Solving Impurity Structures Using Inelastic Neutron Scattering

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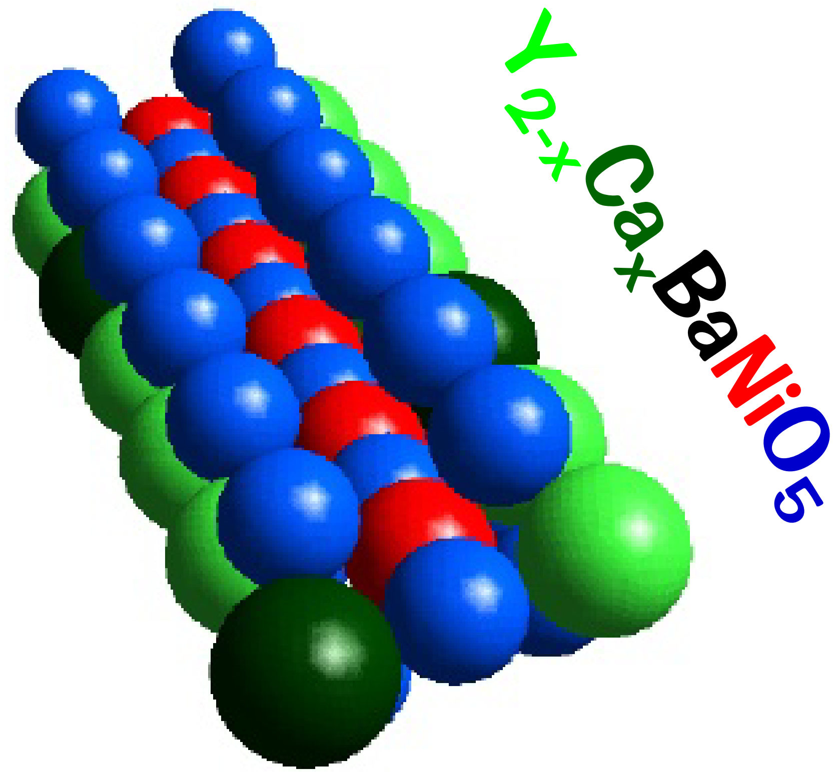
- Quantum Magnetism
  - Pure systems
  - vacancies
  - bond impurities
- Conclusions



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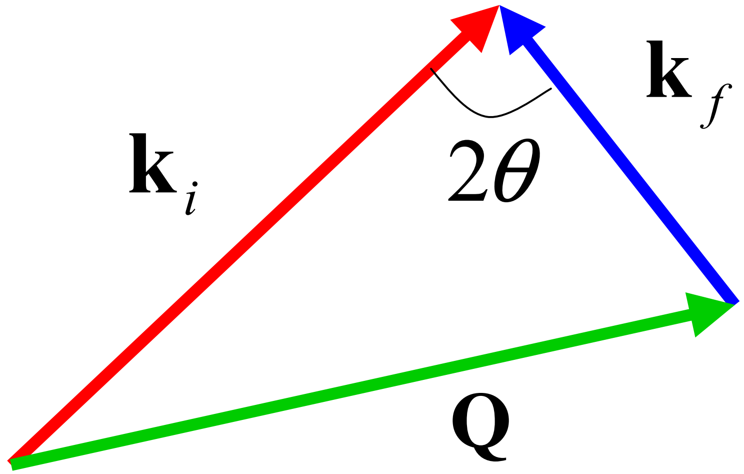
Inelastic Neutron Scattering



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

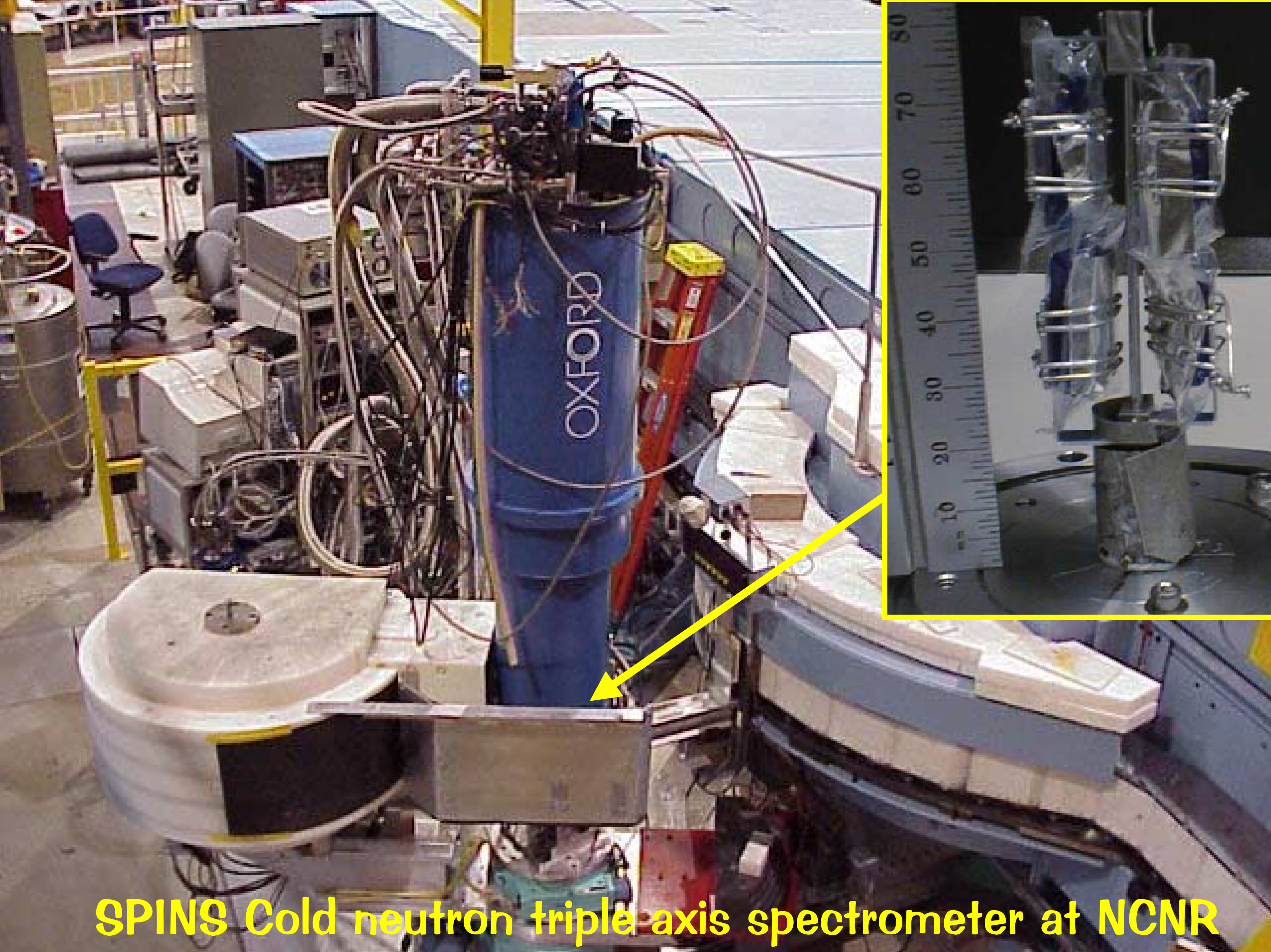
$$\hbar\omega = E_i - E_f$$

Nuclear scattering

$$S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t}\, \frac{1}{N}\left\langle \rho_{\mathbf{Q}}(0)\rho_{-\mathbf{Q}}(t)\right\rangle$$

Magnetic scattering

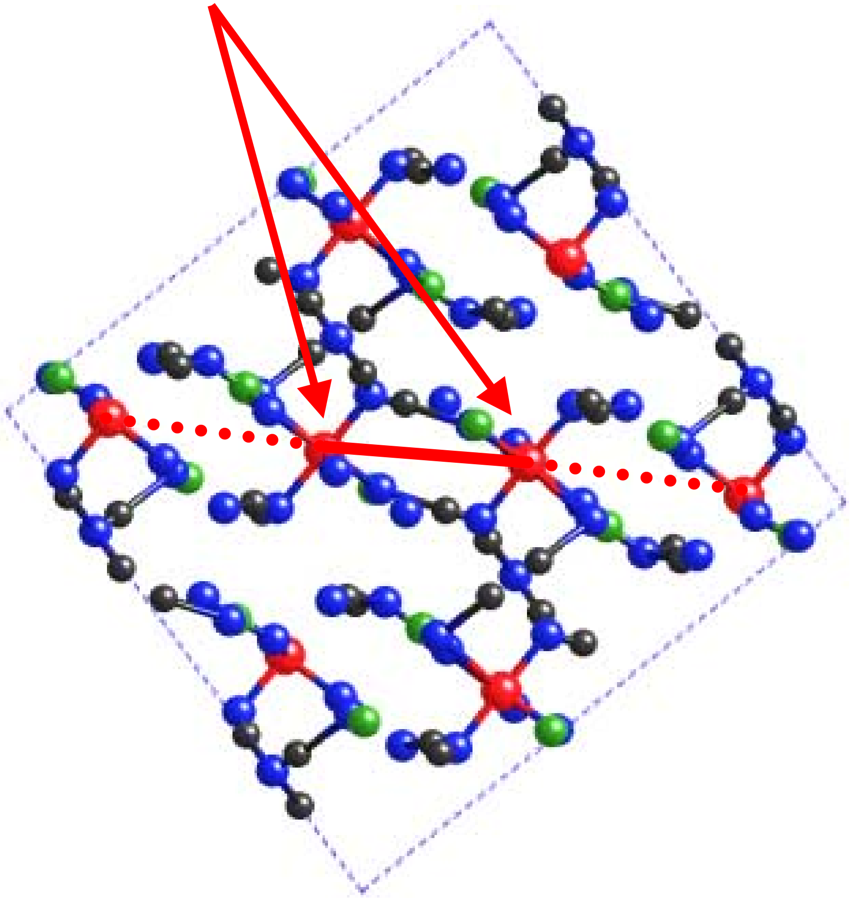
$$S^{\alpha\beta}(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t}\, \frac{1}{N}\sum_{\mathbf{RR'}} e^{i\mathbf{Q}\cdot(\mathbf{R}-\mathbf{R'})} < S^{\alpha}_{\mathbf{R}}(0) S^{\beta}_{\mathbf{R'}}(t) >$$

