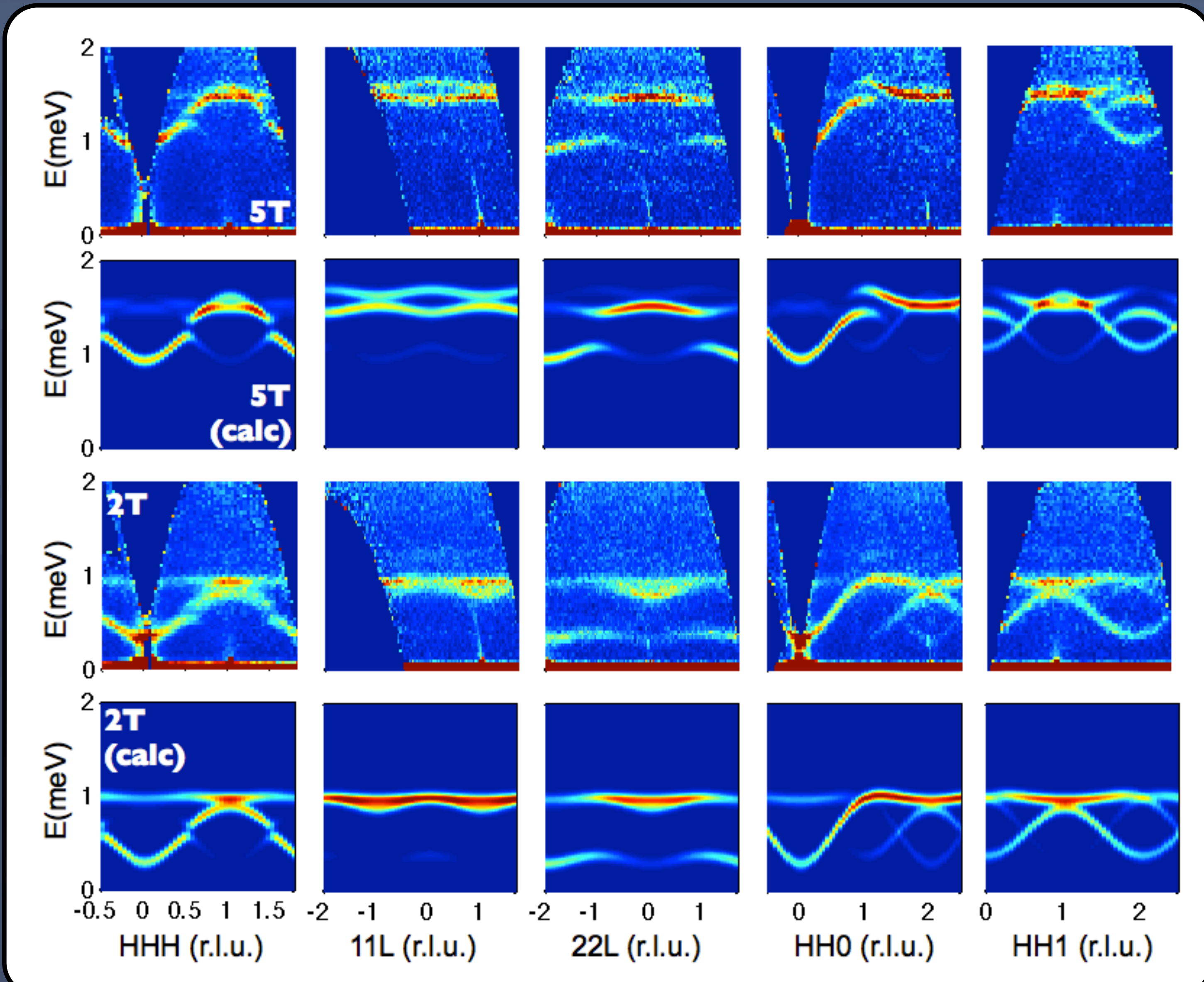
Magnetic Neutron Scattering:

Elucidating Structure and Dynamics of Highly Frustrated Magnets



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E. Kermarrec [1]
J.P. Clancy [1,3]
J.P.C. Ruff [1,4]
K. Fritsch [1,5]
H.A. Dabkowska [1]
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J. Zhang [1]
D.D. Maharaj [1]
J. Gaudet [1]
J.B. Kycia [6]
D. Pomaranski [6]
M.A. White [7]
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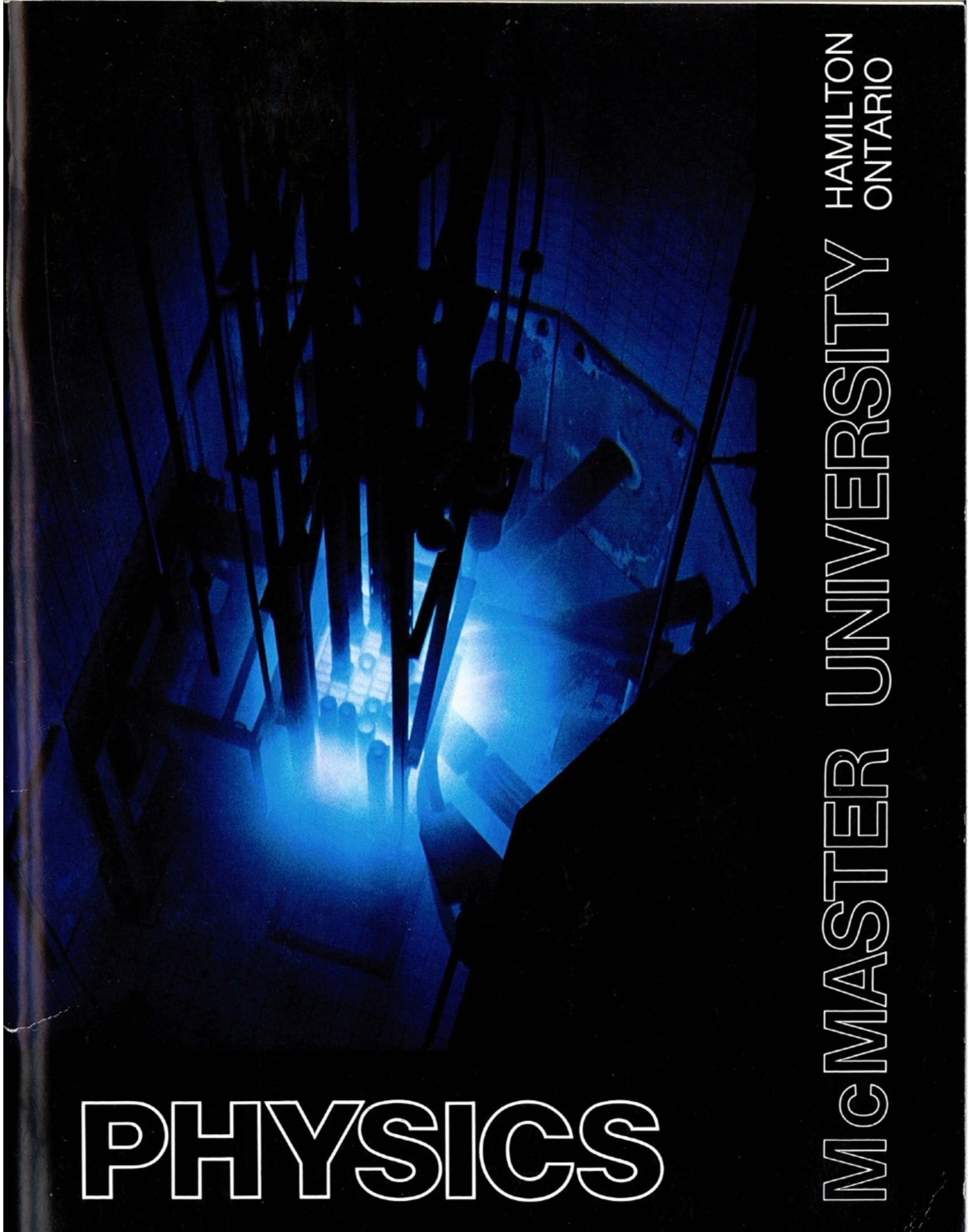


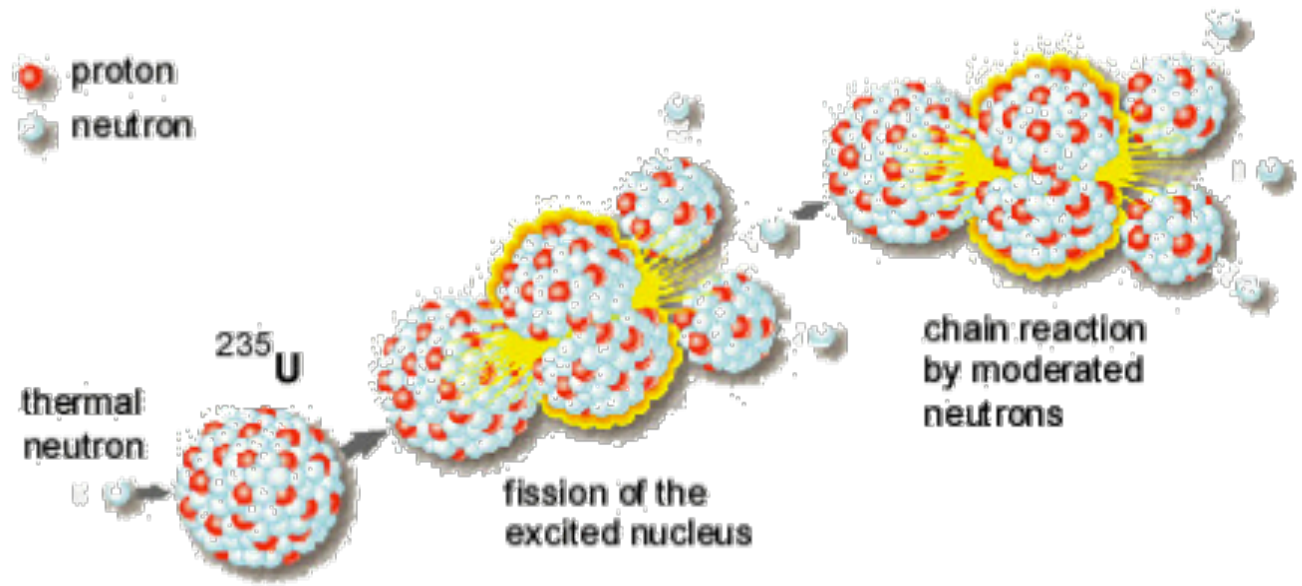
$^{235}U + n$

daughter nuclei +
2-3 n + gammas

neutrons:

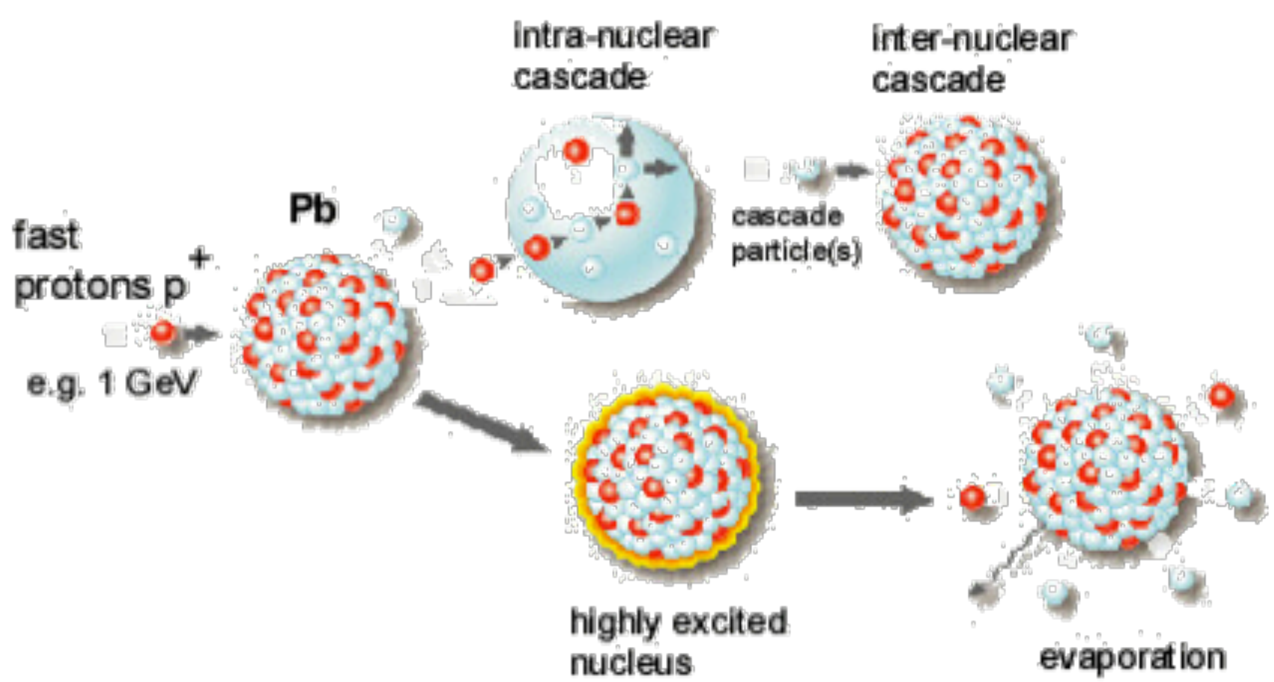
no charge
s=1/2
massive: $mc^2 \sim 1$ GeV

How do we produce neutrons



Fission

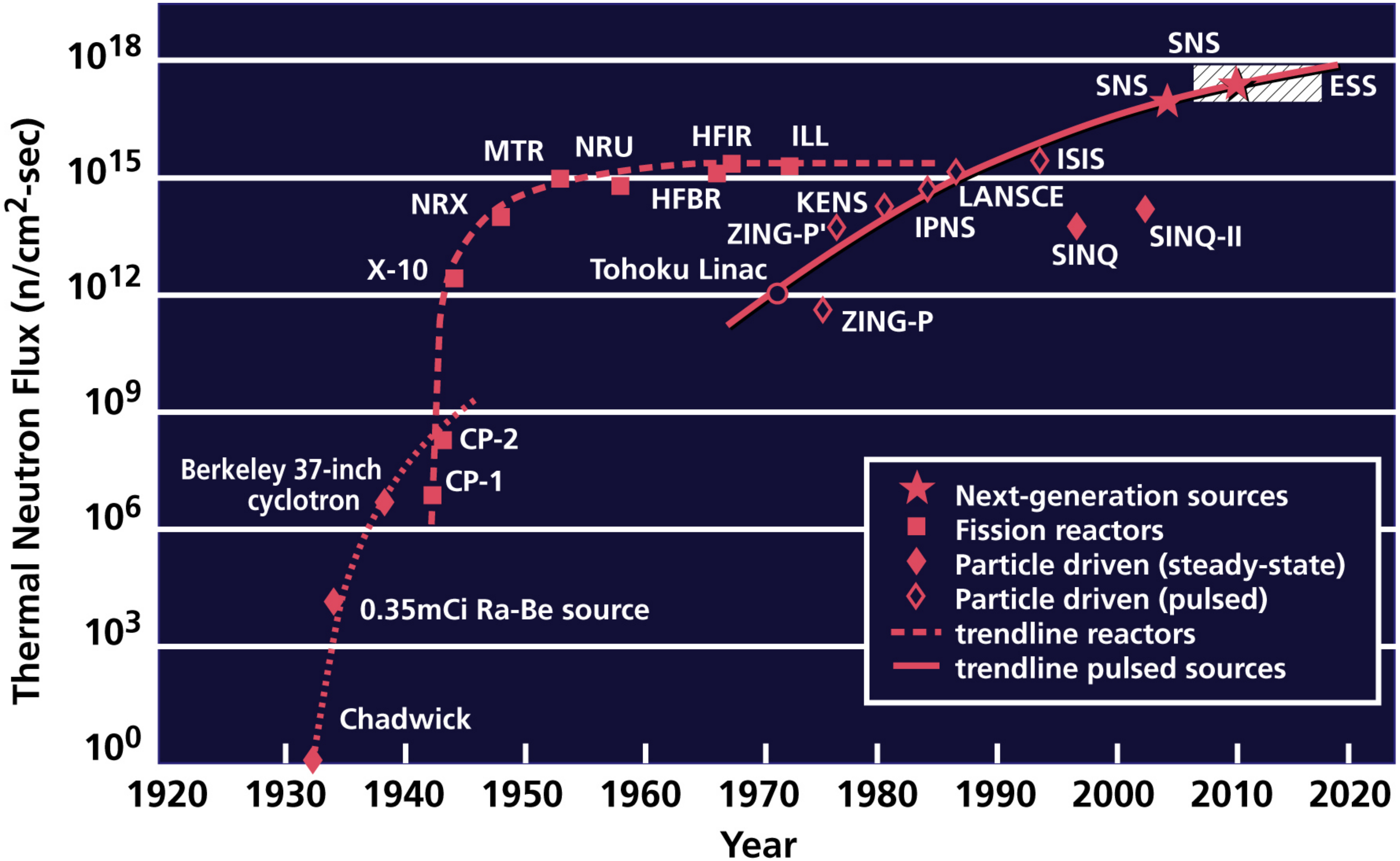
- chain reaction
- continuous flow
- 1 neutron/fission



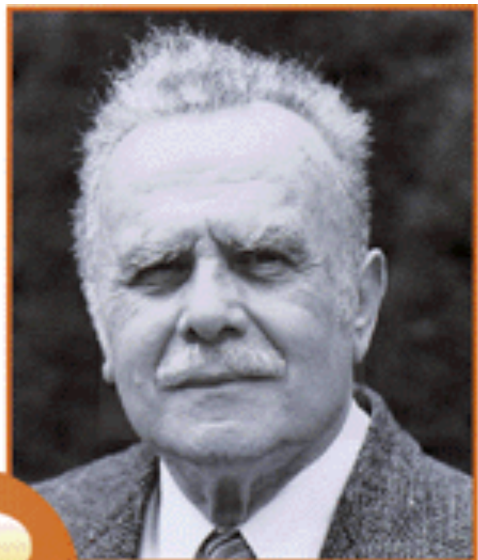
Spallation

- no chain reaction
- pulsed operation
- 30 neutrons/proton

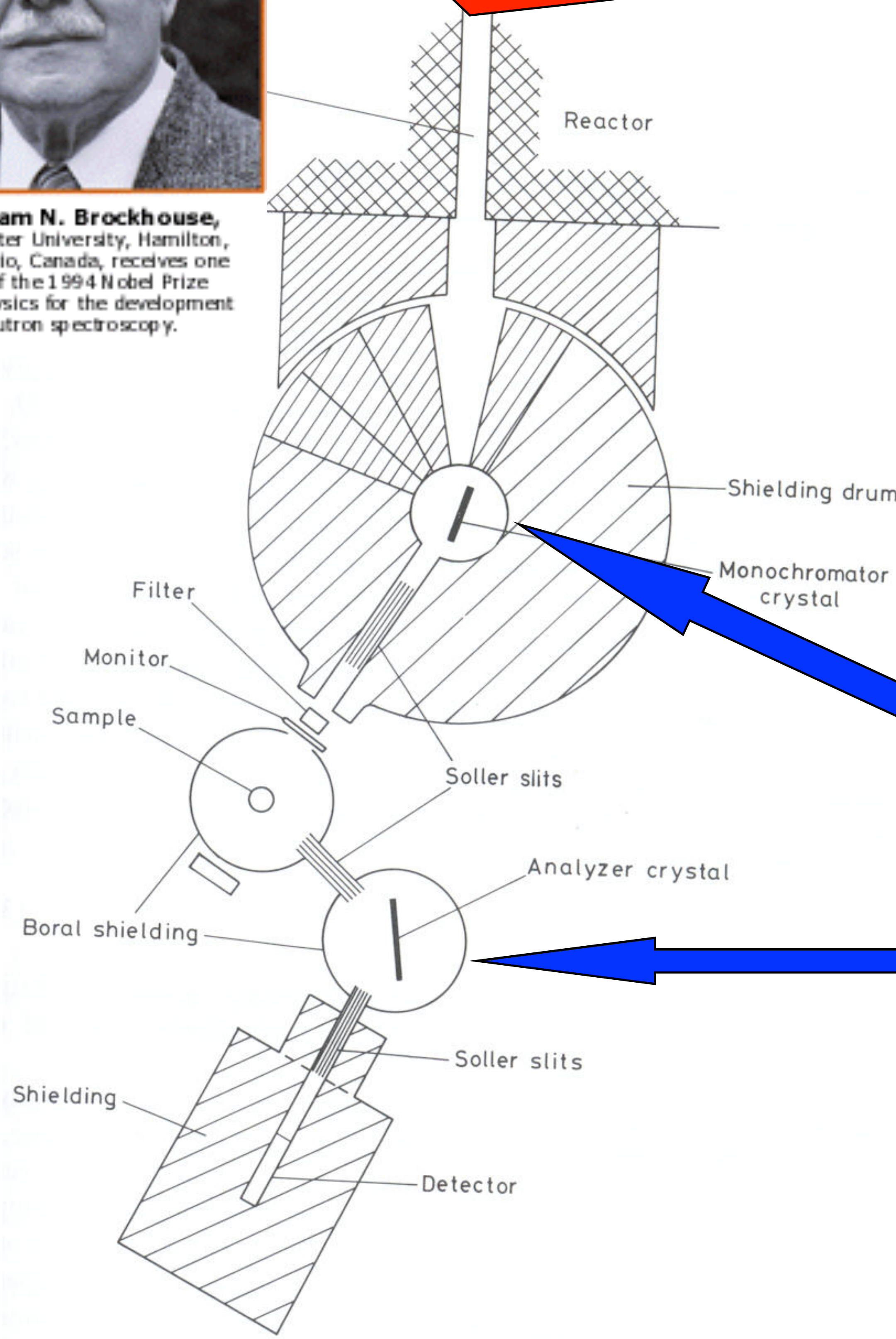
Development of Neutron Science Facilities

