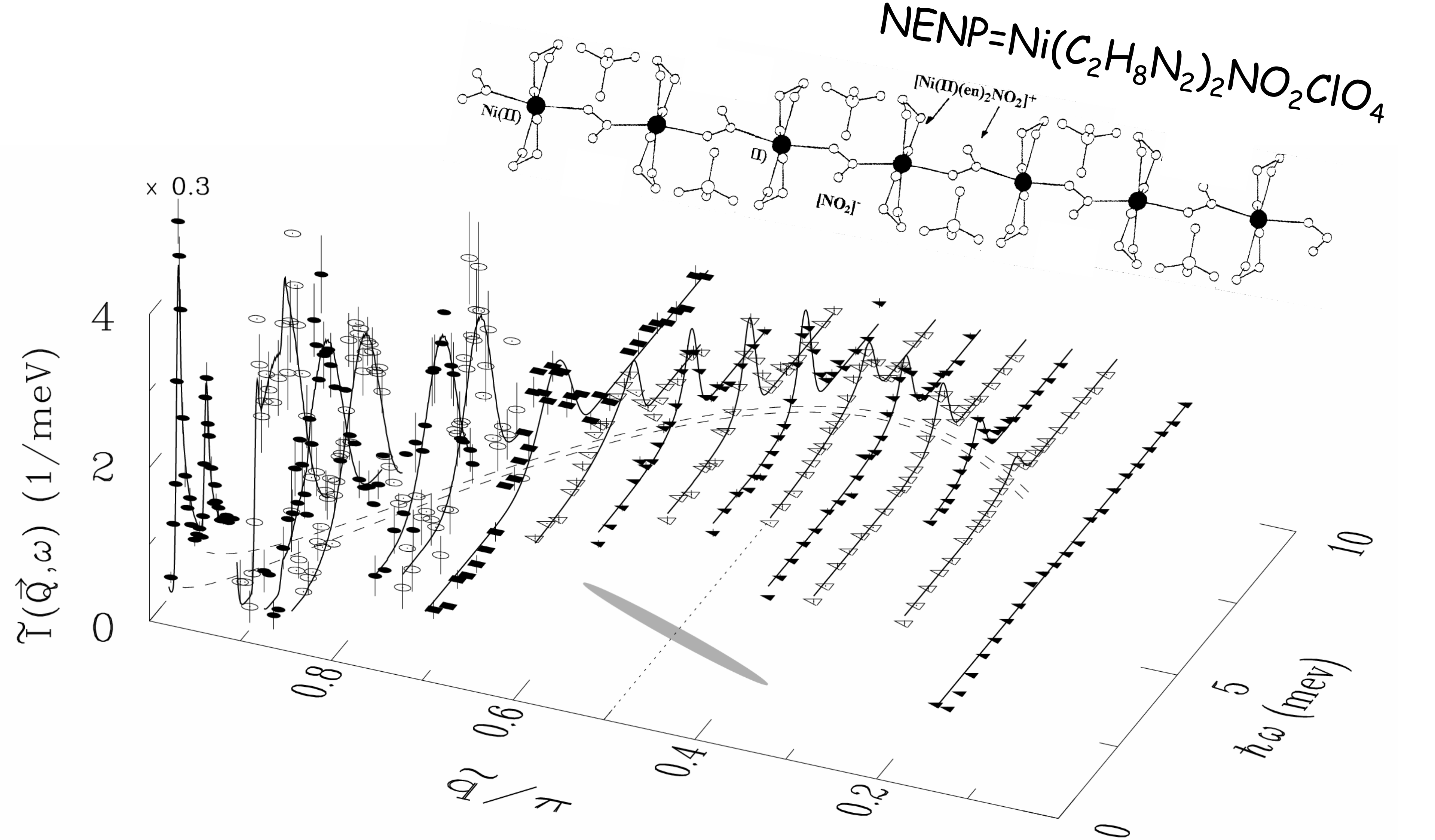
20+20 Channel MACS detection system

Spallation Neutron Source at ORNL, TN

Magnons and their decay in spin-1 chains

Neutrons Create magnons in spin-1 chain

NENP=$Ni(C_2H_8N_2)_2NO_2ClO_4$



Ma et al. PRL (1992)

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 38, NUMBER 7 1 SEPTEMBER 1988

Spin-correlation function of the $S=1$ antiferromagnetic Heisenberg chain at $T=0$

Minoru Takahashi

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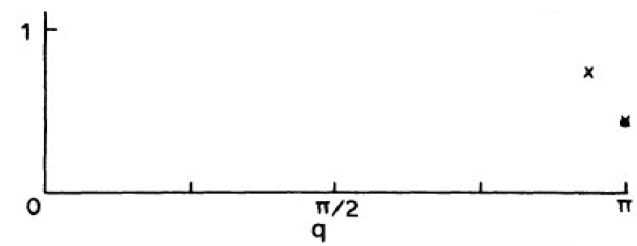
(Received 4 January 1988; revised manuscript received 2 May 1988)

The correlation function $\rho(l)=\langle S_i^z S_{i+l}^z \rangle$ is calculated for the spin-1 Heisenberg antiferromagnetic chain ($H=J\sum_i \mathbf{S}_i \mathbf{S}_{i+1}$, $\mathbf{S}_{N+1}\equiv\mathbf{S}_1$) at the ground state. Using the Monte Carlo method of Hirsch, Sugar, Scalopino, and Blankenbecler, we find that $\rho(l)$ decays exponentially in contrast to the $S=\frac{1}{2}$ case where $\rho(l)$ decays algebraically. This fact coincides with Haldane's prediction and recent numerical calculations. We calculate the upper bound of elementary excitation from the structure factor using a variational method which resembles the Feynman theory for elemen-

FIG. 5. Elementary excitation $\varepsilon(q)$ and $g(q)$ defined in (13) for $S=1$ AFH chain in units of J. Circles are elementary excitation with total spin one and momentum q of the $N=14$ chain which is taken from the Parkinson and Bonner's table in Ref. 6. Crosses are $g(q)$ for the $N=32$ chain.

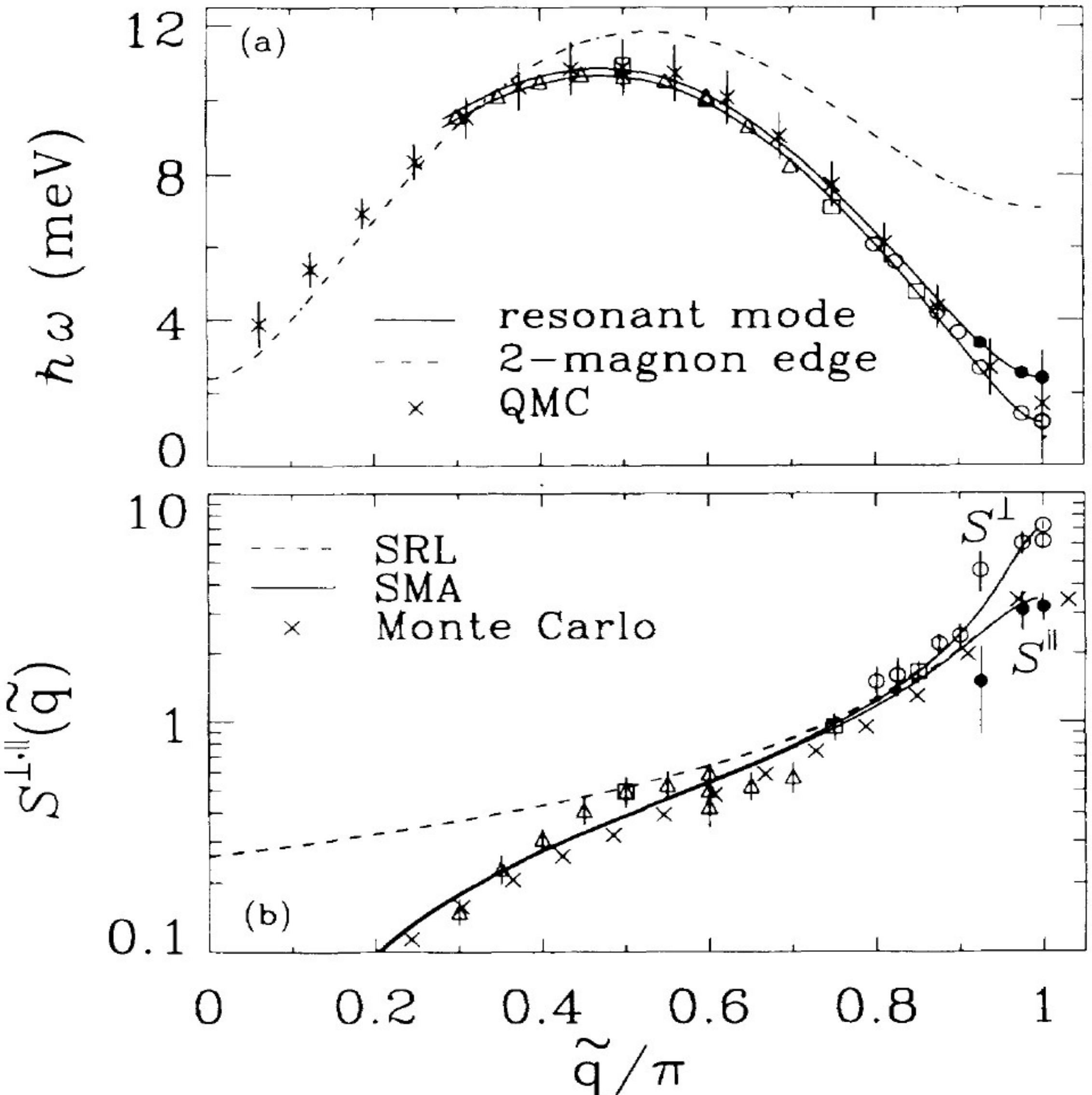


$$\varepsilon(q)=[\varepsilon(q)+\varepsilon(-q)]/2\le\frac{1}{2}\frac{\langle\psi|S^z_{-q}HS^z_q+S^z_qHS^z_{-q}|\psi\rangle}{\langle\psi|S^z_{-q}S^z_q|\psi\rangle}-E_0$$

$$=\frac{1}{2}\frac{\langle\psi|[S^z_{-q},[H,S^z_q]]|\psi\rangle}{\langle\psi|S^z_{-q}S^z_q|\psi\rangle}=\frac{J(1-\cos q)\left(-N^{-1}\sum_i\langle S^x_iS^x_{i+1}+S^y_iS^y_{i+1}\rangle\right)}{S(q)}$$

$$=2J(1-\cos q)[-\rho(1)]/S(q)\equiv g(q)$$

Single mode approximation for spin-1 chain



Ma et al. PRL (1992)