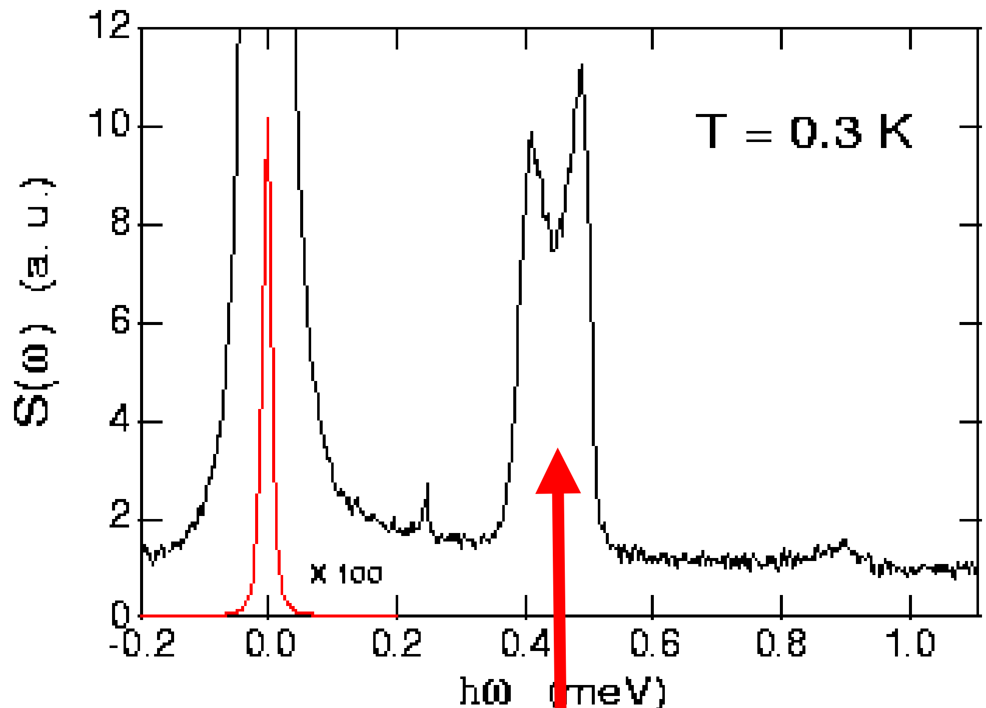


SPINS Cold neutron triple axis spectrometer at NCNR

Simple example of "Quantum" magnet

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

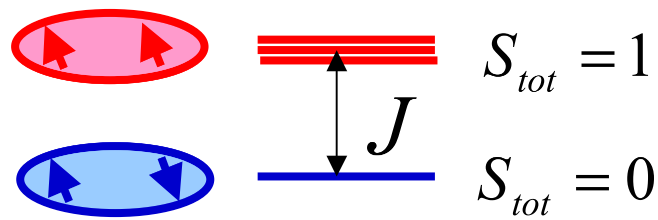




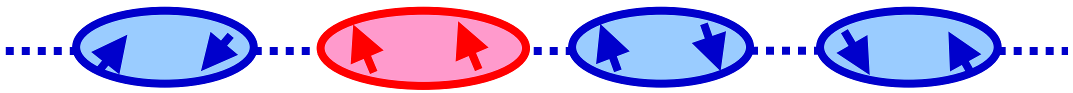
Only Inelastic magnetic scattering

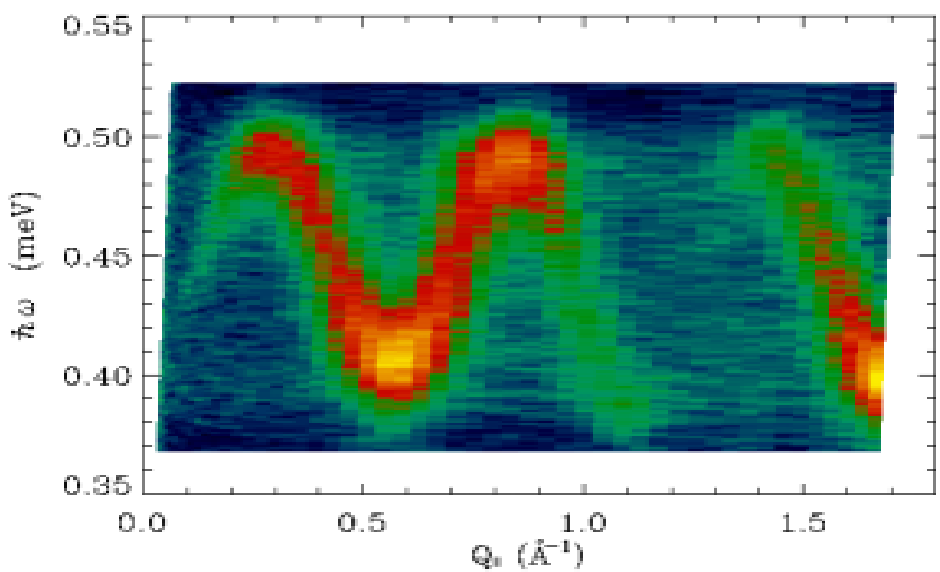
Why dimerized chain is a spin liquid

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



- inter-dimer coupling allows triplet propagation as can be seen from the dispersion of the singlet triplet transition



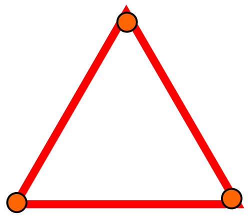


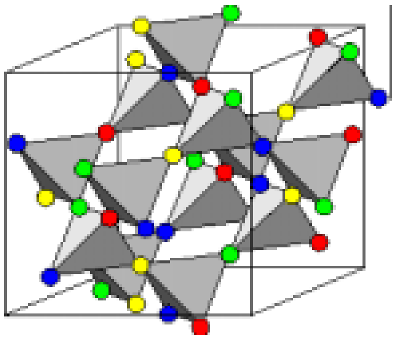
Types of Quantum magnets

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

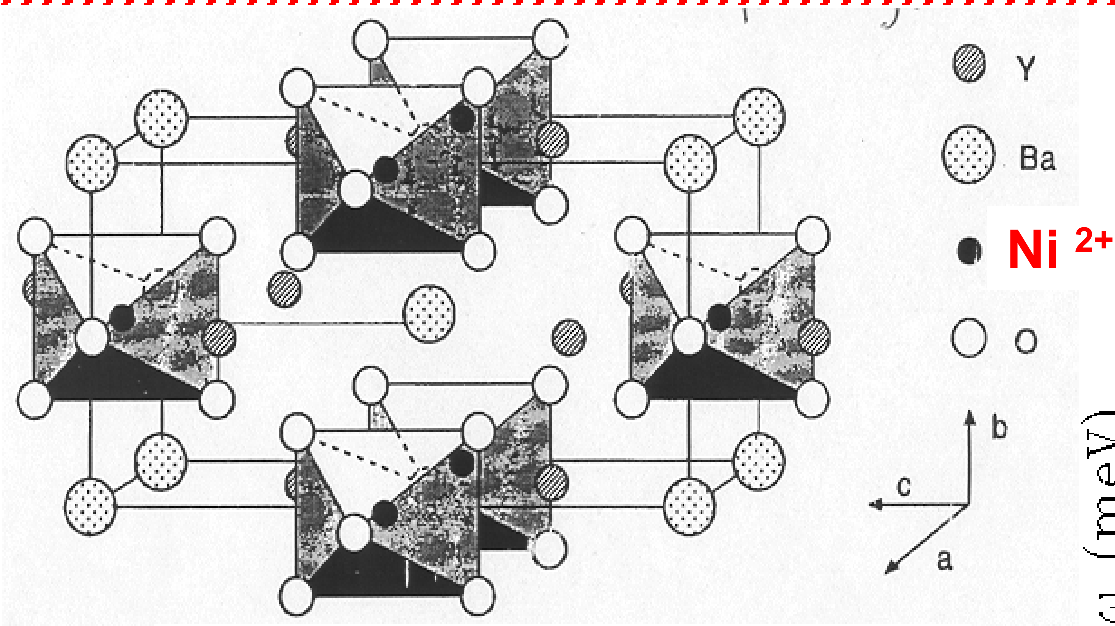
$$\left|\langle \mathbf{S} \rangle\right| << S \quad \text{for} \ \ k_B T << J$$