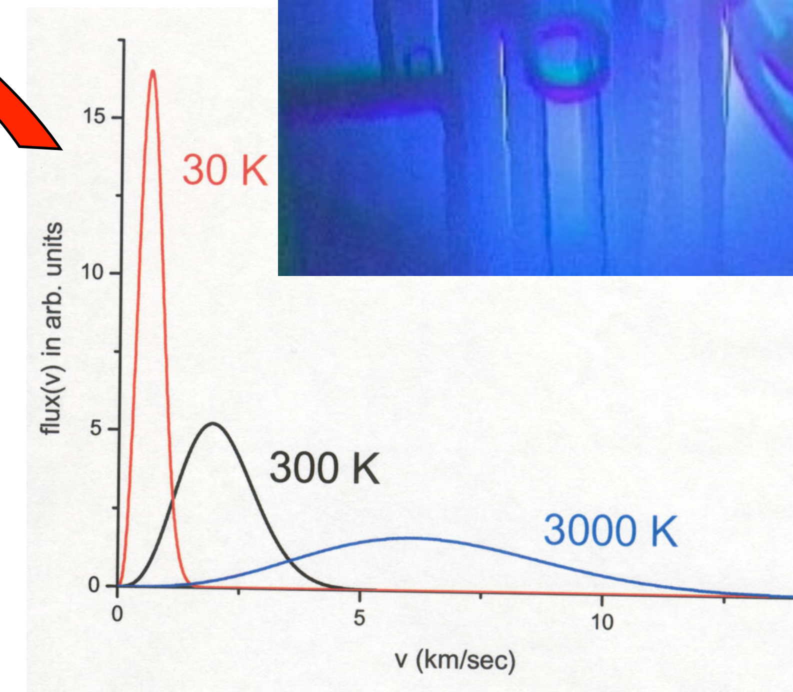


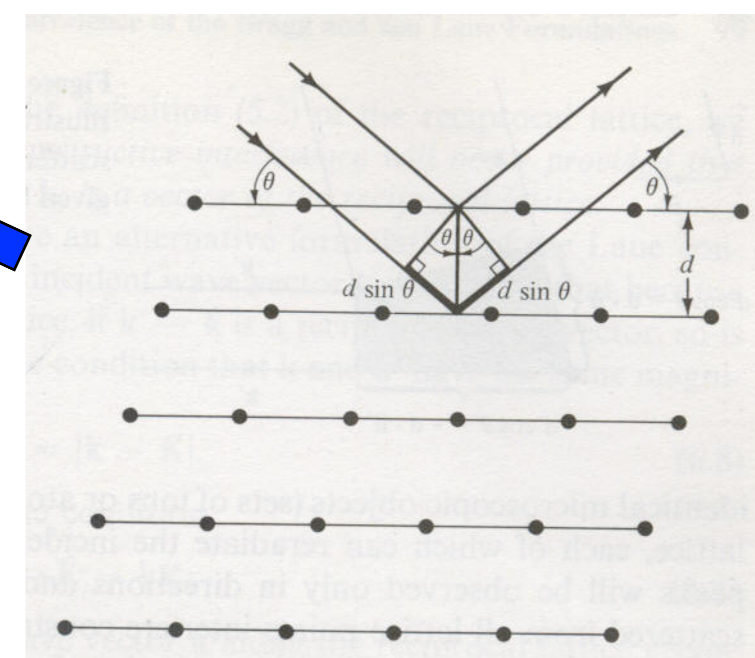
(Updated from *Neutron Scattering*, K. Skold and D. L. Price: eds., Academic Press, 1986)



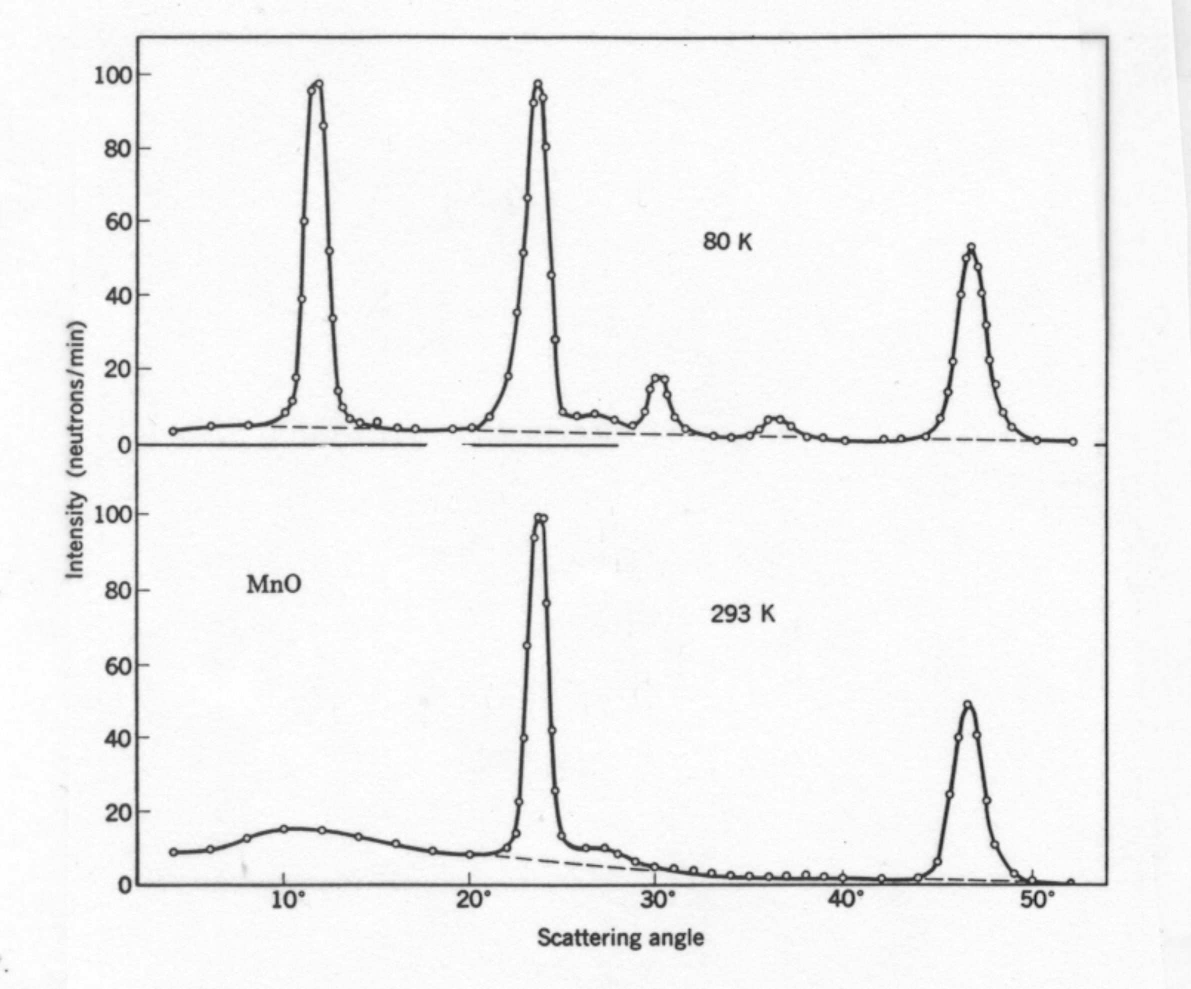
Betram N. Brockhouse, McMater University, Hamilton, Ontario, Canada, receives one half of the 1994 Nobel Prize in Physics for the development of neutron spectroscopy.

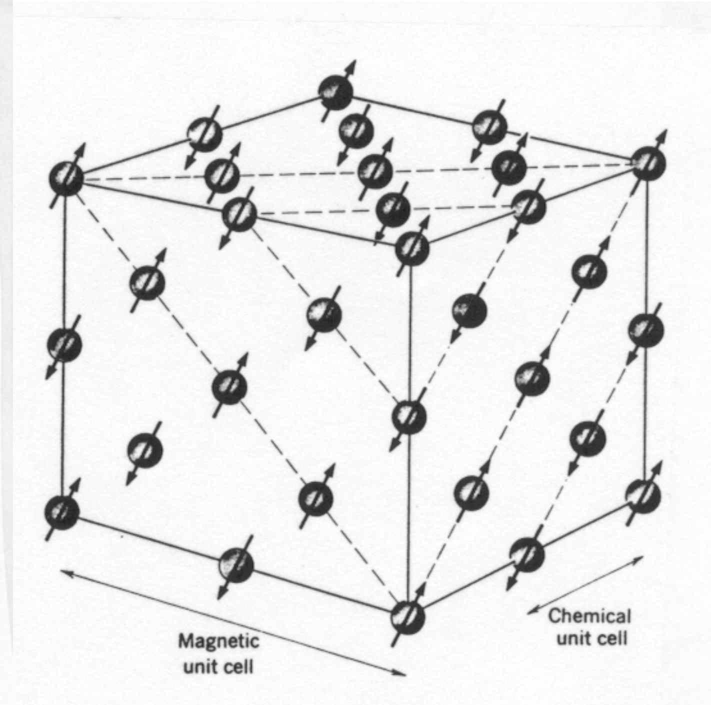




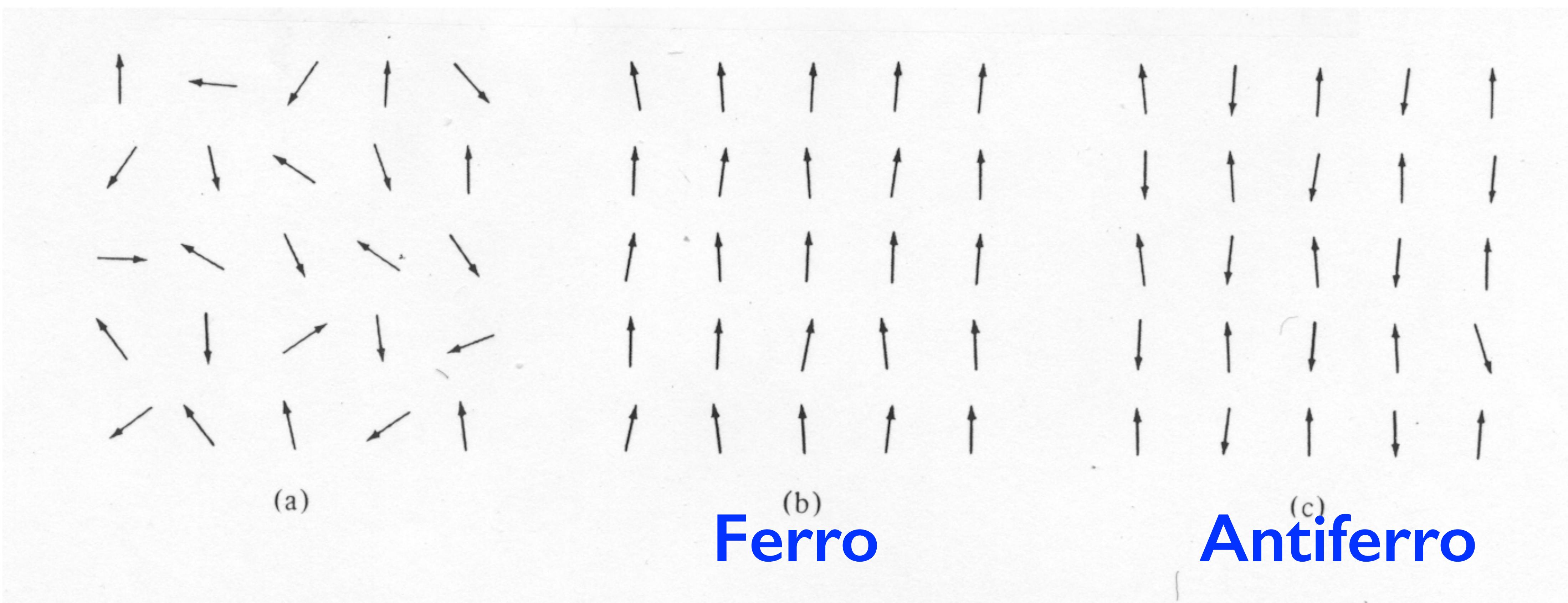


Bragg's Law: nλ = 2d sin(θ)





Clifford G. Shull, MIT, Cambridge, Massachusetts, USA, receives one half of the 1994 Nobel Prize in Physics for development of the neutron diffraction technique.

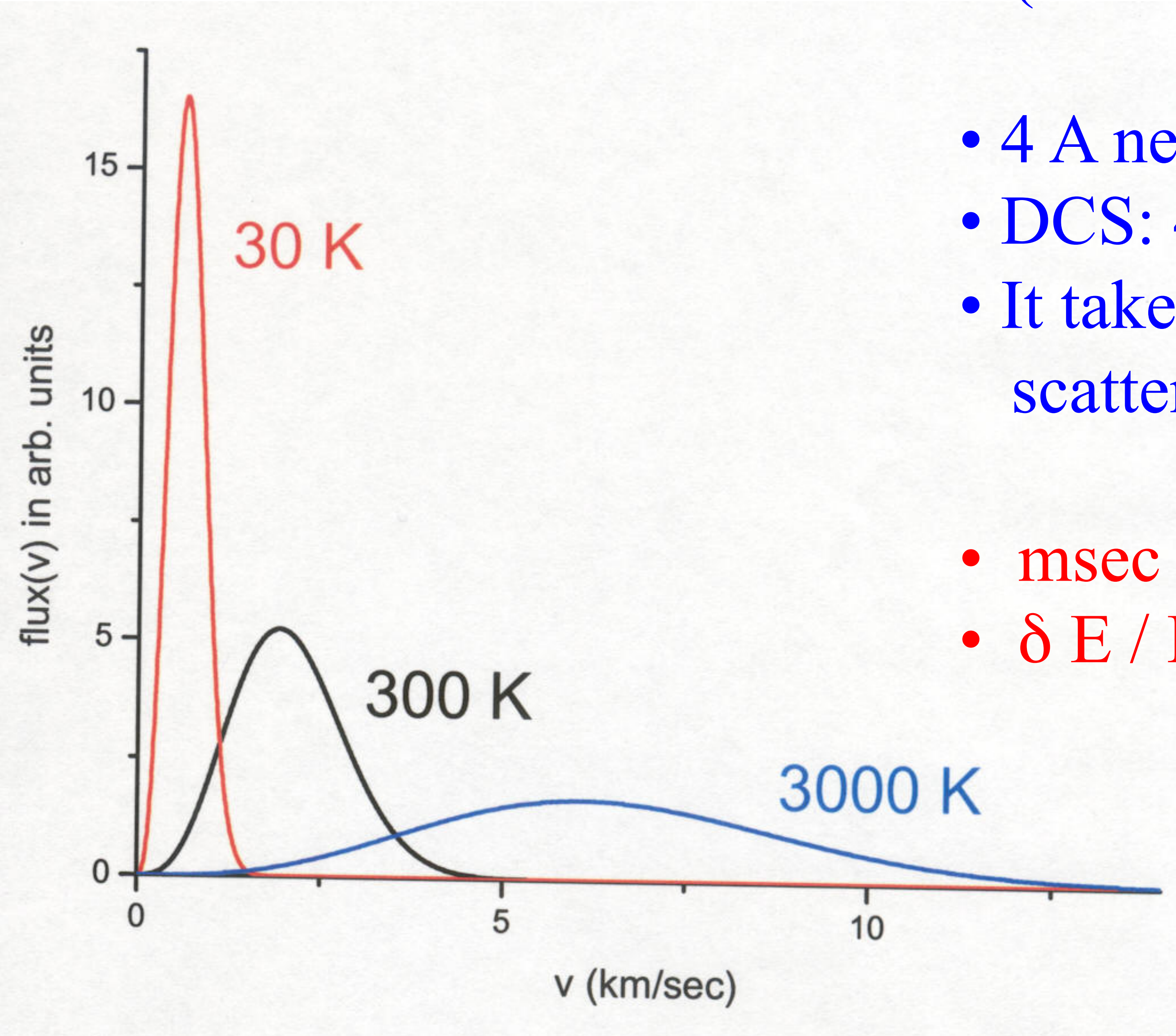


T > Tc

T < Tc

Neutrons have *mass*
so higher energy means faster – lower energy means slower

v (km/sec) = 3.96 / λ (A)

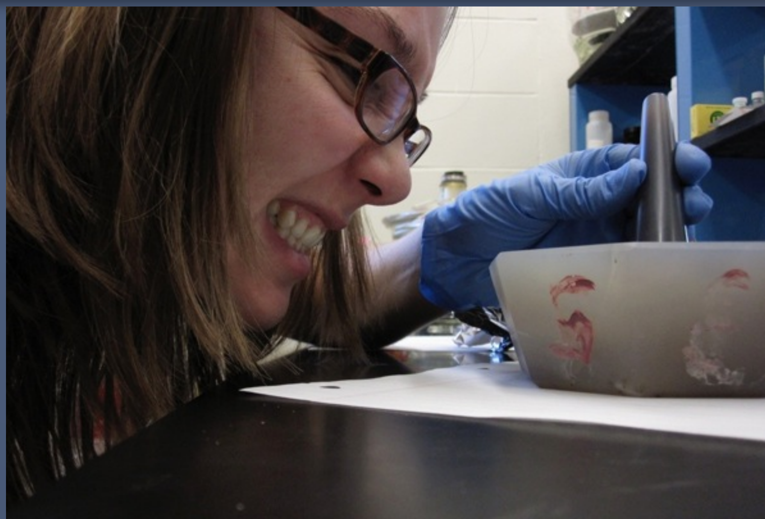


- 4 A neutrons move at ~ 1 km/sec
- DCS: 4 m from sample to detector
- It takes 4 msec for elastically scattered 4 A neutrons to travel 4 m

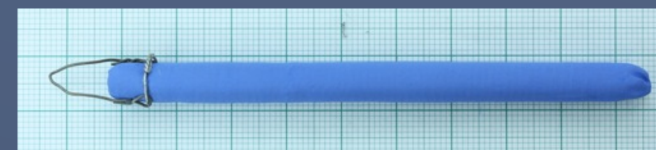
- msec timing of neutrons is easy
- δ E / E ~ 1-3 % - very good !

