Finite Temperature Spin Correlations in Quantum Magnets with a Spin Gap

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Quantum Magnets at T=0

From coherent singlet to paramagnet

- Large gap : Coupled spin-1/2 dimers
- Small gap : Haldane spin-1 chain

Conclusions

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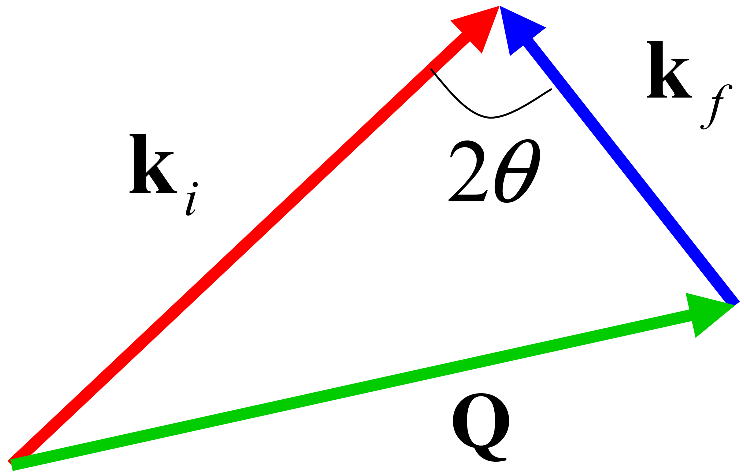
Collaborators