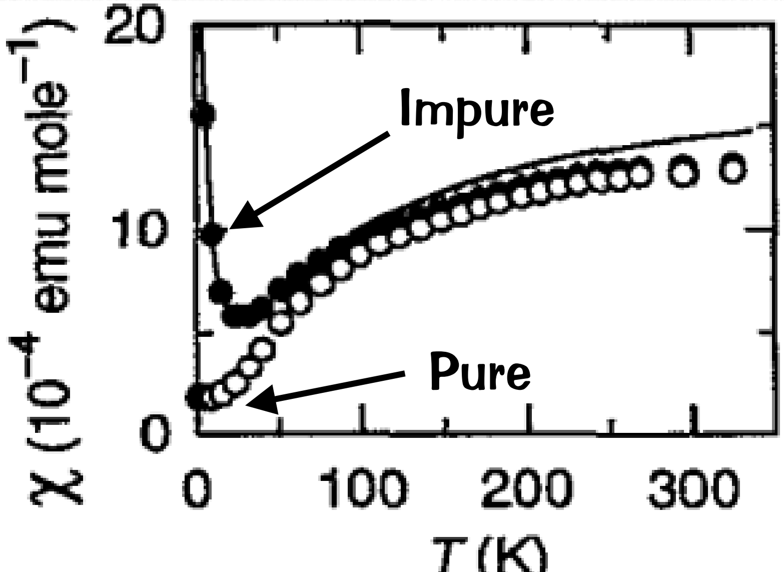
- Conditions that yield quantum magnetism
  - Low effective dimensionality
  - Low spin quantum number
  - geometrical frustration
  - dimerization
  - weak connectivity
  - interactions with fermions
- Novel coherent states
- impurities can induce magnetic polarons

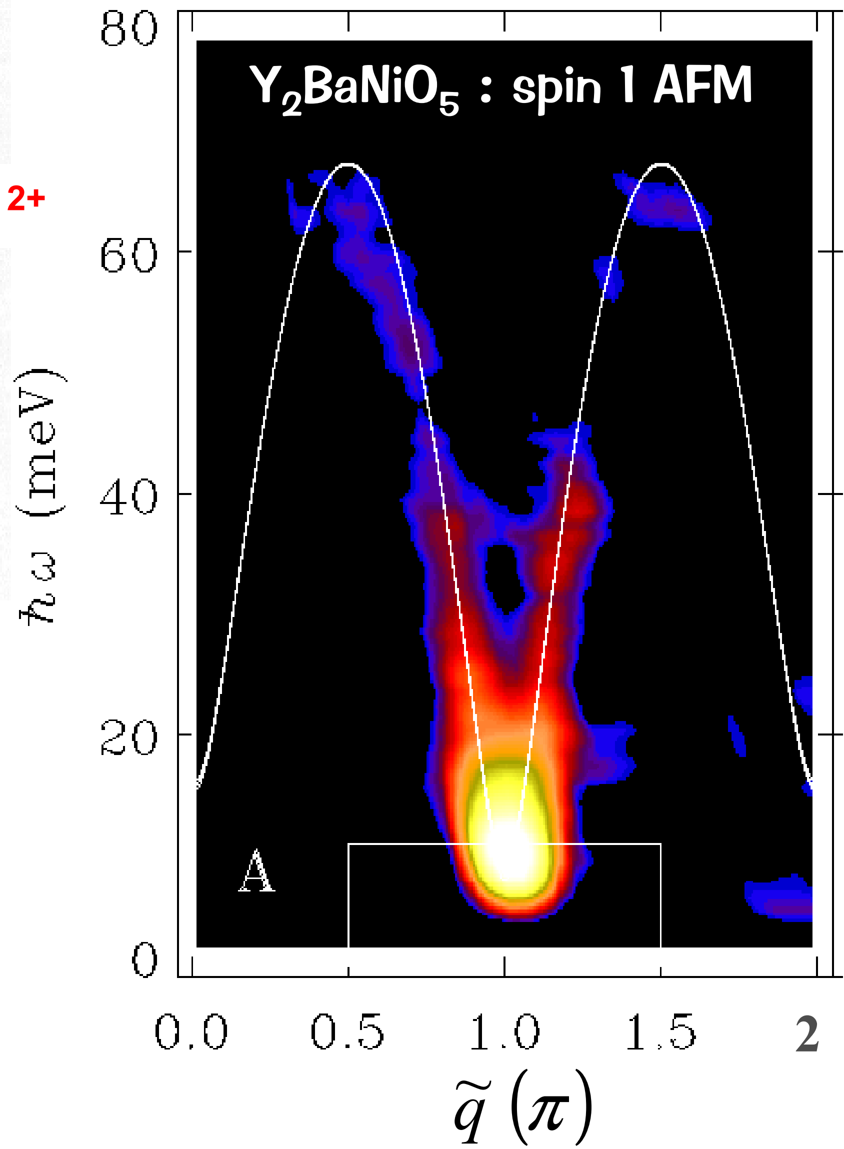




One dimensional spin-1 antiferromagnet Y_2BaNiO_5

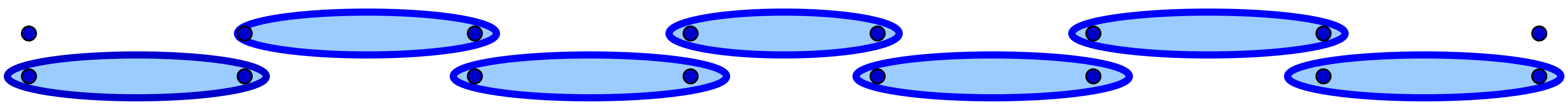






Macroscopic singlet ground state of S=1 chain

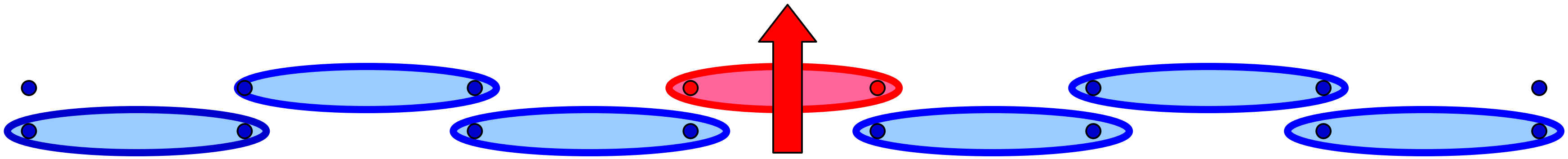
- Magnets with 2S=nz have a nearest neighbor singlet covering with full lattice symmetry.



- This is exact ground state for spin projection Hamiltonian

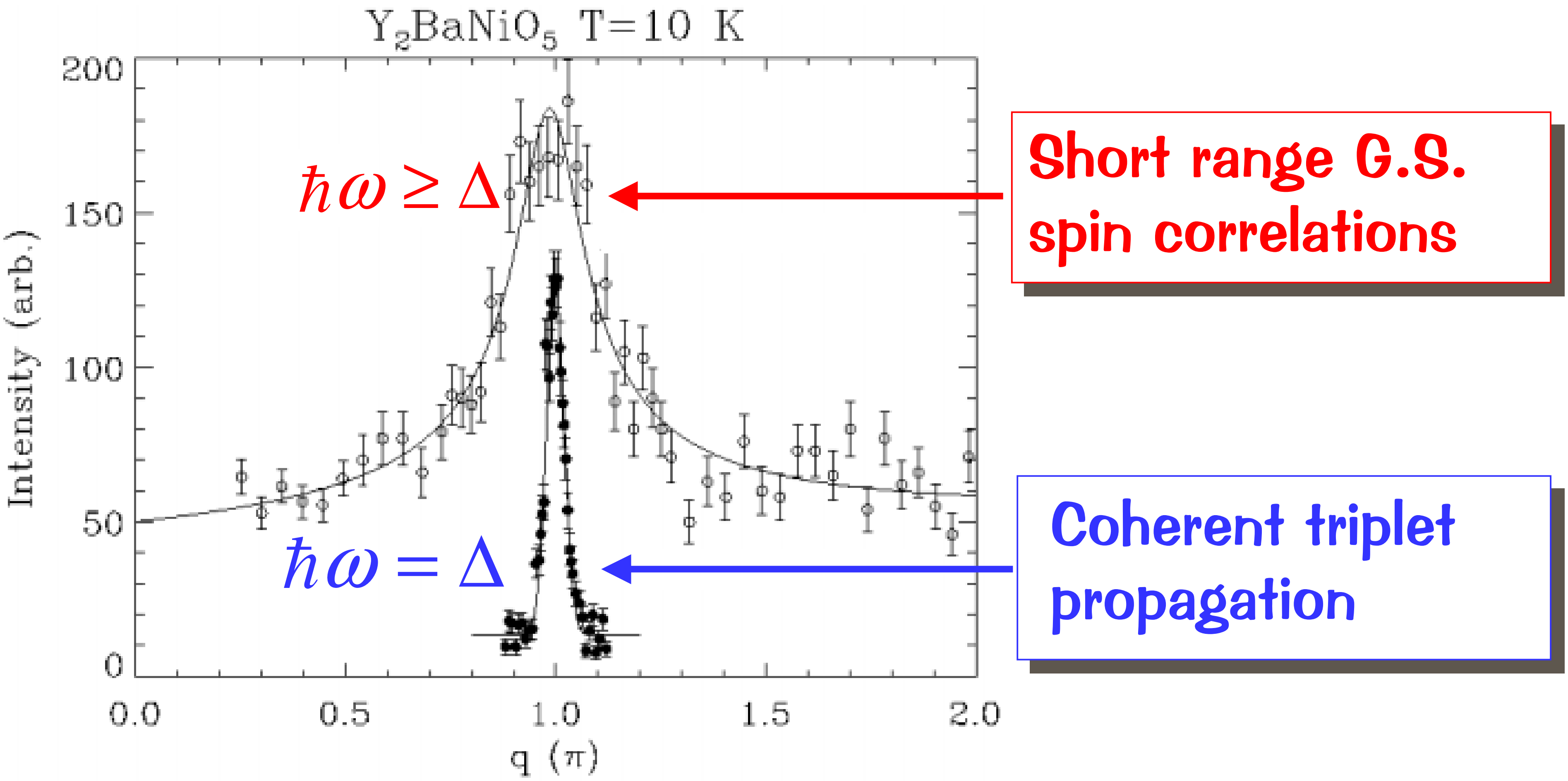
$$\mathscr{H} = \sum_i P_i\left(S_{tot} = 2\right) = \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} - \tfrac{1}{3}\left(\mathbf{S}_i \cdot \mathbf{S}_{i+1}\right)^2\right) \approx \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}$$