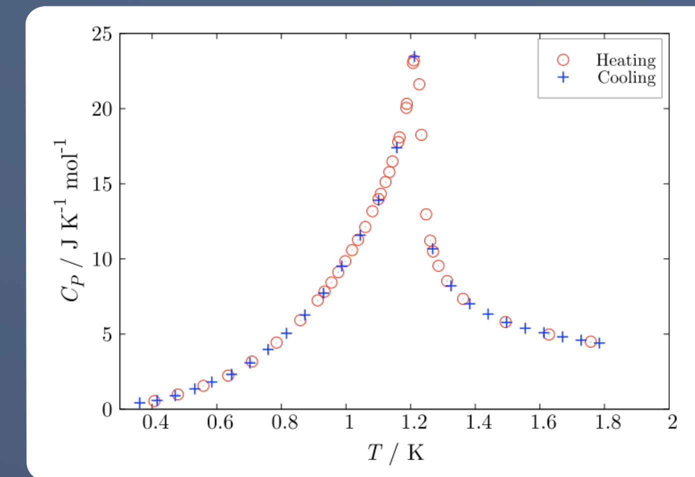
We can measure a neutron's energy, wavelength by measuring its *speed*

Life Cycle of a New Material

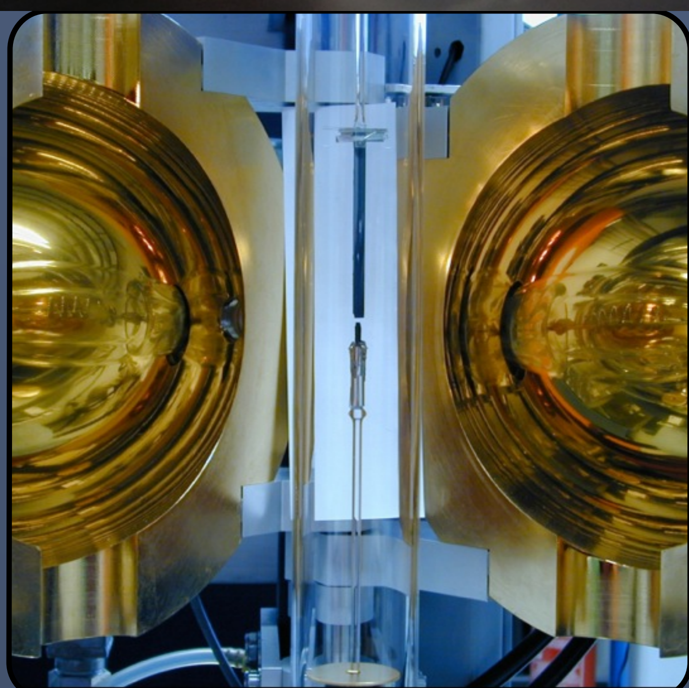


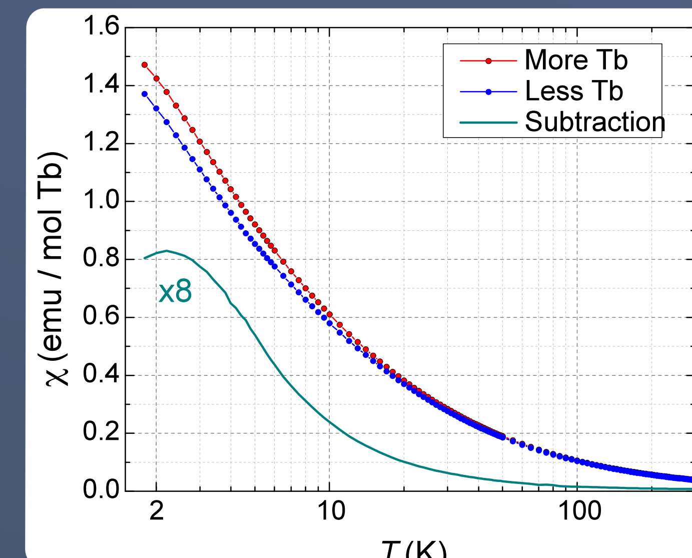
Synthesize Polycrystalline Materials





Characterize Polycrystalline Materials





Grow Single Crystals

Advanced Characterization

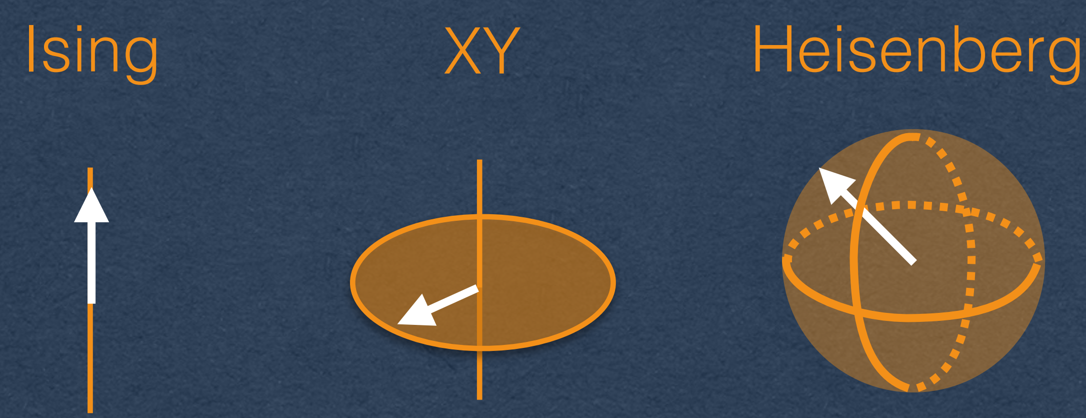
PHYSICAL REVIEW X **1**, 021002 (2011)

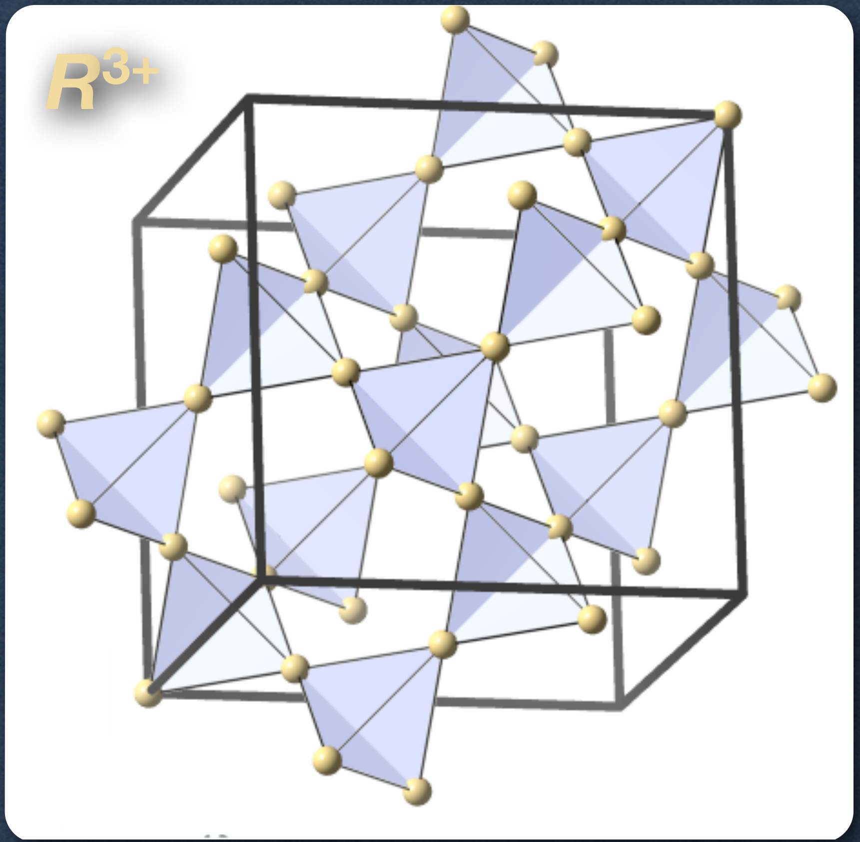
Quantum Excitations in Quantum Spin Ice

Kate A. Ross,[1] Lucile Savary,[2] Bruce D. Gaulin,[1,3,4] and Leon Balents[5,*]

Real Pyrochlores: playgrounds for frustration

$R_2Ti_2O_7$ "Rare earth titanates"

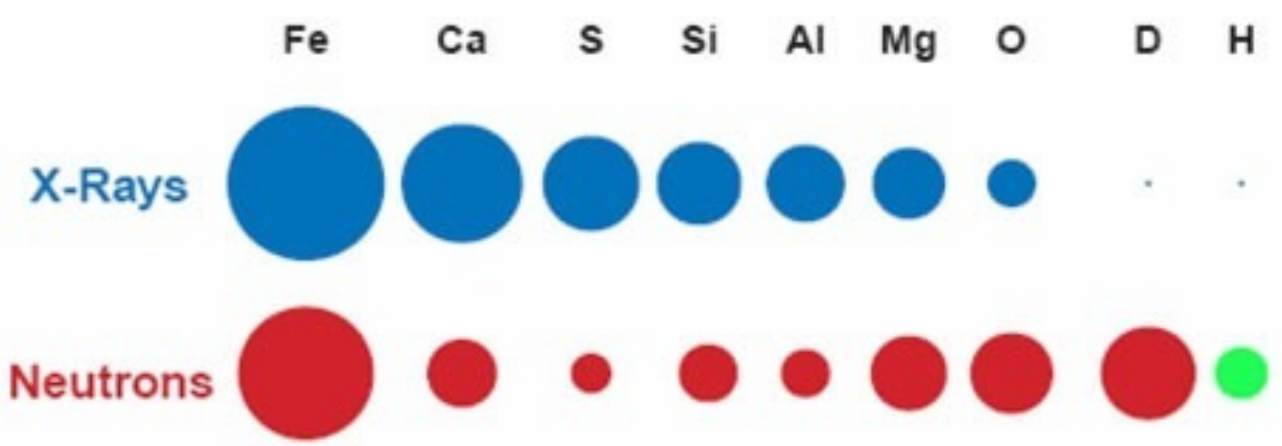


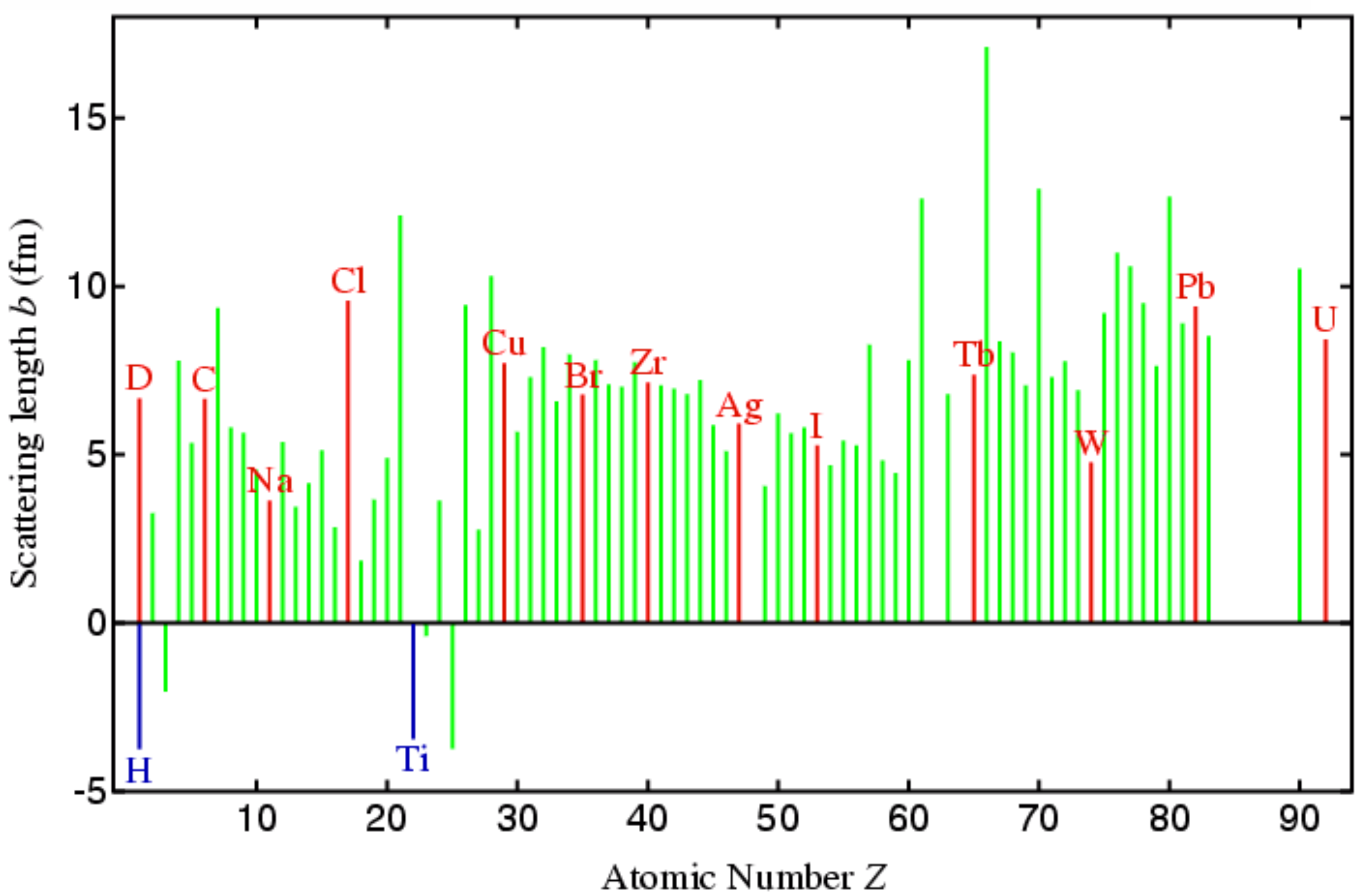


Differences in **Anisotropy** is very important

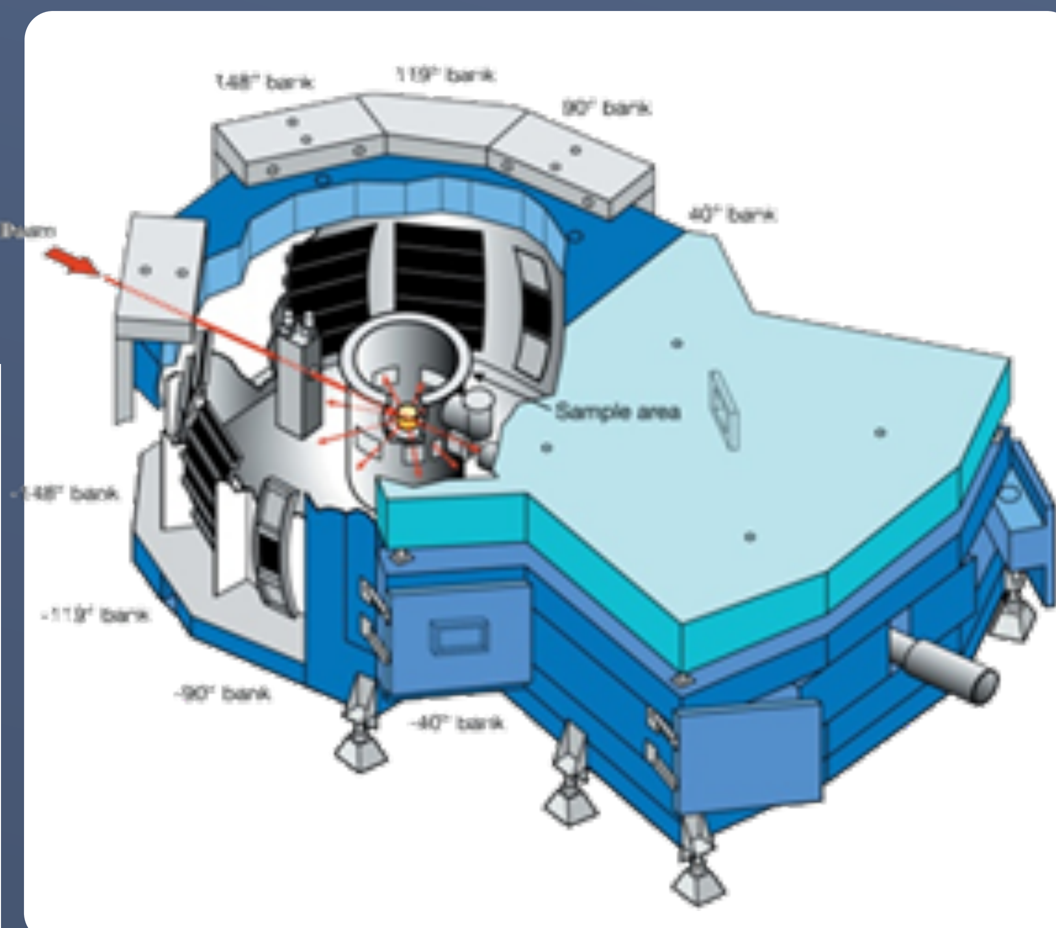
	Single Ion Anisotropy	Interactions	Ground state
Ho, Dy	Ising	FM	spin ice
Tb	Ising	AFM	spin liquid
Gd	Heisenberg	AFM	partial order
Er	XY	AFM	"order by disorder"
Yb	XY	FM	"quantum spin ice"

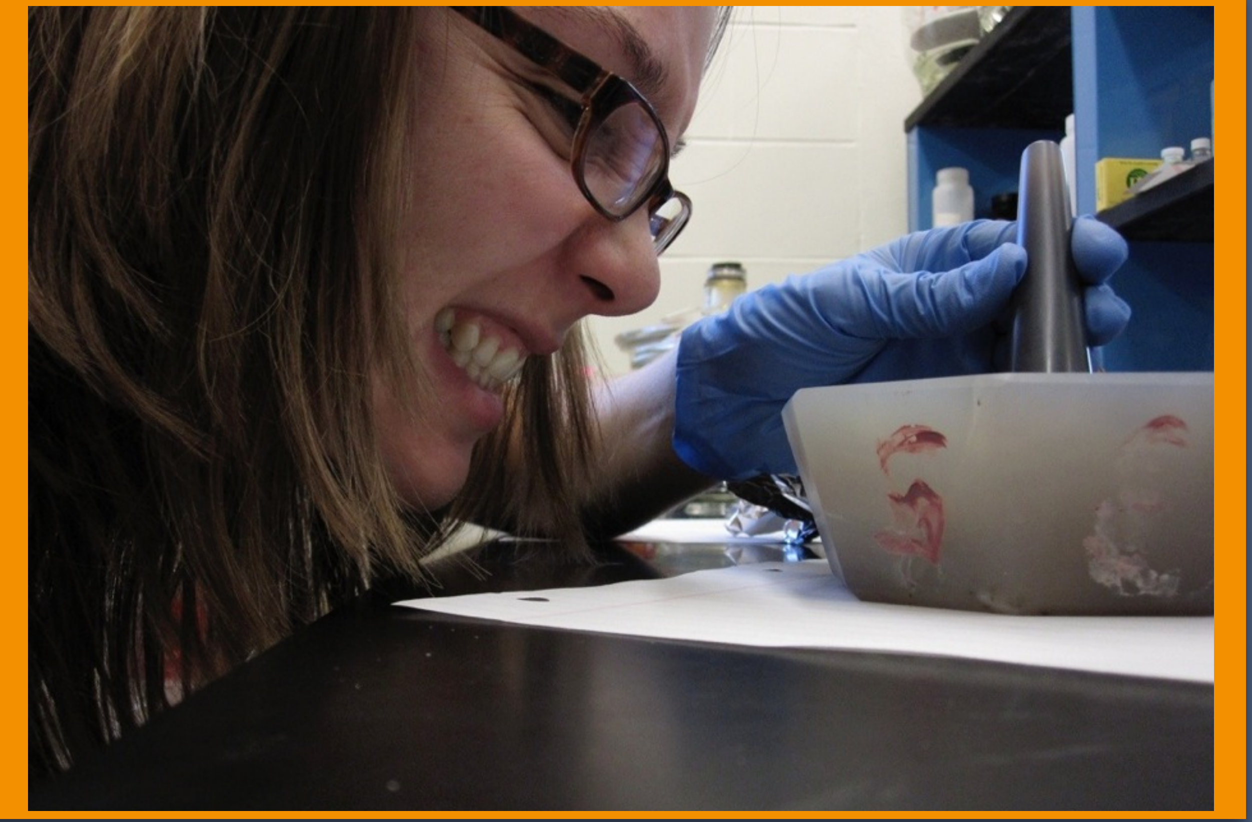
Neutron Diffraction:

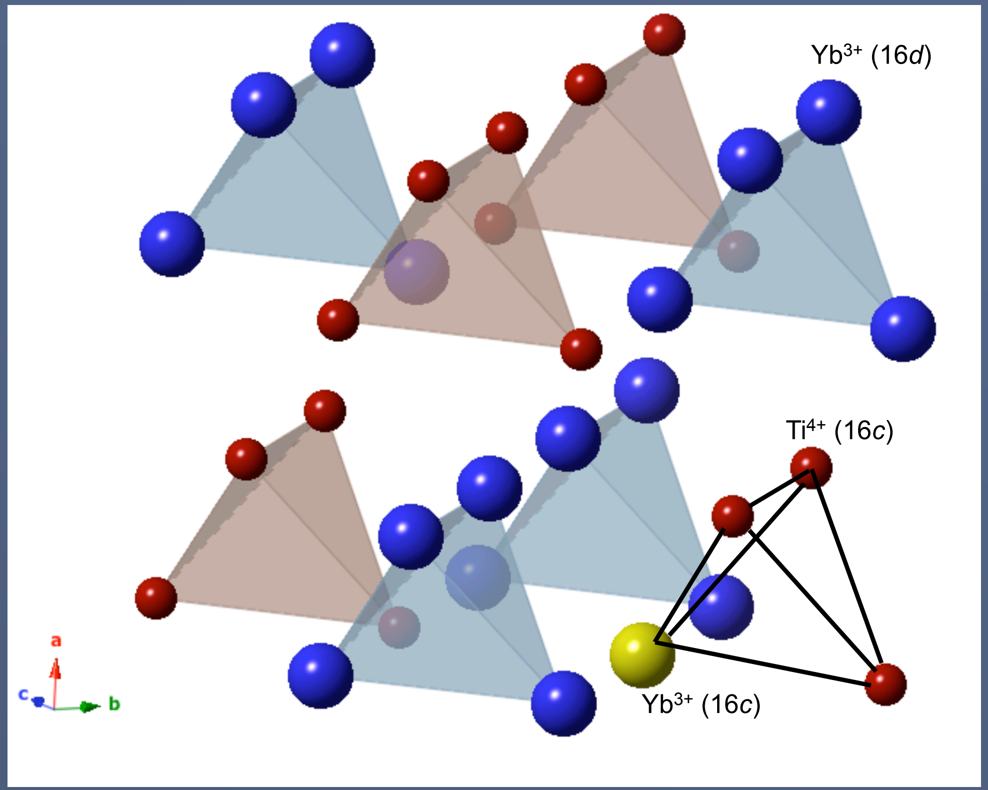




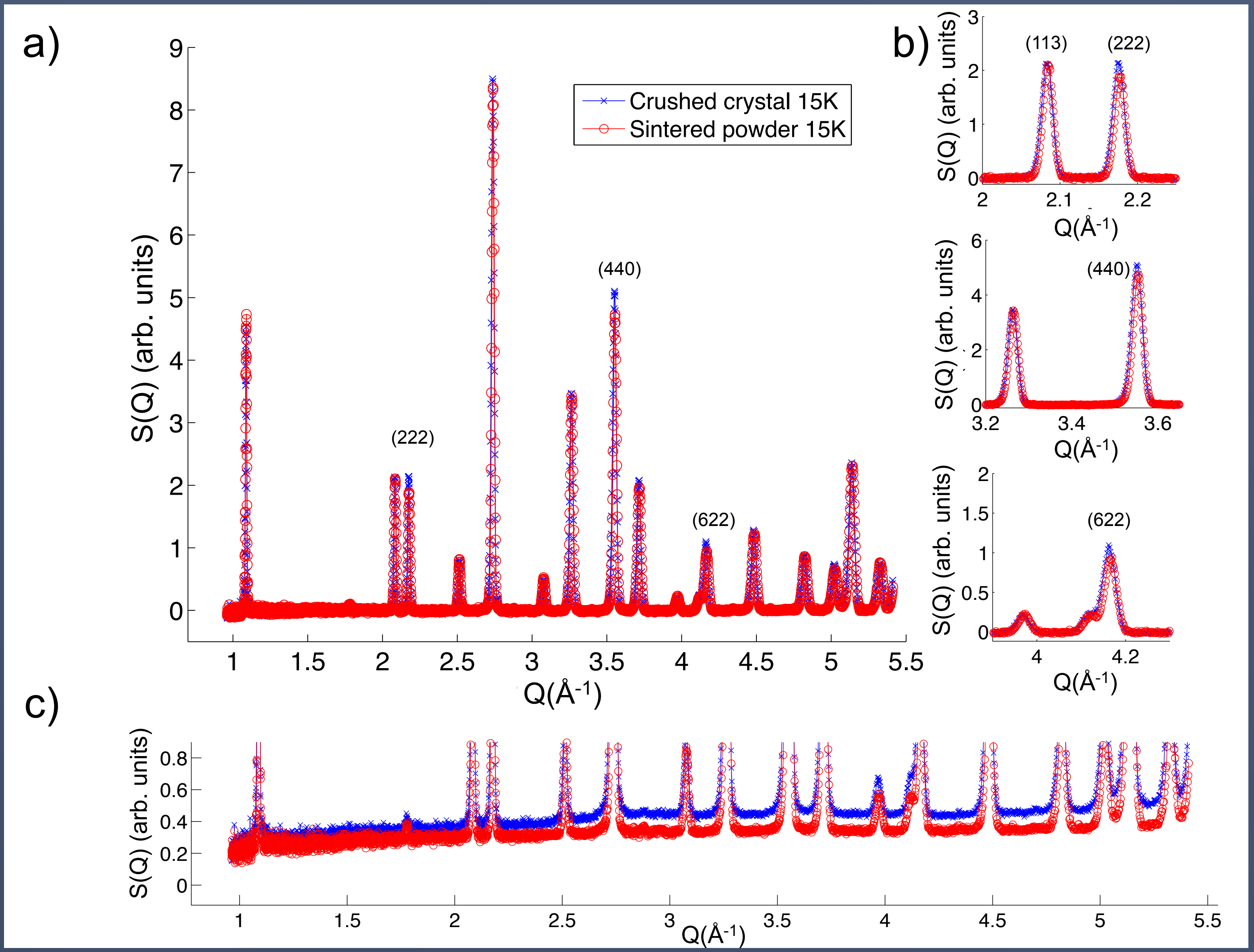
$R_2Ti_2O_7$







Yb3+ (16d)
Ti4+ (16c)
Yb3+ (16c)



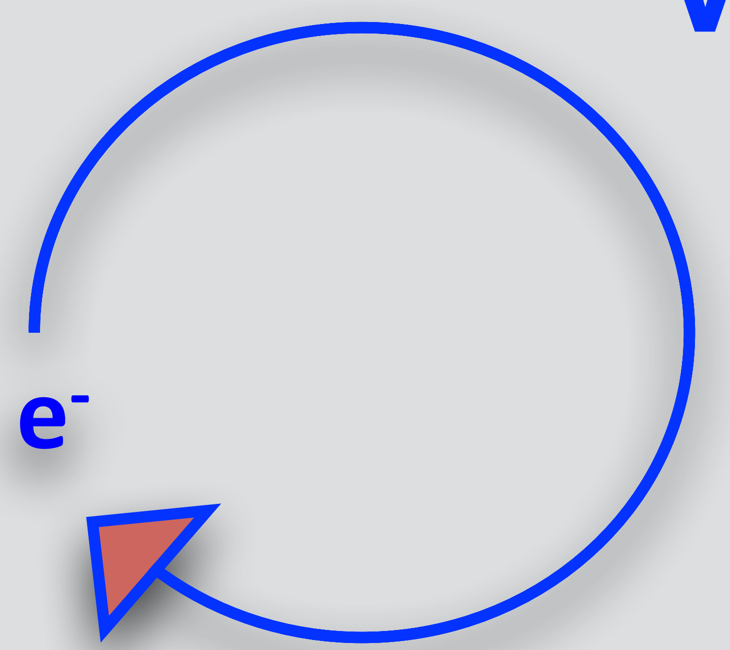
a)
Crushed crystal 15K
Sintered powder 15K
(222)
(440)
(622)
S(Q) (arb. units)
Q(Å-1)
b)
(113)
(222)
(440)
(622)
c)

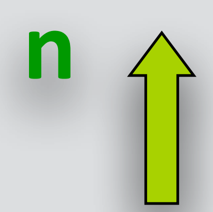
Dipole moment of the neutron interacts with the magnetic field generated by the electron

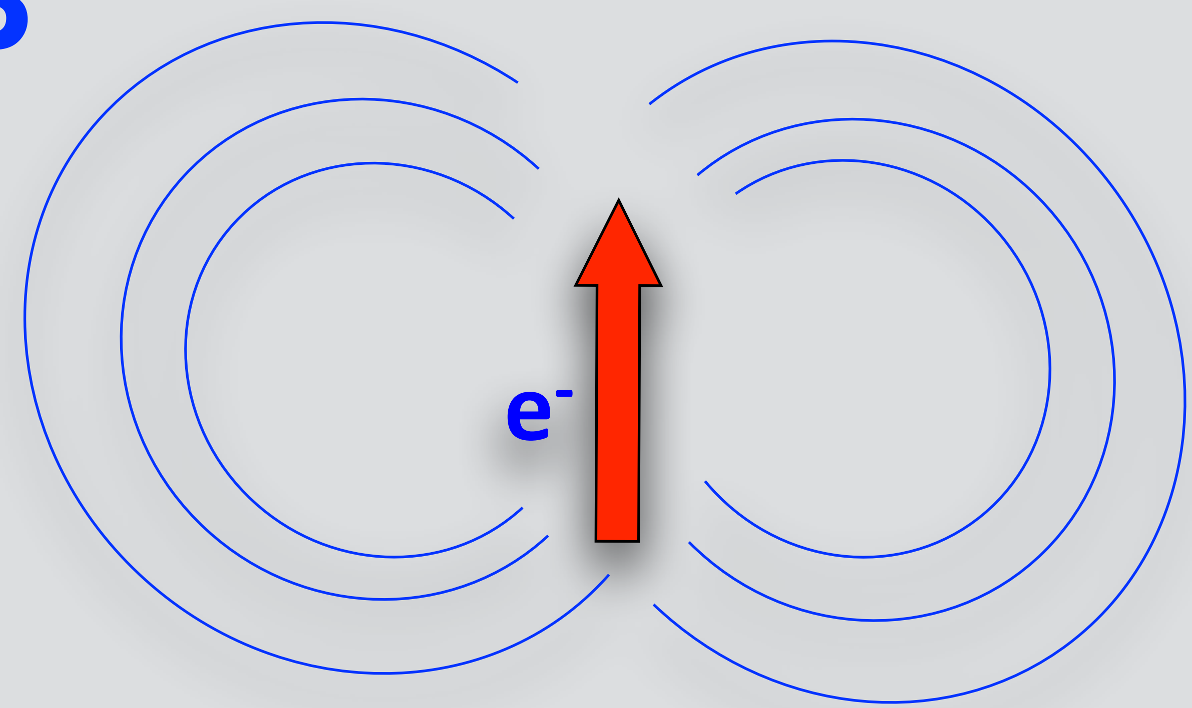
$$\mu_n = -\,\gamma\,\mu_N\,\sigma$$

$\gamma = 1.913$ | nuclear magneton $= e\hbar/2m_n$ | Pauli spin operator

$$V_M = -\mu_n B$$







Dipole field due to orbital currents

Dipole field due to
Spin of the electron(s)

Magnetic neutron scattering cross section:

Magnetic form factor

$$d^2\sigma/d\Omega\, dE' = (\gamma\, r_0)^2/(2\pi\hbar)\quad k'/k\;\; N\{1/2\, g\, F_d(\boldsymbol{\kappa})\}^2$$

$$\times\;\; \Sigma_{\alpha\,\beta}\;\; (\delta_{\alpha\,\beta} - \kappa_\alpha\, \kappa_\beta\,)\; \Sigma_l \exp(i\boldsymbol{\kappa}\cdot\mathbf{l})$$

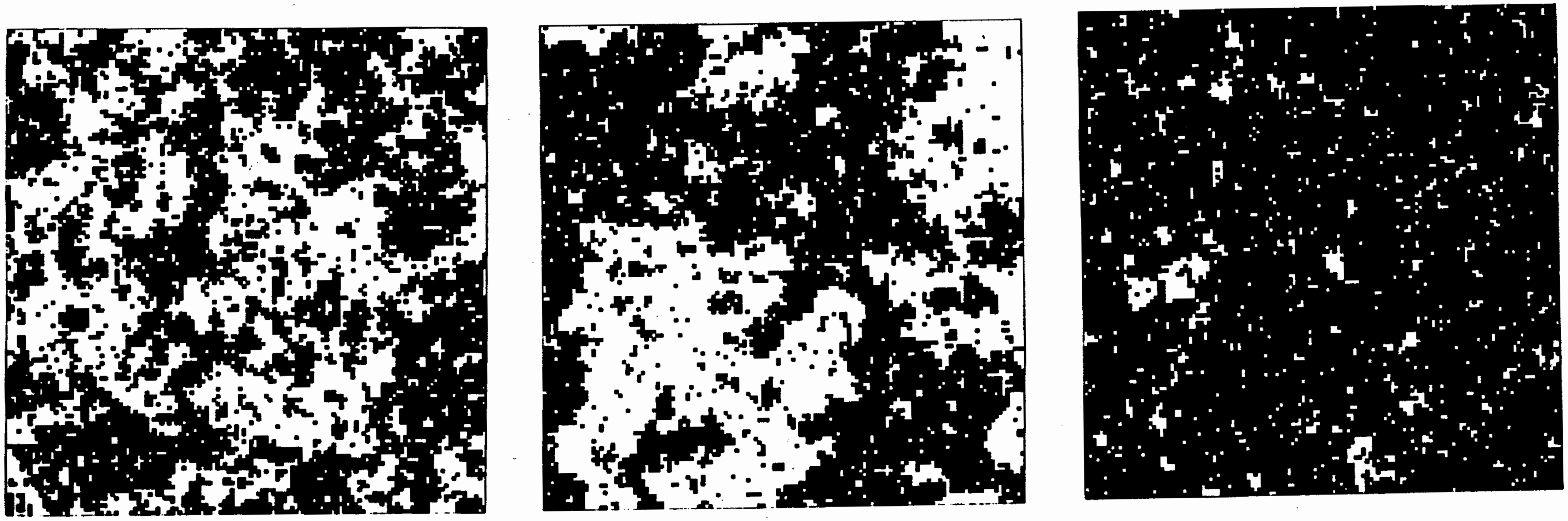
Polarization factor:

neutrons only sense moments perp to Q

$$\times\;\; \int <\exp(-i\boldsymbol{\kappa}\cdot\mathbf{u_0}))\exp(i\boldsymbol{\kappa}\cdot\mathbf{u}_l(t))>$$

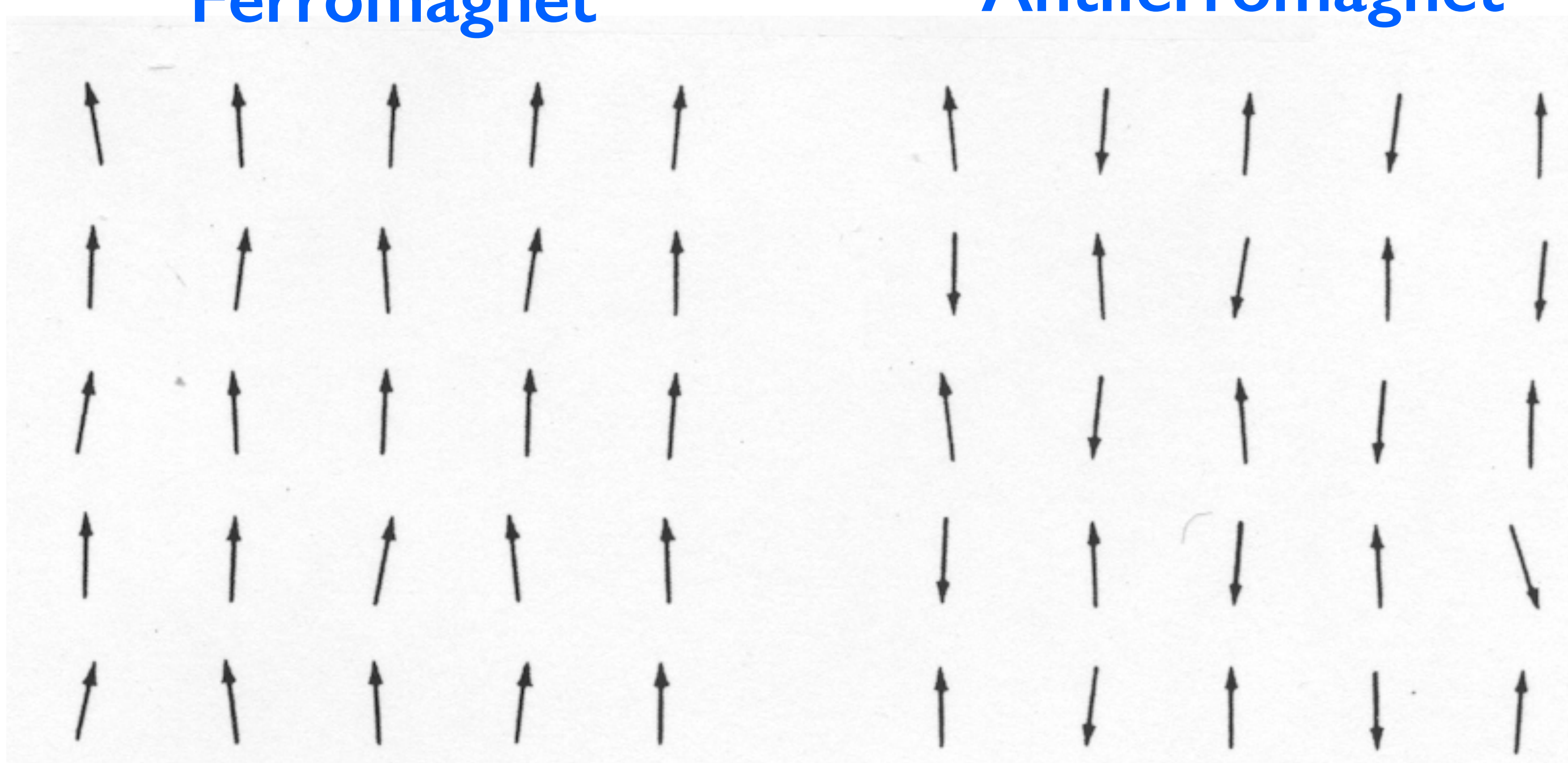
$$\times\;\; <S_0^{\alpha}(0)\; S_l^{\beta}(t)> \exp(-i\omega\, t)\; dt$$