Magnetic Neutron Scattering



$$\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$$

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

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

SPINS Cold neutron triple axis spectrometer at NCNR

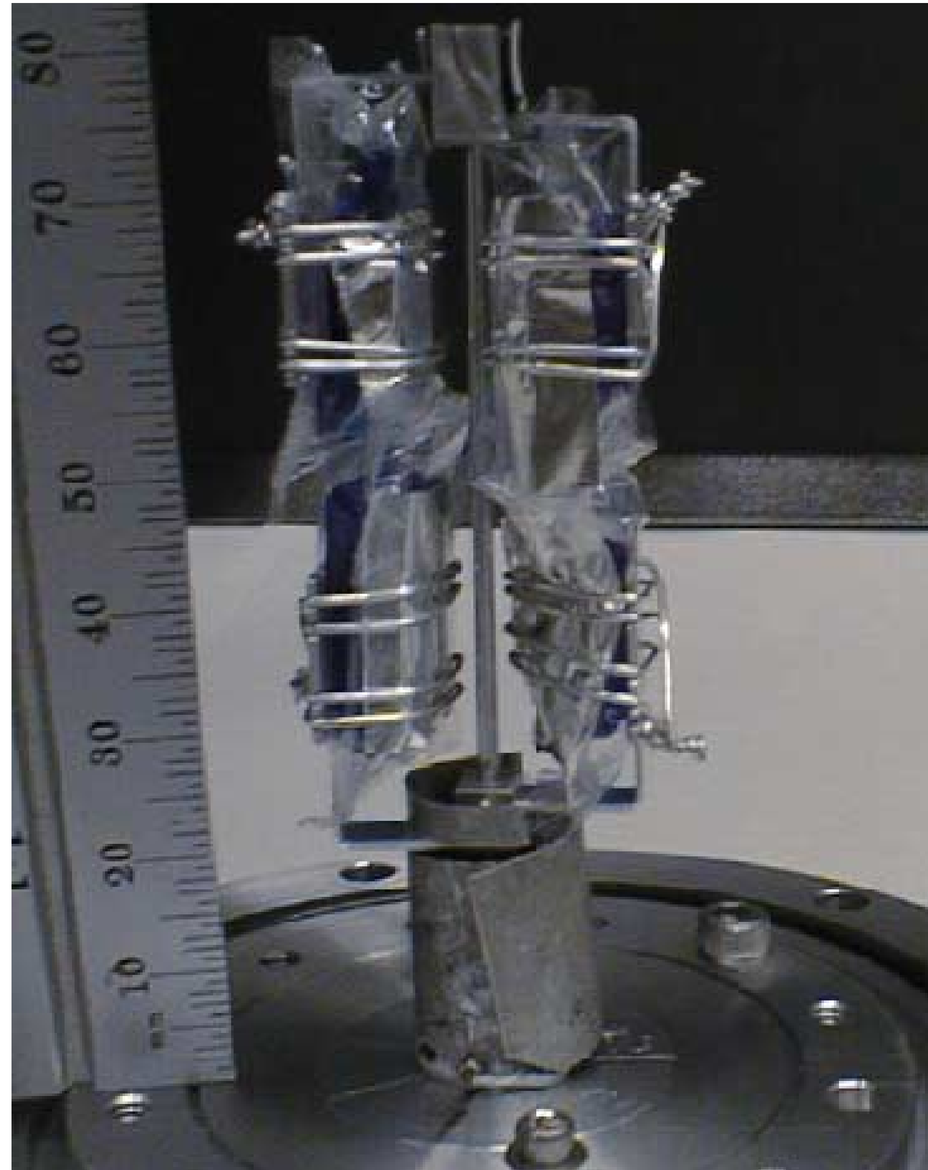
Focusing analyzer system on SPINS

Y_2BaNiO_5

Ito, Oka, and Takagi

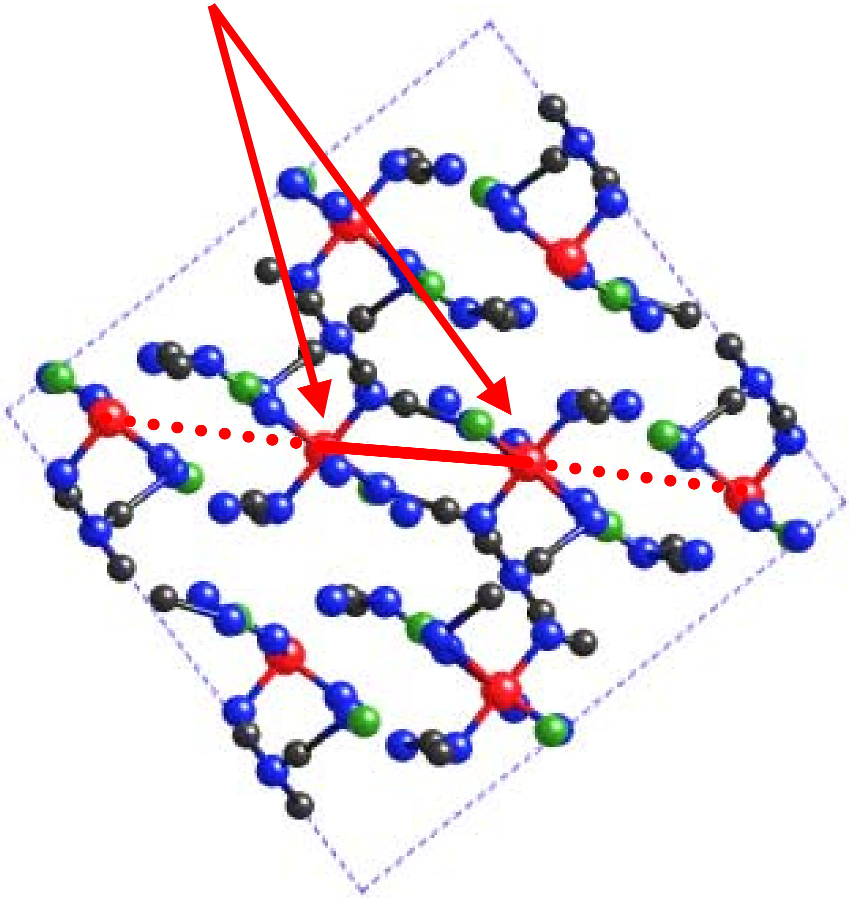
$Cu(NO_3)_2 \cdot 2.5\ D_2O$

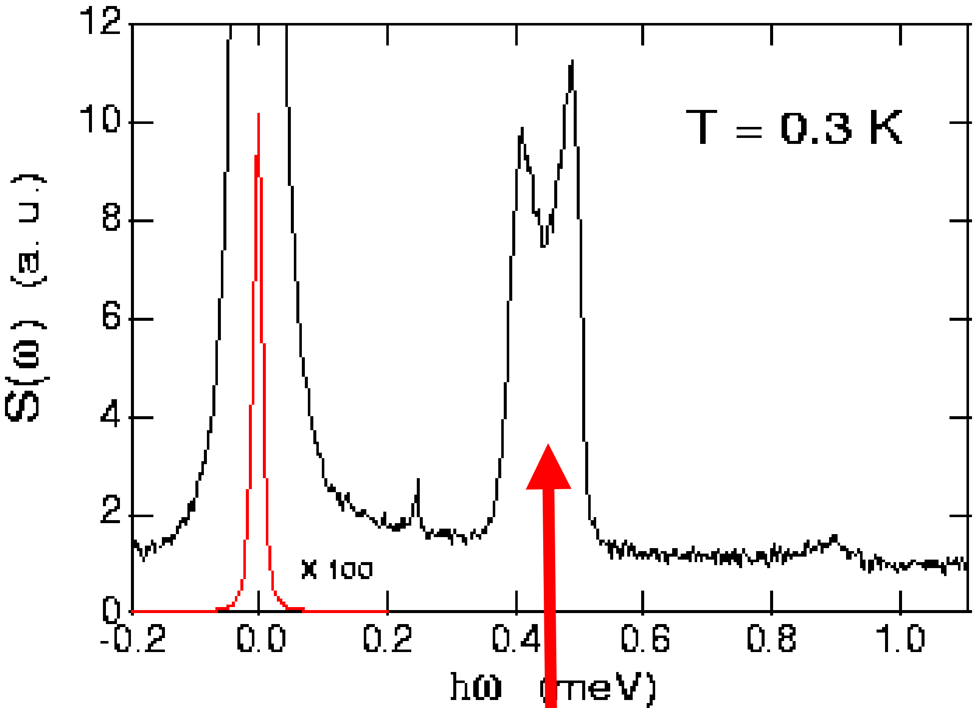
Guangyong Xu



Simple example of "Quantum" magnet

$Cu(NO_3)_2 \cdot 2.5D_2O$: dimerized spin-1/2 system

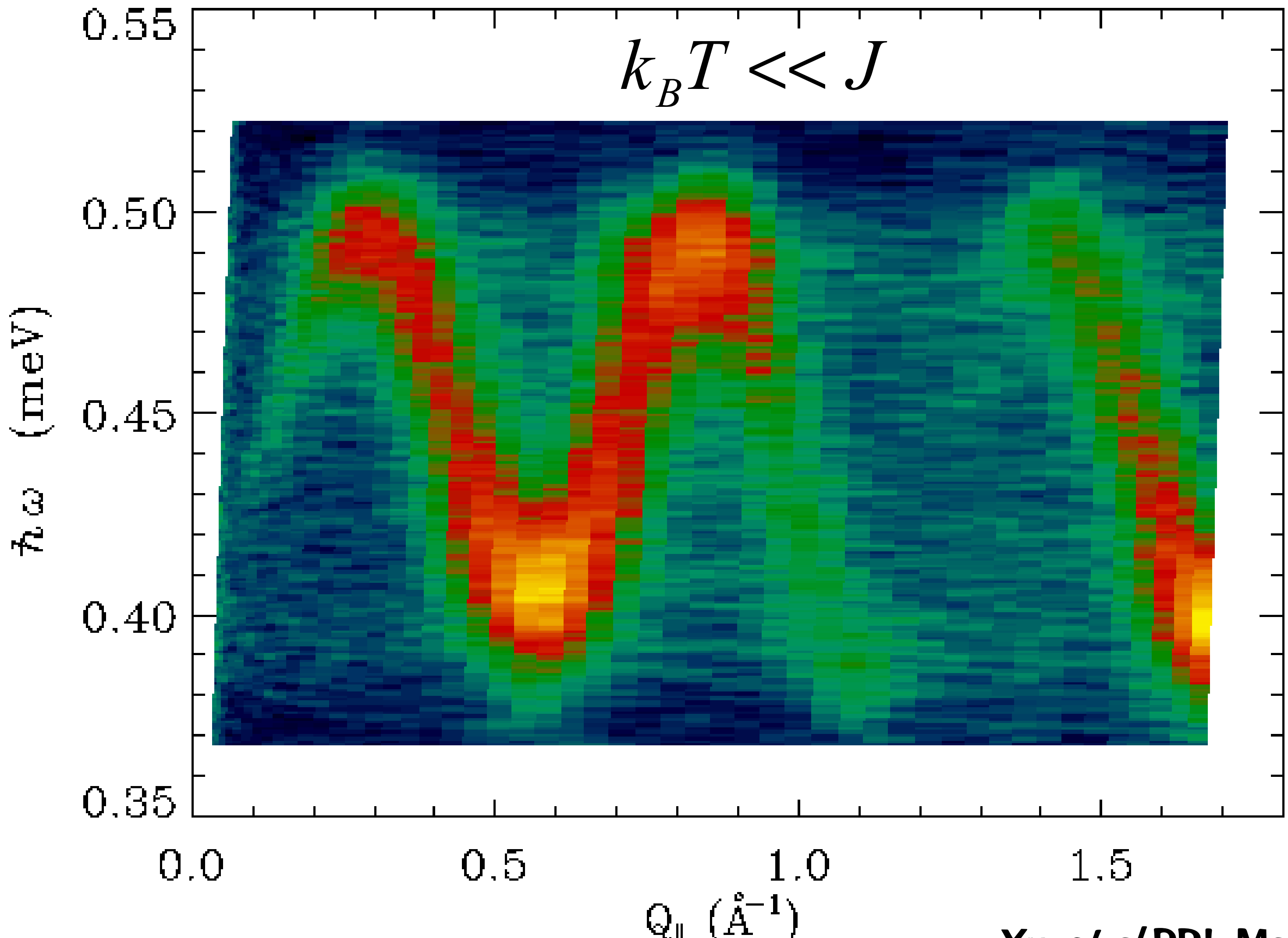




Only Inelastic magnetic scattering

Dispersion relation for triplet waves

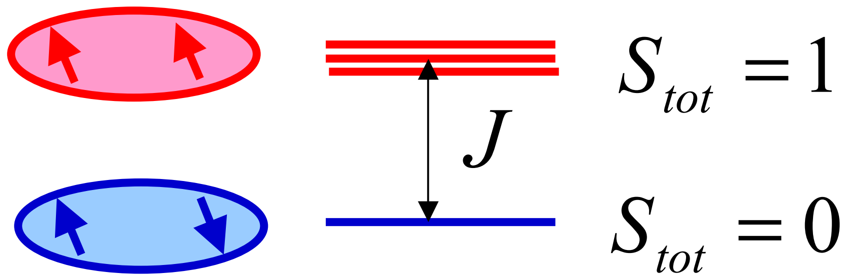
Dimerized spin-1/2 system: copper nitrate



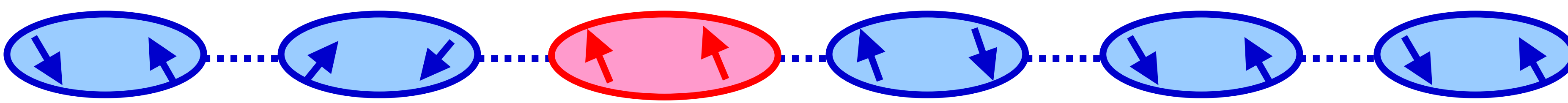
Xu *et al* PRL May 2000

Qualitative description of excited states

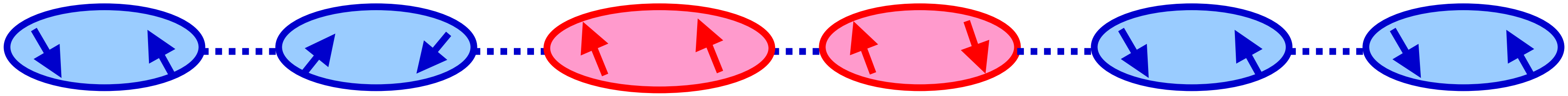
- A spin-1/2 pair with AFM exchange has a singlet - triplet gap:



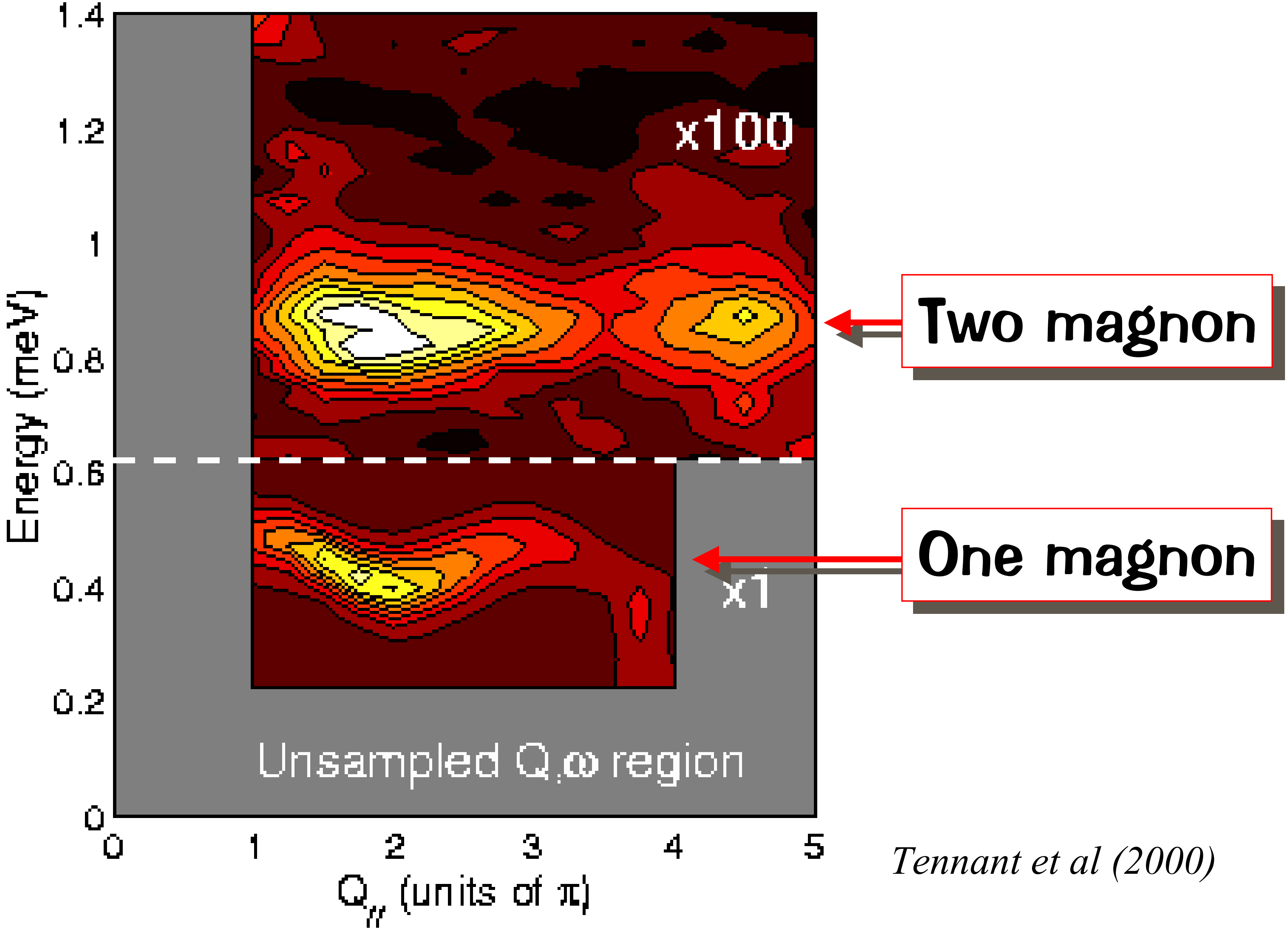
- Inter-dimer coupling allows coherent triplet propagation and produces well defined dispersion relation



- Triplets can also be produced in pairs with total $S_{tot}=1$

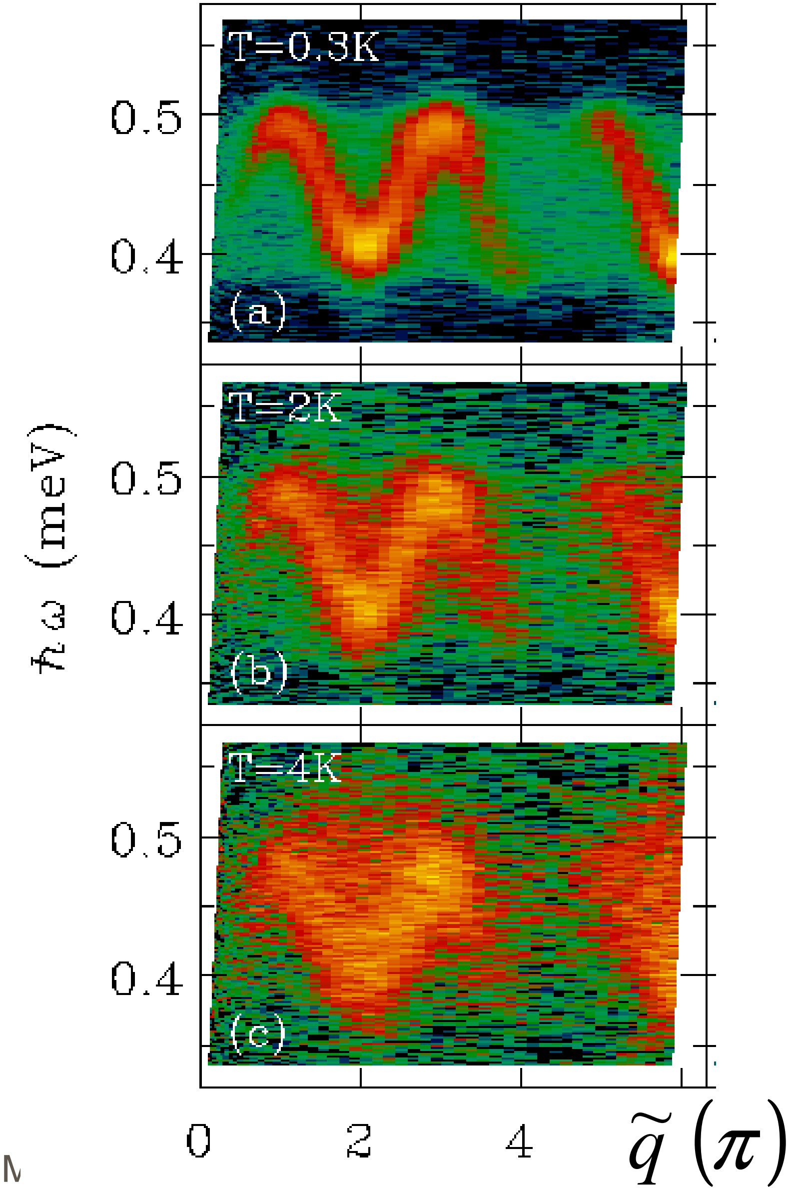


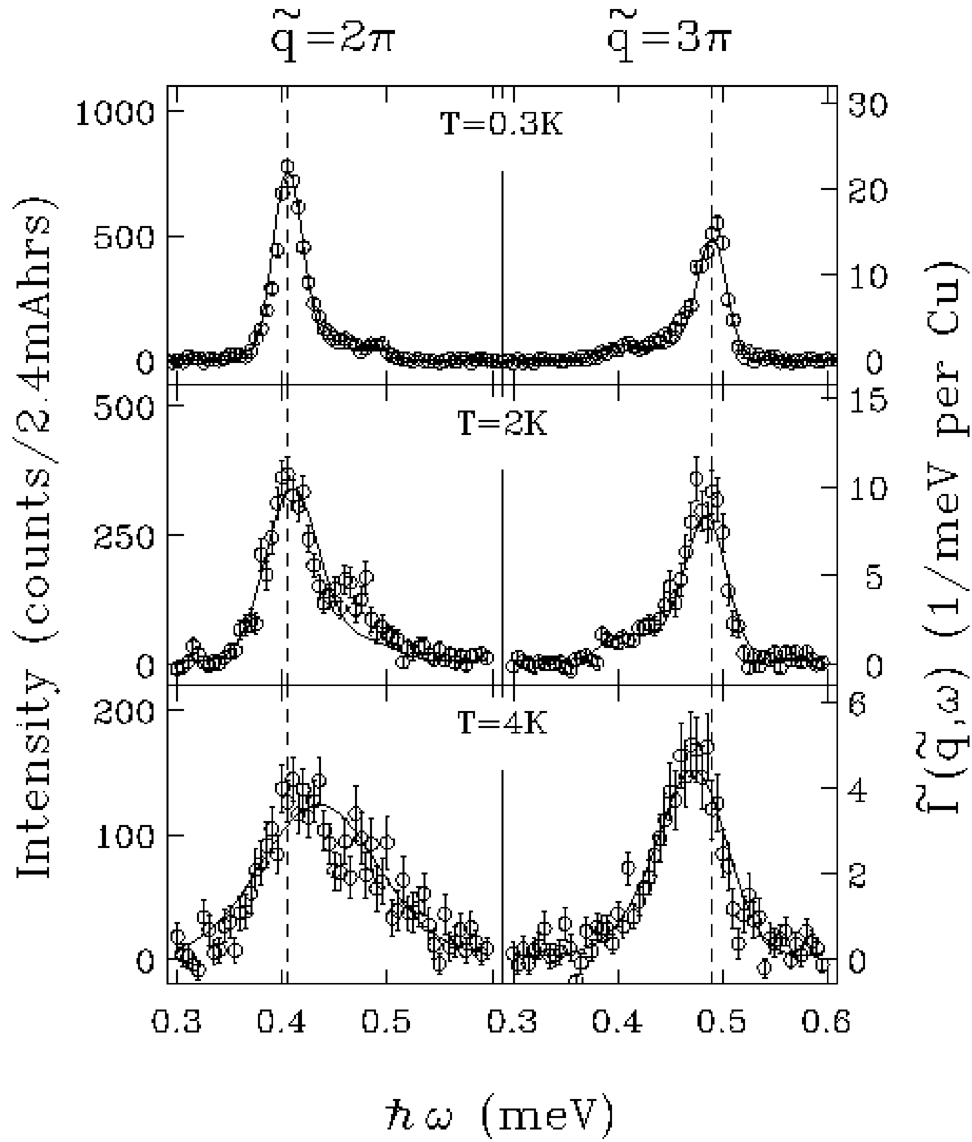
Creating two triplets with one neutron



Tennant et al (2000)

