Excitations in an alternating spin-1/2 chain

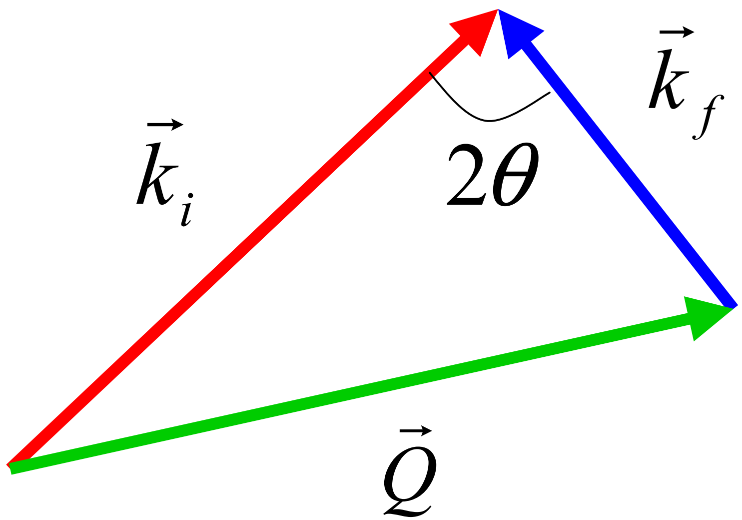
Collin Broholm
Johns Hopkins University and NIST

- Why study an alternating spin chain?
- Excitations for T=0
  - Propagating triplet mode
  - Triplet pair excitations
- Excitations for T>0
  - Damping and band narrowing
- Conclusions

Collaborators

Guangyong Xu	Johns Hopkins University
Daniel H. Reich	Johns Hopkins University
Collin Broholm	Johns Hopkins University
Mark Adams	ISIS facility, RAL

Magnetic Neutron Scattering



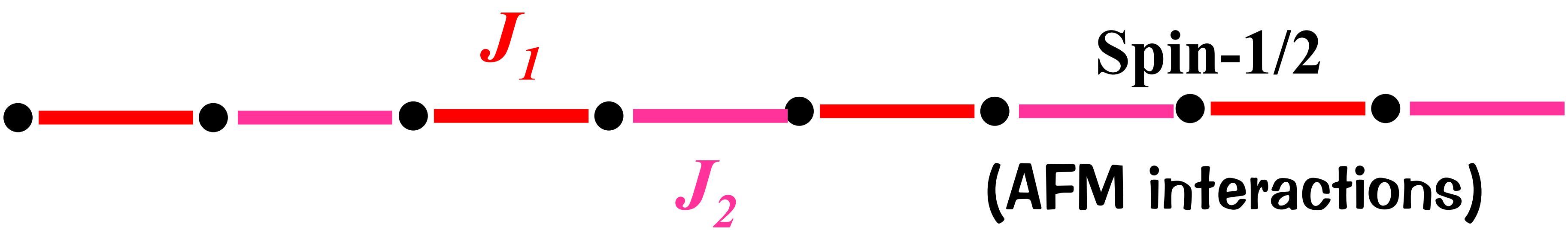
$$\vec{Q} = \vec{k}_i - \vec{k}_f$$

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

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

$$\mathrm{S}^{\alpha\beta}(\vec{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t}\, \frac{1}{N}\sum_{\vec{R}\vec{R}'} e^{i\vec{Q}\bullet(\vec{R}-\vec{R}')} \langle \mathrm{S}^{\alpha}_{\vec{\mathrm{R}}}(t)\,\mathrm{S}^{\beta}_{\vec{R}'}(0) \rangle$$

Alternating spin-1/2 chain "interpolates" between gapfull and gapless quantum magnet



- For J_1=J_2 have gapless uniform spin-1/2 chain
- For J_1>>J_2 have independent spin-1/2 pairs with singlet-triplet transition at $\Delta=J_1$
- Experimental questions:
  - When and how does continuum develop from resonant gapfull spectrum?
  - What are finite T properties of magnet with $\Delta \approx J$