Fourier transform of Spin Pair Correlation Function



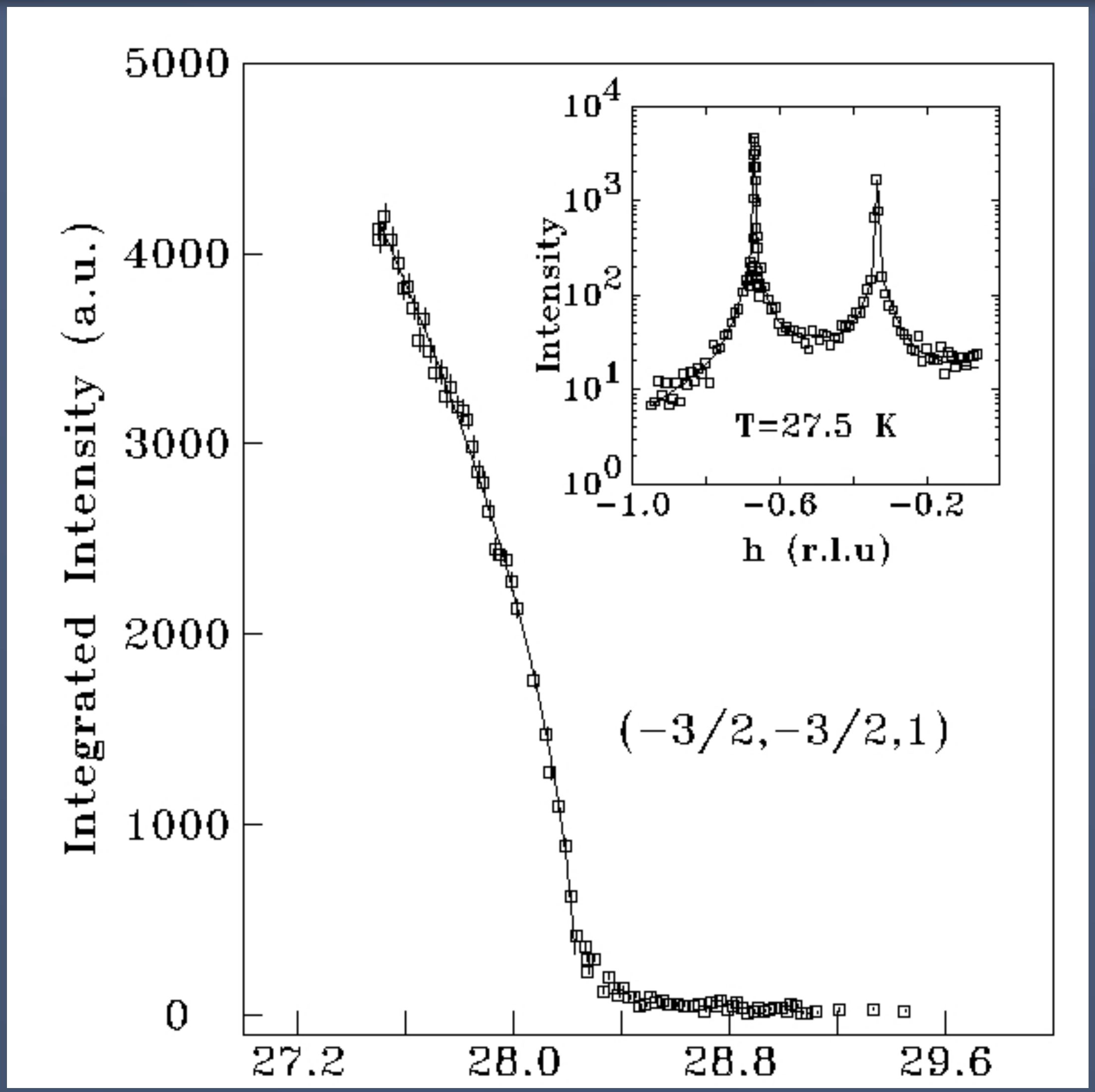
1.1 T_C | T_C | 0.9 T_C

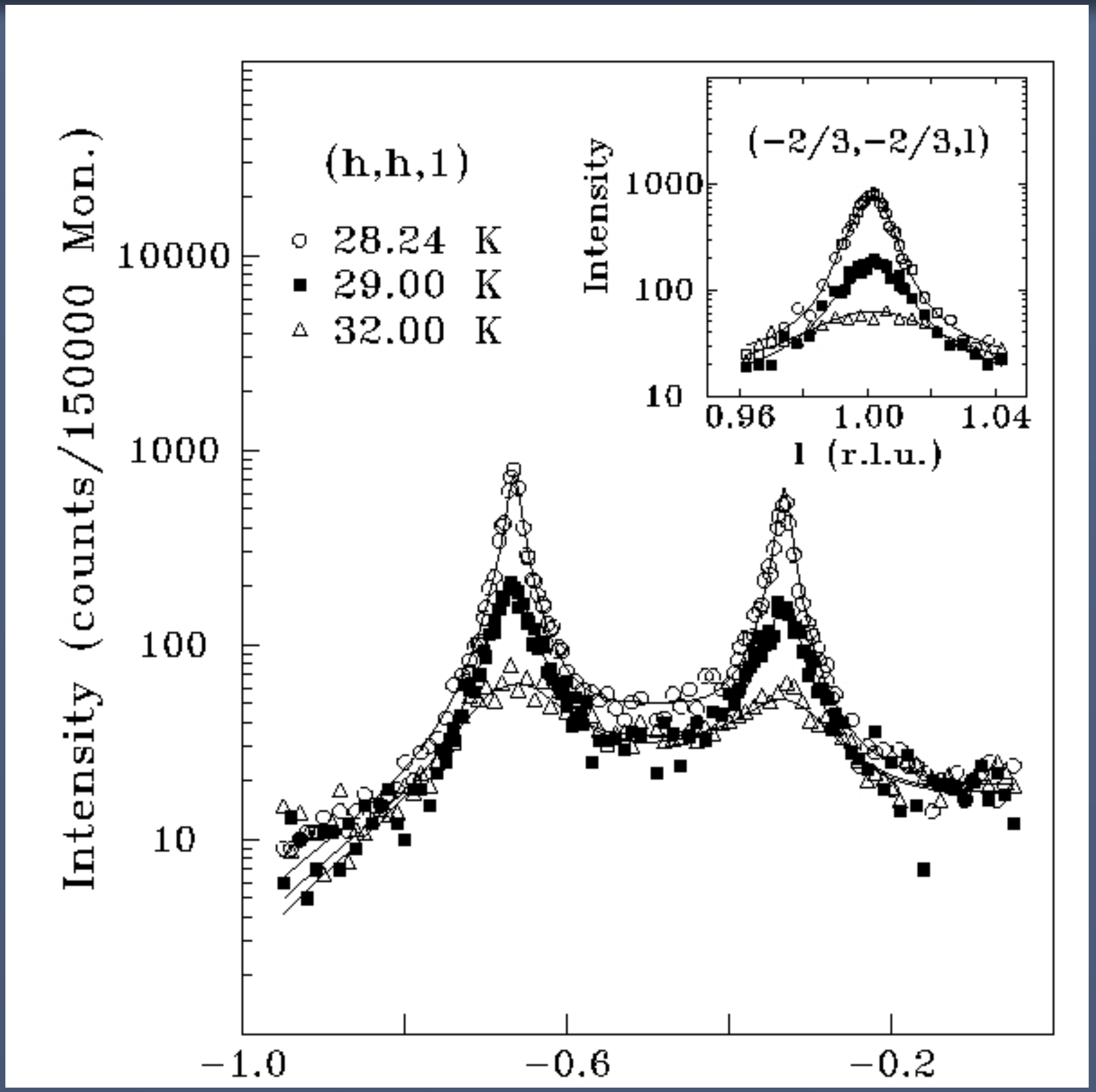
Ferromagnet | Antiferromagnet



$$H = 2J \, \Sigma_{ij} \, \mathbf{S_i} \cdot \mathbf{S_j}$$

Neutron diffraction study of conventional magnetic order





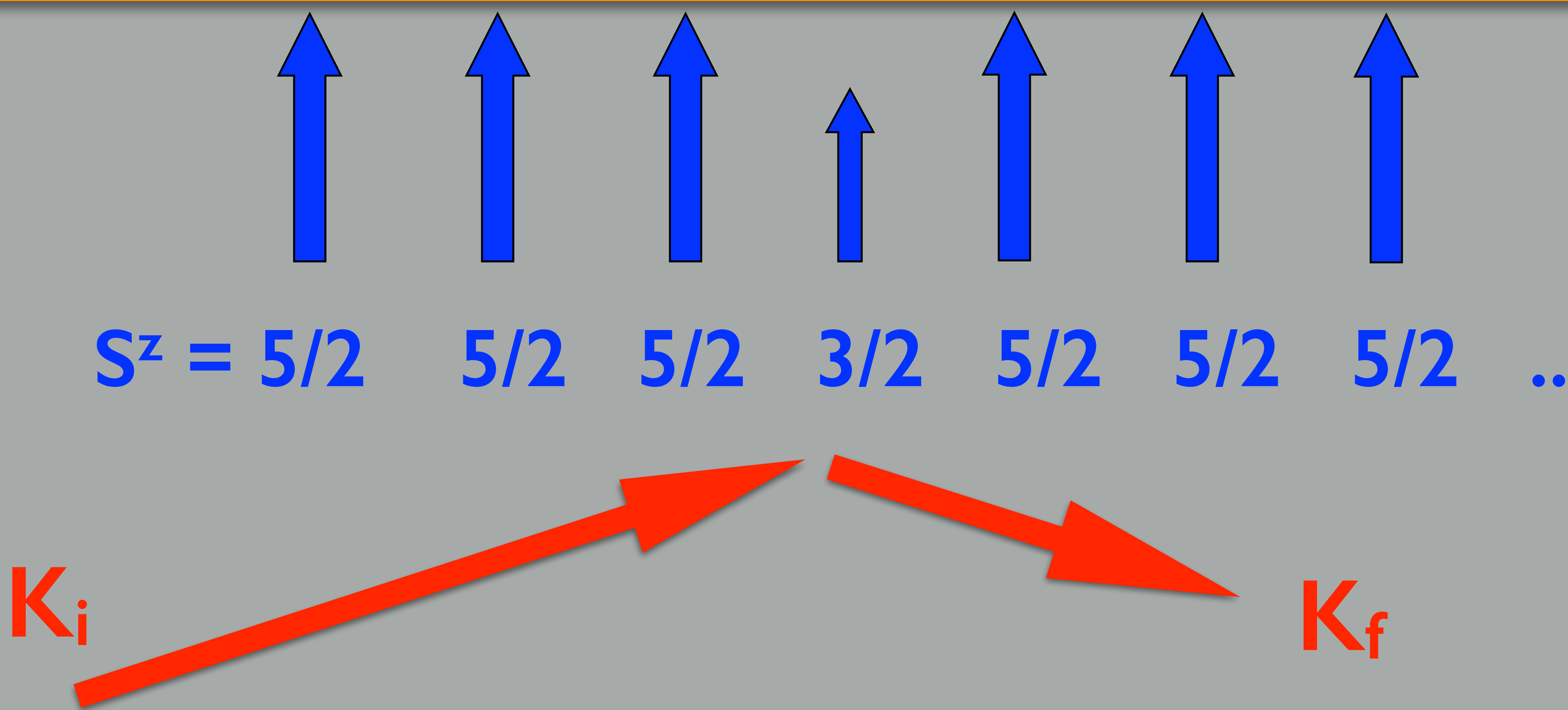
Elastic Bragg scattering

critical diffuse scattering

$CsCoBr_3$

$$\frac{d\sigma(\vec{Q})}{d\Omega} = \frac{\chi(\vec{Q}_{ord})}{1 + \frac{q_a^2 + q_b^2}{\kappa_{ab}^2} + \frac{q_c^2}{\kappa_c^2}},$$

Spin Waves as elementary excitations in ordered magnets



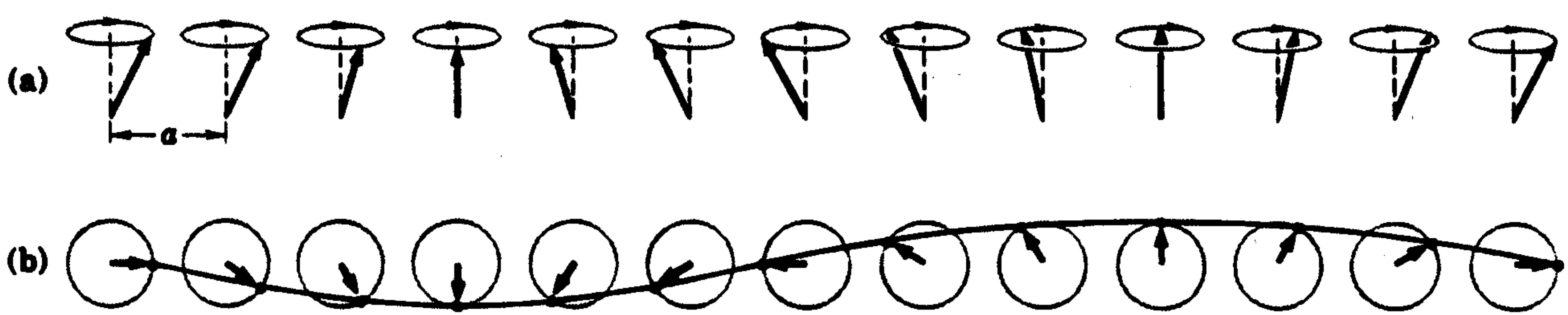
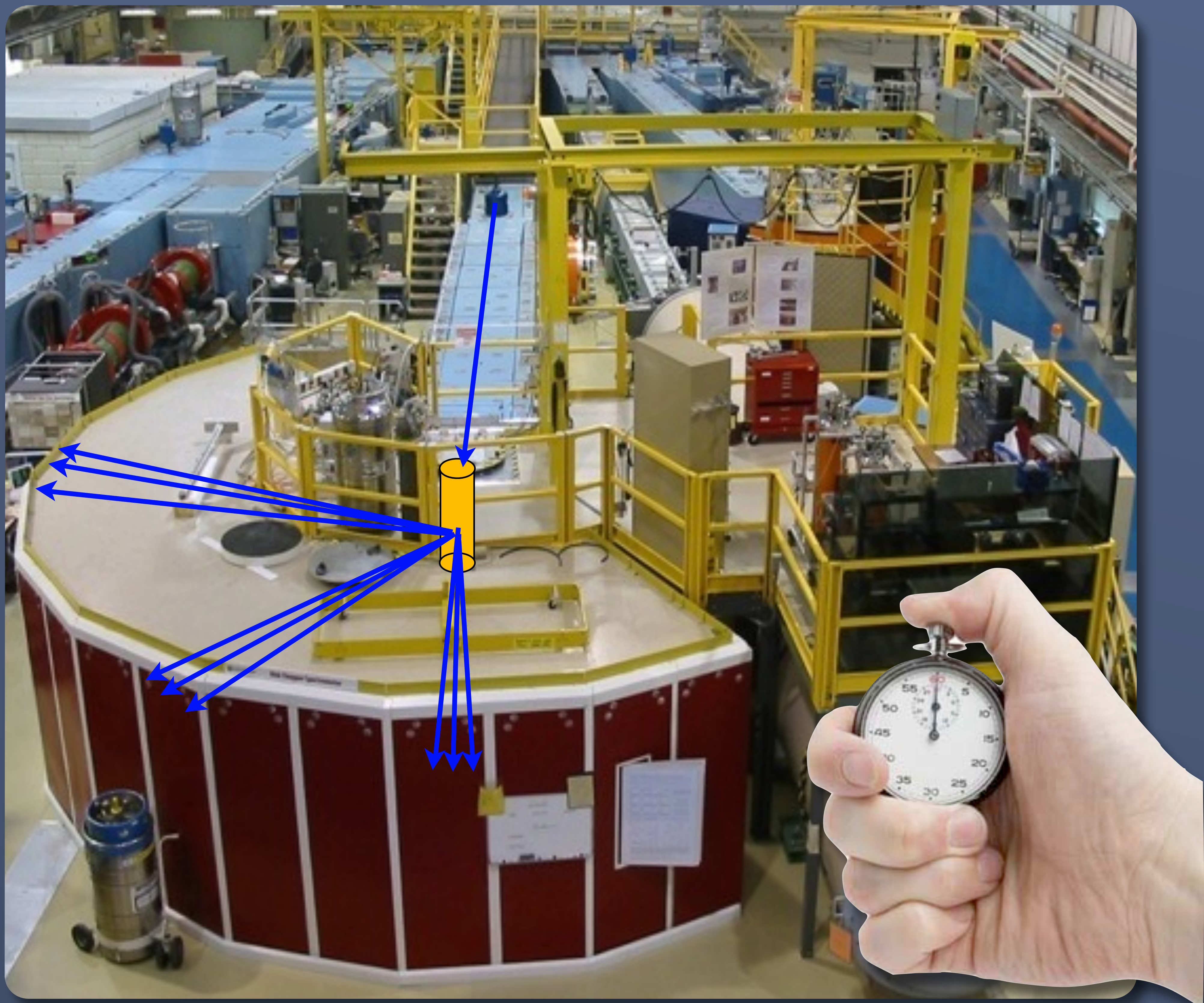


Figure 9 A spin wave on a line of spins. (a) The spins viewed in perspective. (b) Spins viewed from above, showing one wavelength. The wave is drawn through the ends of the spin vectors.

Time of Flight Neutron Scattering

"Disk Chopper Spectrometer" (DCS)