Dispersion relation

Equal time correlation function

PHYSICAL REVIEW B VOLUME 50, NUMBER 5 1 AUGUST 1994-I

Excitation spectra of $S = 1$ antiferromagnetic chains

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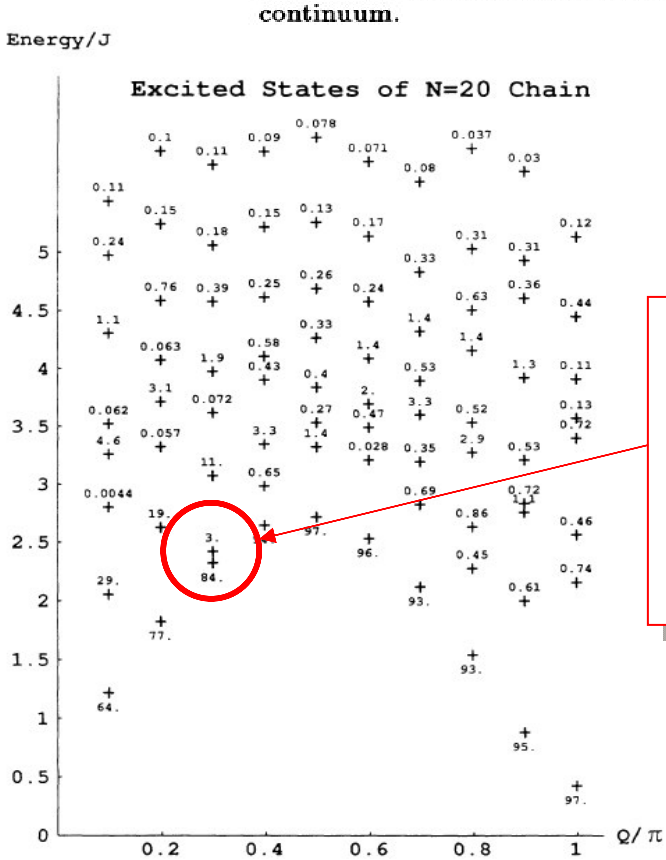
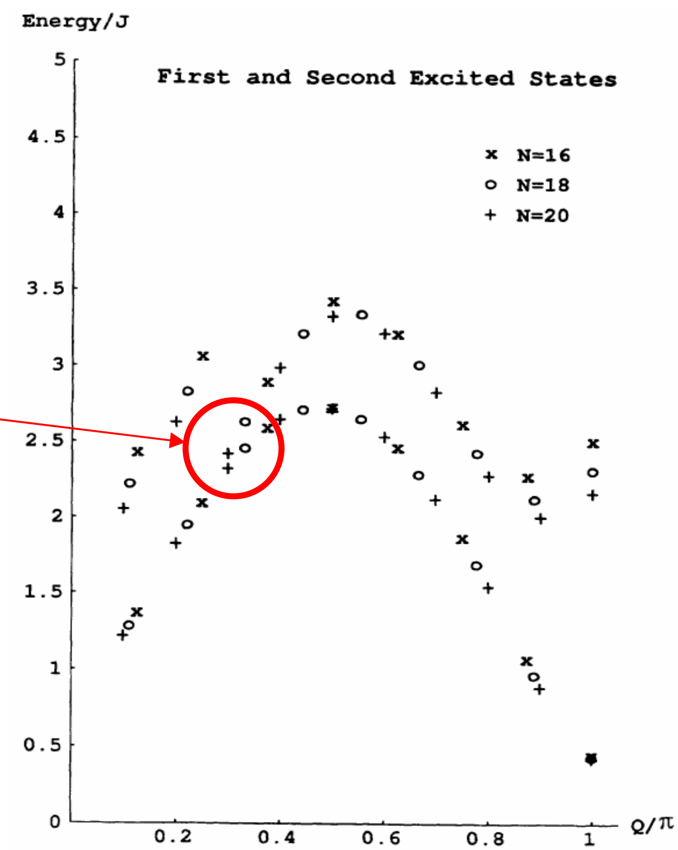
(Received 10 February 1994)

The dynamical structure factor $S(Q,\omega)$ of the $S = 1$ antiferromagnetic Heisenberg chain with length 20 at zero temperature is calculated. The lowest-energy states have the δ-function peak at the region $\pi \geq |Q| > 0.3\pi$. At $|Q| < 0.3\pi$ the lowest-energy states are the lower edge of the continuum of the scattering state, the strength of which decreases for large systems. This gives a reasonable explanation for the experimental fact that no clear peak is observed at the region $Q < 0.3\pi$. This situation is more apparent for the valence-bond solid state. On the contrary for $S = \frac{1}{2}$ antiferromagnetic Heisenberg chain the lowest-energy states are always the edge of the continuum.

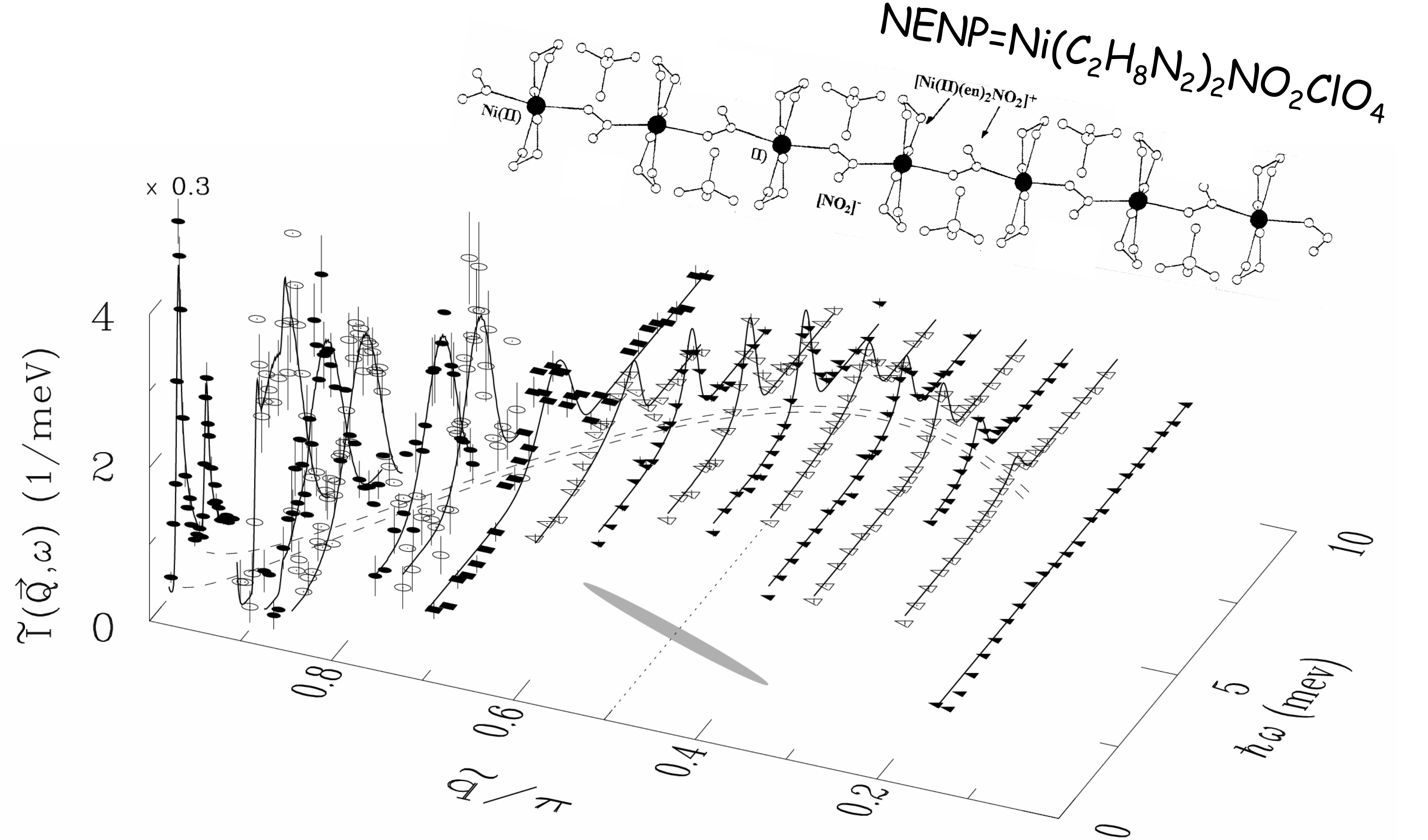


Bound state meets continuum



Neutrons Create magnons in spin-1 chain

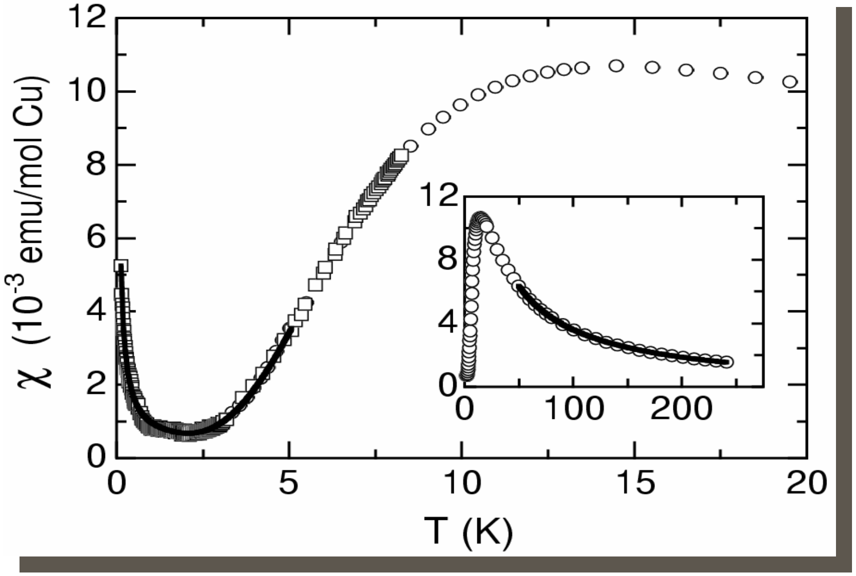
$NENP=Ni(C_2H_8N_2)_2NO_2ClO_4$

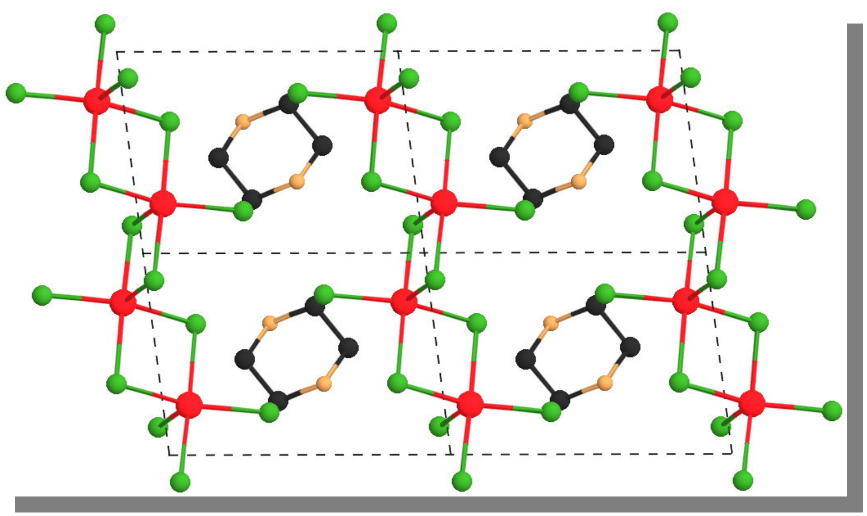


Ma et al. PRL (1992)

