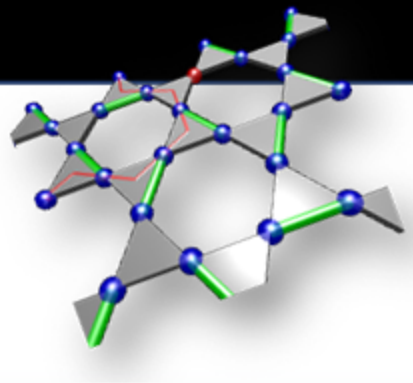


INSTITUTE FOR **QUANTUM MATTER**

A collaboration between
JOHNS HOPKINS UNIVERSITY
and PRINCETON UNIVERSITY

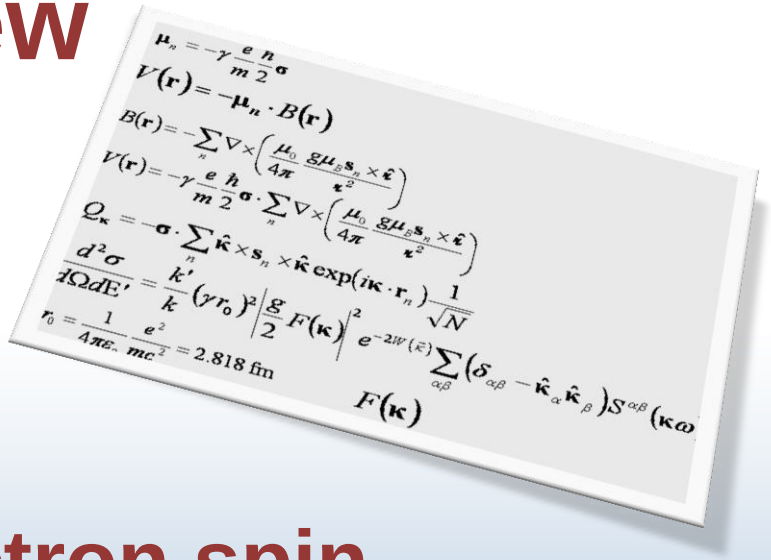
Magnetic Neutron Scattering

Collin Broholm

JOHNS HOPKINS
KRIEGER SCHOOL
of ARTS & SCIENCES

*Supported by U.S. DoE, Basic Energy Sciences,
Materials Sciences & Engineering DE-FG02-08ER46544

Overview



$$\boldsymbol{\mu}_n = -\gamma \frac{e}{m}\frac{\hbar}{2}\boldsymbol{\sigma}$$

$$V(\mathbf{r}) = -\boldsymbol{\mu}_n \cdot B(\mathbf{r})$$

$$B(\mathbf{r}) = -\sum_n \nabla \times \left(\frac{\mu_0}{4\pi} \frac{g\mu_B \mathbf{s}_n \times \hat{\boldsymbol{\kappa}}}{\boldsymbol{\kappa}^2} \right)$$

$$V(\mathbf{r}) = -\gamma \frac{e}{m}\frac{\hbar}{2}\boldsymbol{\sigma} \cdot \sum_n \nabla \times \left(\frac{\mu_0}{4\pi} \frac{g\mu_B \mathbf{s}_n \times \hat{\boldsymbol{\kappa}}}{\boldsymbol{\kappa}^2} \right)$$

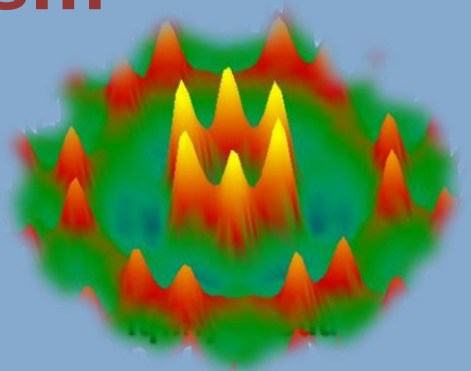
$$Q_{\boldsymbol{\kappa}} = -\boldsymbol{\sigma} \cdot \sum_n \hat{\boldsymbol{\kappa}} \times \mathbf{s}_n \times \hat{\boldsymbol{\kappa}} \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}_n) \frac{1}{\sqrt{N}}$$

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}(\gamma r_0)^2 \left| \frac{g}{2} F(\boldsymbol{\kappa}) \right|^2 e^{-2W(\vec{\kappa})} \sum_{\alpha\beta} (\delta_{\alpha\beta} - \hat{\boldsymbol{\kappa}}_\alpha \hat{\boldsymbol{\kappa}}_\beta) S^{\alpha\beta}(\boldsymbol{\kappa}\omega)$$

$$r_0 = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2} = 2.818 \text{ fm}$$

$$F(\boldsymbol{\kappa})$$

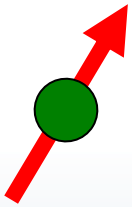
- ❖ Neutron spin meets electron spin
- ❖ Structure : Magnetic diffraction
- ❖ Excitations: Inelastic magnetic scattering
- ❖ Tomorrow : Entangled Magnetism



Magnetic properties of the neutron

The neutron has a dipole moment

$$\vec{\mu}_n = -\gamma \mu_B \frac{m_e}{m} \vec{\sigma}$$



μ_n is 960 times smaller than the electron moment

$$\frac{\mu_e}{\mu_n} = \frac{m}{m_e \gamma} = \frac{1836}{1.913} = 960$$

A dipole in a magnetic field has potential energy

$$V(\mathbf{r}) = -\vec{\mu} \cdot \mathbf{B}(\mathbf{r})$$

Correspondingly the field exerts a torque and a force

$$\vec{\tau} = \vec{\mu} \times \mathbf{B} \qquad \mathbf{F} = \nabla(\vec{\mu} \cdot \mathbf{B})$$

driving the neutron parallel to high field regions

Magnetic Neutron Optics

The combined nuclear and magnetic potential for neutron

$$V = \frac{2p\hbar^2}{m}\left(rb \pm r_0 \vec{M} \times \vec{s}\right)$$

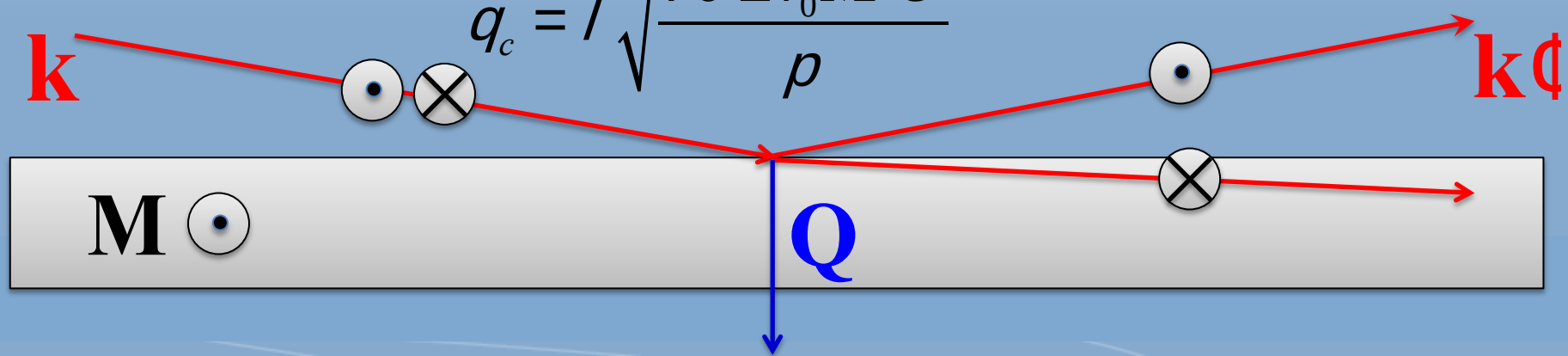
The index of refraction is

$$n = \sqrt{1 - \frac{V}{E}} = \sqrt{1 - \frac{l^2}{p}\left(rb \pm r_0 \mathbf{M} \times \vec{s}\right)}$$

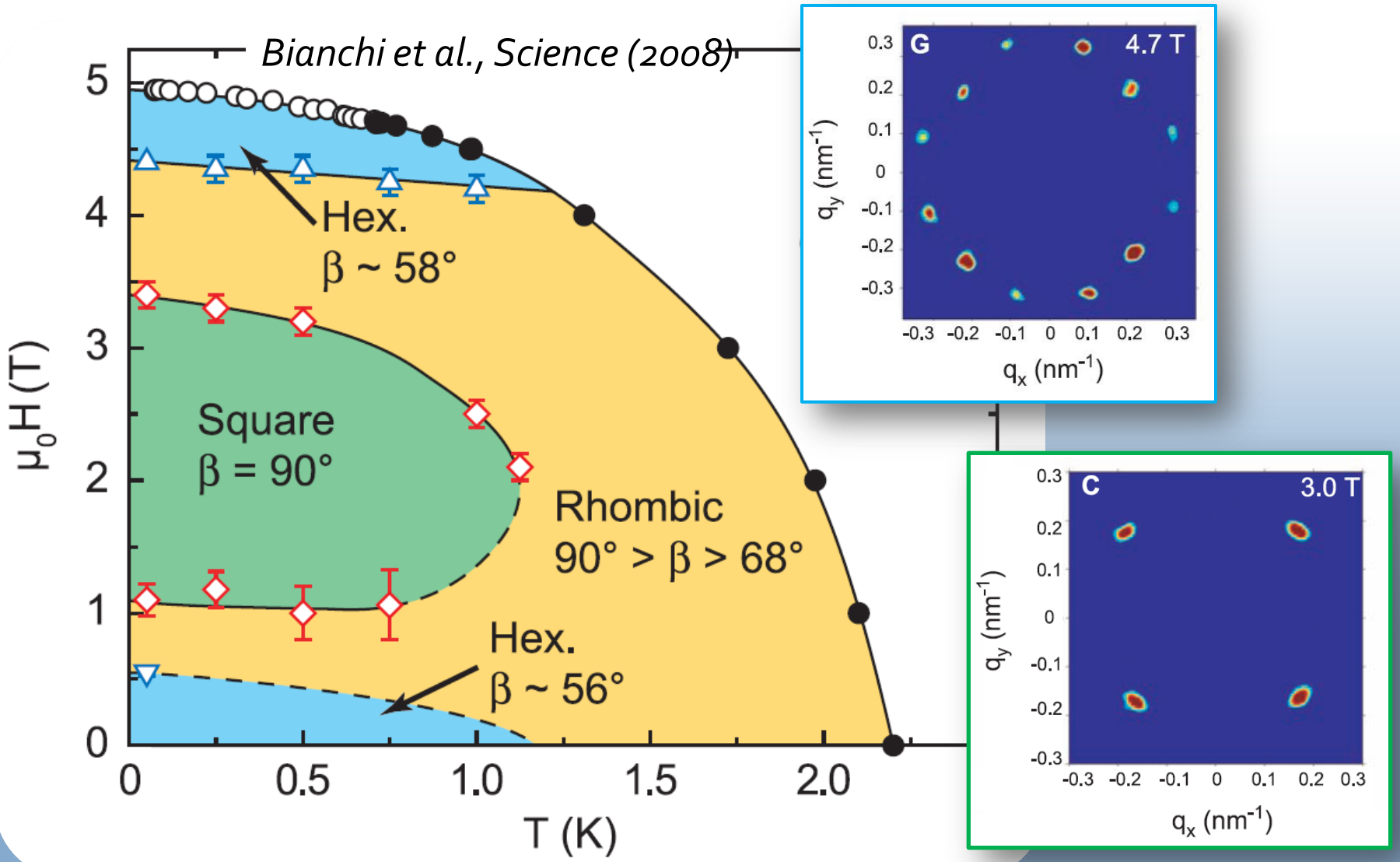
Critical angle for total *external* reflection:

$$q_c = l\sqrt{\frac{rb \pm r_0 \mathbf{M} \times \vec{s}}{p}}$$

Polarized beam!



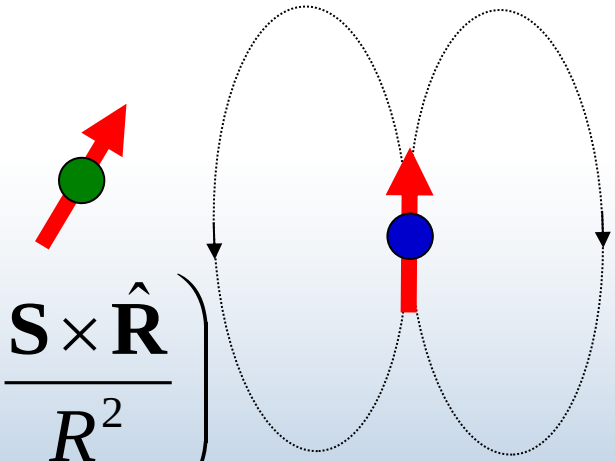
Structure of vortex matter: $CeCoIn_5$



The transition matrix element

The dipole moment of unfilled shells yield inhomog. B-field

$$\mathbf{B} = \nabla \times \left(\frac{\mu_0}{4\pi} \frac{g\mu_B \mathbf{S} \times \hat{\mathbf{R}}}{R^2} \right)$$



The magnetic neutron senses the field

$$V_m(\mathbf{r}) = -\vec{\mu} \cdot \mathbf{B}(\mathbf{r}) = -\frac{\mu_0}{4\pi} g\gamma \frac{m_e}{m} \mu_B^2 \vec{\sigma} \cdot \nabla \times \left(\frac{\mathbf{S} \times \hat{\mathbf{R}}}{R^2} \right)$$

The transition matrix element in Fermi's golden rule

$$\frac{m}{2\pi\hbar^2} \langle \mathbf{k}' s' | V_m | \mathbf{k} s \rangle = -r_0 \frac{g}{2} F(\mathbf{q}) \langle s' | \vec{s} \times \mathbf{S}_{\perp l} | s \rangle \exp(i\mathbf{q} \cdot \mathbf{r}_l)$$

Magnetic scattering length ~ nuclear scattering lengths

$$r_0 = g \frac{\mu_0}{4\pi} \frac{e^2}{m_e} = 0.54 \times 10^{-12} \text{ cm}$$

It is sensitive to atomic dipole moment perp. to $\mathbf{q}$

$$\mathbf{S}_{\perp l} = \mathbf{S}_l - (\mathbf{S}_l \cdot \hat{\mathbf{q}}) \hat{\mathbf{q}}$$

The magnetic scattering cross section

Spin density spread out scattering decreases at high q

$$F(\mathbf{q}) = \int s(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r})\, \mathrm{d}\mathbf{r}$$

The magnetic neutron scattering cross section

$$\left.\frac{\mathrm{d}^2 s}{\mathrm{d}W\mathrm{d}E'}\right|_{s\to s'} = \frac{k'}{k}\left(\frac{m}{2p\hbar^2}\right)^2 \sum_{ll'} p_l \left|\left\langle \mathbf{k}'s'l' \middle| V_m \middle| \mathbf{k}sl \right\rangle\right|^2 d\left(E_l - E_{l'} - \hbar w\right)$$

$$= \frac{k'}{k} r_0^2 \left|\frac{g}{2} F(\mathbf{q})\right|^2 e^{-2W(\vec{k})} \frac{1}{2p\hbar} \int dt\, e^{-iwt} \sum_{ll'} e^{i\mathbf{q}\cdot(\mathbf{R}_l - \mathbf{R}_{l'})}$$

$$\times \left\langle \left\langle s \middle| \vec{s}\cdot\mathbf{S}_{\wedge l}(0) \middle| s' \right\rangle \left\langle s' \middle| \vec{s}\cdot\mathbf{S}_{\wedge l'}(t) \middle| s \right\rangle \right\rangle$$

For unspecified incident & final neutron spin states

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'} = \tfrac{1}{2}\sum_{\sigma\sigma'} \left.\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega\mathrm{d}E'}\right|_{\sigma\to\sigma'}$$

Un-polarized magnetic scattering

Squared form factor

DW factor

Polarization factor

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k} r_0^2 \left| \frac{g}{2} F(\mathbf{q}) \right|^2 e^{-2W(\mathbf{q})} \sum_{ab} \left(d_{ab} - \hat{q}_a \hat{q}_b \right)$$

$$\times \frac{1}{2\pi\hbar} \int dt\, e^{-i\omega t} \sum_{ll'} e^{i\mathbf{q}\cdot(\mathbf{r}_l - \mathbf{r}_{l'})} \left\langle \mathbf{S}_l^a(0) \mathbf{S}_{l'}^b(t) \right\rangle$$

Fourier transform

Spin correlation function

Neutron Scattering in Quantum Condensed Matter Physics

A Multi-University Online Graduate Course

NEW COURSE! FALL 2012

Course Description:

The Neutron Sciences Directorate (NScD) and Joint Institute for Neutron Sciences (JINS) at Oak Ridge National Laboratory (ORNL) are proud to announce a new graduate distance learning course, to be taught collaboratively by expert professors from six contributing universities as well as ORNL scientists. The course provides a solid foundation to understand the use of neutron scattering as a probe of atomic-scale structure and dynamics of quantum condensed matter. The course covers the theoretical background, experimental techniques and methods of analysis. The course will be taught from the lecturers' institutions and will be available on-line with real time interaction for students participating at the live conferencing venues; as well as via streaming. Graduate students and postdocs in the fields of Condensed Matter Physics and Materials Science are invited to enroll or register.

Pre-Requisites:

Quantum Mechanics, Statistical Physics, and Condensed Matter Physics at the graduate level.

Schedule:

Tuesdays and Thursdays 4:00 pm - 5:15 pm, Tuesday 9/4/2012 through Thursday 12/7/2012

Instructors:

- Collin Broholm, Johns Hopkins University (JHU)
- Takeshi Egami, University of Tennessee (UT)/ORNL
- Young S. Lee, Massachusetts Institute of Technology
- Seunghun Lee, University of Virginia
- Stephen Nagler, ORNL/UT
- Roger Pynn, Indiana University
- Sunil K. Sinha, University of California, San Diego

Planning Committee:

- Collin Broholm, JHU
- Takeshi Egami, UT/ORNL
- Meiyun Chang-Smith, Course Coordinator, NScD/JINS, changsmithm@ornl.gov

http://jins.tennessee.edu/course2012

http://neutrons.ornl.gov/education/qcmp

Oak Ridge National Laboratory · Neutron Sciences · JINS · The University of Tennessee UT · University of Virginia · Massachusetts Institute of Technology · Indiana University · UCSD · Johns Hopkins University

Online lectures accessible at:
http://www.sns.gov/education/qcmp/

Magnetic neutron diffraction

Time independent spin correlations elastic scattering

$$\frac{\mathrm{d}s}{\mathrm{d}W} = r_0^2 \left| \frac{g}{2} F(\mathbf{q}) \right|^2 e^{-2W(\mathbf{q})} \sum_{ab} \left(d_{ab} - \hat{q}_a \hat{q}_b \right) \sum_{ll'} e^{i\mathbf{q}\cdot(\mathbf{r}_l - \mathbf{r}_{l'})} \left\langle \mathbf{S}_l^a \right\rangle \left\langle \mathbf{S}_{l'}^b \right\rangle$$

Periodic magnetic structures Magnetic Bragg peaks

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = r_0^2 N_m \frac{(2\pi)^3}{v_m} \sum_{\vec{\tau}_m} \left(\left| \vec{\mathcal{F}}(\mathbf{q}) \right|^2 - \left| \hat{\mathbf{q}} \cdot \vec{\mathcal{F}}(\mathbf{q}) \right|^2 \right) \delta(\mathbf{q} - \vec{\tau}_m)$$

Magnetic primitive unit cell greater than chemical P.U.C.