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



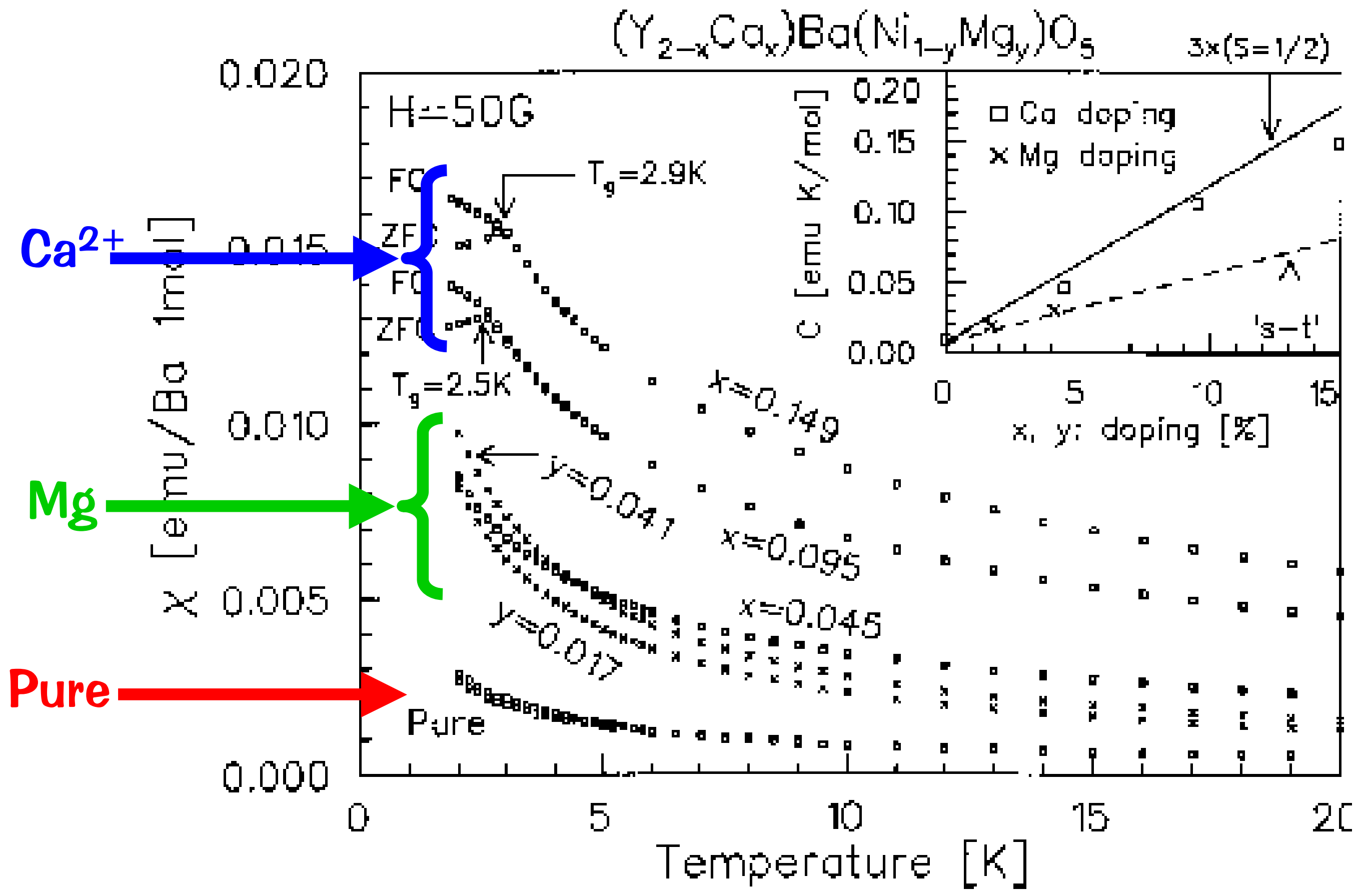
Haldane PRL 1983
Affleck, Kennedy, Lieb, and Tasaki PRL 1987