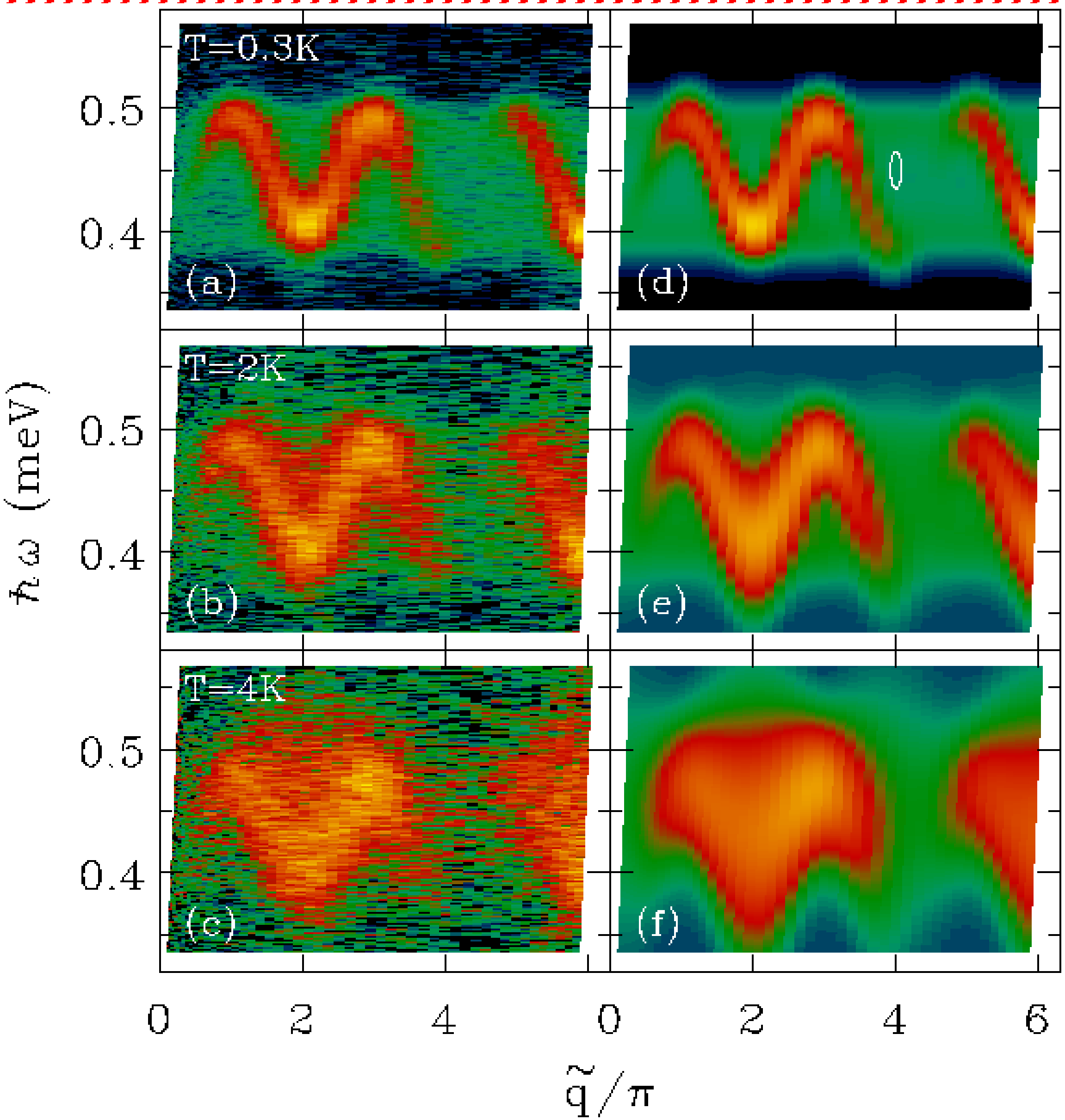
Heating coupled dimers





ICM

SMA fit to scattering data



T-Parameters extracted from fit

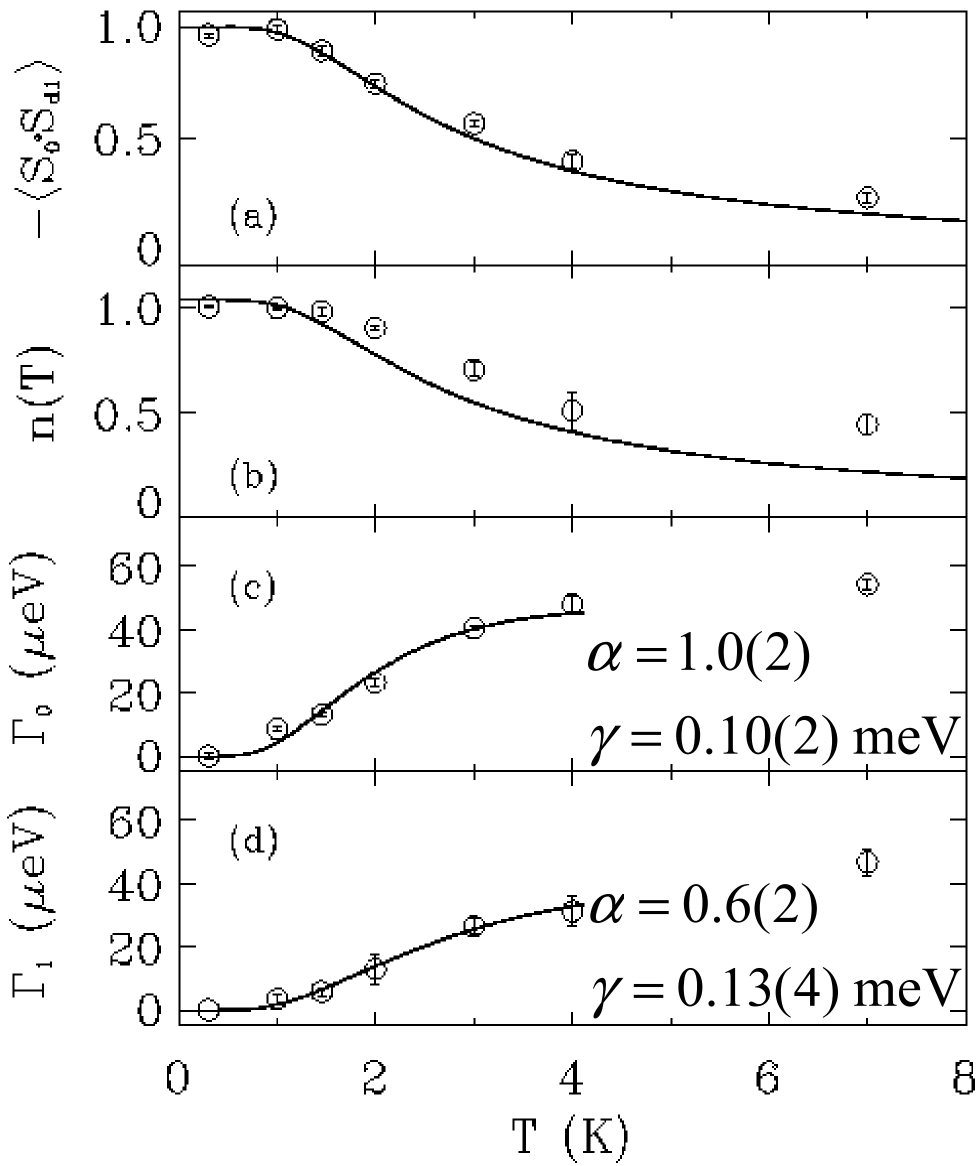
$$\langle S_0 S_d \rangle_T$$

$$\varepsilon(\tilde{q}) = J_1 + n(T)\frac{J_2}{2}\cos\tilde{q}$$

$$\Gamma(\tilde{q}) = \Gamma_0 + \frac{\Gamma_1}{2}\cos\tilde{q}$$

More than 1000 data points per parameter!