Magnetic Brillouin zone smaller than chemical B.Z.

The magnetic vector structure factor is

$$\vec{\mathcal{F}}(\mathbf{q}) = \sum_{\mathrm{d}} \frac{g_{\mathbf{d}}}{2} F_{\mathbf{d}}(\mathbf{q}) e^{-2W_{\mathbf{d}}(\mathbf{q})} \left\langle \mathbf{S}_{\mathbf{d}} \right\rangle e^{i\mathbf{q}\cdot\mathbf{d}}$$

Diffraction from Ferromagnet

Nuclear & magnetic scattering interferes. Effective scatt. length:

$$b + s\, r_0 S_\wedge$$

The structure factor for reciprocal lattice vector, t

$$|F_s|^2 = \left|\sum_{\mathbf{d}} \left(b_{\mathbf{d}} + s\, r_0 S_{\wedge\,\mathbf{d}}\right) e^{i\mathbf{t}\cdot\mathbf{d}}\right|^2$$

$$= \left|\sum_{\mathbf{d}} b_{\mathbf{d}} e^{i\mathbf{t}\cdot\mathbf{d}}\right|^2 + \left|\sum_{\mathbf{d}} s\, r_0 S_{\wedge\,\mathbf{d}} e^{i\mathbf{t}\cdot\mathbf{d}}\right|^2 + 2s \sum_{\mathbf{d}\neq\mathbf{d}'} b_{\mathbf{d}} r_0 S_{\wedge\,\mathbf{d}} e^{i\mathbf{t}\cdot(\mathbf{d}-\mathbf{d}')}$$

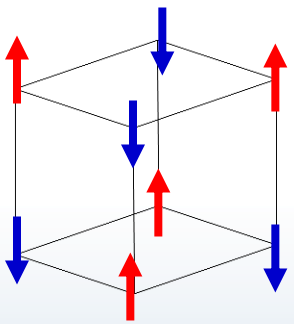
Nuclear | Magnetic | Nuclear-magnetic

The last term vanishes for un-polarized neutrons (s average).

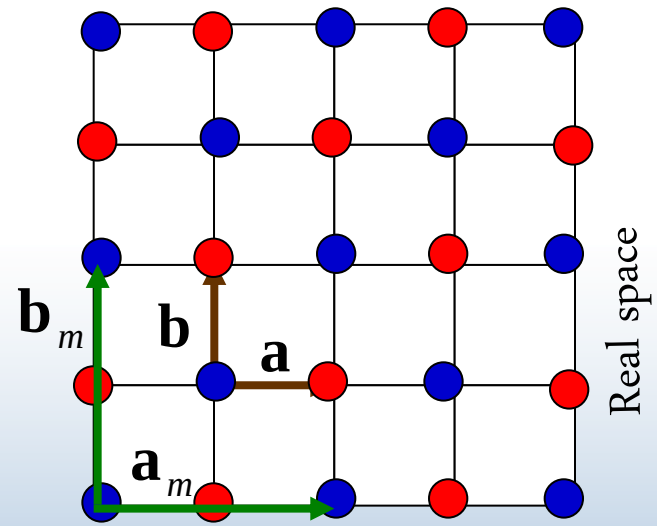
A welcome consequence is that the diffracted beam is polarized!

$$b_{\mathbf{d}} \approx r_0 S_{\wedge\,\mathbf{d}} \Rightarrow |F_\pm|^2 \approx \begin{cases} 4|b_{\mathbf{d}}|^2 & \text{for } s = 1 \\ 0 & \text{for } s = -1 \end{cases}$$

Simple cubic antiferromagnet



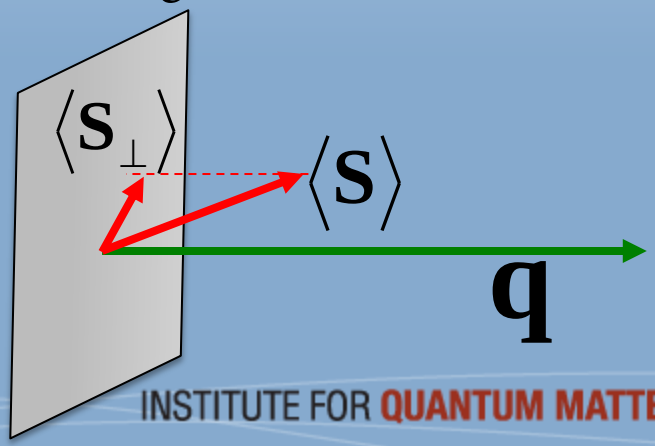
$$g\langle \mathbf{S}\rangle \equiv \frac{m_s}{\mu_B}\hat{\mathbf{z}}$$

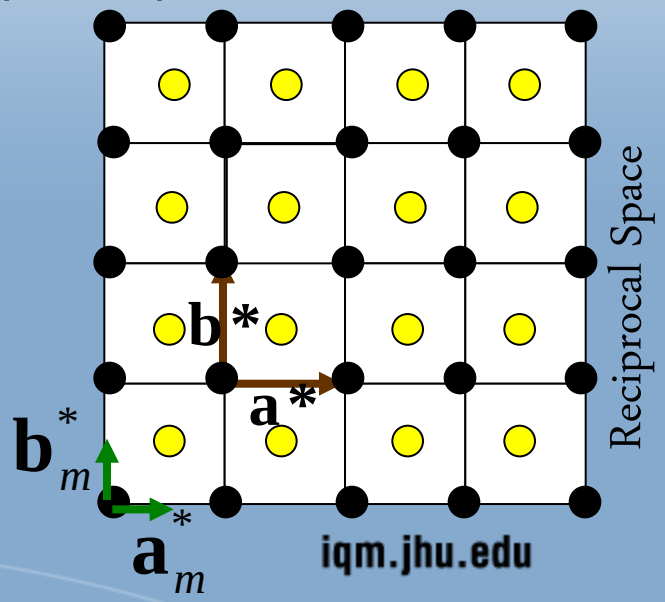


$$\vec{\mathcal{F}}(\vec{\kappa}) = \frac{m_s \hat{\mathrm{z}}}{2\mu_B} F(\mathbf{q}) e^{-2W(\mathbf{q})} 8 \sin \pi h \sin \pi k \sin \pi l$$

$$\frac{\mathrm{d}s}{\mathrm{dW}} = N\left(r_0 \frac{m_s}{2m_B}\right)^2 e^{-2W(\mathbf{q})} \left|F(\mathbf{q})\right|^2 \left(1 - \hat{q}_z^2\right) \frac{(2p)^3}{v} \sum_{\vec{t}_m} d\left(\mathbf{q} - \vec{t}_m\right)$$

No magnetic diffraction for $\mathbf{q} \parallel \langle \mathbf{S}\rangle$

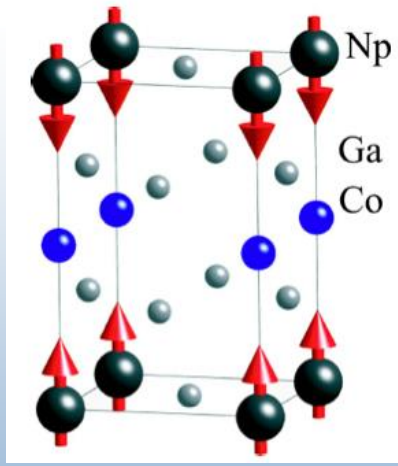


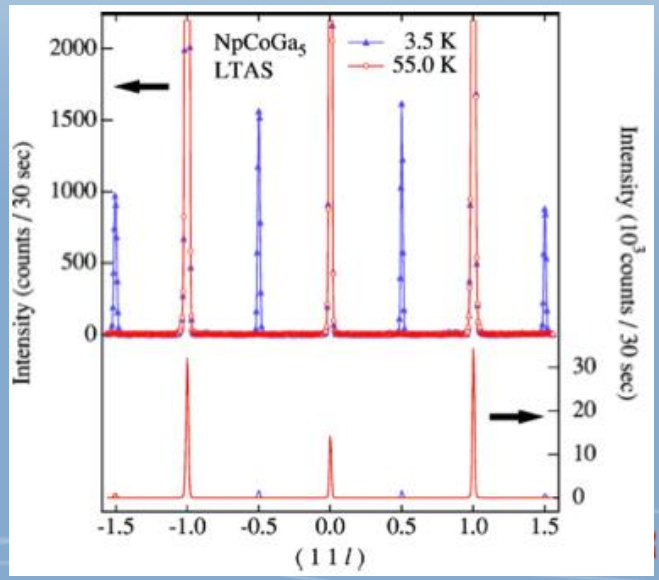


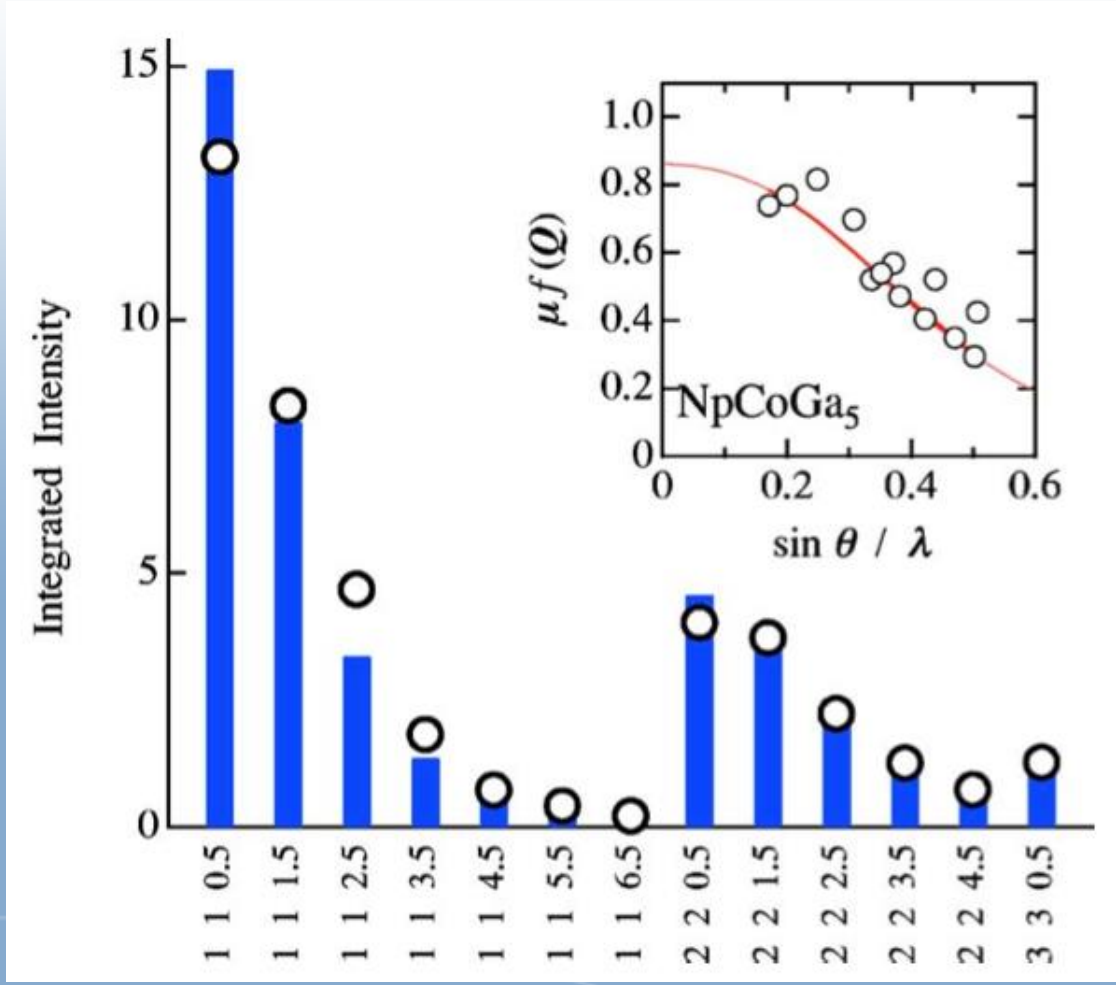
PHYSICAL REVIEW B **72**, 014460 (2005)

Magnetic structure and metamagnetism in single crystals of $NpCoGa_5$

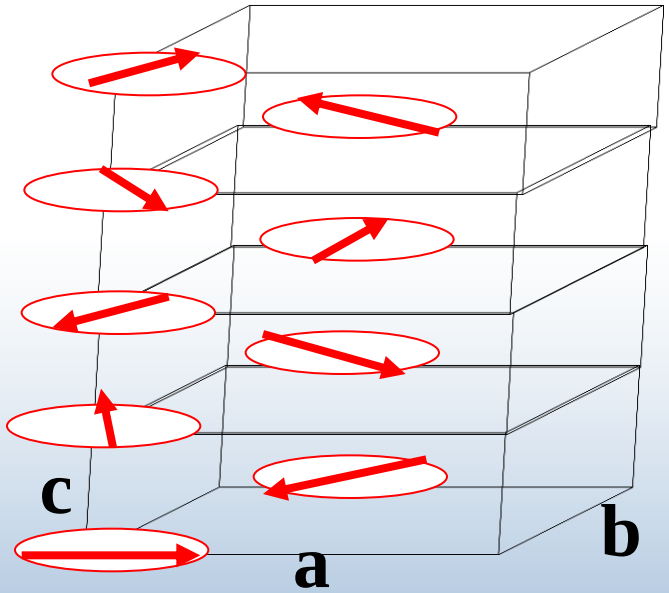
N. Metoki,[1,2,*] K. Kaneko,[1] E. Colineau,[3] P. Javorský,[3,4] D. Aoki,[5] Y. Homma,[5] P. Boulet,[3] F. Wastin,[3] Y. Shiokawa,[1,5] N. Bernhoeft,[6] E. Yamamoto,[1] Y. Ōnuki,[1,7] J. Rebizant,[3] and G. H. Lander[1,3]

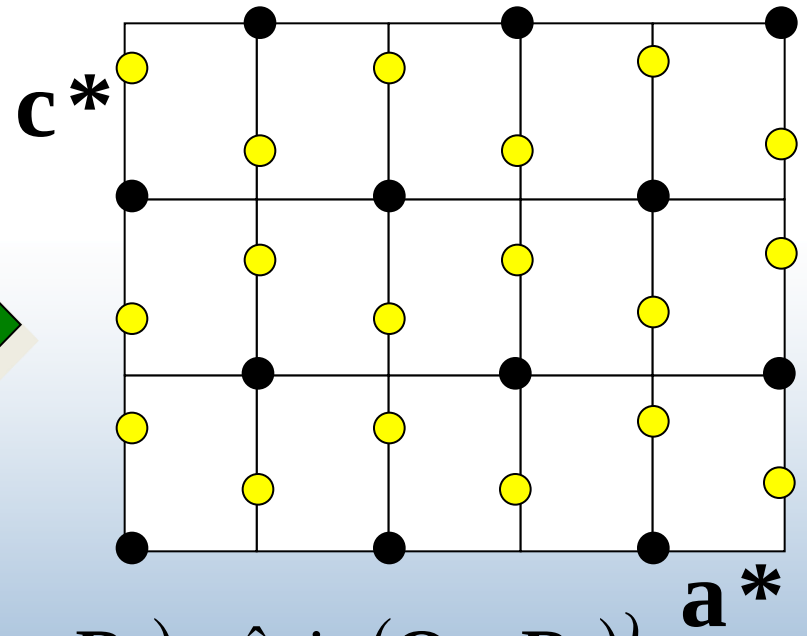






Not so simple Heli-magnet : MnO_2





$$\langle \mathbf{S}_l \rangle = S \exp\left(i\mathbf{w}\cdot\mathbf{R}_l\right)\left\{\hat{\mathbf{x}}\cos\left(\mathbf{Q}_m\cdot\mathbf{R}_l\right)+\hat{\mathbf{y}}\sin\left(\mathbf{Q}_m\cdot\mathbf{R}_l\right)\right\}$$

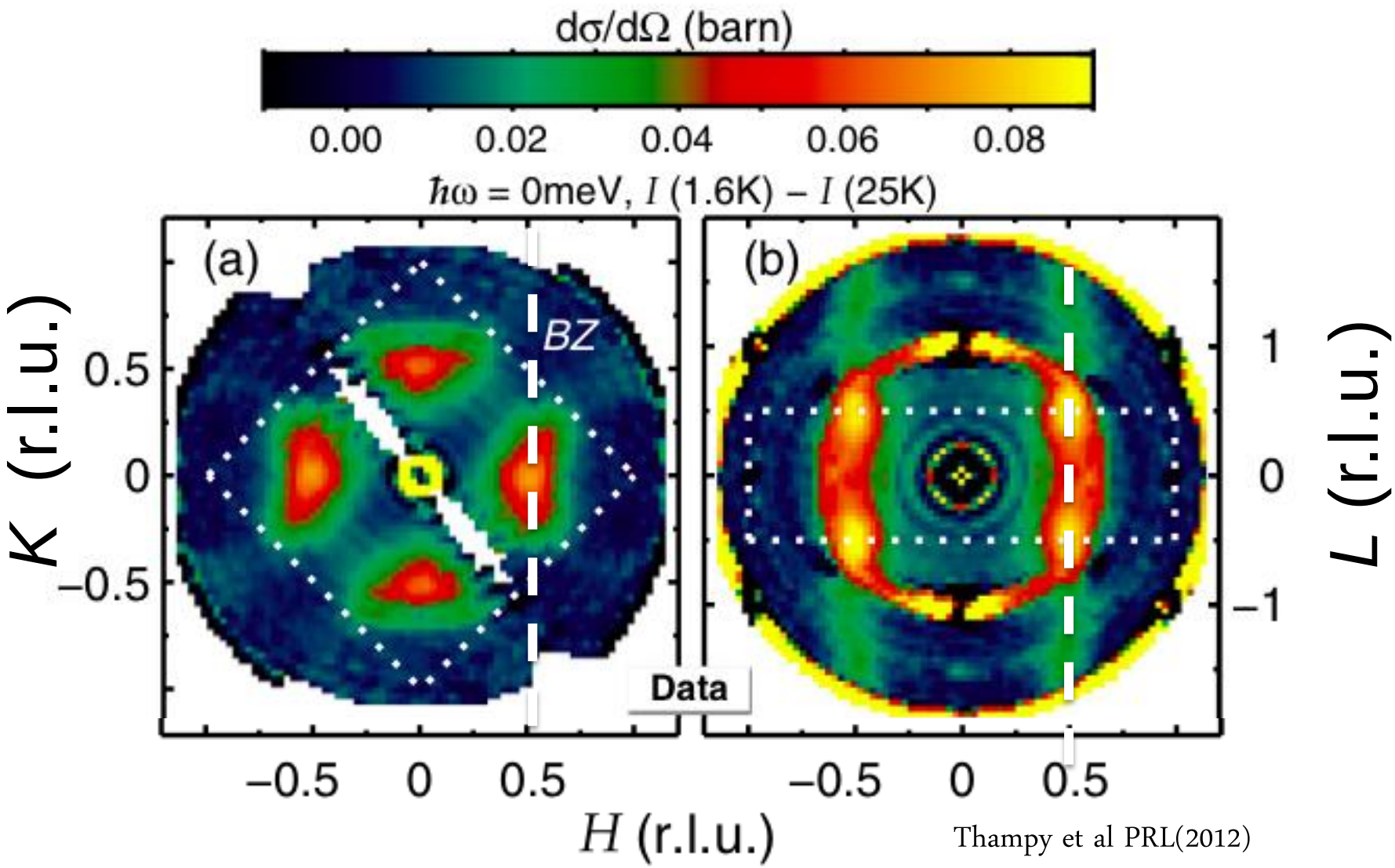
$\mathbf{w} = (111)$ and $\mathbf{Q}_m \approx \left(00\tfrac{2}{7}\right)$ characterize structure