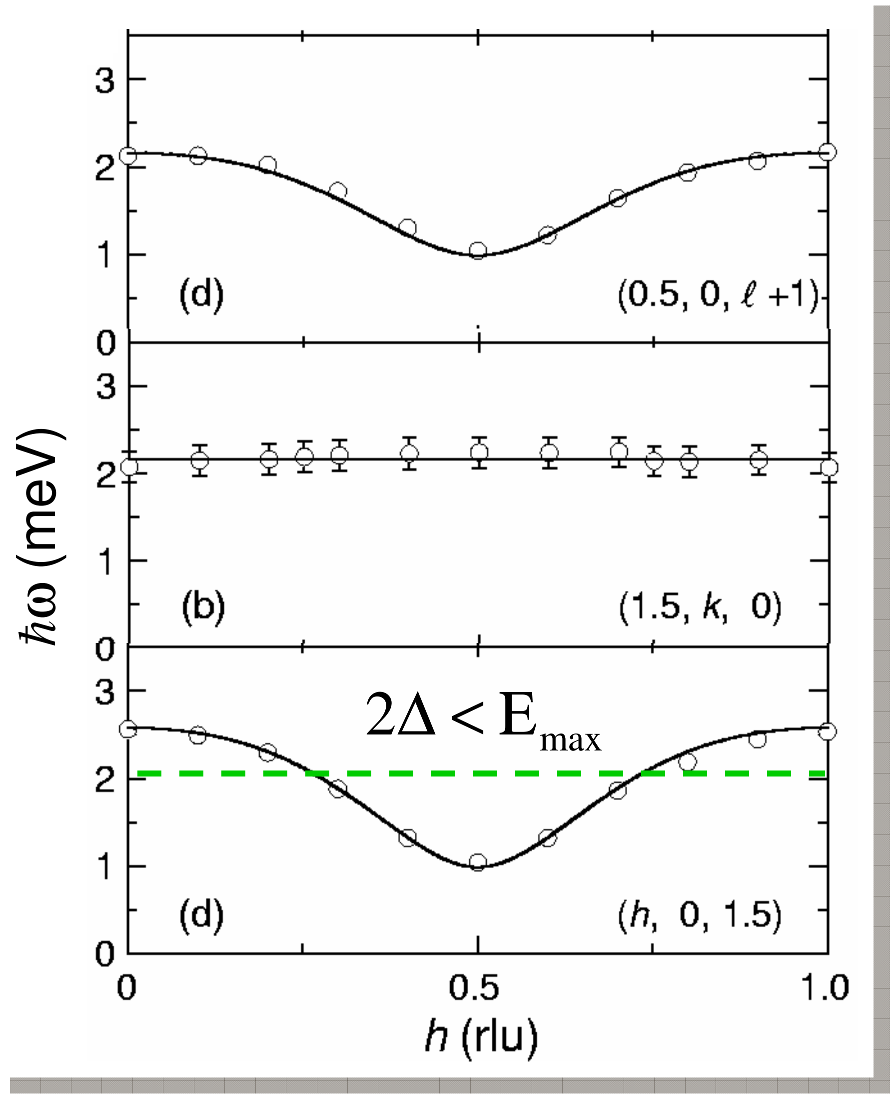
Approaching Quantum Criticality

Strongly Interacting Dimers in PHCC



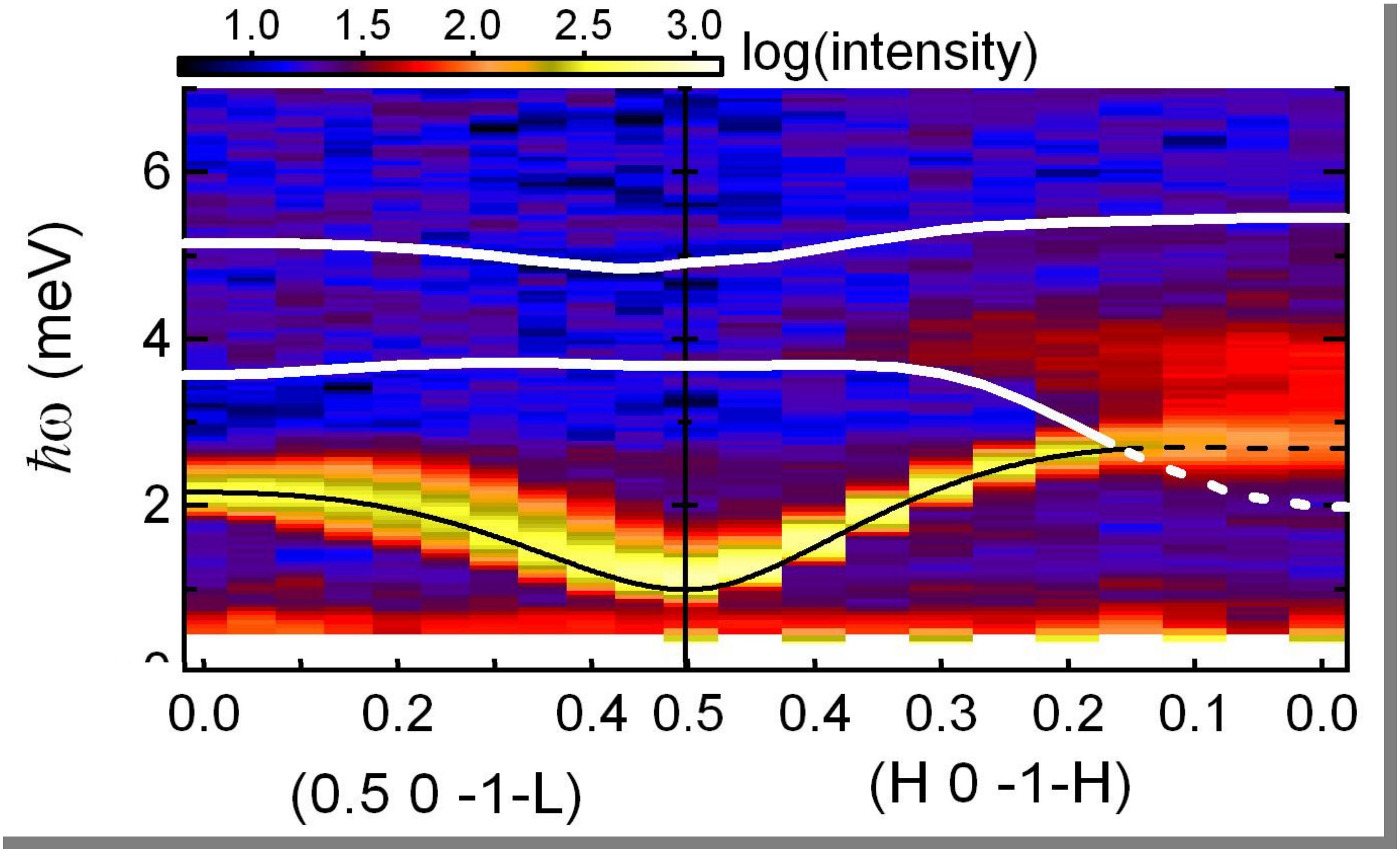


$(C_4H_{12}N_2)Cu_2Cl_6$ (PHCC)



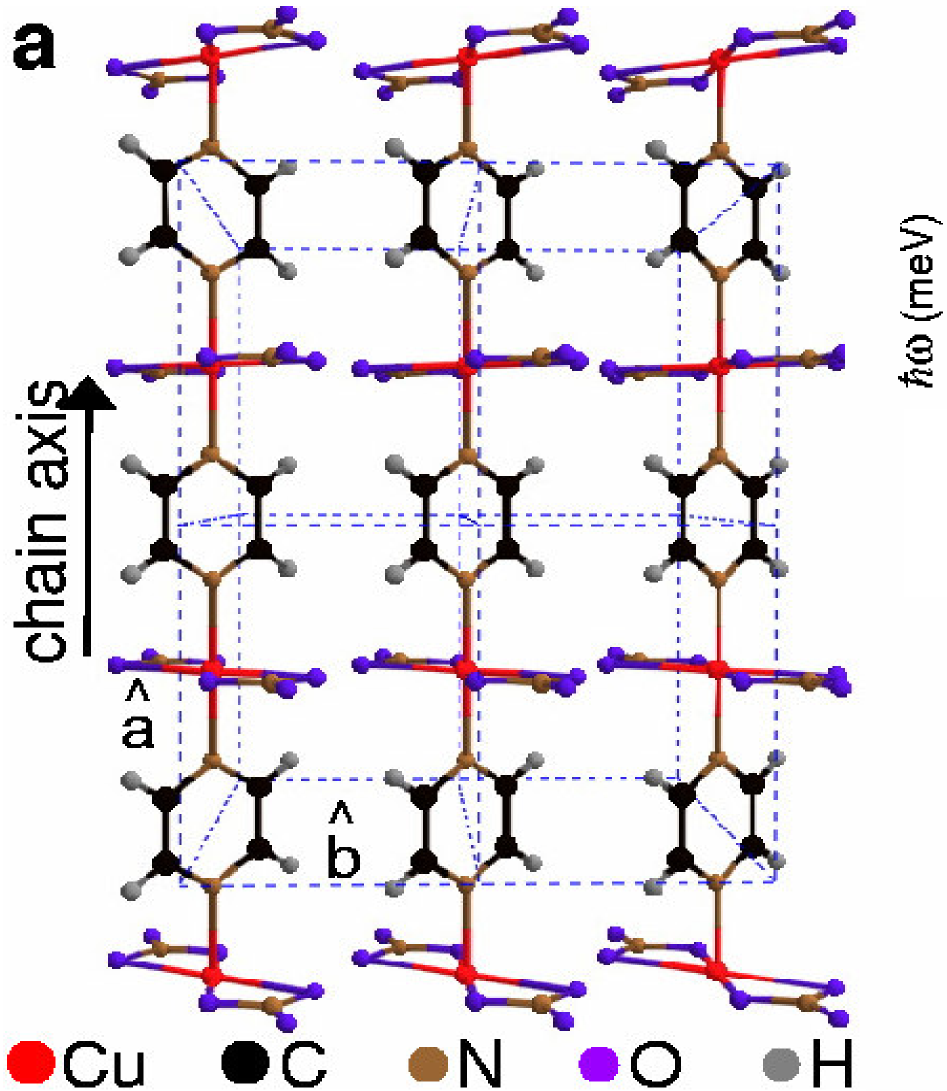
Stone et al. PRB (2001)

Magnon decay in two-magnon continuum

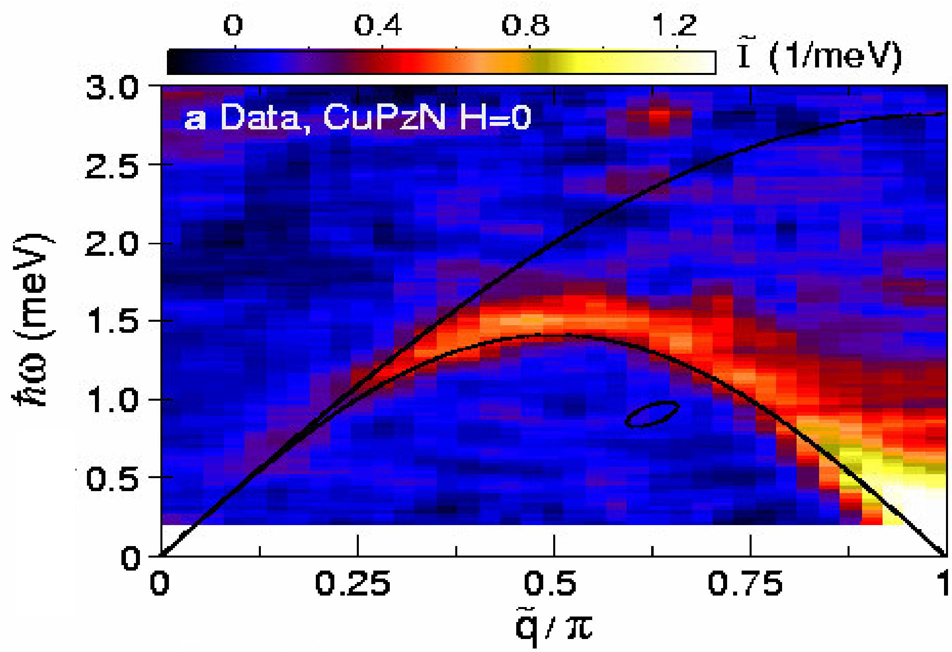


Stone et al. Nature (2006)

Uniform spin chain: Unbound spinons



$Cu(C_4H_4N_2)(NO_3)_2$



Stone et al. (2003).