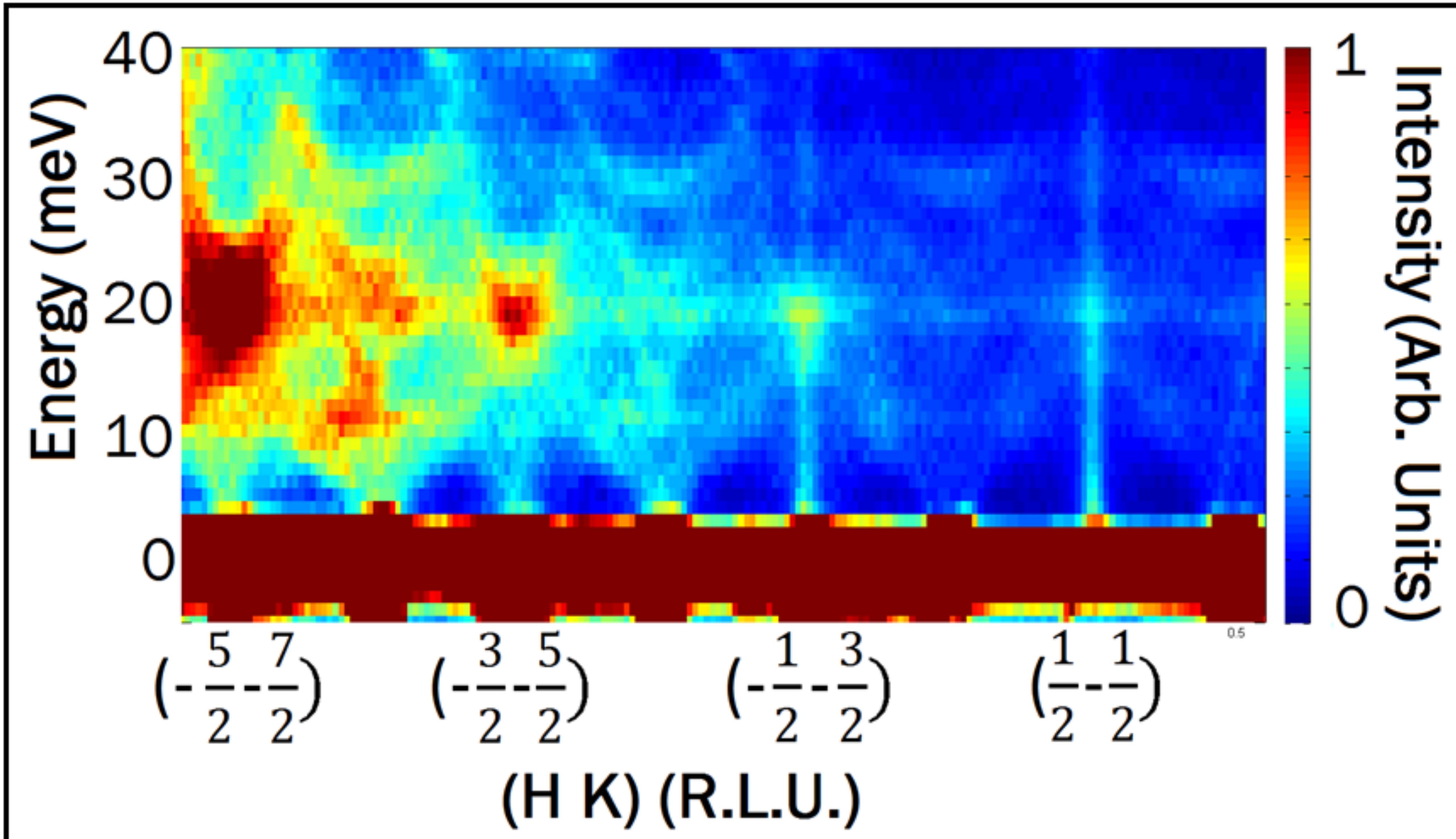
@ NIST Center for Neutron Research



Phonon scattering at large Q

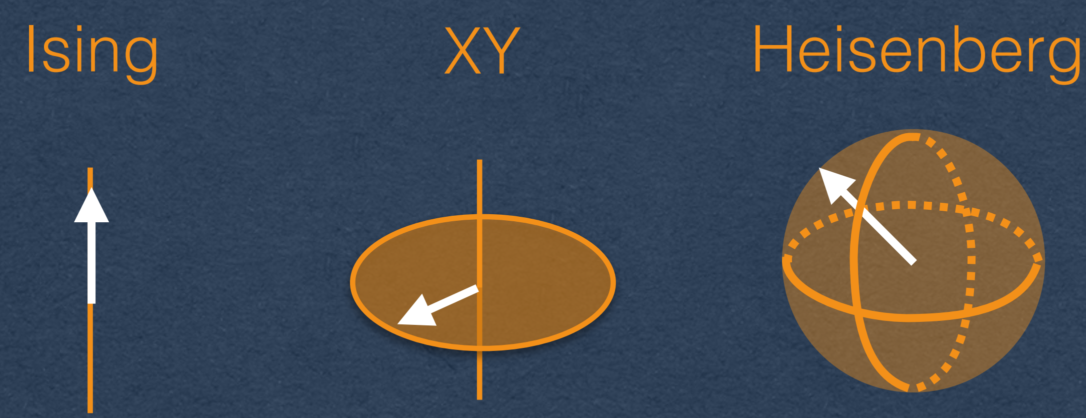
Magnetic scattering at small Q

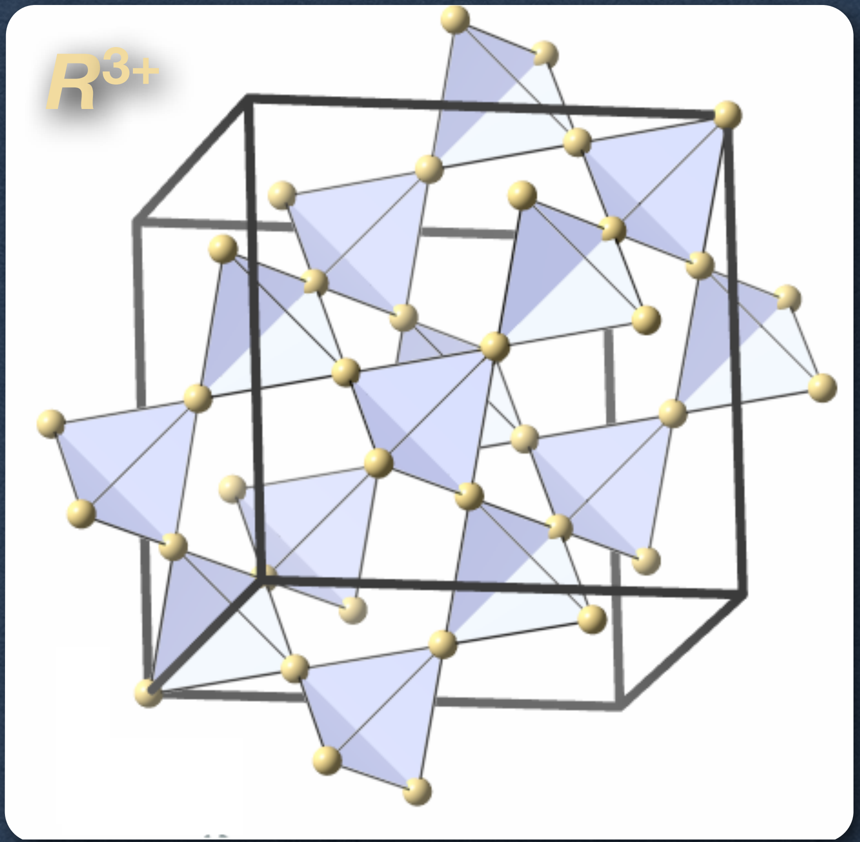
$La_{2-x}Ba_xCuO_4$



Real Pyrochlores: playgrounds for frustration

$R_2Ti_2O_7$ "Rare earth titanates"





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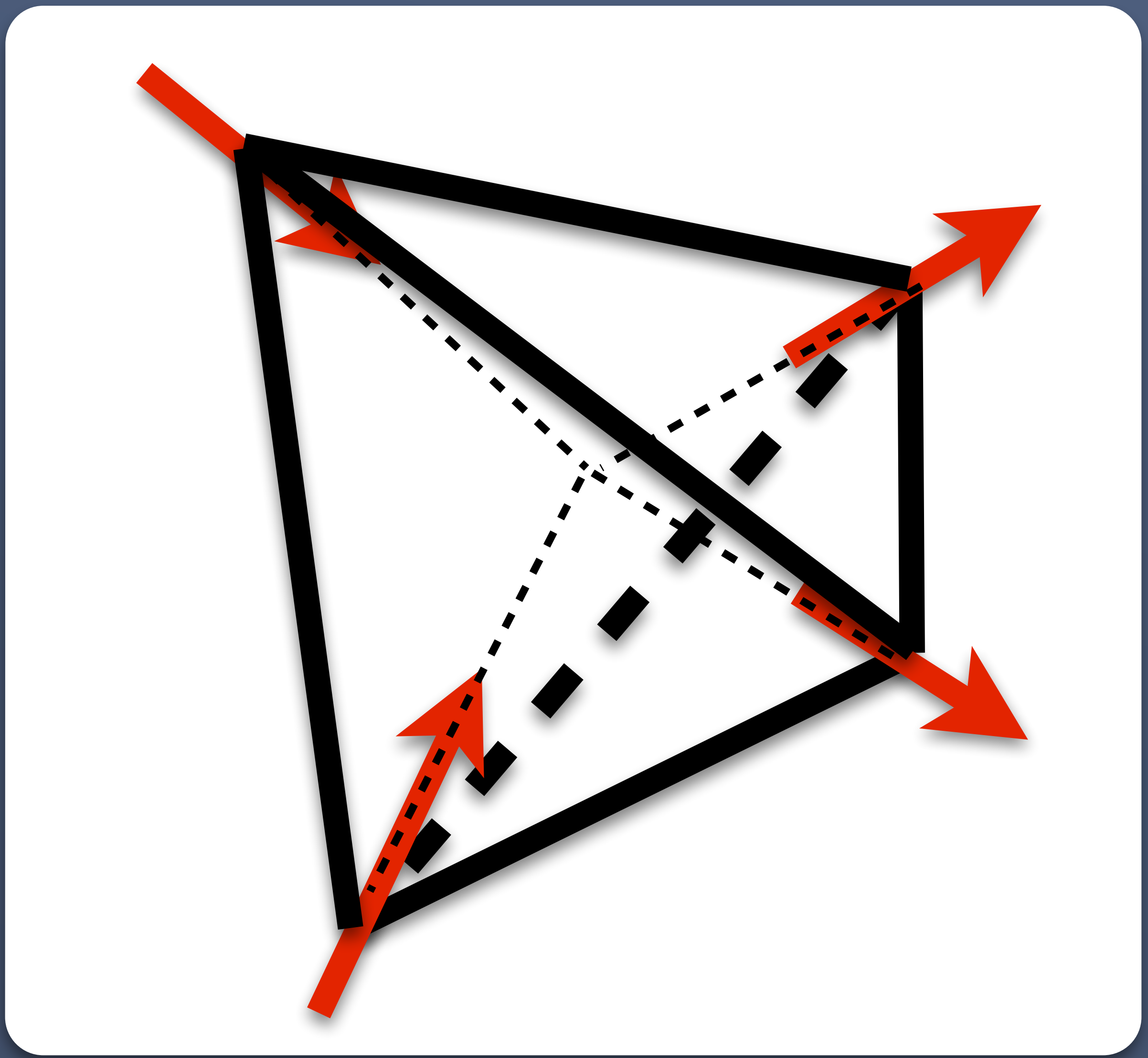
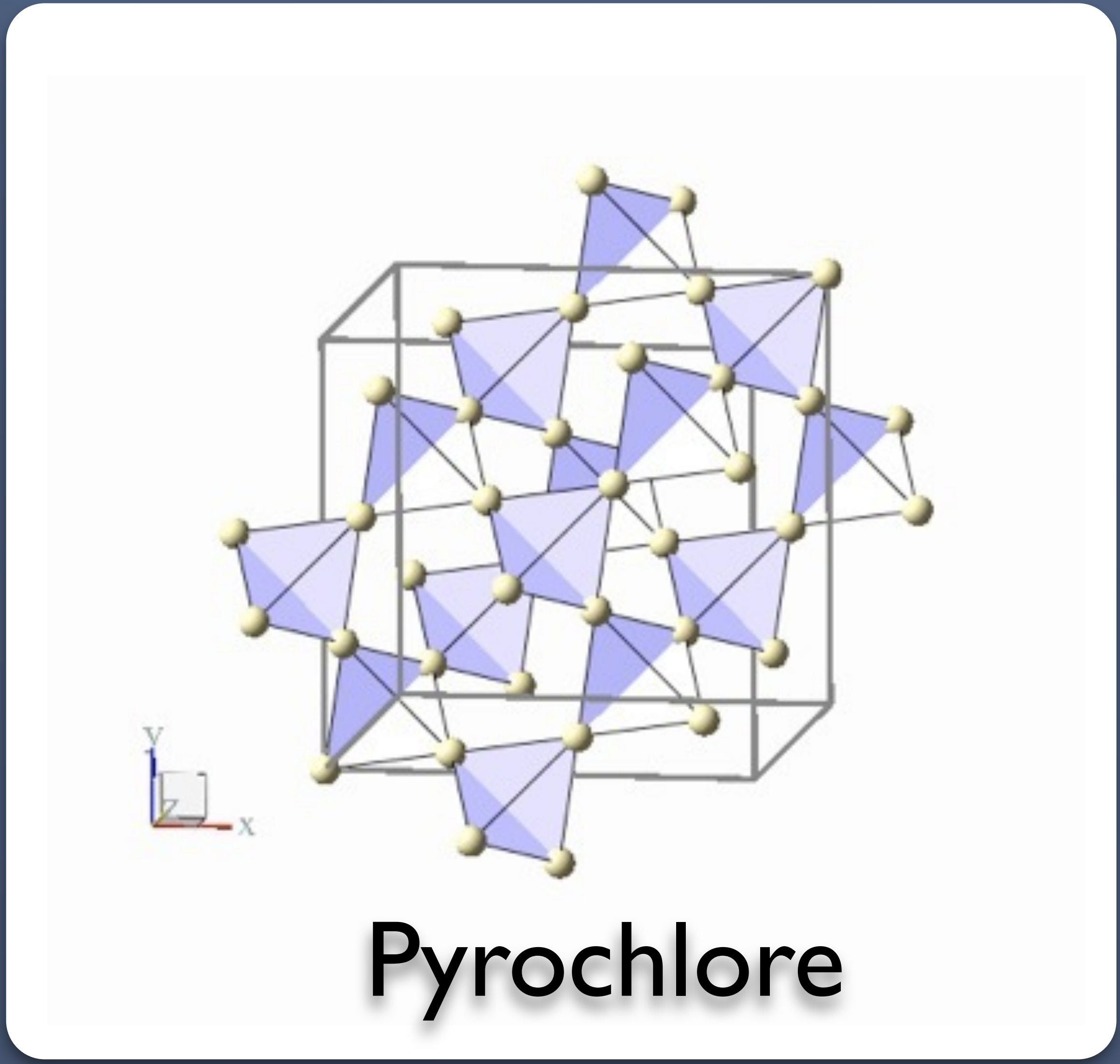
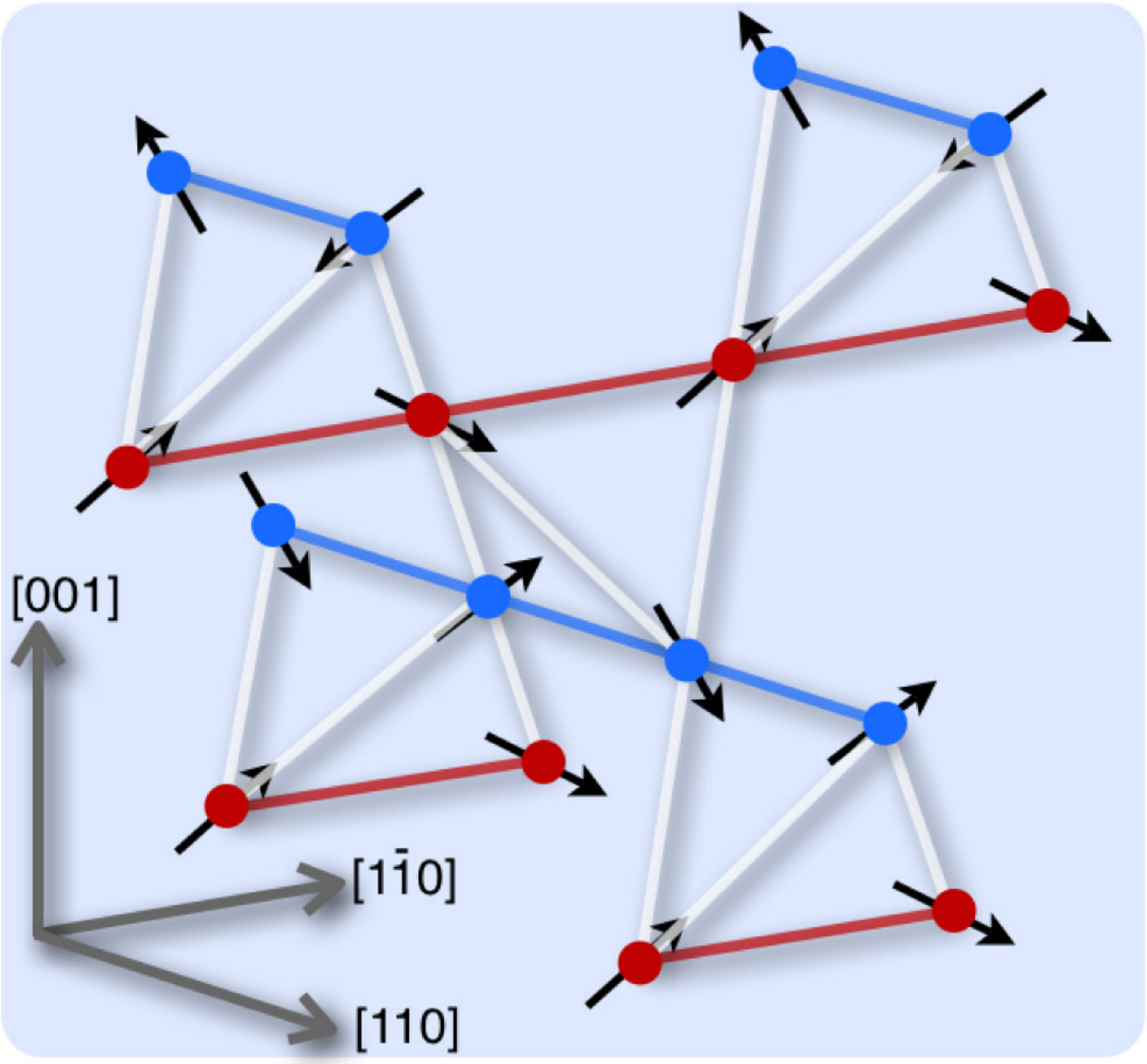
Spin Ice Physics



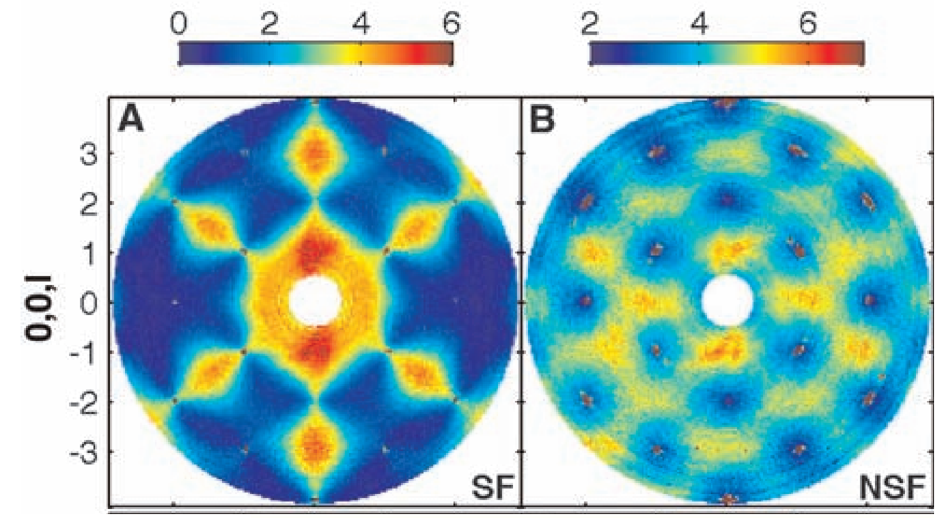


freedom of choice for each tetrahedron leads to a macroscopic degeneracy: **NO Long Range Order**

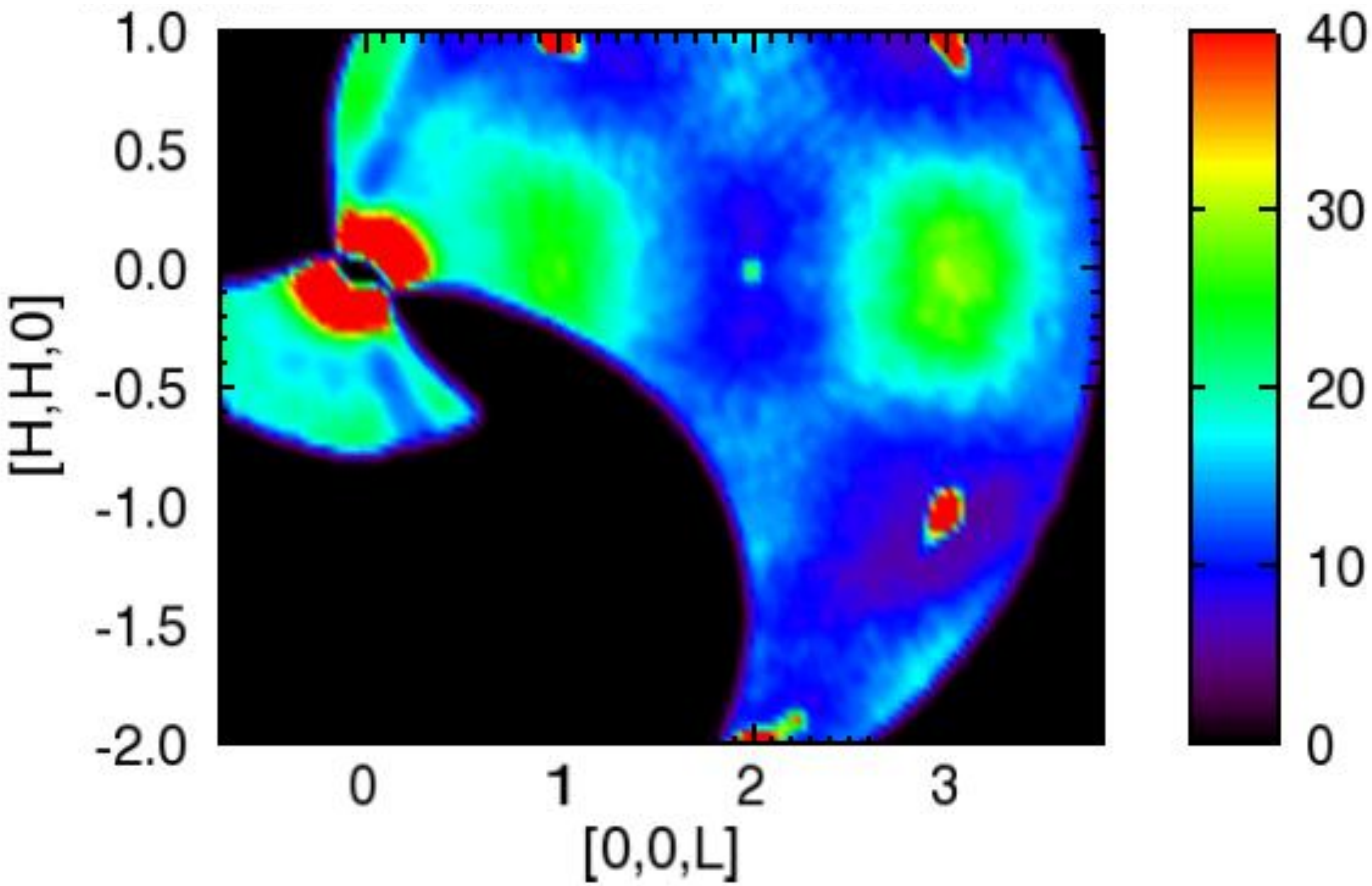


[1-10] Magnetic field should decompose pyrochlore lattice into polarized α chains (red chains) and decoupled qausi-1D β chains (blue chains).