Insert into diffraction cross section to obtain

$$\frac{\mathrm{d}s}{\mathrm{dW}} = N\left(r_0 S\right)^2 e^{-2W(\mathbf{q})}\left|\frac{g}{2}F(\mathbf{q})\right|^2\left(1+\hat{q}_z^2\right)\frac{(2p)^3}{v}$$

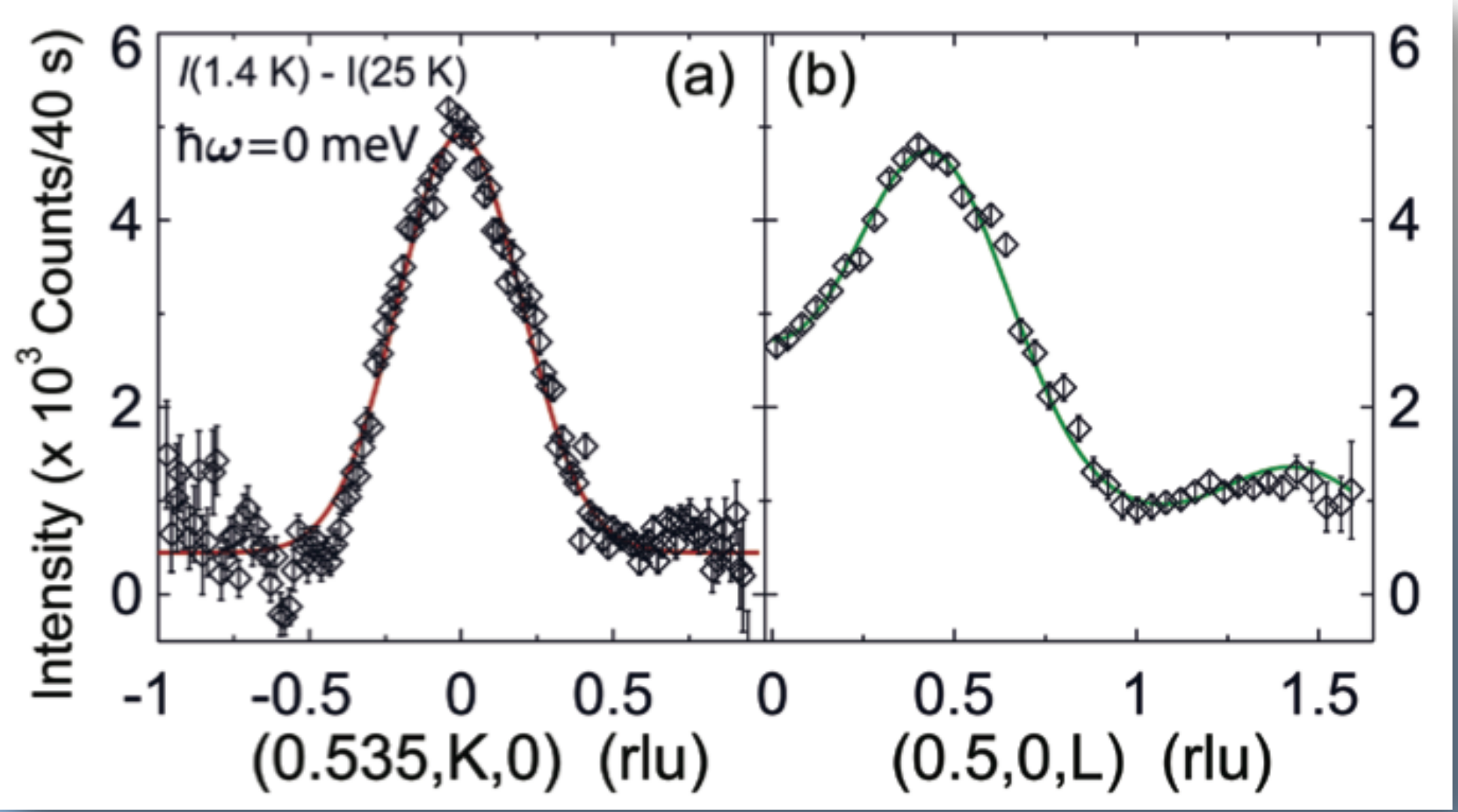
$$\times\sum_{\tau}\left\{d\left(\mathbf{q}+\mathbf{w}-\mathbf{Q}_\mathbf{m}-t\right)+d\left(\mathbf{q}+\mathbf{w}+\mathbf{Q}_\mathbf{m}-t\right)\right\}$$

Diffuse Magnetic Scattering in $FeTe_{0.6}Se_{0.4}$

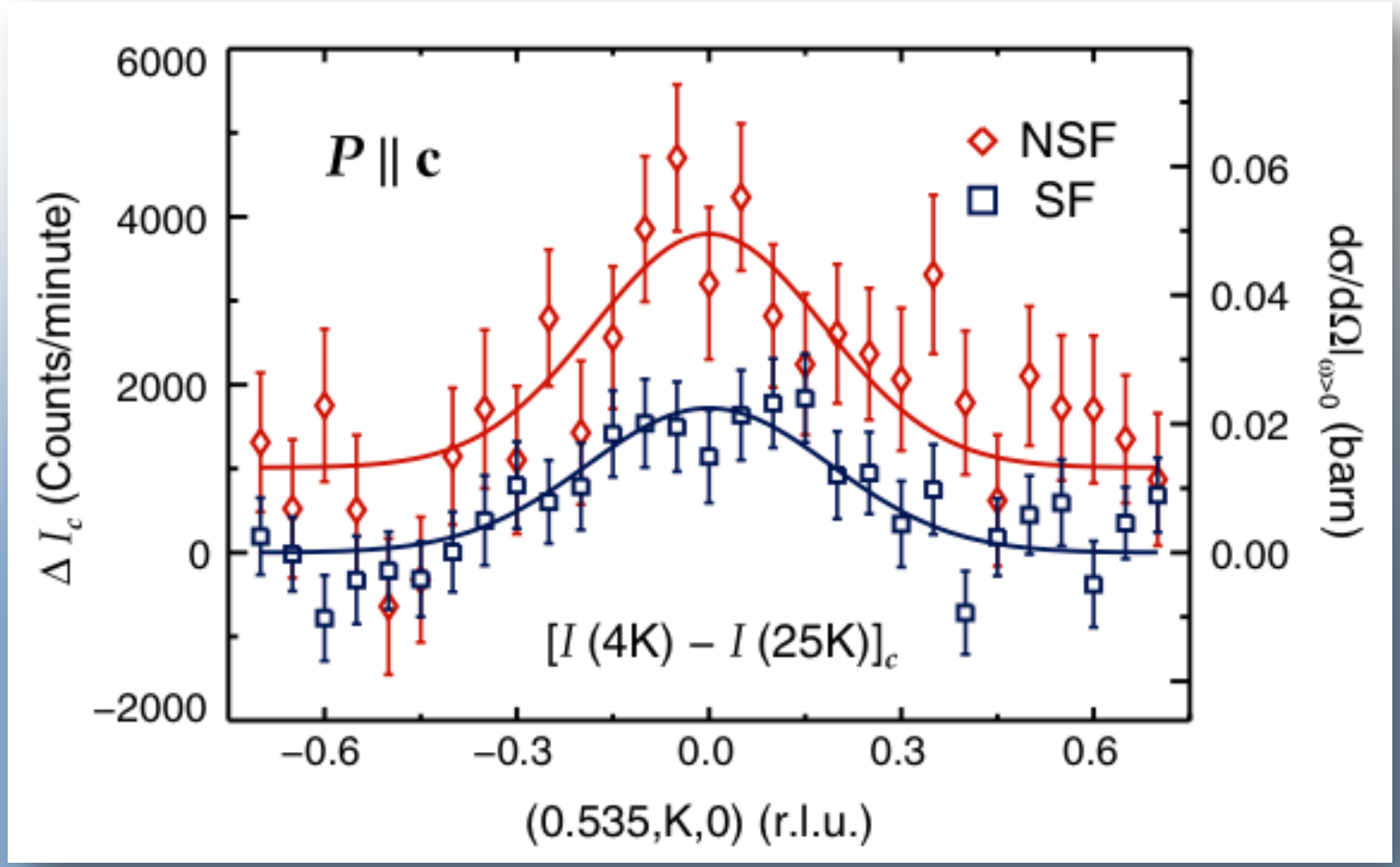


Thampy et al PRL(2012)

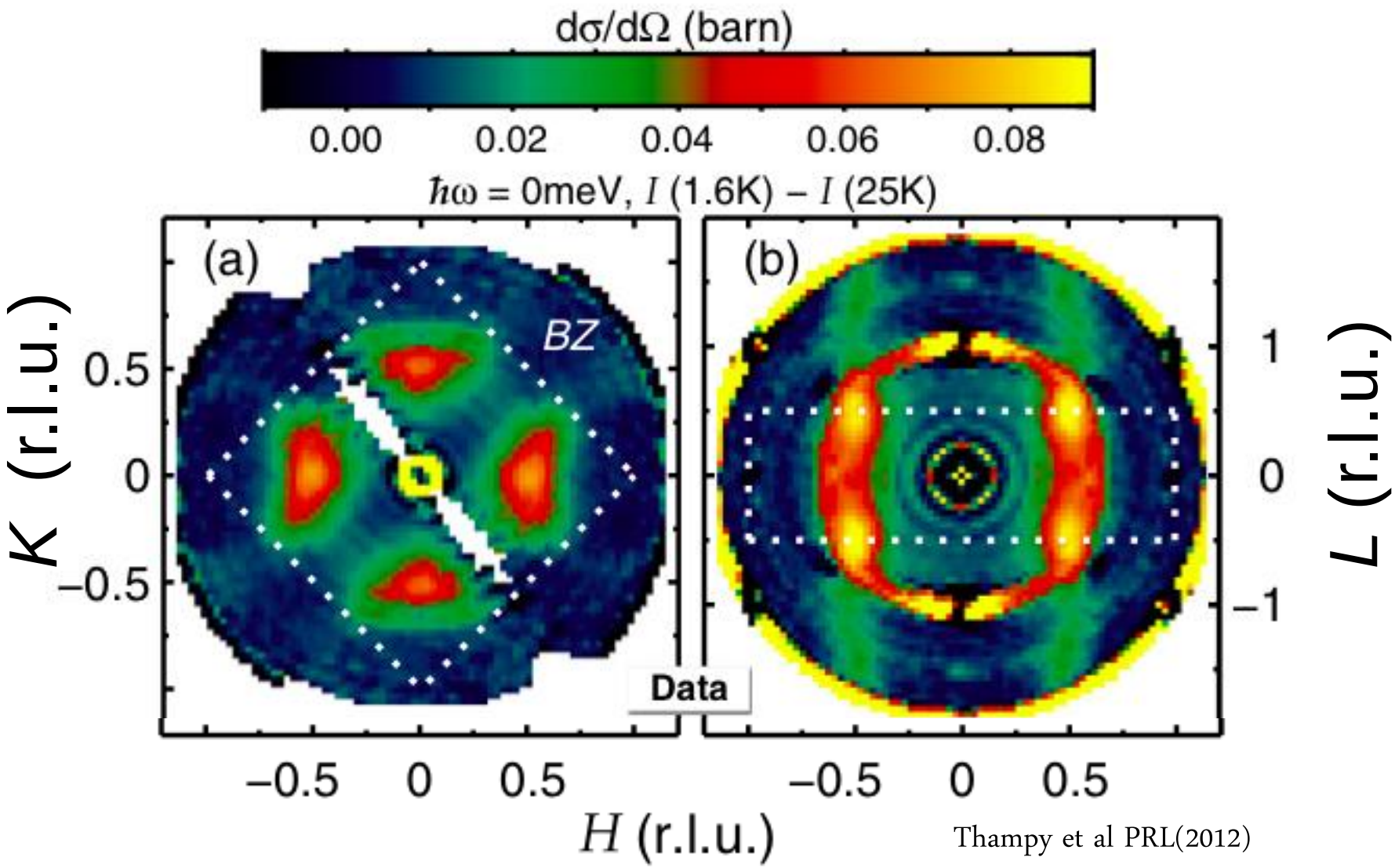
Hypothesis: Ising spins?



Polarized neutrons: isotropic static spin correlations

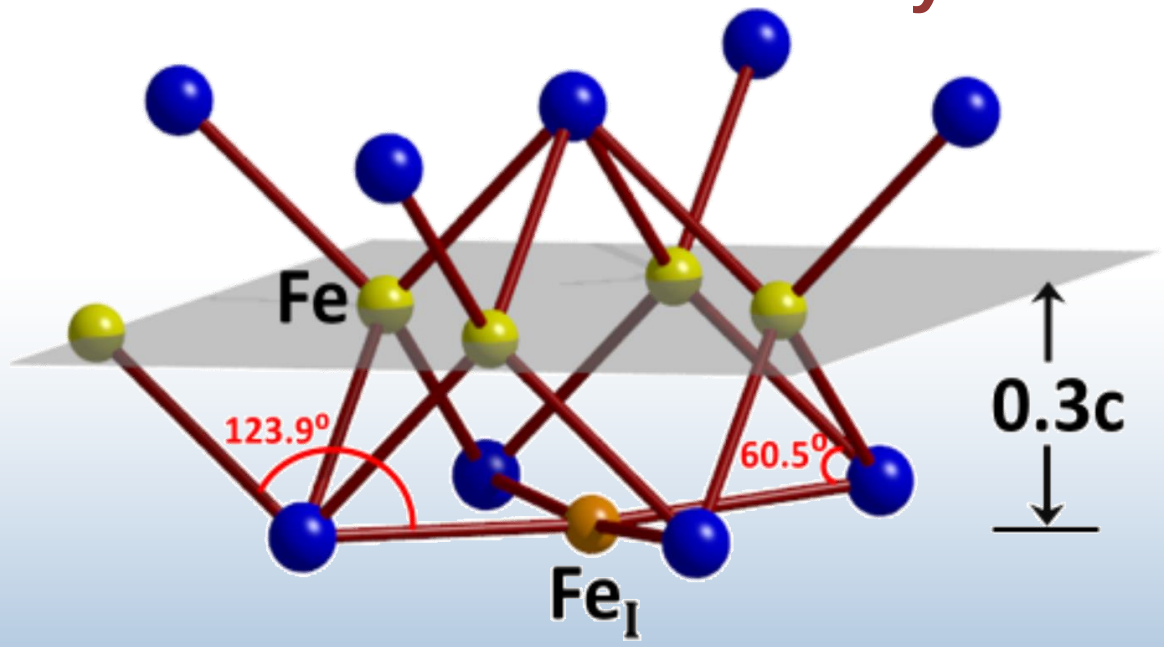


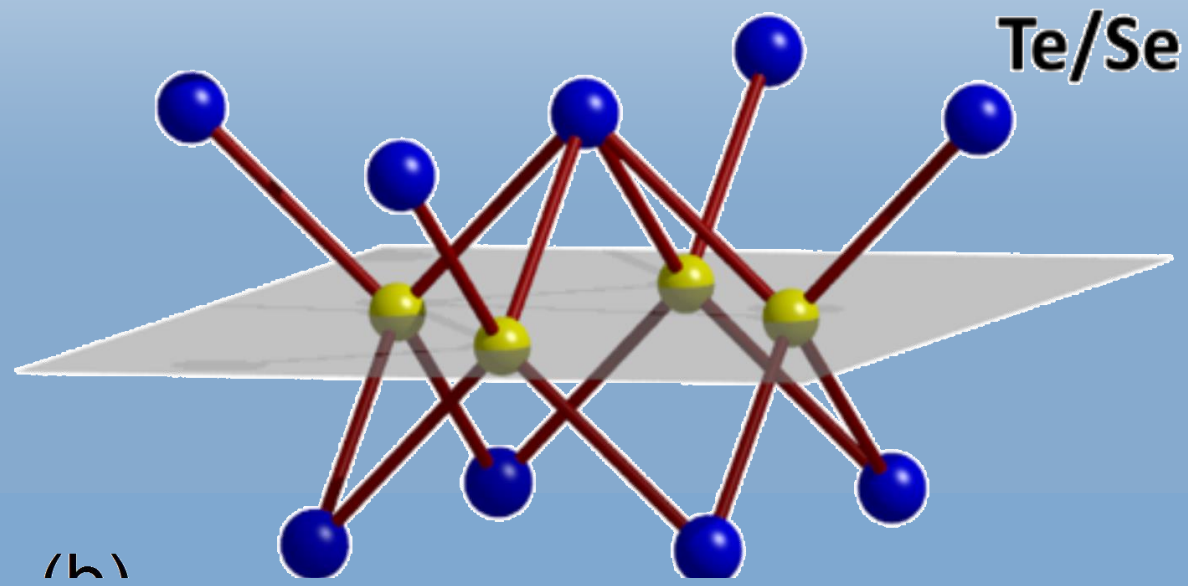
Diffuse Magnetic Scattering in $FeTe_{0.6}Se_{0.4}$



Thampy et al PRL(2012)