Finite T scaling at the QCP

Exact low energy scaling form is known for spin-1/2 chain

$$\chi''(q\omega)=\frac{\pi}{k_BT}\,\mathrm{Im}\left[\rho\left(\frac{\hbar\omega-v(q-\pi)}{4\pi k_BT}\right)\rho\left(\frac{\hbar\omega+v(q-\pi)}{4\pi k_BT}\right)\right]$$

$$\left[\rho(x)=\frac{\Gamma\left(\frac{1}{4}-ix\right)}{\Gamma\left(\frac{3}{4}-ix\right)}\right]$$

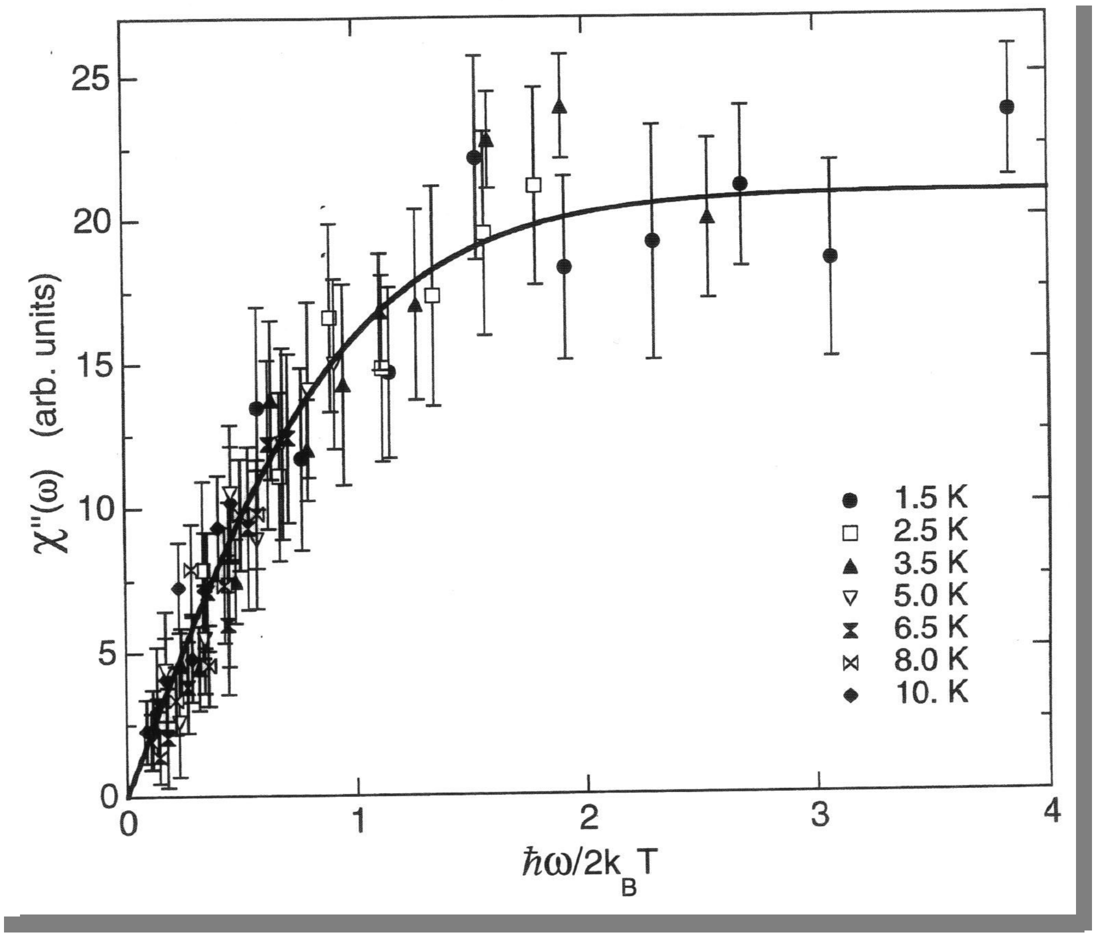
Here we measure the q-integrated "local" response

$$\chi''(\omega)=\int dq\,\chi''(q\omega)\sim\frac{1}{J}\tanh\left(\frac{\hbar\omega}{k_BT}\right)$$

H. J. Schultz PRB (1986)

Local response of spin-1/2 chain

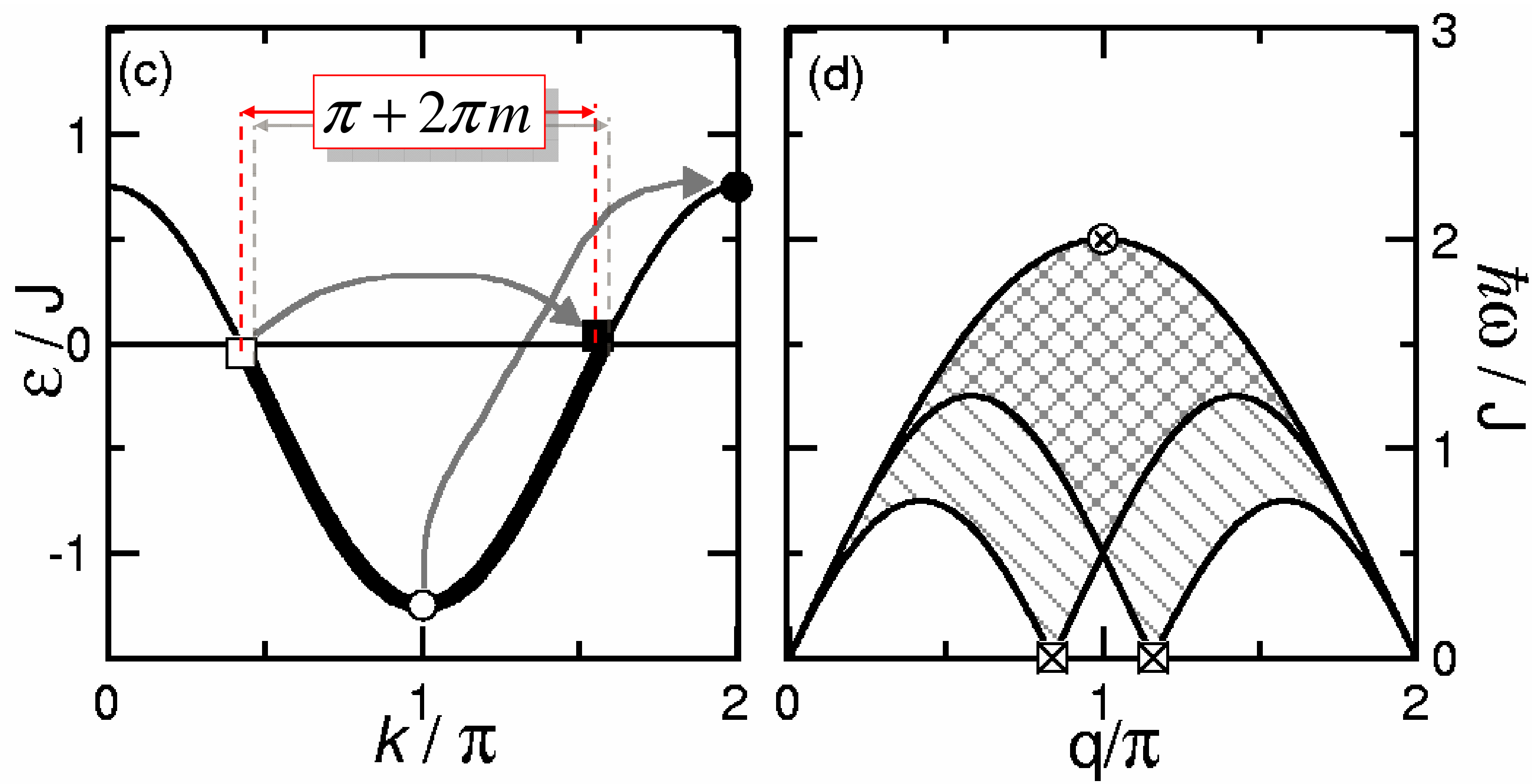
$$\chi''(\omega) = \int dq \chi''(q\omega) \sim \frac{1}{J} \tanh\left(\frac{\hbar\omega}{k_B T}\right)$$



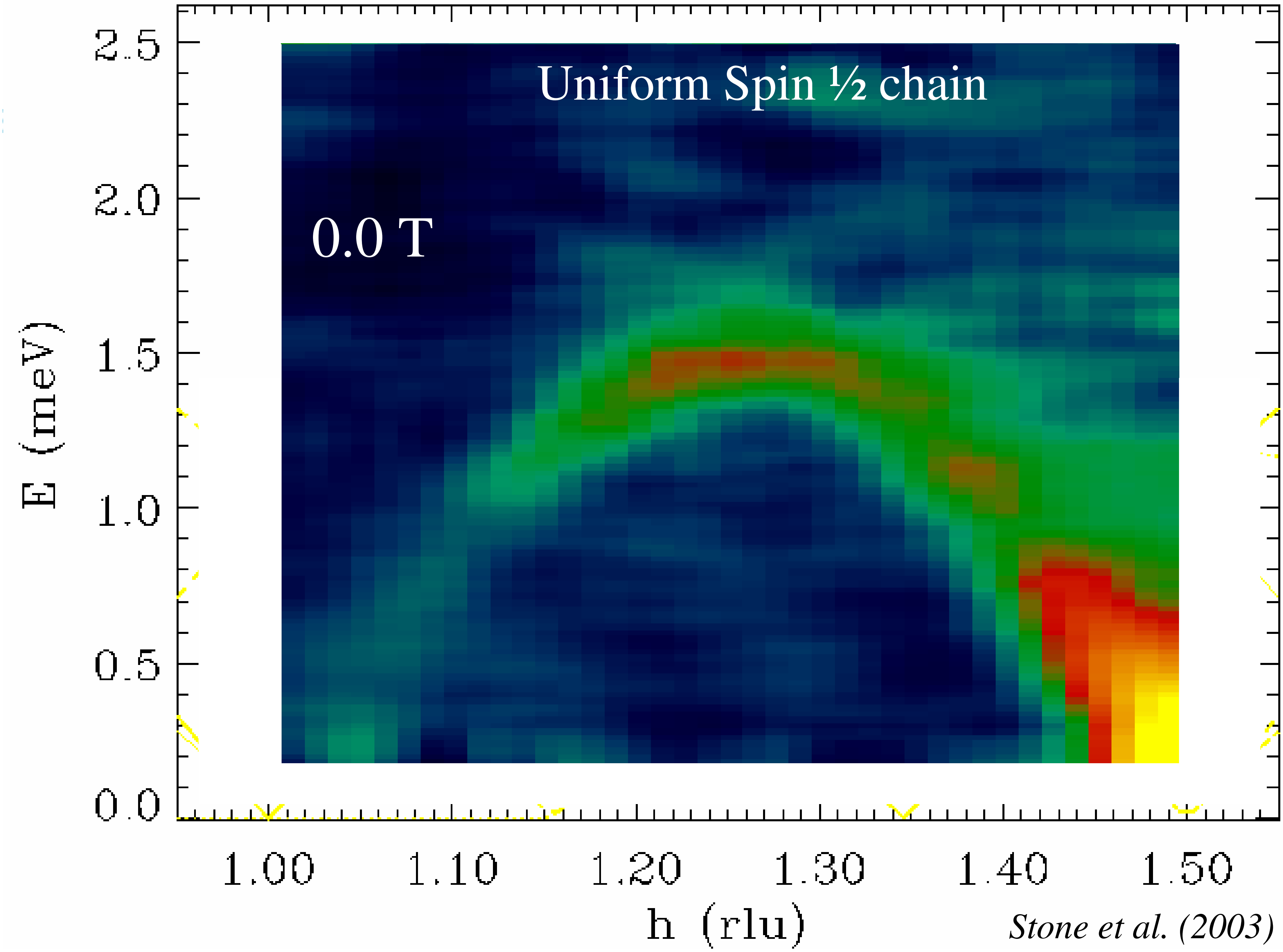
Dender Ph. D. thesis JHU (1997)