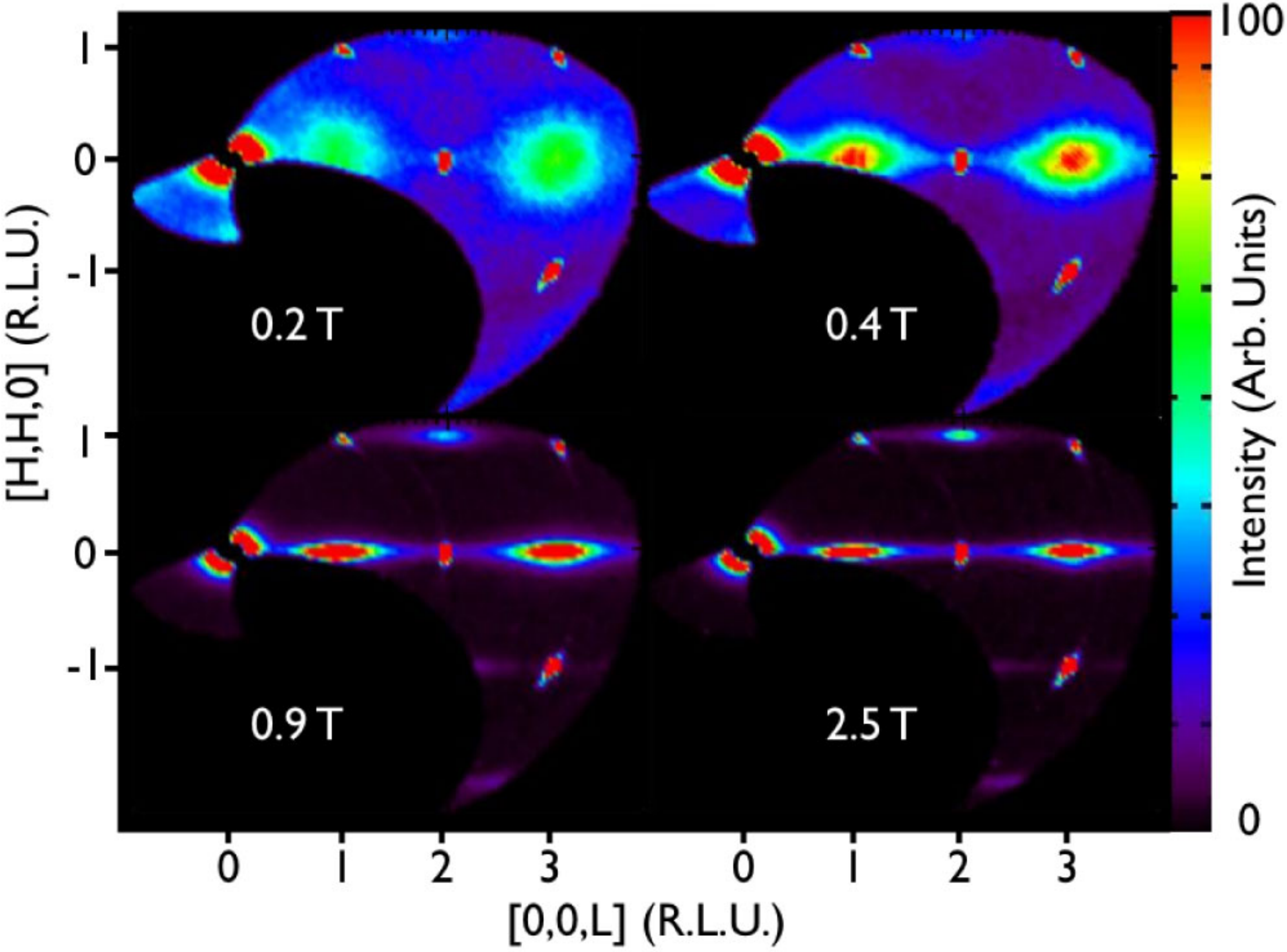
Spin Ice Ground State in $Ho_2Ti_2O_7$



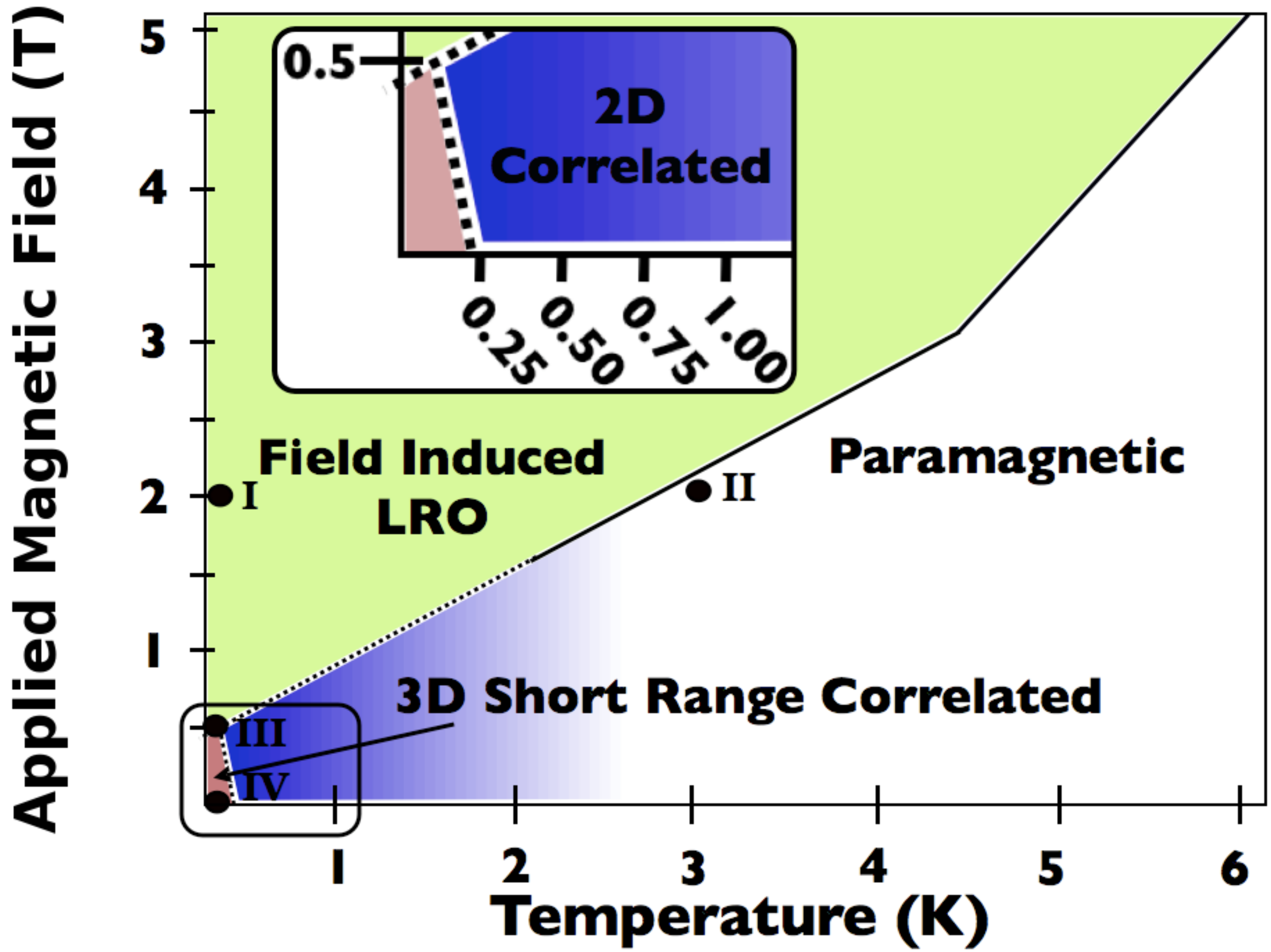
T. Fennell et al.,
Science, 326 (5951): 415-417 (2009)



J. P. Clancy, J. P. C. Ruff, S. R. Dunsiger, Y. Zhao, H. A. Dabkowska,
J. S. Gardner, Y. Qiu, J. R. D. Copley, T. Jenkins, and B. D. Gaulin, Phys. Rev. B 79, 014408 (2009)



0.2 T
0.4 T
0.9 T
2.5 T
[H,H,0] (R.L.U.)
[0,0,L] (R.L.U.)
Intensity (Arb. Units)
100
0
1
0
-1
1
0
-1
0
1
2
3
0
1
2
3

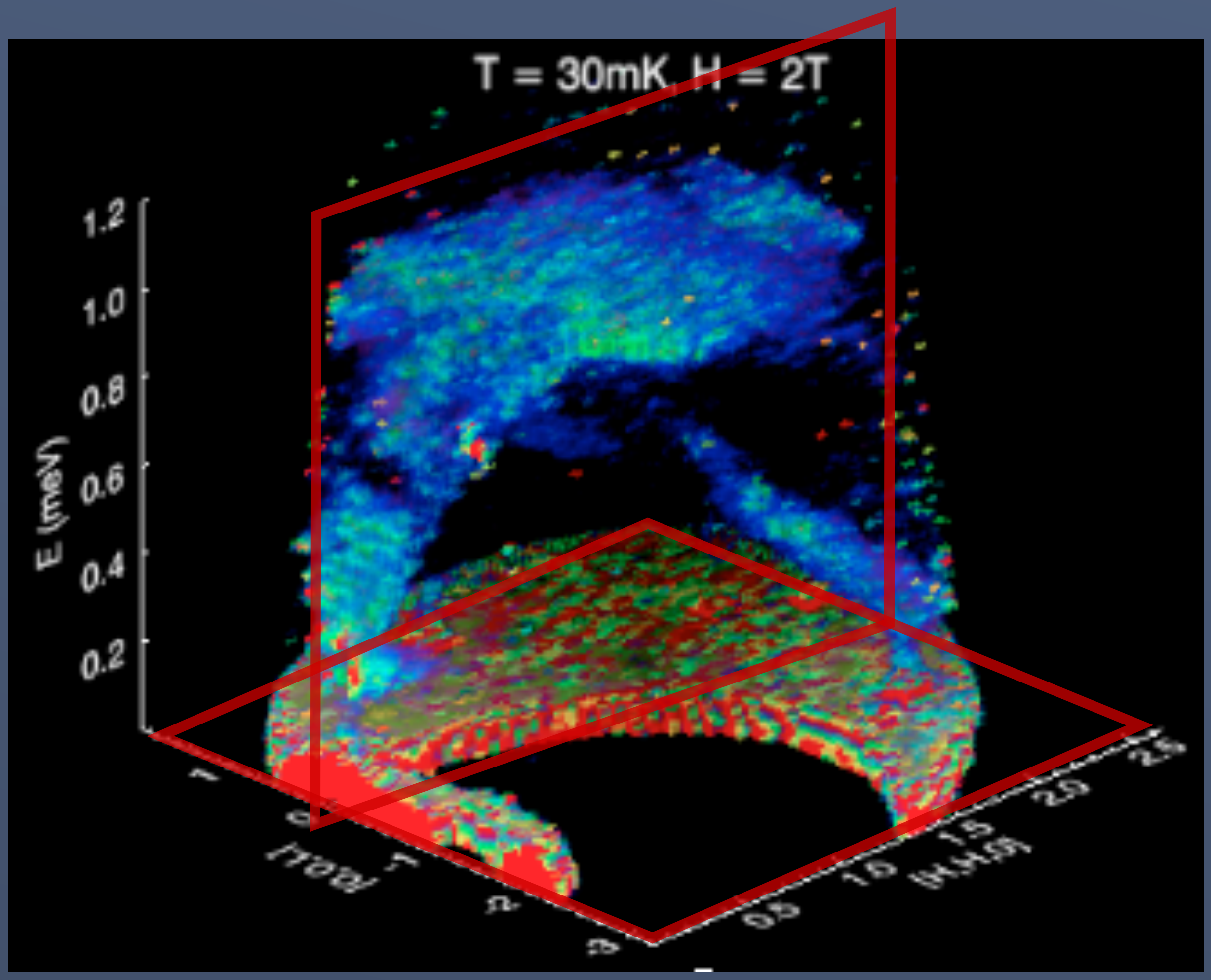


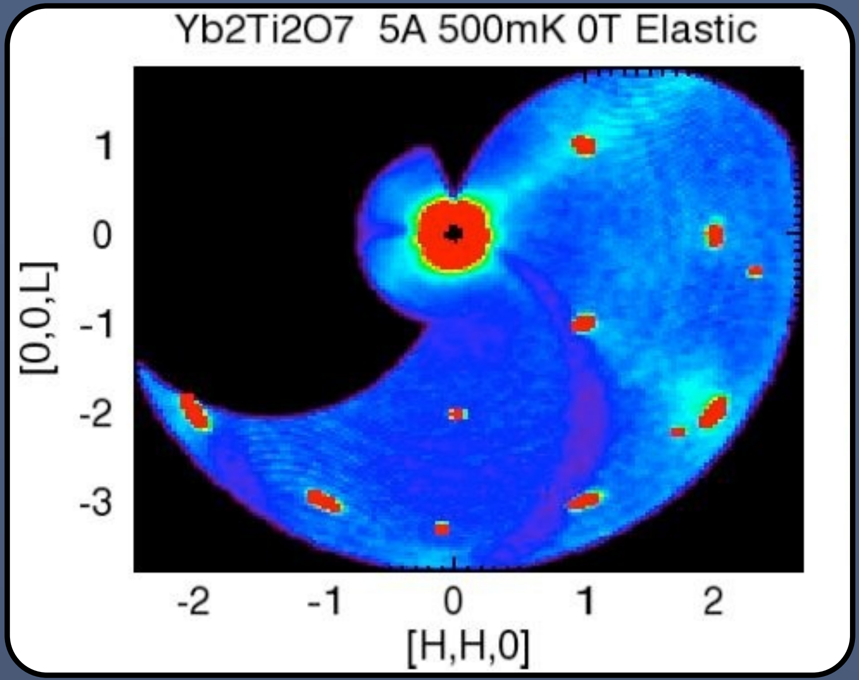
K. A. Ross, J. P. C. Ruff, C. P. Adams, J. S. Gardner, H. A. Dabkowska, Y. Qiu, J. R. D. Copley, and B. D. Gaulin, Phys. Rev. Lett. 103, 227202 (2009)