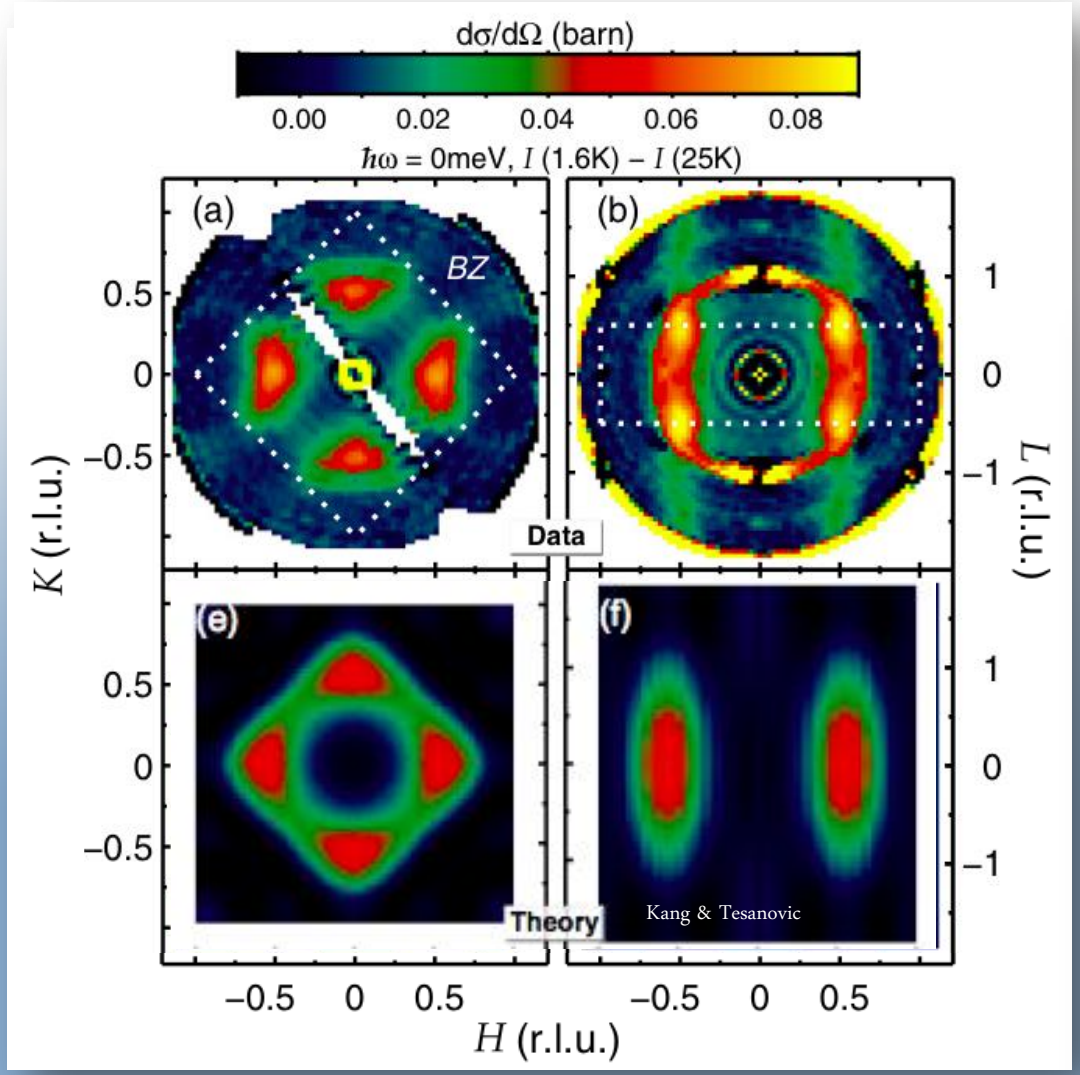
Interstitial Iron in $Fe_{1+y}Te_{1-x}Se_x$





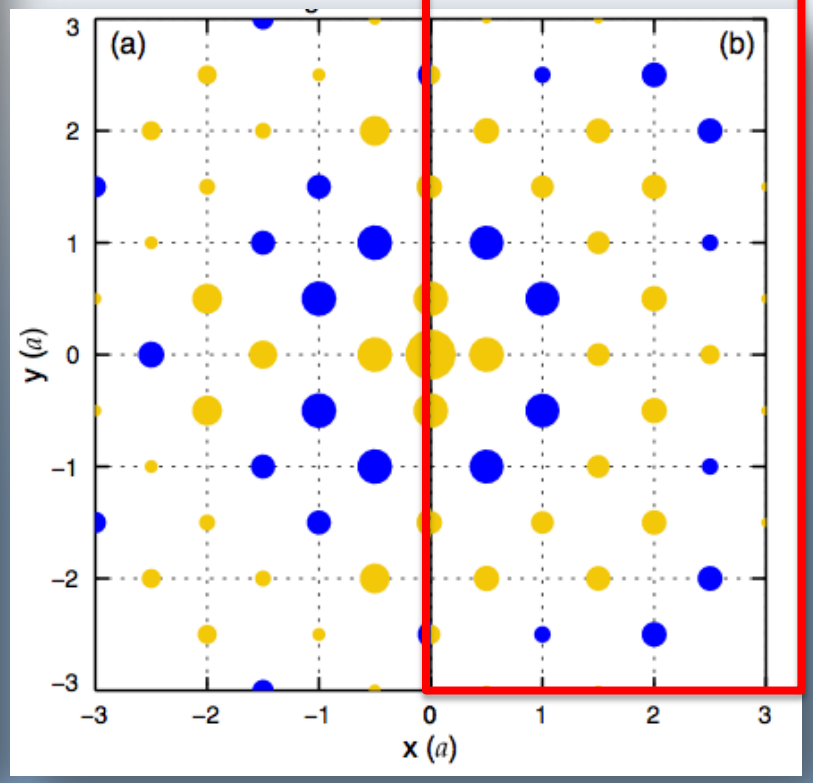
(b)

Extract Local Spin Structure



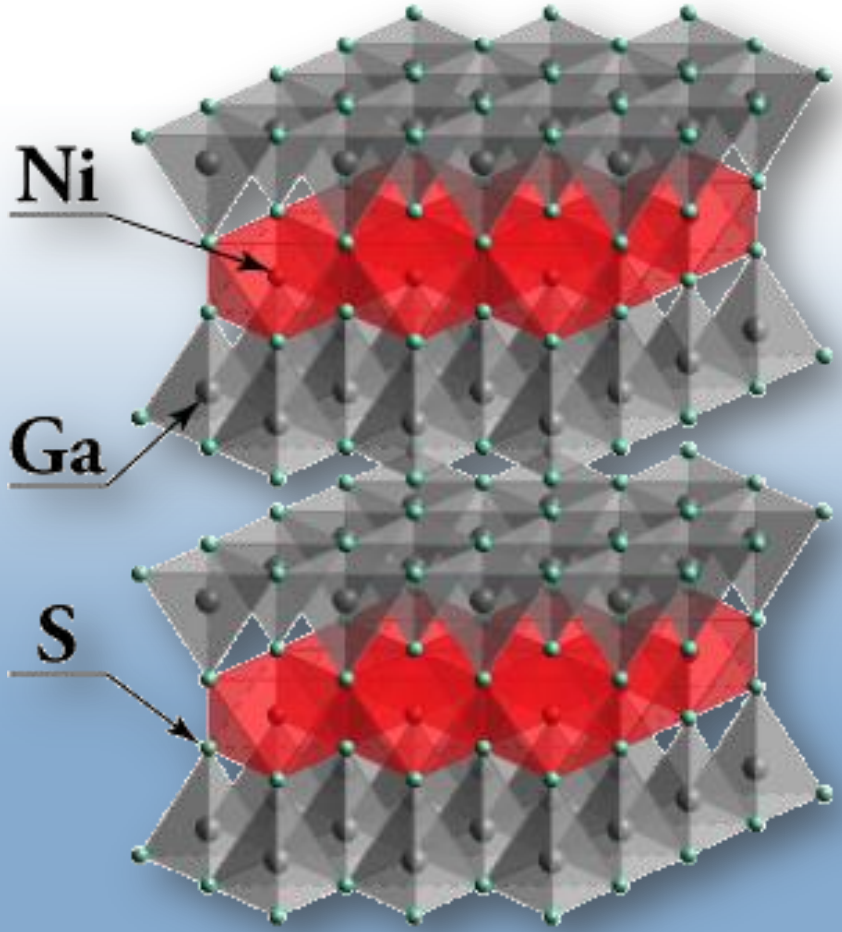
Model by coupling itinerant spin to 5-band model through

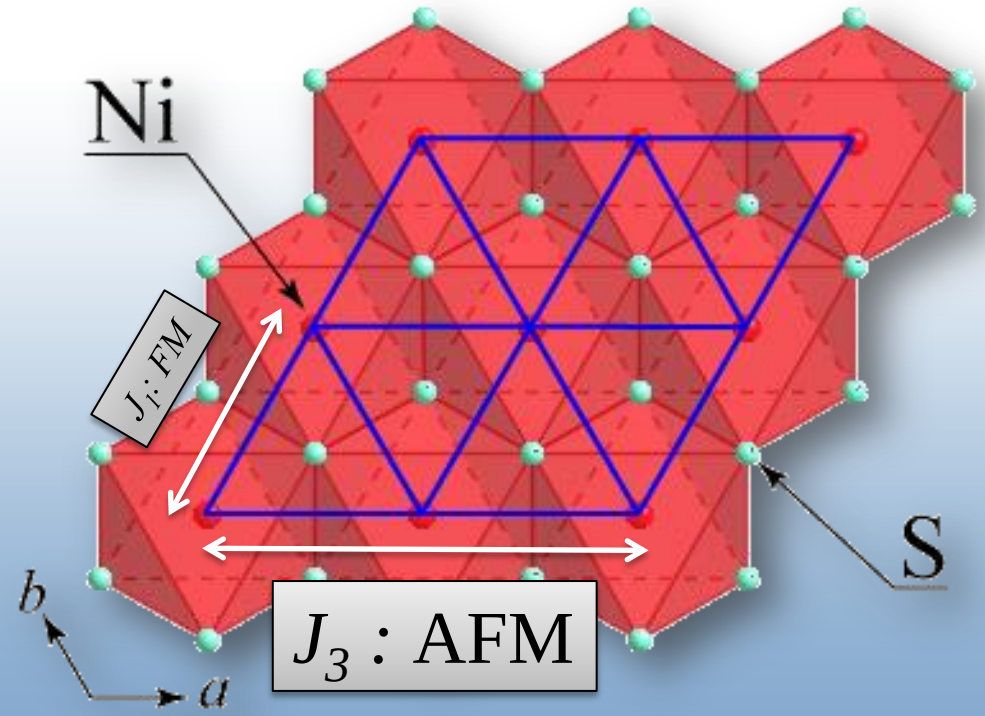
$$\mathcal{H}_{\text{imp}} = J\mathbf{S}\cdot\sum_{i\in\text{NN}}\mathbf{s}_i + J'\mathbf{S}\cdot\sum_{j\in\text{NNN}}\mathbf{s}_j.$$



$NiGa_2S_4$: Spin-1 Triangular Lattice AFM

Nakatsuji et al. Science (2005)

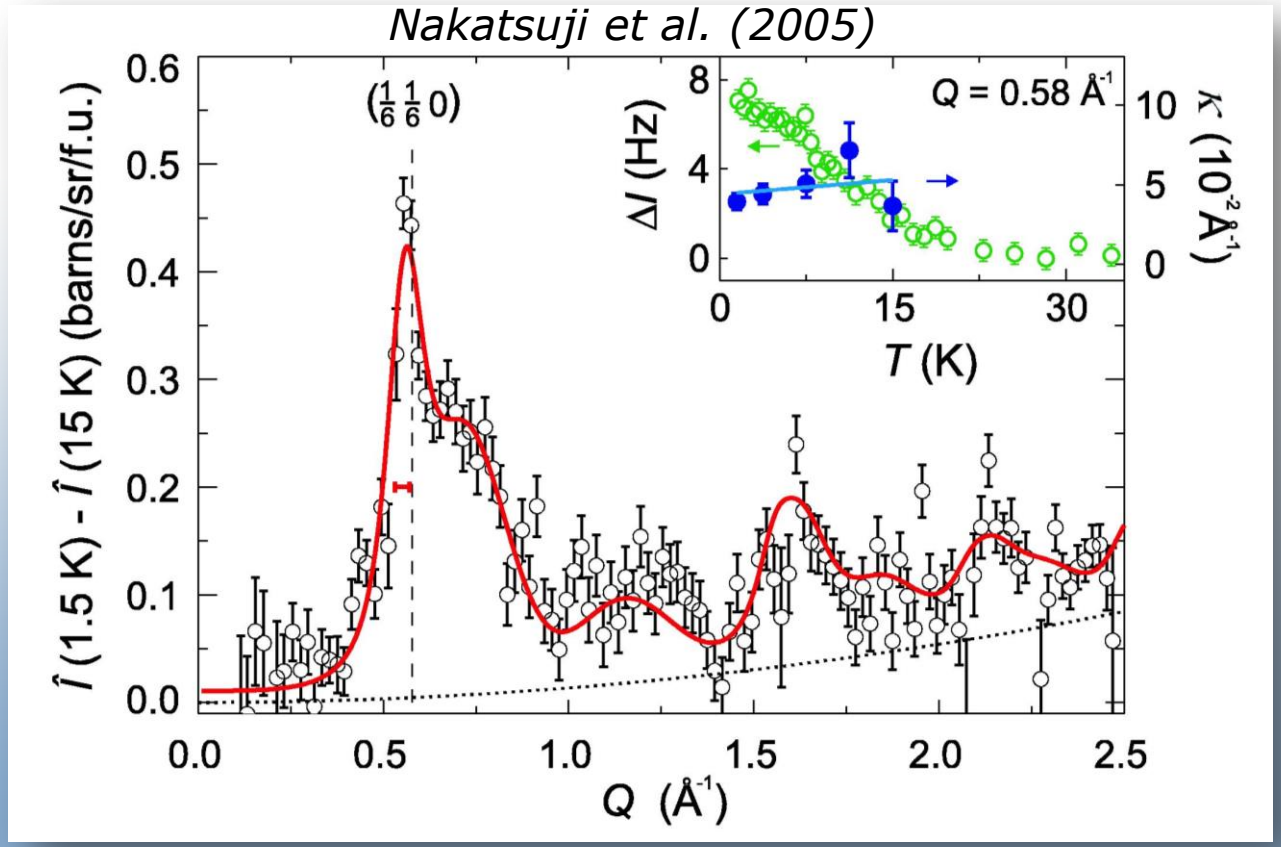




Unusually weak interlayer coupling

Dominant 3rd neighbor interactions
Exact triangular lattice
Weak easy plane anisotropy

Elastic neutron scattering from $NiGa_2S_4$ powder



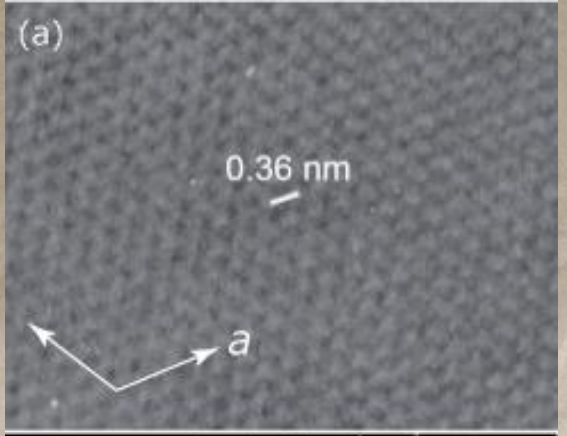
$$\left.\frac{ds}{d\Omega}\right|_{\text{powder}} = \int \frac{d\Omega_Q}{4p} \left.\frac{ds}{d\Omega}\right|_{\text{xtal}}$$

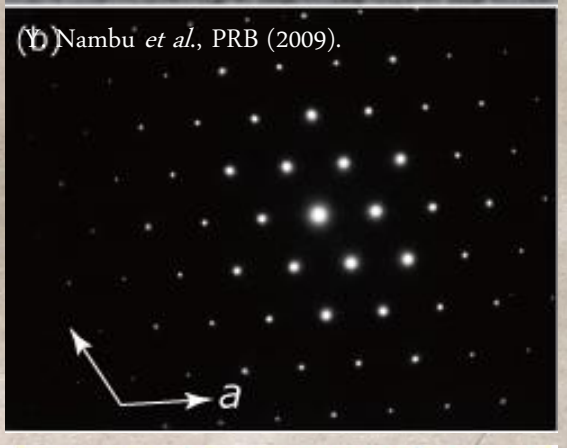
2 Surprises:

$$Q \approx \tfrac{1}{2} Q_{120^o}$$

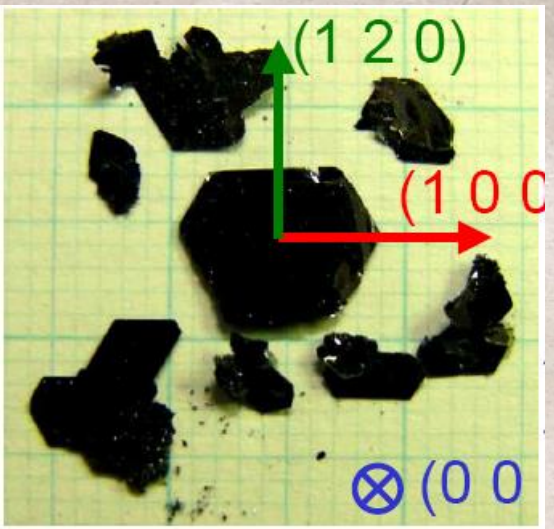
$$\kappa^{-1} = 25(3)\ \text{Å}$$

$$\frac{d\sigma}{d\Omega} = r_0^2 \left|\frac{g}{2} F(Q)\right|^2 N \sum_{\boldsymbol{\tau}} \left(\left|\mathbf{m_q}\right|^2 - \left|\hat{\mathbf{Q}}\cdot\mathbf{m_q}\right|\right)\left(1 + 2\alpha\cos(\mathbf{Q}\cdot\mathbf{c})\right) \frac{A^*\kappa^2/\pi}{\left((\mathbf{Q}-\boldsymbol{\tau}\pm\mathbf{q})^2 + \kappa^2\right)^2}$$

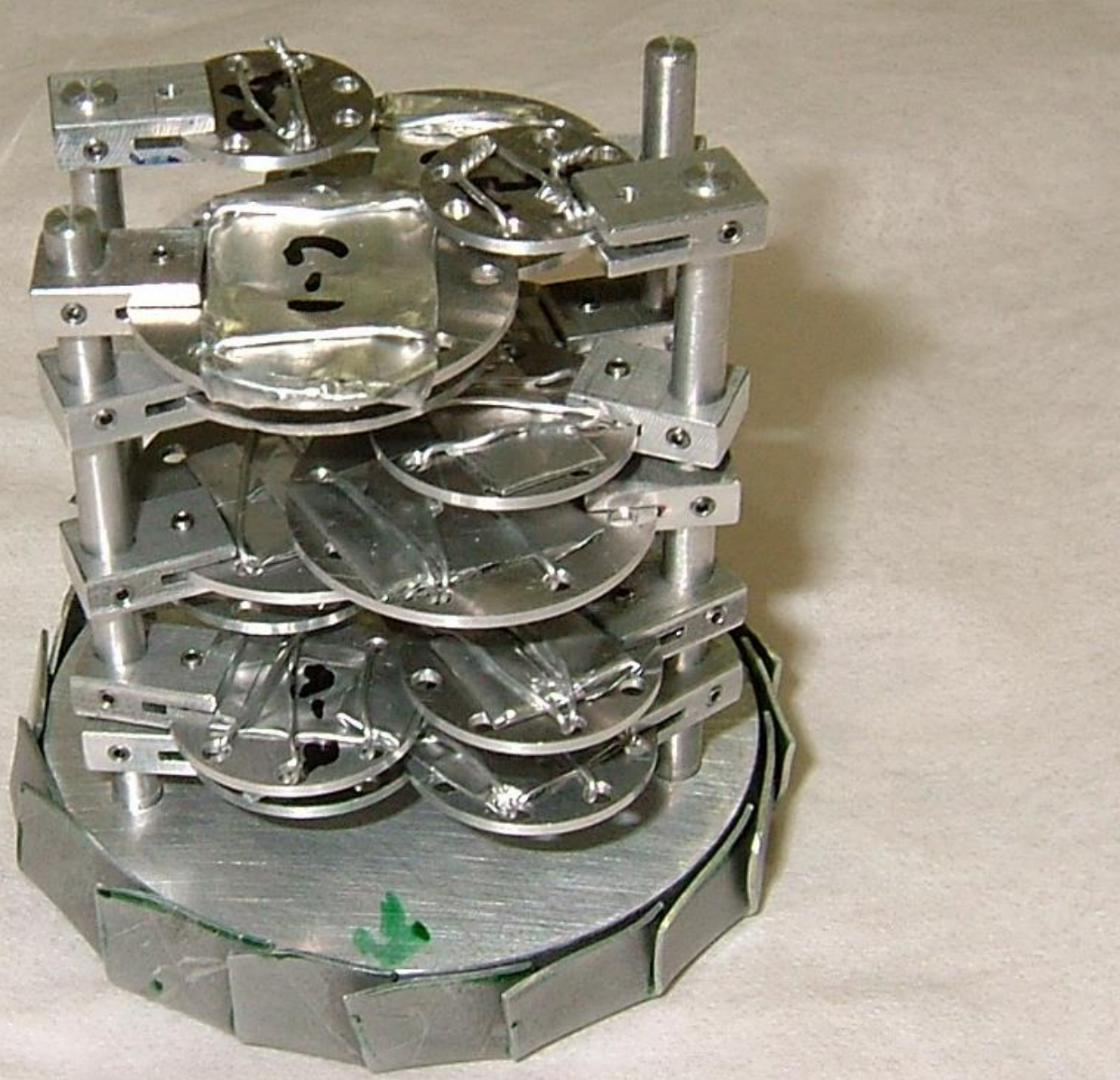




Nambu *et al.*, PRB (2009).