Sum-rules
-and the Single Mode Approximation (SMA)

$$\hbar \int d\omega\, S(\vec{q},\omega) = \frac{1}{N} \sum_{\vec{d}\vec{d}'} < \mathrm{S}_{\vec{d}} \mathrm{S}_{\vec{d}'} > e^{i\vec{q}\cdot(\vec{d}-\vec{d}')} \equiv S(\vec{q})$$

$$\hbar^2 \int \omega \; d\omega\, S(\vec{q},\omega) = -\frac{2}{3}\frac{1}{N} \sum_{\vec{d}\vec{d}} J_{\vec{d}\vec{d}} < \vec{\mathrm{S}}_{\vec{d}} \cdot \vec{\mathrm{S}}_{\vec{d}'} > \left(1 - \cos \vec{q}\cdot\left(\vec{d} - \vec{d}'\right)\right)$$

When a coherent mode dominates the spectrum:

$$S(\vec{q},\omega) \approx S(\vec{q})\,\delta\left(\hbar\omega - \varepsilon(\vec{q})\right)$$

Then sum-rules link S(q) and ε(q)

$$S(\vec{q}) \approx \frac{\hbar^2 \int \omega \; d\omega\, S(\vec{q},\omega)}{\varepsilon(\vec{q})} = -\frac{2}{3}\frac{\frac{1}{N} \sum_{\vec{d}\vec{d}} J_{\vec{d}\vec{d}} < \vec{\mathrm{S}}_{\vec{d}} \cdot \vec{\mathrm{S}}_{\vec{d}'} > \left(1 - \cos \vec{q}\cdot\left(\vec{d} - \vec{d}'\right)\right)}{\varepsilon(\vec{q})}$$

Parameters extracted from low temperature data

- Parameters in a variational dispersion relation

$$\varepsilon(\vec{q}) = J_1 - \frac{1}{2}\sum_{\vec{u}} J_{\vec{u}} \cos \vec{q}\cdot\vec{u}$$

$J_1 = 0.442(2)\,\mathrm{meV}$	-intra dimer exchange
$J_2 = 0.102(2)\,\mathrm{meV}$	-in chain inter dimer exchange
$J_L = 0.012(2)\,\mathrm{meV}$	-out of chain inter-dimer exchange #1
$J_R = 0.018(2)\,\mathrm{meV}$	-out of chain inter-dimer exchange #2

- Equal time intra- and inter-dimer correlations:

$$\left\langle \vec{S}_0 \vec{S}_{\vec{d}_1} \right\rangle_{\mathrm{int}\,er} \Big/ \left\langle \vec{S}_0 \cdot \vec{S}_{\vec{d}_0} \right\rangle_{\mathrm{int}\,ra} = 0.04(8)$$