T-dependence of singlet-triplet mode



$$-\left\langle \mathbf{S}_0 \cdot \mathbf{S}_{\vec{d}_0} \right\rangle_T = S(S+1)\left(\rho_{S=0} - \rho_{S=1}\right)$$

$$n(T) = \rho_{S=0} - \rho_{S=1}$$

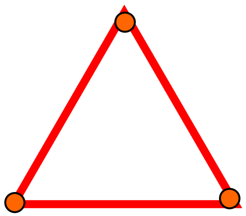
$$\Gamma(T) = \gamma \left(\frac{J_1}{k_B T}\right)^{\alpha} \exp(-J_1/k_B T)$$

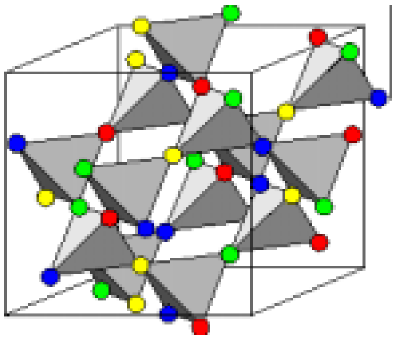
Types of Quantum magnets

- Definition: small or vanishing frozen moment at low T:

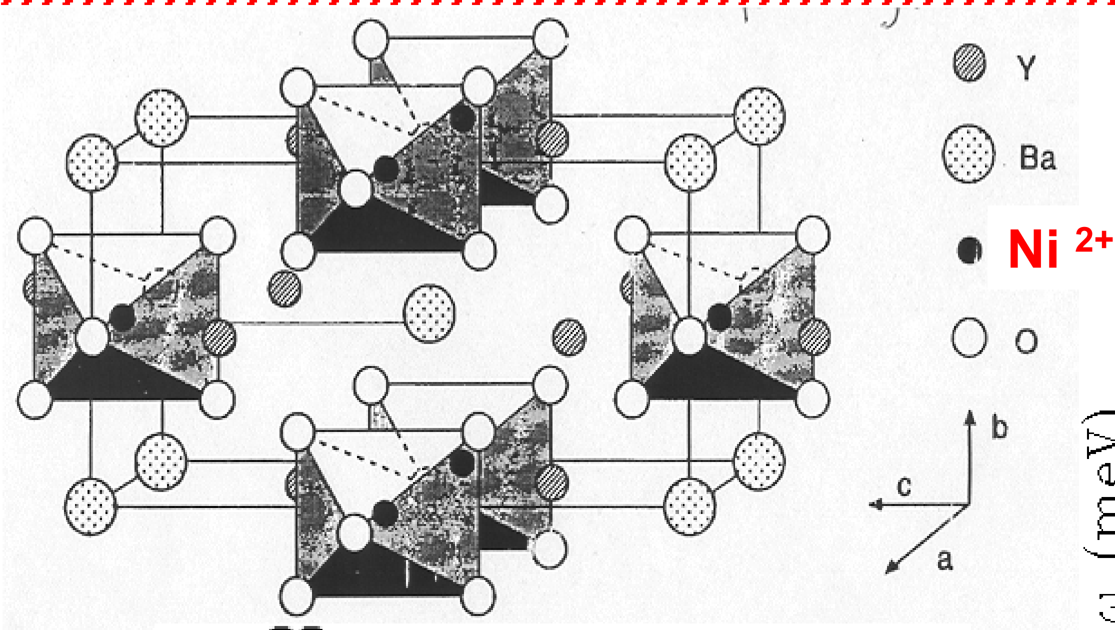
$$\left|\langle \mathbf{S} \rangle\right| << S \quad \text{for} \quad k_B T << J$$

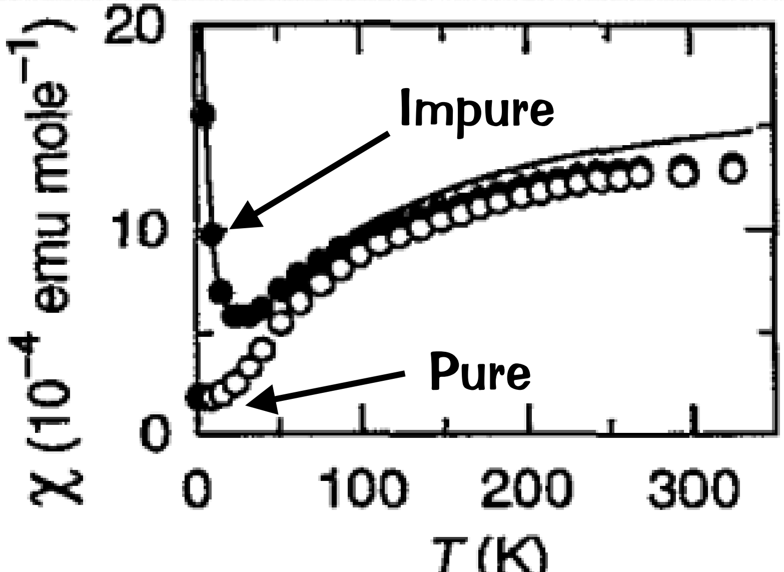
- Conditions that yield quantum magnetism
  - Low effective dimensionality
  - Low spin quantum number
  - geometrical frustration
  - dimerization
  - weak connectivity
  - interactions with fermions
- Novel coherent states