(15 mm X 15 mm X 0.2 mm

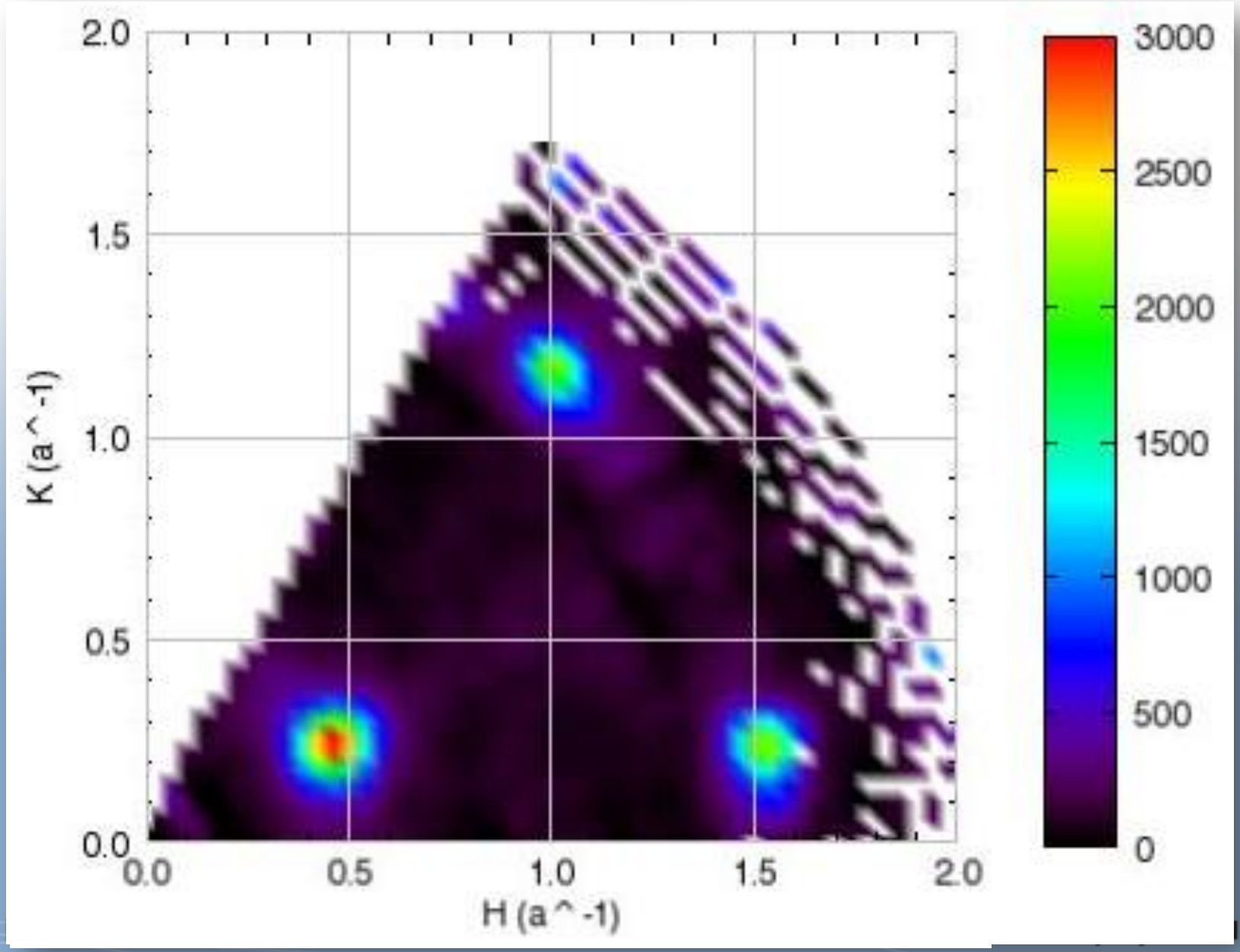


19 $NiGa_2S_4$ crystals

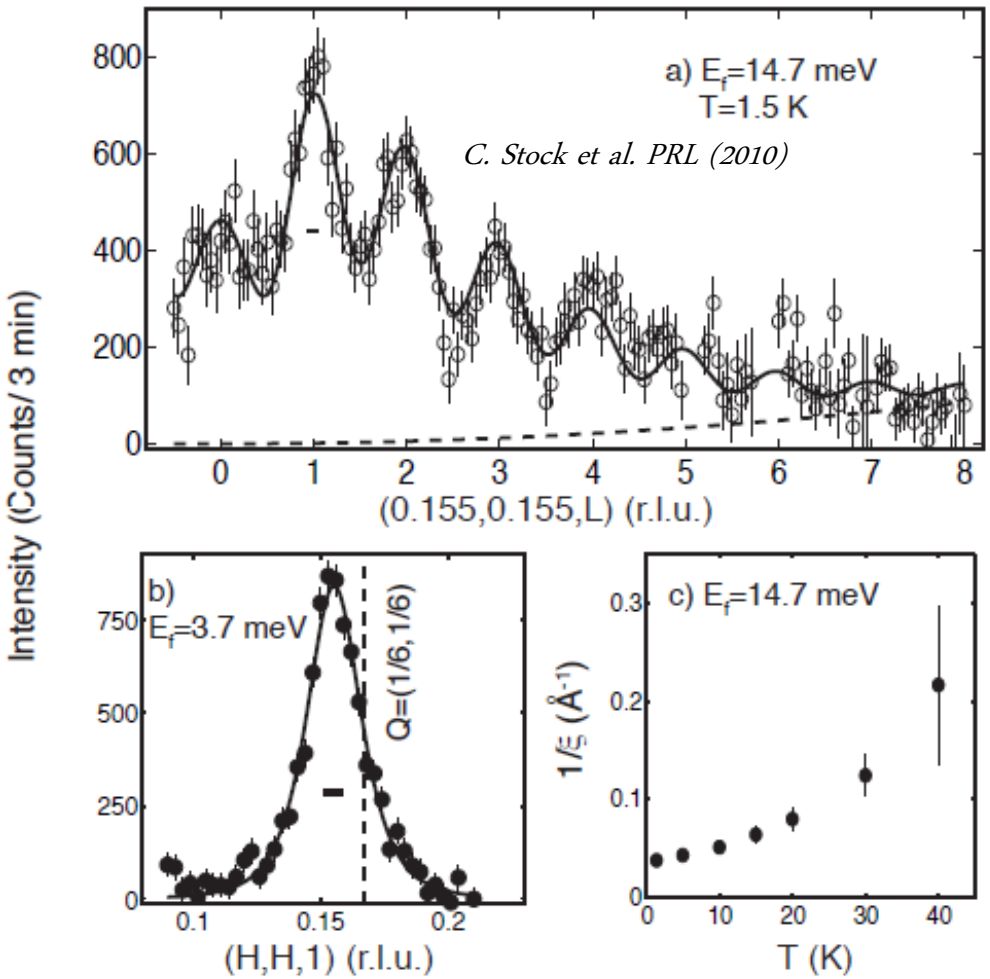
Grown by Yusuke Nambu

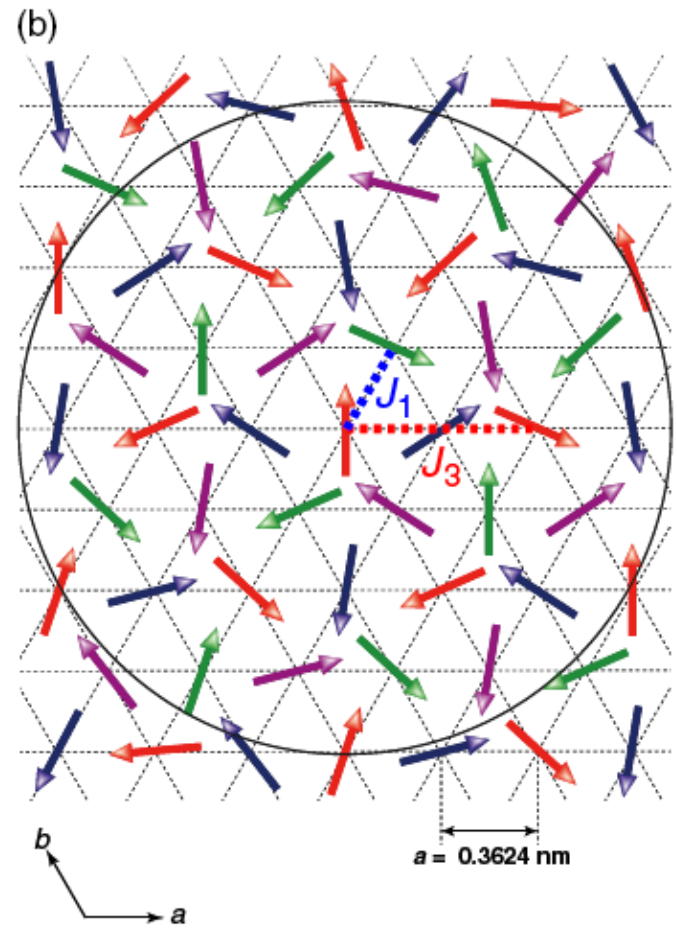
co-aligned by Chris Stock

$NiGa_2S_4$: Elastic Magnetic Scattering



Short range magnetic ordering

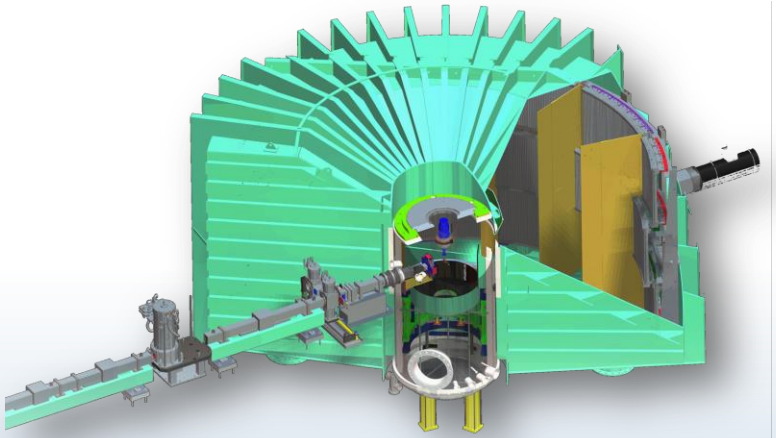




Summary: Diffraction

- **The neutron has a small dipole moment causing scattering from electrons**
- **Magnetic scattering is similar in magnitude to nuclear scattering**
- **Elastic magnetic scattering probes static magnetic structure**
- **Spin direction gleaned from polarization factor (see spin perpendicular to Q)**
- **Periodic structure determined through Bragg intensities**
- **Generally probe magnetic structure on 1-10^4 Å scale:**
  - flux line lattice
  - short range order
    - powder, single crystals, thin films

Inelastic Magnetic Neutron Scattering



$$\boldsymbol{\mu}_n = -\gamma \frac{e}{m}\frac{\hbar}{2}\boldsymbol{\sigma}$$

$$V(\mathbf{r}) = -\boldsymbol{\mu}_n \cdot B(\mathbf{r})$$

$$B(\mathbf{r}) = -\sum_n \nabla \times \left(\frac{\mu_0}{4\pi} \frac{g\mu_B \mathbf{s}_n \times \hat{\boldsymbol{\kappa}}}{\boldsymbol{\kappa}^2} \right)$$

$$V(\mathbf{r}) = -\gamma \frac{e}{m}\frac{\hbar}{2}\boldsymbol{\sigma} \cdot \sum_n \nabla \times \left(\frac{\mu_0}{4\pi} \frac{g\mu_B \mathbf{s}_n \times \hat{\boldsymbol{\kappa}}}{\boldsymbol{\kappa}^2} \right)$$

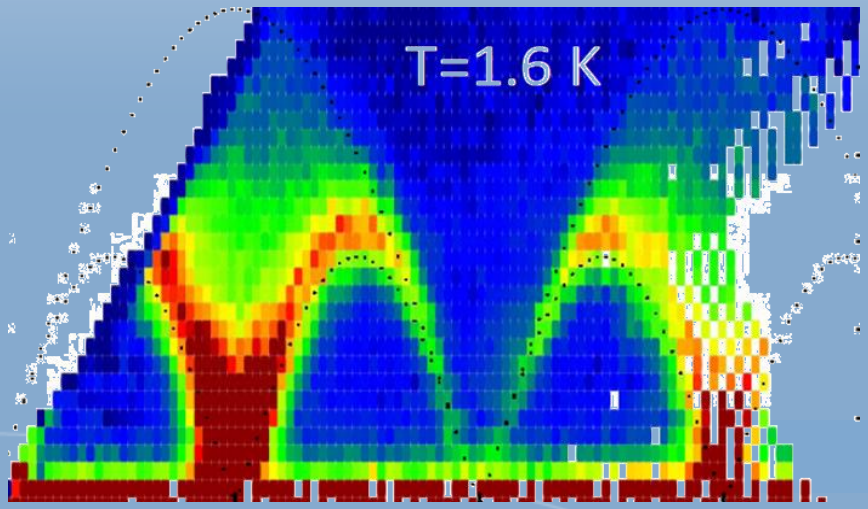
$$Q_{\boldsymbol{\kappa}} = -\boldsymbol{\sigma} \cdot \sum_n \hat{\boldsymbol{\kappa}} \times \mathbf{s}_n \times \hat{\boldsymbol{\kappa}} \exp(i\boldsymbol{\kappa} \cdot \mathbf{r}_n) \frac{1}{\sqrt{N}}$$

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{k'}{k}(\gamma r_0)^2 \left| \frac{g}{2} F(\boldsymbol{\kappa}) \right|^2 e^{-2W(\vec{\kappa})} \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \hat{\boldsymbol{\kappa}}_\alpha \hat{\boldsymbol{\kappa}}_\beta \right) S^{\alpha\beta}(\boldsymbol{\kappa}\omega)$$

$$r_0 = \frac{1}{4\pi\varepsilon_0}\frac{e^2}{mc^2} = 2.818 \text{ fm}$$

$$F(\boldsymbol{\kappa})$$

- Features of the cross section
- The dynamic correlation function
- Fluctuation Dissipation theorem
- Sum-rules
- Examples
- Summary



Understanding Inelastic Magnetic Scattering:

Isolate the "interesting part" of the cross section

$$\frac{d^2\sigma}{d\Omega dE'} \equiv \frac{k'}{k} N r_0^2 \left| \frac{g}{2} F(\mathbf{Q}) \right|^2 e^{-2W(\mathbf{Q})} \sum_{\alpha\beta} \left(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta \right) \mathcal{S}^{\alpha\beta}(\mathbf{Q},\omega)$$

The dynamic correlation function ("scattering law") :

$$\mathcal{S}^{\alpha\beta}(\mathbf{Q},\omega) \equiv \frac{1}{2\pi\hbar} \int dt\, e^{-i\omega t} \frac{1}{N} \sum_{ll'} e^{i\mathbf{Q}\cdot(\mathbf{r}_l - \mathbf{r}_{l'})} \left\langle S_l^\alpha(0) S_{l'}^\beta(t) \right\rangle$$

In thermodynamic equilibrium (detailed balance):

$$\mathcal{S}(\mathbf{Q},\omega) = \exp(\beta\hbar\omega)\, \mathcal{S}(-\mathbf{Q},-\omega)$$

Useful exact sum-rules:

Total moment sum-rule (general result from Fourier analysis)

$$\frac{1}{\int d^3\mathbf{Q}}\sum_{\alpha}\int d^3\mathbf{Q}\int \hbar \mathrm{d}\omega\, \mathcal{S}^{\alpha\alpha}(\mathbf{Q}\omega) = \langle \mathbf{S}(0)\cdot\mathbf{S}(0)\rangle = s(s+1)$$

Correlations in space & time rearrange intensity in space leaving the total scattering scattering unaffected

$\mathbf{Q}$ - w

Definition of the equal time correlation function:

$$\mathcal{S}^{\alpha\alpha}(\mathbf{Q}) \equiv \sum_{ll'}\langle S_l^{\alpha} S_{l'}^{\alpha}\rangle e^{i\mathbf{Q}\cdot(r_l - r_{l'})} = \int \mathcal{S}^{\alpha\alpha}(\mathbf{Q}\omega)\hbar\, d\omega$$

The wave vector dependence of the energy-integrated intensity probe a snap-shot of the fluctuating spin configuration

Fluctuation Dissipation Theorem

Define the following t-dependent "response" function:

$$\Phi_{\mathbf{Q}}(t) = \frac{i}{\hbar}\left\langle\left[S_{\mathbf{Q}}(t), S_{-\mathbf{Q}}\right]\right\rangle$$

The generalized susceptibility can be expressed as:

$$c(\mathbf{Q}w) = -(g\mu_B)^2 \lim_{e\to 0^+}\int_0^\infty dt e^{-i(w-ie)t}\Phi_{\mathbf{Q}}(t)$$