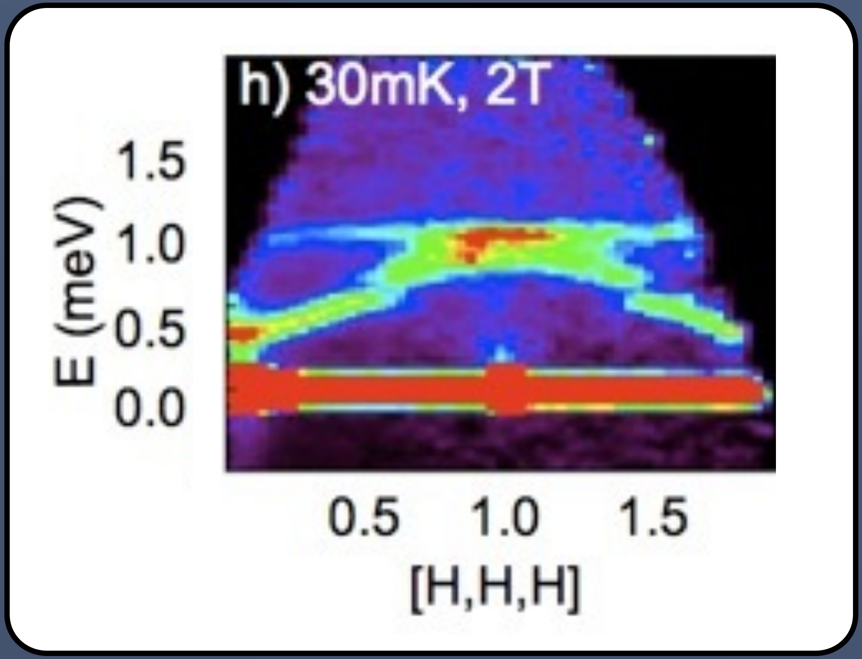
$Yb_2Ti_2O_7$

“Time of Flight” data

Can slice through this volume in several directions

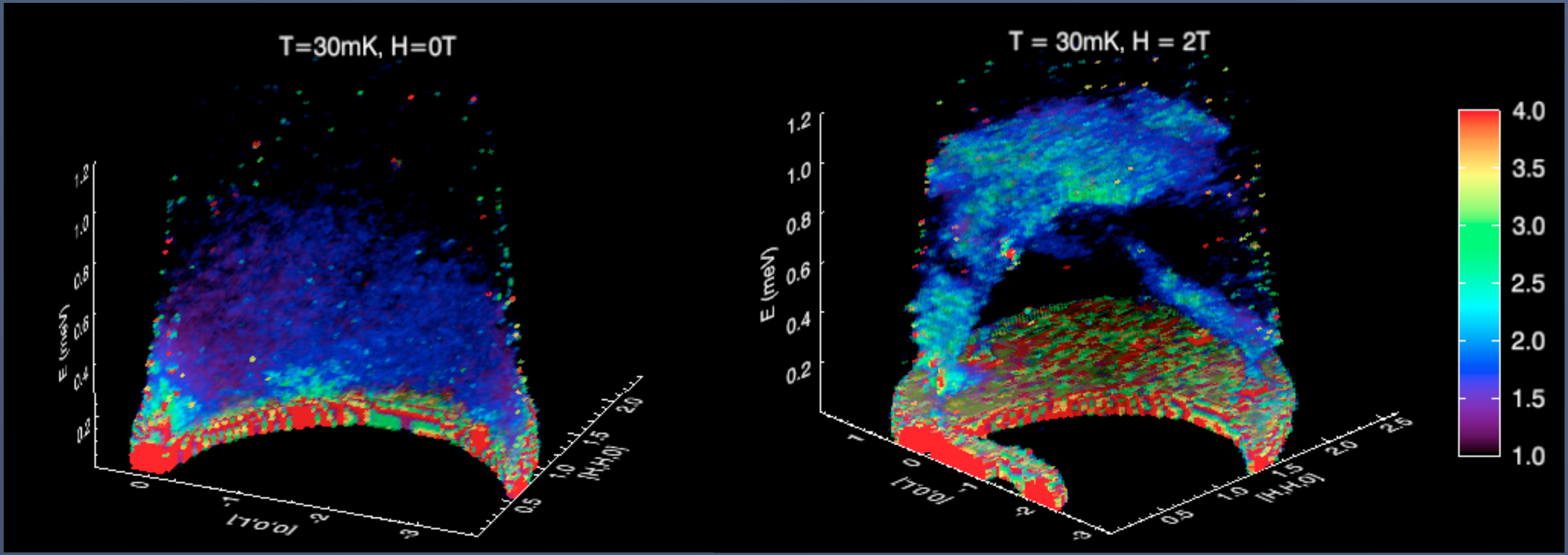






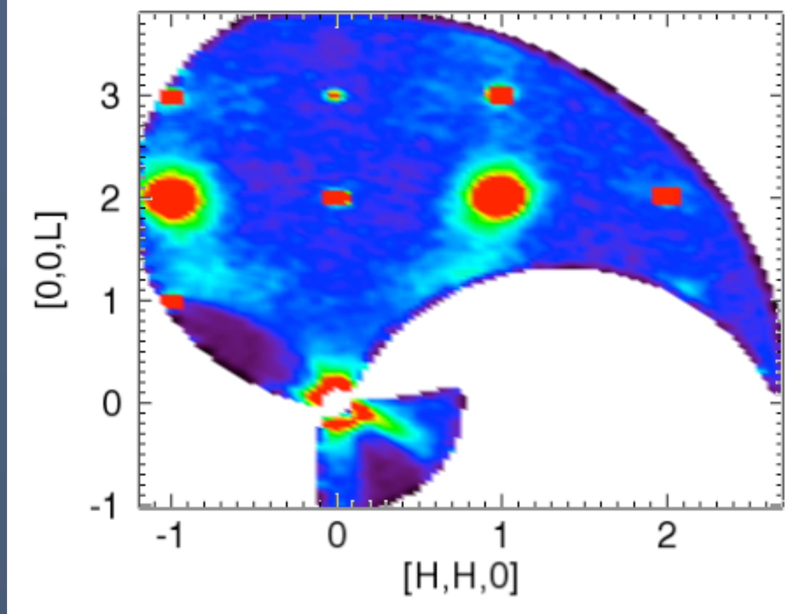
$Yb_2Ti_2O_7$

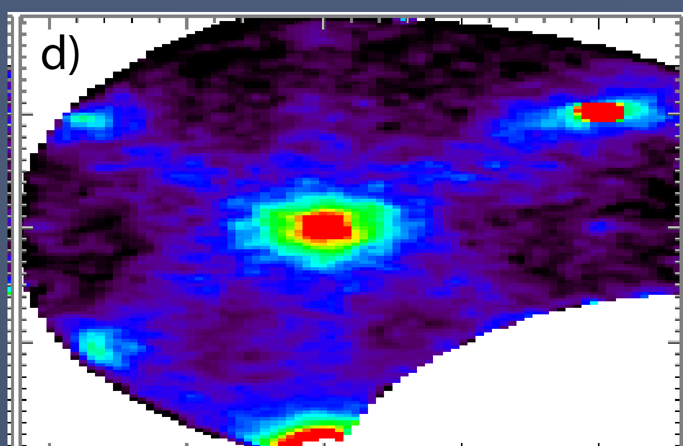
Field Induced Order

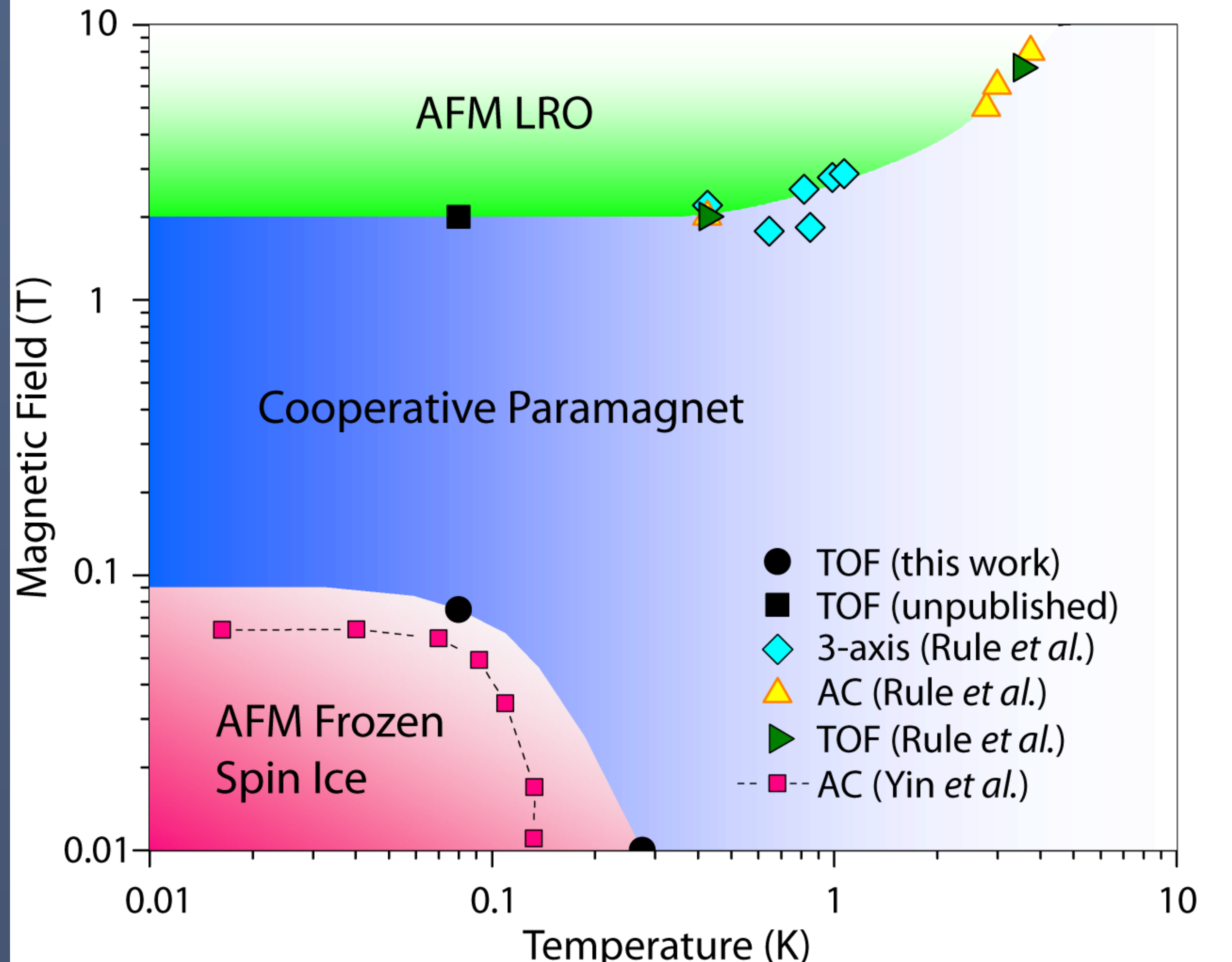


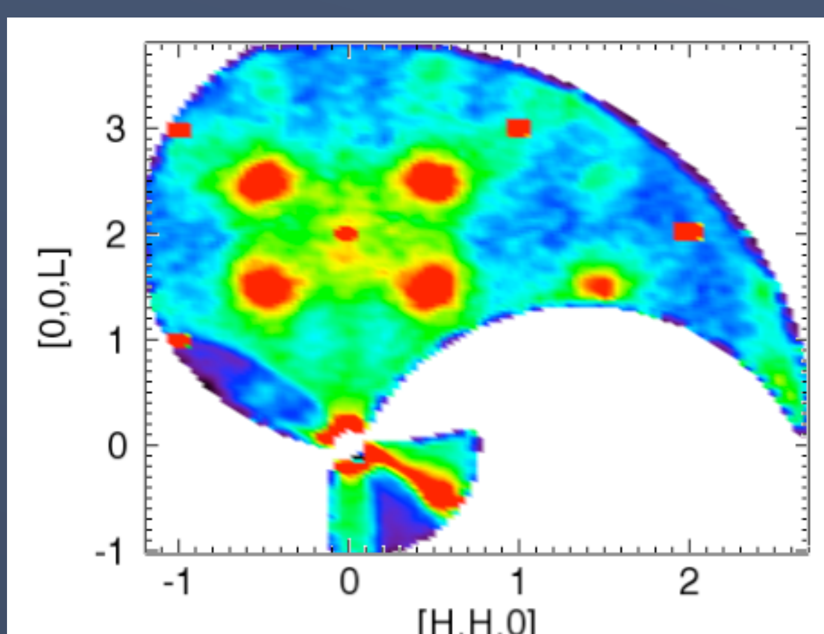
No structure to inelastic scattering

Spin Wave Excitations

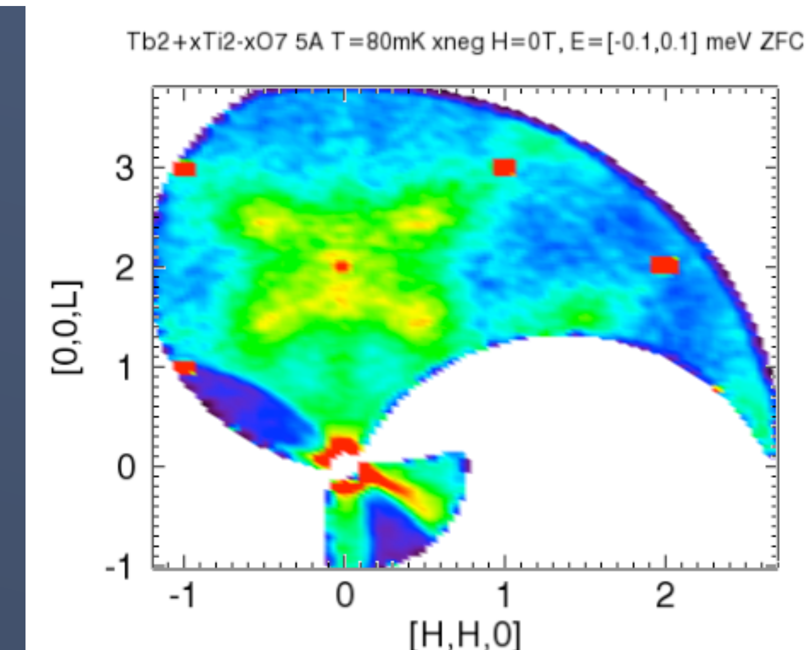

[0,0,L]
[H,H,0]

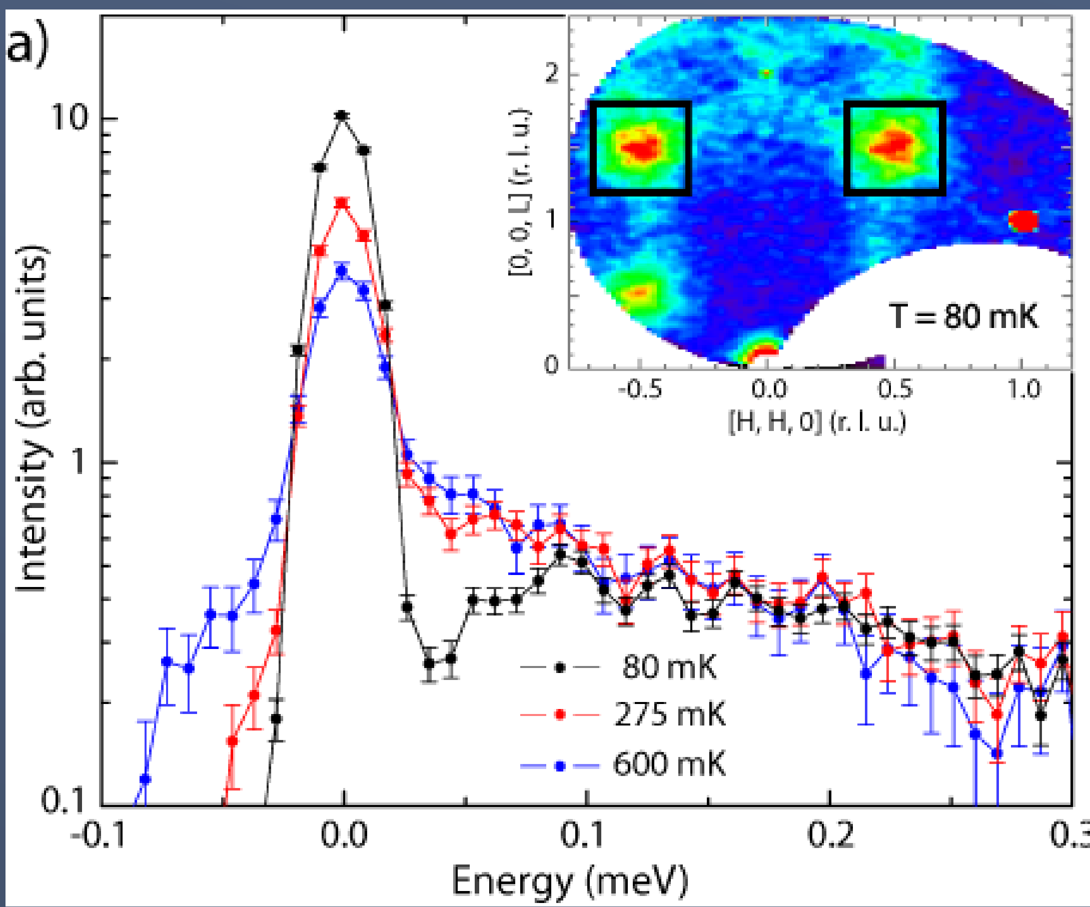

d)


AFM LRO
Cooperative Paramagnet
AFM Frozen
Spin Ice
Magnetic Field (T)
Temperature (K)
TOF (this work)
TOF (unpublished)
3-axis (Rule et al.)
AC (Rule et al.)
TOF (Rule et al.)
AC (Yin et al.)

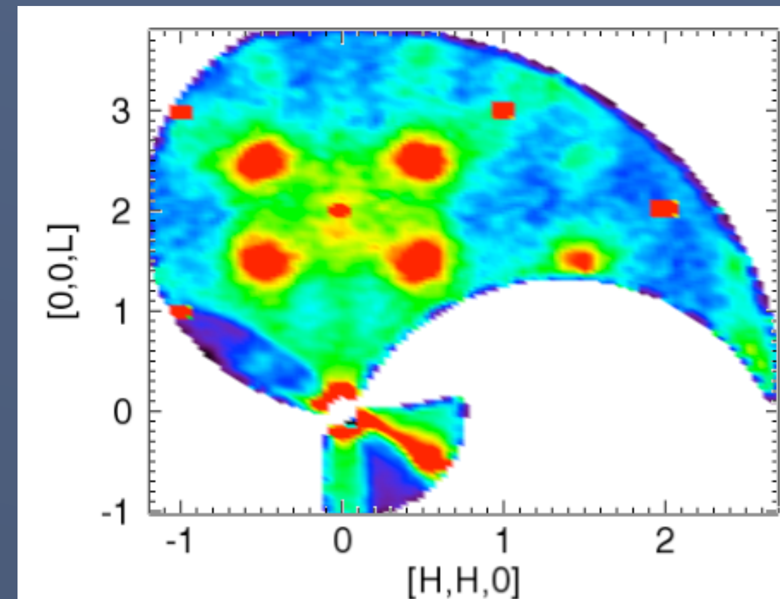

[0,0,L]
[H,H,0]

$Tb_2Ti_2O_7$

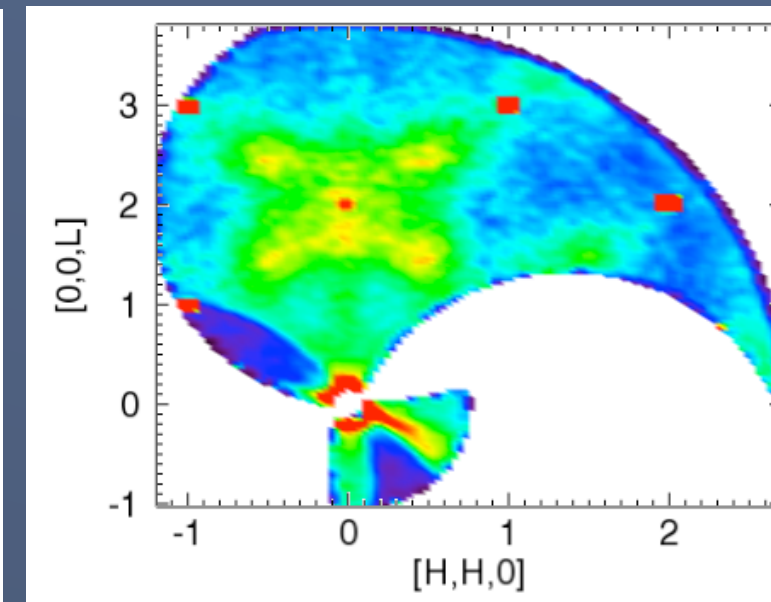

Tb2+xTi2-xO7 5A T=80mK xneg H=0T, E=[-0.1,0.1] meV ZFC
[0,0,L]
[H,H,0]

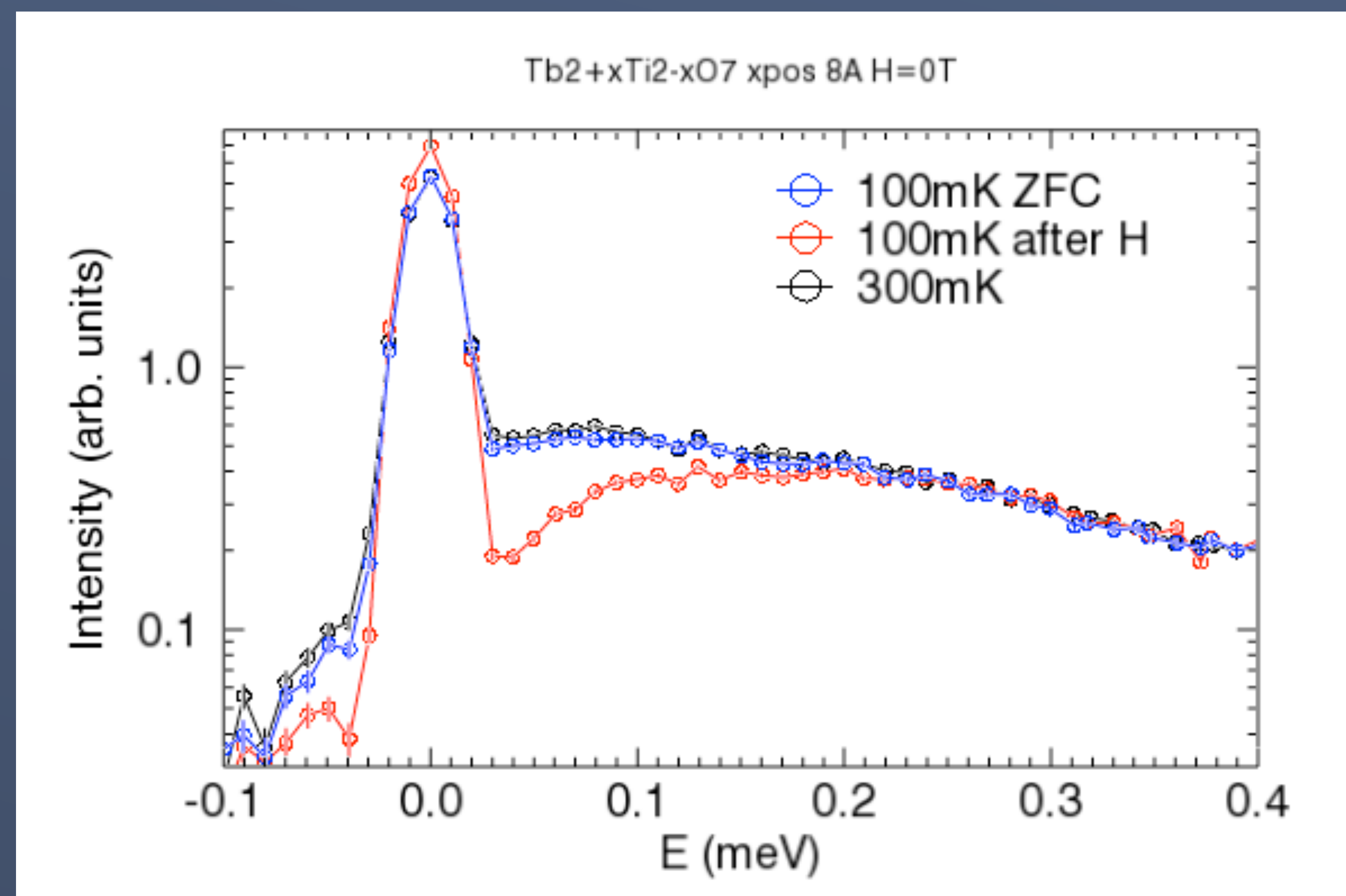


Field Cooled State



Zero-Field Cooled State



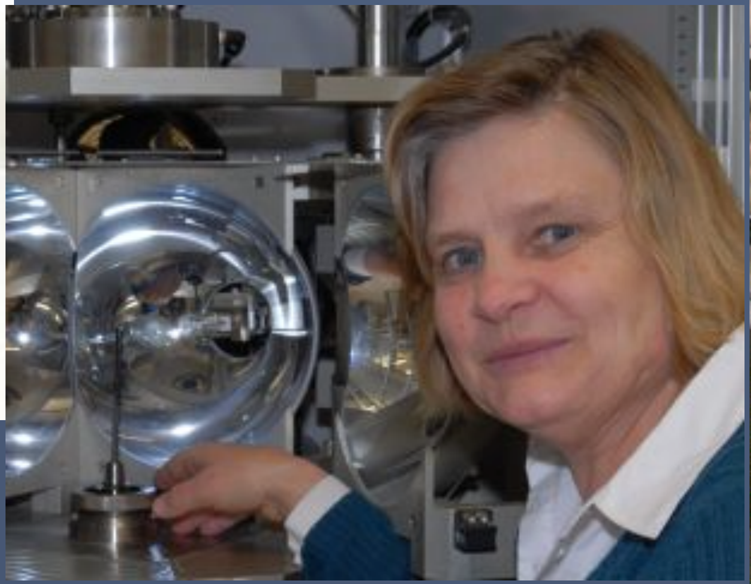


Collaboration

Mary Anne White

Jan Kycia

Hanna Dabkowska



Kate Ross

Pat Clancy

Edwin Kermarrec