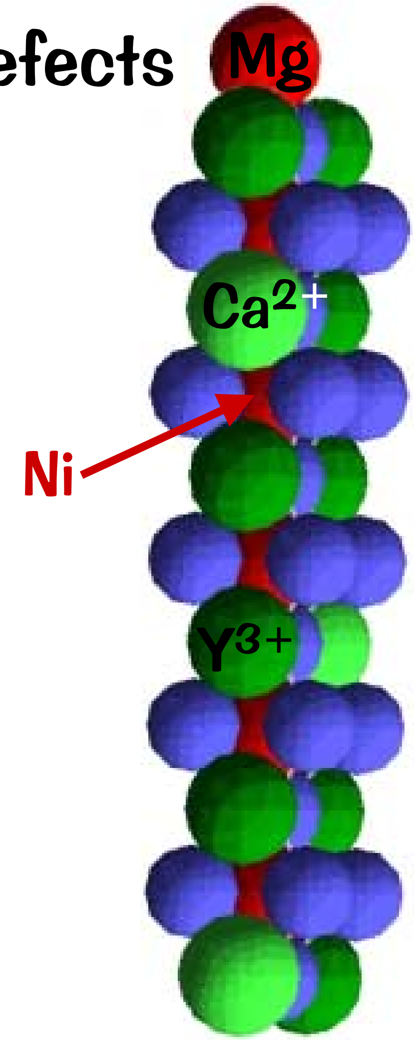
Coherence in a fluctuating system



Impurities in Y_2BaNiO_5

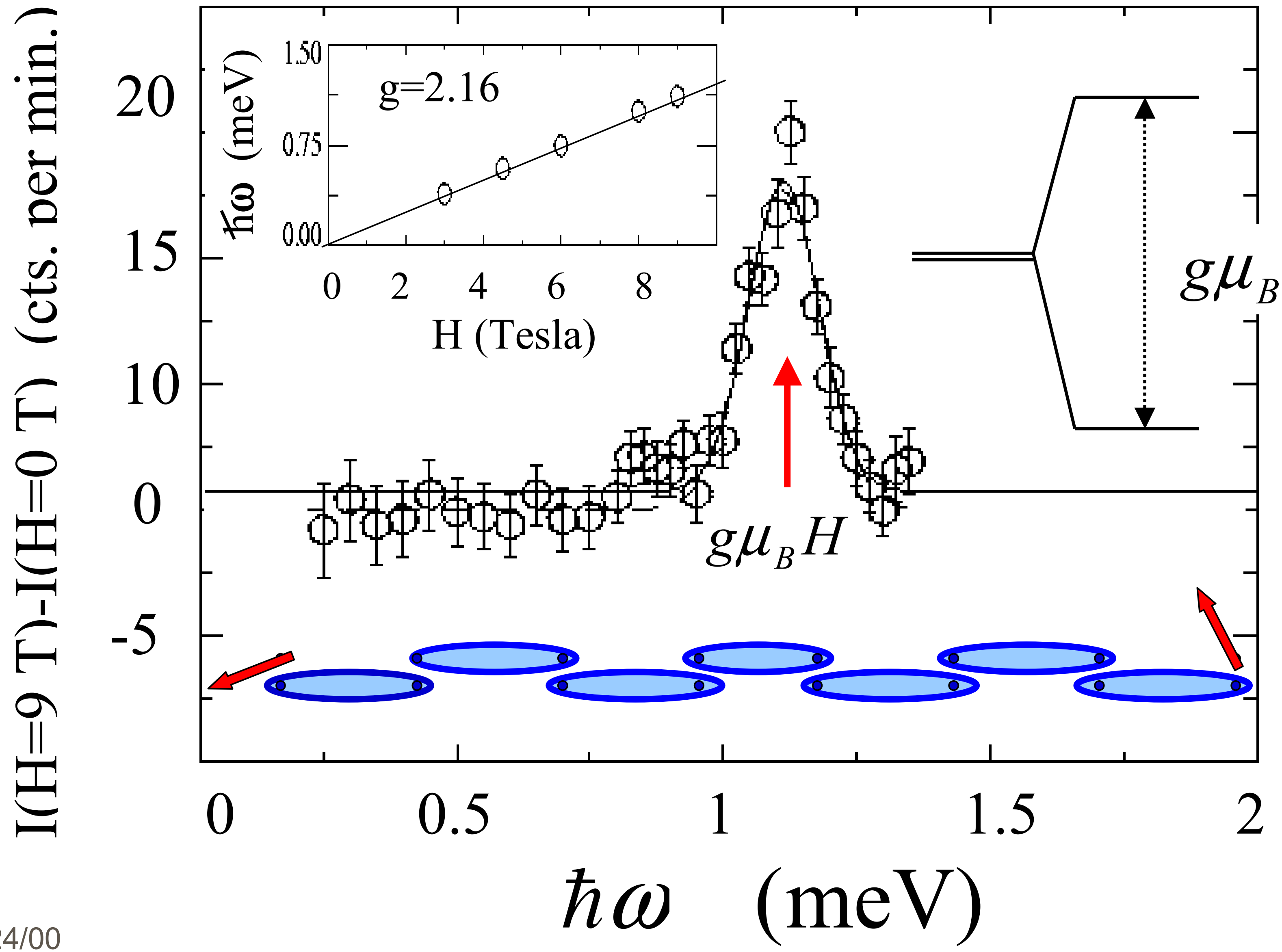
- Mg^{2+} on Ni^{2+} sites → finite length chains
- Ca^{2+} on Y^{3+} sites → mobile bond defects





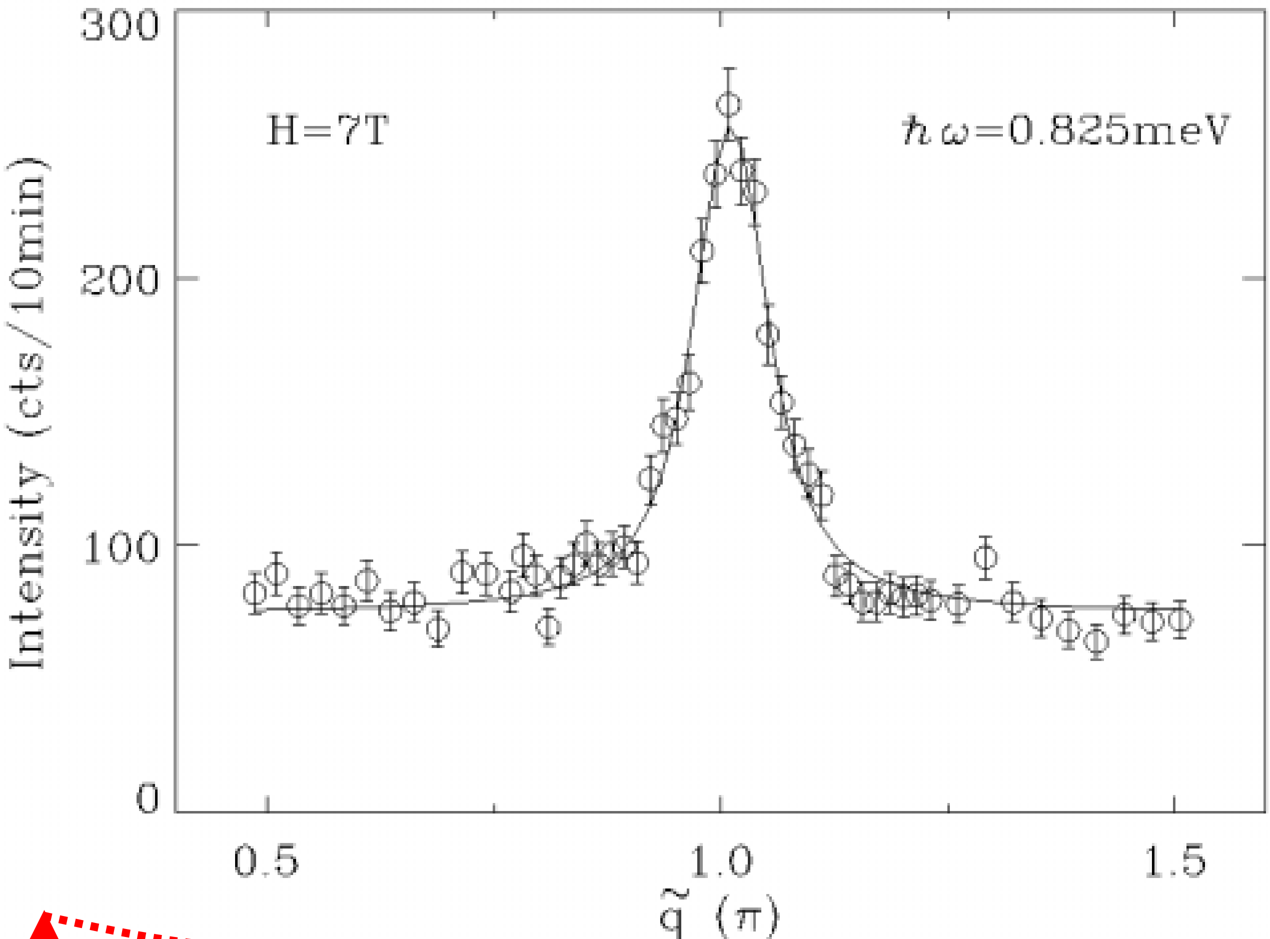
Kojima et al. (1995)

Zeeman resonance of chain-end spins



Form factor of chain-end spins

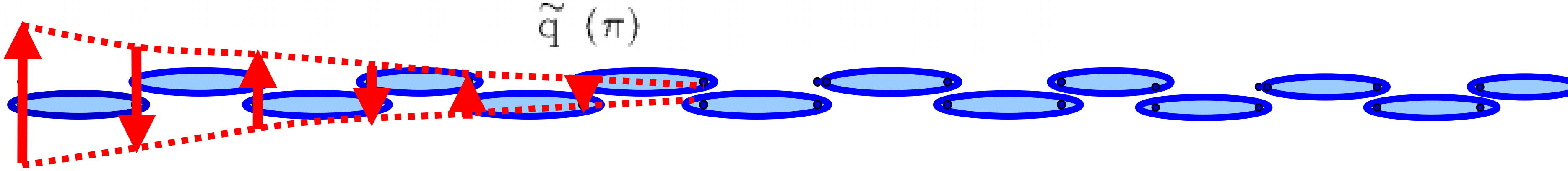
$Y_2BaNi_{1-x}Mg_xO_5$ x=4% $\hbar\omega = g\mu_B H$



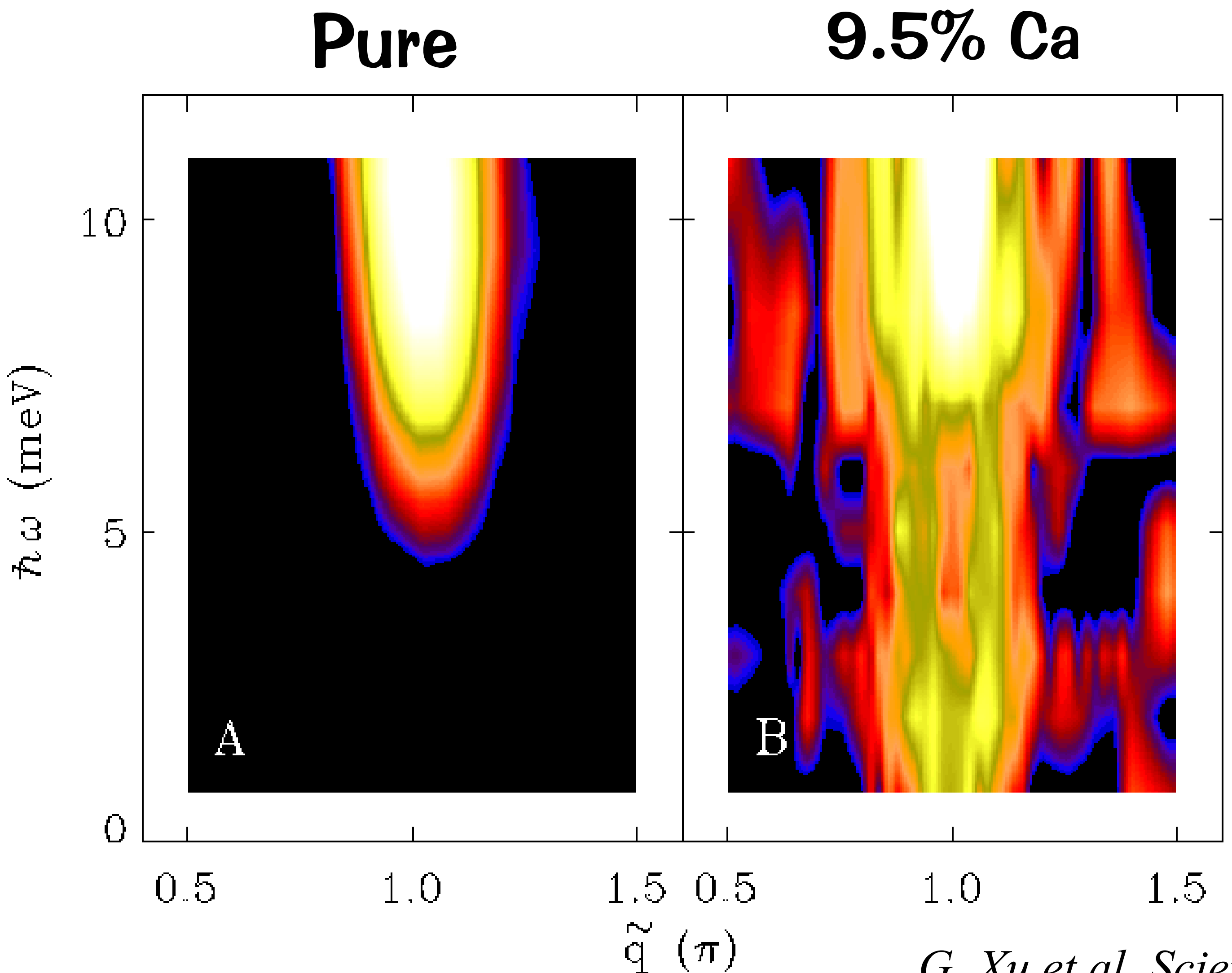
Q-dependence reveals that resonating object is AFM.