The "scattering law" can be expressed as:

$$\mathcal{S}(\mathbf{Q}\omega) = \frac{1}{1-e^{-\beta\hbar\omega}}\frac{1}{2\pi i}\int e^{i\omega t}\Phi_{\mathbf{Q}}(t)dt$$

From which, the "fluctuation-dissipation" theorem:

$$\mathcal{S}(\mathbf{Q}\omega) = \frac{1}{1-e^{-\beta\hbar\omega}}\frac{\chi''(\mathbf{Q}\omega)}{\pi(g\mu_B)^2}$$

First Moment Sum-rule

Fourier transform of expression for scattering law:

$$\Phi_{\mathbf{Q}}(t) = i\int d\omega e^{-i\omega t}\mathcal{S}(\mathbf{Q}\omega)\left(1-e^{-\beta\hbar\omega}\right)$$

Time derivative of left side evaluated for t=0:

$$\partial_t \Phi_{\mathbf{Q}}(t=0) = -\tfrac{1}{2}\left\langle\left[S_{\mathbf{Q}},\left[S_{-\mathbf{Q}},\mathcal{H}\right]\right]\right\rangle$$

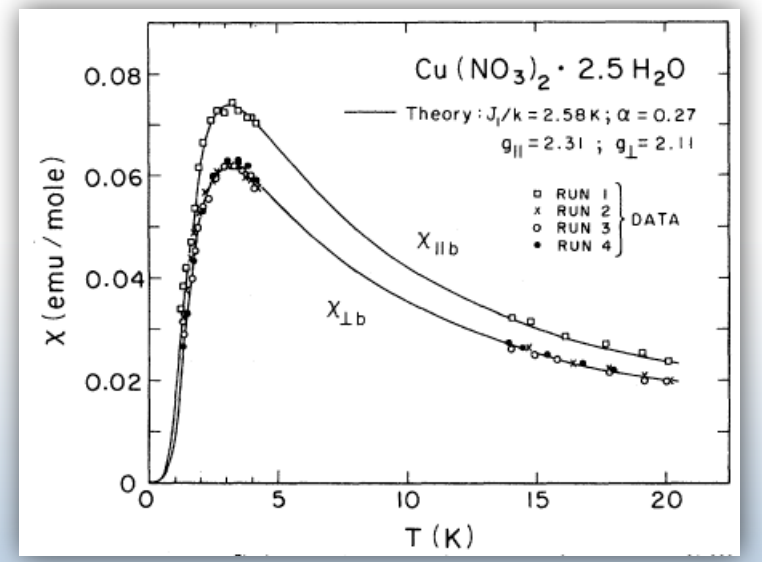
Time derivative of right side evaluated at t=0:

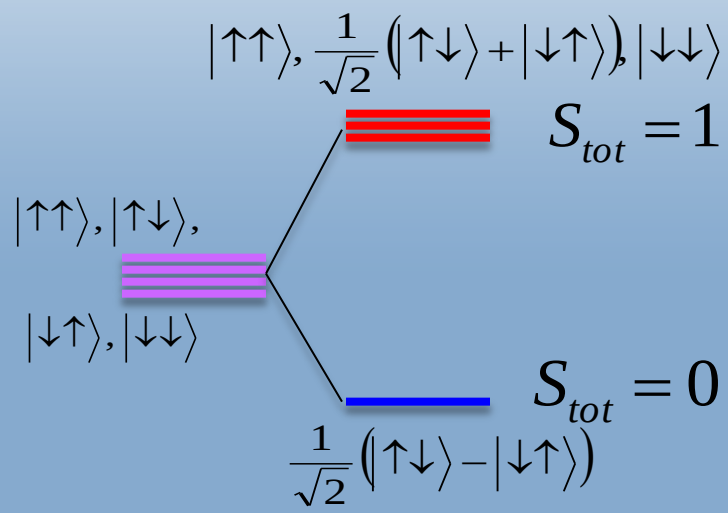
$$\int \omega\, d\omega\, \mathcal{S}(\mathbf{Q}\omega)\left(1-e^{-\beta\hbar\omega}\right) = 2\int \omega\, d\omega\, \mathcal{S}(\kappa\omega)$$

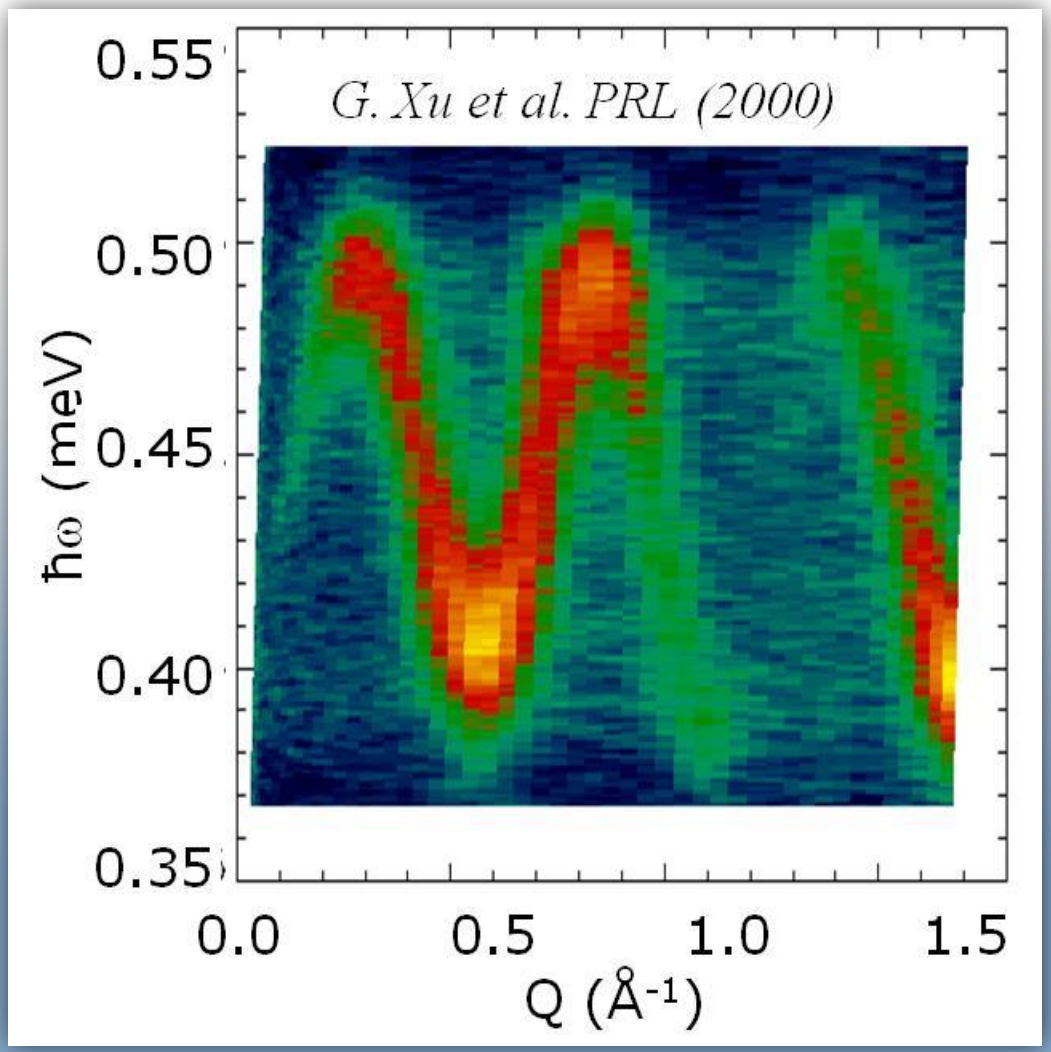
Equating these leads to the first moment sum-rule:

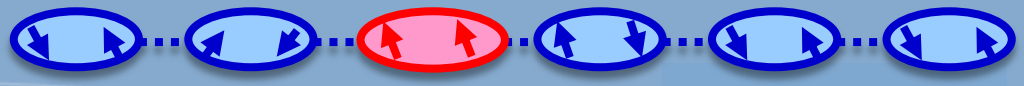
$$\int \hbar\omega\, \hbar\, d\omega\, \mathcal{S}(\mathbf{Q}\omega) = -\tfrac{1}{2}\left\langle\left[S_{\mathbf{Q}},\left[S_{-\mathbf{Q}},\mathcal{H}\right]\right]\right\rangle$$

Weakly Interacting spin-1/2 pairs in Cu-nitrate









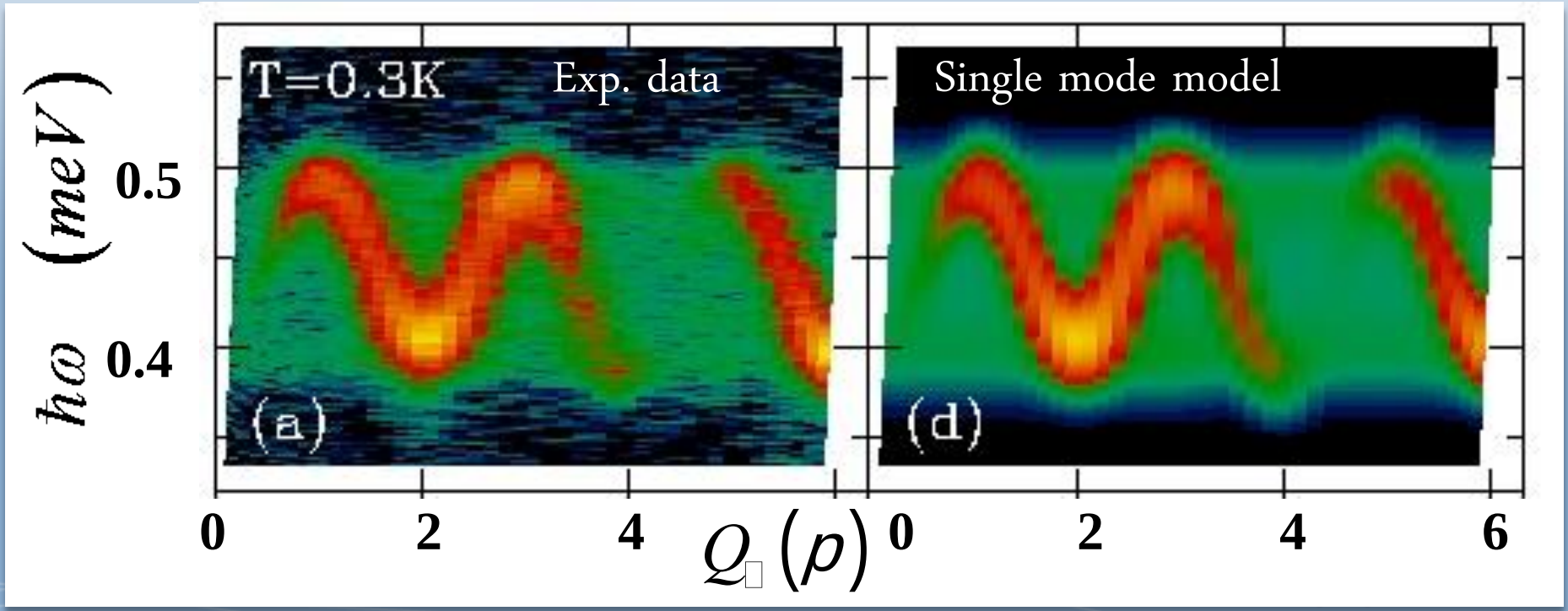
Sum rules and the single mode approximation

When a coherent mode dominates the spectrum:

$$\mathcal{S}(\mathbf{Q},\omega) \approx \mathcal{S}(\mathbf{Q})\delta\left(\hbar\omega - \varepsilon(\mathbf{Q})\right)$$

Sum-rules link $\mathcal{S}(\mathbf{Q})$ and $\varepsilon(\mathbf{Q})$:

$$\mathcal{S}(\mathbf{Q}) \approx \frac{\hbar^2 \int \omega \; d\omega \; \mathcal{S}(\mathbf{Q},\omega)}{\varepsilon(\mathbf{Q})} = -\frac{1}{3}\frac{\frac{1}{N}\sum_{ll'} J_{ll'} \langle \mathrm{S}_l \cdot \mathrm{S}_{l'} \rangle \left(1 - \cos \mathbf{Q}\cdot\left(\mathrm{r}_l - \mathrm{r}_{l'}\right)\right)}{\varepsilon(\mathbf{Q})}$$

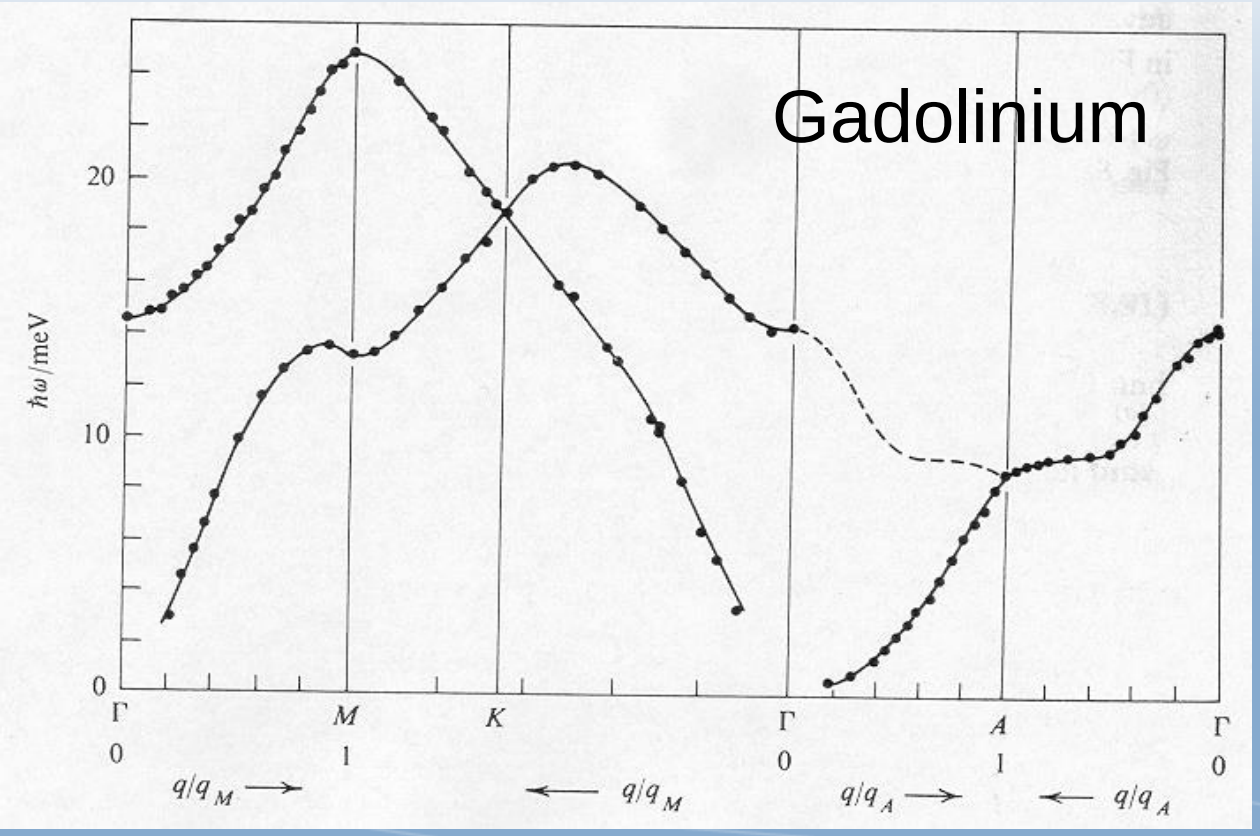


Spin waves in a ferromagnet

$$\mathcal{S}^{\perp}(\mathbf{Q},\omega)=\frac{S}{2}\left\{\delta\left(\varepsilon(\mathbf{Q})-\hbar\omega\right)\left(n(\hbar\omega)+1\right)+\delta\left(\varepsilon(\mathbf{Q})+\hbar\omega\right)n(\hbar\omega)\right\}$$

Magnon creation

Magnon destruction



Dispersion relation

$$\varepsilon(\mathbf{Q})=2S\left(\mathrm{J}(0)-\mathrm{J}(\mathbf{Q})\right)$$

Occupation number

$$n(w)=\frac{1}{e^{b\hbar w}-1}$$

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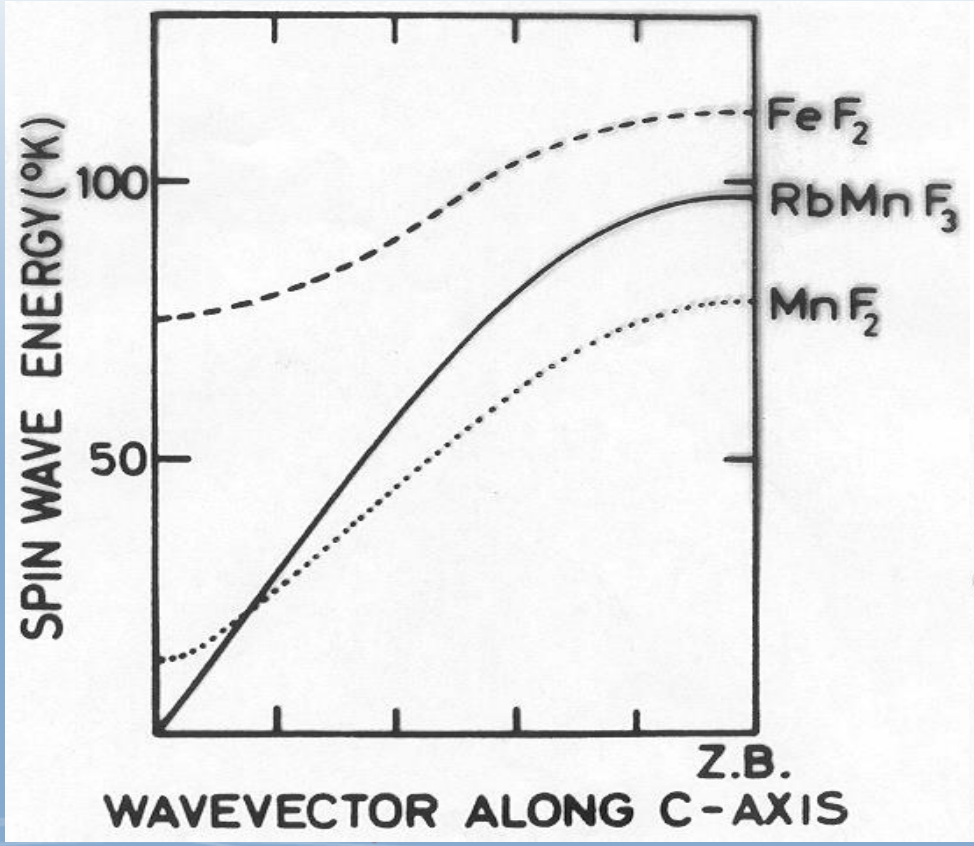
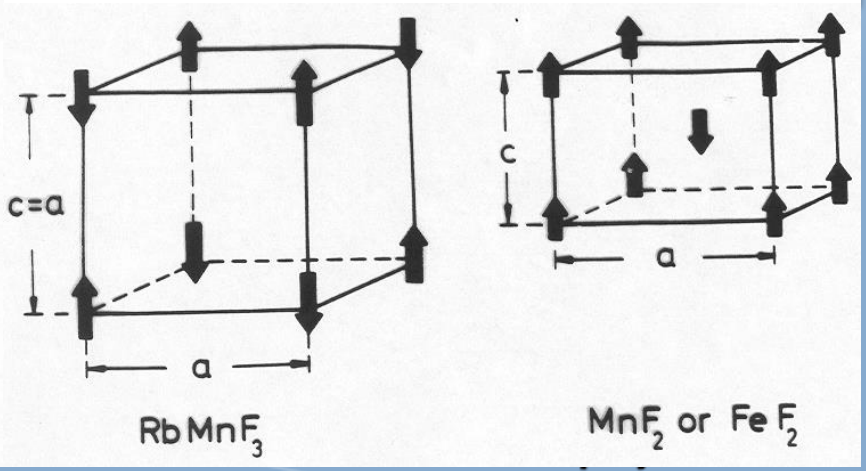
Spin waves in an antiferromagnet

$$\hat{S}(\mathbf{Q},w) = \frac{S}{2}\frac{J\left(1-\frac{1}{z}\sum_{d} e^{i\mathbf{Q}\cdot\mathbf{d}}\right)}{\varepsilon(\mathbf{Q})} \times \left\{\delta\left(\varepsilon(\mathbf{Q})-\hbar w\right)\left(n(\hbar w)+1\right)+\delta\left(\varepsilon(\mathbf{Q})+\hbar w\right)n(\hbar w)\right\}$$