- Relative strength of incoherent double scattering process

Parameters extracted from finite temperature data

- Strength of intra-dimer correlations

$$\left\langle \vec{S}_0 \cdot \vec{S}_{\vec{d}_0} \right\rangle_T$$

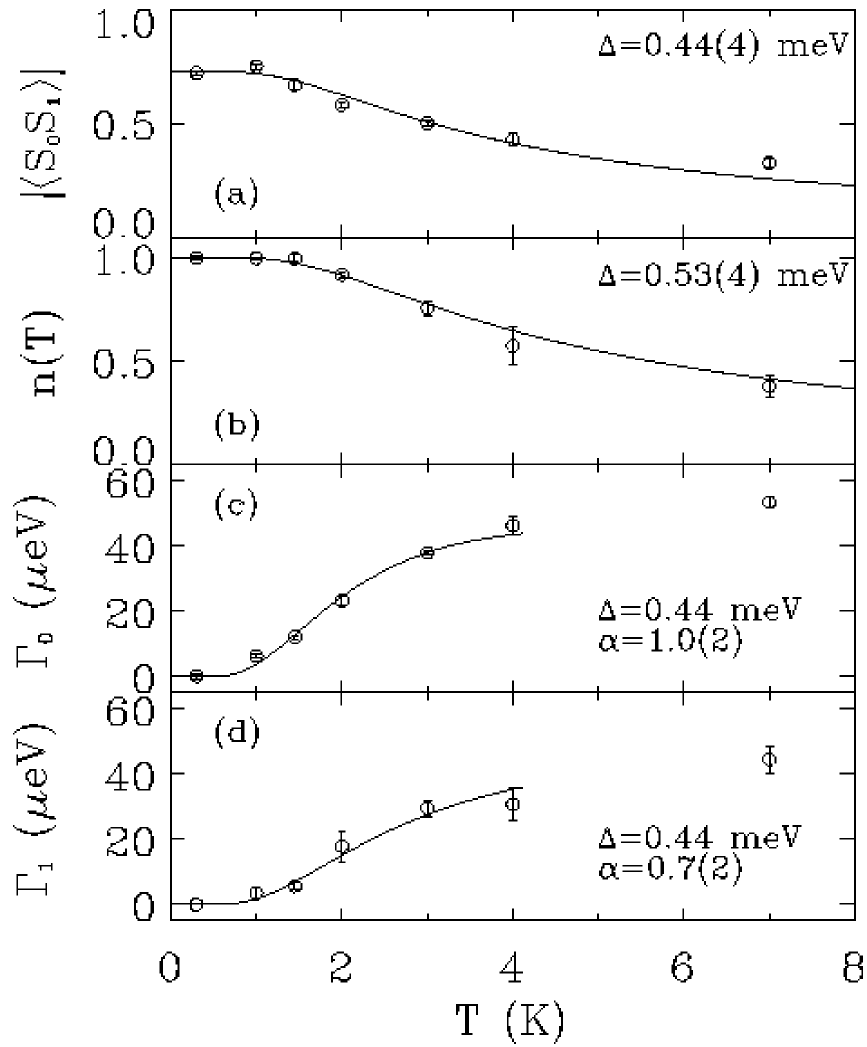
- Overall renormalization parameter $n(T)$ for inter-dimer terms in variational dispersion relation:

$$\varepsilon(\vec{q}) = J_1 - n(T) \cdot \tfrac{1}{2} \sum_{\vec{u}} J_{\vec{u}} \cos \vec{q} \cdot \vec{u}$$

- Parameters in variational q-dependent damping

$$\Gamma(\vec{q}) = \Gamma_0(T) + \tfrac{1}{2} \Gamma_1(T) \cos \vec{q} \cdot \vec{u}_0$$

Temperature dependence of singlet-triplet mode



$$\left|\left\langle \vec{S}_0 \cdot \vec{S}_{\vec{d}_0} \right\rangle\right|_T \propto \tanh \beta\Delta/2$$

$$n(T) = \tanh \beta\Delta/2$$

$$\Gamma_0(T) \propto \frac{1}{T^\alpha} \exp(-J_1/k_B T)$$

$$\Gamma_1(T) \propto \frac{1}{T^\alpha} \exp(-J_1/k_B T)$$

Conclusions about the magnetism of copper nitrate

- Zero temperature excitation spectrum
  - Coherent triplet mode whose contribution to $S(Q,\omega)$ is accounted for by the single mode approximation
  - Weak triplet pair band separated from the coherent triplet mode
- Finite temperature excitation spectrum
  - T-dependence of intensity accounted for by independent spin-pair model.
  - Damping and band-narrowing develop with activated temperature dependence

End Notes

- There does not appear to be a theory which can account for magnetism in the limit relevant for copper nitrate:

$$k_B T \approx \Delta \approx J$$

- With the advent of high power spallation neutron sources complete mapping of $S(Q,\omega,T)$ is now possible. Especially for low Dimensional magnetic dielectrics.