The peak resembles S(Q) for pure system.

Chain end spin carry AFM polarization cloud of length $\xi \approx 7$ Ni-Ni spacings



Sub gap excitations in Ca-doped Y_2BaNiO_5



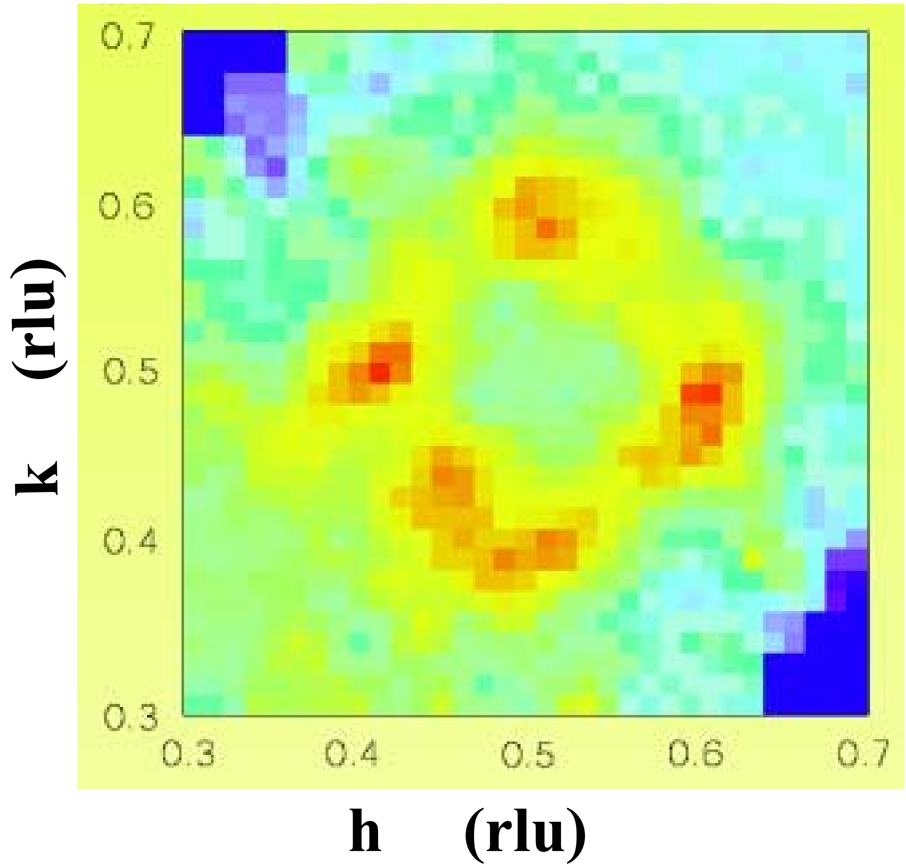
$Y_{2-x}Ca_xBaNiO_5$:

- Ca-doping creates states below the gap
- sub-gap states have doubly peaked structure factor

G. Xu et al. Science (2000)

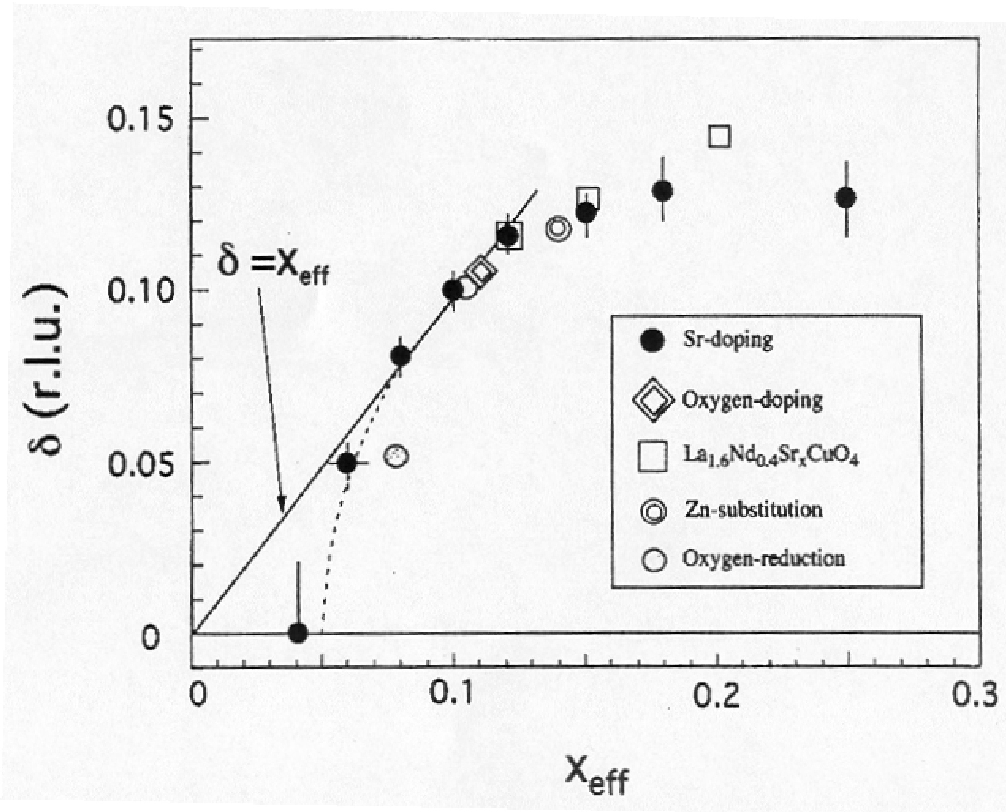
Incommensurate modulations in high T_c superconductors

$YBa_2Cu_3O_{6.6}$ T=13 K E=25 meV



Hayden et al. (1998)

$La_{2-x}Sr_xCuO_4$



Yamada et al. (1998)