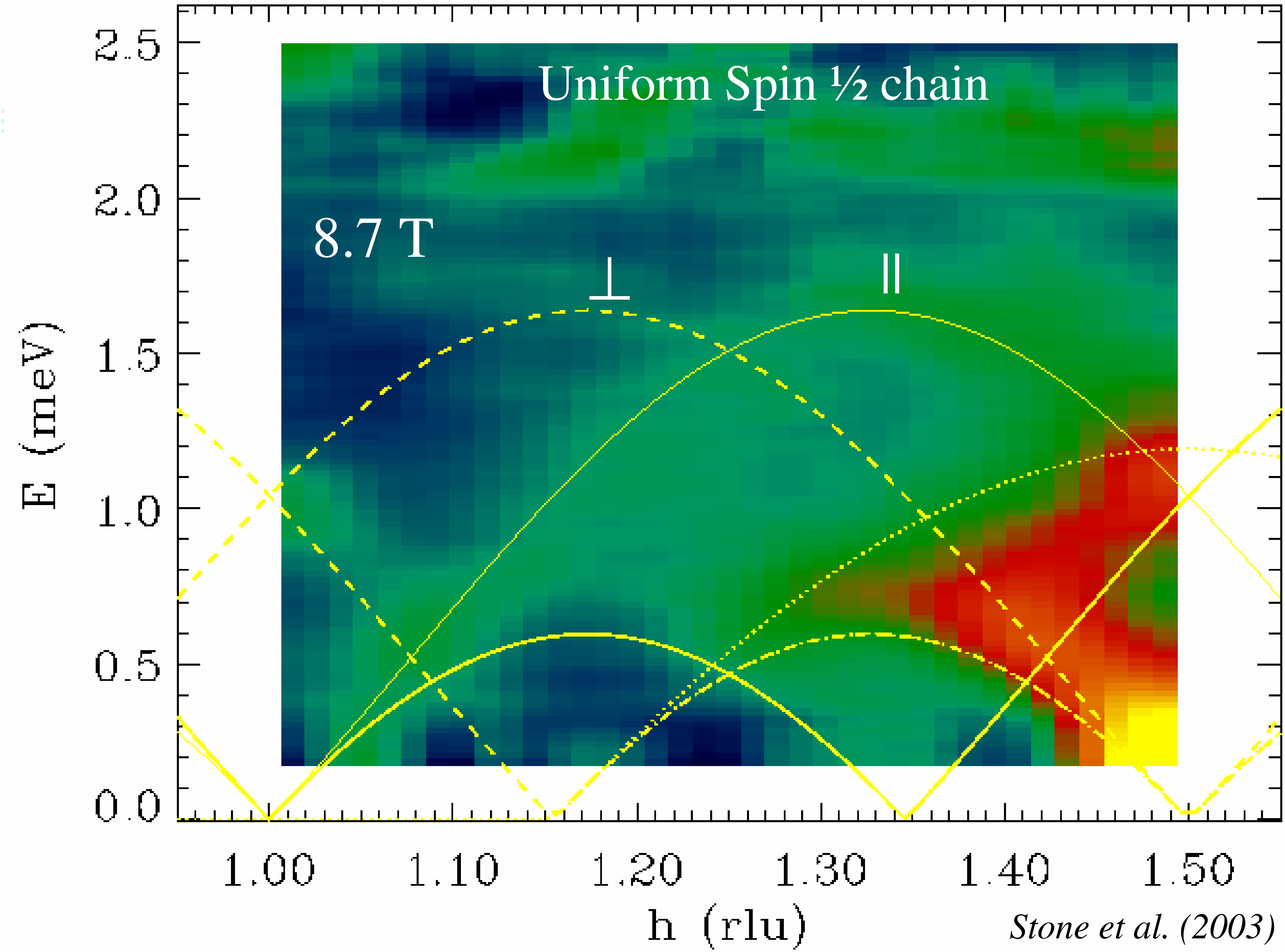
Spin-$\frac{1}{2}$ chain in uniform field

Spinons in magnetized spin-½ chain



(XY case for simplicity)


Uniform Spin ½ chain
0.0 T
E (meV)
2.5
2.0
1.5
1.0
0.5
0.0
1.00
1.10
1.20
1.30
1.40
1.50
h (rlu)
Stone et al. (2003)

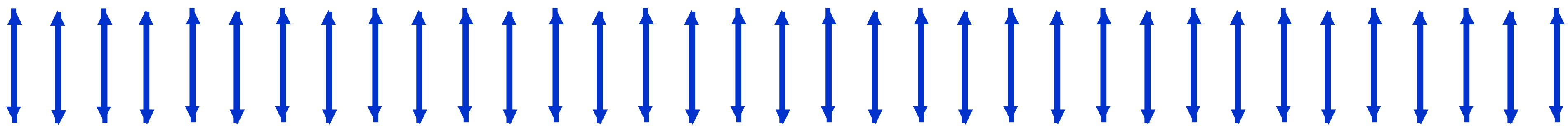


Uniform Spin ½ chain
8.7 T
⊥
∥
E (meV)
2.5
2.0
1.5
1.0
0.5
0.0
1.00
1.10
1.20
1.30
1.40
1.50
h (rlu)
Stone et al. (2003)

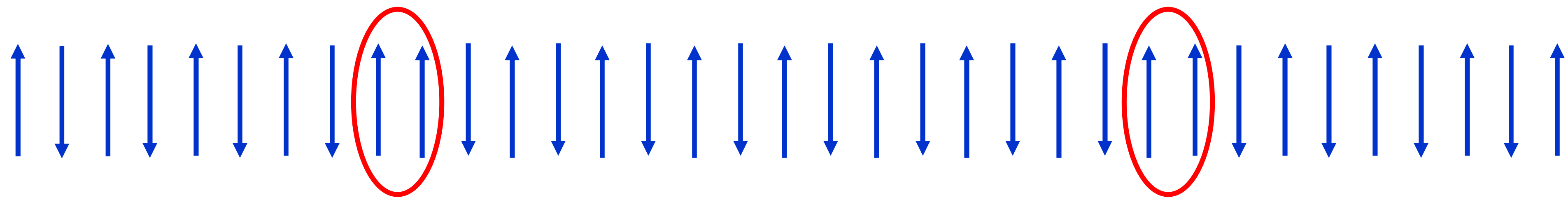
Spin-$\frac{1}{2}$ chain in a staggered field

Why staggered field yields bound states

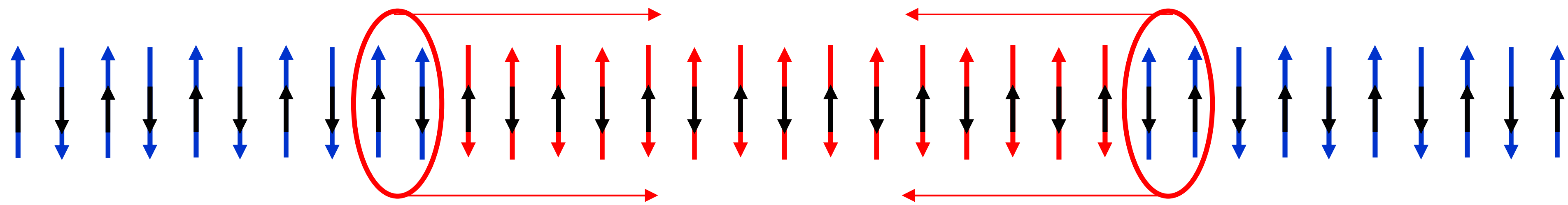
Zero field state quasi-long range AFM order



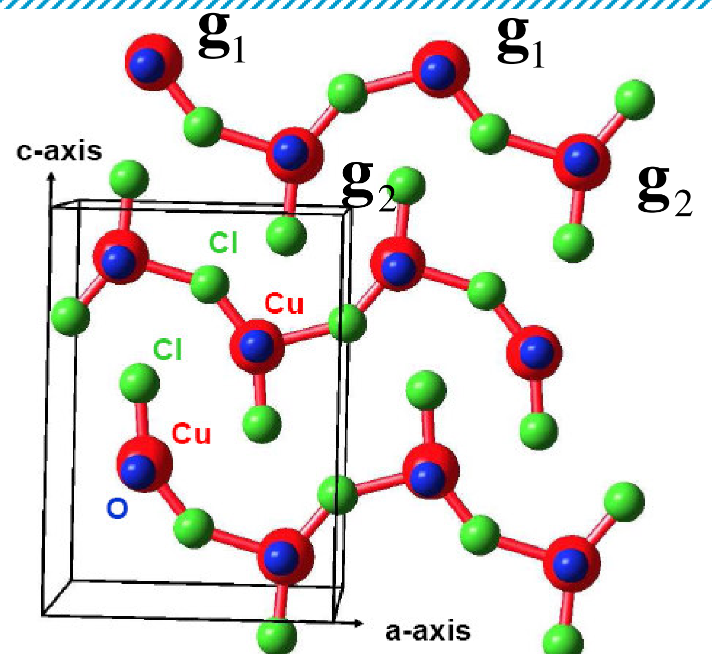
Without staggered field distant spinons don't interact



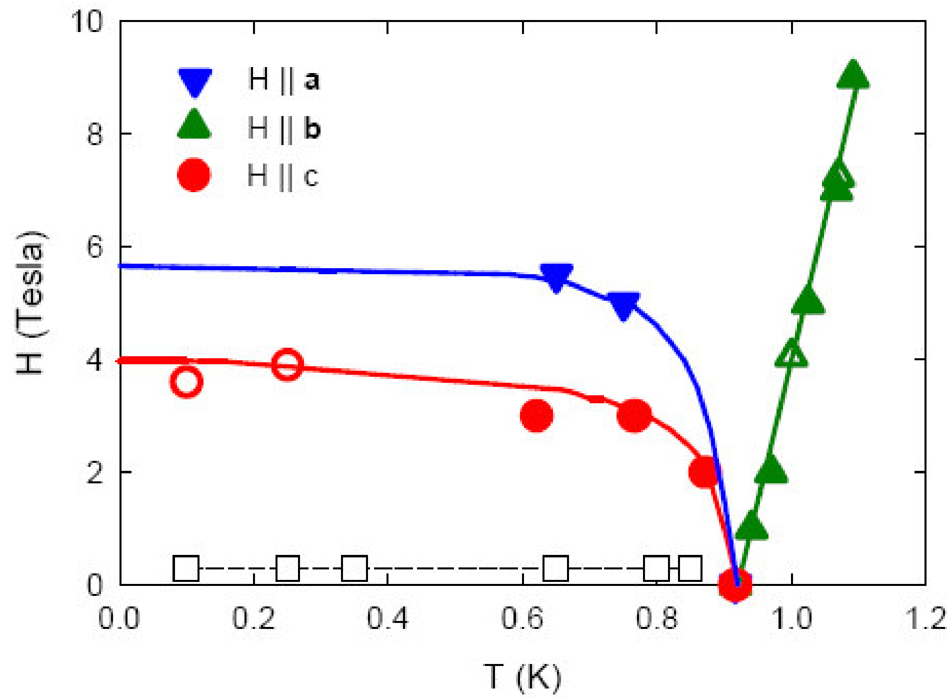
With staggered field solitons separate "good" from "bad" domains, which leads to interactions and bound states