Dispersion relation

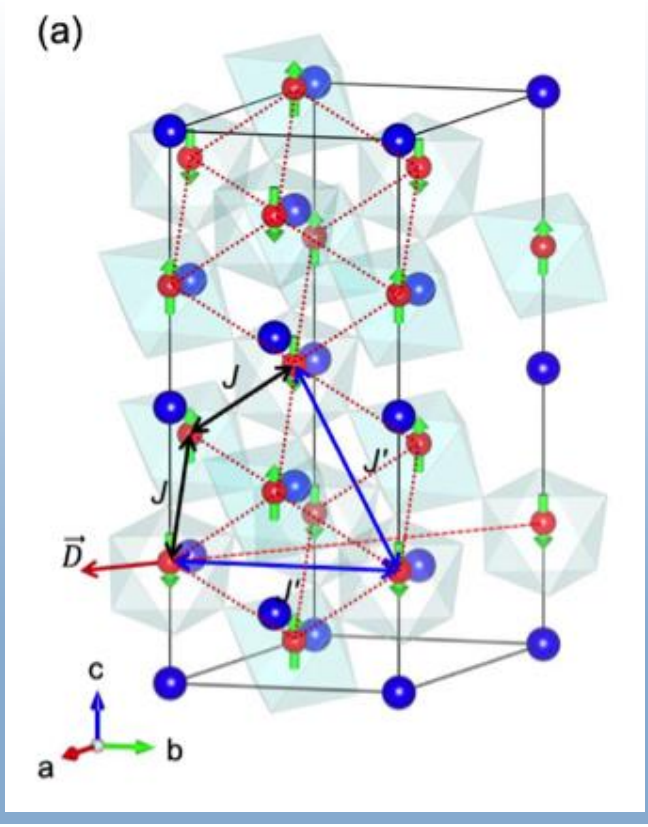
$$\varepsilon(\mathbf{Q}) = 2S\sqrt{J(0)^2 - J(\mathbf{Q})^2}$$

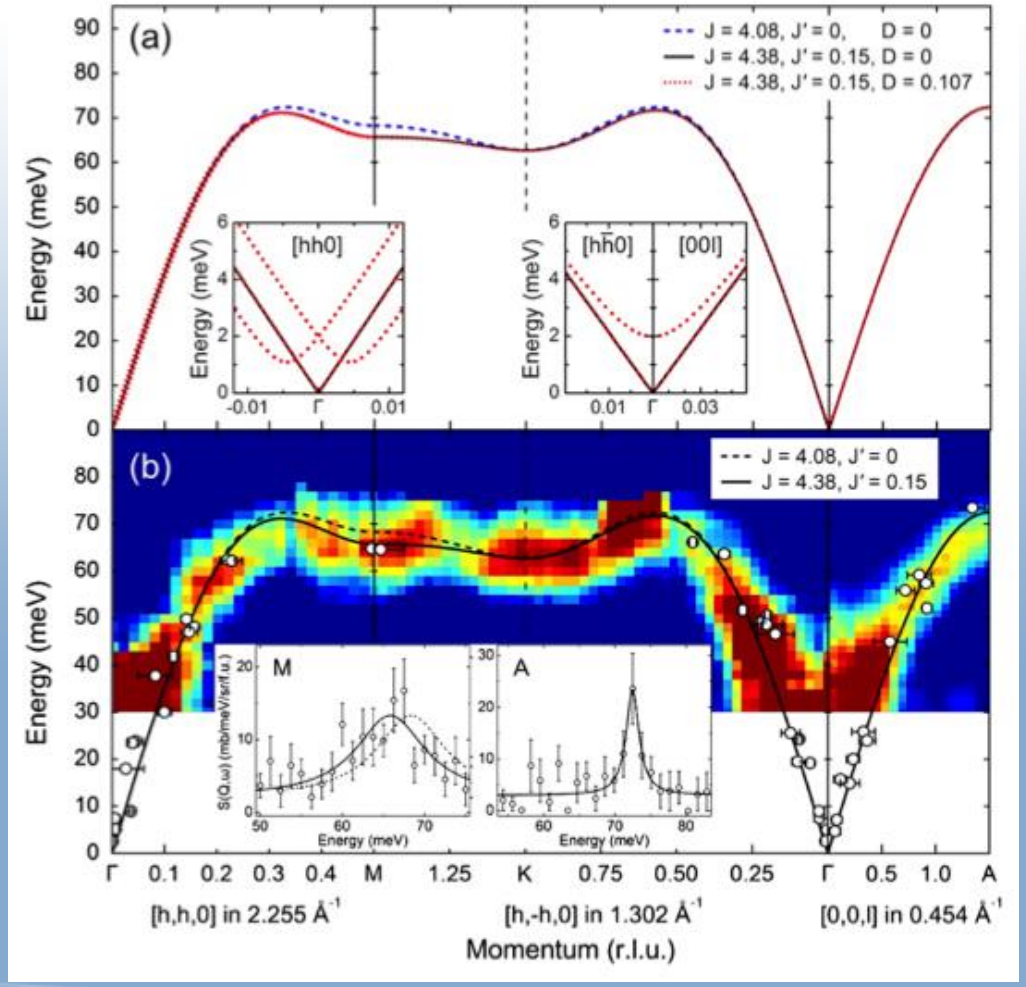


PRL 108, 077202 (2012) PHYSICAL REVIEW LETTERS week ending 17 FEBRUARY 2012

Spin Wave Measurements over the Full Brillouin Zone of Multiferroic $BiFeO_3$

Jaehong Jeong,[1] E. A. Goremychkin,[2] T. Guidi,[2] K. Nakajima,[3] Gun Sang Jeon,[4] Shin-Ae Kim,[5] S. Furukawa,[6] Yong Baek Kim,[6] Seongsu Lee,[5] V. Kiryukhin,[7] S-W. Cheong,[7] and Je-Geun Park[1,8,*]

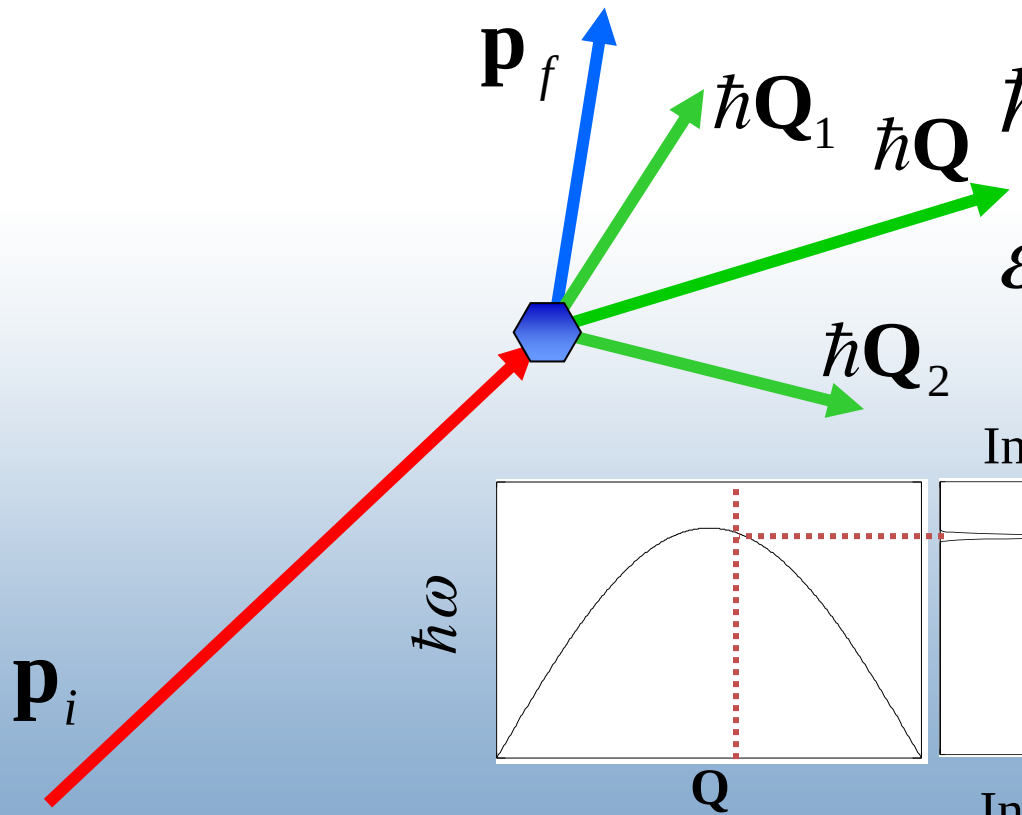




$$H = J\sum_{\mathrm{NN}} \mathbf{S}_i \cdot \mathbf{S}_j + J'\sum_{\mathrm{NNN}} \mathbf{S}_i \cdot \mathbf{S}_j - \mathbf{D} \cdot \sum_i (\mathbf{S}_i \times \mathbf{S}_{i+\hat{\delta}}),$$

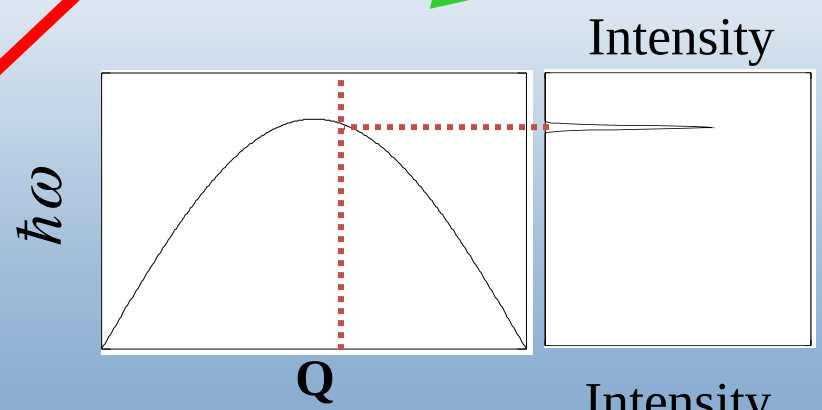
$J = 4.38$ meV J¢= 0.15 meV $D = 0.107$ meV