Origin of incommensurate peaks in doped systems

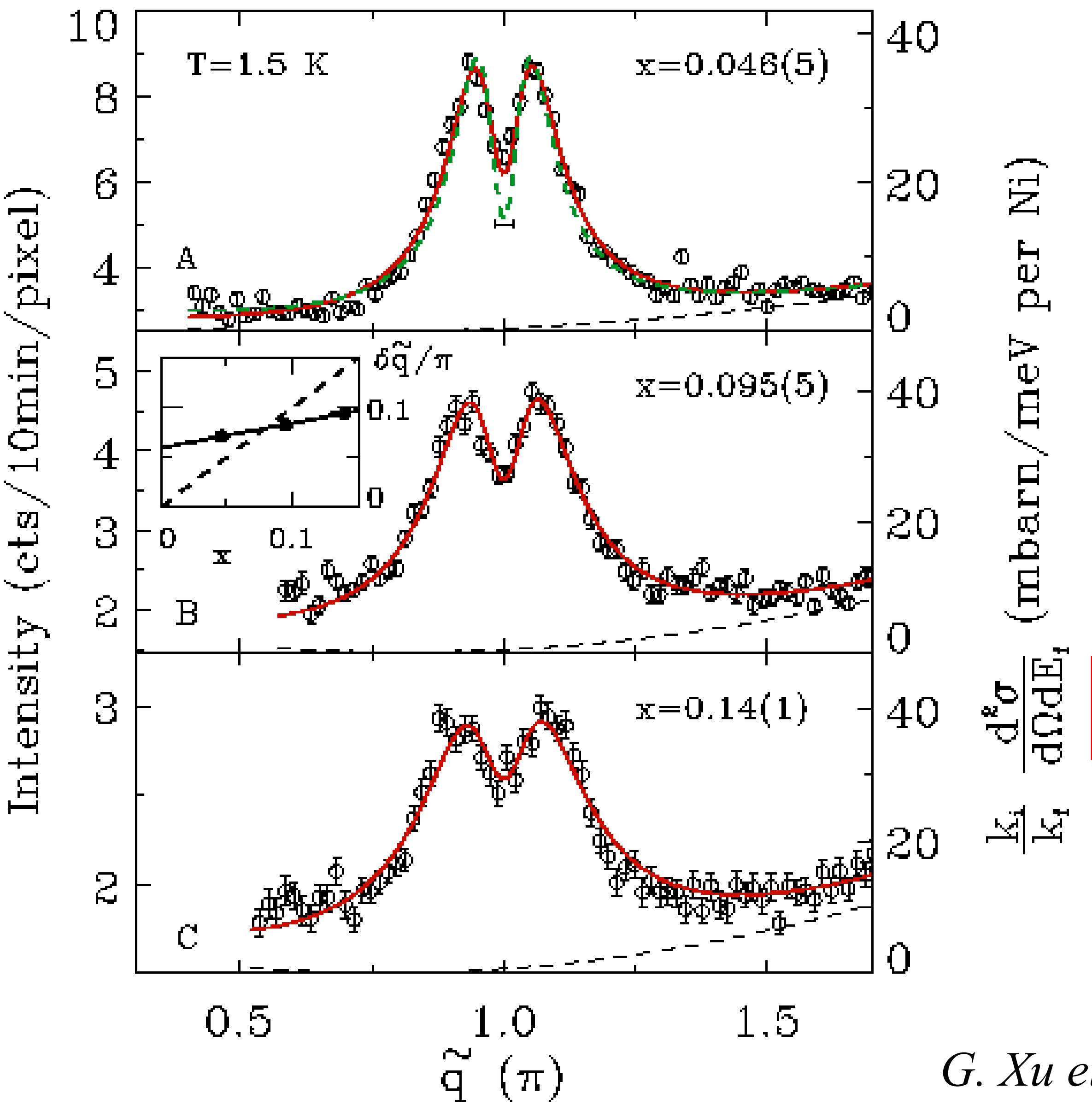
$\delta q \propto x$

- Charge ordering yields incommensurate spin order
- Quasi-particle Quasi-hole pair excitations in Luttinger liquid

δq indep. of x

- Single impurity effect

Does δq vary with calcium concentration?