Spin-½ chain with two spins per chain unit



$CuCl_2$·2(dimethylsulfoxide)



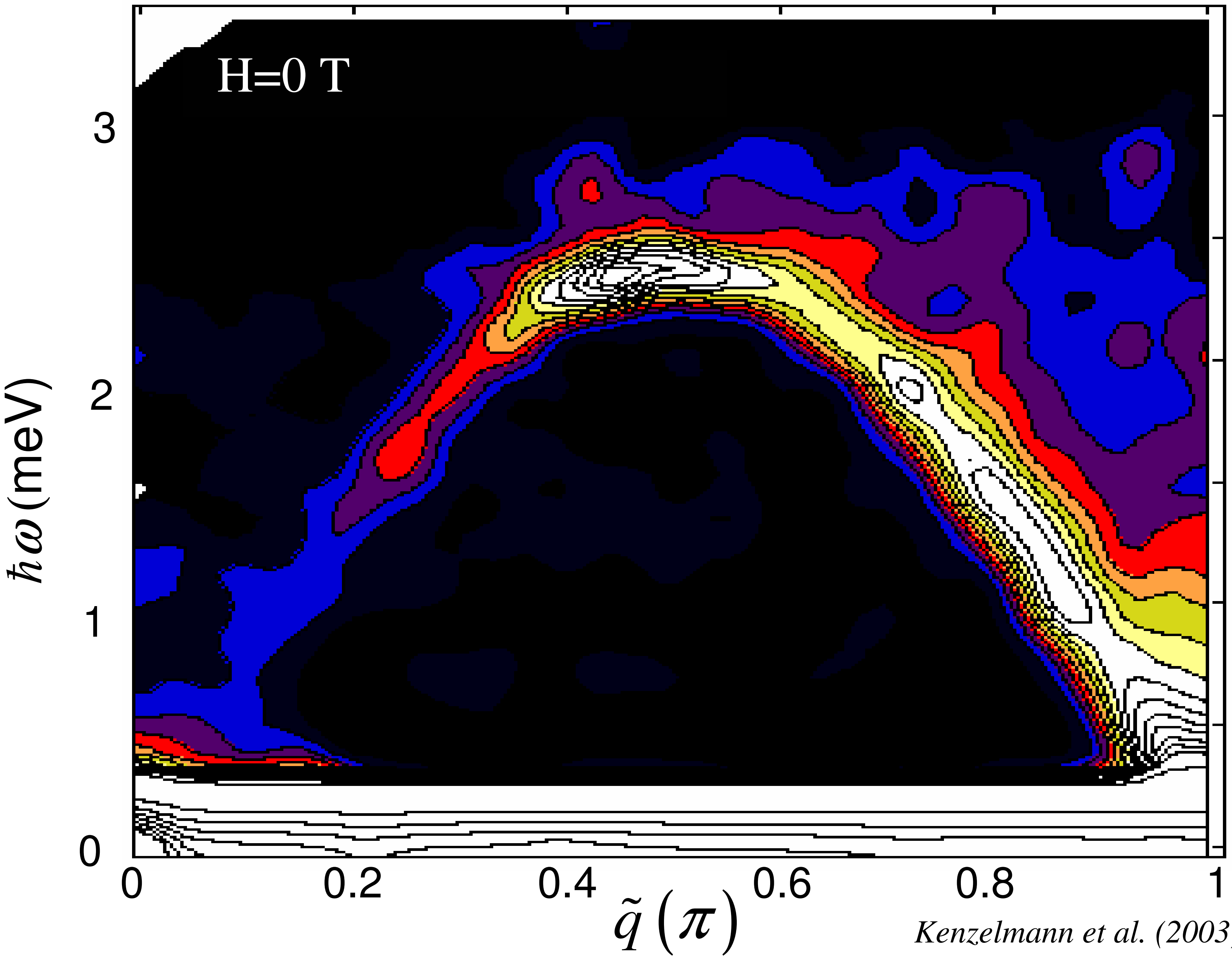
$$\mathrm{H} = \sum_n \left(J\mathbf{S}_n \cdot \mathbf{S}_{n+1} + \mathbf{D}_n \mathbf{S}_n \times \mathbf{S}_{n+1} - \mu_B \mathbf{H} \mathbf{g}_n \mathbf{S}_n \right)$$

$$= \sum_n \left(J\mathbf{S}_n \cdot \mathbf{S}_{n+1} - \tilde{H} S_n^z - h_s (-1)^n S_n^x \right)$$

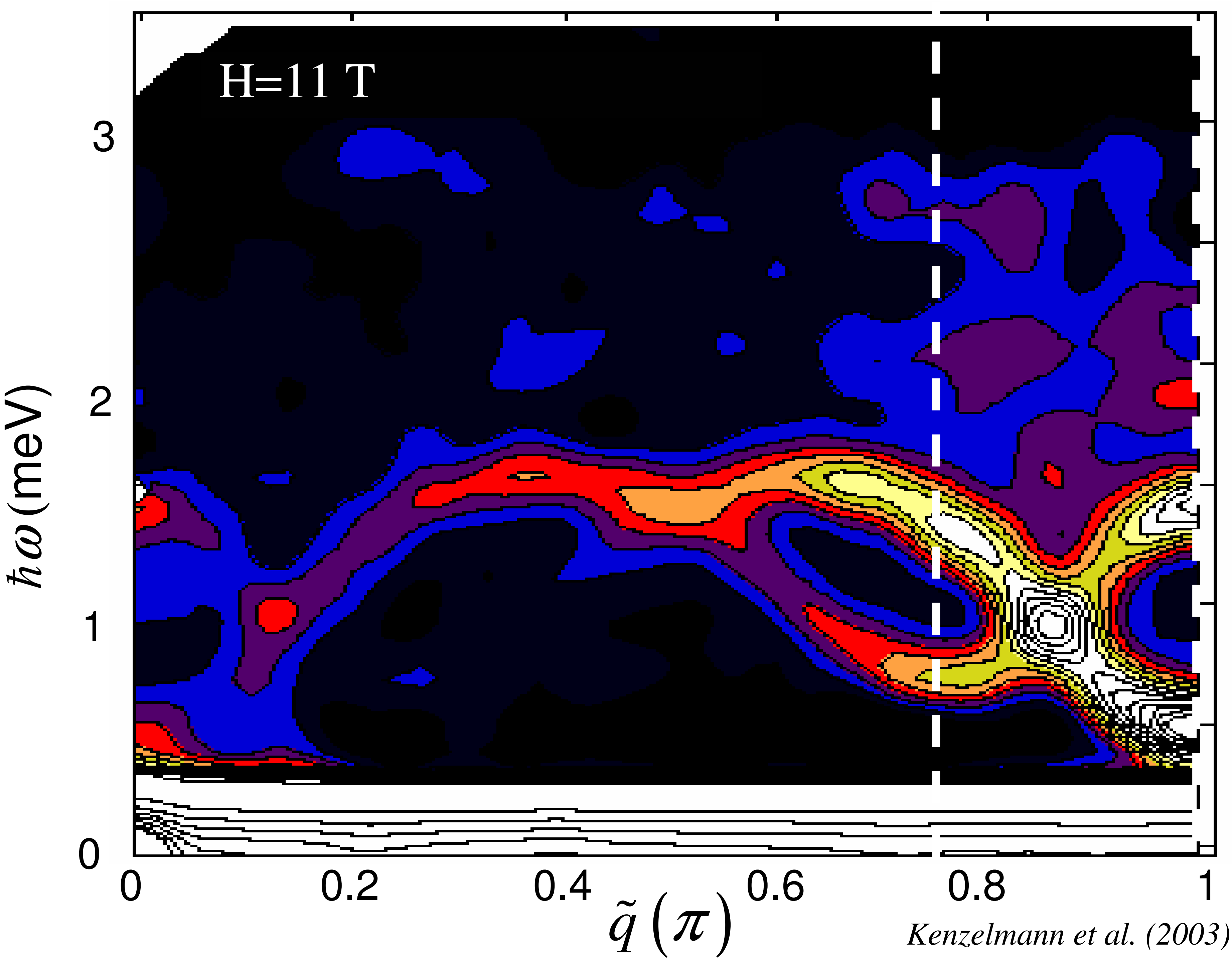
Xia and Riseborough (1988)

$$\mathbf{h}_s \sim \left(\frac{g_1 - g_2}{2} \right) \mathbf{H} + \tfrac{1}{2J} \mathbf{D} \times \left(\frac{g_1 + g_2}{2} \right) \mathbf{H}$$

Oshikawa and Affleck (1997)

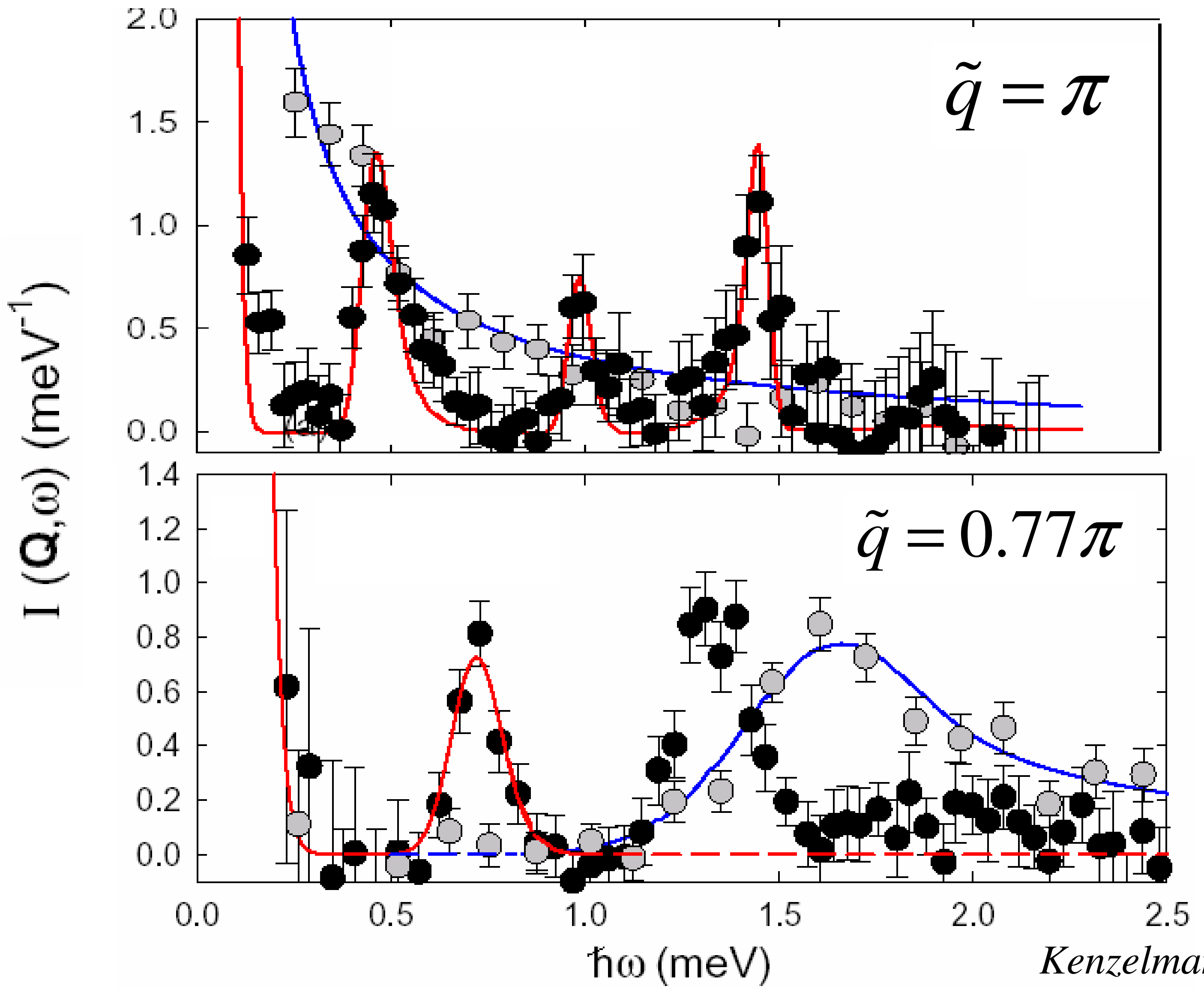


Kenzelmann et al. (2003)