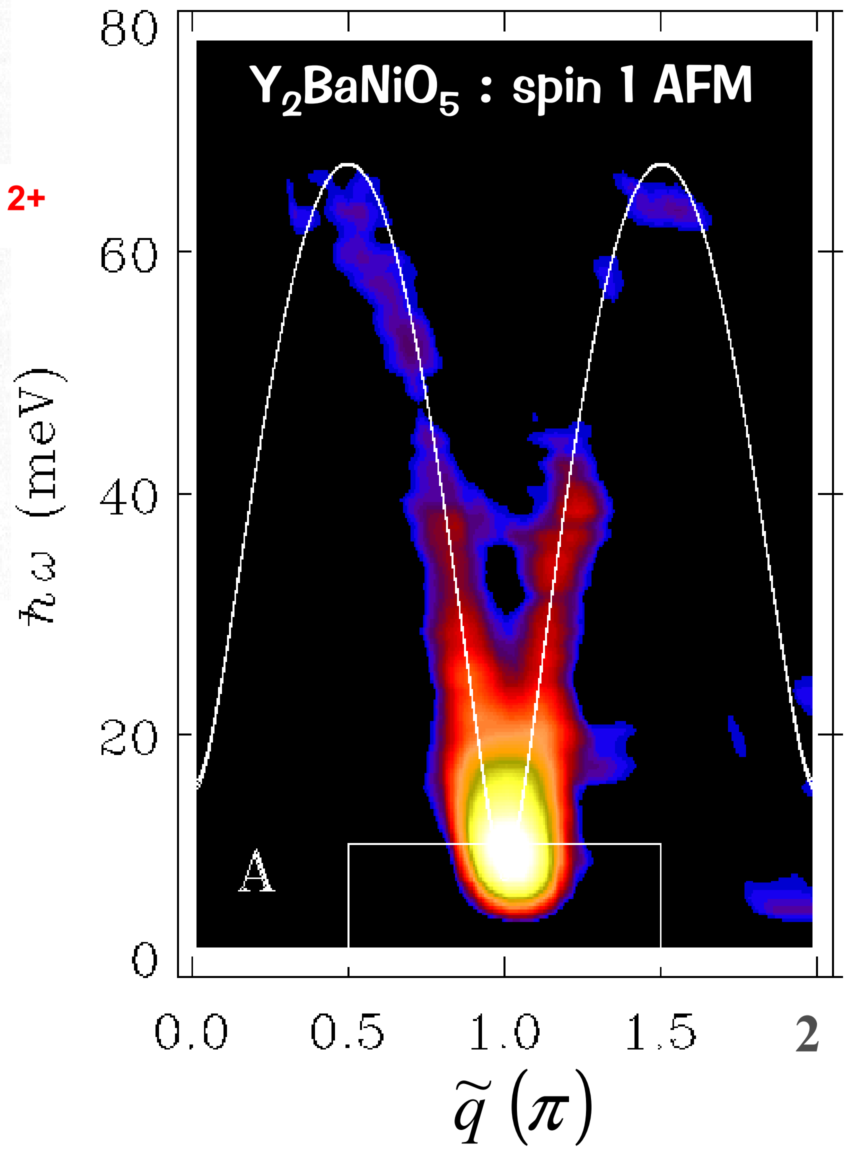




One dimensional spin-1 antiferromagnet Y_2BaNiO_5

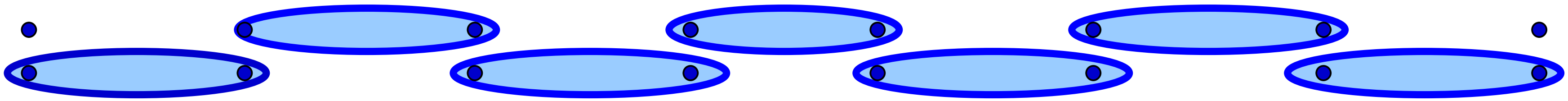






Macroscopic singlet ground state of S=1 chain

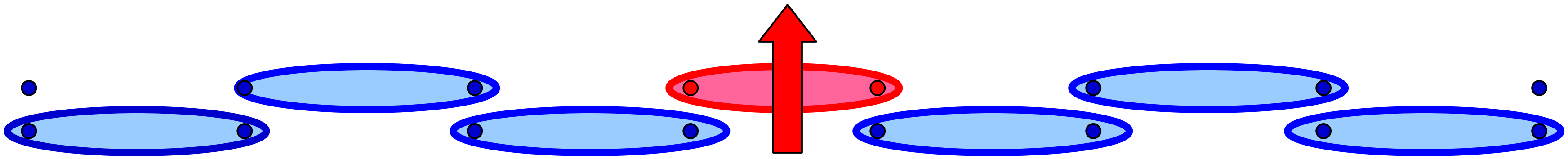
- Magnets with 2S=nz have a nearest neighbor singlet covering with full lattice symmetry.



- This is exact ground state for spin projection Hamiltonian

$$\mathscr{H} = \sum_i P_i\left(S_{tot} = 2\right) = \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \tfrac{1}{3}\left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2\right) \approx \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

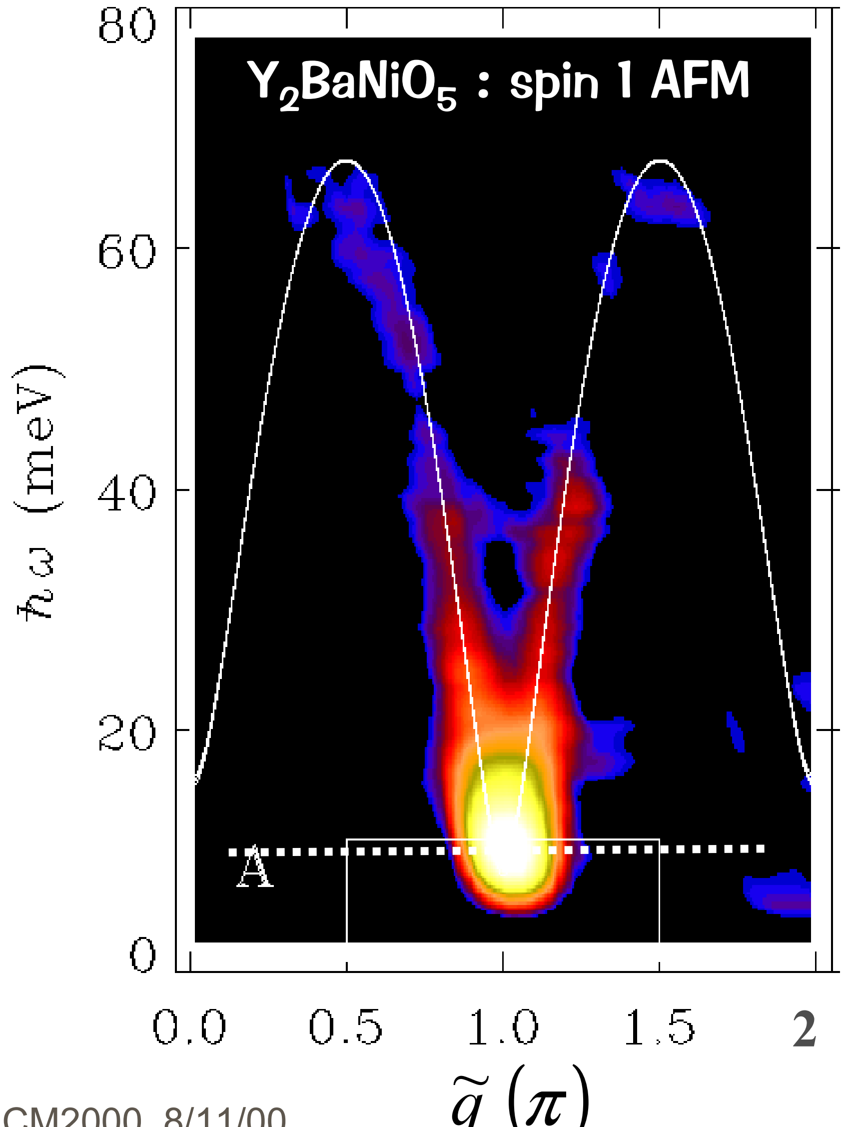
- Excited states are propagating bond triplets separated from the ground state by an energy gap $\Delta \approx J$.



Haldane PRL 1983

Affleck, Kennedy, Lieb, and Tasaki PRL 1987

Two length scales in a quantum magnet



Equal time correlation length

$$S(\tilde{q}) = \hbar \int S(\tilde{q}, \omega)\, d\omega$$

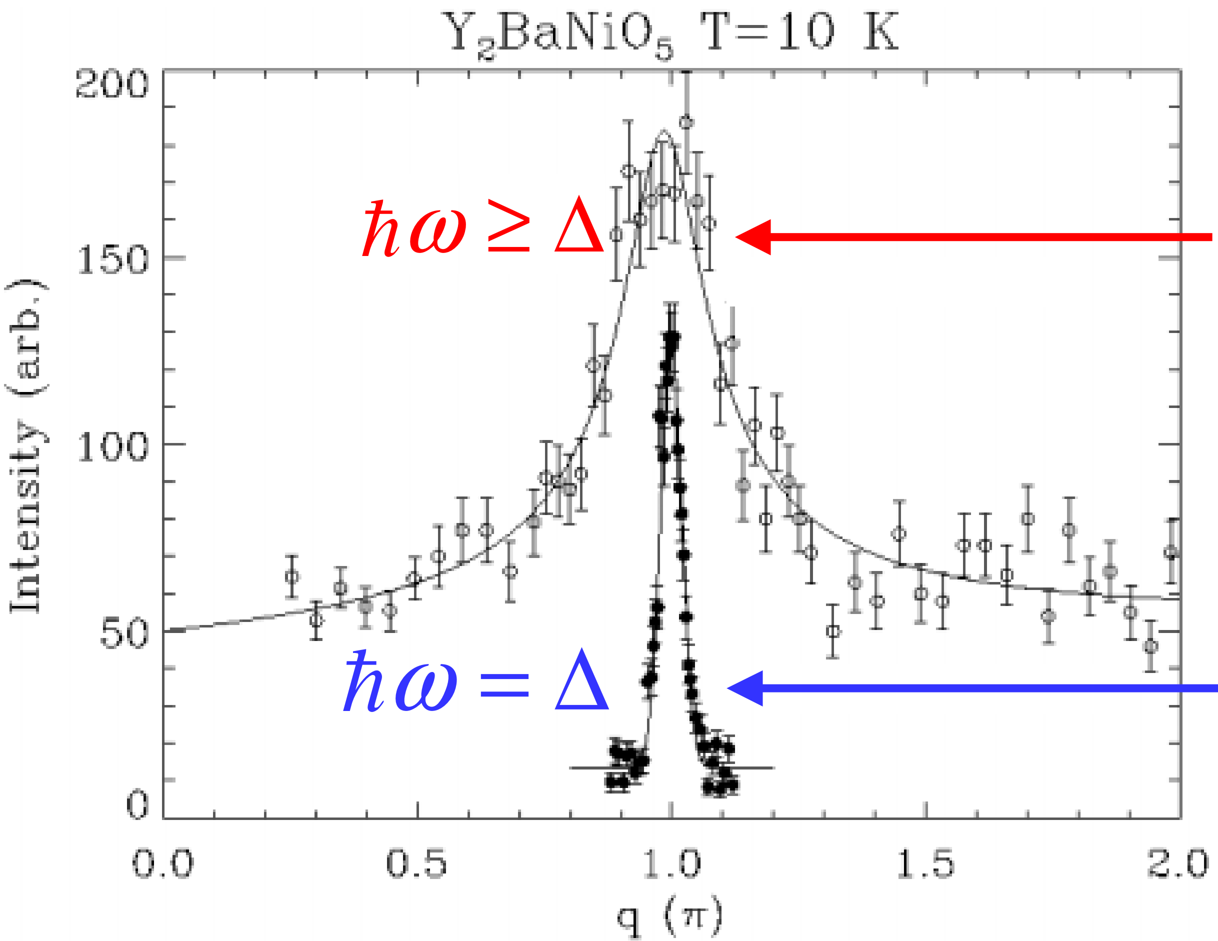
$$S(\tilde{q}) = \frac{1}{N} \sum_{ll'} \langle S_l S_{l'} \rangle \exp(i\tilde{q}(l - l'))$$

$$\langle S_0 S_l \rangle \propto \frac{1}{\sqrt{l}} \exp\left(-\, l / \xi\right)$$