Probing matter through scattering

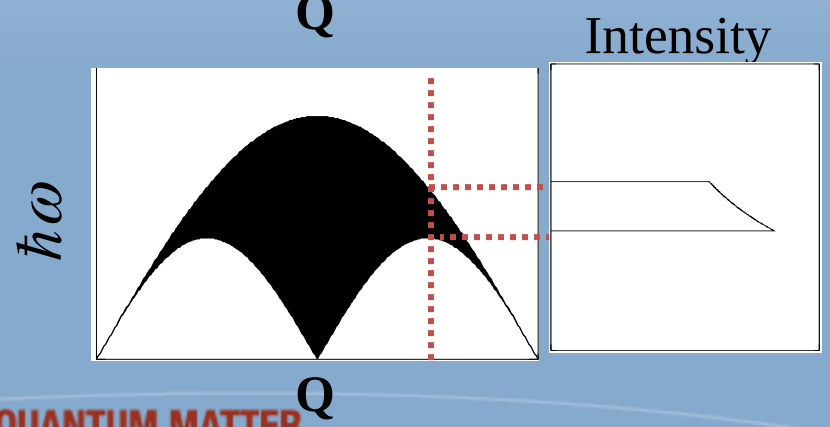


$$\hbar(\mathbf{Q}_1 + \mathbf{Q}_2) = \mathbf{p}_i - \mathbf{p}_f$$

$$\varepsilon(\mathbf{Q}_1) + \varepsilon(\mathbf{Q}_2) = E_i - E_f$$

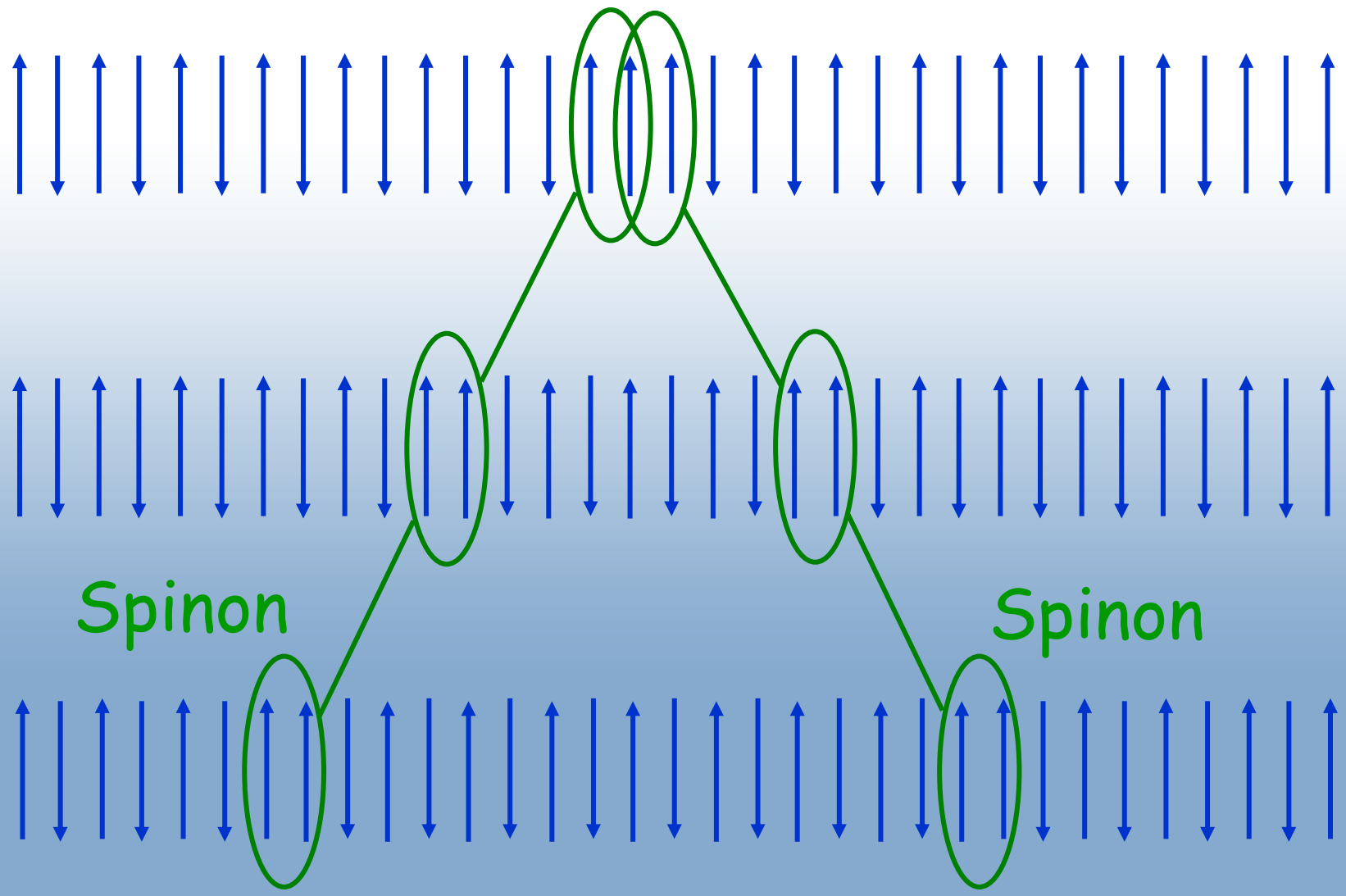


Single Particle Process

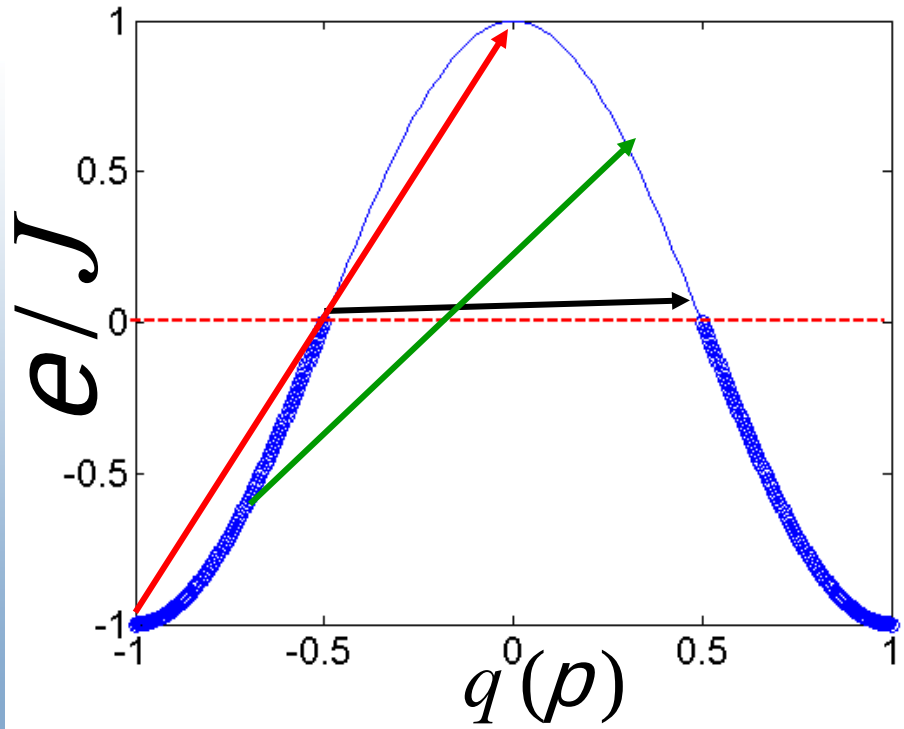


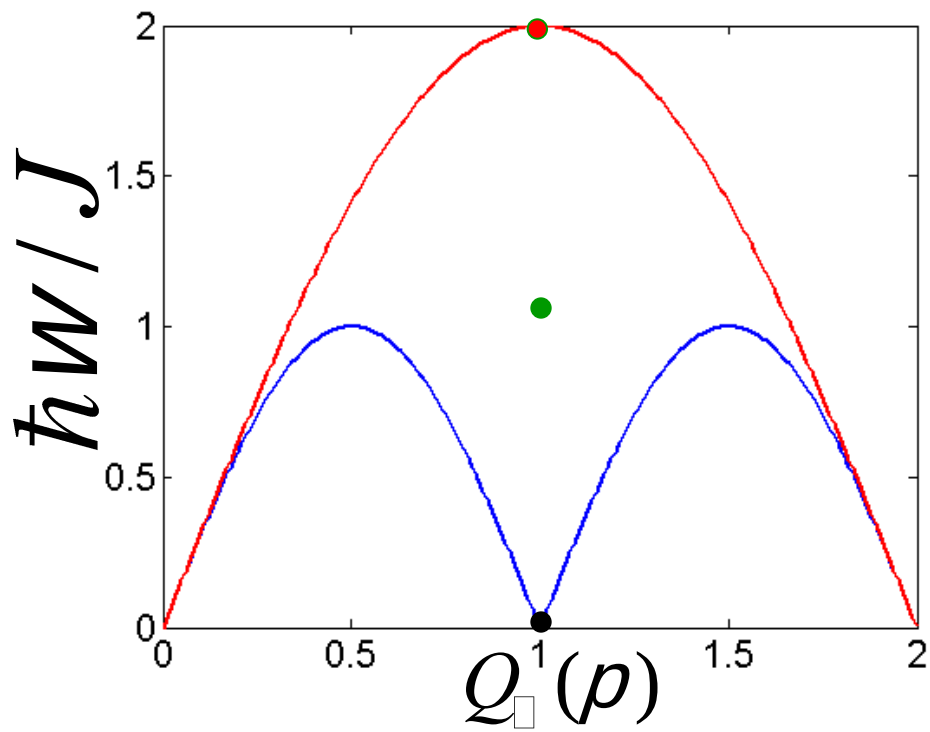
Multi Particle Process

Disintegration of a spin flip in 1D



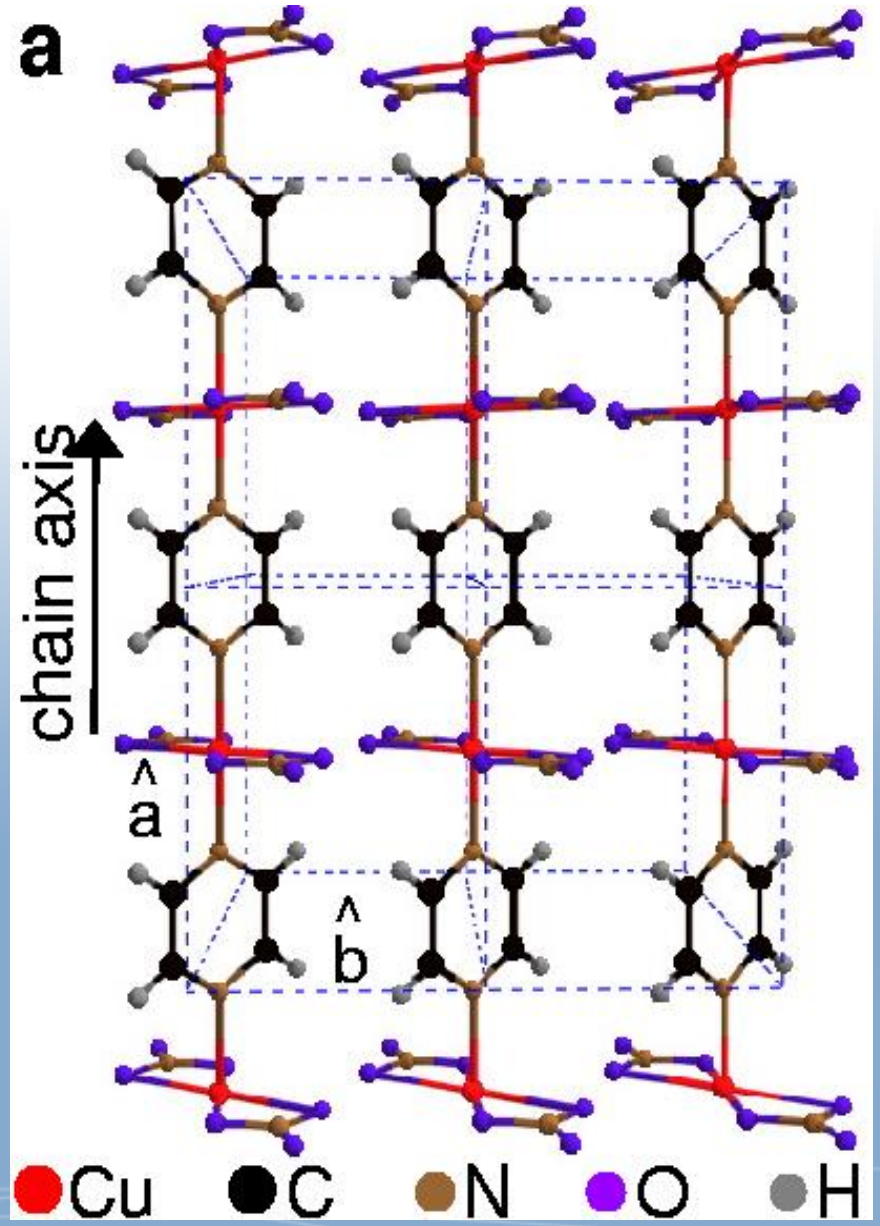
From spinon band-structure to bounded continuum



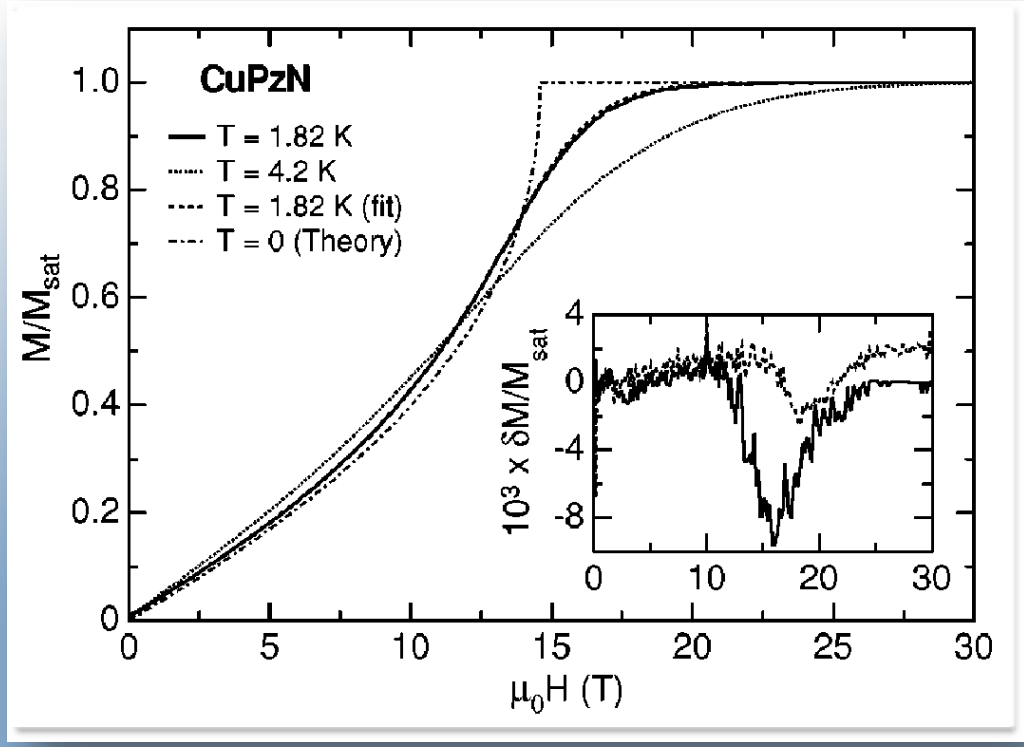


$$S_{\mu\mu}(Q,\omega) = 2\pi \sum_{\lambda} \left| \langle G | S_Q^{\mu} | \lambda \rangle \right|^2 \delta(\omega - \omega_{\lambda})$$

Quantum critical spin-1/2 chain

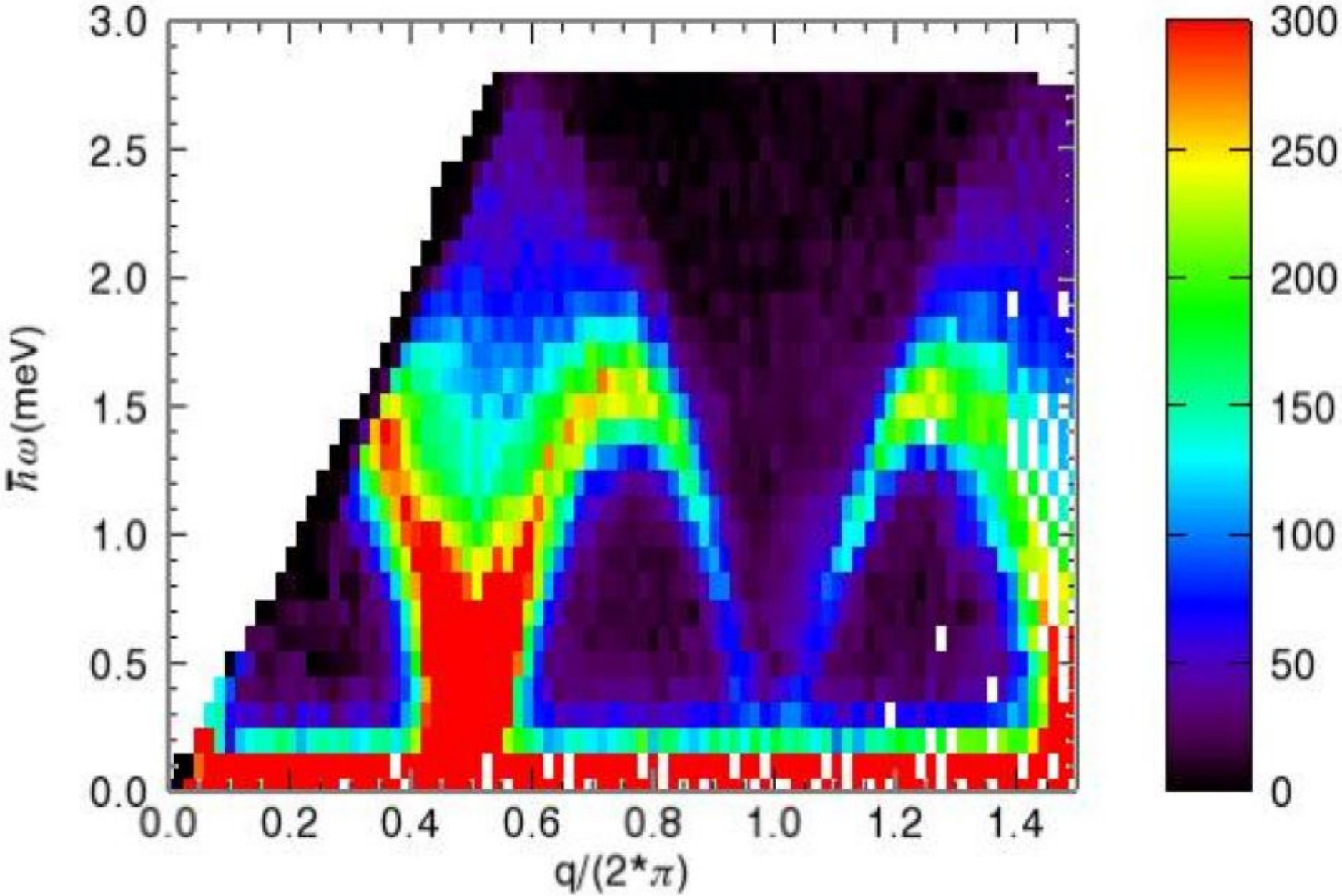


$Cu(C_4H_4N_2)(NO_3)_2$



Hammar et al. (1999)

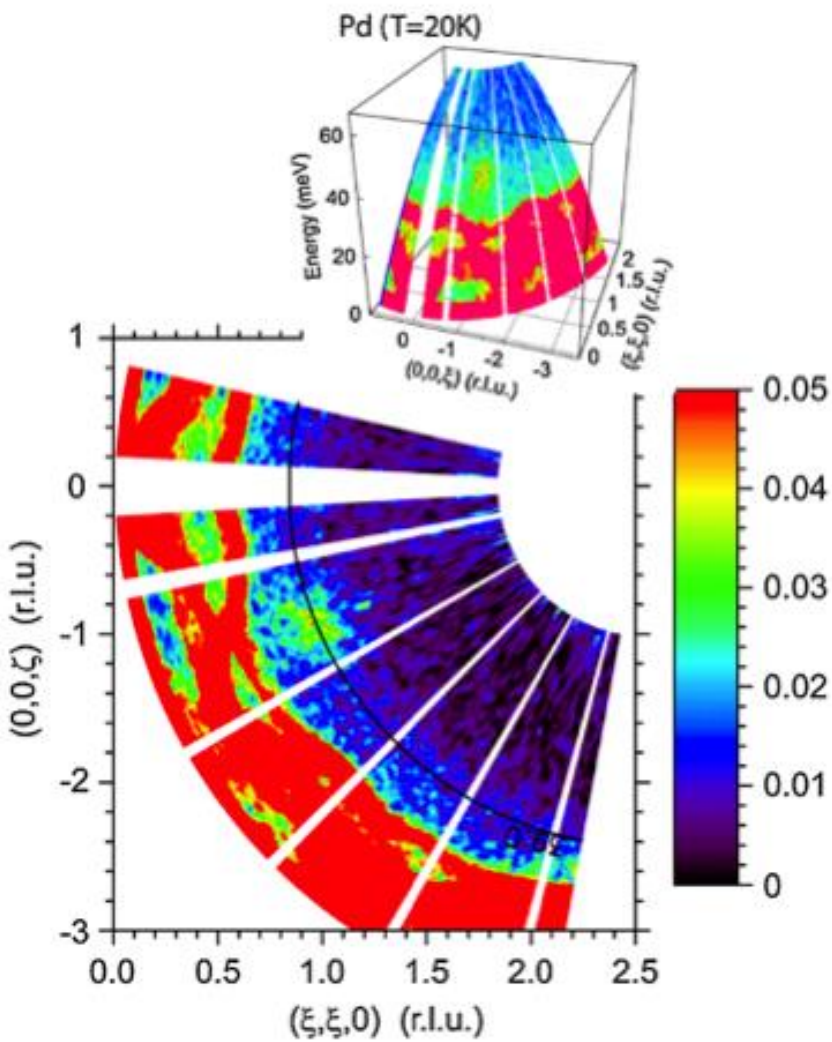
Copper Pyrazine dinitrate

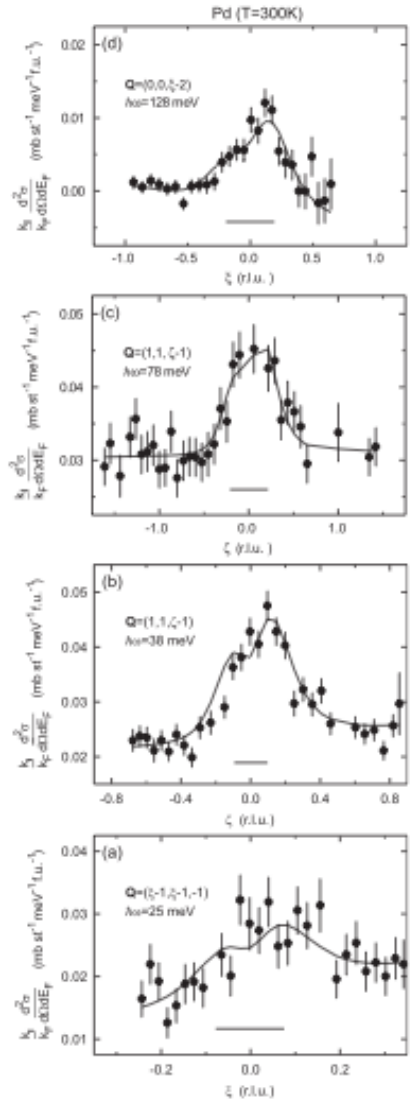


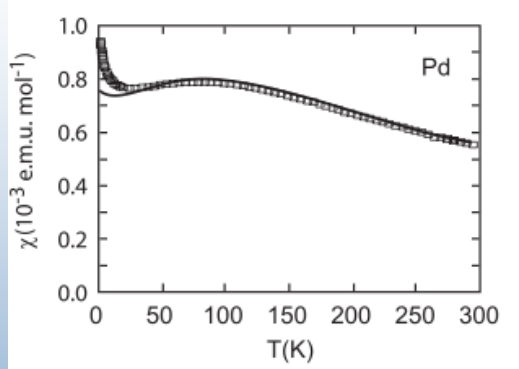
PRL 105, 027207 (2010) PHYSICAL REVIEW LETTERS week ending 9 JULY 2010

Direct Observation of Paramagnons in Palladium

R. Doubble,[1] S. M. Hayden,[1,*] Pengcheng Dai,[2,3] H. A. Mook,[3] J. R. Thompson,[2,3] and C. D. Frost[4]







$$\frac{d^2\sigma}{d\Omega dE} = \frac{2(\gamma r_e)^2}{\pi g^2 \mu_B^2}\frac{k_f}{k_i}|F(\mathbf{Q})|^2 \frac{\chi''(\mathbf{Q},\hbar\omega)}{1-\exp(-\hbar\omega/kT)}, \quad (1)$$

$$\chi''(q,\omega) = \frac{\chi(q)\omega\Gamma(q)}{\Gamma^2(q)+\omega^2}, \quad (2)$$

where the relaxation rate $\Gamma(q)$ is given by

$$\Gamma(q) = \gamma q \chi^{-1}(q) \quad (3)$$

and the wave-vector–dependent susceptibility $\chi(q) = \chi(q, \omega = 0)$ is given by

$$\chi^{-1}(q) = \chi^{-1} + cq^2. \quad (4)$$

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Summary

- **Inelastic Magnetic scattering probes dynamic spin correlation function:**
- **Exact results are critical to interpret data**
- **The full dynamic correlation function as opposed to just the dispersion relation tells the story**
  - Intensity gives equal time correlation function
  - Energy width in resonant excitations probes life time
  - Broad continuum reveals multiparticle excitations
- **Know your sum-rules and happy scattering!**