H=11 T
3
2
1
0
ħω (meV)
0
0.2
0.4
0.6
0.8
1
q̃ (π)
Kenzelmann et al. (2003)

Bound states from 2-spinon continuum



Kenzelmann et al. (2003)

Sine-Gordon mapping of spin-1/2 chain

Effective staggered + uniform field spin hamiltonian

$$\mathrm{H}_{\mathrm{eff}} = \sum_n \left(J\, \tilde{\mathbf{S}}_n \cdot \tilde{\mathbf{S}}_{n+1} - \tilde{H}\tilde{S}_n^z - h_s \left(-1\right)^n \tilde{S}_n^x \right)$$

Spin operators are represented through a phase field $\tilde{\phi}\left(x,t\right)$ relative to incommensurate quasi-long-range order with Lagrangian density

$$\mathrm{L} = \tfrac{1}{2}\left[\left(\partial_t \tilde{\phi}\right)^2 - \left(\partial_x \tilde{\phi}\right)^2 \right] + C h_s \cos\left(2\pi R\left(H\right)\tilde{\phi}\right)$$

This is sine-Gordon model with interaction term proportional to h_s

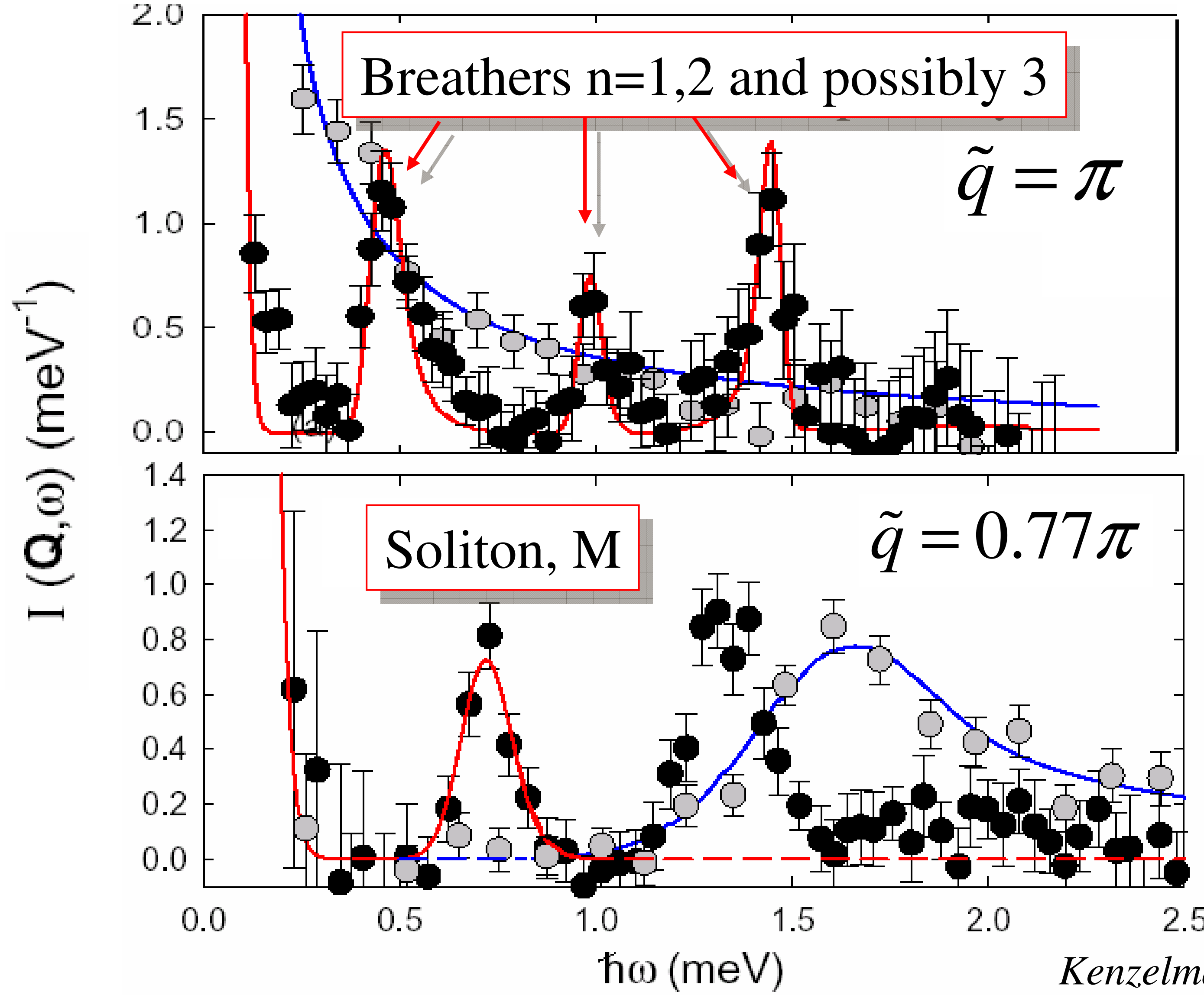
Spectrum consists of

- Solitons, anti-solitons $\quad M = JA \left(\frac{\tilde{H}}{J}\right)\left(\frac{h_s}{J}\right)^{\frac{1}{2-\pi R\left(\tilde{H}\right)^2}}$

- Breather bound states $\quad M_n = 2M \sin\left(n\pi\xi\left(H\right)/2\right)$

Oshikawa and Affleck (1997)

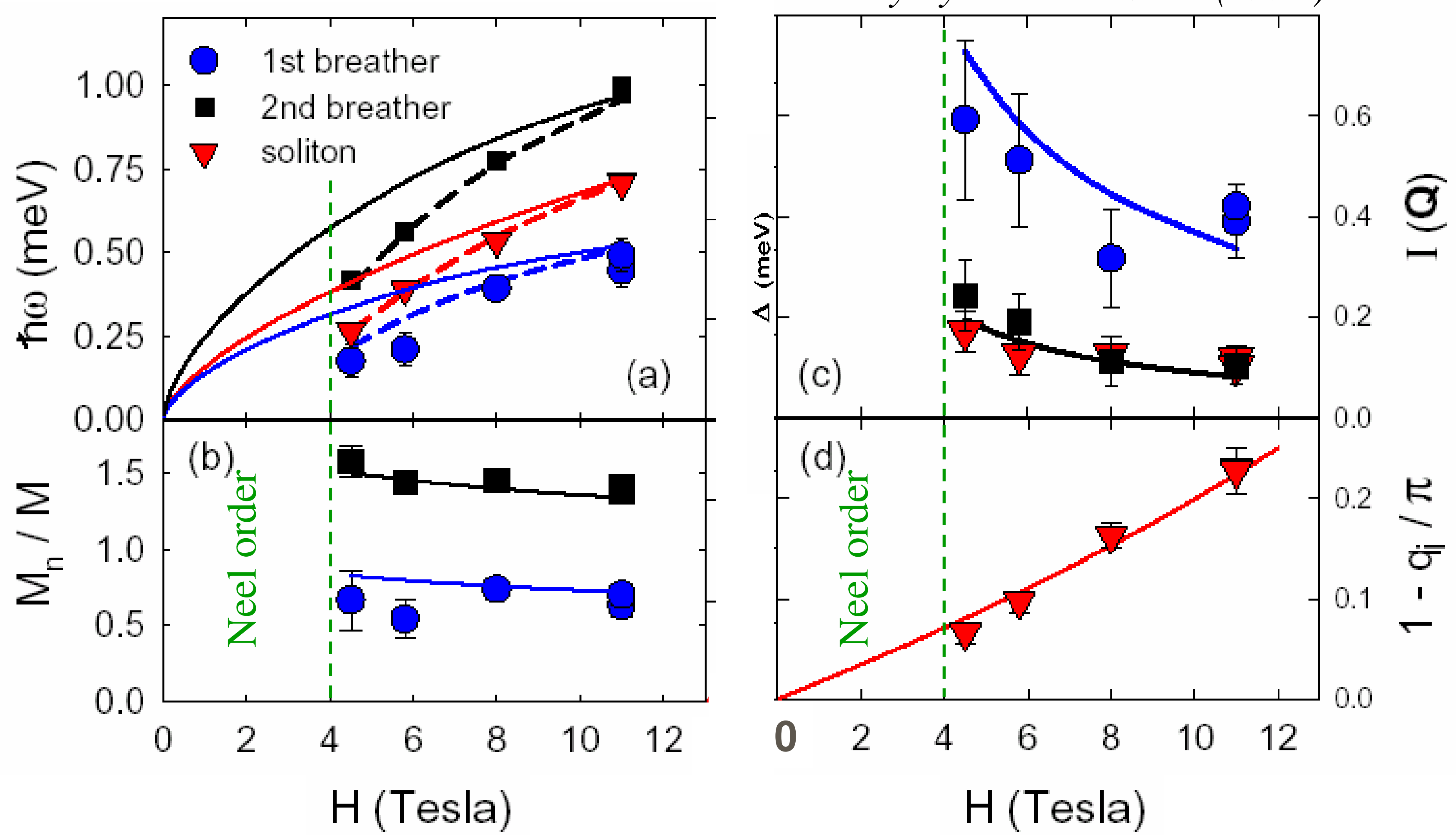
Bound states from 2-spinon continuum



Kenzelmann et al. (2003)

Testing sine-Gordon predictions

Theory by Essler-Tsvelik (1998)



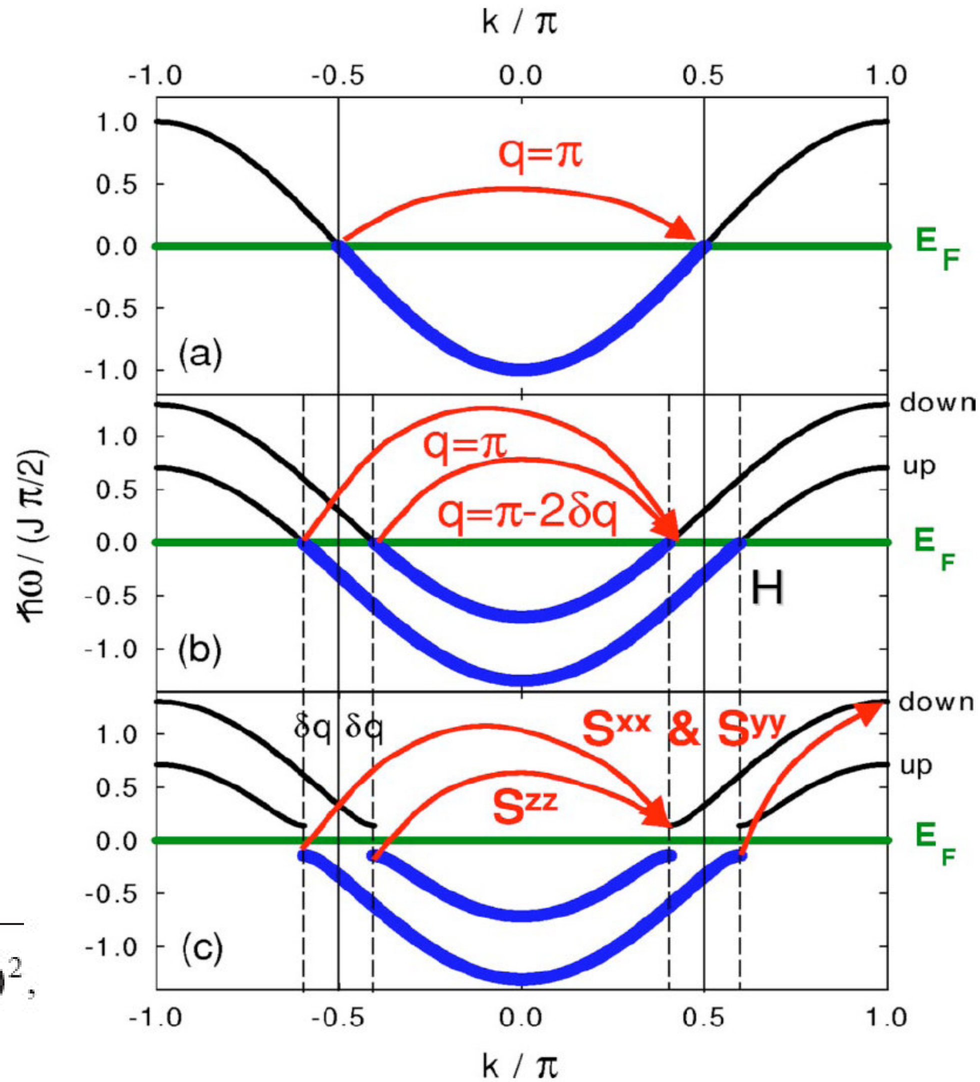
Kenzelmann et al. (2003)