Triplet Coherence length :

length of coherent triplet wave packet

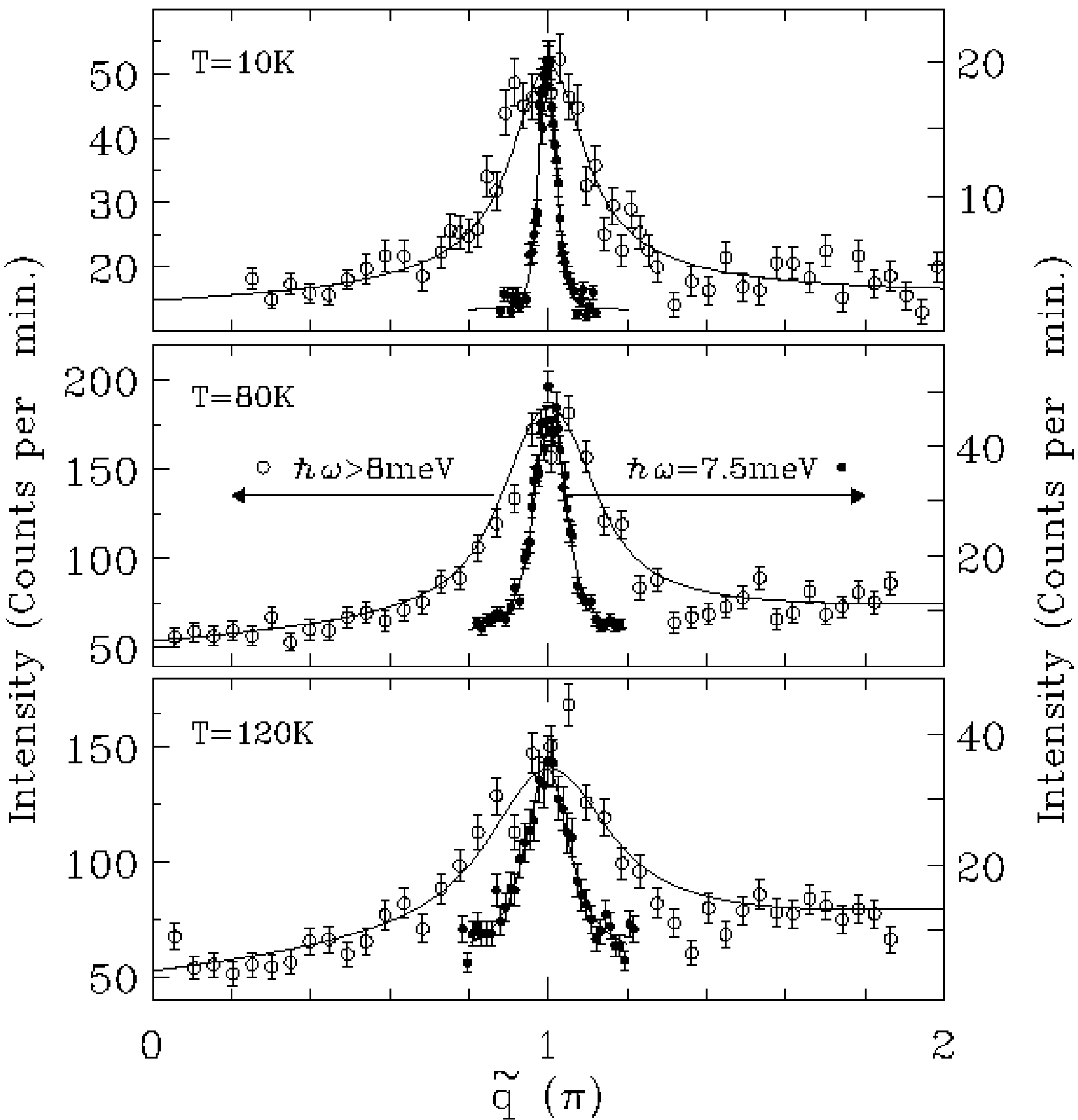
Coherence in a fluctuating system



Short range G.S. spin correlations

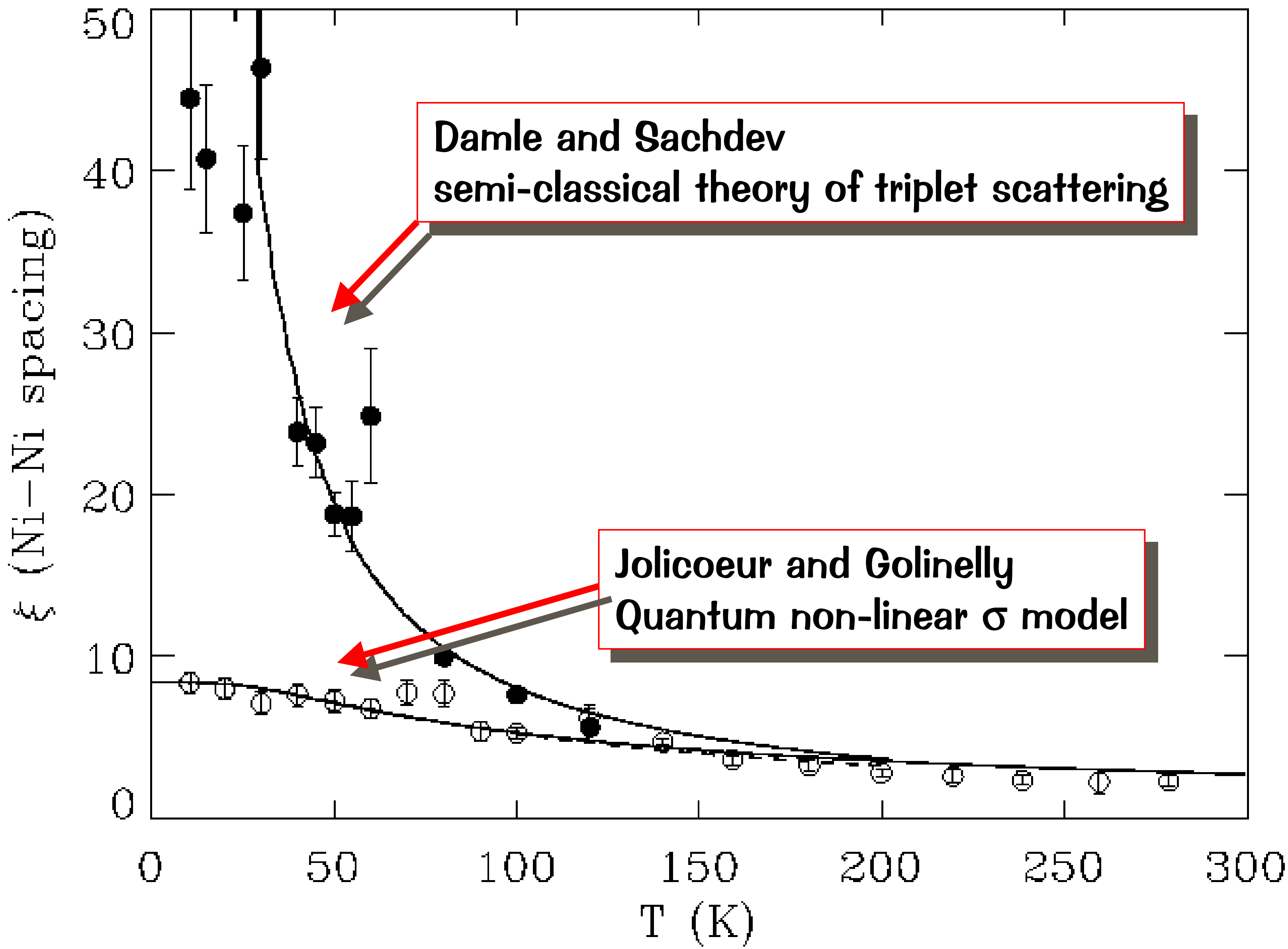
Coherent triplet propagation

Mix in thermally excited triplets



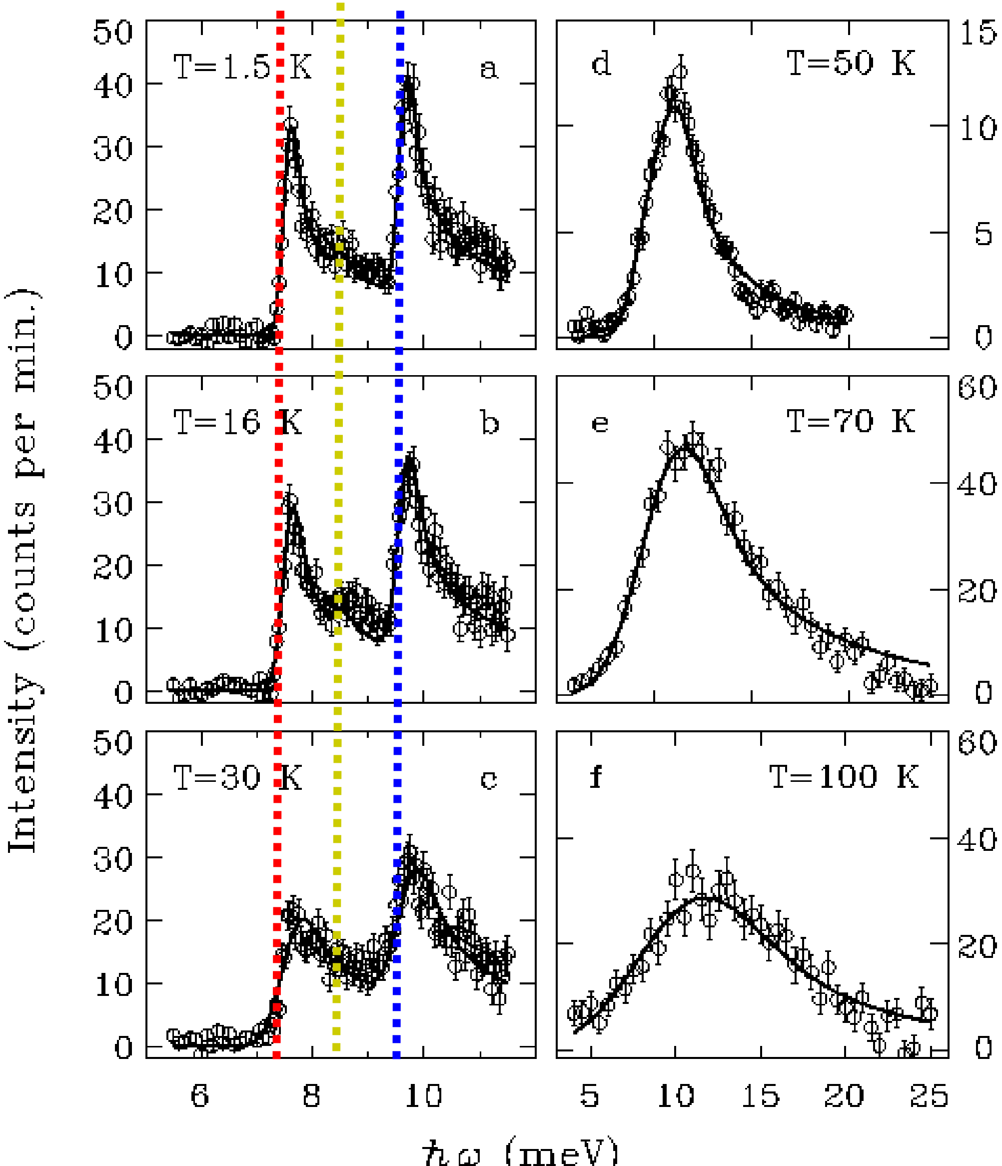
Coherence length approaches Correlation length for $T \approx \Delta / k_B$

Coherence and correlation lengths versus T



q=π Triplet creation spectrum versus T

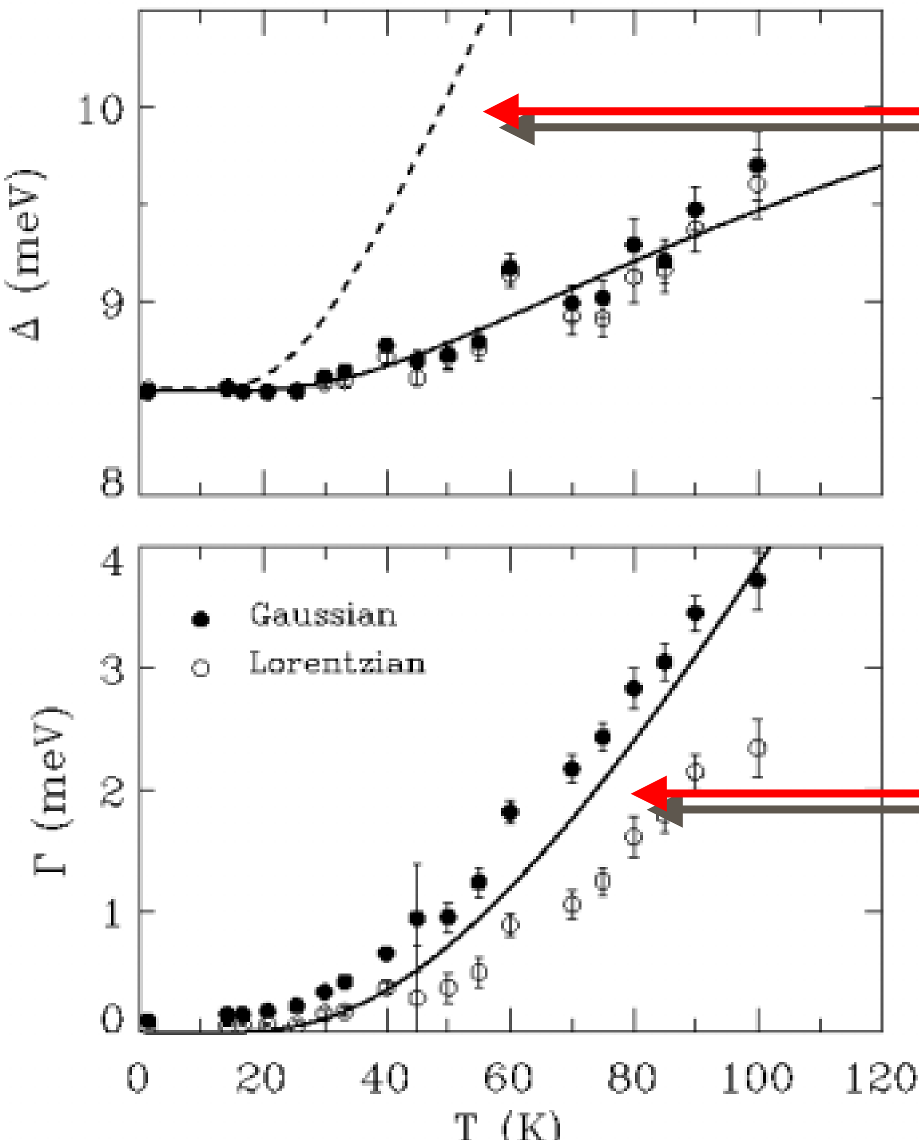
Anisotropy fine structure



Triplet relaxes due to interaction with thermal triplet ensemble

There is slight "blue shift" with increasing T

Resonance energy and relaxation rate versus T



Jolicoeur and Golinelli
Quantum non-linear σ model

Damle and Sachdev

$$\Gamma = \alpha\, \rho_{S=1}(T) \sqrt{\left\langle v^2 \right\rangle_T}$$

$$= \alpha \frac{3 k_B T}{\sqrt{\pi}} \exp\left(- \frac{\Delta}{k_B T} \right)$$

Conclusions

- Strong coupling : Alternating spin chain
  - Thermally activated triplet relaxation
  - Wave-vector dependent relaxation
  - Thermally activated band narrowing
- Weak coupling : Haldane spin-1 chain
  - Coherence length decreases with mean triplet spacing
  - σ model accounts for T-dependent equal-t correlation length
  - Triplet relaxation due to semi classical triplet scattering
  - σ-model over estimates thermally activated blue shift
- Notable strong/weak coupling differences
  - Different power-law pre-factor to T-dependent relaxation rate
  - Theory not yet in place for strong coupling case