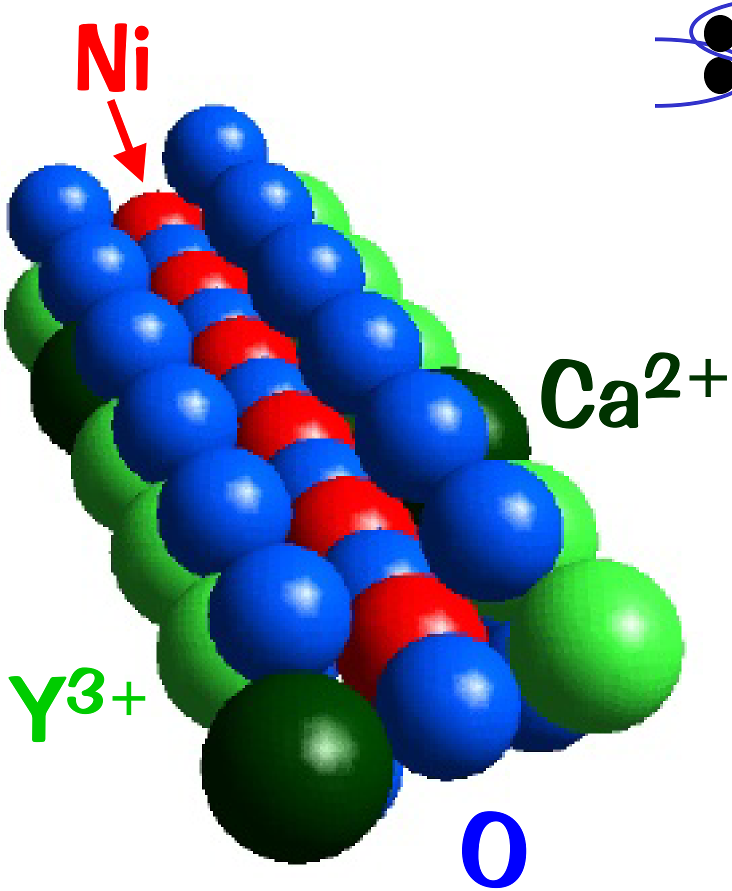


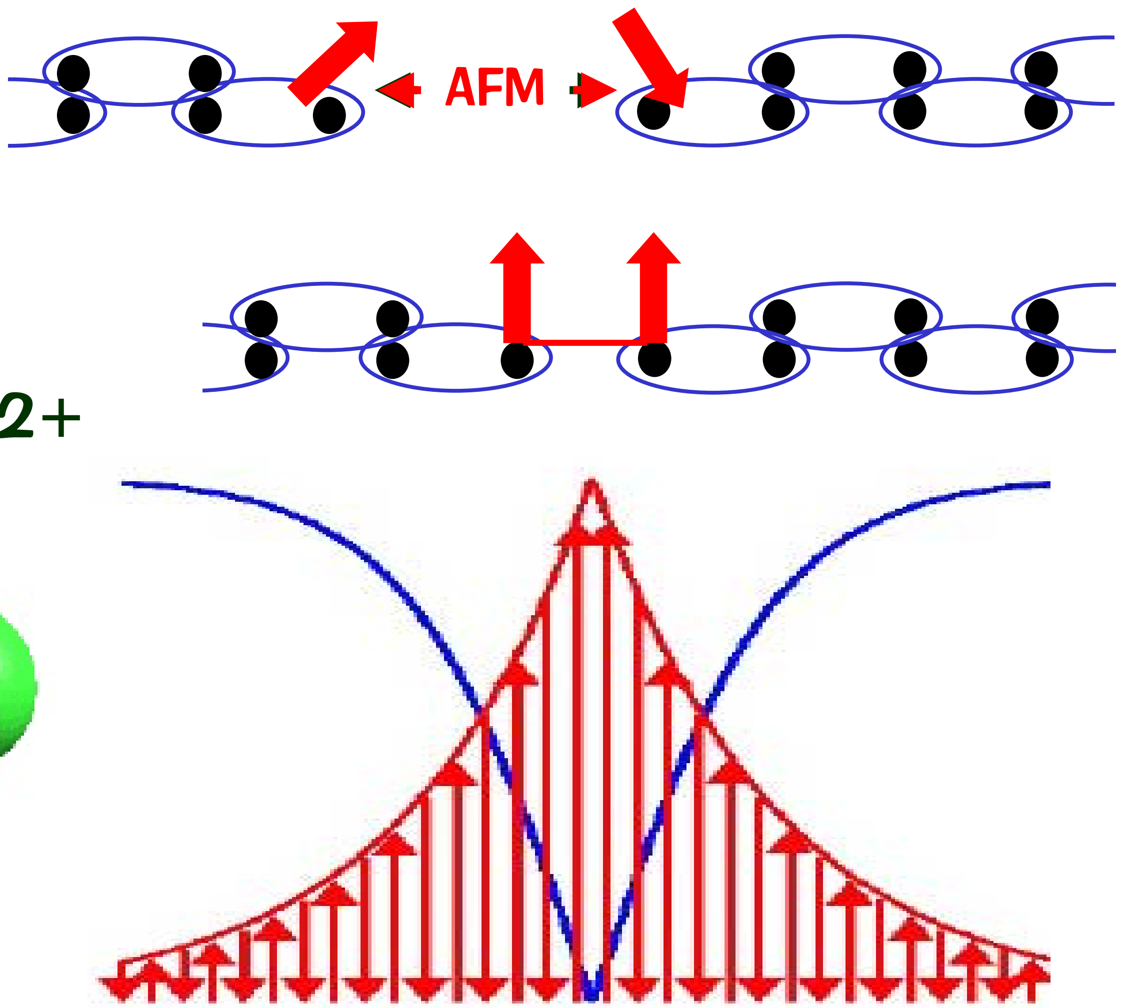
δq not strongly dependent on x

single impurity effect

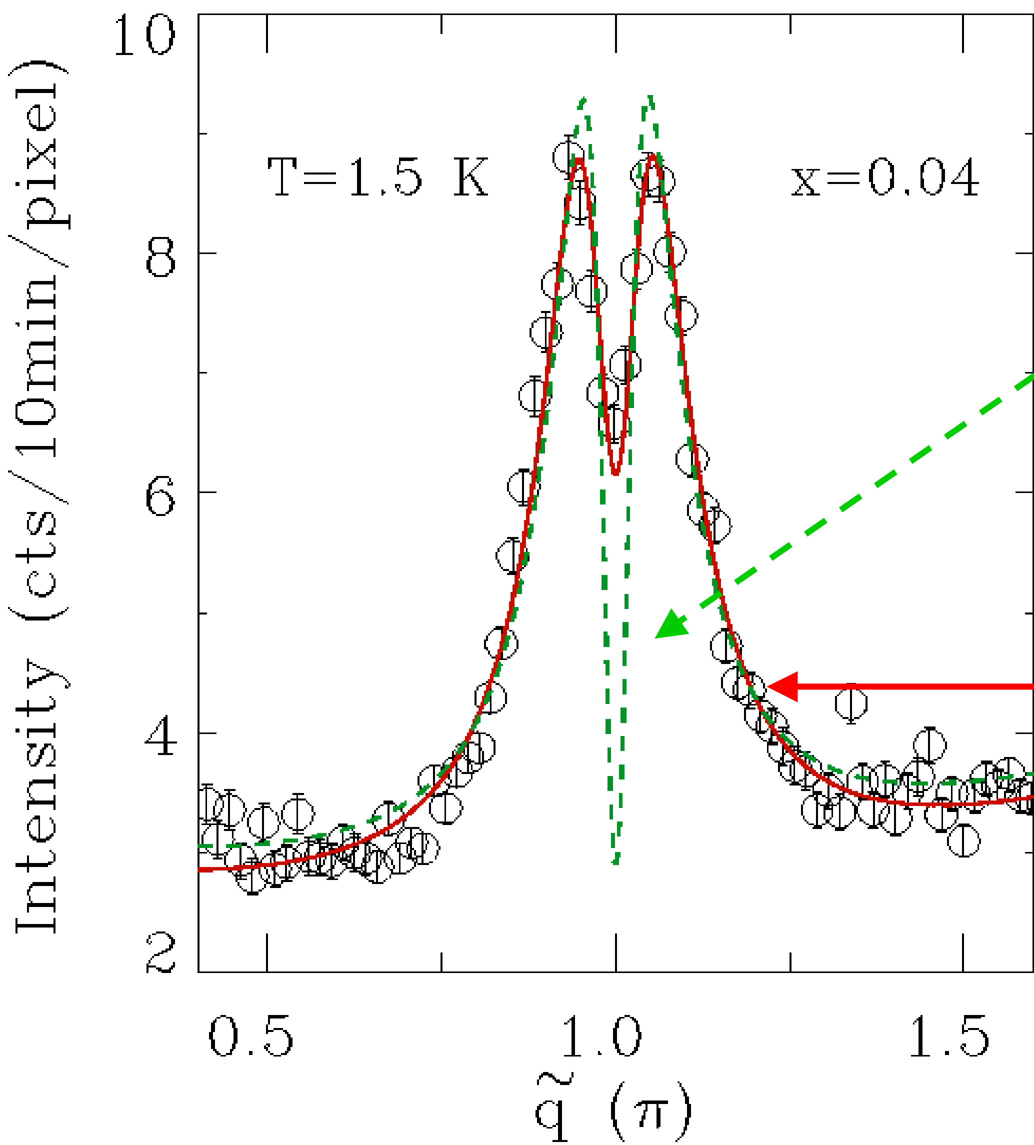
G. Xu et al. Science (2000)

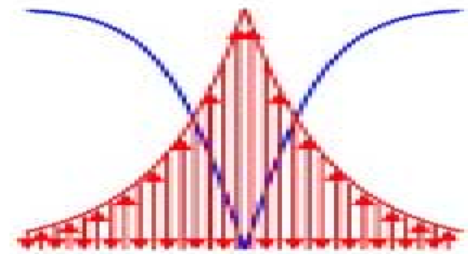
Bond Impurities in a spin-1 chain: $Y_{2-x}Ca_xBaNiO_5$





Form-factor for FM-coupled chain-end spins



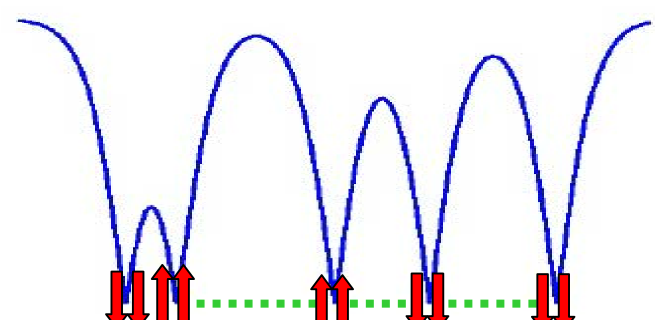


A symmetric AFM droplet

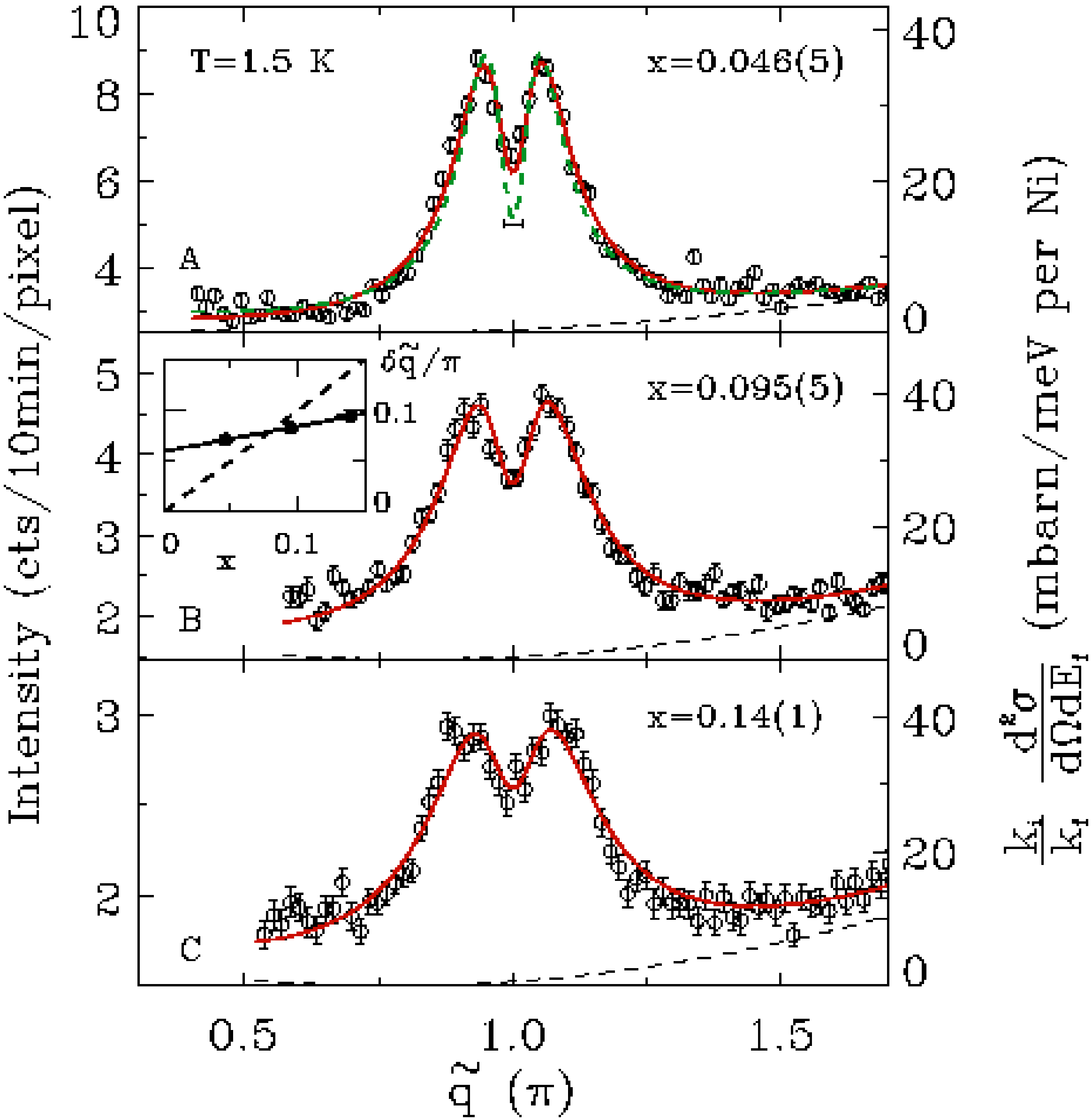
$$S(q) = 2\,\mathrm{Re}\left\{ M_{\infty}(q) e^{iq/2} \right\}$$

Ensemble of independent randomly truncated AFM droplets

$$S(q) = \sum_{ll'} P_{ll'} \left| M_l(q) e^{iq/2} + M_{l'}^{*}(q) e^{-iq/2} \right|^2$$



Consistent description for all concentrations



Parameters:

- background
- amplitude
- droplet size 7.6(5)

G. Xu et al. Science (2000)

Conclusions

- **Quantum Magnets**
  - low dimensional frustrated and/or weakly connected
  - Coherent low T states rather than magnetic order
  - Challenging to describe because fluctuations are essential
- **Impurities in spin-1 chain**
  - They create sup-gap composite spin degrees of freedom
  - Edge states have extended AFM wave function
  - Holes create AFM spin polaron with phase shift π
- **Probing impurities with neutrons**
  - Spectroscopic separation yields unique sensitivity to impurity structures (in quantum magnets) through coherent diffuse inelastic neutron scattering