MFT of fermions in a staggered field

$$\mathcal{H}_{MF} = -\frac{J\gamma}{2}\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + \mathrm{H.c.}) - \frac{g_c}{2}\mu_B H \sum_{i,\sigma}\sigma n_{i\sigma} - \frac{1}{2}(g_a\mu_B H_{\mathrm{st}} + J\delta)\sum_{i,\sigma}(-1)^i c^\dagger_{i\sigma}c_{i\bar{\sigma}} + \lambda\sum_i n_i,$$

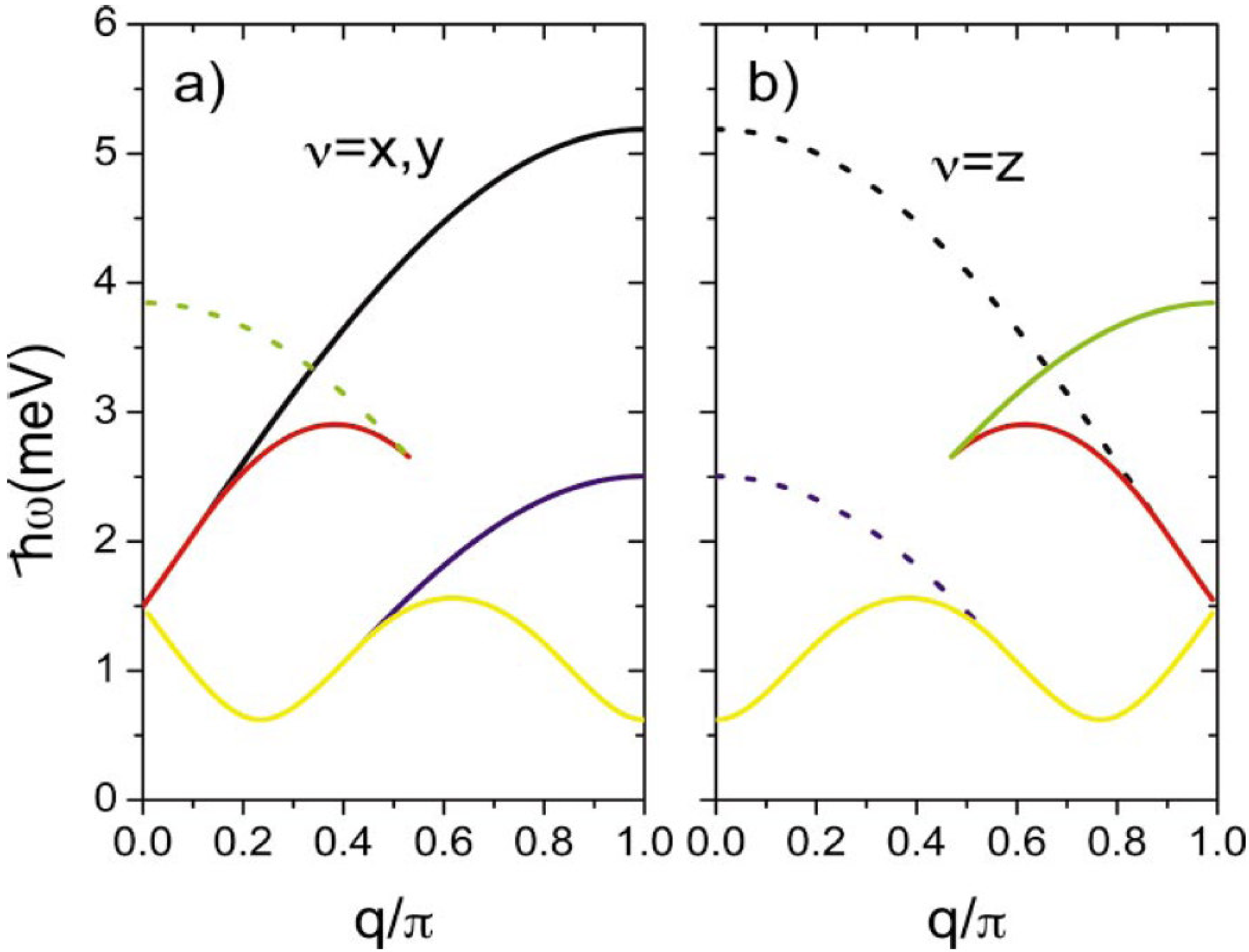
$$\mathcal{H}_{MF} = \sum_{-\pi<k\leq\pi,\sigma}\left[\left(-J\gamma\cos(k) - \frac{\sigma}{2}g_c\mu_B H\right)c^+_{k\sigma}c_{k\sigma} - \frac{1}{2}(g_a\mu_B H_{\mathrm{st}} + J\delta)(c^+_{k+\pi\sigma}c_{k\bar{\sigma}} + c^+_{k\bar{\sigma}}c_{k+\pi\sigma})\right],$$

$$\epsilon^{\pm}_{k\sigma} = \pm\sqrt{\left(J\gamma\cos(k) + \sigma\frac{g_c}{2}\mu_B H\right)^2 + \frac{1}{4}(g_a\mu_B H_{\mathrm{st}} + J\delta)^2},$$

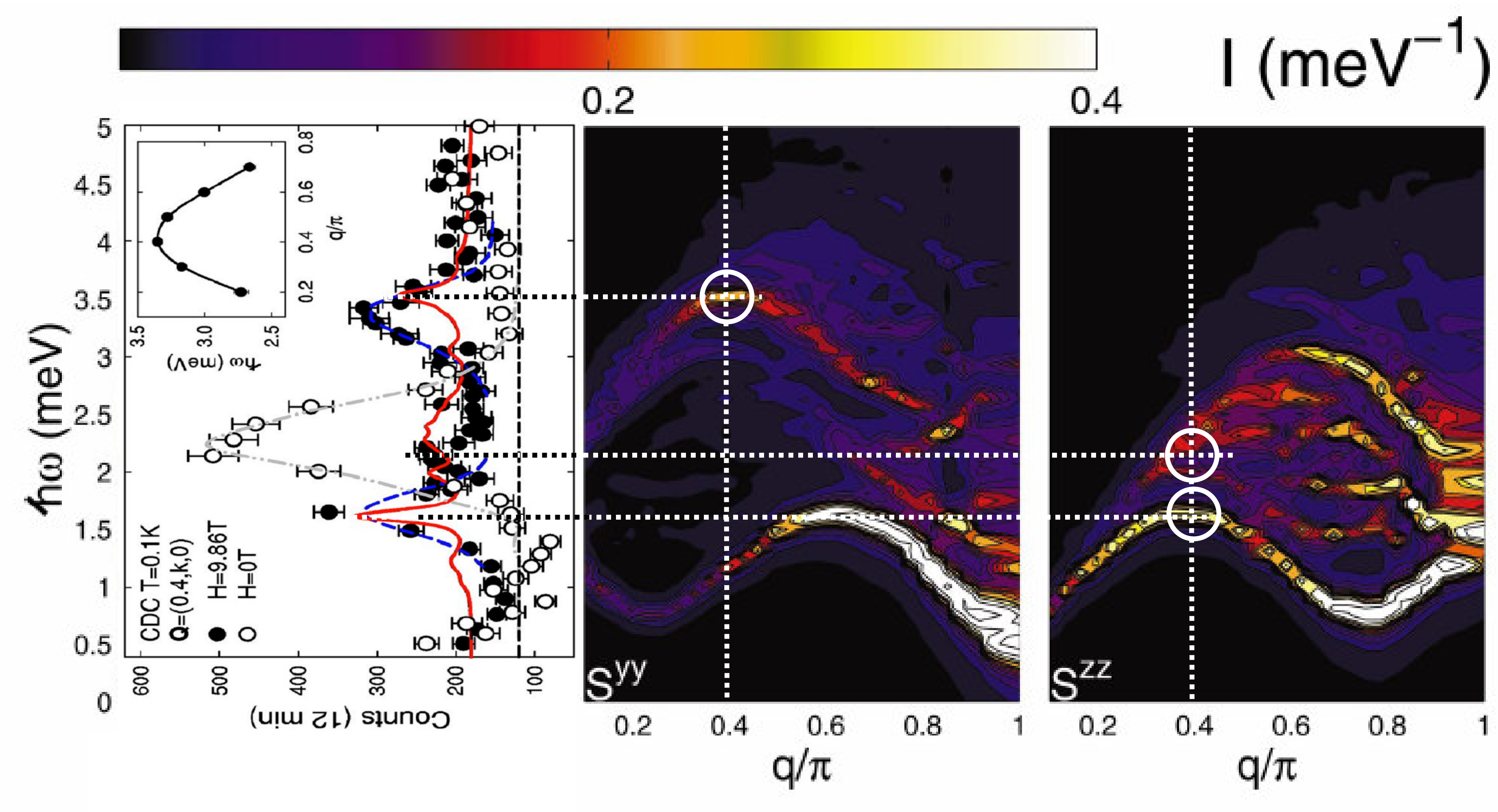


Kenzelmann, Batista, et al. (2005)

Mean Field Dispersion Relations



High energy bound states



Kenzelmann et al. (2005)

Conclusions

- Single mode approximation
  - Good for spin-1 chain when $q>0.3\pi$
  - A versatile tool for experimentalists & theorists
- Decay of bound state in near critical spin-1/2 bi-layer
- Spin-1/2 chains: Physical realization of QCP
- Uniform field exposes extended critical state
- Staggered fields
  - inherent to multi-atom cells
  - produce rich spectrum of bound states
- Sine-Gordon model describes
  - Bound state energies
  - Breather intensities
  - Field dependent incommensurability
- High-E bound states predicted & observed

Some Challenges in Quantum Magnetism

- Identify isotropic D>1 critical phase
  - Isolated critical phase via perturbations
  - Purify known glassy quantum magnets
- "Vortex lattice" in quantum magnet
  - High field phase of spin-1/2 ladder
  - Correlations in magnetization plateau
- Structure & dynamics of quantum impurities in D>1
- Itinerant quantum magnetism
  - Frustration+low D+mobile fermions